Computational Models for Polydisperse Particulate and Multiphase Systems

Providing a clear description of the theory of polydisperse multiphase flows, with emphasis on the mesoscale modeling approach and its relationship with microscale and macroscale models, this all-inclusive introduction is ideal, whether you are working in industry or academia. Theory is linked to practice through discussions of key real-world cases (particle/droplet/bubble coalescence, breakup, nucleation, advection and diffusion, and physical- and phase-space), providing valuable experience in simulating systems that can be applied to your own applications. Practical cases of QMOM, DQMOM, CQMOM, EQMOM, and ECQMOM are also discussed and compared, as are realizable finite-volume methods. This provides the tools you need to use quadrature-based moment methods, choose from the many available options, and design high-order numerical methods that guarantee realizable moment sets. In addition to the numerous practical examples, MATLAB scripts for several algorithms are also provided, so you can apply the methods described to practical problems straight away.

Daniele L. Marchisio is an Associate Professor at the Politecnico di Torino, Italy, where he received his Ph.D. in 2001. He has held visiting positions at the Laboratoire des Sciences du Génie Chimique, CNRS–ENSIC (Nancy, France), Iowa State University (USA), Eidgenössische Technische Hochschule Zürich (Switzerland), and University College London (UK), and has been an invited professor at Aalborg University (Denmark) and the University of Valladolid (Spain). He acts as a referee for the key international journals in his field of research. He has authored more than 60 scientific papers and 5 book chapters, and co-edited the volume Multiphase Reacting Flows (Springer, 2007).

Rodney O. Fox is the Anson Marston Distinguished Professor of Engineering at Iowa State University (USA), an Associate Scientist at the US-DOE Ames Laboratory, and a Senior Research Fellow in the EM2C laboratory at the Ecole Centrale Paris (France). His numerous professional awards include an NSF Presidential Young Investigator Award in 1992 and Fellow of the American Physical Society in 2007. The impact of Fox’s work touches every technological area dealing with multiphase flow and chemical reactions. His monograph Computational Models for Turbulent Reacting Flows (Cambridge University Press, 2003) offers an authoritative treatment of the field.
Computational Models for Polydisperse Particulate and Multiphase Systems

DANIELE L. MARCHISIO
Politecnico di Torino

RODNEY O. FOX
Iowa State University
Daniele L. Marchisio and Rodney O. Fox

Computational models for polydisperse particulate and multiphase systems

© in this web service Cambridge University Press
Cambridge University Press
978-0-521-85848-9 - Computational Models for Polydisperse Particulate and Multiphase Systems
Daniele L. Marchisio and Rodney O. Fox
Frontmatter
More information
a Giampaolo
à Roberte
Contents

Preface xi

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
### Contents

#### 3 Quadrature-based moment methods

3.1 Univariate distributions  
3.1.1 Gaussian quadrature  
3.1.2 The product–difference (PD) algorithm  
3.1.3 The Wheeler algorithm  
3.1.4 Consistency of a moment set  

3.2 Multivariate distributions  
3.2.1 Brute-force QMOM  
3.2.2 Tensor-product QMOM  
3.2.3 Conditional QMOM  

3.3 The extended quadrature method of moments (EQMOM)  
3.3.1 Relationship to orthogonal polynomials  
3.3.2 Univariate EQMOM  
3.3.3 Evaluation of integrals with the EQMOM  
3.3.4 Multivariate EQMOM  

3.4 The direct quadrature method of moments (DQMOM)  

#### 4 The generalized population-balance equation

4.1 Particle-based definition of the NDF  
4.1.1 Definition of the NDF for granular systems  
4.1.2 NDF estimation methods  
4.1.3 Definition of the NDF for fluid–particle systems  

4.2 From the multi-particle–fluid joint PDF to the GPBE  
4.2.1 The transport equation for the multi-particle joint PDF  
4.2.2 The transport equation for the single-particle joint PDF  
4.2.3 The transport equation for the NDF  
4.2.4 The closure problem  

4.3 Moment-transport equations  
4.3.1 A few words about phase-space integration  
4.3.2 Disperse-phase number transport  
4.3.3 Disperse-phase volume transport  
4.3.4 Fluid-phase volume transport  
4.3.5 Disperse-phase mass transport  
4.3.6 Fluid-phase mass transport  
4.3.7 Disperse-phase momentum transport  
4.3.8 Fluid-phase momentum transport  
4.3.9 Higher-order moment transport  

4.4 Moment closures for the GPBE  

#### 5 Mesoscale models for physical and chemical processes  

5.1 An overview of mesoscale modeling  
5.1.1 Mesoscale models in the GPBE  
5.1.2 Formulation of mesoscale models  
5.1.3 Relation to macroscale models  

5.2 Phase-space advection: mass and heat transfer  
5.2.1 Mesoscale variables for particle size  
5.2.2 Size change for crystalline and amorphous particles  
5.2.3 Non-isothermal systems  
5.2.4 Mass transfer to gas bubbles
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
Contents

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
Preface

This book is intended for graduate students in different branches of science and engineering (i.e. chemical, mechanical, environmental, energetics, etc.) interested in the simulation of polydisperse multiphase flows, as well as for scientists and engineers already working in this field. The book provides, in fact, a systematic and consistent discussion of the basic theory that governs polydisperse multiphase systems, which is suitable for a neophyte, and presents a particular class of computational methods for their actual simulation, which might interest the more experienced scholar.

As explained throughout the book, disperse multiphase systems are characterized by multiple phases, with one phase continuous and the others dispersed (i.e. in the form of distinct particles, droplets, or bubbles). The term polydisperse is used in this context to specify that the relevant properties characterizing the elements of the disperse phases, such as mass, momentum, or energy, change from element to element, generating what are commonly called distributions. Typical distributions, which are often used as characteristic signatures of multiphase systems, are, for example, a crystal-size distribution (CSD), a particle-size distribution (PSD), and a particle-velocity distribution.

The problem of describing the evolution (in space and time) of these distributions has been treated in many ways by different scientific communities, focusing on aspects most relevant to their community. For example, in the field of crystallization and precipitation, the problem is described (often neglecting spatial inhomogeneities) in terms of crystal or particle size, and the resulting governing equation is called a population-balance equation (PBE). In the field of evaporating (and non-evaporating) sprays the problem is formulated in terms of the particle surface area and the governing equation is referred to as the Williams–Boltzmann equation. In this and other fields great emphasis has been placed on the fact that the investigated systems are spatially inhomogeneous. Aerosols and ultra-fine particles are often described in terms of particle mass, and the final governing equation is called the particle-dynamics equation. Particulate systems involved in granular flows have instead been investigated in terms of particle velocity only, and the governing equation is the inelastic extension to multiphase systems of the well-known Boltzmann equation (BE) used to describe molecular velocity distributions in gas dynamics.

Although these apparently different theoretical frameworks are referred to by different names, the underlying theory (which has its foundation in classical statistical mechanics) is exactly the same. This has also generated a plethora of numerical methods for the solution of the governing equations, often sharing many common elements, but generally with a specific focus on only part of the problem. For example, in a PBE the distribution representing the elements constituting the multiphase system is often discretized into classes or sections, generating the so-called discretized population-balance equation (DPBE). Among the many methods developed, one widely used among practitioners in computational fluid dynamics (CFD) is the multiple-size-group (MUSIG) method. This approach resembles,
in its basic ideas, the discretization carried out for the BE in the so-called discrete-velocity method (DVM). Analogously, the method of moments (MOM) has been used for the solution of both PBE and BE, but the resulting closure problem is overcome by following different strategies in the two cases. In the case of the BE the most popular moment closure is the one proposed by Grad, which is based on the solution of a subset of 13 or 26 moments, coupled with a presumed functional form for the velocity distribution. In contrast, in the case of a PBE the closure strategy often involves interpolation among the known moments (as in the method of moments with interpolative closure, MOMIC). Given the plethora of approaches, for the novice it is often impossible to see the connections between the methods employed by the different communities.

