Analysis of gas-solid flow using particle-resolved direct numerical simulation: flow physics and modeling

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Analysis of gas-solid flow using particle-resolved direct numerical simulation: flow physics and modeling

by

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Gas-solid flows are encountered in many industrial processes such as pneumatic conveying, fluid catalytic cracking, $\text{CO}_2$ capture and fast pyrolysis process. In spite of several experimental and numerical studies performed to understand the physics governing observed phenomena in gas-solid flows, and to propose accurate closure models for computational fluid dynamics (CFD) simulations using the averaged conservation equations, there are several challenges in gas-solid flows that yet need to be addressed. In many of the industrial processes, the solid-to-fluid density ratio is of the order of 100 to 1000, and the particle diameter ranges from 50 to 500 $\mu$m. The interaction of heavy and large particles with the carrier phase leads to the formation of a boundary layer around each particle that in turn gives rise to interphase momentum transfer at the fluid-solid interface. The rate of work done by the carrier flow to sustain the interphase transfer of momentum leads to generation of velocity fluctuations in both the gas phase and the solid phase. Gas-phase velocity fluctuations enhance gas-particle heat transfer and the mixing of chemical species. Additionally, fluctuating motion of solid particles together with microscale hydrodynamic instabilities give rise to formation of mesoscopic particle clusters in gas-solid flows. The particle clusters then modify the hydrodynamic field and then the interconnected phenomena mentioned above dynamically modify the response of the system. Furthermore, if there exists a particle size distribution in the dispersed phase, the differences in the gas-particle and particle-particle drag forces lead to the segregation phenomenon.

In this study, particle-resolved direct numerical simulation (PR-DNS) is used to address some aspects of the challenges noted above, and to propose closure models for device-scale CFD calculations. First, the level of gas-phase velocity fluctuations is quantified, and its dependence on flow parameters is explained. An algebraic Reynolds stress model is proposed by decomposing the Reynolds stress into isotropic and deviatoric parts. Also the interaction of solid particles with isotropic turbulent flow has been addressed using PR-DNS. In addition, in
this study the slip velocity between two particle size classes in a bidisperse mixture is quantified, which is the key signature of segregation of particle size classes. The predictive capability of two-fluid closure models in predicting the slip velocity between particle size classes is also assessed. PR-DNS is used to propose a bidisperse gas-particle drag model that improves the prediction of the mean slip velocity between the two particle size classes. In addition, the mechanism of transfer of kinetic energy from the mean flow to fluid-phase and particle velocity fluctuations in a homogeneous bidisperse suspension is explained. This mechanism of transfer of energy is important because particle velocity fluctuations affect the particle-particle drag, which jointly with the gas-particle drag on each particle class determines the mean slip velocity between the two particle classes. In this study we have also used PR-DNS to quantify the mean drag force on particle clusters that are statistically consistent with those observed in experiments. A clustered particle drag model has been proposed based on our PR-DNS results. To address the effect of filtering the hydrodynamic field on flow statistics, which is used in LES of gas-solid flows, we have shown that the source and sink of kinetic energy in particle velocity fluctuations obtained from the PR-DNS are different from those predicted by the LES approach. These differences lead to a different level of kinetic energy in the solid phase obtained from the two approaches, and thus the flow characteristics that depend on solid-phase kinetic energy, such as formation and evolution of particle clusters, may not be comparable between the PR-DNS and LES approaches. In this study we have also used PR-DNS to quantify the growth rate of mixing length in a particle-laden mixing layer, and the corresponding mechanism is identified by using a scaling analysis.
CHAPTER 1. INTRODUCTION

1.1 Background

Multiphase flow is a system in which several phases such as solid, liquid and gas coexist and interact with each other. Multiphase flows are very common in nature. Motion of raindrops and snowflakes in air, sand storms, eruption of volcanic ashes, and the sedimentation process in rivers are examples of natural occurrences of multiphase flows. These flows are also very common in industrial applications. For instance, in an internal combustion engine, fuel is injected into the combustion chamber.

A complex interplay of hydrodynamic forces, surface tension, and turbulence in the fuel stream leads to primary breakup of the jet into coarse ligaments. These coarse structures experience a secondary breakup, and then micro-droplets are formed which are essential for fast evaporation and mixing of the fuel with air. The quality of the fuel-air mixture then determines the efficiency of the combustion process. In fluidized bed combustors, solid fuel particles are suspended by upward blowing jets of air during the combustion process, providing an effective chemical reaction. In the fluid catalytic cracking process, a fluidized powdered catalyst converts high-molecular-weight hydrocarbons of crude oil into gasoline, olefin, and other products (Speight, 2006). In the CO$_2$ capture process, the exhaust gas from a combustion process is directed to a fluidized bed with dry sorbent particles. These particles absorb the carbon dioxide from the exhaust gas, and the remaining gas free of CO$_2$ is purged to the atmosphere. These examples indicate that multiphase flow is a general name that encompasses several types of flows that can be characterized with different kind of interactions and flow regimes. In the current study, we narrow down the scope of our study to gas-solid flows.
In industrial applications of gas-solid flows, the particle to fluid density ratio $\rho^{(p)}/\rho^{(f)}$ is of the order of 100 to 1000 and particle diameter $d_p$ ranges from 50 to 500 $\mu$m, which is usually larger than the Kolmogorov length scale $\eta$. These particles are associated with high particle Stokes number, which is the ratio of the particle response time $\tau_p = \rho^{(p)} d_p^2/18 \rho^{(f)} \nu^{(f)}$ to the fluid characteristic timescale $\tau^{(f)}$. When carrier flow blows over a collection of such particles, they cannot instantly respond to flow structures due to the difference between the particle response time and the fluid characteristic timescale. As a result, a slip velocity forms from the difference between the gas-phase and particles velocities. The interaction of the viscous carrier flow with inertial particles gives rise to formation of a boundary layer around each particle surface. Therefore, each particle experiences a hydrodynamic force originating from pressure and viscous stresses. The particles accelerate and gain momentum and energy under the influence of the hydrodynamic force. If the solid phase is not too dilute, particles may collide with other particles. This collision gives rise to the collisional force, in addition to the hydrodynamic force. Particle collisions result in redistribution of momentum and energy among solid particles. Due to the large particle size and high mass density, there is a two-way fluid-solid interaction in the suspension. This means that not only are particles influenced by the hydrodynamic forces originating from the carrier flow, the pressure and velocity fields in the fluid phase can also be modified by the motion of particles. This two-way coupling at the scale of individual particles (microscale) is very important because it determines the meso/macroscopic interactions and quantities of the gas-solid flow. Therefore, *detailed understanding of the microscale interactions between the gas-phase and the solid phase, accurate quantification of meso/macroscopic quantities, and discovering the coupling across these scales is essential.*

Due to the lack of detailed understanding of gas-solid interactions at moderate Reynolds numbers (Stokes flow is well studied), the design, optimization and scale-up of industrial devices currently rely on empirical correlations. These correlations do not correctly incorporate the effect of microscale interactions on macroscopic quantities. Therefore, these correlations usually lead to over-design, low product yield and low process efficiency. Recently, due to the increasing power of computational resources and advances in numerical methods, compu-
tational fluid dynamics (CFD) simulation has become an alternative approach for the design process in industrial applications. Device-scale CFD simulations of gas-solid flow mainly rely on either Lagrangian-Eulerian (LE) or Eulerian-Eulerian (EE) approaches. In the LE approach, the trajectory of each particle is tracked in response to collisional and hydrodynamic forces, while the carrier flow is represented in an Eulerian frame. Although this method provides useful information about the solid particles, it is still limited to small systems of thousands of particles due to the demanding computational expenses for tracking individual solid particles. In contrast, in the EE approach, both phases are considered as inter-penetrating continua that are represented in an Eulerian frame. In both LE and EE approaches, the continuous fields are represented by averaged conservation equations of mass, momentum and energy. The averaging process gives rise to mean interphase transfer terms and also correlations of fluctuating quantities. All these terms are unclosed in the level of averaged equation. Therefore, accurate and predictive closure models are required for reliable CFD calculations of gas-solid flow.

Theoretical studies can be used to propose closure models for interphase transfer terms (Carman, 193; Hasimoto, 1959; Acrivos et al., 1980; Sangani and Acrivos, 1982), and to investigate the stability limits of a gas-solid suspension (Koch and Sangani, 1999; Wylie and Koch, 2000; Valiveti and Koch, 1999). However, these models are limited to the Stokes flow regime where the effect of nonlinear convective terms in the momentum transport equation can be neglected. In real gas-solid flow devices, the existence of a finite slip velocity between the gas phase and the solid phase prohibits the applicability of analytical solutions of inertia-less Stokes flow. This arises from the nonlinearity of the Navier-Stokes equations.

Experimental studies are useful for developing closure models of interphase transfer terms. In this approach, measured data are used for the budget analysis (global balance) of transport equations in order to indirectly quantify, for instance, the interphase momentum transfer (Ergun, 1952; Richardson and Zaki, 1954) or the interphase heat transfer (Gunn, 1978). Nevertheless, this experimental technique is not able to provide detailed information of microscale interactions in gas-solid flows. To gain insight into the microscale interactions of a gas-solid flow, precisely controlled non-intrusive experimental measurements, such as laser doppler velocimetry (LDV) and particle image velocimetry (PIV) have been developed. However, the
applicability of these techniques is restricted to dilute gas-solid flows or pseudo two-dimensional suspensions due to the limited optical access in dense suspensions.

Particle-resolved direct numerical simulation (PR-DNS) is an alternative approach well-suited for discovering the flow physics in gas-solid flows, as well as model development for unclosed terms in EE and LE averaged transport equations (Tenneti and Subramaniam, 2014). Several PR-DNS techniques have been developed and successfully tested in the context of gas-solid flows. These techniques rely on either body-fitted-mesh solvers (Burton and Eaton, 2005) or Cartesian-mesh solvers based on Lattice-Boltzmann method (Hill et al., 2001a; van der Hoef et al., 2005), immersed boundary method (Uhlmann, 2008; Tenneti et al., 2010) and spherical harmonics expansions (Zhang and Prosperetti, 2005). In spite of the capability of PR-DNS in providing detailed spatio-temporal information of the flow field, this method is currently limited to idealized problems in small domains which do not have the geometrical complexity of a real gas-solid flow. **In the current study we choose PR-DNS as our primary tool to discover flow physics and propose closure models for unclosed terms used in averaged equations of motion.** This approach is also used to address some of the challenges in gas-solid flow that yet need to be addressed. These challenges are described in detail in the following sub-section.

### 1.2 Challenges in gas-solid flow analysis

There are many challenges associated with gas-solid flows that have not been considered in current modeling attempts. Some of these challenges are listed below:

- **Generation of particle-induced gas-phase velocity fluctuations:** Interaction of the carrier flow with solid particles through the no-slip and no-penetration boundary conditions gives rise to formation of *pseudo-turbulent* velocity fluctuations that are different in nature from high Reynolds number turbulence in the gas phase that we refer to as *intrinsic* turbulence. These pseudo-turbulent gas-phase velocity fluctuations originate from microscale interactions (Mehrabadi et al., 2015) that manifest themselves in the form of turbulent kinetic energy (TKE). Since the separation of these pseudo-turbulent...
fluctuations from intrinsic turbulent fluctuations is non-trivial, in most of gas-solid flow modeling, modified versions of single-phase turbulence models are used to represent these fluctuations. Nevertheless, the difference in the mechanism of generation of gas-phase pseudo-turbulence from intrinsic turbulence suggests developing a physics-based model that accounts for this difference.

- **Polydispersity of solid particles:** In industrial applications of gas-solid flow, there exists a particle size distribution. Additionally, there may be particles with different mass densities in the mixture as well. Therefore, the gas-particle interaction between the gas phase and solid particles with different size or mass density is not identical. This variety in particle size and density gives rise to segregation of particle classes and substantially affects particle mixing. Therefore, a better understanding of mechanisms leading to particle segregation is essential.

- **Instability of gas-solid flows:** Particle configurations in a gas-solid flow are prone to formation and growth of instabilities that manifest themselves in the formation and breakup of particle clusters. These particle clusters range in size from 10 to 100 particle diameters, and form a local dense region compared to a uniformly distributed state. These particle clusters substantially alter gas-particle interaction by changing the exchange of momentum, energy and heat and mass transfer between the gas-phase and the solid phase. Although understanding the origin and characterization of these particle clusters has been attempted, there is no consensus on the mechanisms responsible for formation and breakup of particle clusters in gas-solid flows. Therefore, identifying the corresponding mechanisms and their effects on flow hydrodynamics and energy transfer is essential.

In a gas-solid flow, these phenomena are interconnected, meaning that any variation in one of them affect the others. As shown in Fig. 1.1, the interaction of the carrier flow with solid particles generates gas-solid drag force. The rate of work done by the mean flow to overcome this hydrodynamic drag force results in production of kinetic energies in both gas and solid phases (Xu and Subramaniam, 2007; Mehrabadi et al., 2015). The kinetic energy in the fluid phase manifest itself in the level of gas-phase velocity fluctuations, while the kinetic energy
in the solid phase appears is the level of solid-phase granular temperature. If particles move towards each other as a result of hydrodynamic forces, electrostatic attractions, cohesion, etc., then particle clusters form which are distinguished by a region of high particle number density surrounded by a voidage. In the meantime, the interaction between the fluid phase and the solid phase changes from the fluid-particle interface to cluster-voidage interface. The particle structures now modify the hydrodynamic flow field by enforcing the drag force (interphase momentum transfer) to be adjusted to the new particle configuration. As a consequence, the rate of transfer of energy to the fluctuating velocities in the gas phase and the solid phase changes as well. If the particles are polydisperse, the rate of transfer of momentum and energy to each particle class depends on particle diameter and mass density. These differences may lead to either segregation or mixing of particle classes in the mixture which add more complexity to the interplay of mechanisms shown in Fig. 1.1.
Understanding the physics underlying the dynamics of these phenomena and their effects on the mass, momentum and energy interphase transfer terms require utilization of precise tools and modern techniques for their analysis. Incorporation of these challenges in gas-solid flow models has substantial effect on predictive capability of models used in industrial applications. In the following section, we summarize studies that have investigated the phenomena mentioned above.

1.3 Existing work

In this section, we review the gas-solid flow literature that addresses some aspects of the challenges noted in the foregoing section.

1.3.1 Particle-induced gas-phase velocity fluctuations modeling

Gas-phase pseudo-turbulence generated from the interaction of carrier flow with solid particles gives rise to gas-phase velocity fluctuations. It is also evident that the existence of solid particles in a turbulent flow can either attenuate or enhance the level of gas-phase velocity fluctuations (Gore and Crowe, 1989; Elghobashi, 1994). Therefore, the differences in the mechanisms as well as the role of particles in altering the level of gas-phase turbulence should be accounted for in gas-solid flow modeling.

In early CFD calculations of gas-solid flow, in the absence of any quantitative measurement for the level of gas-phase velocity fluctuations, the transport of the gas-phase Reynolds stress is sometimes neglected in dense gas-solid flow on the grounds that the dominant forces in the gas-phase momentum balance are the pressure drop and drag force (Sinclair and Jackson, 1989; Ding and Gidaspow, 1990; Pita and Sundaresan, 1993; Gidaspow, 1994; Hrenya and Sinclair, 1997). Similarly, due to the lack of data for the gas-phase Reynolds stress at low volume fractions, this term is also neglected in some CFD simulations of dilute gas-solid flow (Agrawal et al., 2001). In contrast, the hot wire measurements of Moran and Glicksman (2003) indicate that the level of gas-phase velocity fluctuations can be significant in a circulating fluidized bed riser at dilute solid-phase volume fraction. Therefore, the transport of gas-phase pseudo-turbulent Reynolds stress cannot be neglected in a gas-solid flow.
In an attempt to model gas-phase velocity fluctuations in gas-solid flows, Elghobashi and Abou-Arab (1983) and Chen and Wood (1985) used a time-averaging technique on the volume-averaged velocity field to derive a transport equation for the fluctuating velocities. This approach results in an inconsistency since the fluctuations obtained from the time averaging do not correspond to velocity fluctuations in the volume-averaged field. Besnard and Harlow (1988) developed a model that accounted for modulation of turbulence by only considering the gas-particle interaction through the interphase momentum transfer term, while disregarding the effect of viscous stresses in the fluid phase on the dissipation. Kataoka and Serizawa (1989), Hwanc and Shen (1993) and Liljegren and Foslein (1996) used ensemble-averaging and developed energy equations for the fluctuating velocities that incorporated a source term arising from the work done by particles on the fluid phase. Louge et al. (1991) and Bolio et al. (1995) used the eddy viscosity hypothesis to propose, respectively, one-equation and two-equation models for dilute systems of large particles. These models are similar to those of single-phase turbulence that are modified to account for presence of particles in a gas-solid flow. Bolio and Sinclair (1995) also extended the model of Bolio et al. (1995) to account for the enhancement of gas-phase turbulence in a gas-solid flow. They incorporated an enhancement mechanism in their model inspired by the work of Yuan and Michaelides (1992) in which they associated the turbulence enhancement with formation of wakes behind solid particles. Bolio and Sinclair (1995) showed that their model compared well with experimental data of Tsuji et al. (1984). Subsequently, more sophisticated models such as the four-equation \(k-\varepsilon\) model of Simonin (1996) were proposed for gas-solid flow CFD simulations.

The main focus of the studies noted above was to derive a transport equation for the fluid-phase velocity fluctuations (and also a dissipation rate equation in \(k-\varepsilon\) approaches) for averaged equations of motion. These equations rely on model functions and model constants that cannot be determined with further information about the unresolved flow field. The success of direct numerical simulation (DNS) methodology in single-phase turbulence that provides detailed information of the flow field offers the promise of further discovery as well as model development in gas-solid flow as well. In early gas-solid flow DNS studies, particles were assumed to be much smaller than the Kolmogorov length scale. Therefore, particles were represented as point
particles. This gave rise to the emergence of point-particle direct numerical simulation (PP-DNS) with the one-way coupling approach in which low Stokes number particles do not disturb the fluid field (Riley and Patterson, 1974; Squires and Eaton, 1991b; Elghobashi and Truesdell, 1992), two-way coupling approach in which disturbance of the fluid phase with high Stokes number particles is considered by adding a force to the Navier-Stokes equations (Squires and Eaton, 1990; Elghobashi and Truesdell, 1993; Ferrante and Elghobashi, 2003), and four-way coupling in which the solid phase is dense enough that the particle-particle interactions cannot be neglected (Vance et al., 2006). These PP-DNS studies were used mostly to gain insight into some of phenomena observed in turbulent gas-solid flows, such as formation of particle clusters, particle dispersion, and modulation of turbulence, although the use of an implied particle acceleration model is taken granted. In spite of its potential, the limited applicability of PP-DNS approach to dilute regimes with particles smaller than the Kolmogorov length scale prohibits the use of this methodology in studying practical gas-solid flow regimes where particles are relatively larger and heavier, and the suspension is more packed (Balachandar and Eaton, 2010).

Increasing availability of computational resources in the last decade has offered the promise of using model-free particle-resolved direct numerical simulation (PR-DNS) in which the flow around each particle is exactly resolved, and the particle acceleration is directly computed by integrating the stress tensor at the particle surface. This method has been used to discover mechanisms underlying the generation of particle-induced gas-phase velocity fluctuations in homogeneous gas-solid suspension (Uhlmann, 2008; Uhlmann and Doychev, 2014) and channel flow (Kidanemariam et al., 2013) with finite size heavy particles. Nevertheless, quantifying the pseudo-turbulent gas-phase velocity fluctuations over a wide range of flow parameters and proposing a physics-based gas-phase Reynolds stress model is lacking. Further understanding of these velocity fluctuations that coexist with the intrinsic gas-phase turbulence is yet to be addressed.
1.3.2 Polydispersity of solid particles

In real-gas solid flows, the dispersed phase is generally polydisperse, meaning that there is a distribution in the particle size and mass density. These distributions lead to a complex interplay of various gas-particle and particle-particle interactions that in turn give rise to mass flux of one particle class with respect to another class. This mass flux is the key signature of the segregation phenomenon observed in gas-solid suspensions.

