Instantaneous particle acceleration model for gas-solid suspensions at moderate Reynolds numbers

Sudheer Tenneti  
*Iowa State University*, sudheert@gmail.com

Rodney O. Fox  
*Iowa State University*, rofox@iastate.edu

Shankar Subramaniam  
*Iowa State University*, shankar@iastate.edu

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Keywords
Immersed boundary method, DNS, drag laws, granular temperature

Disciplines
Biomechanical Engineering | Catalysis and Reaction Engineering | Chemical Engineering | Mechanical Engineering

Comments

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Instantaneous particle acceleration model for gas–solid suspensions at moderate Reynolds numbers

S. Tenneti*, R. O. Fox† and S. Subramaniam∗

* Department of Mechanical Engineering, Iowa State University, Ames, IA 50011, USA
† Department of Chemical and Biological Engineering, Iowa State University, Ames, IA 50011, USA
sudheert@iastate.edu, rofox@iastate.edu, shankar@iastate.edu

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Abstract

Gas–solid flows are encountered in many industrial applications such as fluidized beds and coal gasification. The design and scale-up of such industrial devices requires a better understanding of the characteristics of gas–solid suspensions. Device-scale computational fluid dynamics (CFD) simulations that solve for average quantities such as solid volume fraction and phasic mean velocity fields are being extensively used in the industrial design process. The capability of these simulations to accurately predict the characteristics of gas–solid flow depends upon the accuracy of the models for unclosed terms that appear in the equations for mass, momentum and energy conservation. Hrenya and Sinclair (1997) show that the particle granular temperature (particle velocity variance) plays an important role in the prediction of the core annular structure in riser flows. In statistically homogeneous suspensions undergoing elastic collisions, the particle acceleration–velocity covariance alone governs the evolution of granular temperature. This acceleration–velocity covariance can be decomposed into a source and dissipation of granular temperature due to hydrodynamic forces. Koch and co-workers (Koch 1990; Koch and Sangani 1999) quantified the hydrodynamic source and dissipation terms in the granular temperature evolution using a combination of kinetic theory closure and multipole expansion simulations at very low Reynolds numbers (Stokes flow regime). At moderate Reynolds numbers, particle-resolved direct numerical simulation (DNS) is as a viable tool to quantify the hydrodynamic source and dissipation. In this study, DNS of freely evolving gas–solid suspensions are performed using the Particle-resolved Uncontaminated-fluid Reconcilable Immersed Boundary Method (PURelIBM) that has been developed at Iowa State University to simulate flow past fixed particle assemblies (Garg et al. 2009) and freely evolving suspensions (Tenneti et al.). Analysis of DNS results shows that the fluctuations in the particle acceleration that are aligned with the fluctuations in the particle velocity give rise to source in the granular temperature. It is found that simple extension of a class of mean particle acceleration models to their corresponding instantaneous versions does not predict the correct joint acceleration–velocity statistics that are obtained from DNS. Also such models do not give rise to any source in the granular temperature due to hydrodynamic effects. This motivates the development of better instantaneous particle acceleration models. It is found that a Langevin equation for the increment in the particle velocity reproduces the DNS results for particle velocity autocorrelation in freely evolving suspensions.

Introduction

Particle–laden flows are very common in many industrial applications like fluidized bed combustors, coal gasification, pneumatic transport lines etc. In addition to the industrial significance of gas–solid flows, the complexity of the physical mechanisms that govern these flows attracts the attention of many researchers. Furthermore, a fundamental understanding of gas–solids flow is relevant due to increasing interest in carbon–neutral energy generation technologies such as chemical looping combustion (Li and Fan 2008).

Computational fluid dynamics (CFD) simulations that solve for the averaged equations of multiphase flow are a cost-effective solution for rapid evaluation of design and scale up of industrial devices like fluidized beds. Device-scale CFD simulations are usually based on the Eulerian–Eulerian two-fluid approach in which averaged equations for conservation of mass, momentum and energy are written for each phase, with coupling terms representing the interphase interactions. These equations contain unclosed terms that need to be modeled. For example, 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. Therefore, the predictive capability of multiphase CFD simulations depends on the models for interphase exchange of species, momentum, and heat. In this work we only consider closure models for the interphase momentum transfer.