This book provides a consistent treatment of these issues that is based on a general theoretical framework. This, in turn, stems from the generalized population-balance equation (GPBE), which includes as special cases all the other governing equations previously mentioned (e.g. PBE and BE). After discussing how this equation originates, the different computational models for its numerical solution are presented. The book is structured as follows.

- Chapter 1 introduces key concepts, such as flow regimes and relevant dimensionless numbers, by using two examples: the PBE for fine particles and the KE for gas–particle flow. Subsequently the mesoscale modeling approach used throughout the book is explained in detail, with particular focus on the relation to microscale and macroscale models and the resulting closure problems.

- Chapter 2 provides a brief introduction to the mesoscale description of polydisperse systems. In this chapter the many possible number-density functions (NDF), formulated with different choices for the internal coordinates, are presented, followed by an introduction to the PBE in their various forms. The chapter concludes with a short discussion on the differences between the moment-transport equations associated with the PBE, and those arising due to ensemble averaging in turbulence theory.

- Chapter 3 provides an introduction to Gaussian quadrature and the moment-inversion algorithms used in quadrature-based moment methods (QBMM). In this chapter, the product–difference (PD) and Wheeler algorithms employed for the classical univariate quadrature method of moments (Q MOM) are discussed, together with the brute-force, tensor-product, and conditional QMOM developed for multivariate problems. The chapter concludes with a discussion of the extended quadrature method of moments (EQMOM) and the direct quadrature method of moments (DQMOM).

- In Chapter 4 the GPBE is derived, highlighting the closures that must be introduced for the passage from the microscale to the mesoscale model. This chapter also contains an overview of the mathematical steps needed to derive the transport equations for the moments of the NDF from the GPBE. The resulting moment-closure problem is also thoroughly discussed.

- Chapter 5 focuses on selected mesoscale models from the literature for key physical and chemical processes. The chapter begins with a general discussion of the mesoscale modeling philosophy and its mathematical framework. Since the number of mesoscale models proposed in the literature is enormous, the goal of the chapter is to introduce examples of models for advection and diffusion in real and phase space.
Preface

and zeroth-, first-, and second-order point processes, such as nucleation, breakage, and aggregation.

- Chapter 6 is devoted to the topic of hard-sphere collision models (and related simpler kinetic models) in the context of QBMM. In particular, the exact source terms for integer moments due to collisions are derived in the case of inelastic binary collisions between two particles with different diameters/masses, and the use of QBMM to overcome the closure problem is illustrated.

- Chapter 7 is devoted to solution methods of the spatially homogeneous GPBE, including class and sectional methods, MOM and QBMM, and Monte Carlo methods. The chapter concludes with a few examples comparing solution methods for selected homogeneous PBE.

- Chapter 8 focuses on the use of moment methods for solving a spatially inhomogeneous GPBE. Critical issues with spatially inhomogeneous systems are moment realizability and corruption (due to numerical advection and diffusion operator) and the presence of particle trajectory crossing (PTC). These are discussed after introducing kinetics-based finite-volume methods, by presenting numerical schemes capable of preserving moment realizability and by demonstrating with practical examples that QBMM are ideally suited for capturing PTC. The chapter concludes with a number of spatially one-dimensional numerical examples.

- To complete the book, four appendices are included. Appendix A contains the MATLAB scripts for the most common moment-inversion algorithms presented in Chapter 3. Appendix B discusses in more detail the kinetics-based finite-volume methods introduced in Chapter 8. Finally, the key issues of PTC in phase space, which occurs in systems far from collisional equilibrium, and moment conservation with some QBMM are discussed in Appendix C and Appendix D, respectively.

The authors are greatly indebted to the many people who contributed in different ways to the completion of this work. Central in this book is the pioneering research of Dr. Robert L. McGraw, who was the first to develop QMOM and the Jacobian matrix transformation (which is the basis for DQMOM) for the solution of the PBE, and brought to our attention the importance of moment corruption and realizability when using moment methods. The authors are therefore especially grateful to Professor Daniel E. Rosner, who in 1999 directed their attention to the newly published work of Dr. McGraw on QMOM. They would also like to thank Professor R. Dennis Vigil for recognizing the capability of QMOM for solving aggregation and breakage problems, and Professor Prakash Vedula for providing the mathematical framework used to compute the moment source terms for hard-sphere collisions reported in Chapter 6.

A central theme of the solution methods described in this book is the importance of maintaining the realizability of moment sets in the numerical approximation. On this point, the authors are especially indebted to Professor Marc Massot for enlightening them on the subtleties of kinetics-based methods for hyperbolic systems and the general topic of particle trajectory crossings. Thanks to the excellent numerical analysis skills of Professor Olivier Desjardins and a key suggestion by Dr. Philippe Villedieu during the 2006 Summer Program at the Center for Turbulence Research, Professor Massot’s remarks eventually pointed us in the direction of the realizable finite-volume schemes described in Chapter 8. In this regard, we also want to acknowledge the key contributions of Professor Z. J. Wang
Preface

in the area of high-order finite-volume schemes and Dr. Varun Vikas for the development and implementation of the realizable quasi-high-order schemes described in Appendix B.

The idea of publishing this book with Cambridge University Press is the result of the interest shown in the topic by Professor Massimo Morbidelli. The contribution of many other colleagues is also gratefully acknowledged, among them Antonello A. Barresi, Marco Vanni, Giancarlo Baldi, Miroslav Soos, Jan Sefcik, Christophe Chalons, Frédérique Laurent, Hailiang Liu, Alberto Passalacqua, Venkat Raman, Julien Reveillon, and Shankar Subramaniam. All the graduate students and post-doctoral researchers supervised by the authors in the last ten years who have contributed to the findings reported in this book are gratefully acknowledged and their specific contributions are meticulously cited.

The research work behind this book has been funded by many institutions and among them are worth mentioning the European Commission (DLM), the Italian Ministry of Education, University, and Research (DLM), the ISI Foundation (DLM, ROF), the US National Science Foundation (ROF), the US Department of Energy (ROF), the Ecole Centrale Paris (ROF), and the Center for Turbulence Research at Stanford University (ROF). The constant stimulus and financial support of numerous industrial collaborators (ENI, Italy; BASF, Germany; BP Chemicals, USA; Conoco Phillips, USA; and Univation Technologies, USA) are also deeply appreciated.
Notation

Upper-case Roman

\( A \)
generic particle acceleration due to buoyancy, gravity, and drag
\( A \)
coefficient matrix in DQMOM and brute-force QMOM for
determining the quadrature approximation
\( A \)
coefficient matrix constituted by mixed moments for calculating
velocity parameters \( u_i \) in inhomogeneous systems

\( A_D \)
particle cross-section surface area
\( A_{eq} \)
area of equivalent sphere
\( A_H \)
Hamaker parameter
\( A_p \)
particle surface area

\( A_f \)
fluid acceleration due to body forces
\( A_{bp} \)
pure particle acceleration due to fluid–particle momentum exchange
\( A_p \)
pure particle acceleration due to body forces
\( A_{pf} \)
mean particle-acceleration term
\( A_{pf} \)
pure fluid acceleration due to fluid–particle momentum exchange