Rowe and Nienow (1976) explained the mechanism of segregation from a series of experimental studies they conducted in early 1970’s. They reported that formation of bubbles in a fluidized bed plays a key role in the segregation process. Their observations showed that once a bubble passes through the bed with a mixture of light and heavy particles, it carries lighter particles upward since the bubble rise velocity is greater than the fluidization velocity of light particles. Meanwhile, the heavier particles fall into the bubble and move downwards because their fluidization velocity is greater than the bubble rise velocity. Continuous formation and rise of bubbles eventually lead to segregation of the binary mixture. They also found that the increase of the inlet gas velocity increases the chance of fluidization of heavier particles, and therefore the mixing phenomenon becomes more dominant. Furthermore, they proposed a correlation for the gas-phase velocity above which the segregation starts in a binary mixture of solid particles. Nienow et al. (1987) also tried to investigate the effect of the gas distributor at the bottom a circular fluidized bed on segregation and mixing. To study more complex systems, Wang and Chou (1995) analyzed patterns of segregation and mixing in a ternary mixture particles with different sizes, densities and shapes, and proposed a minimum fluidization velocity based on their data. Goldschmidt et al. (2003) used a non-intrusive digital image analysis technique to study a pseudo two-dimensional bidisperse fluidized bed to study the segregation and bubbles dynamics in the bed, and also provide and experimental benchmark for validation of closure models developed for CFD of gas-solid flows. Bokkers et al. (2004) used particle image velocimetry (PIV) to measure the segregation rate of a bidisperse mixture, and to evaluate the performance of CFD-DEM approach when compared to experimental results. They reported that the CFD-DEM results strongly depend on the choice of the gas-solid drag model. They
also showed that the segregation rate from CFD-DEM compares favorably with their experimental data when the drag model of Ergun (1952) together with the model of Wen and Yu (1966) is used. Chew et al. (2011) tested particle segregation in a circulating fluidized bed using a binary mixture as well as a continuous size distribution. They observed particle segregation in both radial and axial directions in the riser. They also found that heavier particles tend to segregate towards the walls which is consistent with earlier experimental observations (Tartan and Gidaspow, 2004; Biggs et al., 2008) as well as simulations (Huilin et al., 2003; Benyahia, 2008; Songprawat and Gidaspow, 2010).

Experimental investigations of bi/polydisperse gas-solid flow, including those mentioned above provide information about the macroscopic behavior of the suspension such as the mean rate of segregation and particle class density profile. Nevertheless, these approaches cannot reveal further detail about the microscale gas-particle and particle-particle drag forces, and their individual contributions to segregation and mixing. Since these contributions can be quantified from a PR-DNS, this methodology is a suitable tool for addressing segregation and mixing phenomena.

van der Hoef et al. (2005) used PR-DNS to propose a drag model for monodisperse gas-solid flow in the Stokes regime using fixed particle assemblies. They also performed PR-DNS of bidisperse gas-solid flow at low Reynolds number regime in an attempt to extend their model applicable to bi/polydisperse systems, and proposed a correlation that relates the equivalent monodisperse drag force to the drag force experienced by each particle size class in a polydisperse suspension. Beetstra et al. (2007) used fixed particle assemblies to incorporate the effect of finite mean slip Reynolds number into the low-Reynolds-number monodisperse drag model of van der Hoef et al. (2005), and also examined the validity of the polydisperse drag model at the inertial flow regime. Sarkar et al. (2009) then confirmed the applicability of this polydisperse drag correlation at extreme particle size ratios up to 1 : 10. Yin and coworkers (Yin and Sundaresan, 2009; Holloway et al., 2010) reasoned that the relative motion of particles in a suspension indirectly affects the hydrodynamic force experienced by neighboring particles through the lubrication forces. They used frozen particle configurations in their PR-DNS setup with assigned mean velocity to each particle class which gave rise to evolution of flow motion through
implementation of the no-slip and no-penetration boundary condition at particle surface. With this scheme, they explored the effect of indirect particle-particle interaction through the carrier flow, and proposed a new gas-particle drag model for mono/polydisperse suspensions.

All of the aforementioned bidisperse PR-DNS exploited fixed or frozen particle assemblies as an approximation to gas-solid suspensions with heavy particles. However, the significance of relative motion between pair of particles as well as the effect of different slip velocities on the gas-particle drag in a freely moving particles has not been reported, to the best of our knowledge. In addition, it is unknown a priori if particle size ratio is alone adequate to characterize the mean gas-particle drag, and how well this assumption holds in freely evolving suspensions.

1.3.3 Instability of gas-solid flows

Gas-solid flows in industrial devices such as fluidized beds exhibit non-uniform and heterogeneous structures known as particle clusters. It is hypothesized that hydrodynamic instabilities at the microscale play a key role in formation, growth and breakup of the particle clusters. These particle clusters substantially affect the flow field by modifying the interphase transfer of mass, momentum and energy compared with uniformly distributed particles in gas-solid flow. Therefore, predicting the formation of particle clusters and their effect on the flow field should be embedded in closure models that are used for CFD calculations.

It is well-known from the kinetic theory of granular gases (KTGG) that inelastic particle collisions give rise to formation of particle clusters in a granular flow. In a granular flow, in the absence of interstitial fluid, if the particles undergo inelastic collisions, the corresponding energy loss gives rise to the formation of a locally “cool” region in the suspension with a lower particle pressure. This region with a relative negative pressure attracts more particles from the surrounding area, and therefore the particle concentration increases. Increase of particle concentration accelerates the local cooling process and finally particle clusters form in the granular cooling gas.

Although KTGG describes formation of particle clusters in a granular flow, the clustering mechanism becomes much more complicated when the interaction of solid particles with the
interstitial fluid becomes significant. Theoretical analysis has been used to provide a stability regime in gas-solid flows. Batchelor (1988) established a one-dimensional mean equation of motion for solid particles from physical arguments. He then showed that this equation jointly with the conservation equation of mass is adequate to determine the stability limits of a gas-solid suspension. He pointed out that the inertia of particles amplifies disturbances in the particulate phase while particle diffusion provides a damping mechanism. He then provided a critical particle Froude number beyond which instability occurs.

The linear stability analysis approach of single-phase flow has also been used in gas-solid flow to provide stability limits. Jackson (193) and Anderson and Jackson (1968) applied this approach to a fluidized bed in a statistically homogeneous and stationary base state. They reported that the state of motion of a flow through a particle assembly is unconditionally unstable to vertically travelling waves. They also showed that instabilities form and grow as fluctuations in the voidage. Koch (1990) used an \(N\)-particle distribution function to derive the governing equations of a gas-solid suspension in a Stokes flow. These equations were separately derived for the collision-dominated regime as well as for the regime in which viscous forces are important compared with the collisional forces. He then used the linearized stability analysis approach to determine the stability limits of a very dilute suspension with high Stokes number particles in the Stokes regime. He started with the mean equations of mass, momentum, and energy of the solid phase with interphase transfer terms being solely a function of the solid-phase volume fraction. He showed that with massive particles where the system is collision-dominated, the suspension is always unstable, while for moderately massive particles the system is stable. Koch and Sangani (1999) extended the scope of this study to dense suspensions and provided a critical Stokes for the onset of instabilities in gas-solid suspensions.

When the inertial forces are non-negligible in both phases, the analytical Stokes flow instability map does not hold. This is mainly due to the nonlinearity of inertial terms in the momentum equations and the multiscale nature of interactions in a gas-solid flow. Numerical simulations of gas-solid flow is a promising route to analyzing the instability phenomenon in gas-solid flows. Agrawal et al. (2001) used a continuum representation of the governing equations of motion and performed a series of highly-resolved CFD calculations of the two-fluid
equations for a dilute sedimenting gas-solid flow in an attempt to identify the source of cluster formation. They observed that in the absence of a macroscale shear rate, micro structures form, although the effect of interphase momentum transfer due to microscale interphase interactions was closed by an assumed drag law. Even in the presence of low macroscale shear rates, the instabilities are dominated by the microscale instabilities. Nonetheless, these instabilities are significantly influenced when a high macroscale shear rate exists. Similarly, Andrews et al. (2005) and Igci et al. (2008) showed that capturing the microscale hydrodynamics has profound effect on mesoscale structures as well as the macroscale quantities. These analyses are based on the averaged equations of motion in which the unclosed microscale interactions are incorporated using closure models. These models are based on experimental and numerical correlations that are independent of particle structures. However, it is well known that once these structures form, they significantly affect the interphase transfer of mass, momentum and energy. Therefore, a more sophisticated approach is required for mapping out the instability limits of gas-solid suspensions.

High fidelity numerical simulations of gas-solid suspensions have been used to study stability limits by observing the formation of particle clusters. Wylie and Koch (2000) simulated the dynamics of a gas-solid suspension with elastic and high Stokes number particles in a Stokes flow. Particles were initialized with a Maxwellian velocity distribution, and the interstitial fluid was solved using a multipole technique. They observed formation of particle clusters by quantifying the nearest neighbor distance. They reported that initial clustering occurs at scales comparable to a particle diameter. In addition, the viscous dissipation from the interstitial fluid plays a key role in the formation of particle clusters. Yin et al. (2013) used quasi two-dimensional particle-resolved direct numerical simulation to study the importance of viscous versus collisional dissipation in formation of particle clusters. The particles in their simulations were initialized with a Maxwellian velocity distribution dispersed in a quiescent flow. They observed that viscous dissipation accelerates formation of particle clusters compared to a granular flow with no interstitial fluid with the same level of inelasticity in particle collisions. They also mentioned that once the particle clusters are formed, the level of dissipation counter-intuitively decreases. Although these studies provide detailed information about the mechanisms driving
the formation of particle structures, they are limited to the Stokes flow where the effect of fluid inertia is neglected.

Capecelatro et al. (2014a) used large eddy simulation (LES) approach in an attempt to simulate formation of particle clusters in a gas-solid suspension with a finite mean slip velocity between the two phases. They showed that starting from a uniform particle assembly, the solid-phase volume fraction probability density function resembles a log-normal distribution once particle clusters form. Although LES is capable of capturing mesoscale interactions as well as predicting the formation of particle structures in a gas-solid suspension, the microscale subgrid interactions such as gas-particle drag and gas-phase Reynolds stress, are represented by closure models. It is hypothesized that in the absence of a wall-induced or a mean shear rate in the carrier flow, the mesoscale structures appearing in a homogeneous gas-solid flow originate from microscale hydrodynamics instabilities that are not longer available in the filtered hydrodynamic field. Therefore, the effect of LES filtering on prediction of mesoscale particle clusters should be addressed.

Tenneti (2013) performed PR-DNS of freely evolving suspensions of initially clustered particle assemblies in a homogeneous flow with a finite mean slip velocity. He used the radial distribution function as a measure of particle clustering and reported that during the course of simulation, the particles rearrange themselves in a fashion similar to a uniform particle assembly. It is argued that the lack of particle clusters in these simulations is associated with the length of the computational domain which is of the order of $10d_p$, whereas the Agrawal et al. (2001) and Capecelatro et al. (2014a) mentioned that the computational domain should be of the order of $\mathcal{L} \sim \mathcal{O}(\tau_p^2g) = \mathcal{O}(100d_p)$.

1.4 Research objectives and approaches

The principal goal of this study is to use PR-DNS to obtain detailed spatio-temporal information of gas-solid flows in a homogeneous configuration in order to gain insight into the challenging aspects noted in the preceding section. We also use this method to propose predictive closure models that can be used in EE and LE simulations of gas-solid flows. The specific research objectives of this study that address these principal goals are as follows:
1. Develop a scalable PR-DNS solver for homogeneous gas-solid flow simulations

2. Quantify the gas-phase Reynolds stress corresponding to pseudo-turbulence over a wide range of flow parameters

3. Address the interaction of solid particles with intrinsic turbulent motion in a turbulent gas-solid flow

4. Address particle segregation in gas-solid flows by quantifying the particle mass flux in bidisperse gas-solid flow

5. Quantify the interphase transfer of momentum in the presence of particle clusters

6. Address the importance of microscale gas-particle and particle-particle interactions that lead to formation and growth of instabilities in gas-solid flows

These specific objectives are explained below in more detail.

1.4.1 Development of a scalable PR-DNS solver

PR-DNS of gas-solid flow with the presence of mesoscale particle structures exchanging momentum and energy with the carrier flow requires enormous computational and storage resources that are only provided by computer clusters. In these clusters, the computational and storage loads are distributed over thousands of computational nodes. Therefore, to utilize the computer clusters that are capable of handling such calculations, a well-established numerical method scalable on distributed memory architectures is required. An in-house PR-DNS code based on the particle-resolved uncontaminated fluid reconcilable immersed boundary method (PUReIBM) of Tenneti et al. (2010) has been developed to simulate homogeneous gas-solid flow suspensions. This code is based on a two-dimensional pseudo-spectral one-dimensional finite difference formulation (Garg et al., 2010c) known as PS2D-FD1D PUReIBM. The trajectories of solid particles in this code are tracked by Newton’s laws of motion using a discrete element method (DEM) that uses a spring-dashpot model to represent particle collisions. This code is parallelized by domain decomposition along the coordinate direction in which the equations are discretized using the finite difference approach (slab-like decomposition). This parallelization
strategy makes the code suitable for PR-DNS of domains where one dimension of the computational domain is much larger than the other two dimensions. Tenneti (2013) showed excellent scale-up of the code up to 12,288 processors on the Jaguarpf computer cluster at the Oak Ridge Leadership Computing Facility. Nevertheless, the scalability of this one-dimensional domain decomposition strategy for a computational cube with \( N^3 \) grid points is limited to \( N \) processors if the maximum number of grid points fitting on the memory of a processor in a slab-like sub-domain is \( N^2 \).

To further extend the scalability of the code, in the current study a new hydrodynamic solver based on a three dimensional pseudo-spectral method, known as PS3D PUReIBM, is developed. This is parallelized using a two-dimensional domain decomposition strategy (pencil-like decomposition). This pencil-like decomposition extends the scalability of the code to \( N^4 \) processors for a computational domain with \( N^6 \) grid points when the maximum number of grid points fitting on the memory of a processor in a pencil-like sub-domain is \( N^2 \). The convergence and accuracy as well as the scalability of the code on available computer clusters is tested.

1.4.2 Quantification of pseudo-turbulent gas-phase Reynolds stress

Device-scale CFD calculations of gas-solid flow requires physics-based model development for unclosed terms in the average transport equations. We used PR-DNS to quantify the particle-induced pseudo-turbulent gas-phase Reynolds stress over a wide range of solid-phase volume fraction \( (0.1 \leq \phi \leq 0.5) \) and mean slip Reynolds number \( (0.01 \leq Re_m \leq 300) \) in a homogeneous gas-solid suspension. The behavior of the gas-phase Reynolds stress with respect to flow parameters is explained by decomposing it into isotropic and deviatoric parts. Correlations are proposed for each of these parts that provide an algebraic gas-phase Reynolds stress model that can be used in CFD of gas-solid flows.

1.4.3 Modulation of turbulence in particle-laden turbulent flows

PP-DNS has been widely used to study the interaction of small scale particles with a turbulent flow. This approach requires a particle acceleration model to account for the gas-particle interaction. However, the accuracy of using acceleration models for PP-DNS of particle-
laden turbulent flows has not been tested. In the current study, PR-DNS is used in a regime that also satisfies the assumptions underlying PP-DNS. We then compare flow quantities such as the kinetic energy in the gas phase and the solid phase as well as the viscous dissipation to assess the accuracy of the results from PP-DNS.

1.4.4 Segregation of particles in a bidisperse gas-solid flow

Segregation and mixing of solid particles are two competing phenomena in a bidisperse fluidized bed. The characteristics of segregation and mixing are associated with both gas-particle and particle-particle interactions in a suspension. In order to isolate the effect of these interactions, a bidisperse assembly of particles in a homogeneous gas-solid flow is investigated using PR-DNS. Our calculations show that there exists a mean slip velocity between the two particle classes in a homogeneous gas-solid flow. The mean slip velocity can be interpreted as particle mass flux that in turn gives rise to segregation in a inhomogeneous flow setup. We assess the ability of current gas-particle drag models in predicting this slip velocity between the particle classes, and try to improve the predictions by improving the gas-particle drag model in a bidisperse gas-solid flow.

The role of particle-particle drag in segregation of particle size classes cannot be neglected. Therefore, control of particle segregation for design and optimization of industrial devices requires a better understanding of the role of particle-particle drag in segregation as well. Particle-particle drag depends, on one hand, on the mean slip velocity between the two particle size classes, and on the other hand, on the level of kinetic energy in particle velocity fluctuations. Given the importance of particle velocity fluctuations in the particle-particle drag, especially in dense regimes, it is important to understand the mechanism of transfer of energy from one phase to another due to interphase interactions. By deriving the governing conservation equations from statistical approaches for bidisperse suspensions, we explain that the power required to sustain the relative mean velocities between any of the two phases in the suspension leads to generation of velocity fluctuations in the two corresponding phases. We also address the role that particle-particle drag plays in the partitioning of kinetic energy between size classes.
1.4.5 Quantification of interphase momentum transfer terms in the presence of particle clusters

Once particle clusters form in gas-solid flow, the macroscopic quantities such as the mean pressure drop, bed expansion height, heat and transfer change. These modifications are attributed to the change in transfer of mass, momentum and energy at micro/mesoscales. Since CFD of gas-solid flow rely on closure models for interphase transfer terms, the accuracy of CFD predictions strongly depend on the ability of such models to predict the formation of particle clusters in a computational domain. The majority of current closure models have been proposed for uniform particle configurations. One exception is the EMMS drag model (Yang et al., 2004) that incorporates the effect of clusters by conditioning the drag force on the minimum energy required for the flow pass through solid particles. Although this model is useful, a more accurate physics-based clustered drag model is required. In addition, the effect of particle clusters on heat and mass transfer as well the pseudo-turbulent gas-phase velocity fluctuations is yet to be discovered. In this study, particle clusters are generated based on experimental measures (Cocco et al., 2010). These clusters are then used as static particle configurations in PR-DNS over a range flow parameters to quantify drag force. These data are finally used to propose a closure drag model for CFD of gas-solid flow with particle clusters.

1.4.6 Instability analysis in gas-solid flow

Microscale instabilities in gas-solid flow are believed to initiate mesoscale instabilities in homogeneous gas-solid flow. Although formation of mesoscale instabilities have been shown by two-fluid CFD simulations (Agrawal et al., 2001) and LES approach (Capecelatro et al., 2014a), the instabilities obtained from these averaged/filtered hydrodynamic fields may not represent the origin of microscale instabilities. PR-DNS is an appropriate tool to analyze the effect of microscale interactions on mesoscale instabilities. However, the computational resources required for mesoscale PR-DNS of gas-solid flow is prohibitively demanding. The aim of this study is to understand the role of microscale interactions in the formation of particle clusters, provided that computational resources are available. Also, the effect of LES filtering/averaging
of microscale hydrodynamics on flow quantities will be addressed. This analysis may shed light on the nature of mesoscale instabilities observed in LES/CFD approaches. In addition, the growth of instability in a particle-laden mixing layer will be studied. This analysis provides the mechanism of instability growth in regions where a dense region of solid particles is in proximity of a voidage. This region can be found near the edge of a cluster or gas bubble in a gas-solid bubbly flow, or near the gas-phase orifice through which the air is blown into a fluidized bed Halvorsen and Mathiesen (2002).

1.5 Accomplishments and future works

The completed tasks associated with the objectives mentioned in the preceding section are listed in Table 1.1.

