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.

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Frontmatter
More Information

Contents

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 (QMOM) 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 throughly 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 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 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.

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