\( A^{(n)} \)
acceleration acting on \( n \)th particle due to body forces
(for particles in vacuum)
\( A^{(n)}_f \)
acceleration acting on the fluid in the neighborhood of the
\( n \)th particle due to pressure, body, and viscous forces
\( A^{(n)}_{bp} \)
acceleration acting on the \( n \)th particle
due to fluid–particle forces
\( A^{(n)}_p \)
acceleration acting on the \( n \)th particle due to body forces
(for particles suspended in a fluid)
\( A^{(n)}_{pf} \)
acceleration acting on the fluid in the neighborhood of the
\( n \)th particle due to fluid–particle forces

\( A^*_{bp} \)
global particle acceleration due to fluid–particle momentum
exchange (including diffusion terms)
\( A^*_i \)
coefficient matrix constituted by moments \( m_{i,j}^{*} \) for calculating
velocity parameters \( u_i \) in inhomogeneous systems with FVM
\( A_{ij}^{*} \)
collision frequencies between particle-velocity classes in DVM

\( \langle A_f \rangle_1 \)
multi-particle conditional expected fluid acceleration
due to body forces
\( \langle A_{bp} \rangle_1 \)
multi-particle conditional expected particle acceleration
due to fluid–particle forces
Notation

⟨\(A_p\)\rangle_1 \quad \text{multi-particle conditional expected particle acceleration due to field forces}

⟨\(A_{pf}\)\rangle_1 \quad \text{multi-particle conditional expected fluid acceleration due to fluid–particle forces}

⟨\(A_{fp}(n)\)\rangle \quad \text{single-particle conditional expected continuous particle acceleration due to fluid–particle forces}

⟨\(A_{p}(n)\)\rangle \quad \text{single-particle conditional expected continuous particle acceleration due to field forces}

[\(A_f\)] \quad \text{total acceleration of the fluid seen by the particles due to forces in the fluid phase}

[\(A_g\)]_N \quad \text{total acceleration acting on monodisperse particles (of constant size and mass) due to drag, lift, and pressure forces}

[\(A_p\)]_p \quad \text{total acceleration acting on particles due to body forces}

[\(A_{fp}\)]_f \quad \text{total acceleration of fluid seen by the particles due to momentum transfer between phases}

\(\text{Ar}_p\) \quad \text{Archimedes number for disperse phase}

\(\beta(x, y)\) \quad \text{beta function}

\(\beta(g, x)\) \quad \text{hard-sphere collision kernel}

\(B_{ij}\) \quad \text{rate of change of the particle-number density in intervals } I_i^{(1)} \text{ and } I_j^{(0)} \text{ due to a generic point process (in CM for bivariate systems)}

\(P_{agg}^i\) \quad \text{rate of change of the particle number in interval } I_i \text{ due to aggregation (in CM for univariate systems)}

\(P_{break}^i\) \quad \text{rate of change of the particle number in interval } I_i \text{ due to breakage (in CM for univariate systems)}

\(B_{\gamma\gamma}\) \quad \text{coefficient matrix constituted by mixed moments for calculating velocity parameters } u_{\gamma} \text{ (in inhomogeneous systems)}

\(B_{\gamma\xi}\) \quad \text{mixed phase-space diffusion tensor for fluid velocity and particle internal coordinate}

\(B_{\xi\xi}\) \quad \text{pure phase-space diffusion tensor for fluid velocity and fluid internal coordinate}

\(B_{\gamma\xi}\) \quad \text{mixed phase-space diffusion tensor for particle velocity and fluid internal coordinate}

\(B_{\xi\xi}\) \quad \text{mixed phase-space diffusion tensor for particle velocity and particle internal coordinate}

\(B_{\psi\psi}\) \quad \text{mixed phase-space diffusion tensor for particle velocity and fluid velocity}

\(B_{\psi\xi}\) \quad \text{mixed phase-space diffusion tensor for particle velocity and fluid internal coordinate}

\(B_{\psi\xi}\) \quad \text{mixed phase-space diffusion tensor for fluid velocity and fluid internal coordinate}

\(B_{\psi}\) \quad \text{Bond number (equal to Eötvös number)}

\(C\) \quad \text{constant appearing in the parabolic daughter distribution function for particle breakage}

\(C(\psi)\) \quad \text{collisional source term for monodisperse system}
Notation

\( C_1 \) coefficient appearing in definition of the fluid effective (laminar plus turbulent) viscosity \( \mu_{eff} \)

\( C_{1-7} \) constants appearing in breakage kernel

\( C_D \) particle-drag coefficient

\( C_D' \) particle-drag coefficient including the Cunningham correction factor for rarefied continuous phase

\( C_i \) concentration of the potential-determining ions

\( C_L \) lift-force coefficient

\( C_m \) momentum exchange coefficient appearing in thermophoretic force

\( C_s \) thermal slip coefficient appearing in thermophoretic force appearing in thermophoretic force

\( C_{vm} \) virtual-mass force coefficient identifying the fraction of fluid volume moving with a particle

\( C_a \) coefficients appearing in the functional expansion of the NDF

\( C_{a\alpha\beta}(\psi) \) collisional source term for polydisperse system (particles of types \( \alpha \) and \( \beta \))

\( C_{a\alpha\beta}^{\gamma}(\psi) \) terms appearing in the expansion of the collisional source term for polydisperse systems (particles of types \( \alpha \) and \( \beta \))

\( C_{ij,k}^{\gamma} \) approximate collision source term for velocity moments of global order \( \gamma \) (monodisperse systems)

\( C_{ij,k\alpha}^{\gamma} \) approximate collision source term for velocity moments of global order \( \gamma \) of particle type \( \alpha \) (polydisperse systems)

\( C \) generic collisional source term

\( C_{a\alpha\beta} \) collisional source term for particles of types \( \alpha \) and \( \beta \)

\( C_{N_p} \) \( N_p \)-particle collision operator

\( C_{f\xi} \) mixed phase-space diffusion tensor for fluid internal coordinate and particle internal coordinate

\( C_{v\xi} \) mixed phase-space diffusion tensor for fluid internal coordinate and particle velocity

\( C_{p\xi} \) mixed phase-space diffusion tensor for particle internal coordinate and fluid internal coordinate

\( C_{p\xi} \) mixed phase-space diffusion tensor for particle internal coordinate and fluid velocity

\( C_{p\xi} \) mixed phase-space diffusion tensor for particle internal coordinate and fluid internal coordinate

\( C_{p\xi}^{\alpha\beta} \) concentration of potential determining ions at point of zero charge

\( C_{D}^{\alpha\beta} \) pure phase-space diffusion tensor for fluid internal coordinate

\( C_{p\xi}^{\alpha\beta} \) mixed phase-space diffusion tensor for particle internal coordinate and particle velocity

\( C_{p\xi}^{\alpha\beta} \) mixed phase-space diffusion tensor for particle internal coordinate and fluid velocity

\( C_{p\xi}^{\alpha\beta} \) mixed phase-space diffusion tensor for particle internal coordinate and fluid internal coordinate

\( C_{p\xi}^{\alpha\beta} \) concentration of potential determining ions at point of zero charge

\( C_{D}^{\alpha\beta} \) drag coefficient for the \( \alpha \)th particle

\( C_{D}^{\alpha\beta} \) rate of change of the internal coordinate vector for the fluid surrounding the \( \alpha \)th particle due to discontinuous events

\( C_{p\xi}^{\alpha\beta} \) rate of change of velocity for the \( \alpha \)th particle due to collisions (particles suspended in fluid)
Notation

$C_{\xi}^{(n)}$: rate of change of particle internal coordinate vector for $n$th particle due to collisions (particles suspended in fluid)