1.6 Outline

The outline of this thesis is as follows. In Chapter 2 the code development efforts for a petascale-capable PR-DNS code is described. In Chapter 3, the quantification of pseudo-turbulent gas-phase Reynolds stress is presented, which is followed by Chapter 4 that describes the interaction of solid particles with a turbulent flow. In Chapter 5 the importance of gas-particle drag model in predicting particle segregation in a bidisperse gas-solid suspension is presented. In Chapter 6 the mechanism of kinetic energy transfer from mean flow to velocity fluctuations in bidisperse gas-solid flow is explained. In Chapter 7 a gas-particle drag model for clustered particles in gas-solid flow based on PR-DNS of fixed clustered assemblies is proposed. In Chapter 8 the importance of microscale hydrodynamics in growth of instabilities in gas-solid flow is studied, followed by Chapter 9 where the development of a particle-laden mixing layer is analyzed. Finally, in Chapter 10 some of the possible future directions to pursue the current research are suggested.
Table 1.1: Accomplishments corresponding to research objectives

<table>
<thead>
<tr>
<th>Objectives</th>
<th>Results</th>
<th>Conclusions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mesoscale PR-DNS</td>
<td>A scalable hydrodynamic solver based on 3D pseudo-spectral method was developed</td>
<td>The code is shown to be accurate and convergent</td>
</tr>
</tbody>
</table>
| Particle-induced gas-phase velocity fluctuations | 1. Compared the level of gas-phase velocity fluctuations when the flow is initialized with a uniform flow compared to a case when the initial flow is an isotropic turbulence  
2. Quantified the level of gas-phase Reynolds stress over a wide range of flow parameters  
3. Compared the level of gas-phase velocity fluctuations in freely evolving suspensions to that of fixed particle assemblies  
4. Identified the mechanism of transfer of energy from the mean flow to fluctuating velocities  
5. Identified the regime of flow | 1. Gas-phase velocity fluctuations are mainly originated the gas-particle interactions. A turbulent flow with a very high turbulent Reynolds number is needed to dominate the particle-induced turbulence  
2. For high Stokes number particle, the level of gas-phase velocity fluctuations does not significantly change if particle assemblies are fixed or moving  
3. An algebraic gas-phase Reynolds stress model is proposed for a wide range of flow parameters  
4. The power used by the mean flow to sustain a mean slip velocity is partitioned into TKE source terms of the gas phase and the solid phase  
5. The gas-solid flow with a finite mean slip is viscous dominant if initialized with $Re_T = 0$ |
<table>
<thead>
<tr>
<th>Objectives</th>
<th>Results</th>
<th>Conclusions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Particle-laden turbulent flow</td>
<td>1. Gas-phase TKE is not significantly in the PP-DNS and PR-DNS</td>
<td>1. The difference at early fact that particles times arises due to the have not equilibrated to the surrounding fluid</td>
</tr>
<tr>
<td>modulation</td>
<td>2. Evolution of solid-phase TKE is different at early times</td>
<td>2. At later times, particles equilibrate with the surrounding fluid and thus the difference is not noticeable afterwards</td>
</tr>
<tr>
<td></td>
<td>3. Evolution of the viscous dissipation is significantly different at early times</td>
<td>3. Inaccuracy of the particle acceleration model in PP-DNS at early times gives rise to the differences observed at early times</td>
</tr>
<tr>
<td>Particle segregation in a</td>
<td>1. There exists a slip velocity between particle size classes in a bidisperse gas-solid flow</td>
<td>1. The slip velocity between two particle size classes arises due the differences in gas-particle and particle-particle drag forces</td>
</tr>
<tr>
<td>bidisperse gas-solid flow</td>
<td>2. Gas-particle drag and particle-particle drag contribute to the mean slip velocity between the two particle size classes</td>
<td>2. Improvement in drag models is required for better prediction of the slip velocities</td>
</tr>
<tr>
<td></td>
<td>3. Existing two-fluid drag models cannot predict this slip velocity</td>
<td>3. A new gas-particle drag model based on existing models improves predicting the slip velocity</td>
</tr>
<tr>
<td></td>
<td></td>
<td>4. Particle-particle drag originating from particle velocity fluctuations can be better understood by considering the mechanism of transfer of energy from the mean flow to velocity fluctuations</td>
</tr>
</tbody>
</table>
Table 1.1 continued

<table>
<thead>
<tr>
<th>Objectives</th>
<th>Results</th>
<th>Conclusions</th>
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</thead>
<tbody>
<tr>
<td>Influence of particle clusters on macroscale</td>
<td>1. Fixed assemblies of particle clusters are exposed to a predefined mean slip Reynolds number</td>
<td></td>
</tr>
<tr>
<td>quantities</td>
<td>2. Mean gas-particle drag force reduces compared to a uniformly distributed particle assembly</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1. When particle clusters form, the local fluid velocity inside the particle cluster reduces which gives rise to reduction in magnitude of the gas-phase velocity gradient a particle surface</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2. This gives rise to reduction of viscous stress at particle surface as well as the drag force</td>
<td></td>
</tr>
<tr>
<td>Instability analysis of gas-solid flow</td>
<td>1. LES filtering of the hydrodynamics field leads to inaccurate prediction of particle acceleration</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2. If sub-grid particle accelerations are not modeled correctly, the source and dissipation of particle granular temperature are not correctly accounted for</td>
<td></td>
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<tr>
<td></td>
<td>3. Particle granular temperature from a filtered field does not match that of a PR-DNS</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1. Mesoscale instabilities in a gas-solid flow originating from microscales strongly depend on the appropriateness of the particle acceleration model</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2. If the effect of the filtered field on particle acceleration model is not accounted for, the onset of mesoscopic particle clusters and the corresponding configurations may not be physical</td>
<td></td>
</tr>
<tr>
<td>Particle-laden mixing layer</td>
<td>1. A particle laden mixing layer is approximated by an number density profile initially distributed as a step function</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2. The setup is exposed to gravity and particles are gradually entrained into the voidage</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1. Evolution of particle number density and particle velocity profiles are self-similar</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2. Development of the mixing length is a diffusion process</td>
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</table>
CHAPTER 2. DIRECT NUMERICAL SIMULATION OF GAS-SOLID FLOW WITH PUReIBM

In this chapter, the formulation of Particle-Resolved Uncontaminated-fluid Reconcilable Immersed Boundary Method (PUReIBM) is introduced. The method is a legacy of Mohd-Yusof (1996) which was used to simulate the interaction of a single particle with a turbulent flow. It was then developed by Tenneti et al. (2010) to simulate homogeneous gas-solid suspensions with random distribution of particles for both fixed beds and freely evolving suspensions.

2.1 Introduction

Although gas-solid flows have been studied for several decades, design of devices utilizing gas-solid suspensions, such as circulating fluidized beds and coal gasifiers, is still a challenge in industrial applications. Recently, computational fluid dynamics (CFD) has played a key role in such device-scale designs due to the increasing power of computational resources. CFD involves solving averaged conservation equations of mass, momentum and energy for both carrier and dispersed phases. These equations include unclosed interphase transfer terms and sub-grid velocity fluctuation correlations. In modeling, the focus is to relate the unclosed terms to averaged flow quantities. PR-DNS of gas-solid suspensions in canonical flows is the best approach to developing accurate models for unclosed terms (Balachandar and Eaton, 2010) in two-fluid theory. Accordingly, several PR-DNS methods have been developed by various research groups. In the current study, we use PUReIBM based on the immersed boundary method.
2.2 Numerical method

PUReIBM is a robust and highly accurate method for PR-DNS of gas-solid flows. The method is clearly described elsewhere (Garg, 2009; Tenneti et al., 2010). However, for the sake of completeness the method is summarized here.

One of the advantages of PUReIBM over other PR-DNS methods is its flexibility in simulating freely evolving suspensions with arbitrary physical parameters. In numerical investigations of freely evolving suspensions, the sedimentation of particles have usually been studied under the influence of gravity, which leads to a balance between the drag force and the weight of particles (Yin and Koch, 2007). In these simulations, the Reynolds number reaches a unique value dependant upon physical parameters such as fluid and particle densities, and gravitational acceleration. The formulation of PUReIBM in an accelerating frame of reference enables us to simulate arbitrary mean slip Reynolds numbers, while keeping other parameters constant. This feature lets us study the effect of each parameter on a freely evolving gas-solid suspension. In PUReIBM a mean pressure gradient is established along the flow direction to balance the drag force exerted on particles, and also supply the required body force to maintain desired mean slip velocity. Since hydrodynamic forces from the fluid phase cause particles to experience a mean acceleration, the mean pressure gradient should subsequently increase to maintain a constant mean slip velocity between the two phases. Therefore, a steady state solution in the laboratory frame is non-existent. The continuous growth of characteristic velocities in the laboratory frame decreases the time stepping of the numerical method due to the Courant number criterion. Thus, the simulation of freely evolving suspensions in the laboratory frame would be prohibitively restricted to short periods of evolution time.

In PUReIBM, the velocity, pressure, and tensor fields are continuous. However, particle presence is represented by implementing the no-slip and no-penetration boundary conditions at the surface of particles. The strategy is similar to conventional CFD approaches where the boundaries are satisfied by considering a ghost cell beyond the physical domain (Patankar 1980), and reversing the flow so the relative velocity between the two faces becomes zero at the interface. In PUReIBM, the required immersed boundary forcing is only effective to the com-
Figure 2.1: Schematic of the computational with multiple particles in PUReIBM. The volumes of fluid and solid phases are denoted by $V^{(f)}$ and $V^{(s)}$, respectively. The boundary surfaces of the fluid and solid phases are denoted by $\partial V^{(f)}_{\text{ext}}$ and $\partial V^{(p)}_{\text{ext}}$, respectively. The fluid and solid interface in computational domain is indicated by $\partial V_{\text{int}}$.

Computational nodes inside the particles. Thus, the fluid-phase solution remains uncontaminated compared to conventional immersed boundary methods (Peskin, 2002). This approach enables us to directly compute the drag force by integrating the stress tensor over the particle surface.

In PUReIBM, an Eulerian description is used for the carrier phase and a Lagrangian description is used for the dispersed phase. Governing equations are solved over a Cartesian grid, providing simplicity and generality of the numerical method, compared to body fitted grid methods encompassing huge computational remeshing loads. The conservation equations of mass and momentum in the laboratory and accelerating frames are related to each other. If the laboratory frame and non-inertial frame are denoted by $E$ and $\bar{E}$ respectively, the velocity, position and time between these two frames are transformed as

$$
\mathbf{u} = \mathbf{u} - \mathbf{V}_f, \\
\mathbf{x} = \mathbf{x} - \int_0^t \mathbf{V}_f(t') dt', \\
\bar{t} = t,
$$

where $\mathbf{V}_f$ is the accelerating frame velocity, $\mathbf{x}$, $t$, and $\mathbf{u}$ are position, time and velocity in the laboratory frame, and those with a bar corresponding to quantities in the accelerating frame.
The governing equations of the fluid phase are conservation equations of mass and momentum, solved for both carrier and dispersed phases with periodic boundary conditions. Figure 2.1 shows a schematic periodic configuration of the simulation setup. Continuity and momentum equations in the accelerating frame $E$ are, respectively, given as (Pope, 2000)

\[ \nabla \cdot \mathbf{u} = 0, \tag{2.1} \]

\[ \frac{\partial \mathbf{u}}{\partial t} + \mathbf{S} = -\frac{1}{\rho(f)}\mathbf{g} + \nu(f)\nabla^2 \mathbf{u} + \frac{1}{\rho(f)}\mathbf{f} - A_f, \tag{2.2} \]

where $\mathbf{u}$ is the instantaneous velocity, $\mathbf{S} = \nabla \cdot \langle \mathbf{uu} \rangle$ is the convective term in conservative form, $\mathbf{g}$ is the pressure gradient, $\mathbf{f}$ is the immersed boundary forcing in response to the presence of particles satisfying the boundary condition at the particle-fluid interface, and $A_f$ is the frame acceleration.

The instantaneous quantities can be divided into into mean and fluctuating components. Thus, for a given quantity $Q(x,t)$, we have

\[ Q(x,t) = \langle Q(t) \rangle_V + Q'(x,t), \tag{2.3} \]

with $Q'$ being the fluctuating component, and $\langle \cdot \rangle$ denoting the ensemble average. In statistically homogeneous fields, ensemble average is equivalent to the volumetric average, that is

\[ \langle Q(t) \rangle_V = \frac{1}{V} \int_V Q(x,t) dV. \tag{2.4} \]

The mean conservation equations of mass and momentum can be obtained by using the above averaging process in Eqs. 2.1 and 2.2, and integrating them over the computational volume. The resulting equations are

\[ \nabla \cdot \langle \mathbf{u} \rangle_V = 0, \tag{2.5} \]

\[ \frac{\partial \langle \mathbf{u} \rangle_V}{\partial t} = -\frac{1}{\rho(f)}\langle \mathbf{g} \rangle_V + \frac{1}{\rho(f)}\langle \mathbf{f} \rangle_V - A_f, \tag{2.6} \]

for the mean conservation of mass and momentum, respectively. Subtracting the above equations from Eqs. 2.1 and 2.2 results in the fluctuating conservation equations of mass and momentum, given as

\[ \nabla \cdot \mathbf{u}' = 0 \tag{2.7} \]
\[
\frac{\partial \mathbf{u}'}{\partial t} + \mathbf{S} = -\frac{1}{\rho(f)} \mathbf{g}' + \nu(f) \nabla^2 \mathbf{u}' + \frac{1}{\rho(f)} \mathbf{r}'. \tag{2.8}
\]

As mentioned earlier, the system’s driving force is the mean pressure gradient balancing the drag force exerted on particles, and maintaining a constant mean slip velocity between the two phases. To obtain an expression for the evolution of mean pressure gradient, the phasic mean momentum equation of the fluid phase is determined by integrating Eq. 2.2 over the fluid phase, providing
\[
\frac{d}{dt} \langle \mathbf{u}(f) \rangle = -\frac{1}{\rho(f)} \langle \mathbf{g} \rangle_V - \frac{1}{\rho(f)} V(f) \oint_{\partial V(p)} \left( -\psi' \delta + \mu(f) \nabla \mathbf{u} \right) \cdot \mathbf{n}^{(p)} dA - A_f, \tag{2.9}
\]
where \( \psi' \) is the fluctuating pressure, \( \delta \) is the Kronecker delta, \( V(f) \) is the fluid volume, \( \partial V(p) \) is the solid surface boundaries, and \( \mathbf{n}^{(p)} \) is the normal vector at the particle surface pointing outward toward the fluid phase. Rearrangement of the above equation leads to an expression for the mean pressure gradient as
\[
-\frac{1}{\rho(f)} \langle \mathbf{g} \rangle_V = \frac{d}{dt} \langle \mathbf{u}(f) \rangle + \frac{1}{\rho(f)} V(f) \oint_{\partial V(p)} \left( -\psi' \delta + \mu(f) \nabla \mathbf{u} \right) \cdot \mathbf{n}^{(p)} dA + A_f. \tag{2.10}
\]

The mean pressure gradient cannot be determined since the frame acceleration is not specified. Thus, one would need to deduce the phasic mean momentum equation of the solid phase to obtain an expression for this quantity. Accordingly, the governing equation of motion for particles in the laboratory frame (with Lagrangian description) is
\[
m \frac{d \mathbf{V}^{(m)}}{dt} = \int_{\partial \mathbf{V}^{(m)}(t)} \left( -\psi \delta + \mu_f \nabla \mathbf{u} \right) \cdot \mathbf{n}^{(m)} dA \tag{2.11}
\]
where \( m \) is the mass of each particle, \( \psi \) is the pressure, and the superscript \( (m) \) denotes the \( m^{th} \) sphere in the particle assembly. By transforming the velocity of the \( m^{th} \) particle into the accelerating frame by \( \mathbf{V}^{(m)}(t) = \mathbf{V}^{(m)}(t) - \mathbf{V}_f(t) \), and using \( \langle \mathbf{u}^{(p)} \rangle = \langle \mathbf{u}^{(p)} \rangle - \mathbf{V}_f(t) \) as an averaging operator, the phasic mean momentum equation of the solid phase is obtained as
\[
\frac{d}{dt} \langle \mathbf{u}^{(p)} \rangle = -\frac{1}{\rho^{(p)}} \langle \mathbf{g} \rangle_V - \frac{1}{\rho^{(p)}} V^{(p)} \oint_{\partial V^{(p)}} \left( -\psi' \delta + \mu(f) \nabla \mathbf{u} \right) \cdot \mathbf{n}^{(p)} dA - A_f, \tag{2.12}
\]
where \( \rho^{(p)} \) is the particle density and \( V^{(p)} \) is the solid-phase volume. Rearrangement of the above equation leads to another mean pressure gradient expression as
\[
-\frac{1}{\rho^{(p)}} \langle \mathbf{g} \rangle_V = \frac{d}{dt} \langle \mathbf{u}^{(p)} \rangle + \frac{1}{\rho^{(p)}} V^{(p)} \oint_{\partial V^{(p)}} \left( -\psi' \delta + \mu(f) \nabla \mathbf{u} \right) \cdot \mathbf{n}^{(p)} dA + A_f. \tag{2.13}
\]
In Eqs. 2.10 and 2.13, the integral term is the total drag force acting on particles (denoted as $\overline{F}_D$ from hereon) reconcilable to the average interphase momentum transfer $\left\langle \tau_{ji}^{(f)} n_{ji} (x - x^{(f)}) \right\rangle$ in the two-fluid theory (Drew, 1983). Eliminating the frame acceleration between these two equations gives a general closed expression for the mean pressure gradient

$$\left( \frac{1}{\rho^{(f)}} - \frac{1}{\rho^{(p)}} \right) \langle \overline{g} \rangle_{\mathcal{V}} = \frac{d}{dt} \langle \overline{u}^{(p)} \rangle - \frac{d}{dt} \langle \overline{u}^{(f)} \rangle - \frac{\overline{F}_D}{V} \left\{ \frac{1}{\phi \rho^{(p)}} + \frac{1}{(1 - \phi) \rho^{(f)}} \right\}.$$  \hspace{1cm} (2.14)

Since the mean solid velocity is zero in the accelerating frame of reference, the solid-phase unsteady term in this equation is zero. Additionally, the fluid-phase unsteady term at each time step is estimated by a finite difference expression, enabling the mean fluid velocity to attain a desired value $\langle \overline{u}^{(f)} \rangle^d$, determined by the Reynolds number. Hence, the unsteady term in Eq. 2.14 is discretized as

$$\frac{d}{dt} \langle \overline{u}^{(f)} \rangle^{k+1} = \langle \overline{u}^{(f)} \rangle^d - \langle \overline{u}^{(f)} \rangle^k \Delta t,$$  \hspace{1cm} (2.15)

where superscripts $k$ and $k+1$ denote the $k^{th}$ and $k+1^{th}$ time steps, respectively. Therefore, the mean pressure gradient is estimated as

$$\left( \frac{1}{\rho^{(f)}} - \frac{1}{\rho^{(p)}} \right) \langle \overline{g} \rangle_{\mathcal{V}}^{k+1} = -\frac{\langle \overline{u}^{(f)} \rangle^d - \langle \overline{u}^{(f)} \rangle^k}{\Delta t} - \frac{\overline{F}_D}{V} \left\{ \frac{1}{\phi \rho^{(p)}} + \frac{1}{(1 - \phi) \rho^{(f)}} \right\},$$  \hspace{1cm} (2.16)

Accordingly, by knowing the mean pressure gradient, the frame acceleration is determined from Eq. 2.13, that is

$$\mathbf{A}_f^{k+1} = \frac{1}{\rho^{(p)}} \left( -\langle \overline{g} \rangle_{\mathcal{V}}^{k+1} + \frac{\overline{F}_D}{\phi V} \right).$$  \hspace{1cm} (2.17)

Although these formulations are derived for freely evolving suspensions, the fixed particle assembly equations are recovered (Garg et al., 2010c) in the limiting case of massive particles ($1/\rho^{(p)} \rightarrow 0$).

In PUReIBM, due to the periodicity of the fluctuating fields, a pseudo-spectral method is used with Crank-Nicolson scheme for the viscous terms and an Adams-Bashforth scheme for the convective terms. A fractional time-stepping method based on the approach proposed by Kim and Moin (1985) is used to advance the fluctuating velocities in time. Garg et al. (2010c) and Tenneti et al. (2011) have shown that PUReIBM is numerically convergent and accurate in describing the drag force for DNS of gas-solid flows. The method is validated through
a comprehensive set of tests: (i) flow past an isolated sphere (ii) Stokes flow past SC and
FCC arrangements (ranging from dilute to close-packed limit) compared with the boundary-
integral method of Zick and Homsy (1982), (iii) Stokes flow past random arrays of monodisperse
spheres compared with LBM simulations of van der Hoef et al. (2005), (iv) moderate to high
Reynolds numbers ($Re_m = 300$) in SC and FCC arrangements compared with LBM simulations
of Hill et al. (2001b), and (v) high Reynolds number flow past random arrays of monodisperse
spheres with ANSYS–FLUENT CFD package. It is also shown that PUReIBM is numerically
convergent for gas-phase velocity fluctuations (Mehrabadi et al., 2015).

