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Recent advances in well-posed Eulerian models for polydisperse multiphase flows

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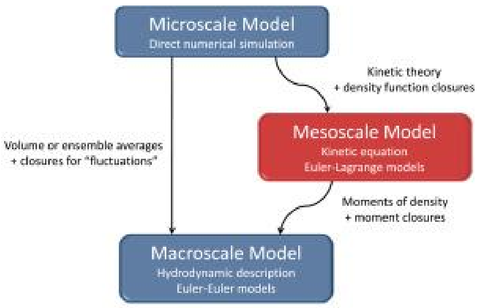
Highlights

- Kinetic-based modeling of polydisperse multiphase flows is reviewed.
- A multiscale modeling framework consisting of micro-, meso- and macroscale models is proposed.
- The links between the micro- and mesoscale and the meso- and macroscale models are described using gas–particle flow.
- The importance of verifying that the model is well-posed as each scale is emphasized.
- The multiscale modeling approach is shown to reproduce the correct physics over a wide range of parameters.

Abstract

The current state-of-the-art for computational modeling of polydisperse multiphase flows is reviewed and future research directions are discussed. Physics-based computational models at three distinct levels of abstraction: the microscale, mesoscale and macroscale; are discussed and compared. Special emphasis is placed on the relationship between the models at different scales and on how information from the finer scales is used to provide closures at the coarser scales. For disperse multiphase flows, it is argued that the passage from a direct-numerical simulation at the microscale to the kinetic description at the mesoscale is the crucial step for ensuring the validity of the macroscale model. In particular, the passage from the microscale to the mesoscale requires physics-based closures, while the passage from the mesoscale to the macroscale requires mathematical closures. The choices made in the physical and mathematical closures of the spatial fluxes and coupling terms will determine whether the Eulerian model is well-posed. In addition, the use of quadrature-based moment methods for polydisperse particles is presented as an efficient macroscale closure when dealing with a distribution of particle sizes. Examples of monodisperse and polydisperse multiphase flows are provided for cases where the fluid phase is compressible (high speed) and incompressible (low speed).

Graphical abstract



Mesoscale model incorporates more microscale physics in closures!

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Introduction

Polydisperse multiphase flows exist in many different forms and occur in numerous applications (Balachandar and Eaton, 2010, Guazzelli and Hinch, 2011, Deike, 2022, Brandt and Coletti, 2022, Morris, 2020, Capecelatro and Wagner, 2024, Capecelatro, 2022, Risso, 2018, Prosperetti, 2017, Voth and Soldati, 2017, Dufek, 2016). For the purposes of this work, a *disperse* multiphase flow consists of a disperse phase (gas, liquid or solid) and a continuous phase (gas or liquid). The individual elements making up the disperse phase are referred to as *particles* (e.g., bubbles, droplets, solid spheres, etc.). Furthermore, if the disperse phase is made up of particles with identical physical properties (volume, shape, density, temperature, composition, surface tension, etc.), then the flow is *monodisperse*. Otherwise, if some properties vary from particle to particle, then the flow is *polydisperse*. In either case, the particle velocities are allowed to be different for each particle, varying inside the flow due to surface stresses in the continuous phase and body forces acting on the particles. Other important subcategories for the particles are *deformable* and *non-deformable* and, for the continuous phase, *Newtonian* and *non-Newtonian* fluids. For clarity, in this work, the main focus is on monodisperse and non-deformable two-phase flows with Newtonian fluids, but the extension to polydisperse particles is also discussed (Fox et al., 2024). In any case, the modeling approaches are also applicable for more complex cases where, for example, the particles' shapes change due to hydrodynamic forces (as in the example in Fig. 1). Such polydisperse cases require additional variables (beyond mass and velocity) to describe the state of a particle (Marchisio and Fox, 2013, Essadki et al., 2019, Fox et al., 2024). This extension is briefly described for polydisperse gas–particle flows in Section 4.2.

The primary objective of this work is to provide a high-level overview of recent advances in formulating Eulerian models for polydisperse multiphase flow. In the literature, this type of model is referred to as a two-fluid (monodisperse) or a multi-fluid (polydisperse) model. Mathematically, such models consist of (at a minimum) continuum balances for the mass and momentum of the two phases (disperse, continuous) that are coupled together through various interfacial force terms. As shown in Fig. 2, there are at least two methods commonly used to derive these balance equations for polydisperse multiphase flows. However, one very important mathematical property needed for a well-posed two-fluid model is that the system of (inviscid) balance equations be *hyperbolic* (Lhuillier et al., 2013). In practice, the main cause of ill-posed multiphase flow equations is the Archimedes' force exerted by the continuous phase on the disperse phase, particularly for flows where the fluid material density ρ_f is larger than the particle density ρ_p (e.g., bubbly flows). As discussed in detail below, one of the most important recent advances is a globally hyperbolic Eulerian model based on a kinetic theory accounting for particle–particle interactions transmitted by the continuous fluid phase (Fox et al., 2020), which are referred to as the particle–fluid–particle (pfp) (Wang et al., 2021) or hydrodynamic (Spelt and Sangani, 1998) stresses.