$C_{\xi}^{(n)}$: rate of change of velocity for the $n$th particle due to discontinuous particle collisions (in vacuum)

$C_{\xi}^{(n)}$: rate of change of particle internal coordinate vector for $n$th particle due to particle collisions (in vacuum)

$C_{\xi}^{(n)}$: single-particle collision operator

$C_{l_1l_2l_3}^\xi$: collision source terms for integer moments of orders $l_1$, $l_2$, and $l_3$ with respect to the three velocity components

$D$: solute molecular diffusion coefficient

$D_b$: diameter of a stable bridge between two aggregating particles

$D_f$: particle fractal dimension

$D_0$: average size of objects constituting a porous medium

$D$: symmetric $N \times N$ diffusion matrix

$\tilde{D}$: volume-average symmetric $N \times N$ diffusion matrix

$D^*$: dimensionless normalized diffusion matrix

$D_a$: aggregation Damköhler number

$D_{ab}$: breakage Damköhler number

$E$: bubble aspect ratio

$E_{\alpha\beta}$: energy scaling factor in polydisperse systems (particle types $\alpha$ and $\beta$)

$E_p$: total particle granular energy

$E_o$: Eötvös number

$F$: inter-particle force

$F(\zeta)$: dimensionless normalized NDF

$F_i$: cumulative probability distribution for the quiescence time in MC methods

$F^\gamma_{i,l_1l_2l_3}$: $i$th component of spatial flux for moment of global order $\gamma$

$F^\gamma_{i,l_1l_2l_3}$: $i$th component of spatial flux for moment of global order $\gamma$

$F^\gamma_{i,l_1l_2l_3}$: $i$th component of spatial flux for moment of global order $\gamma$

$F^\gamma_{i,l_1l_2l_3}$: $i$th component of spatial flux for moment of global order $\gamma$

$F(\mathbf{M})$: generic moment flux function

$F_{\gamma\beta}$: drag and buoyancy fluid–particle force

$F_{l_1l_2l_3}^\gamma$: spatial flux for moment of global order $\gamma$

$F_{l_1l_2l_3}^\gamma$: spatial flux for moment of global order $\gamma$

$F_{l_1l_2l_3}^\gamma$: spatial flux for moment of global order $\gamma$

$F_{l_1l_2l_3}^\gamma$: spatial flux for moment of global order $\gamma$

$F_{i,l_1l_2l_3}^\gamma$: $i$th component of spatial flux for moment of global order $\gamma$

$F_{i,l_1l_2l_3}^\gamma$: $i$th component of spatial flux for moment of global order $\gamma$

$F_{i,l_1l_2l_3}^\gamma$: $i$th component of spatial flux for moment of global order $\gamma$

$F_{i,l_1l_2l_3}^\gamma$: $i$th component of spatial flux for moment of global order $\gamma$

$F_{i,l_1l_2l_3}^\gamma$: $i$th component of spatial flux for moment of global order $\gamma$

$F_l$: flow number for particle aggregation

$F_{\gamma\ell}$: Froude number for the continuous phase

$G(n_s, n_r)$: numerical flux function for inhomogeneous systems discretized with FVM

$G_{\ell}$: fluid shear rate
Notation

\( G_i \) gain rate of particles with velocity \( \xi_i \) due to collisions in DVM
\( G_{i|k,\phi|\phi} \) Gaussian moments with mean velocity \( U_{\phi\phi} \) and
 covariance matrix \( \sigma_{\phi\phi} \)
\( G_L \) continuous rate of change of particle size (growth rate)
\( G_{L,k} \) average particle growth rate for moment of order \( k \)
\( G_m(\psi) \) component \( m \) of the collisional-flux term
\( G_{m,l_1,l_2,l_3} \) collisional-flux term for integer moments of orders \( l_1, l_2, \) and \( l_3 \)
 with respect to the three velocity components
\( G_p \) pure advection component for the rate of change of crystal size
\( G_{p,\alpha} \) correction for fluid-dynamic interactions between particles
\( G_{\alpha} \) coefficients appearing in the calculation of the velocity parameters \( u_e \)
 for inhomogeneous systems
\( \bar{G}_p \) global rate of change of crystal size
\( G_{p,\alpha} \) mass-transfer rate from fluid to particle

\( G \) vectorial numerical flux function for inhomogeneous systems
discretized with FVM
\( G(\phi) \) collisional-flux term for monodisperse systems
\( G_f \) pure mesoscale advection model for the fluid internal coordinate
\( G_{l_1,l_2,l_3} \) collisional-flux vector for velocity moment of order \( l_1,l_2,l_3 \)
\( G_p \) pure mesoscale advection model for particle internal coordinate
\( G_{\alpha\beta}(\psi) \) collisional-flux term for polydisperse systems constituted by
 particle types \( \alpha \) and \( \beta \)

\( G^{(n)} \) continuous rate of change of the internal coordinate vector
 for the \( n \)th particle (particles in vacuum)
\( G^{(n)}_f \) continuous rate of change of the internal coordinate vector
 for the fluid surrounding the \( n \)th particle
\( G^{(n)}_p \) continuous rate of change of the internal coordinate vector
 for the \( n \)th particle (particles suspended in fluid)
\( G^{(n)}_{\alpha\beta}(\psi) \) terms appearing in the expansion for the collisional-flux term
 for polydisperse systems with particle types \( \alpha \) and \( \beta \)

\( \langle G_f \rangle_1 \) multi-particle conditional expected continuous rate of change
 of fluid internal coordinate vector
\( \langle G^{(n)}_f \rangle_1 \) single-particle conditional expected continuous rate of change
 of fluid internal coordinate vector
\( \langle G_p \rangle_1 \) multi-particle conditional expected continuous rate of change
 of particle internal coordinate vector
\( \langle G^{(n)}_p \rangle_1 \) single-particle conditional expected continuous rate of change
 of particle internal coordinate vector

\[ [G_f] \] rate of change of fluid-phase mass density due to
 continuous processes
\[ [G_p] \] rate of change of disperse-phase mass density due to
 continuous processes
\[ [G_f]_V \] rate of change of fluid-phase volume fraction due to
 continuous processes
\[ [G_p]_V \] rate of change of disperse-phase volume fraction due
 to continuous processes
\[ [G^\star_f]_r \] global fluid momentum rate of change due to mass transfer
 from fluid phase
Notation

\[ [G_p]_{p} \] global particle momentum rate of change due to mass transfer from liquid phase

\[ H(\xi) \] Heaviside step function

\[ \mathcal{H} \] functional appearing in the general definition of the pair distribution function (function of the moments)

\[ H_{a,b} \] distance between two primary particles within an aggregate

\[ H_{o} \] symmetric change of variable involving \( l_{12}^{(m)} \)

\[ I \] finite \( i \)th internal coordinate interval used in CM

\[ I_{(m)}^{(j)}(x) \] indicator function equal to unity if \( x \in [x_1, x_2] \) and zero otherwise

\[ I_{(m)}^{(j)} \] finite \( i \)th interval for the \( j \)th internal coordinate in CM when extended to multivariate problems

\[ I_{l_{1}l_{2}l_{3}}^{(m)} \] factor appearing in collision term for integer velocity moments of orders \( l_{1}, l_{2}, \text{and } l_{3} \)

\[ I_{l_{1}l_{2}l_{3}}^{(p,q)} \] factor appearing in the collision term for polydisperse systems for integer velocity moments of orders \( l_{1}, l_{2}, \text{and } l_{3} \)

\[ J \] molar flux of solute molecules at particle surface

\[ J(\phi) \] rate of particle formation

\[ J(\tilde{\eta}, \eta) \] Jacobian of variable transformation relating phase-space variables before and after collision