In any statistical closure problem, an important modeling question is the adequacy of the mathematical representation to capture physical phenomena. Hreya and Sinclair (1997) show that it is necessary to solve the transport equation for the particle granular temperature to predict the core–annular structure observed in riser flows. This shows that closure only at the level of the mean momentum is not adequate, but a closure at the level of second moment of particle velocities is necessary. But it is not clear if closure at the level of second moments is adequate for predictive CFD simulations.

The objective of this work is to use direct numerical simulations (DNS) to propose a particle acceleration model that provides a closure for all moment equations. In order to achieve this objective we consider the evolution of the one–particle distribution function. The advantage of this approach is that closure at the level of the one–particle distribution function implies a closure for all the moment equations. Tennen et al. discussed in detail the evolution equation of the one–particle distribution function for gas–solids flow and analyzed existing models used to close the conditional expectation of the particle acceleration term that appears in the evolution equation. They showed that simple extension of mean particle acceleration models does not predict the correct particle acceleration–velocity covariance obtained from DNS. A consequence of the use of such models in CFD codes is that the granular temperature will decay to zero resulting in physically incorrect behavior and triggering numerical instabilities.

For statistically homogeneous gas–solids flow with perfectly elastic solid particles, the particle granular temperature evolves only due to the correlation between the fluctuating particle acceleration and the fluctuating particle velocity. For dilute suspensions in the Stokes flow regime Koch (1990) decomposed the particle acceleration–velocity covariance into source and sink contributions arising due to hydrodynamic interactions and derived the corresponding analytical expressions for these terms. Later Koch and Sangani (1999) used an approximate multipole expansion method to specify the source and sink terms for higher solid volume fractions in the Stokes flow regime. At moderate mean flow Reynolds numbers, Tennen et al. reported DNS results that confirm Koch’s observation (in the Stokes flow regime) that particle velocity fluctuations correlate with particle acceleration fluctuations to generate a source in the granular temperature.

In this study, DNS of freely evolving gas–solid suspensions are performed using the Particle–resolved Uncontaminated-fluid Reconcilable Boundary Method (PUREIBM) that has been developed at Iowa State University to simulate flows past fixed particle assemblies (Garg et al. 2009) and freely evolving suspensions (Tennen et al.). PUREIBM is a particle-resolved direct numerical simulation approach for gas–solid flow with the following features that distinguish it from other immersed boundary method approaches:

1. Uncontaminated fluid: In PUREIBM the immersed boundary (IB) forcing is solely restricted to those grid points that lie in the solid phase, and therefore the flow solution in the fluid phase is uncontaminated by the IB forcing. Consequently the velocity and pressure in the fluid phase is a solution to the unmodified Navier-Stokes equations (in contrast to IB implementations that smear the IB forcing on to grid points in the fluid phase adjoining solid boundaries, resulting in solution fields that do not correspond to unmodified Navier–Stokes equations).

2. Reconcilable: In PUREIBM the hydrodynamic force experienced by a particle is computed directly from the stress tensor at the particle surface that is obtained from this uncontaminated fluid flow solution (in contrast to IB implementations that calculate the hydrodynamic force from the IB forcing field). This feature of PUREIBM enables us to directly compare the DNS solution with any random-field theory of multiphase flows. In particular, for statistically homogeneous suspensions it is shown that (Garg et al. 2009) if the volume-averaged hydrodynamic force exerted on the particles by the fluid is computed from a PUREIBM simulation, it is a consistent numerical calculation of the average interphase momentum transfer term \( \left\{ \tau_{ij}^{(p)} \delta (x - x^\Gamma) \right\} \) in the two-fluid theory (Drew 1983). This reconciles DNS results with multiphase flow theory.