It must be emphasized that kinetic-based models can only be applied to the disperse phase when it is made up of discrete particles, for example, with bubbles (Spelt and Sangani, 1998), droplets (Essadki et al., 2019), or solids (Gidaspow, 1994, Simonin et al., 1993). Thus, the Eulerian models described in this work are a subset of the two-fluid models used in the literature (Drew and Passman, 1999). For example, 1-D two-fluid models developed for (turbulent and/or segregated) gas–liquid flow in pipelines do not fall into the subset of kinetic-based Eulerian models. Another important distinction is that the kinetic-based models do not employ Reynolds averaging as is done in single-phase turbulence models. Thus, at high-enough Reynolds numbers, the flow predicted by a kinetic-based model will be turbulent at length scales much larger than the particle size. Therefore, in the limit where the volume fraction of the disperse phase α_p is very small, the continuous phase will be governed by the Navier–Stokes (or Euler) equation. In this sense, its numerical solution is a direct-numerical simulation (DNS) of the kinetic-based model. Nonetheless, a kinetic-based two-fluid model can also be Reynolds averaged or spatially filtered to develop a multiphase turbulence model (Fox, 2014, Fox, 2021, Ozel et al., 2013). However, this step is completely separate from the kinetic-based modeling discussed in this work.

As shown in Fig. 2, particle-resolved DNS (PR-DNS) is referred to as the *microscale* solution (Tenneti and Subramaniam, 2014, Elghobashi, 2019, Maxey, 2017), DNS of the kinetic-based model as the *mesoscale* solution, and DNS of the hyperbolic conservation equations derived from the kinetic-based model (i.e., the two-fluid model) as the *macroscale* solution. At each level of description, the number of conserved variables will be smaller as details at the finer level appear as constitutive equations at the coarser level. For example, the continuous-phase stresses at any point on a particle surface are known at the microscale, but are represented as a fluid–particle drag force for each particle at the mesoscale (i.e., averaging the point-wise stresses over the particle's surface). At the macroscale, only the fluid–particle drag force for the *average* particle velocity appears in the momentum balances. The modeling challenge is then to make the descriptions at the different levels be consistent with each other, especially for flows wherein the disperse-phase volume fraction is large enough to have strong particle–particle interactions.

The flow physics of polydisperse multiphase flows exhibit a strong dependence on the material density ratio $\mathscr{Z} = \rho_f/\rho_p$ and the disperse-phase volume fraction α_p. Generally speaking, it is more difficult to model flows with $\mathscr{Z} \gg 1$ (e.g., bubbly flows Spelt and Sangani, 1998) than with $\mathscr{Z} \ll 1$ (e.g., gas–solid flows Gidaspow, 1994). This is primarily because with larger $\mathscr{Z}$, the role of the fluid in determining the spatial fluxes and interfacial stresses is more important and multifaceted. For example, in gas–solid flows the principal coupling term is the fluid drag force on the particles, and particle-phase stresses arise due to particle–particle collisions. For these flows the added mass and lift forces (which scale with ρ_f) can usually be neglected. On the other hand, for bubbly flows the added-mass and lift forces are much larger than direct particle–particle collisions. Moreover, the pfp stresses (which scale with ρ_f Bulthuis et al., 1995) must be taken into account when $\mathscr{Z} > 0.1$ (e.g., solid–liquid sedimentation).

The mass loading, defined by $\varphi = \rho_p \alpha_p / \left(\rho_f \alpha_f\right)$ with continuous-phase volume fraction $\alpha_f = 1 - \alpha_p$, is also an important parameter that determines the multiphase flow regime. For example, with $\varphi \ll 1$, the continuous-phase momentum balance is weakly dependent on the disperse phase, while for $\varphi \geq 1$ most of the flow momentum is present in the disperse phase. Finally, another important quantity is the phasic slip velocity $\mathbf{u}_{pf} = \mathbf{u}_p - \mathbf{u}_f$ where $\mathbf{u}_p$ and $\mathbf{u}_f$ are the average velocities in the particle and fluid phases, respectively. For very small particles (i.e., Stokes number St near zero), the slip velocity can be neglected so that only the continuous-phase momentum balance must be solved, in which case the model is almost always well-posed. However, a very small, but finite, slip velocity leads to ill-posed models when $\mathscr{X} \gg 1$. In the kinetic-based approach, all important terms observed in PR-DNS can, in principle, be included so that the macroscale model will be applicable and well-posed for arbitrary values of $\mathbf{u}_{pf}$, φ, $\mathscr{X}$ and α_p.