\[ J_{l} \] rate of particle formation

\[ J_{l}^{*} \] volume-average rate of particle formation

\[ J_{k} \] \( k \)th moment of the rate of particle formation in univariate GPBE

\[ J_{k}^{*} \] \( k \)th moment of the rate of particle formation in multivariate GPBE

\[ J^{*} \] dimensionless and normalized rate of particle formation

\[ K_B \] history-force kernel

\[ k_{\theta}^{(m)} \] integral over collision angles

\[ k_{\theta}^{(j)} \] coefficients appearing in the third integral over collision angles

\[ K \] exponent matrix used to build the quadrature approximation

\[ K \] moment vector used in the definition of the moment set \( \mathbf{M} \)

\[ K_{n}^{*} \] reconstructed \( K \) in the \( i \)th cell at time step \( m \) employed in FVM

\[ K_{i}^{*} \] \( K \) evaluated with \( v_{i,j}^{*} \) or \( v_{i,j} \)

\[ K_{n} \] Knudsen number for continuous phase (relative to particle diameter)

\[ K_{n}^{*} \] Knudsen number for continuous phase (relative to particle radius)

\[ K_{n,p} \] Knudsen number for disperse phase

\[ L \] characteristic length of the system under investigation

\[ L \] particle length

\[ L_{s} \] loss rate of particles with velocity \( \xi \) due to collisions in DVM

\[ L_{s} \] latent heat of evaporation

\[ L_{10} \] number-average mean particle length

\[ L_{32} \] area-average mean particle length or Sauter diameter

\[ L_{43} \] volume-average mean particle length

\[ L \] transformation matrix between laboratory and collision frames

\[ Le \] Lewis number
**Notation**

- $M$ number of internal coordinates appearing in the NDF
- $M$ number of sections or classes used in CM and DVM
- $M_f$ number of fluid internal coordinates appearing in the NDF
- $M_G$ ratio between particle and collector size
- $M_k$ number of intervals used for the $k$th internal coordinate in multivariate CM
- $M_i$ mass of the particles in the interval $I_i$ in CM
- $M_p$ number of particle internal coordinates appearing in the NDF
- $M_p$ particle mass
- $M_w$ molecular weight (relative molecular mass) of chemical species
- $M_{w1}$ molecular weight of the evaporating component
- $M_{w2}$ molecular weight of the stagnant component
- $M_{agg}$ rate of change of particle mass in interval $I_i$ due to aggregation in CM
- $M_{break}$ rate of change of particle mass in interval $I_i$ due to breakage in CM
- $M_{\gamma}^{\gamma}$ velocity distribution moment of global order $\gamma = i + j + k$
- $M_{\gamma}^{\gamma,*}$ velocity equilibrium moment of global order $\gamma = i + j + k$
- $M_{\gamma}^{\gamma,\alpha}$ velocity distribution moment of global order $\gamma = i + j + k$ for particles of type $\alpha$ in polydisperse systems
- $M_{ij/z, f}$ positive integer moment of the velocity distribution in the $i$th direction
- $M_{ij/z, f}$ negative integer moment of the velocity distribution in the $i$th direction
- $\mathbf{M}$ vector defining the tracked moment set
- $\mathbf{M}^+$ positive half-moment set (integration for positive velocity)
- $\mathbf{M}^-$ negative half-moment set (integration for negative velocity)
- $\mathbf{M}^m$ volume-averaged moment set in the $i$th cell at time step $m$ defined in FVM for a 1D grid
- $\mathbf{M}^m_{ij/k}$ volume-averaged moment set at cell $\Omega_{ij/k}$ and time step $m$ defined in FVM for a structured 3D grid
- $\mathbf{M}^m_{ij/k,p}$ updated moment set at cell $\Omega_{ij/k}$ and time step $m$ defined in FVM for a structured 3D grid calculated with permutation $p$
- $\mathbf{M}^{(1)}_{ij/k}$ first-stage moment set in the $i$th cell at time step $m$ defined in FVM for a 1D grid
- $\mathbf{M}^{(2)}_{ij/k}$ positive half-moment set at cell $\Omega_{ij/k}$ in FVM (3D)
- $\mathbf{M}^{(2)}_{ij/k}$ negative half-moment set at cell $\Omega_{ij/k}$ in FVM (3D)
- $\mathbf{M}^{(3)}_{ij/k}$ second-stage moment set in the $i$th cell at time step $m$ defined in FVM for a 1D grid
- $M_a$ Mach number for continuous phase
- $M_{ap}$ Mach number for disperse phase
- $M_o$ Morton number
- $N$ order of the quadrature approximation
- $N^2$ number of quadrature nodes used in the calculation of the positive and negative fluxes
<table>
<thead>
<tr>
<th>Notation</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>(N(t, x))</td>
<td>total particle-number concentration (or density)</td>
</tr>
<tr>
<td>(N(V</td>
<td>V'))</td>
</tr>
<tr>
<td>(N(\xi'</td>
<td>\xi))</td>
</tr>
<tr>
<td>(N_d)</td>
<td>global number of degrees of freedom of the multiphase system</td>
</tr>
<tr>
<td>(N_i)</td>
<td>number of particles belonging to the (i)th interval in CM and DVM</td>
</tr>
<tr>
<td>(N_{ij})</td>
<td>number of particles belonging to intervals (I(i)) and (I(j)) for bivariate CM</td>
</tr>
<tr>
<td>(N_i)</td>
<td>number density of particles with velocity equal to (\xi_i) in DVM</td>
</tr>
<tr>
<td>(N_p)</td>
<td>number of primary particles forming a fractal object</td>
</tr>
<tr>
<td>(N_t)</td>
<td>total particle-number density</td>
</tr>
<tr>
<td>(N')</td>
<td>number of weights and abscissas for Laguerre-polynomial recursion coefficients in EQMOM</td>
</tr>
<tr>
<td>(\text{Nu})</td>
<td>Nusselt number</td>
</tr>
<tr>
<td>(P(\xi'</td>
<td>\xi))</td>
</tr>
<tr>
<td>(P_\alpha(\xi))</td>
<td>polynomial of order (\alpha) orthogonal to the NDF</td>
</tr>
<tr>
<td>(P_{ij})</td>
<td>elements of the matrix used in the PD algorithm</td>
</tr>
<tr>
<td>(P_{ij})</td>
<td>components of the second-order pressure tensor</td>
</tr>
<tr>
<td>(P)</td>
<td>matrix used in the PD algorithm</td>
</tr>
<tr>
<td>(P_{\alpha})</td>
<td>total particle stress tensor and second-order pressure tensor</td>
</tr>
<tr>
<td>(P_{\alpha,\beta})</td>
<td>second-order pressure tensor in polydisperse systems for particles of type (\alpha)</td>
</tr>
<tr>
<td>(\text{Pe})</td>
<td>Péclet number</td>
</tr>
<tr>
<td>(\text{Pr})</td>
<td>Prandtl number</td>
</tr>
<tr>
<td>(Q^+)</td>
<td>positive moment flux (integration for positive velocity)</td>
</tr>
<tr>
<td>(Q^-)</td>
<td>negative moment flux (integration for negative velocity)</td>
</tr>
<tr>
<td>(R)</td>
<td>ideal-gas constant</td>
</tr>
<tr>
<td>(R_g)</td>
<td>radius of gyration of the particle</td>
</tr>
<tr>
<td>(\text{Re}_g)</td>
<td>continuous (gas)-phase Reynolds number</td>
</tr>
<tr>
<td>(\text{Re}_p)</td>
<td>disperse (particulate)-phase Reynolds number</td>
</tr>
<tr>
<td>(\text{Re}_m)</td>
<td>critical particle Reynolds number</td>
</tr>
<tr>
<td>(\text{Re}_m^\text{crit})</td>
<td>meta-critical particle Reynolds number</td>
</tr>
<tr>
<td>(\text{Re}_p^\text{mod})</td>
<td>modified disperse-phase Reynolds number</td>
</tr>
<tr>
<td>(S)</td>
<td>supersaturation</td>
</tr>
<tr>
<td>(S)</td>
<td>comprehensive source term in the GPBE including drift, diffusion, and point processes</td>
</tr>
<tr>
<td>(S_c)</td>
<td>particle collisional cross-sectional area</td>
</tr>
<tr>
<td>(S_{kl})</td>
<td>reconstructed slope in the (k)th cell for the solution of the moment transport equation discretized with FVM (1D)</td>
</tr>
<tr>
<td>(S_{n_{ijkl}})</td>
<td>reconstructed slope in the (i)th cell at time instant (n) from EQMOM discretized with FVM (1D)</td>
</tr>
<tr>
<td>(S)</td>
<td>moment set source term</td>
</tr>
<tr>
<td>(S)</td>
<td>generic source term due to discontinuous events for the GPBE</td>
</tr>
<tr>
<td>(S_{fv})</td>
<td>source term due to discontinuous events for the fluid-phase volume fraction</td>
</tr>
<tr>
<td>(S_M)</td>
<td>source term due to discontinuous events for the disperse-phase mass density</td>
</tr>
</tbody>
</table>
### Notation

