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Filtered sub-grid constitutive models for fluidized gas-particle flows constructed from 3-D simulations

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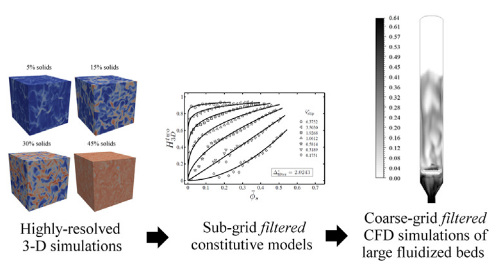
HIGHLIGHTS

- New coarse-grained *filtered* models for gas-particle flows.
- Filtered corrections for fluid-particle drag and solid/gas-phase stresses.
- More accurate CFD fluidized-bed predictions afforded using coarse grids.
- Filtered models validated using NETL/PSRI challenge problem.

GRAPHICAL ABSTRACT



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ABSTRACT

The accuracy of fluidized-bed CFD predictions using the two-fluid model can be improved significantly, even when using coarse grids, by replacing the microscopic kinetic-theory-based closures with coarse-grained constitutive models. These coarse-grained constitutive relationships, called *filtered* models, account for the unresolved gas-particle structures (clusters and bubbles) via sub-grid corrections. Following the previous 2-D approaches of Igci et al. [AIChE J., 54(6), 1431–1448, 2008] and Milioli et al. [AIChE J., 59(9), 3265–3275, 2013], new closures for the filtered inter-phase drag and stresses in the gas and particle phases are constructed from highly-resolved 3-D simulations of gas-particle flows. These new closure relations are then validated through the bubbling-fluidized-bed challenge problem presented by National Energy Technology Laboratory and Particulate Solids Research Inc.

1. Introduction

Gas-particle flows in fluidized and fast-fluidized beds manifest persistent fluctuations in particle volume fraction and phase velocities that span a wide range of length and time scales. These fluctuations are associated with clusters and streamers of particles in dilute flows and bubble-like voids at higher particle volume fractions. Although the formation of such structures, which can be as small as a few particle diameters, is predicted by two-fluid models supplemented with simple phenomenological relationships (Glasser et al., 1996, 1997; Glasser et al., 1998) or more elaborate kinetic theory-based closures for particle phase stress (Ding and Gidaspow, 1990; Gidaspow, 1994), resolving them explicitly

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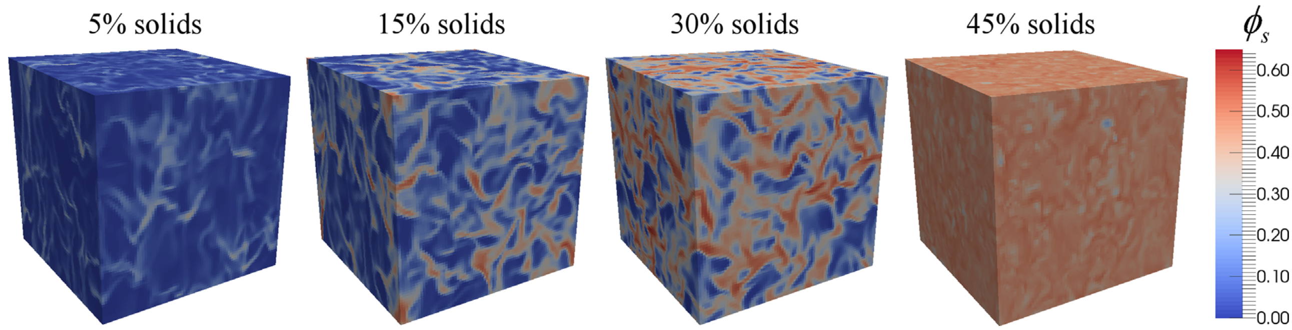

Fig. 1. Snapshots of particle volume fraction fields obtained in highly resolved, 3-D simulations of gas-fluidization in periodic domains for different domain-averaged solids loading (5, 15, 30 and 45 vol%). The color corresponds to local solid fraction ϕ_s. Results from such highly resolved simulations are analyzed to construct coarse-grained constitutive relations for filtered two-fluid models. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

using a sufficiently fine grid is impractical: $O(10^6)$ cells would be required for two-dimensional (2-D) simulations and $O(10^9)$ cells for three-dimensional (3-D) simulations of commercial-scale devices, which are well beyond current computational capabilities (Sundaresan, 2000).

Filtered two-fluid models suitable for coarse-grid simulations seek to account for the effects of fine-scale (unresolved) particle clusters and gas bubbles on the resolved flow via coarse-grained closure models. This approach is similar to large-eddy simulations of single-phase turbulent flows (Pope, 2000). As discussed below, several research groups have sought to formulate coarse closures on the basis of statistics generated by systematically filtering results from highly resolved simulations of flows in model geometries. Our research group has previously published constitutive models deduced from highly resolved flows simulations of fluidization in 2-D periodic domains (e.g., see Igci and Sundaresan (2011a), and Milioli et al. (2013)).