Owing to these specific advantages, it is shown elsewhere (Garg et al. 2009; Garg 2009) that PUREIBM is a numerically convergent and accurate particle-resolved DNS method for gas–solids flow. Its performance has been validated in a comprehensive suite of tests (i) Stokes flow past simple cubic (SC) and face centered cubic (FCC) arrangements (ranging from dilute to close-packed limit) with the boundary–integral method of Zick and Hornsby (1982), (ii) Stokes flow past random arrays of monodisperse spheres with LBM simulations of van der Hoef et al. (2005) (iii) moderate to high Reynolds numbers (Re_m \( \lesssim 300 \)) in SC and FCC arrangements with LBM simulations of Hill et al. (2001)
and (iv) high Reynolds number flow past random arrays of monodisperse spheres with ANSYS–FLUENT CFD package. It has also been extended to study passive scalar transport, and validated for heat transfer from a single isolated sphere (Garg 2009; Garg et al.). In this work, the DNS methodology based on PUReIBM developed by Tenneti et al. to simulate freely evolving suspensions is used to propose an instantaneous particle acceleration model that incorporates the effect of particle velocity fluctuations and hydrodynamic effects of neighboring particles.

The rest of the paper is organized as follows. First the instantaneous particle acceleration model is described. Results from the simulations of freely evolving suspensions and verification of the Langevin model are discussed next. Finally, a procedure for determining the coefficients of the acceleration model is described.

**Instantaneous particle acceleration model**

We propose the following stochastic model for the increment in the particle velocity:

\[ dv_i = -\beta \langle W_i \rangle dt - \gamma v_i^n dt + BDW_i, \]  \hspace{1cm} (1)

The above equation is an isotropic form of the general Langevin model developed by Tanneti and Subramaniam. In the above equation \( dv_i \) is the increment in the particle velocity, \( v_i^n \) is the fluctuation in the particle velocity and \( dW_i \) is a Wiener process increment. Fluctuations in the particle velocity are defined about the mean particle velocity, i.e., \( v_i^n \equiv v_i - \langle v_i \rangle \). The first term on the right hand side of Eq. 1 accounts for the effect of the mean slip velocity. The mean slip velocity, defined as \( \langle W \rangle = \langle v \rangle - \langle u_f \rangle \), is the relative velocity between the solid phase mean velocity and the fluid phase mean velocity. The second term accounts for the fluctuation in the particle velocity and the last term models the effect of the hydrodynamic interaction of the neighboring particles. The coefficient \( \gamma \) is the inverse of the Lagrangian particle velocity autocorrelation time. It quantifies how long a particle retains memory of its initial velocity. These coefficients are functions of volume fraction \( \phi \), mean flow Reynolds number \( Re_m \) and particle to fluid density ratio \( \rho_p/\rho_f \). To extract a functional form for the Langevin model coefficients, simulations of freely evolving suspensions where the motion of the particles is affected by the surrounding fluid, are performed using the DNS methodology developed by Tenneti et al. Results from the simulations freely evolving suspensions are presented in the following section.

**Results**

IBM simulations of freely evolving suspensions are performed for solid volume fractions between 0.1 and 0.4 and for mean flow Reynolds numbers between 10 and 100. The Reynolds number based on the mean slip velocity between the fluid and particulate phase is defined as

\[ Re_m = \frac{(1 - \phi) \rho_f |\langle v \rangle - \langle u_f \rangle| \varsigma_f}{\mu_f}, \]  \hspace{1cm} (2)

where \( \phi \) is the solid volume fraction, \( \rho_f \) and \( \mu_f \) are the density and dynamic viscosity of the fluid phase respectively, and \( \varsigma_f \) is the particle diameter. When characterizing the effect of particle velocity fluctuations it is useful to define a Reynolds number based on the granular temperature \( Re_T \) as:

\[ Re_T = \frac{\rho_f \varsigma_f T^{1/2}}{\mu_f}, \]  \hspace{1cm} (3)