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_N$</td>
<td>source term due to discontinuous events for the total disperse-phase number density</td>
</tr>
<tr>
<td>$S_V$</td>
<td>source term due to discontinuous events for the disperse-phase volume fraction</td>
</tr>
<tr>
<td>$S_1$</td>
<td>generic source term due to discontinuous events for GPBE</td>
</tr>
<tr>
<td>$S_t$</td>
<td>viscous and pressure stress tensor for fluid phase</td>
</tr>
<tr>
<td>$\overline{S}_k$</td>
<td>source term for the $k$th moment of the NDF</td>
</tr>
<tr>
<td>$\overline{S}_k$</td>
<td>source term for the moment of order $k$ of the multivariate NDF</td>
</tr>
<tr>
<td>$S_{i,j,k}$</td>
<td>source term of the moments of orders $i$, $j$, and $k$ with respect to the particle-velocity components for the NDF</td>
</tr>
<tr>
<td>$S_{\gamma}$</td>
<td>factor appearing in the collision term for velocity moments of the NDF of orders $l_1$, $l_2$, and $l_3$ with respect to the three components</td>
</tr>
<tr>
<td>$S_{\gamma}^{(m)}$</td>
<td>source terms for moment of global order $\gamma = l_1 + l_2 + l_3$</td>
</tr>
<tr>
<td>$\left[ S \right]_{ij}$</td>
<td>rate of change for particle momentum due to discontinuous events</td>
</tr>
<tr>
<td>$\mathcal{S}^{*}$</td>
<td>collision cross section</td>
</tr>
<tr>
<td>$S_c$</td>
<td>Schmidt number</td>
</tr>
<tr>
<td>$S_h$</td>
<td>Sherwood number</td>
</tr>
<tr>
<td>$S_t$</td>
<td>Stokes number</td>
</tr>
<tr>
<td>$S_{tp}$</td>
<td>particle Stokes number</td>
</tr>
<tr>
<td>$T_f$</td>
<td>continuous (fluid) phase temperature</td>
</tr>
<tr>
<td>$T_p$</td>
<td>disperse (particulate) phase temperature</td>
</tr>
<tr>
<td>$T_{ref}$</td>
<td>reference temperature for liquid boiling</td>
</tr>
<tr>
<td>$T_s$</td>
<td>temperature on particle surface</td>
</tr>
<tr>
<td>$T_{sat}$</td>
<td>saturation temperature for the continuous phase</td>
</tr>
<tr>
<td>$U$</td>
<td>characteristic continuous phase velocity</td>
</tr>
<tr>
<td>$U(\xi)$</td>
<td>particle velocity conditioned on particle size $\xi$</td>
</tr>
<tr>
<td>$U_0$</td>
<td>characteristic particle velocity</td>
</tr>
<tr>
<td>$U_g$</td>
<td>continuous phase velocity</td>
</tr>
<tr>
<td>$U_p$</td>
<td>mean particle velocity</td>
</tr>
<tr>
<td>$U_r$</td>
<td>impact, or relative, velocity for fragmenting particles</td>
</tr>
<tr>
<td>$U_\infty$</td>
<td>particle terminal velocity</td>
</tr>
<tr>
<td>$U_f$</td>
<td>mean fluid velocity field</td>
</tr>
<tr>
<td>$U_{fV}$</td>
<td>volume-average fluid velocity</td>
</tr>
<tr>
<td>$U_M$</td>
<td>mass-average particle velocity</td>
</tr>
<tr>
<td>$U_{mix}$</td>
<td>mass-average mixture velocity</td>
</tr>
<tr>
<td>$U_N$</td>
<td>number-average particle velocity</td>
</tr>
<tr>
<td>$U_p$</td>
<td>mean particle velocity</td>
</tr>
<tr>
<td>$U_{p,2}$</td>
<td>second-order particle velocity-moment tensor</td>
</tr>
<tr>
<td>$U_{p,\xi}$</td>
<td>conditional particle velocity for $\xi_p = \xi_{\phi}$</td>
</tr>
<tr>
<td>$U_{PM}$</td>
<td>fluid-mass-average particle velocity</td>
</tr>
<tr>
<td>$U_V$</td>
<td>volume-average particle velocity</td>
</tr>
<tr>
<td>$U_{gp}$</td>
<td>mean velocities for polydisperse Gaussian distributions</td>
</tr>
<tr>
<td>$U_{\gamma}$</td>
<td>characteristic disperse-phase velocity</td>
</tr>
<tr>
<td>$U_0^{(n)}$</td>
<td>velocity of the $n$th particle (in vacuum)</td>
</tr>
<tr>
<td>$U_f^{(n)}$</td>
<td>fluid velocity in the neighborhood of the $n$th particle</td>
</tr>
<tr>
<td>Notation</td>
<td>Description</td>
</tr>
<tr>
<td>---------------</td>
<td>-----------------------------------------------------------------------------</td>
</tr>
<tr>
<td>$\mathbf{U}_f$</td>
<td>mesoscale variable describing fluid velocity</td>
</tr>
<tr>
<td>$\mathbf{U}_p(n)$</td>
<td>velocity of the $n$th particle</td>
</tr>
<tr>
<td>$\mathbf{U}_p$</td>
<td>mesoscale variable describing particle velocity</td>
</tr>
<tr>
<td>$\langle \mathbf{U}_f \rangle$</td>
<td>Reynolds-average fluid velocity field</td>
</tr>
<tr>
<td>$\langle \mathbf{U}_p</td>
<td>\xi = \zeta \rangle$</td>
</tr>
<tr>
<td>$\langle \mathbf{U}_p</td>
<td>\xi_p \rangle$</td>
</tr>
<tr>
<td>$\left[ \mathbf{U}_f \right]_p$</td>
<td>particle-mass-average fluid velocity</td>
</tr>
<tr>
<td>$V$</td>
<td>particle volume</td>
</tr>
<tr>
<td>$V_f$</td>
<td>fluid volume seen by the particle</td>
</tr>
<tr>
<td>$V_L$</td>
<td>length-based volume density function</td>
</tr>
<tr>
<td>$V_p$</td>
<td>particle volume</td>
</tr>
<tr>
<td>$V_W$</td>
<td>sample volume used in the estimation of the NDF</td>
</tr>
<tr>
<td>$V_{\alpha\beta}^{\text{adj}}$</td>
<td>particle velocity with EQMOM in the $i$th cell after the advection step when using FVM (1D) with time splitting</td>
</tr>
<tr>
<td>$V_{\alpha\beta}^r$</td>
<td>particle velocity with EQMOM in the $i$th cell after the advection step when using FVM (1D) with time splitting</td>
</tr>
<tr>
<td>$V$</td>
<td>dimensionless and normalized particle velocity</td>
</tr>
<tr>
<td>$V_f$</td>
<td>fluid-velocity space for fluid surrounding the $n$th particle</td>
</tr>
<tr>
<td>$V_p$</td>
<td>particle-velocity space for the $n$th particle</td>
</tr>
<tr>
<td>$W(t)$</td>
<td>generic Wiener process</td>
</tr>
<tr>
<td>$W_{\alpha\beta}^{\text{adj}}$</td>
<td>product of $w_{\alpha}$ and $w_{\alpha\beta}$ in EQMOM and calculated after the advection step with time splitting</td>
</tr>
<tr>
<td>$W_{\alpha\beta}^r$</td>
<td>product of $w_{\alpha}^r$ and $w_{\alpha\beta}^r$ in EQMOM</td>
</tr>
<tr>
<td>$W(t)$</td>
<td>generic vectorial Wiener process</td>
</tr>
<tr>
<td>$W_\alpha$</td>
<td>Weber number</td>
</tr>
<tr>
<td>$X$</td>
<td>dimensionless and normalized spatial coordinate</td>
</tr>
<tr>
<td>$X^T$</td>
<td>abscissa (or node) matrix</td>
</tr>
<tr>
<td>$X^{(0)}$</td>
<td>center of mass of the $n$th particle</td>
</tr>
<tr>
<td>$X_p$</td>
<td>mesoscale variable describing particle position</td>
</tr>
<tr>
<td>$Y_{f1}$</td>
<td>molar fraction of evaporating component in the gas phase</td>
</tr>
<tr>
<td>$Y_{i1}$</td>
<td>molar fraction of evaporating component on droplet surface</td>
</tr>
<tr>
<td>$Y_f$</td>
<td>gas-phase molar fraction of evaporating component</td>
</tr>
<tr>
<td>$Y_2$</td>
<td>gas-phase molar fraction of stagnant component</td>
</tr>
<tr>
<td>$Y_f$</td>
<td>fluid-phase species mass fractions</td>
</tr>
<tr>
<td>$Y_p$</td>
<td>particle species mass fractions</td>
</tr>
<tr>
<td>$Y_w = w_{\alpha}\xi $</td>
<td>weighted node (or abscissa) of the $M$-dimensional quadrature approximation</td>
</tr>
<tr>
<td>$Y^T$</td>
<td>weighted-abscissa (or weighted-node) matrix</td>
</tr>
</tbody>
</table>