In the present study, highly resolved simulations of gas-particle flows have been performed in 3-D periodic domains (Fig. 1), and analyzed to construct new 3-D filtered models for gas-particle drag, as well as stresses in the gas and particle phases. Comparison of these models with previously developed 2-D corrections exposes the similarities and differences. The present study also proposes a new model for the solids stress anisotropy. The influence of solids-phase material properties on the closures is briefly explored by performing a few additional simulations with smaller and denser particles. Coarse-grid simulations of the National Energy Technology Laboratory (NETL)/ Particulate Solids Research Inc. (PSRI) bubbling fluidized bed challenge problem (Shadle et al., 2011) are then performed to assess the predictions afforded by the filtered closure relations proposed in this study.

2. Background

It is straightforward to coarse-grain the two-fluid model and obtain the general form of the filtered two-fluid model (Fox, 2014; Igci et al., 2008; O'Brien, 2014). One is then left with the task of developing coarse-grained closure relations for the fluid-particle interaction force and the effective stresses in the gas and particle phases. From a budget analysis, Parmentier et al. (2012) identified the correction to the gas-particle drag to be the most significant, with the effective stresses playing a lesser role. Indeed, modified drag coefficients that account for the effects of clusters have been proposed much earlier in the literature (Li and Kwauk, 1994), while deducing coarse-grained closures through systematic filtering of highly resolved simulation results is relatively more recent (Andrews et al., 2005; Igci et al., 2008; Igci and Sundaresan, 2011a; Milioli et al., 2013). The highly resolved simulations can be grouped into different categories: fluidization in (i) periodic domains (Andrews et al., 2005; Igci et al., 2008; Igci and Sundaresan, 2011a; Milioli et al., 2013), (ii) small beds including gas entrance, bounding walls, and gas exit (Igci and Sundaresan, 2011b; Parmentier et al., 2012), and (iii) periodic segment of a riser (Özel et al., 2013). Most studies focused on 2-D simulations, while few have considered 3-D systems. Although some quantitative differences are found in the closures obtained through these different test problems, the general characteristics of coarse closures remain very similar. More recently, Sarkar et al. (2013, 2014b) extended this method and developed the filtered drag models for fluidized beds with immersed cooling tube arrays.

Not surprisingly, the filter size Δ_{filter} (see Fig. 2) is a key parameter in the coarse-grained closures. Additionally, the filtered particle volume fraction, $\bar{\phi}_s$, emerges as an important marker characterizing the sub-filter scale structures in every model proposed thus far. Models involving only $\bar{\phi}_s$ to characterize the sub-filter scale (Igci et al., 2008; Igci and Sundaresan, 2011a; Parmentier et al., 2012; Ozel et al., 2013; Sarkar et al., 2013) are henceforth referred to as *one-marker* models. It should be noted that the model by Parmentier et al. (2012) includes a dynamic correction, which could be viewed as an implicit second marker. Although verification (Igci and Sundaresan, 2011b; Sarkar et al., 2014b) and validation (Igci et al., 2012) studies with the

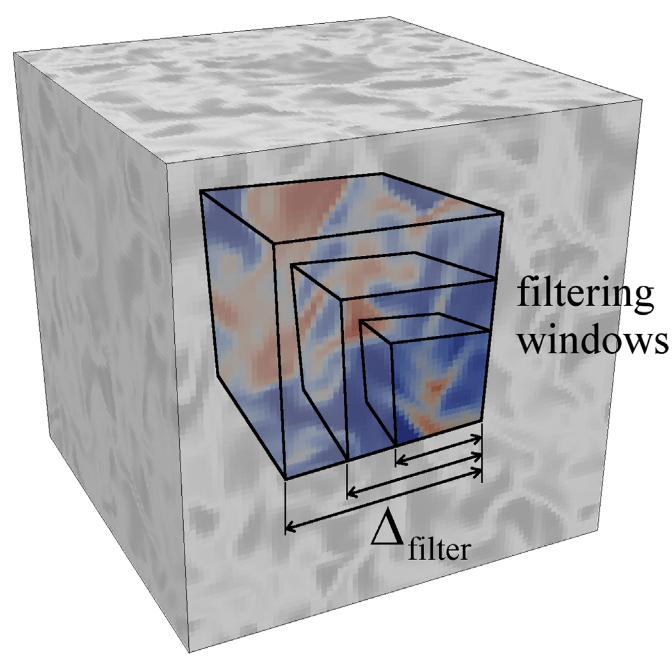

Fig. 2. Schematic of the filtering procedure, showing filtering windows of different sizes constructed within the periodic domain. For each snapshot, windows of varying sizes and at various locations are constructed to gather filtered statistics.