2.3 Development of a three-dimensional pseudo-spectral PUReIBM

In the earlier version of PUReIBM called PS2D-FD1D, the fluctuating fields are advanced
in time using a two-dimensional pseudo-spectral technique perpendicular to the mean flow in
conjunction with a finite difference technique along the mean flow direction. This implementa-
tion easily allows parallelization of the computational domain along the mean flow direction
using a one-dimensional domain decomposition. Tenneti (2013) reported that the PS2D-FD1D
code scales well up to 12,000 processors using a pencil-like domain.

The limitations on scalability of PS2D-FD1D arising from the one-dimensional domain de-
composition approach (cf. Section 1.4.1) motivated us to develop another version of PUReIBM
based on three-dimensional pseudo-spectral method that utilizes the domain decomposition
strategy in more than one dimension. This version of the code is called PS3D and is described
in detail in the following sections.

2.3.1 Implementation of PS3D PUReIBM

Using a pseudo-spectral solver enables us to exploit the high accuracy of spectral methods for
solving the conservation equations. In pseudo-spectral methods, Fourier transforms of the fluid
velocity and pressure fields are needed at each time step. Therefore, the performance of pseudo-
spectral codes strongly depends on the method chosen for Fourier transform. In our code, we
use the FFTW3 library (Frigo and Johnson, 2005) that is based on the discrete fast Fourier
transform method proposed by Cooley and Tukey (1965). Although very efficient in Single
Instruction-Single Data (SISD) implementations, this method is only weakly scalable for Single Instruction-Multiple Data (SIMD) applications. This is because this algorithm requires access to the whole data that is spread over several computational nodes in SIMD implementations. This limitation of the fast Fourier transform limits the scalability of pseudo-spectral codes as well.

In fast Fourier transforms of multi-dimensional data, the Fourier transformation along one coordinate is independent of the transform along other coordinates. A recent version of the FFTW3 library has exploited this property to provide a one-dimensional parallelization of the fast Fourier transform. Given multi-dimensional data, for instance a three-dimensional dataset $M_x \times M_y \times M_z$ with $M_x = M_y = M_z$, which is distributed over $P_x$ processors along the first coordinate, each processor has a chunk of data with size $(M_x/P_x) \times M_y \times M_z$. To perform the Fourier transform, first $(M_x/P_x)$ two-dimensional transforms of the size $M_y \times M_z$ along the last two coordinates are performed on each processor since the required data is local to each processor. After a global data transposition, data will become decomposed along the second coordinate, i.e. $M_x \times (M_y/P_y) \times M_z$. Then, $M_y M_z/P_x$ one-dimensional Fourier transforms of the size $M_x$ are performed along the first coordinate. Although, this approach extends the scalability of the fast Fourier transform, the maximum utilization of available computational resources is limited to $P_x = M_x$ processors, and other processors remain idle while a fast Fourier transform is being performed.

Recently, some fast Fourier transform packages such as 2DECOMP (Li and Laizet, 2010), P3DFFT (Pekurovsky, 2012), and PFFT (Pippig, 2013) have been developed that enable a domain-decomposition strategy along more than one coordinate. In these packages, the data is decomposed along the first two coordinates, i.e. $(M_x/P_x) \times (M_y/P_y) \times M_z$, and thus the data along the last coordinate is local to each processor. This enables $M_x M_y/P_x P_y$ executions of one-dimensional Fourier transforms along the last coordinate. A global data transposition then rearranges the data structure as $(M_x/P_x) \times M_y \times (M_z/P_y)$ that is followed by $M_x M_z/P_x P_y$ executions of one-dimensional transforms along the second coordinate. Finally, a similar data transposition and transform along the first coordinate results in the full representation of the data in Fourier space. This approach extends the scalability of the fast Fourier transform to a
Figure 2.2: (a) Comparison of the mean drag force per particle between the PS3D and PS2D-FD1D PURelIBM codes for a FCC particle configuration with $\phi = 0.3$ and $Re_m = 20$. (b) The relative error in the drag force when compared with the highest grid resolution $D_m = 70$.

maximum of $p_x p_y = M_x M_y$ processors that enables us to simulate much bigger simulations in the SIMD implementation.

We use FFTW3 (Frigo and Johnson, 2005) along with PFFT (Pippig, 2013) to facilitate the performance of fast Fourier transforms in our code for better scalability of the code in massively parallel PR-DNS applications. The salient feature of PFFT is that it can also facilitates three-dimensional data domain decomposition in physical space, unlike other packages. This enables even higher utilization of processors in pseudo-spectral codes.

2.3.2 Validation

The PS2D-FD1D PURelIBM code has been extensively validated (Garg et al., 2010c; Tenneti et al., 2011) by comparing the drag force obtained from PURelIBM with available experimental and simulation data in the literature in a comprehensive suite of test cases. Therefore, it is legitimate to validate the accuracy of PS3D by comparing the results of this code with those obtained from PS2D-FD1D.

Figure 2.2 shows the comparison of the mean drag force obtained from the PS3D with those of the PS2d-FD1D normalized by the Stoked drag force for a FCC particle configuration with solid-phase volume fraction $\phi = 0.3$ and mean slip Reynolds number $Re_m = 20$. These results also indicate the convergence behavior of the drag force with respect to the grid resolution
Figure 2.3: (a) Comparison of the mean drag force per particle between the PS3D and PS2D-FD1D PUReIBM codes for a random particle configuration with $\phi = 0.3$ and $Re_m = 20$. (b) The relative error in the drag force when compared with the highest grid resolution $D_m = 50$. It is evident from Fig. 2.2(a) that the mean drag forces obtained from both codes are almost the same. In addition, when the relative error is calculated with respect to the highest grid resolution result, the convergence behavior of the mean drag force with respect to grid resolution obtained from both codes is the same, as observed in Fig. 2.2(b). Similarly, comparison of the drag force between the PS3D and the PS2d-FD1D in Fig. 2.3(a) for a random particle configure with $L/d_p = 5$, $\phi = 0.3$ and $Re_m = 20$ shows that the difference in the drag force between the two codes is less than 1%. Furthermore, the convergence behavior of the two codes with respect to $D_m$ for this random particle configuration is the same, as shown in Fig. 2.3(b). These results in conjunction with other validation tests that are not presented here indicates that the PS3D version of PUReIBM is as accurate and numerically convergent as the PS2D-1D.

2.3.3 Scalability

In order to check effective scaling of the PS3D PUReIBM code, its weak scaling performance have been tested on CyEnce and Condo clusters in Iowa State University as well as the Stampede cluster in XSEDE computing facility. The week scaling problem is selected such that the grid resolution on each processor be $150^3$. In addition, the solid-phase volume fraction is $\phi = 0.3$ with particles uniformly distributed in the domain. This configuration setup
Figure 2.4: Weak scaling speedup of the PS3D PURelIBM on CyEnce and Condo clusters in Iowa State University and Stampede cluster in XSEDE computing facility. These speedup profiles are compared with the ideal linear speedup shown in dashed line.

occupying about 1.5 GB of RAM on each processor guarantees that the computational load and memory usage are evenly distributed among all processors. In addition, the computational load remains constant in the scaleup process. Figure 2.4 compares the overall speedup of the PS3 code on CyEnce, Condo and Stampede clusters when the simulations with 64 processors are selected as the reference. It is observed that the speedup on Condo cluster is close to the ideal linear speedup. Although the speedup profiles on other clusters are not as close to the linear speedup as the Condo cluster profile does, they represent an acceptable speedup (about 60% on Stampede) when compared to other CFD codes.
CHAPTER 3. PSEUDO-TURBULENT GAS-PHASE VELOCITY FLUCTUATIONS IN HOMOGENEOUS GAS-SOLID FLOW: FIXED PARTICLE ASSEMBLIES AND FREELY EVOLVING SUSPENSIONS


Abstract

Gas-phase velocity fluctuations due to mean slip velocity between the gas and solid phases are quantified using particle-resolved direct numerical simulation (PR-DNS). These fluctuations are termed pseudo-turbulent because they arise from the interaction of particles with the mean slip even in ‘laminar’ gas-solid flows. The contribution of turbulent and pseudo-turbulent fluctuations to the level of gas-phase velocity fluctuations is quantified in initially ‘laminar’ and turbulent flow past fixed random particle assemblies of monodisperse spheres. The pseudo-turbulent kinetic energy (PTKE) $k^f$ in steady flow is then characterized as a function of solid volume fraction $\phi$ and the Reynolds number based on the mean slip velocity $Re_m$. Anisotropy in the Reynolds stress is quantified by decomposing it into isotropic and deviatoric parts, and its dependence on $\phi$ and $Re_m$ is explained. An algebraic stress model is proposed that captures the dependence of the Reynolds stress on $\phi$ and $Re_m$. Gas-phase velocity fluctuations in freely evolving suspensions undergoing elastic and inelastic particle collisions are also quantified. The flow corresponds to homogeneous gas-solid systems, with high solid to gas density ratio and particle diameter greater than dissipative length scales. It is found that for the parameter
values considered here, the level of pseudo-turbulence differs by only 15% from the values for equivalent fixed beds. The principle of conservation of interphase turbulent kinetic energy transfer is validated by quantifying the interphase transfer terms in the evolution equations of kinetic energy for the gas-phase and solid-phase fluctuating velocity. It is found that the collisional dissipation is negligible compared to the viscous dissipation for the cases considered in this study where the freely evolving suspensions attain a steady state starting from an initial condition where the particles are at rest.

3.1 Introduction

Gas-solid flows are encountered in industrial devices such as fluidized beds and in pneumatic conveying. It is generally agreed that the interaction of gas-phase velocity fluctuations with solid particles, as well as particle-particle interactions, play an important role in the formation of complex flow structures such as the core annular structure (Miller and Gidaspow, 1992) that is observed in circulating fluidized beds. Gas-phase velocity fluctuations also affect gas-particle and particle-wall heat transfer, and the mixing of chemical species inside the fluidized bed. This motivates the current study that is focused on understanding the origin and mechanisms responsible for the generation of gas-phase velocity fluctuations in fluidized beds. Furthermore, quantifying the level of gas-phase velocity fluctuations in canonical gas-solid flows is an important step towards understanding and modeling gas-solid flow in industrial devices.

Device-scale calculations using computational fluid dynamics (CFD) simulations of multiphase flow are a promising route to inexpensive design and scale-up of industrial process equipment (Halvorsen et al., 2003; Kashiwa and Gaffney, 2003; Sun et al., 2007). CFD of multiphase flow involves solving the averaged equations for mass, momentum and energy in both the solid and fluid phases. In every grid cell, conservation equations for averaged quantities such as volume fraction and velocity are solved for both phases. These conservation equations are obtained using a statistical averaging procedure (Anderson and Jackson, 1967; Drew and Passman, 1998), and hence the solution to these averaged two-fluid equations involves modeling the unclosed terms that represent interphase interactions.
The mean gas-phase velocity \( \langle u^{(f)} \rangle \) obtained by averaging the instantaneous momentum equation (Drew and Passman, 1998; Pai and Subramaniam, 2009) evolves as

\[
\frac{\partial}{\partial t} \left\{ \rho^{(f)} (1 - \phi) \langle u_i^{(f)} \rangle \right\} + \frac{\partial}{\partial x_j} \left\{ \rho^{(f)} (1 - \phi) \left( \langle u_j^{(f)} \rangle \langle u_i^{(f)} \rangle \right) \right\} = - (1 - \phi) \langle g_i \rangle + \frac{\partial I^{(f)} \tau_{ji}}{\partial x_j} - \frac{\partial}{\partial x_j} \left\{ \rho^{(f)} \left( I^{(f)} u_j^{(f)} u_i^{(f)} \right) \right\} - \left\{ \tau_{ji} n_j^{(p)} \delta (x - x^{(f)}) \right\},
\]

where \( I^{(f)} (x, t) \) is the indicator function of the fluid (or gas) phase, which is unity if the point \( x \) lies in the fluid-phase and zero otherwise. In this equation, \( u_i^{(f)} = u_i - \langle u_i^{(f)} \rangle \) denotes the fluctuations in the fluid velocity field with respect to the phase-averaged fluid velocity, \( \phi \) is the average volume fraction of the fluid phase, \( \rho^{(f)} \) is the material density of the fluid-phase, \( n^{(p)} \) is the unit normal vector pointing outward from the solid phase into the gas phase, and \( \delta (x - x^{(f)}) \) is the Dirac delta function representing the gas-solid interface.

In Eq. (3.1), \( g \) represents the body forces (hydrostatic pressure gradient, acceleration due to gravity etc) acting per unit volume of an infinitesimal fluid element, while \( \tau \) represents the surface stresses (both pressure and viscous stresses) acting on the surface of an infinitesimal fluid element. The first two terms on the right-hand side are the average body force density, and divergence of the average fluid-phase stress respectively. The last two unclosed terms that need to be modeled are the transport of fluid-phase velocity fluctuations (fluid-phase Reynolds stress), and the average interphase momentum transfer respectively. The average interphase momentum transfer \( \langle \tau_{ji} n_j^{(p)} \delta (x - x^{(f)}) \rangle \) has been extensively studied and there is a general consensus on the closure models for this term (Ergun, 1952; Wen and Yu, 1966; Syamlal, M. and O’Brien, T. J., 1987; Gidaspow, 1994; Hill et al., 2001a,b; van der Hoef et al., 2005; Beetstra et al., 2007; Reddy et al., 2010; Tenneti et al., 2011). However, the gas-phase Reynolds stress \( \langle I^{(f)} u_i^{(f)} u_j^{(f)} \rangle \) has not been comprehensively quantified in the parameter range corresponding to fluidized beds. Note that this pseudo-turbulent gas-phase velocity fluctuation is naturally incorporated in any PR-DNS of gas-solid flow that is used to derive drag expression.

In the absence of such comprehensive quantification, the transport of the gas-phase Reynolds stress \( R_{ij}^{(f)} = \langle I^{(f)} u_i^{(f)} u_j^{(f)} \rangle \) is sometimes neglected in CFD simulations of dense gas-solid flow.
on the grounds that the dominant forces in the gas-phase momentum balance are the pressure drop and drag force. Similarly, due to the lack of data for \( R^{(f)}_{ij} \) at low volume fractions, this term is also neglected in some CFD simulations of dilute gas-solid flow (Agrawal et al., 2001).

Nevertheless, there is evidence to indicate that gas-phase velocity fluctuations can be significant. Hot wire measurements by Moran and Glicksman (2003) indicate that the level of gas-phase velocity fluctuations can be significant in a circulating fluidized bed riser at dilute solid volume fraction. Moreover, CFD simulations of dilute gas-solid flow based on the Reynolds-averaged Navier-Stokes (RANS) equations that incorporated a model for the transport of the gas-phase Reynolds stress generally showed better agreement for mean flow velocity profiles with experiments in particle laden pipe flows (Bolio et al., 1995; Bolio and Sinclair, 1995; Crowe, 2000; Zhang and Reese, 2003). These observations, along with the measurements of Moran and Glicksman (2003), indicate that quantification and modeling of the gas-phase Reynolds stress over a range of solid volume fraction and mean slip Reynolds number (based on the mean slip velocity between solid and gas-phase) is necessary.

In industrial applications of gas-solids flow such as fluidized beds, the solid-to-fluid-density ratio is of the order of 1000, and the particle diameter \( d_p \) ranges from 50 to 500 \( \mu \)m. Therefore particle inertia is significant. Furthermore, the particle diameter is usually larger than the Kolmogorov length scale \( \eta \). In such flows the mean slip velocity between the solid and the gas-phase becomes an important parameter. The mean slip velocity causes an asymmetric pressure distribution around the particles and also results in the formation of boundary layers around the particle surface. The pressure asymmetry results in the formation of wake structures and contributes to gas-phase velocity fluctuations that interact with the particles downstream. These velocity fluctuations are generated in the gas-phase even in “laminar” gas-solid flows. They add to the inherent turbulent velocity fluctuations in the gas-phase, and contribute significantly to the gas-phase Reynolds stress. In this paper, we denote local, particle-scale gas-phase velocity fluctuations generated by the presence of particles as pseudo-turbulent velocity fluctuations, and the kinetic energy associated with these fluctuations is called the pseudo-turbulent kinetic energy (PTKE). Most closure models for the gas-phase Reynolds stress do not distinguish between the pseudo-turbulent and inherent turbulent velocity fluctuations in the flow.
This is because both these mechanisms essentially manifest themselves as a non-zero Reynolds stress in the gas-phase. However, the length and time scales associated with the turbulent and pseudo-turbulent contributions can be different. Therefore, it is useful from a modeling viewpoint to distinguish pseudo-turbulence from the turbulent velocity fluctuations intrinsic to the gas-phase in gas-solid suspensions. Note that due to the nonlinearity of the Navier-Stokes equations, it is likely that although the mechanisms responsible for the generation of PTKE and inherent turbulence are different, their effect could be coupled.

The fluctuations in gas-phase velocity that contribute to the gas-phase Reynolds stress $R_{ij}^{(f)}$ arise from fluid motions over a range of length scales. In device-scale two-fluid RANS calculations, the closure model for $R_{ij}^{(f)}$ can be termed a macroscale closure that represents these fluid motions over the entire range of length scales. In a RANS closure, the PTKE contribution can be simply taken as additive to the closure for the turbulent contribution. Currently we are not aware of any evidence from particle-resolved simulations that validates the additive approach, or indicates the need for more sophisticated models. There are several reasons for this. One is that it is non-trivial to perform PR-DNS simulation of a homogeneous turbulent particle-laden flow where there is sustained inherent turbulence as well as PTKE, without artificially forcing the flow. While in single-phase turbulence one can force at the large scales and simulate the natural dynamics of the energy cascade, current computational limitations do not permit the dynamic range needed to access this range of scales using PR-DNS. Furthermore, inertial particles dynamically interact with fluid eddies of a much larger scale and it is well established that the presence of inertial particles modifies the fluid velocity spectra at large scales. In particle-laden flows, such artificial forcing can contaminate the natural dynamics of the system. An alternative to artificial forcing in single-phase turbulence is to perform homogeneous shear simulations to sustain turbulence level. However, our analysis indicates that subjecting the fluid phase to linear shear does not ensure that the gas-solid flow will remain statistically homogeneous.

In the absence of viable options to sustain inherent turbulence in current PR-DNS of homogeneous flows, it is difficult to arrive at a definitive conclusion on this point. Therefore, the simple additive approach is a first approximation that could be improved by using a weighted
This approach may by legitimate since in a RANS closure there is no distinction on the basis of length or time scales.

In large eddy simulations (LES) of gas-solid flows (Capecelatro and Desjardins, 2013), the gas-phase velocity is partitioned into resolved (meso) scales, and unresolved (micro) scales that need to be modeled. The gas-phase momentum equation with no interphase mass transfer in such LES (Capecelatro and Desjardins, 2013) reads

$$\frac{\partial}{\partial t} \left( \rho^{(f)} (1 - \phi) \tilde{u}^{(f)} \right) + \nabla \cdot \left( \rho^{(f)} (1 - \phi) \tilde{u}^{(f)} \tilde{u}^{(f)} \right) = \nabla \cdot (\tilde{\tau} - R_u) + \rho^{(f)} (1 - \phi) g - F_{\text{inter}},$$

(3.2)

where \( \tilde{u}^{(f)} \) is the filtered gas-phase velocity, \( \tilde{\tau} \) is the filtered viscous stress tensor, \( R_u = \rho^{(f)} (1 - \phi) \tilde{u}^{(f)} \tilde{u}^{(f)} \) is the unresolved gas-phase Reynolds stress, \( g \) is the body force, and \( F_{\text{inter}} \) is the interphase momentum transfer due to the drag force. If one considers an ensemble-average of the term \( \tilde{u}^{(f)} \tilde{u}^{(f)} \), then this term contains \( \langle u^{(f)} \rangle \langle u^{(f)} \rangle \) and the mesoscale portion of \( R_{ij}^{(f)} \). If the LES filter width is of the order of 10 particle diameters then the unresolved gas-phase Reynolds stress \( R_u \) is dominated by PTKE, which can be interpreted as the microscale contribution to \( R_{ij}^{(f)} \). Note that in general, \( R_u \) could contain microscale turbulent contributions if there is a mechanism to sustain them. Therefore, PTKE may account for only a portion of the \( R_u \), rather than the entire contribution. However, the relative magnitude of these two contributions is not known in homogeneous particle-laden turbulent flow for the reasons already noted. A rough analysis based on single-phase turbulent scaling reveals that relatively a high turbulence Reynolds number \( R_{e\lambda} \) is needed to generate inherent turbulent kinetic energy that is comparable to PTKE. Based on this reasoning, we believe that PTKE will be a dominant contributor to the fluid-phase velocity fluctuations at the microscale. Therefore, it is appropriate to use PR-DNS to quantify the PTKE and infer closure laws for these unresolved gas-phase velocity fluctuations \( R_u \) in LES. Such a closure may also be meaningfully interpreted as a closure for the microscale portion of \( R_{ij}^{(f)} \).