### Lower-case Roman

- $a$: aggregation kernel
- $a$: breakage kernel (Chapter 7)
- $a_0$: constant-breakage kernel (Chapter 7)
Notation

\( a_{ij} \)  
affinity parameter for \( i-j \) aggregation (with \( i = A, B \) and \( j = A, B \))

\( a_\alpha \)  
coefficients of recursive formula for orthogonal polynomials

\( a_\alpha \)  
source term for the evolution equation of weight \( w_\alpha \) in DQMOM

\( \bar{a}_i \)  
coefficients of recursive formula appearing in Wheeler algorithm

\( a_{m} \)  
volume-average aggregation kernel

\( a_{ijk} \)  
slope vector employed in second-order spatial reconstructions for FVM (3D)

\( b \)  
frequency of first-order process (breakage kernel)

\( b(\xi' | \xi) \)  
daughter distribution function (Chapter 7)

\( b_{i,\alpha} \)  
source term for the evolution equation of weighted node \( \alpha \) for the \( i \)th internal coordinate in DQMOM

\( b_\alpha \)  
coefficients of recursive formula for orthogonal polynomials

\( b_\alpha \)  
source term for the evolution equation of weighted node \( \alpha \) in univariate DQMOM

\( b_\alpha^* \)  
coefficients of recursive formula appearing in Wheeler algorithm

\( b^* \)  
dimensionless and normalized kernel for first-order process

\( \hat{b} \)  
volume-average frequency of first-order process

\( \langle b \rangle \)  
volume-average breakage kernel

\( \bar{b}_\alpha \)  
moment transform of order \( k \) of the daughter distribution function for \( \xi_\alpha \) in univariate problems

\( \overline{\bar{b}}_\alpha \)  
moment transform of order \( k \) of the daughter distribution function for \( \xi_\alpha \) in multivariate problems

\( b_{\text{tvf}} \)  
response vector coefficient for fluid fluctuations

\( b_t \)  
response vector for third-order differences to a unit increment

\( b_{\text{pvi}} \)  
particle-velocity coefficient for fluid fluctuations

\( c_{\text{eq}} \)  
equilibrium solute concentration

\( c_{\text{ref}} \)  
self-diffusion component of crystal size growth rate

\( c_{\text{ref}} \)  
constant appearing in the definition of the pair distribution function

\( c^\alpha \)  
coefficients appearing in upwind reconstruction schemes

\( c^f \)  
specific heat of fluid phase

\( c_p \)  
particle specific heat

\( c_\alpha \)  
lattice velocities used in LBM

\( d \)  
degree of accuracy of the quadrature approximation

\( d \)  
molecular diameter of a solute molecule

\( d_o \)  
diameter of primary particles in an aggregate

\( d_p \)  
particle size

\( d_{10\%} \)  
size corresponding to 10% of the smaller particles

\( d_{90\%} \)  
size corresponding to 10% of the larger particles

\( d_\alpha \)  
size of the particles of type \( \alpha \) taking part in a collision

\( d_\beta \)  
size of the particles of type \( \beta \) taking part in a collision

\( d_{\alpha\beta} \)  
arithmetic average of colliding particle size (polydisperse systems)

\( d_r \)  
characteristic particle length

\( d_{ij}^\alpha \)  
net flux of particles for the \( k \)th internal coordinate due to phase-space diffusion in bivariate CM

\( d \)  
vector containing the moments source terms in DQMOM

\( d_n \)  
difference vector of order \( n \) of natural logarithm of NDF moments
## Notation

- $e$: coefficient of restitution for particle–particle collisions
- $e$: elementary charge
- $e_i$: particle specific energy for the $i$th velocity component
- $e_p$: particle specific energy
- $e_{\alpha\beta}$: restitution coefficient in polydisperse systems for collisions between particles of types $\alpha$ and $\beta$

- $f(t, x, v)$: particle-velocity NDF for monodisperse system
- $f(\xi_1, \ldots, \xi_{M-1})$: marginal NDF used in CQMOM
- $f(\xi_a|\ldots)$: conditional NDF used in CQMOM
- $f_\gamma$: shape function for colliding particles
- $f_0$: one-point PDF for the fluid
- $f_{\alpha\beta}$: volume distribution of the fluid shear rate
- $f_0$: multi-particle joint PDF
- $f_e$: probability density function for the quiescence time in MC methods
- $f_{eq}$: equilibrium velocity NDF

