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Direct numerical simulation of gas–solid suspensions at moderate Reynolds number: Quantifying the coupling between hydrodynamic forces and particle velocity fluctuations

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ABSTRACT

Predictive device-level computational fluid dynamics (CFD) simulation of gas–solid flow is dependent on accurate models for unclosed terms that appear in the averaged equations for mass, momentum and energy conservation. In the multifluid theory, the second moment of particle velocity represents the strength of particle velocity fluctuations and is known to play an important role in the prediction of core-annular flow structure in risers (Hrenya and Sinclair, AIChEJ, 43 (4) (1994) [5]). In homogeneous suspensions the evolution of the second velocity moment is governed by the particle acceleration–velocity covariance. Therefore, fluctuations in the hydrodynamic force experienced by particles in a gas–solid flow affect the evolution of particle velocity fluctuations, which in turn can affect the mean and variance of the hydrodynamic force. This coupling has been studied in the limit of Stokes flow by Koch and co-workers using a combination of kinetic theory and multipole expansion simulations. For Reynolds numbers beyond the Stokes limit, direct numerical simulation is a promising approach to quantify this coupling. Here we present direct numerical simulation (DNS) results for the evolution of particle granular temperature and particle acceleration variance in freely evolving homogeneous gas–solid suspensions. It is found that simple extension of a class of mean particle acceleration models to their corresponding instantaneous versions does not recover the correlation of particle acceleration with particle velocity. This study motivates the development of better instantaneous particle acceleration models that are able to accurately capture the coupling between particle acceleration and velocity.

1. Introduction

Gas–solid flows are commonly encountered in energy generation and chemical processing. The design and scale-up of industrial devices motivate a better understanding of gas–solid flow characteristics and transport phenomena. A fundamental understanding of gas–solid flow is increasingly relevant with renewed interest in zero-carbon and carbon-negative energy generation technology such as chemical looping combustion.

Computational fluid dynamics (CFD) simulations that solve for averaged equations of multiphase flow are being increasingly used in the design process because they provide detailed information about the solid volume fraction and phasic mean velocity fields in gas–solid flow [1]. Most CFD codes for device-level simulations of gas–solid flow are based on the Eulerian–Eulerian (EE) multifluid approach because these are computationally less expensive than Lagrangian–Eulerian (LE) simulations. In the EE multifluid approach both the solid and fluid phases are treated as interpenetrating continua, and averaging techniques [2–4] are used to derive the equations governing the conservation of average mass and momentum in the fluid and particle phases. This results in a closure problem similar to that encountered in the statistical theory of single-phase turbulence because the averaging procedure results in unclosed terms that need to be modeled. For instance, the mean momentum conservation equation in the particle phase requires closure of the average fluid–particle interaction force (mean drag force) and the average stress in the solid particle phase. Accurate models for these unclosed terms are needed for predictive CFD simulation of gas–solid flow.

As with all statistical closures, an important modeling question is the adequacy of the mathematical representation to capture physical phenomena of engineering relevance. For instance, it is now established that the prediction of core-annular structure in riser flows requires solving the transport equation for the particle granular temperature or pseudo-thermal energy [5]. This informs us that a closure at the level of mean quantities is not adequate to predict important flow characteristics such as core-annular structure, but a

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closure at the level of second moments is necessary. However, it is not clear that closure at the level of the second moments is sufficient for predictive CFD simulation that will facilitate design and scale-up. Closure at the level of third-order moments has been attempted by some researchers [6,7].

An alternative approach to the closure of moment transport equations is to consider the evolution of the one-particle distribution function. Just as closure at the level of the transport equation for the probability density function (PDF) in single-phase turbulent reactive flow implies a closure for all moment equations, similarly a kinetic equation that achieves a closure for the one-particle distribution function in kinetic theory implies a closure for all moment equations. In particular, a closure at the one-particle distribution level automatically implies closure of the mean momentum and particle velocity second moment equations. Furthermore, closures at the one-particle distribution level are guaranteed to satisfy realizability criteria, whereas special care is needed to ensure the same in the case of moment closures. These considerations motivate the development of models for the unclosed terms in the transport equation for the one-particle distribution function corresponding to gas–solid flow.

While there is considerable work on kinetic theory of granular flows where the interaction with ambient fluid is neglected, the kinetic theory of gas–solid flow is still being developed. For low Reynolds number flow in the Stokes regime, Koch and co-workers [8,9] developed a kinetic theory closure with a model for the conditional particle acceleration that accounts for the presence of ambient fluid in the term transporting the distribution function in velocity space. This theoretical framework allows us to consider two coupled effects: (i) the effect of particle velocity fluctuations on the mean drag, and (ii) the effect of fluctuating particle acceleration on particle velocity fluctuations or granular temperature. Wylie et al. [10] studied the effect of particle velocity variance on the mean drag for the limiting case of high Stokes number where the particles move under elastic collisions but are unaffected by hydrodynamic forces. They showed that particle velocity fluctuations do not affect the mean drag in Stokes flow. This result is not surprising because in Stokes flow the particle acceleration is a linear function of instantaneous particle velocity. However, at moderate mean slip Reynolds numbers the drag law is nonlinear and Wylie et al. [10] showed that particle velocity fluctuations do affect the mean particle acceleration. They proposed a modified drag law in terms of volume fraction ϕ, mean flow Reynolds number Re_m and Reynolds number based on particle granular temperature Re_T. The focus of this paper is on the second effect: the effect of fluctuating hydrodynamic forces on granular temperature.