where \( T \) is the granular temperature which is given by \( T = \frac{1}{2} \langle v_i^n v_i^n \rangle \). Estimation of granular temperature from DNS of freely evolving suspensions is discussed in detail by Tenneti et al.. The evolution of \( Re_T \) for a freely evolving suspension at a volume fraction of 0.1 and solid to fluid density ratio of 100 is shown in Fig. 1. Firstly, we observe that for all mean flow Reynolds numbers, the granular temperature attains a statistical steady state. From the figure we can also see that at a given solid to fluid density ratio, the steady state granular temperature
increases with increasing mean flow Reynolds number. This result can be explained based on the fact that the particles pick up energy from the fluid and the energy in the system increases with increasing Re_m. To the authors’ knowledge, this is the first report of the effect of mean flow Reynolds number on granular temperature. Similar behavior of the steady granular temperature with Re_m is observed for all the volume fractions studied (φ = 0.1, 0.2, 0.3 and 0.4). The Langevin model for the particle acceleration is verified by computing the particle velocity autocorrelation function after the granular temperature reaches a steady state.

Verification of Langevin model. In this section, verification of the Langevin model for the instantaneous particle acceleration is presented. For this purpose we consider the increment in the particle velocity fluctuations:

$$d\nu^n_1 = -\gamma \nu^n_1 dt + B \nu^n_1.$$

(4)

As described earlier, in the above equation the model coefficient $\gamma$ is the inverse of the integral time scale of the particle velocity autocorrelation. The particle velocity autocorrelation function $\rho(s)$ is defined as follows:

$$\rho(s) = \frac{\langle \nu^n_1(t_0) \nu^n_1(t_0+s) \rangle}{\langle \nu^n_1(t_0) \nu^n_1(t_0) \rangle}$$

where $s$ is the separation in time. The integral time scale for the autocorrelation function is defined as $T_\rho = \int_0^\infty \rho(s) ds$. Using this definition, we computed the integral time scale from DNS after the granular temperature reached a steady state. If a stochastic process obeys the Langevin equation with an integral time scale of $T_\rho$, then its autocorrelation function should decay exponentially, i.e., $\rho(s) = e^{-s/T_\rho}$. We extracted the autocorrelation function from the DNS and compared it with the exponential function predicted by the Langevin model. This comparison is shown in Fig. 2. We can see that for both density ratios considered, the evolution of the autocorrelation function obtained from DNS matches with the exponential decay predicted by the Langevin model.

We established that Langevin model predicts the dynamics of a freely evolving suspension very well after the granular temperature reaches steady state. However, at a given volume fraction, mean flow Reynolds number and solid to fluid density ratio, we need to specify the coefficients as a function of the granular temperature so that we can predict the evolution of the suspension using the Langevin model. In order to do this, we have to identify the source and dissipation of granular temperature from the DNS data. In the next section, a method to identify source and dissipation of granular temperature from DNS is presented.

Identification of source and dissipation from DNS. Using the Langevin model for the increment in the particle velocity fluctuations (cf. Eq. 2), we can derive the evolution equation for the modeled granular temperature $T^*$ as:

$$\frac{dT^*}{dt} = -2\gamma T^* + B^2.$$

(5)

In the above equation, we can clearly identify that the source for the granular temperature is $B^2$ and that the dissipation is $2\gamma T^*$. For a statistically homogeneous suspension, the evolution equation for the granular temperature can be written as:

$$\frac{dT}{dt} = \frac{2}{3} \langle A^n_1 \nu^n_1 \rangle.$$
where the source is,

\[
S = -\frac{2}{3} \frac{1}{N_p} \sum_{n=1}^{N_p} \zeta^{(n)} \nu^{(n)} \nu^{(n)}
\]

and the dissipation is

\[
\Gamma = -\frac{2}{3} \frac{1}{N_p} \sum_{n=1}^{N_p} \zeta^{(n)} \nu^{(n)} \nu^{(n)}
\]

In the above expressions for source and dissipation, \( \zeta^{(n)} = \frac{1}{2} (\zeta^{(n)} + |\zeta^{(n)}|) \) and \( \nu^{(n)} = \frac{1}{2} (\zeta^{(n)} - |\zeta^{(n)}|) \).