In most of the studies that employ gas-solid flow CFD using the two-fluid approach, \( R_{ij}^{(f)} \) is modeled using an eddy viscosity (Ahmadi and Ma, 1990b; Bolio and Sinclair, 1995; Balzer et al., 1998; Benyahia et al., 2005) in a fashion similar to single-phase turbulence. The computation
of the eddy viscosity in such an approach requires the knowledge of both the kinetic energy associated with the gas-phase velocity fluctuations $k^{(f)}$ and the dissipation rate $\varepsilon^{(f)}$. In some works (Ahmadi and Ma, 1990b,a; Bolio and Sinclair, 1995; Balzer et al., 1998; Benyahia et al., 2005) a two-equation approach with transport equations for $k^{(f)}$ and $\varepsilon^{(f)}$ that are modified to account for the presence of solid particles is used to infer the eddy viscosity. There are also a few studies in which only a transport equation for $k^{(f)}$ is solved (one-equation approach), and $\varepsilon^{(f)}$ is modeled using single-phase turbulence models for dissipation rate (Ahmadi and Ma, 1990b,a; Kenning and Crowe, 1997; Crowe, 2000). A review of existing multiphase turbulence models can be found in Crowe et al. (1996). It is worthwhile to note that the algebraic models, and the one-equation approaches require the quantification of $k^{(f)}$ as well as the dissipation rate $\varepsilon^{(f)}$.

In dense gas-solid flows, non-intrusive measurements to quantify the level of gas-phase velocity fluctuations are difficult because of limited optical access, and the effect of intrusive instrumentation could alter the flow considerably. Therefore, simulations are a suitable alternative for quantifying gas-phase velocity fluctuations. A popular numerical approach that has been widely used to understand the effect of particles on the flow turbulence is the point particle direct numerical simulation (PP-DNS) methodology (Squires and Eaton, 1991a; Elghobashi and Truesdell, 1993; Boivin et al., 1998; Sundaram and Collins, 1999; Mashayek and Taulbee, 2002; Calzavarini et al., 2009). In PP-DNS, the particles are treated as point sources of momentum and the effect of the particles on the gas-phase is represented by a force applied at the particle center. This approach is valid only when the particle diameter $d_p$ is much smaller compared to the Kolmogorov length scale $\eta$. However, as noted earlier, in industrial applications of gas-solids flow the particle diameter is usually larger than the Kolmogorov length scale (Moran and Glicksman, 2003).

When the particle size is larger or comparable to the Kolmogorov length scale, it is important to resolve the boundary layers around the particle. In this regime, the appropriate numerical approach is the particle-resolved direct numerical simulation (PR-DNS) methodology in which all the scales of the inherent turbulence and the flow scales introduced by the presence of large particles are resolved. PR-DNS has been used to study the interaction of a
single particle with decaying (Bagchi and Balachandar, 2003; Burton and Eaton, 2005) and sta-
tionary (Naso and Prosperetti, 2010) isotropic turbulence. PR-DNS has also been employed to
study the effect of a collection of particles on decaying homogeneous isotropic turbulence (Lucci
et al., 2011; Subramaniam et al., 2014), particle-laden turbulent channel flow (Uhlmann, 2008;
Kidanemariam et al., 2013) as well as gas-solid flow with upstream turbulence (Xu and Sub-
ramaniam, 2010). This methodology has also been used to assess the ability of point-particle
models in predicting particle acceleration when Faxen correction is considered in the drag model
for particle diameter $2 \leq d_p/\eta \leq 14$ (Homann and Bec, 2010). It is worthwhile to note that un-
derstanding the generation of gas-phase velocity fluctuations using PR-DNS has been identified
as one of the future directions in the review article by Balachandar and Eaton (2010). Tenneti
and Subramaniam (2014) also argued that PR-DNS is a first-principles approach for developing
accurate models for unclosed terms in statistical representations of multiphase flows, including
kinetic theories of gas-solid flows (Garzó et al., 2012).

In this work, we use PR-DNS to quantify the level of gas-phase velocity fluctuations in flow
through a statistically homogeneous fixed assembly of monodisperse spheres to determine the
relative contribution of turbulent and pseudo-turbulent gas-phase velocity fluctuations to the
steady level of $k^{(J)}$. We first study the relaxation of gas-phase velocity fluctuations in initially
turbulent gas-solid flow. We then focus on quantifying the steady PTKE in a laminar flow.
We also quantify the dissipation rate of PTKE by considering the energy balance equation,
in a manner similar to the work of Kenning and Crowe (1997). To differentiate between the
pseudo-turbulent gas-phase velocity fluctuations and the inherent turbulence present in the
flow field, we consider “laminar” gas-solid flow to quantify the PTKE. In the context of this
work, “laminar” flow implies that there is no inherent turbulence in the flow field i.e. in the
absence of particles, the flow field is not turbulent.

In fixed-bed simulations the particles are held stationary and a steady flow is established
by imposing a pressure gradient that corresponds to the desired flow rate. Use of the fixed-
bed simulation setup for gas-solid flow model development is justified on the grounds that
the configuration of massive particles changes very slowly when compared to the time it takes
to attain mean momentum balance (Hill et al., 2001b; Tenneti et al., 2011). The fixed-bed
simulation setup has been successfully used to extract computational drag laws (Hill et al., 2001a,b; van der Hoef et al., 2005; Beetstra et al., 2007; Tenneti et al., 2011) as well as to understand the effect of particle clusters on gas-phase turbulence (Xu and Subramaniam, 2010). Xu and Subramaniam (2010) argued that the timescale over which the particle configuration changes depends on $Re_T = d_p T^{1/2}/\nu^{(f)}$, which is the Reynolds number based on the particle fluctuating velocity characterized by the particle granular temperature $T = 2k^{(p)}/3$, and $k^{(p)}$ is the level of energy in solid-phase velocity fluctuations. Since both experiment (Cocco et al., 2010) and PR-DNS (Tenneti et al., 2010) of gas-solid flows show that $Re_T$ is low for high Stokes number suspensions, fixed-particle assemblies have been used as a good approximation to freely evolving suspensions.

Recent PR-DNS of gas-solid flows (Uhlmann, 2008; Xu and Subramaniam, 2010) indicate that the gas-phase Reynolds stress is strongly anisotropic. In industrial gas-solid flows, the anisotropy of the velocity fluctuations results in anisotropic heat and scalar transport even in statistically homogeneous suspensions (Tenneti et al., 2013). This motivates us to quantify the level of anisotropy in gas-solid flows extracted from our PR-DNS data. These anisotropy results in conjunction with a model for gas-phase velocity fluctuations are used to propose an algebraic stress model for the gas-phase Reynolds stress in gas-solid flows.

Although the assumption of fixed particle assemblies is a good approximation to freely moving particles with high Stokes number, in reality however, particles move and collide freely in particle-laden flows. This may in turn affect the level of gas-phase velocity fluctuations. In order to account for these effects, we report PR-DNS of freely evolving homogeneous gas-solid suspensions with a finite mean slip velocity. Numerical simulations of freely evolving suspensions have been performed (Yin and Koch, 2007) to study the sedimentation of particles under gravity in the presence of fluid. In these studies, the steady mean flow Reynolds number attains a unique value that depends on problem parameters (gas and particle densities, solid volume fraction, gravitational acceleration, etc.). Therefore, in sedimenting suspensions it is not possible to simulate arbitrary Reynolds numbers. However, the simulation of freely evolving suspensions in an accelerating frame of reference (Tenneti et al., 2010) enables us to simulate suspensions at arbitrary Reynolds numbers while maintaining other parameters at fixed values.
Using this methodology, gas-phase velocity fluctuations of freely evolving suspensions are compared for selected problem parameters \((R_{em} = 20, \phi = 0.1 \text{ and } 0.2, \rho^{(p)}/\rho^{(f)} = 100 \text{ and } 1000)\) with data from fixed particle assemblies at the same solid volume fraction and Reynolds number that has not been previously reported to the best of our knowledge. This direct comparison gives us insight into the effect of freely moving particles on gas-phase velocity fluctuations. In addition, we verify the validity of the fixed bed approximation to freely evolving suspensions of particles with high Stokes number.

The rest of the paper is organized as follows. In section 3.2 we define the ensemble-averaged quantities that are computed from PR-DNS. We then briefly describe our PR-DNS approach and its validation in sections 3.3 and 3.4, respectively. The flow setup is then described in detail in section 3.5. The evolution of an initially turbulent gas phase in steady mean flow through homogeneous particle assemblies is addressed in section 3.6. Then the results quantifying the level of PTKE in terms of solid volume fraction and mean slip Reynolds number are presented in section 3.7. Subsequently, in section 3.8 the anisotropy of the Reynolds stress is examined, and an algebraic stress model is proposed. We continue our discussion with gas-phase velocity fluctuations in freely evolving suspensions in section 3.9. Quantification of the dissipation is summarized in section 3.10, followed by conclusions in section 3.11.

### 3.2 Gas-phase velocity variance

In the Eulerian two-fluid theory the fluid-phase Reynolds stress is defined as a phasic average, which is an average conditional on the presence of the fluid phase (Drew, 1983; Drew and Passman, 1998; Pai and Subramaniam, 2009). If \(Q(x,t)\) is any field, then its phasic average \(\langle Q^{(f)}(x,t) \rangle\) referred to as its fluid-phase mean, is defined as:

\[
\langle Q^{(f)}(x,t) \rangle = \frac{\langle I^{(f)}(x,t)Q(x,t) \rangle}{\langle I^{(f)}(x,t) \rangle},
\]

(3.3)

where \(I^{(f)}\) is the fluid-phase indicator function defined in section 3.1.

Using this definition, the ensemble-averaged kinetic energy in the fluid phase \(\langle E^{(f)} \rangle\) is defined as

\[
\langle E^{(f)} \rangle = \frac{1}{2} \frac{\langle I^{(f)}u_i u_i \rangle}{\langle I^{(f)} \rangle},
\]

(3.4)
where $\boldsymbol{u}$ is the fluid velocity. It is easy to see that the average kinetic energy in the fluid phase is the sum of the kinetic energy in the mean fluid motion $\bar{E}(f)$ and the average kinetic energy in the fluctuating motions $k(f)$. The average kinetic energy in the mean fluid motion is given by $\bar{E}(f) = \frac{1}{2} \left\langle u_i^{(f)} \right\rangle \left\langle u_i^{(f)} \right\rangle$, where the quantity $\left\langle u_i^{(f)} \right\rangle$ is the phase-averaged fluid velocity. The average kinetic energy in the fluctuating motion of the fluid is given by

$$k(f) = \frac{1}{2} \frac{1}{\left\langle I(f) \right\rangle} \left\langle I(f) u_i^{(f)} u_i^{(f)} \right\rangle,$$  \hspace{1cm} (3.5)

where fluctuations in the fluid velocity field are defined with respect to the phase-averaged fluid velocity i.e., $u_i^{(f)} = u_i - \left\langle u_i^{(f)} \right\rangle$. We now describe the procedure to compute $k(f)$ from the solution of the flow past statistically homogeneous suspensions using PR-DNS.

### 3.2.1 Quantifying gas-phase velocity variance from PR-DNS

In PR-DNS, a single realization from the ensemble of events that contribute to the phasic average in Eq. 3.5 is simulated (cf. figure 3.1). The set $\{X^{(i)}, V^{(i)}, i = 1, \ldots, N_p\}$ denotes the positions and velocities of a random configuration of $N_p$ particles that represents a realization $\omega$ of gas-solid flow in the event space $\Omega$. Let $\boldsymbol{u}(\boldsymbol{x}, t; \omega)$ be the fluid velocity field obtained from PR-DNS of flow past this configuration of particles. The ensemble-averaged fluid-phase velocity field is defined as (Subramaniam, 2000):

$$\left\langle u^{(f)} \right\rangle (\boldsymbol{x}, t) = \frac{1}{\Omega} \int \Omega f^{(f)}(\boldsymbol{x}, t; \omega) \boldsymbol{u}(\boldsymbol{x}, t; \omega) \, dP_\omega,$$  \hspace{1cm} (3.6)

where $P_\omega$ is the probability measure that is defined on $\Omega$. This concept is explained schematically in figure 3.1. The average gas-phase velocity and volume fraction that are solved in the CFD calculations are obtained by averaging over all possible realizations. Fluctuations in the gas-phase velocity are defined as departures of the instantaneous velocity field from the average gas-phase velocity.

If the flow is statistically homogeneous, ensemble-averaged quantities can be approximated by taking the volumetric mean of the solution fields, e.g. the volumetric mean of the velocity field over the fluid region is defined as:

$$\left\langle u^{(f)} \right\rangle_V (t; \omega) = \frac{1}{V(f)} \int_V f^{(f)}(\boldsymbol{x}, t; \omega) \boldsymbol{u}(\boldsymbol{x}, t; \omega) \, dV,$$  \hspace{1cm} (3.7)
Figure 3.1: Schematic showing the concept of the average fluid-phase velocity. The average fluid-phase velocity that is solved in gas-solid CFD simulations is obtained by averaging over all possible realizations.

where $V^{(f)}$ is the volume of the region occupied by the fluid-phase. It has been shown by Tenneti et al. (2011) that a statistically homogeneous gas-solid flow is well approximated by flow past a random configuration of particles in a periodically repeating unit cell. Therefore, volume averages are used here to estimate the true mathematical expectation. The volumetric mean approaches the ensemble average in the limit of infinite box size (i.e., $V \rightarrow \infty$). Periodic boundary conditions can be used in a computational domain with finite box size provided the two-point correlations in the particle and the fluid phases decay to zero within the box length. This is simply the two-phase extension of the criterion given by Pope (2000) for single-phase turbulent flows. Later we show that the Eulerian two-point correlation of fluid velocity does indeed decay to zero within 3 to 4 particle diameters for different grid resolutions, box sizes and Reynolds numbers. However, a box of finite length does not completely account for the statistical variability arising from different particle configurations. In order to estimate the ensemble-averaged quantities from finite box sizes more accurately, we simulate fixed particle assemblies and average over different configurations. For fixed particle assemblies, the ensemble-average is estimated by averaging over different configurations or realizations i.e.,

$$\left\{ \langle u^{(f)} \rangle \right\}_{\nu,M} (t) = \frac{1}{M} \sum_{\mu=1}^{M} \langle u^{(f)} \rangle_{V,\nu}(t; \omega_{\mu}). \quad (3.8)$$
In the above equation \( \{ u^{(f)} \}_{\nu,M} \) denotes an estimate to the true expectation \( \langle u^{(f)} \rangle \) and \( M \) denotes the number of independent realizations. Similarly, for each realization of the gas-solid flow we compute the kinetic energy in the fluctuating motions using volume averaging:

\[
\begin{aligned}
    k^{(f)}_{\mu} &= \frac{1}{V^{(f)}} \int_{V^{(f)}} \frac{1}{2} \left( u(x,t,\omega_{\mu}) - \{ u^{(f)} \} \right) \cdot \left( u(x,t,\omega_{\mu}) - \{ u^{(f)} \} \right) \, dV.
\end{aligned}
\]  

(3.9)

The value of \( k^{(f)}_{\mu} \) obtained from a single realization (cf. Eq 3.9) is averaged over multiple independent simulations (MIS) to obtain an estimate for the ensemble-averaged kinetic energy \( k^{(f)} \):

\[
\begin{aligned}
    k^{(f)} &= \frac{1}{M} \sum_{\mu=1}^{M} k^{(f)}_{\mu}.
\end{aligned}
\]  

(3.10)

A similar approach is used to calculate the gas-phase Reynolds stress tensor \( R^{(f)}_{ij} \) in section 3.8.

In the next section, we describe the PR-DNS approach that is used in this work to quantify \( k^{(f)} \) in steady flow past both fixed assemblies of spheres and freely evolving suspensions.

### 3.3 Numerical Method

Several numerical methods have been developed for PR-DNS of gas-solid suspensions (Johnson and Tezduyar, 1997; Peskin, 2002; Prosperetti and Oguz, 2001). The PR-DNS methodology employed in this work is called Particle-resolved Uncontaminated-fluid Reconcilable Immersed Boundary Method (PUReIBM).

In PUReIBM, the entire physical domain is discretized using a uniform Cartesian grid and the governing equations of fluid flow are solved on all the grid points (including those lying inside the particles). The governing equations that are solved in PUReIBM are the continuity and the Navier-Stokes equations equation that are respectively given as

\[
\begin{aligned}
    \nabla \cdot u &= 0, \quad (3.11) \\
    \rho^{(f)} \frac{\partial u}{\partial t} + \rho^{(f)} S &= -g_{\text{IBM}} + \mu^{(f)} \nabla^2 u + f - \rho^{(f)} A_f. \quad (3.12)
\end{aligned}
\]

Here \( u \) is the instantaneous velocity field, \( S = \nabla \cdot (uu) \) is the convective term in conservative form, \( g_{\text{IBM}} \) is the pressure gradient, and \( A_f \) accounts for the acceleration of the frame of
reference (Tenneti et al., 2010). The simulation of freely evolving suspension in PUReIBM is carried out in an accelerating frame of reference that moves with the mean velocity of particles. The formulation of PUReIBM in an accelerating frame of reference enables the simulation of not just sedimenting suspensions, but arbitrary mean slip values while maintaining average particle motion at rest in the accelerating frame. In other words, the use of accelerating frame of reference facilitates examining the influence of each flow parameter while maintaining other parameters constant.

The no-slip and no-penetration conditions on the fluid velocity at the particle surfaces is imposed via the additional immersed boundary (IB) force term \( f \) in Eq. (3.12). The full details of the computation of the IB force can be found in the work of Tenneti et al. (2011). To compute the IB force, the surface of the sphere is represented by a discrete number of points called the boundary points that are parametrized in spherical coordinates. Two additional sets of points, termed as exterior and interior points are generated by projecting the boundary points onto spheres of radii \( r + \Delta r \) and \( r - \Delta r \) respectively, with \( \Delta r \) chosen to be equal to the grid spacing.