For statistically homogeneous gas–solid flows, the correlation between the particle fluctuating velocity and its acceleration fluctuation determines the evolution of the particle velocity second moment. In the limiting case of Stokes flow, Koch [8,9] analyzed the granular temperature, which is the trace of the particle velocity second moment, and decomposed the particle acceleration–velocity covariance as the sum of source and sink contributions. Particle granular temperature decreases due to inelastic collisions and viscous interactions with the ambient fluid, and these effects are represented by the sink term. If particle collisions are elastic or flow past fixed particle assemblies is considered, then the granular temperature decreases only due to viscous interactions with the ambient fluid. In the Stokes flow regime the sink term simply relaxes the granular temperature to zero on the viscous relaxation time scale. In Koch's decomposition of the acceleration–velocity covariance into source and sink terms [9], the source term due to hydrodynamic interactions with neighboring particles can balance the sink term leading to a steady state granular temperature in stable homogeneous suspensions. For moderate Reynolds number, there is no unique decomposition of the particle acceleration–velocity covariance as the sum of source and sink contributions.

The source term in the granular temperature equation plays an important role in sustaining a nonzero value of the granular temperature. In its absence the granular temperature in a homogeneous suspension would simply decay to zero, leading to an infinite Mach number in the particle phase. Not only is this problematic from a numerical standpoint for CFD simulations, but it is also unphysical over a wide range of mean flow Reynolds number and volume fraction. The origin of the source term lies in the hydrodynamic interactions that each particle experiences with its neighbors, and the range of this interaction depends on the mean flow Reynolds number and the solid volume fraction. It is well known that a sphere sedimenting in a fluid can have a “drafting” effect on its neighbors and draw them into its wake. The draft, kiss and tumble phenomena are well documented in [11]. These physical mechanisms can manifest as a source in particle velocity fluctuations by changing each particle's velocity. This effect is quantified through DNS of freely evolving suspensions in this work.

Although Koch's analysis is useful in the Stokes flow regime, it is difficult to extend the analysis to moderate Reynolds number cases. At moderate Reynolds number, DNS offers a promising approach to quantify unclosed terms in the transport equations for particle velocity moments, or the transport equation for the one-particle distribution function. This naturally leads to an evaluation of existing models. We use DNS of gas–solid flow at moderate Reynolds number to evaluate a class of acceleration models. The results indicate the need for improved instantaneous particle acceleration models that are capable of capturing the coupling between particle velocity fluctuations and hydrodynamic forces in gas–solid flow.

The next section describes pertinent details of the statistical modeling approach that motivate this study. This is followed by a description of the Particle-resolved Uncontaminated-fluid Reconcilable Immersed Boundary Method (PUReIBM) that is used to perform DNS of gas–solid flow. Then the simulation details for fixed particle assemblies and freely moving suspensions are presented. Results that quantify the coupling are reported, and a class of particle acceleration models is evaluated. Finally, the conclusions of this study are summarized.

2. Statistical models

The averaged equations for mean momentum conservation and transport of the second moment of particle velocity in the multifluid theory can be derived using either the Eulerian–Eulerian or Lagrangian–Eulerian approach. A comprehensive summary of the relations between the moment equations obtained from these statistical approaches can be found in [12]. Here we choose the Lagrangian–Eulerian approach with the one-particle distribution function as our starting point because it naturally leads to an explicit connection with the moment equations.

2.1. One-particle distribution function

The one-particle distribution function, which is the number density of particles in an appropriately defined phase space, is the fundamental quantity of interest in the kinetic theory of granular and multiphase flow [8,14–17]. It is also referred to as the droplet distribution function in spray theory [18]. For monodisperse particles the distribution function $f(\mathbf{x}, \mathbf{v}, t)$ is defined in a position–velocity space, and evolves by the following transport equation:

$$\frac{\partial f}{\partial t} + \nabla_{\mathbf{x}} \cdot (\mathbf{v} f) + \nabla_{\mathbf{v}} \cdot (\langle \mathbf{A} | \mathbf{x}, \mathbf{v}; t \rangle f) = \dot{f}_{\mathrm{coll}}, \tag{1}$$

where $\boldsymbol{\nabla}_{\mathbf{x}}$ and $\boldsymbol{\nabla}_{\mathbf{v}}$ denote the gradient operators in the position and velocity space, respectively, and $\dot{f}_{\mathrm{coll}}$ is the collisional term that can depend on higher-order statistics. A closure model for the collisional term results in a kinetic equation. This well-known equation has been extensively studied in the context of granular flows where collisions