From these equations, it is clear that the particles whose fluctuating acceleration is aligned with the fluctuating velocity contribute to the source in granular temperature. Particles with the fluctuating acceleration aligned in a direction opposite to that of the fluctuating velocity contribute to the dissipation in granular temperature. This can be easily visualized from the scatter plot shown in Fig. 3. For illustration, in this figure we show the scatter plot of fluctuating particle acceleration and fluctuating particle velocity obtained from the DNS of flow past a fixed particle array \((\phi = 0.2, \text{Re}_{m} = 20 \text{ and } \text{Re}_{T} = 16) \). The symbols that lie in the first and the third quadrants denote the particles whose fluctuating acceleration is aligned with the fluctuating velocity. Hence, these particles contribute to the source in granular temperature. Similarly, the symbols in the second and fourth quadrants contribute to the dissipation in granular temperature. Tenny et al. show that a simple extension of mean particle acceleration model applied to any particle velocity distribution does not produce any scatter in the first and third quadrants. They demonstrate that such instantaneous acceleration models do not produce any source in the granular temperature evolution equation. On the other hand, a stochastic acceleration model (cf. Eq. 1) always results in a finite source term for the particle granular temperature for non-zero \( B \).

We wish to know if the steady state attained by the suspension is a stable attractor. We can verify this by studying suspensions with different initial conditions. Using the formulas given by Eq. 6 and Eq. 7, we extracted the source and dissipation from the DNS data and plotted them versus the granular temperature in Fig. 4 as a phase space plot. The state of the system is characterized by the granular temperature \( T \) and in phase space plots, the rate of change of the state variable \( \frac{dT}{dt} \) is plotted versus the state variable \( T \). But the rate of change of granular temperature is simply the difference between the source \( S \) and dissipation \( \Gamma \). To understand the behavior of source and dissipation separately, we plot both \( S \) and \( \Gamma \) versus \( T \) in the plots shown in Fig. 4. Source and dissipation are plotted for two sets of simulations differing only in their initial conditions. For both cases, the solid volume fraction is 0.2, mean flow Reynolds number is 20 and solid to fluid density ratio is 100. Triangular symbols are the data for a suspension in which the particles initialized with zero granular temperature. In this case, the particles pick up energy from the fluid and hence we note that the source term is greater than dissipation at initial time. Square symbols show the source
Figure 3: Scatter plot showing the fluctuating particle acceleration versus the fluctuating particle velocity obtained from the DNS of flow past a fixed particle assembly at a volume fraction of 0.2, mean flow Reynolds number of 20 and Reynolds number based on granular temperature of 16. From the analysis on the extraction of source and dissipation from the DNS, we can see that the symbols that lie in the first and the third quadrant contribute to source and the symbols that lie in the second and the fourth quadrant contribute to the dissipation.

and dissipation data for a suspension initialized with a granular temperature corresponding to $Re_T = 4$. In this case, the particles have higher energy and thus they lose their energy to fluid. So for this case the dissipation is initially greater than the source term. A key observation from the figure is that both suspensions attain the same steady granular temperature. This shows that the steady state behavior of a statistically homogeneous gas–solids suspension is independent of the initial temperature. Finally we note that for both suspensions, the source and dissipation are equal at steady state. These observations verify the expressions for the source and dissipation presented earlier and show that this is a viable approach to propose the acceleration model.

Conclusions

Evolution of the particle granular temperature in gas-solids suspensions at moderate Reynolds numbers is studied by DNS of freely evolving suspensions using PUREBM. DNS results show that the steady granular temperature increases with the mean flow Reynolds number. This steady granular temperature is independent of the initial granular temperature of the suspension. A key finding that emerges from this work is that at steady state the particle velocity autocorrelation function decays exponentially thus motivating the use of a Langevin–like model to describe the increment in particle velocity. A Langevin equation is proposed to model the instantaneous particle acceleration in gas–solid suspensions at moderate Reynolds numbers. Expressions to compute the source and sink of granular temperature from DNS are derived. Previous work by Tenne et al. shows that simple extension of mean particle acceleration models does not recover the joint acceleration–velocity statistics that are obtained from DNS. Using the expressions for source and dissipation derived in this work it is also shown that such models do not produce any source for the particle granular temperature which justifies the use of Langevin–like models to model the instantaneous particle acceleration.

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References