The remainder of this work is organized as follows. In Section 2, the multi-scale modeling approach for polydisperse flows is discussed, as well as the important physical parameters that must be accounted for at the three different scales (microscale, mesoscale, macroscale). In Section 3, examples of the models developed at each of the scales are provided in order to familiarize the reader with the modeling challenges encountered at each scale and with how information from finer scales is used at the coarser scales. The two most common types of mesoscale models (Euler–Lagrange, kinetic equation) are also compared. In Section 4, a specific example of kinetic-based modeling of gas–particle flow is presented in sufficient detail to introduce the reader to this critical modeling step. Then, in Section 5, this kinetic model is employed to find the unclosed macroscale model equations, which are subsequently closed using quadrature-based moment methods (QBMM). Finally, in Section 6, example applications of the macroscale models are provided to demonstrate the wide range of physics that can be captured using well-posed Eulerian models. Conclusion are drawn in Section 7.

Section snippets

Computational modeling of polydisperse multiphase flow

Before going into details with specific examples, in this section, a bit more information about the modeling approach used for disperse multiphase flows is presented. In particular, the physical distinctions between the models used at the different scales are clearly discussed. Note that the term 'particle' is used to denote the property of a single particle, and 'particle-phase' to denote the average property of all particles. For example, at the microscale, the particle velocity $\mathbf{U}(t)$ and…

Examples of models at different scales

In this section, some specific examples of models used at the three scales shown in Fig. 2 are provided. Since it is the essential starting point for developing well-posed macroscale models, the mesoscale model based on kinetic theory is described in more detail than the microscale and macroscale models. Furthermore, the numerical methods needed to solve each type of model are briefly mentioned. Most importantly, the key conceptual points to understand from this section are (1) how the unclosed …

Mesoscale models for gas–particle flow

As shown in the previous section, a mesoscale model for gas–particle flow can be written as either an Euler–Lagrange model or as a kinetic model. In this section, specific examples of kinetic models are presented for gas–particle flow with added mass, starting with the monodisperse case. The kinetic model governs the mass-weighted NDF $f(t, \mathbf{x}, \mathbf{u})$

including added mass (Boniou et al., 2023), which is defined by $f(t, \mathbf{x}, \mathbf{u}) = \beta(t, \mathbf{x}) m_p n(t, \mathbf{x}, \mathbf{u}) = m_p^\star n(t, \mathbf{x}, \mathbf{u})$. Here, as before, $n(t, \mathbf{x}, \mathbf{u})$ is the number-based NDF,…

Macroscale models for gas–particle flow

In Section 3.3, a brief overview was presented on how a macroscale model is found from a mesoscale kinetic equation. Here, through the specific example of gas–particle flow from Section 4, further details are provided on how closure of the velocity moment equations leads to a closed macroscopic model. In addition, the issue of well-posed models is discussed, as well as how this property is verified using the macroscopic model equations for the particle and fluid phases. In the context of…

Example applications of macroscale models

In this section a few example applications of the macroscale models described in the previous section are provided. Each example is selected to highlight a particular aspect of the flow physics such as the frictional pressure and the pfp stresses. Results for both the monodisperse and the polydisperse models are presented. Because it is assumed that the flows are spatially homogeneous in directions normal to the flow direction, all the example applications can be simulated using the 1-D…

Conclusions

The kinetic-based approach for modeling polydisperse multiphase flows introduces an intermediate step between PR-DNS at the microscale and the Eulerian two-fluid model at the macroscale. In this work, the relationships between the models at the three different scales have been discussed. From a physical-modeling standpoint, the transition from the microscale to the mesoscale model is the critical step. In general, the most difficult challenge for this transition is the successful modeling of…

CRediT authorship contribution statement

Rodney O. Fox: Conceptualization, Data curation, Formal analysis, Funding acquisition, Investigation, Methodology, Project administration, Resources, Software, Supervision, Validation, Visualization, Writing – original draft, Writing – review & editing.…

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.…

Acknowledgments

Due to the huge number of high-quality scientific publications dealing with the topics covered in this work, I was unable to cite many significant contributions by numerous colleagues working in polydisperse multiphase flows. Despite this obvious shortcoming, I hope to have been able to have transmitted the general philosophy of kinetic-based modeling approaches to readers new to this field, and possibly to have inspired future research to bridge the scales identified in Fig. 2 and in…

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