- $f_a$: weights used in reconstructing the NDF in LBM
- $f_\alpha(t, x, v)$: particle velocity NDF for particle type $\alpha$
- $f_\beta(t, x, v)$: particle velocity NDF for particle type $\beta$
- $f_e$: volume distribution of the fluid turbulent dissipation rate

- $f^{(2)}$: pair correlation velocity NDF
- $f^*(v)$: equilibrium distribution function in the BGK kinetic model and in Grad’s moment closure
- $f_1^{(\alpha)}$: single-particle joint PDF
- $f_i^*$: net flux of particles for the $i$th internal coordinate due to phase-space drift in bivariate CM
- $f_a^*$: weights used in LBM corresponding to the equilibrium NDF

- $g$: gravity acceleration constant
- $g(\epsilon)$: Kuwabara function for particle deposition in porous media
- $g_0(\alpha_p/\alpha_p^*)$: particle radial distribution function
- $g_{\alpha\beta}$: pair correlation function for particles of types $\alpha$ and $\beta$
- $g_{\omega}(\xi)$: constant appearing in the pair correlation function
- $g_\alpha(\xi)$: velocity parameters used in conjunction with EQMOM
- $g(\gamma)$: mean velocity difference used to approximate $|v_1 - v_2|$

- $h$: size of the regular discretization used in CM
- $h_i(\xi)$: function used to model the second-order tensor for mixed advection
- $h_i(\xi)$: numerical NDF in the $i$th cell for FVM (1D)
- $h_L$: discontinuous event term for length-based formulation
- $h_{L,k}$: moment of order $k$ of source term for discontinuous event
- $h_W$: constant kernel function used as filter to estimate NDF
- $h_i$: particle collisional acceleration term
- $h^*$: rate of particle formation due to discontinuous events
- $h^-$: rate of particle disappearance due to discontinuous events

- $i$: index vector identifying a discrete particle velocity in DVM

- $k$: order of moment for univariate NDF
- $k_\alpha$: particle surface shape factor
Notation

- \( k_B \): Boltzmann constant
- \( k_c \): corrective growth crowding factor
- \( k_{\infty} \): coordination number for an aggregate
- \( k_d \): particle mass-transfer coefficient
- \( k_T \): fluid-phase turbulent kinetic energy
- \( k_T \): fluid-phase thermal conductivity
- \( k_f \): fractal scaling factor of order unity
- \( k_h \): particle heat-transfer coefficient
- \( k(\xi) \): polynomial used to represent the NDF in the \( I_i \) interval in CM
- \( k_p \): thermal conductivity of particle
- \( k_v \): particle volumetric shape factor
- \( k_A^* \): equivalent particle surface shape factor
- \( k_V^* \): equivalent particle volumetric shape factor
- \( k \): exponent vector for the order of moment in multivariate NDF
- \( k_{\xi} \): internal coordinate exponent vector
- \( m \): particle mass (used in daughter NDF for breakage)
- \( m(k) \): moment of order \( k \) of univariate NDF
- \( m(k) \): moment of order \( k = (k_1, \ldots, k_M) \) of multivariate NDF
- \( m_n \): mass of newly formed particle (nucleus mass)
- \( m_{i,j,k} \): moment of order \( i, j, \) and \( k \) with respect to the three velocity components of the particle velocity NDF
- \( m_{L,k} \): \( k \)th moment of length-based NDF
- \( m_{M,k} \): \( k \)th moment of mass-based NDF
- \( m_{U,k} \): \( k \)th moment of velocity-based NDF
- \( m_{V,k} \): \( k \)th moment of volume-based NDF
- \( m_{\xi,k} \): moment of order \( k = (k_1, \ldots, k_M) \) of the multivariate NDF
- \( m_{\alpha} \): mass of particle of type \( \alpha \) taking part in collision
- \( m_{\beta} \): mass of particle of type \( \beta \) taking part in collision
- \( m_{\xi}^* \): moment definition used in EQMOM
- \( m_{\xi}^* \): reconstructed moment for the \( i \)th cell at time instant \( n \) in FVM
- \( m_{\xi,j,k}^* \): mixed moment of order \( j \) and \( k \) for the \( i \)th cell in FVM when using time splitting after convection
- \( m_{\xi,j,k}^* \): mixed moment of orders \( j \) and \( k \) for the \( i \)th cell in FVM when using time splitting after drag
- \( n \): generic NDF appearing in GPBE
- \( n_{eq} \): equilibrium NDF
- \( n_L \): length-based NDF
- \( n_M \): mass-based NDF
- \( n_V \): velocity-based NDF
- \( n_V \): volume-based NDF
- \( n_{\xi} \): generic NDF
- \( \langle n_{\xi} \rangle \): Reynolds-average NDF
- \( \hat{n} \): volume-average NDF
Notation

\( n^* \) reconstructed NDF

\( n^\alpha \) equilibrium Maxwellian NDF

\( n_{\alpha}^{[13]} \) NDF reconstructed in Grad’s 13-moment closure

\( n_m^{n}(\xi) \) NDF in the \( n \)th cell at time step \( m \) reconstructed in FVM (1D) from \( M^\alpha \)

\( n_{m}^{\pm}(\alpha) \) weights of the quadrature approximation calculated from the positive and negative moments of the velocity distribution

\( n_{i,k}^{n}(h) \) NDF in \( \Omega_{i,k} \) updated after advection in the \( h \) direction for FVM

\( n_{i,k}^{m} \) NDF in cell \( \Omega_{i,k} \) at time \( t = m \Delta t \) for FVM

\( n_{i,k}^{+) \) contribution for updating the NDF due to advection from positive velocity in cell \( \Omega_{i,k} \) for FVM

\( n_{i,k}^{-} \) contribution for updating the NDF due to advection from negative velocity in cell \( \Omega_{i,k} \) for FVM

\( p_f \) pressure of the fluid phase

\( p_{f1} \) partial pressure of evaporating component in gas phase

\( p_g \) pressure of the gas phase

\( p_{\text{ref}} \) reference pressure for boiling liquid

\( p_{\alpha} \) partial pressure of evaporating component on droplet surface

\( p_{\alpha} \) orthogonal polynomials of order \( \alpha \) used in functional expansion of NDF

\( p_{a} \) granular pressure of particles of type \( \alpha \)

\( q \) heat flux to surface of particle

\( q_{i} \) skewness of the NDF with respect to the \( i \)th velocity component

\( q \) total particle energy flux

\( s \) specific surface area of the porous medium

\( s \) ratio of geometric grids employed in CM

\( s \) particle surface area

\( t_{\alpha \beta} \) abscissa computed from Laguerre-polynomial recursion coefficients used in EQMOM

\( u \) generic known disperse-phase velocity (1D)

\( u(\xi) \) known particle velocity conditioned on internal coordinate \( \xi \)

\( u_{k} \) (with \( k = 0, 1, 2 \)) flow-dependent velocity parameters

\( u_{\alpha} \) velocity node \( \alpha \) of the quadrature approximation

\( u_{i,j}^{+} \) positive \( i \)-component of velocity evaluated at left face of cell \( \Omega_{i,j} \) in FVM (1D)

\( u_{i,j}^{-} \) negative \( i \)-component of velocity evaluated at right face of cell \( \Omega_{i,j} \) in FVM

\( [u_{i},u_{j}] \) disperse-phase stress tensor

\( v \) disperse-phase velocity (1D)

\( v_{l} \) fluid-phase velocity (1D)

\( v_{i}^{+} \) positive \( i \)-component of velocity evaluated at left face of cell \( \Omega_{i,j} \) in FVM

\( v_{i}^{-} \) negative \( i \)-component of velocity evaluated at right face of cell \( \Omega_{i,j} \) in FVM