In PUReIBM, the IB force is computed at the interior points so that a desired velocity \( u^{(d,k)} \) is obtained at the \( k^{th} \) interior point. Following the direct forcing method proposed by Mohd-Yusof (1996) the IB force \( f^{(k)} \) at the \( k^{th} \) interior point is specified to cancel the remaining terms in the momentum conservation, and to force the velocity to its desired value \( u^{(d,k)} \):

\[
f^{(k)} = \rho^{(f)} \frac{u^{(d,k)} - u^{(k,n)}}{\Delta t} + \rho^{(f)} \nabla \cdot [\mu^{(f)} \nabla u^{(k,n)}] + g^{(k,n)} - \mu^{(f)} \nabla \cdot u^{(k,n)} + \frac{\rho^{(f)} \mathbf{A}}{\Delta t^{(f)}}.
\] (3.13)

Note that all the terms in the above equation are evaluated at the \( k^{th} \) interior point. The desired velocity \( u^{(d,k)} \) depends on the velocity of the particle. For instance, for a fixed particle the desired velocity at the interior point is equal in magnitude but opposite in direction of the fluid velocity at the corresponding exterior point so that the velocity at the boundary point is zero. The IB force so computed at all the interior points is interpolated to the neighboring grid nodes that do not include those lying in the fluid phase to get \( f \).
The governing equations in PUReIBM are solved in terms of fluctuating variables and periodicity conditions are imposed on the appropriate fluctuating fields. The velocity field is decomposed into a spatially uniform mean flow \( \langle u \rangle_V(t) \) and a fluctuating velocity \( u'(x,t) \), i.e.,

\[
  u(x,t) = \langle u \rangle_V(t) + u'(x,t),
\]

where the volumetric mean velocity is obtained by averaging the velocity field over the entire computational domain. Similar decompositions are written for the convective term \( S \), pressure gradient \( g \), and IB forcing \( f \) terms. Substituting the above decompositions in Eqs. (3.11) and (3.12), followed by averaging over the entire computational domain yields the volume averaged mass and momentum conservation equations (detailed equations are given by Tenneti et al. (2011)). Evolution equations for the fluctuating variables are derived by subtracting the volume averaged equations from their instantaneous counterparts. The resulting equations for the fluctuating variables are solved using a pseudo-spectral method, with the Crank-Nicolson scheme for the viscous terms, and an Adams-Bashforth scheme for the convective terms. A fractional time-stepping method that is based on Kim and Moin’s approach (Kim and Moin, 1985) is used to advance the fluctuating velocity fields in time.

In the case of fixed assemblies, the no-slip and no-penetration boundary conditions on \( u \) are imposed at the fixed particle surfaces. For freely evolving suspension, the particles in PUReIBM move under the influence of hydrodynamic and collisional forces, and are represented in a Lagrangian frame of reference at time \( t \) by \( \{X^{(i)}(t), V^{(i)}(t) \ i = 1...N_p\} \), with \( X^{(i)}(t) \) and \( V^{(i)}(t) \) being the position and velocity of the \( i^{th} \) particle, respectively, and \( N_p \) being the total number of particles. The position and translational velocity of the \( i^{th} \) particle evolve according to Newton’s second law as

\[
  \frac{dX^{(i)}(t)}{dt} = V^{(i)}(t),
\]

\[
  m \frac{dV^{(i)}(t)}{dt} = B + F^{(h)}_{i}(t) + \sum_{j=1 \atop j \neq i}^{N_p} F^{(c)}_{ij}(t)
\]

where \( B \) is any external body force, \( F^{(h)}_{i} \) is the hydrodynamic force (calculated from the velocity and pressure fields at the particle surface) and \( F^{(c)}_{ij} \) is the contact force on the \( i^{th} \) particle as a
result of collision with $j^{th}$ particle. Particle-particle interactions are treated using a soft-sphere model originally proposed by Cundall and Strack (1979). In the soft-sphere approach, the contact mechanics between two overlapping particles is modeled by a system of springs and dashpots in both normal and tangential directions. The spring causes colliding particles to rebound, and the dashpot mimics the dissipation of kinetic energy due to inelastic collisions. The spring stiffness coefficients in the tangential and normal directions are $k_t$ and $k_n$, respectively. Similarly, the dashpot damping coefficients in the tangential and normal directions are $\eta_t$ and $\eta_n$, respectively. The spring stiffness and dashpot damping coefficients are related to the coefficient of restitution and the coefficient of friction (Garg et al., 2010a).

The particles considered in this study are assumed to be frictionless. This implies that the tangential component of the contact force is zero, and thus rotation of particles is not accounted for in this study. Therefore, only the normal component of the contact force $F_{n_{ij}}$ is considered at time $t$, and it is given by

$$F_{n_{ij}} = k_n \delta_{ij} n_{ij} - \frac{m}{2} \eta_n V_{n_{ij}},$$

where $\delta_{ij}$ is the overlap between the particles computed using the relation

$$\delta_{ij} = d_p - |X^{(i)} - X^{(j)}|,$$

and $V_{n_{ij}}$ is the relative velocity in the normal direction that is defined using

$$V_{n_{ij}} = \left[ \left( V^{(i)} - V^{(j)} \right) \cdot \hat{r}_{ij} \right] \hat{r}_{ij}.$$  

The normal vector $\hat{r}_{ij}$ is the unit vector along the line of contact pointing from particle $i$ to particle $j$. The hydrodynamic and contact forces computed at each time step are then used to evolve the position and translational velocity of particles by Eqs. 3.15 and 3.16, respectively.

The salient feature that distinguishes PUReIBM from other immersed boundary method approaches (including the original implementation of Mohd-Yusof (1996)) is that the IB forcing is restricted to those grid points that lie in the solid. Consequently, the velocity and pressure fields in the fluid phase are a solution to the unmodified Navier-Stokes equations with the appropriate boundary conditions. Since a flow field that is contaminated by additional forcing affects the calculation of $k^{(f)}$ and its dissipation rate, the uncontaminated flow field of PUReIBM is
better suited for quantification of \( k^{(f)} \) and its dissipation rate. Another consequence of the non-contamination of the fluid flow solution by the IB forcing is that the evolution equation of the volume averaged fluid velocity exactly corresponds to that of the ensemble-averaged fluid-phase velocity. Therefore, it is possible to reconcile the solution obtained from PR-DNS with any random field theory of multiphase flow.

### 3.4 Validation

The PUReIBM PR-DNS methodology has been extensively validated (Garg et al., 2010c; Tenneti et al., 2011) by comparing the drag force obtained from PUReIBM with available experimental and simulation data in the literature in a comprehensive suite of test cases:

1. Drag acting on a single sphere (Garg et al., 2010c; Garg, 2009) with experimental correlation of Schiller and Naumann (1935)

2. Drag acting on simple cubic and face-centered cubic arrangements (Tenneti et al., 2011) of particles in Stokes flow regime with those reported by Zick and Homsy (1982) using the Boundary Integral method (semi-analytic solution)

3. Drag acting on simple cubic (SC) and face-centered cubic (FCC) arrangements (Tenneti et al., 2011) of particles at moderate Reynolds numbers with the results published by Hill et al. (2001b) using lattice Boltzmann method (LBM)

4. Mean drag acting on a random arrangement (Tenneti et al., 2011) of particles in the Stokes flow regime with the results published by Hill et al. (2001a) and van der Hoef et al. (2005) using LBM

5. High Reynolds number flow past random arrays of monodisperse spheres with ANSYS-FLUENT CFD package

In addition to the comprehensive validation of the PUReIBM method (Tenneti et al., 2011; Garg et al., 2010c), we present selected additional validation tests to establish the numerical convergence and accuracy of PUReIBM near solid boundaries in figure 3.2. The first plot (see
Figure 3.2: (a) Variation of the coefficient of pressure $C_p$ along the surface of the sphere. Symbols are the data obtained from PUReIBM simulations for a Reynolds number of 10, while the solid line is that reported in the book authored by Clift, Grace and Weber (CGW) (Clift et al. 1978). (b) Comparison of the velocity profile in a square duct obtained from PUReIBM simulations at a Reynolds number of 20 with the analytical solution (Cornish 1928). Note that the walls are generated using the immersed boundary method.

Figure 3.2(a) shows a comparison of the pressure coefficient along the surface of a sphere obtained from our PR-DNS with that reported by Clift et al. (1978) (CGW) for an isolated sphere at a Reynolds number of 10. Figure 3.2(a) shows an excellent agreement of the coefficient of pressure profile on the surface of the sphere with the data reported in CGW. The second plot (see figure 3.2(b)) shows a comparison of the velocity field in a square duct at a Reynolds number of 20 with the analytical solution given by Cornish (1928). We can see that the velocity profile obtained from PUReIBM is numerically converged and accurate. These plots show that in addition to computing the total drag accurately, our method also computes the correct contributions of pressure and viscous drag forces. In the following section we describe the simulation setup used to compute the level of gas-phase velocity fluctuations and also discuss the choice of the numerical parameters needed to ensure numerically converged results.

### 3.5 Simulation Setup

In our simulation setup the particles are held stationary and a steady flow is established by imposing a pressure gradient that corresponds to the desired mean slip Reynolds number. A typical simulation of flow past random arrangement of particles with contours of local kinetic
energy \( \left( \frac{1}{2} u_i^{(f)} u_i^{(f)} \right) \) normalized by the mean energy is shown in Fig. 3.3. In all the simulations the mean flow is directed along the positive \( x \)-axis.

For flow past homogeneous particle assemblies, a Reynolds number based on the magnitude of mean slip velocity between the two phases is defined as

\[
Re_m = \frac{(1 - \phi)|\langle W \rangle| d_p}{\nu^{(f)}},
\]

where \( |\langle W \rangle| \) is the magnitude of the mean slip velocity, \( d_p \) is the particle diameter and \( \phi \) is the solid volume fraction. The mean slip velocity \( \langle W \rangle = \langle u \rangle^{(p)} - \langle u \rangle^{(f)} \) is defined as the difference between the average solid and gas-phase velocities. In the simulations, the mean slip Reynolds number (or the desired flow rate) is specified as an input and since for fixed assemblies \( \langle u^{(p)} \rangle = 0 \), the desired fluid-phase mean velocity \( \langle u^{(f)} \rangle \) is known in terms of the input Reynolds number and other physical properties. The mean pressure gradient evolves in time until it attains the value required to drive the fluid at the desired flow rate.

Particles are initialized corresponding to a specified mean solid volume fraction \( \phi \). The particles are fixed in a random equilibrium configuration they attain following elastic collisions (in the absence of ambient fluid) starting from a lattice arrangement with a Maxwellian velocity distribution. The elastic collisions are simulated using a soft-sphere discrete element model (Cundall and Strack, 1979; Garg et al., 2010a).

The computational domain used is a cube with sides of length \( L \) which is discretized using a regular Cartesian grid with \( M \) grid cells in each direction so that \( \Delta x = L/M \) is the size of each
Table 3.1: Numerical parameters (number of particles $N_p$, number of MIS $M$, particle diameter in grid units $D_m$ and the ratio of the length of the box to the particle diameter $L/d_p$) used for random arrays in PUReIBM simulations. Different numerical parameters are used for $Re_m \leq 100$ and $Re_m > 100$. These are separated by “/”. Numbers before the “/” correspond to $Re_m \leq 100$ while numbers after the “/” correspond to $Re_m > 100$. At volume fraction 0.5 PUReIBM simulations are performed only up to a Reynolds number of 100.

<table>
<thead>
<tr>
<th>$\phi$</th>
<th>$N_p$</th>
<th>$M$</th>
<th>$D_m$</th>
<th>$L/d_p$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>80/41</td>
<td>5</td>
<td>20/30</td>
<td>7.5/6</td>
</tr>
<tr>
<td>0.2</td>
<td>161/34</td>
<td>5</td>
<td>20/40</td>
<td>7.5/4.5</td>
</tr>
<tr>
<td>0.3</td>
<td>71/26</td>
<td>5</td>
<td>30/50</td>
<td>5/3.6</td>
</tr>
<tr>
<td>0.4</td>
<td>95/20</td>
<td>5</td>
<td>30/60</td>
<td>5/3</td>
</tr>
<tr>
<td>0.5</td>
<td>61/–</td>
<td>5</td>
<td>40/–</td>
<td>4/–</td>
</tr>
</tbody>
</table>

grid cell. The spatial resolution is represented by the number of grid cells across the diameter of a particle, which is denoted $D_m = d_p/\Delta x$. For random arrangements of particles, the ratio $L/d_p$ is an independent parameter. The minimum box length is determined by the criterion that the spatial autocorrelation of flow statistics must decay to zero within the box. This is to prevent the periodicity of the numerical solution from leading to unphysical flow fields. The numerical parameter $L/d_p$ also determines the number of particles $N_p$ in the box such that for a given volume fraction $\phi$ it is given by

$$N_p = \left[ \frac{6\phi}{\pi} \left( \frac{L}{d_p} \right)^3 \right],$$

(3.21)

where the square brackets denote the nearest integer. The various numerical parameters used in the simulations are reported in table 3.1.

The convergence of $k^{(f)}/\bar{E}^{(f)}$ with respect to the grid resolution $D_m$ for a solid volume fraction of 0.3 and mean slip Reynolds number of 20 is shown in figure 3.4. The grid resolutions used in the PUReIBM simulations (see table 3.1) have been chosen such that they yield numerically converged solutions. The values provided in table 3.1 guarantee that particle mean drag force is also converged (Tenneti et al., 2011). The level of $k^{(f)}/\bar{E}^{(f)}$ for a specific random particle assembly clearly shows numerical convergence as the grid resolution is increased.

The convergence of the ensemble-averaged $k^{(f)}$ with 65 realizations for the case $\phi = 0.4$ and $Re_m = 100$ is shown in figure 3.5. This figure indicates that the ensemble-averaged mean obtained with 65 realizations lies within the 95% confidence intervals obtained with 5
Figure 3.4: Convergence characteristics of $k^{(f)}/\bar{E}^{(f)}$ with grid resolution $d_p/\Delta x$ for flow past a random particle configuration at $\phi = 0.3$ and $Re_m = 20$. The random configuration is the same for all grid resolutions.

Figure 3.5: Convergence characteristics of $k^{(f)}/\bar{E}^{(f)}$ with number of realizations for flow past random arrays of spheres at $\phi = 0.4$ and $Re_m = 100$. The error bars denote 95% confidence intervals in the estimation of the average $k^{(f)}$. The filled symbol represents the level of $k^{(f)}$ corresponding to 5 realizations.
realizations (highlighted as the filled symbol in figure 3.5). Also the 95% confidence intervals for 5 realizations represent less than 5% deviation from the evaluated average. Therefore, 5 independent realizations were simulated for all the cases shown in table 3.1.

Besides convergence with grid resolution and number of realizations, it is also important to check whether the box size is adequate or not. The box size is deemed adequate if the two-point correlation functions in the fluid-phase decay to zero within the box length. To check this, the two-point velocity correlation function for the streamwise component of velocities has been computed for the highest Reynolds number simulated. The fluid-phase velocity autocorrelation $\rho_{u||}(r)$ is defined as

$$\rho_{u||}(r) = \frac{\langle I(f)(x) u_{\parallel}(f)(x) I(f)(x + r) u_{\parallel}(f)(x + r) \rangle}{\langle I(f) u_{\parallel}(f)(x) u_{\parallel}(f)(x) \rangle}.$$

where $r = |r|$, and $u_{\parallel}(f)$ is the streamwise component of gas-phase velocity fluctuation. Figure 3.6(a) shows convergence of the fluid-phase velocity autocorrelation function with grid resolution as well as box size for a random configuration of particles at a solid volume fraction of 0.2 and Reynolds number of 20. The autocorrelation function has also been computed for the highest Reynolds number that we simulated and is shown in figure 3.6(b). These results clearly indicate that the numerical parameters used in our simulation are adequate to obtain numerically converged results for $k^{(f)}$. We now present the results obtained from PUReIBM simulations of flow past monodisperse fixed particle assemblies.

### 3.6 Gas-phase velocity fluctuations in steady flow past fixed particle assemblies

While the evolution of gas-phase velocity fluctuations due to particles has been studied for zero mean slip (Cate et al., 2004; Zhang and Prosperetti, 2005; Lucci et al., 2010), the mean slip velocity between the phases is non-zero in fluidized beds. Xu and Subramaniam (2010) studied the interaction of a turbulent upstream flow with a fixed particle assembly in an attempt to reproduce the experimental findings of Moran and Glicksman (2003). In their study the upstream flow is initialized with isotropic turbulence and drawn through a uniform
configuration of fixed particles by imposing a mean constant pressure gradient. This flow is inhomogeneous in the mean flow direction but gas-phase velocity fluctuations reach a constant value within three particle diameters of entering the bed. The significant result of this study is the enhancement of turbulence as it interacts with solid spheres of the fixed bed.

In the current study we simulate initially turbulent flow in fixed particle assemblies to quantify the relative magnitude of gas-phase velocity fluctuations arising from turbulent and pseudo-turbulent sources. Note that the initial isotropic turbulence is not sustained by artificial forcing and decays in time. The particle configurations correspond exactly to the uniformly distributed particle configurations of Xu and Subramaniam (2010). These configurations are uniform distributions of non-overlapping spheres generated using the Matérn hard-core point process (Stoyan et al., 1995). This process is essentially a Poisson point process for particle centers from which overlapping spheres have been removed using an approach called dependent thinning. To address the level of turbulent and pseudo-turbulent gas-phase velocity fluctuations we consider three types of simulations:
Figure 3.7: Evolution of $k^{(f)}$ normalized by mean flow $\bar{E}^{(f)}$ energy versus time normalized by the characteristic flow timescale $d_p/|\langle W \rangle|$. Symbols (▽) correspond to the simulation initialized with an isotropic turbulence. Symbols (△) represent simulation of perturbed velocity field. Symbol (○) shows the steady value of gas-phase pseudo-turbulence.

1. Case I initialized with a non-turbulent uniform laminar flow

2. Case II initialized with an isotropic turbulent flow

3. Case III initialized with the steady solution of Case I to which the initial isotropic turbulence of Case II is added

The simulations start by imposing a mean pressure gradient along the mean flow such that the Reynolds number reaches the desired value. The mean slip Reynolds number is 50 with 4 realizations for all cases. Detailed information of flow parameters is provided in table 3.2.

Table 3.2: Numerical and physical parameters of turbulent/pseudo-turbulent simulations: solid-phase volume fraction $\phi$, mean slip Reynolds number $Re_m$, Taylor microscale turbulent Reynolds number $Re_\lambda$, particle diameter to dissipative lengthscale ratio $d_p/\eta$, particle diameter in grid units $d_p/\Delta x$, computational box length to particle diameter ratio $L/d_p$, and number of particles $N_p$.

<table>
<thead>
<tr>
<th></th>
<th>$\phi$</th>
<th>$Re_m$</th>
<th>$Re_\lambda$</th>
<th>$d_p/\eta$</th>
<th>$d_p/\Delta x$</th>
<th>$L/d_p$</th>
<th>$N_p$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case I: pseudo-turbulent</td>
<td>0.05</td>
<td>50</td>
<td>–</td>
<td>–</td>
<td>20</td>
<td>12.8</td>
<td>200</td>
</tr>
<tr>
<td>Case II: turbulent</td>
<td>0.05</td>
<td>50</td>
<td>12</td>
<td>5</td>
<td>20</td>
<td>12.8</td>
<td>200</td>
</tr>
<tr>
<td>Case III: Case I_{s.s.}+iso. turb.</td>
<td>0.05</td>
<td>50</td>
<td>–</td>
<td>–</td>
<td>20</td>
<td>12.8</td>
<td>200</td>
</tr>
</tbody>
</table>
described by Rogallo (1981) for a Taylor microscale turbulent Reynolds number $Re_\lambda$ of 12 with the energy spectrum function given by Pope (2000). The corresponding Kolmogorov length scale is selected such that the ratio $d_p/\eta$ is 5. Although the $Re_\lambda$ obtained from scaling analysis in experimental studies could be relatively high (turbulent Reynolds number $Re_\lambda$ is about 50 in the work of Moran and Glicksman (2003)), we are naturally limited by computational resources to lower initial $Re_\lambda$ because particle-resolved simulations for $d_p/\eta > 1$ impose additional computational overhead. This is because the mean slip velocity generates flow structures that need to be resolved in PR-DNS (for estimates of computational cost, see for instance Xu and Subramaniam (2010)).

Figure 3.7 also indicates that for Case II, the level of $k^{(f)}$ starts from the specified initial isotropic turbulence level and increases to the steady state pseudo-turbulent value. The data reveal that the velocity fluctuations arising from the presence of particles in flow with nonzero mean slip velocity are much higher than the turbulent velocity fluctuations for $Re_\lambda = 12$, and the principal contribution to the gas-phase velocity fluctuations is the pseudo-turbulent part.

Since in this study the configurations and simulation parameters are the same as those chosen by Xu and Subramaniam (2010), we can compare the $k^{(f)}$ values between these homogeneous PURReIBM simulations and the inflow/outflow simulations of Xu and Subramaniam (2010). In their study, the flow is inhomogeneous along the flow direction and $k^{(f)}$ is reported along the mean flow direction. The level of $k^{(f)}$ increases from the beginning of the bed and represents a 100% increase from the entrance of particle bed and reaches a constant value after an entrance length of $3d_p$. Our homogeneous simulation results are similar for Case II where normalized $k^{(f)}$ starts from an initial value of 0.1 and reaches approximately twice its initial value (0.19) at steady state. This indicates that the enhancement observed by Xu and Subramaniam (2010) is mainly due to the pseudo-turbulent velocity fluctuations, an observation corroborated by experiment (Moran and Glicksman, 2003).

