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A drag model for filtered Euler–Lagrange simulations of clustered gas–particle suspensions

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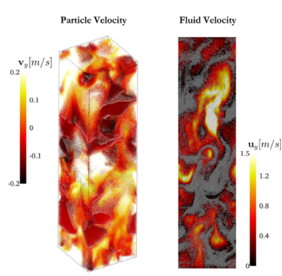
HIGHLIGHTS

- We use data from EL simulations to assemble a model for the filtered drag force.
- Corrections to gas–particle drag lead to superior predictions.
- We identify an approximate characteristic length scale of particle clusters.

GRAPHICAL ABSTRACT

Snapshots for the particle distribution colored by the vertical particle velocity (left, the gray surface indicates an isocontour at $\phi_p = 0.54$) and the vertical fluid velocity (right, a thin cross section through the computational domain is shown; $\langle \phi_p \rangle = 0.25$).



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ABSTRACT

Fluidized gas–particle systems are inherently unstable and they manifest structures on a wide range of length and time scales. In this article we present for the first time in the literature a coarse-grained drag force model for Euler–Lagrange (EL) based simulations of fluidized gas–particle suspensions. Two types of coarse graining enter into consideration: coarse fluid grids as well as particle coarsening in the form of parcel-based simulations where only a subset of particles is simulated. We use data from well-resolved EL simulations to assemble a model for the filtered drag force that examines fluid and particle coarsening separately. We demonstrate that inclusion of correction to gas–particle drag to account for fluid coarsening leads to superior predictions in a test problem. We then present an ad hoc modification to account for particle coarsening, which improves accuracy of simulations involving both fluid and particle coarsening. We also identify an approximate characteristic length scale that can be used to collapse the results for different gas–particle systems.

1. Introduction

Fluidized gas–particle suspensions play a key role in a variety of industrial processes, such as chemical looping combustion (Adanez et al., 2012), cracking of hydrocarbons (House et al., 2004), or granulation and coating processes relevant for the food and pharmaceuticals industry (Toschkoff and Khinast, 2013). Inhomogeneous flow structures that take the form of particle clusters and streamers or bubble like voids readily form in such systems (Agrawal et al., 2001; Glasser et al., 1998; Sundaresan, 2003), and affect key process characteristics such as the particle hold-up, the rate of heat and mass transfer, or the overall reaction rate (Agrawal et al., 2001; Holloway and Sundaresan, 2012; Igci and Sundaresan, 2010; Igci et al., 2008; Li et al., 2013).

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In process-scale simulations, it is computationally expensive to fully resolve the meso-scale structures, which span a wide range of length and time scales. There is now ample evidence that failure to resolve or account for the effects of meso-scale structures is one reason for inaccurate predictions afforded by coarse-grid simulations of Euler–Euler Two-Fluid-Models (Anderson and Jackson, 1967). Filtered suspension flow models, supplemented with suitably coarse-grained constitutive models for effective drag and stresses which strive to account for the effects of unresolved flow structures, are being developed and tested as candidates for coarse-grid simulations (Heynderickx et al., 2004; Igci and Sundaresan, 2010; Milioli et al., 2013; Ozel et al., 2013; Parmentier et al., 2012; Schneiderbauer and Pirker, 2014; Schneiderbauer et al., 2013; Wang et al., 2008; Zhang and van der Heyden, 2002). There is now a broad consensus on the structure and benefits of coarse-grained drag models for TFMs (Igci and Sundaresan, 2011; Parmentier et al., 2012; Wang et al., 2010; Yang et al., 2003). Recently, coarse-grained models for effective heat and mass transfer between particles and gas (Agrawal et al., 2013), as well as effective reaction rate in clustered gas–particle suspensions have also been proposed (Holloway and Sundaresan, 2012, 2010). A brief overview of the recent studies addressing the development of coarse-grained drag models is summarized in Table 1.