Case III is basically used to examine the relaxation of turbulence in particle-laden flows. The evolution of $k^{(f)}$ for Case III in figure 3.7 shows that the excess amount of $k^{(f)}$ decays and the pseudo-turbulent steady state level of $k^{(f)}$ is recovered. These results showing both attenuation and enhancement of turbulence depending on the initial level of velocity fluctuations indicate
that for this choice of $\phi$ and $Re_m$, initial turbulent motions in the gas-phase do not influence the steady value of $k^{(f)}$, which corresponds to the pseudo-turbulent fluctuations arising from the interaction of particles with the mean flow. Since the mechanism for generation and dissipation of these contributions to $k^{(f)}$ are different, this provides useful information for the development of predictive multiphase turbulence models in this regime of gas-solid flow. Therefore, in following sections we focus on quantifying the level of pseudo-turbulence and the corresponding dissipation rate over a wide range of flow parameters.

3.7 Quantification of PTKE from PR-DNS

We performed PUReIBM DNS of flow past fixed assemblies of monodisperse spheres over a wide range of solids volume fraction ($0.1 \leq \phi \leq 0.5$) and mean slip Reynolds number ($0.01 \leq Re_m \leq 300$) to quantify the level of PTKE in terms of $\phi$ and $Re_m$. All simulations start with the initial condition of uniform fluid velocity. We have shown in the previous section that initializing the simulations with a homogeneous isotropic turbulent velocity field does not affect the steady value of $k^{(f)}$ attained by the system. Therefore the steady state value of $k^{(f)}$ obtained in a fixed particle assembly depends only on the solids volume fraction and the mean slip Reynolds number. Figure 3.8(a) shows the variation of $k^{(f)}/\bar{E}^{(f)}$ with solids volume fraction for different mean slip Reynolds numbers while figure 3.8(b) shows the variation of $k^{(f)}/\bar{E}^{(f)}$ with mean slip Reynolds number for different solid volume fractions. As evident from figure 3.8(a), the
PTKE normalized by the mean energy in the gas-phase increases dramatically with volume fraction. As shown in figure 3.8(b), at a given volume fraction \( k(f) / \bar{E}(f) \) decreases rapidly with increasing mean slip Reynolds number up to \( Re_m = 50 \) and beyond \( Re_m = 50 \) it has a weak power law dependence on \( Re_m \). This behavior is a result of the normalization of \( k(f) \) by \( \bar{E}(f) \). It implies that the variance of gas velocity increases approximately as the square of the mean slip Reynolds number. Since the total kinetic energy of the gas increases with increasing mean flow Reynolds number, we expect the strength of gas-phase velocity fluctuations to also increase. Using the data obtained from PUReIBM DNS we found that the following function fits the data for PTKE with an average deviation of 5%:

\[
\frac{k(f)}{\bar{E}(f)}(\phi, Re_m) = 2\phi + 2.5\phi(1 - \phi)^3 \exp(-\phi Re_m^{1/2}) , \quad 0.1 \leq \phi \leq 0.5,
\]

\[
0.01 \leq Re_m \leq 300. \quad (3.23)
\]

As shown in Eq. 3.23, the correlation is proposed from simulations in the range \( 0.1 \leq \phi \leq 0.5 \) and \( 0.01 \leq Re_m \leq 300 \). The value of \( k(f) / \bar{E}(f) \) from Eq. (3.23) tends to appropriate values in the limit of infinite dilution and creeping flow. In the limiting case of infinite dilution i.e. \( \phi \to 0 \) the value of \( k(f) / \bar{E}(f) \) is zero. This limiting value is consistent with the fact that in the absence of particles the flow field is uniform. In the Stokes flow regime \( (Re_m \to 0) \) the value of \( k(f) / \bar{E}(f) \) reaches an asymptote and depends only on the solid volume fraction. This behavior is consistent with the fact that the mean drag (which is shown to be the source of \( k(f) \) in the next section) acting on the particles is linear in the Stokes flow regime and thus the normalized quantity \( k(f) / \bar{E}(f) \) is independent of Reynolds number.

Although our study is for homogeneous gas-solid suspensions, the dependence of \( k(f) \) on the solid volume fraction and mean slip Reynolds number has implications for transport of the gas-phase Reynolds stress in inhomogeneous flows also. The strong dependence of \( k(f) \) on \( \phi \) suggests that the transport of \( k(f) \) could be significant in statistically inhomogeneous flows with spatial variation of \( \phi \). The quantification of the dissipation of PTKE in the gas-phase is discussed in the following section.
3.8 Reynolds stress tensor of pseudo-turbulent gas-phase velocity fluctuations

The gas-phase Reynolds stress is defined as

$$R_{ij}^{(f)} = \frac{\langle I^{(f)} u_i^{(f)} u_j^{(f)} \rangle}{\langle I^{(f)} \rangle},$$

(3.24)

and its trace represents the level of gas-phase velocity fluctuations $k^{(f)}$. The presence of particles introduces anisotropy in the gas-phase Reynolds stress that in turn modifies the structure of the carrier phase by extending them along the mean flow (Uhlmann, 2008; Xu and Subramaniam, 2010). The gas-phase anisotropy tensor

$$b_{ij}^{(f)} = \frac{R_{ij}^{(f)}}{2k^{(f)}} - \frac{1}{3} \delta_{ij},$$

(3.25)

which is computed along the streamwise (parallel to mean slip) and spanwise (perpendicular to mean slip) directions and presented in figures 3.9(a) and 3.9(b), respectively. The results indicate that the cross-correlation of velocity fluctuations $b^{(f)}_{||,\perp}$ is negligible (not shown here), and the normal component in the parallel direction $b^{(f)}_{||}$ is dominant compared to the component in the perpendicular direction $b^{(f)}_{\perp,\perp}$. Hence, the state of pseudo-turbulent gas-phase velocity fluctuations is axisymmetric (Pope, 2000).
Figure 3.10: Symbols show length scale of gas-phase velocity fluctuations $L_{||,||}$, while the straight lines show the corresponding local interparticle spacing $L_{int}$. The shaded region shows where the maximum anisotropy occurs.

Figure 3.9 indicates that the level of anisotropy increases with $Re_m$ from Stokes flow to moderate Reynolds numbers (ranging from 10 to 40) and then smoothly decreases. We hypothesize that this variation in anisotropy is related to the ratio of the length scale associated with gas-phase velocity fluctuations to the local average interparticle spacing. These length scales are quantified using our simulations.

Increase of Reynolds number from low $Re_m$ flow initiates the separation of boundary layer around particles and a standing eddy forms behind spheres with a characteristic length (Pruppacher et al., 1970), which is a source of anisotropy in gas-phase Reynolds stress (Mohd-Yusof, 1996; Uhlmann, 2008). However, defining an appropriate length scale for gas-phase velocity fluctuations in a random particle assembly is not straightforward since the wakes are affected by the presence of neighbor particles. We use the Eulerian two-point correlation of gas-phase velocity fluctuations to define a characteristic length for gas-phase velocity fluctuations $L_{||,||}$ as follows:

$$L_{||,||} = \frac{1}{R^{(f)}_{||,||}(0)} \int_{0}^{\infty} R^{(f)}_{||,||}(r) dr,$$  \hspace{1cm} (3.26)

where $R^{(f)}_{||,||}(r)$ is

$$R^{(f)}_{||,||}(r) = \frac{1}{V(f)} \int_{V(f)} u''_{||}(x)u''_{||}(x+r) dV,$$  \hspace{1cm} (3.27)
the two-point correlation in the parallel direction. This length scale of gas-phase velocity fluctuations shown in figure 3.10 decreases with $Re_m$ due to the fact that the flow structures become finer and less correlated to other surrounding structures. In addition, increase of solid volume fraction makes the gas-phase velocity fluctuations less spatially correlated due to the influence of nearby particles, and hence the length scale decreases.

We use the radial distribution function $g(r)$ to define a characteristic local interparticle spacing within a neighborhood of a test particle. Note that other studies used a similar approach to compute the nearest neighbor distance for point particles (Hertz, 1909) and finite size particles (Torquato et al., 1990) in random particle arrangements. The radial distribution function is shown in figure 3.11 for different volume fractions. The radial distribution is the probability of finding a particle at separation $r$ given that there is a particle at the coordinate origin. By assuming a spherical shell of volume $4\pi r^2 \delta r$ at separation $r$, the number of particles in the shell is $2\pi N_p n g(r) r^2 \delta r$. Thus, we compute the local interparticle spacing of the suspension using the expression

$$L_{int} \frac{d_p}{d_p} = \frac{1}{d_p} \int_{d_p}^{R} g(r) r^2 f(l) \, dr \int_{d_p}^{R} g(r) r^2 f(l) \, dr,$$

which is a weighted average of distances among particles in a spherical shell between the minimum separation $d_p$ and $R$. In Eq. 3.28, $l$ is the surface to surface distance defined as $r - d_p$, and $f(l)$ is a weight function. We choose $R$ as the second peak of $g(r)$, which includes
all particles in the local neighborhood of the test particle. The weight function is assumed
to have the form $1/l^p$ with $p \geq 0$. Note that the choice of $p = 0$ causes $L_{\text{int}}$ to be equally
weighted by neighbor particles, while choosing higher values for $p$ preferentially weights the
most proximate particles. We select $p = 1$, a value that takes into account the importance of
all particles in the region between $d_p$ and $R$ in a manner where proximate particles contribute
more to the local interparticle spacing.

The results indicate that the local interparticle spacing (shown as straight lines in figure 3.10) intersect
the length scales of gas-phase velocity fluctuations at the Reynolds numbers
where the anisotropy starts to decrease (figure 3.9). At low Reynolds numbers, flow structures
formed behind particles elongate with $Re_m$ that give rise to the increase of anisotropy. At
moderate Reynolds numbers ($10 \leq Re_m \leq 40$) the wakes become as large as the gaps among
particles and are broken up due to interaction with neighbor spheres. Thus, the anisotropy is
characterized by the ratio of gas-phase velocity fluctuations length scale to local interparticle
spacing. The breakup of elongated structures redistributes the fluctuating velocities energy
among Reynolds stress components and decreases the anisotropy.

It is also observed that the increase of solid volume fraction causes an attenuation in the
level of anisotropy. Increase of solid volume fraction lessens the local interparticle gaps and does
not allow the formation of distinct wake structures (Reddy et al., 2013), leading to a decrease
in anisotropy. This is confirmed in figure 3.10 since the length scale of gas-phase velocity
fluctuations decreases with volume fraction. Breault et al. (2008) also reported that the axial
solid dispersion coefficient of particles in a particle-laden flow decreases with volume fraction,
which is interpreted as decrease of $R_{||}$ while $R_{\perp\perp}$ increases, and our data is in agreement
with this trend observed in experiments.

Using the gas-phase anisotropy data obtained from our PR-DNS and considering the afore-
mentioned physics explaining the behavior of gas-phase anisotropy, we found that the following
function fits the data for the gas-phase anisotropy

$$b_{||}(\phi, Re_m) = \frac{a}{1 + b \exp(-c Re_m)} \exp \left( \frac{-d \phi}{1 + e \exp(-f Re_m)} \right)$$

$$b_{\perp\perp}(\phi, Re_m) = \frac{-b_{||}(\phi, Re_m)}{2},$$

where $a$, $b$, $c$, $d$, and $e$ are fitted parameters.
which is plotted in figure 3.9 with solid lines. The model constants in Eq. 3.29 are given as \( a = 0.523, b = 0.305, c = 0.114, d = 3.511, e = 1.801, \) and \( f = 0.005 \). This model asymptotically reaches a constant value for a fixed \( \phi \) (not shown here) that guarantees the normal components of the gas-phase anisotropy remain non-zero. This model and the model proposed for \( k^{(f)} \) in Eq. 3.23 can be used together to propose an algebraic stress model (ASM) for the pseudo-turbulent gas-phase Reynolds stress in the form of

\[
\frac{R^{(f)}_{ij}}{\bar{E}^{(f)}} = 2 \left( b^{(f)}_{ij} + \frac{1}{3} \delta_{ij} \right) \frac{k(f)}{\bar{E}^{(f)}}. \tag{3.31}
\]

Comparison of this ASM with PR-DNS data as shown in figure 3.12 indicates that the model appropriately predicts the non-zero components of the pseudo-turbulent gas-phase Reynolds stress. A noteworthy feature of this model is that in the limit of \( \phi \to 0 \), the gas-phase Reynolds stress becomes zero and the system reduces to a laminar single-phase flow without any pseudo-turbulent velocity fluctuations.

### 3.9 Gas-phase velocity fluctuations in freely evolving suspensions

Although fixed beds are good approximations to particle-laden flows at high particle Stokes number, in reality each sphere moves with an acceleration arising from hydrodynamic and collisional forces. Simulation of freely evolving suspensions enables us to study the effect of
physical parameters such as solid to gas density ratio and coefficient of restitution, in addition to solid volume fraction and Reynolds number that are used to characterize fixed bed simulations. Note that these freely evolving simulations complement the study of Yin et al. (2013) by exploring the $Re_m$ axis of the parameter space, whereas their work explores granular temperature dependence for zero $Re_m$.

In our freely evolving suspension study, a mean pressure is imposed along the mean flow direction such that a desired mean slip Reynolds number is achieved. All our simulations are performed at mean slip Reynolds number $Re_m = 20$ with five independent realizations for each case. Detailed information of particle configurations is provided in table 3.3. The influence of solid volume fraction is studied by simulating two volume fractions $\phi = 0.1$ and 0.2. The simulations are initialized with a uniform mean flow for the gas phase and zero granular temperature for the solid phase, and are carried out until a steady value of $k^{(f)}$ is attained.

Table 3.3: The numerical and physical parameters of freely evolving suspensions.

<table>
<thead>
<tr>
<th>$\phi$</th>
<th>$Re_m$</th>
<th>$d_p/\Delta x$</th>
<th>$L/d_p$</th>
<th>$N_p$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.1</td>
<td>20</td>
<td>20</td>
<td>7.5</td>
<td>80</td>
</tr>
<tr>
<td>0.2</td>
<td>20</td>
<td>20</td>
<td>7.5</td>
<td>161</td>
</tr>
</tbody>
</table>

Figure 3.13: Evolution of $k^{(f)}$ normalized by mean flow energy for elastic particles with different $\phi$ and $\rho^{(p)}/\rho^{(f)}$. Fixed bed values at $\phi = 0.1$ and 0.2 are shown for comparison.
3.9.1 Effect of particle-to-fluid density ratio

To investigate the effect of particle to gas density ratio we simulated two density ratio values of $\rho(p)/\rho(f) = 100$ and 1000. These density ratios are associated with particle Stokes numbers (the ratio of the particle response time $\tau_p = \rho(p)d_p^2/(18\rho(f)\nu(f))$ to the fluid characteristic timescale $\tau_f = d_p/|\langle W \rangle|$) in the range of 123 to 1390 for the cases considered in this study. The comparison of $k(f)$ for the two density ratios with elastic particles indicates that the level of gas-phase velocity fluctuations is not significantly influenced by particle densities as shown in figure 3.13. In this figure, $k(f)$ increases rapidly and then attains a relatively constant value. The evolution of $k(f)$ is also compared with fixed bed results at the same Reynolds number and solid volume fractions represented by dashed lines in the figure. The difference of $k(f)$ in freely evolving suspensions from its value in the corresponding fixed bed is less than 10%. This establishes the validity of using fixed bed simulations as an approximation to high Stokes number suspensions undergoing elastic collisions, which was employed in earlier studies (Xu and Subramaniam, 2010; Tenneti et al., 2010).

Traditionally it has been assumed that the energy in the gas-phase velocity fluctuations is at best a small fraction of the energy in the particle velocity fluctuations and the energy associated with mean flow. Therefore, it is of interest to quantify the relative magnitude of kinetic energy in the fluctuating velocities of gas and solid phases, as shown in figure 3.14.
Figure 3.15: Comparison of $k^{(f)}$ normalized by mean flow energy for freely evolving suspensions undergoing elastic collisions (COR=1) with those undergoing inelastic collisions (COR<1).

for density ratios $\rho^{(p)}/\rho^{(f)} = 100$ and 1000. These density-weighted energies are computed as $\tilde{e}^{(f)} = \rho^{(f)}(1-\phi)k^{(f)}$ in the gas phase and $\tilde{e}^{(p)} = \rho^{(p)}\phi k^{(p)}$ in the solid phase, normalized by the kinetic energy in the mean slip $\tilde{E}^{(f)} = \rho^{(f)}\bar{E}^{(f)}$. The energy $k^{(p)}$ in the solid-phase fluctuating velocities $k^{(p)}$ is defined as $\langle \langle u''^{(p)} \cdot u''^{(p)} \rangle \rangle / 2$, where $u''^{(p)} = u^{(p)} - \langle u^{(p)} \rangle$ is the solid-phase velocity fluctuation. Figure 3.14 shows that the amount of energy in the gas-phase velocity fluctuations $\tilde{e}^{(f)}$ is comparable to that in the solid-phase and both are significant compared to the energy of the mean slip. In other words, the kinetic energy of the gas phase is as important as the kinetic energy of the solid phase, and cannot be neglected in modeling of gas-solid flows.

3.9.2 Effect of coefficient of restitution in particle collisions

In freely evolving suspensions with inelastic particle collisions, the energy of the system is dissipated by collisional dissipation among particles as well as viscous dissipation of the carrier flow. We compare the effect of the coefficient of restitution (COR) on $k^{(f)}$ in figure 3.15 for three values of COR: 1.0, 0.9, and 0.7. Figure 3.15 shows that $k^{(f)}$ is not very sensitive to COR and the differences are not statistically significant, especially for the lower volume fraction. In addition, as figures 3.15(a) and 3.15(b) show, the density ratio has negligible effect on the level of $k^{(f)}$ for inelastic particles. Similar to the results of elastic particles, the level of $k^{(f)}$ is in good agreement with those of fixed beds (refer to figure 3.13), with a maximum difference of
15\% for the higher volume fraction. The weak dependence of $k(f)$ on the inelasticity of particles further strengthens the validity of using fixed beds as an approximation to high Stokes number suspensions.

The independence of $k(f)$ with respect to COR suggests that these suspensions belong to a regime that is dominated by viscous dissipation, as opposed to the collisionally dissipative regime (Sangani et al., 1996). To precisely characterize the regime of the gas-solid flows examined in this study, we quantify the ratio of time taken by gas-phase forces to affect particle motions $t_{\text{hydro}}$, to the average time between collisions $t_{\text{coll}}$ (Wylie et al., 2003). The timescale over which the particle responds to hydrodynamic forces is defined as

$$t_{\text{hydro}} = \frac{\sqrt{3T}}{\sigma_A},$$

where $T = \langle u^{\nu(p)} \cdot u^{\nu(p)} \rangle / 3$ is the granular temperature, and $\sigma_A$ characterizes the standard deviation in particle accelerations. In order to calculate the mean collisional timescale from our PR-DNS data, we first compute $\bar{N}_{\text{coll}}$, the mean number of collisions per particle in the domain and then divide the corresponding sampling time $\bar{t}$ by this mean value, i.e. $t_{\text{coll}} = \bar{t} / \bar{N}_{\text{coll}}$. Wylie et al. (2003) reported that the flow is collision-dominant if the hydrodynamic to collisional timescale ratio is much larger than 1, i.e. $t_{\text{hydro}} / t_{\text{coll}} \gg 1 \sim O(10)$. Figure 3.16 indicates that this ratio is less than unity for the cases simulated in this study. This confirms that the time required for the gas-phase stresses to influence particle motions is less than the mean.
time between the collisions \((t_{\text{hydro}} < t_{\text{coll}})\). In other words, these gas-particle systems are dominated by viscous forces, and therefore the energy loss due to collisional dissipation does not significantly affect the evolution of \(k^{(f)}\). Consequently, the energy of gas-phase fluctuating velocities evolves in a manner similar to fixed particle assemblies.