Similar issues arise in the case of Euler–Lagrange (EL) simulations as well, where either all the particles or a sub-set of representative particles (a.k.a. parcels) are tracked. Although some studies simply apply the microscopic drag model to simulate full-scale fluidized beds (Snider et al., 2011), recent work clearly indicates that an effective (filtered) drag model is necessary for EL simulations as well (Benyahia and Sundaresan, 2012). In fact, an ad hoc modification of the drag law to model the effective drag can be found even in the early work of Helland et al. (2007, 2005). Although some studies have used the filtered drag law designed for TFM-based simulations in coarse-grid EL simulations (Li et al., 2012; Ozarkar et al., 2013; Zou et al., 2008), questions remain. For example, when coarse-graining TFMs, one filters both the fluid and particle phase equations simultaneously and to the same spatial extent. In contrast, in EL simulations, the fluid and the particles can be coarsened separately. For example, one can opt to solve the locally-averaged fluid-phase equation using different fluid grid sizes while solving for the motion of all the particles in the system using a particle-scale fluid–particle interaction force model. Particle–particle collisions can then be modeled using, for example, the Discrete Element Method (Cundall and Strack, 1979). In EL simulations of this kind, the fluid–particle interaction force model should depend on the fluid grid resolution in order to capture the effect of sub-grid fluid flow structures; henceforth, we refer to this as fluid coarsening. Note, that such a fluid coarsening (for EL simulations) is not identical to the coarsening performed when using a filtered TFM-based simulation approach. Unfortunately, we could not find a conclusive model of how to correct for fluid coarsening in EL simulations in the literature.

Analogously, simulating only a subset of particles (parcels) can be thought of "particle coarsening", where each simulated particle is a proxy for a prescribed number of real particles (a.k.a. parcel size); in this case, the filtered drag law and the rules according to which the parcels interact with each other should, at least in principle, depend on parcel size, again to reflect the effect of fine-scale particle structure lost through the coarsening. As fluid and particle coarsening can be done independently, effective constitutive models (such as the drag law) should account for them independently, but, to the best of our knowledge, this issue is not addressed in the literature.

This consideration motivates the present study where we first examine how the drag law must be corrected to reflect fluid coarsening by systematically filtering the results from "well-resolved" simulations. The computational data to be filtered can be generated through (i) fully-resolved direct numerical simulations (Derksen and Sundaresan, 2007), or (ii) well-resolved EL simulations that use a particle-scale drag model commonly referred to as "CFD–DEM" (Hoomans et al., 1996; Zhou et al., 2010). Here we focus on the latter approach so that we can track several million particles in order to gather enough statistics on the meso-scale structures that form in fluidized gas–particle mixtures. Through systematic filtering of the data from such well-resolved simulations, we formulate a model for corrections to the gas–particle drag to capture the effect of fluid coarsening. We then demonstrate that simulations with coarse fluid grids can predict the average sedimentation velocity observed in the well-resolved simulations, provided fluid coarsening is accounted for in the drag model.

We then perform particle-coarsened (i.e. parcel-based) simulations, using the Discrete Particle Model (Patankar and Joseph, 2001), and a fluid-coarsened drag model. These CFD–DPM simulations revealed that the predicted average sedimentation velocity depends on parcel size, demonstrating that corrections for particle coarsening must also be accounted for in the gas–particle drag model. In this study we have not attempted to formulate a particle-coarsened drag model through systematic filtering (which will be a topic for a future study); instead, we will discuss the

Table 1
Overview of recent studies on drag modifications for coarse-grid simulations of sedimenting gas–particle suspensions (in chronological order).

Authors	*Year of publication*	*Type of simulation*	*Approach*	*Key influence parameter(s)*
Schneiderbauer et al.	2013–2014	Two-Fluid Model	Filtering and assumed cluster size distribution	Filtered volume fraction, slip velocity, and filter size; distinguish between resolved and unresolved clusters
Ozel et al., Parmentier et al.	2012–2013		Filtering of resolved simulation data	Filtered volume fraction and filter size; various flavors of structural models
Milioli et al., Igci et al.	2008–2013		Filtering of resolved simulation data	Filtered volume fraction, slip velocity, and filter size
Wang et al.	2010		Assumed porosity of the emulsion phase	Filtered volume fraction
Wang et al., Yang et al.	2003–2008		Assumed cluster size distribution	
Heynderickx et al.	2004		Assumed porosity of clusters	
Zhang and van der Heyden	2002		Filtering of resolved simulation data	Constant correction factor
Zou et al.	2008	Euler–Lagrange	Assumed cluster size distribution	Filtered volume fraction
Helland et al.	2005–2007		Ad hoc modification	