### 3.9.3 Energy transfer from mean flow to velocity fluctuations

The principle of conservation of interphase turbulent kinetic energy (TKE) transfer proposed by Xu and Subramaniam (2007) states that \(\Pi^{(m)}\), the rate of work done by the mean pressure gradient in moving the flow at the prescribed mean slip velocity, is partitioned into sources of interphase TKE transfer in the fluid phase \(\Pi^{(f)}\) and the solid phase \(\Pi^{(p)}\), such that

\[
\Pi^{(m)} = \langle \mathbf{W} \rangle \cdot \langle \mathbf{S}^{(f)}_M \rangle = \Pi^{(f)} + \Pi^{(p)},
\]

where \(\langle \mathbf{S}^{(f)}_M \rangle = \langle \tau_{ji} n_j^{(f)} \delta(\mathbf{x} - \mathbf{x}^{(f)}) \rangle\) is the average momentum transfer between the gas and the solid phase that balances the mean pressure gradient at steady state. The source terms \(\Pi^{(f)}\) and \(\Pi^{(p)}\) appear in the evolution equations for \(k^{(f)}\) and \(k^{(p)}\), respectively, and these are given below. While in fixed beds \(\Pi^{(p)} = 0\), the solid-phase interphase TKE transfer is non-zero in freely evolving suspensions.

The evolution of \(k^{(f)}\) for a homogeneous suspension is given by (Xu and Subramaniam, 2007; Pai and Subramaniam, 2009)

\[
\rho^{(f)}(1 - \phi) \frac{dk^{(f)}}{dt} = \left[ u_i^{(f)} \tau_{ji} n_j^{(f)} \delta(\mathbf{x} - \mathbf{x}^{(f)}) \right] + \left[ u_i^{(f)} \frac{\partial (I^{(f)} \tau_{ji})}{\partial x_j} \right],
\]

where \(n^{(f)}\) is the unit normal vector pointing outward from the gas phase into the solid phase. The gas-phase interphase TKE transfer \(\Pi^{(f)}\) in Eq. 3.34 arises from the fluctuating velocity-stress tensor covariance only at the gas-solid interface, while it is zero in the bulk flow due to the Dirac delta function. The second term on the right-hand side of Eq. 3.34 is the covariance of the fluctuating fluid velocity field and the gradient of the stress tensor in the fluid phase. For statistically homogeneous flows this term simplifies (cf. Appendix A) to \(-2\mu^{(f)} \langle I^{(f)} s_{ij} s_{ij} \rangle\), where \(\varepsilon^{(f)} = 2\mu^{(f)} \langle I^{(f)} s_{ij} s_{ij} \rangle\) can be identified as the dissipation that is strictly non-negative.
Re$^T = 0$  

Re$^T = 2$  

Figure 3.17: Quantification of interphase TKE transfer terms in Eq. 3.33 normalized by $\mu^{(f)}(|\langle W \rangle|/d_p)^2$ in unsteady flows for a single realization. The scales on the left vertical axes indicate values of mixture interphase TKE transfer $\Pi^{(m)}$ and gas-phase interphase TKE transfer $\Pi^{(f)}$, while the scales on the right vertical axes indicate values of solid-phase interphase TKE transfer $\Pi^{(p)}$ as well as the error in the conservation law $\varepsilon_{\Pi}$.

Here $s_{ij} = \frac{1}{2} \left( \frac{\partial u''^{(f)}_i}{\partial x_j} + \frac{\partial u''^{(f)}_j}{\partial x_i} \right)$ is the strain rate of the fluctuating fluid velocity field.

On the other hand, the evolution equation for the solid-phase fluctuating kinetic energy $k^{(p)}$ in a homogeneous system is

$$\rho^{(p)} \phi \frac{dk^{(p)}}{dt} = \left\{ u''^{(p)}_i \tau_{ji}^{(p)} \delta (x - x^{(I)}) \right\} - \Gamma_{\text{coll}}.$$  

(3.35)

Note that the unit normal vectors are related to each other as $n^{(p)} = -n^{(f)}$. It has been shown that the correlation of the fluctuating particle acceleration with the fluctuating particle velocity $\Pi^{(p)}$ can be partitioned into a source and a sink of particle kinetic energy arising from hydrodynamic interactions (Koch, 1990; Koch and Sangani, 1999; Tenneti et al., 2010).

It is of interest to validate the conservation of interphase TKE transfer (Xu and Subramaniam, 2007) by quantifying the terms in Eq. 3.33. Figures 3.17(a) and 3.17(b) show the budget analysis of the terms in Eq. 3.33 for a single realization of a freely evolving suspension with $\phi = 0.1$, $Re_m = 20$, and $\rho^{(p)}/\rho^{(f)} = 100$. In order to illustrate the fact that the solid-phase interphase TKE transfer term can appear as either a source or a sink term in Eq. 3.35, the case in Figure 3.17(a) is initialized with particles at rest ($Re_T = 0$ where $Re_T = \sqrt{T}d_p/\nu^{(f)}$), while the case in Figure 3.17(b) is initialized with particle granular temperature higher than the steady value of $T$ that the suspension eventually relaxes to. The errors in the conservation
Figure 3.18: Quantification of interphase TKE transfer terms in Eq. 3.33 normalized by $\mu^{(f)} (|\langle W \rangle | / dp)^2$: $\Pi^{(m)}$ (○), $\Pi^{(f)}$ (△), $\Pi^{(p)}$ (●); hollow symbols ($\phi = 0.1$), filled symbols ($\phi = 0.2$). The error in the conservation of interphase TKE transfer $\varepsilon_\Pi$ is indicated by diamond symbols (⋄). The scale on the left vertical axis indicates values of $\Pi^{(m)}$ and $\Pi^{(f)}$, while the scale on the right vertical axis indicates values of $\Pi^{(p)}$ and $\varepsilon_\Pi$. The error bars, representing 95% confidence intervals, are inside the symbols for most cases since the errors are small.

Of interphase TKE transfer, defined as $\varepsilon_\Pi = \Pi^{(m)} - (\Pi^{(f)} + \Pi^{(p)})$, are represented by the right-hand-side vertical axes in these figures. The error is exactly zero for both cases, indicating that the conservation principle is satisfied correctly in our PR-DNS.

As noted earlier, the solid-phase interphase TKE transfer $\Pi^{(p)}$ can appear as a source and sink of energy in the evolution of $\tilde{e}_p$ (Koch, 1990; Koch and Sangani, 1999; Tenneti et al., 2010). Figure 3.17(a) shows that $\Pi^{(p)}$ is positive for the case initialized with $Re_T = 0$, and then relaxes to zero at steady state. The origin of this source of energy is $\Pi^{(m)}$, which is the rate of work done by the mean flow in generating velocity fluctuations that is partitioned into $\Pi^{(f)}$ and $\Pi^{(p)}$. In contrast, $\Pi^{(p)}$ is negative in the transient interval for the case initialized with $Re_T = 2$ in figure 3.17(b). This level of solid-phase velocity fluctuations is much higher than the corresponding steady value. This excess energy in the fluctuating velocities of the solid phase transfers to the fluid-phase velocity fluctuations. Therefore, the gas-phase interphase TKE transfer term $\Pi^{(f)}$ is higher than $\Pi^{(m)}$ since it receives additional rate of energy from the solid phase.
Quantification of the terms in Eq. 3.33 at steady state for all cases considered in this study is shown in figure 3.18, which indicates that the conservation principle is also satisfied on average since the error \( \varepsilon_{\Pi} \) is exactly zero. In addition, a comparison of the fluid and solid interphase TKE transfer terms in figures 3.17 and 3.18 indicates that the bulk of \( \Pi^{(m)} \) goes to \( \Pi^{(f)} \) (see left vertical axis for the scale), while \( \Pi^{(p)} \) is about two orders of magnitude smaller (see right vertical axes for the scale). This is due to the fact that in these cases the granular temperature is low \( (Re_T/Re_m \approx 0.1) \), and the kinematic condition \( u''^{(f)} = \langle W \rangle + u''^{(p)} \) (Xu and Subramaniam, 2007) that determines the level of gas-phase velocity fluctuations at the gas-particle interface shows them to be of the same magnitude as the mean slip velocity. This gives rise to the imbalance in partitioning of the rate of energy transfer to the gas phase and the solid phase. As a result, more than 95% of \( \Pi^{(m)} \) is partitioned to \( \Pi^{(f)} \), while only the remaining small portion goes to \( \Pi^{(p)} \). This imbalance in the partitioning of energy causes the level of gas-phase velocity fluctuations to attain a steady value over a much smaller timescale as compared to that of the solid phase (see figure 3.14).

The kinetic energy of the two-phase mixture \( e^{(m)} \) is defined as \( \rho^{(f)}(1 - \phi)k^{(f)} + \rho^{(p)}\phi k^{(p)} \). The mixture kinetic energy evolution equation is obtained by adding Eqs. 3.34 and 3.35:

\[
\frac{de^{(m)}}{dt} = \Pi^{(f)} + \Pi^{(p)} - \varepsilon^{(f)} - \Gamma_{\text{coll}} = \langle W \rangle \cdot \left\langle S^{(f)}_M \right\rangle - \varepsilon^{(f)} - \Gamma_{\text{coll}},
\]  

(3.36)

where the last equality stems from the conservation principle of interphase TKE transfer (Xu and Subramaniam, 2007) (cf. Eq. 3.33). If the mean slip velocity is aligned with the mean interphase momentum transfer (Hill et al., 2001b; Tenneti et al., 2010), the mixture interphase TKE transfer \( \Pi^{(m)} \) is positive and represents a source of energy, while the viscous dissipation and the collisional dissipation are sinks of energy. At steady state, the terms on the right-hand-side of Eq. 3.36 should balance each other. The \( \Pi^{(m)} \) term is computed directly from the DNS data by taking the inner product of the mean slip and the mean drag force computed by integration of the stress tensor at particle surface. The viscous dissipation is also computed directly from the DNS by the expression

\[
\varepsilon^{(f)} = \frac{1}{V} \int_V I^{(f)}2\mu^{(f)}s_{ij}s_{ij}dV.
\]

(3.37)
The collisional dissipation of the system is estimated from the expression given by Sangani et al. (1996) as
\[ \Gamma_{\text{coll}} = \frac{24}{d_p \pi^{1/2}} (1 - e) \rho^{(p)} \phi^2 g(d_p) T^{3/2}, \] (3.38)
where \( e \) is the COR.

The budget analysis of Eq. 3.36 in figure 3.19 indicates that for these suspensions where the particles start from rest and attain a relatively low steady state granular temperature \( (Re_T/Re_m \approx 0.1) \), the principal balance of terms is between \( \Pi^{(m)} \) and \( \varepsilon^{(f)} \), while \( \Gamma_{\text{coll}} \) is smaller by one to two orders of magnitude. The balance of energy implies that the magnitude of collisional dissipation in gas-solid suspensions with low granular temperature is not significant compared to the magnitude of interphase TKE transfer and viscous dissipation. We also simulated cases with higher initial granular temperature (twice the steady Reynolds number based on granular temperature; results not shown here) and found that although \( \Gamma_{\text{coll}} \) is initially higher than at the steady state, it does not affect the steady \( k^{(f)} \) and \( k^{(p)} \). The analysis presented in this section explains why the inelasticity of particles does not influence the overall level of energy in the system, and why the magnitude of \( k^{(f)} \) does not change significantly with the COR. It also suggests that the model for steady \( k^{(f)} \) for fixed beds in Eq. 3.23 is applicable to freely evolving suspensions of gas-solid flow as well.
3.10 Quantification of the dissipation rate of PTKE

Viscous dissipation can be understood by analyzing the evolution equation of the mixture energy in statistically homogeneous gas-solid flow given by Eq 3.36. In this simple flow, the steady $e^{(m)}$ results from a balance of mixture interphase TKE transfer and viscous dissipation, bearing in mind that collisional dissipation is negligible. An expression for the mixture interphase TKE transfer $\Pi^{(m)}$ can be derived by its representation in terms of the average drag force acting per particle:

$$\Pi^{(m)} = \langle W \rangle \cdot \left( \text{S}_{M}^{(f)} \right) = \frac{18\phi(1-\phi)^{2}\mu^{(f)}}{d_{p}^{2}} F(\phi, Re_{m}) \mid \langle W \rangle \mid^{2}. \quad (3.39)$$

In the above expression, $F(\phi, Re_{m})$ is the normalized average drag force per particle given by

$$F = \frac{\mid \langle F \rangle \mid}{F_{\text{Stokes}}}, \quad (3.40)$$

where $\mid \langle F \rangle \mid$ is the average hydrodynamic force per particle and $F_{\text{Stokes}} = 3\pi\mu^{(f)}d_{p}(1-\phi) \mid \langle W \rangle \mid$ is the Stokes drag acting on an isolated sphere moving with a slip velocity of $d_{p}(1-\phi) \mid \langle W \rangle \mid$.

The expression in Eq. (3.39) for the source of $e^{(m)}$ due to interphase transfer of kinetic energy, is similar to the one derived by Crowe (2000). While Crowe (2000) used the single sphere drag correlation for $F(\phi, Re_{m})$, here we obtain this value directly from the PR-DNS. An accurate correlation for $F(\phi, Re_{m})$ has been developed using the data obtained from PUReIBM simulations (Tenneti et al., 2011). The drag correlation is summarized below for the sake of completeness. The average normalized drag force acting per particle in flow past a random assembly of monodisperse spheres is given by

$$F(\phi, Re_{m}) = \frac{F_{\text{isol}}(Re_{m})}{(1-\phi)^{3}} + F_{\phi}(\phi) + F_{\phi,Re_{m}}(\phi, Re_{m}) \quad (3.41)$$

where, $F_{\text{isol}}$ is the drag force acting on an isolated sphere moving in an unbounded medium. The drag on an isolated sphere is taken to be the correlation proposed by Schiller and Naumann (1935). The remaining two terms in Eq. 3.41 are given by

$$F_{\phi}(\phi) = \frac{5.81\phi}{(1-\phi)^{3}} + 0.48 \frac{\phi^{1/3}}{(1-\phi)^{4}},$$

$$F_{\phi,Re_{m}}(\phi, Re_{m}) = \phi^{3} Re_{m} \left( 0.95 + 0.61\phi^{3} \right).$$
The dissipation rate of PTKE can be quantified by noting that the source and sink of $e^{(m)}$ must balance each other at steady state, i.e.,

$$\Pi^{(m)} = \varepsilon^{(f)}. \quad (3.42)$$

Since the source of $e^{(m)}$ depends only on the average interphase momentum transfer and the mean slip velocity, knowledge of the average drag force acting on the particles is enough to quantify the dissipation. At any solid volume fraction and mean slip Reynolds number, the dissipation rate can be readily inferred from Eqs. 3.42 and 3.39 and by using a drag correlation (eg., Eq. (3.41)).

Note that these expressions for mixture interphase TKE transfer and viscous dissipation have been developed using a drag model obtained from PR-DNS of uniformly distributed, fixed particle assemblies. However, in practical systems where particle clustering is observed and in unsteady and inhomogeneous flows where the particle granular temperature is far from its steady value, these expressions may not be applicable in two-fluid RANS calculations. Nevertheless, these expressions are still valuable for modeling the residual fluid stresses in LES calculations that are able to resolve mesoscale features of the flow such as particle clustering.

### 3.11 Conclusions

In this work we quantify the contribution of turbulent and pseudo-turbulent gas-phase velocity fluctuations to the steady value of turbulent kinetic energy in gas-solid flows with nonzero mean slip velocity using PR-DNS of steady flow past fixed particle assemblies. We employ the Particle-resolved Uncontaminated-fluid Reconcilable Immersed Boundary Method (PURelIBM) to perform PR-DNS of flow past fixed particle assemblies. The evolution of initially isotropic turbulence in a fixed particle bed with mean slip reveals that for the solid volume fraction and Reynolds number considered in this study, the gas-phase velocity fluctuations arising from the presence of particles always relax to their pseudo-turbulent level, irrespective of the level of initial turbulence. Therefore, the level of gas-phase velocity fluctuations in particle-laden flows with $d_p/\eta > 1$ arising from the interaction of gas and solid phases through the mean slip velocity is not influenced by the initial velocity field. We also quantify the
strength of pseudo-turbulent gas-phase velocity fluctuations in gas-solid flows as a function of solids volume fraction and Reynolds number based on mean slip velocity using PR-DNS of steady flow past fixed particle assemblies. We observe that the presence of particles in mean slip generates high level of fluctuations in the gas velocity. The pseudo-turbulent kinetic energy in the fluctuating motions \( k^{(f)} \) can be as high as the kinetic energy in the mean motion \( \bar{E}^{(f)} \), especially for systems with higher solid volume fraction greater than 0.4. The ratio \( k^{(f)}/\bar{E}^{(f)} \) increases with the solids volume fraction and decreases with mean slip Reynolds number. Based on the PUReIBM PR-DNS data, we propose a correlation for \( k^{(f)}/\bar{E}^{(f)} \) in terms of solid volume fraction and mean slip Reynolds number. The current study confirms previous findings (Uhlmann, 2008; Xu and Subramaniam, 2010) that the Reynolds stress is highly anisotropic and axisymmetric along the mean slip. Over a wide range of volume fraction \( 0.1 \leq \phi \leq 0.4 \) the anisotropy increases with Reynolds number as the flow structures form and elongate in the mean slip direction. As \( Re_m \) increases in the range \( 10 \leq Re_m \leq 40 \), these structures are affected by neighbor particles that causes them to decorrelate over length scales smaller than local interparticle spacing, resulting in attenuation of anisotropy. Increase of the solid volume fraction also decreases the local interparticle gaps and flow structures are broken up leading to attenuation of anisotropy. The insight into the nature of gas-phase velocity fluctuations in gas-solid flows gained from PR-DNS is used to propose an algebraic stress model for the pseudo-turbulent gas-phase Reynolds stress in homogeneous suspensions.

We extended our PR-DNS to freely evolving suspensions in an attempt to mimic real flow conditions wherein particles are allowed to move under hydrodynamic and collisional forces. Our data indicates that the level of \( k^{(f)} \) in freely evolving suspensions with highly inertial particles is similar to those obtained from fixed particle assemblies at the same solid-phase volume fraction and mean slip Reynolds number. In addition, changes in the particle density for these high Stokes number particles do not significantly change the level of \( k^{(f)} \), since the time required for the particle configuration to change is longer than the momentum relaxation time. This suggests that the model proposed for \( k^{(f)} \) in fixed particle assemblies is also applicable to freely evolving suspensions with high Stokes number particles.
Quantification of interphase TKE transfer terms and the error in partitioning of energy from $\Pi^{(m)}$ to $\Pi^{(f)}$ and $\Pi^{(p)}$ indicates that this error is zero, which validates the principle of conservation of interphase TKE transfer (Xu and Subramaniam, 2007). It also shows that most of the rate of work done by the mean flow in generating fluctuations ($\Pi^{(m)}$) goes into $\Pi^{(f)}$ to generate fluid velocity fluctuations, while $\Pi^{(p)}$ is considerably smaller in the cases considered. This finding justifies the short timescale associated with the growth of $\dot{\epsilon}^{(f)}$ to its steady value, as compared to the corresponding timescale for $\dot{\epsilon}^{(p)}$. In addition, a comparison of the timescale over which particles respond to hydrodynamic forces with the average time between collisions reveals that these flows are dominated by viscous dissipation, unlike gas-solid suspensions with high granular temperature that are characterized as collision dominant. It is also found that the estimated collisional dissipation is negligible compared to viscous dissipation, and thus variation in particle inelasticity does not substantially affect $k^{(f)}$.

3.12 Acknowledgments

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CHAPTER 4. DEVELOPING IMPROVED LAGRANGIAN POINT PARTICLE MODELS OF GAS-SOLID FLOW

This chapter is an article titled “Developing improved Lagrangian point particle models of gas-solid flow” published in *Studying Turbulence Using Numerical Simulation Databases-XV, Proceedings of the CTR 2014 Summer Program* authored by S. Subramaniam, M. Mehrabadi, J. Horwitz, and A. Mani (Subramaniam et al., 2014).

Abstract

Lagrangian point-particle models are widely used to model particle-laden flows in Reynolds Average Navier-Stokes (RANS) simulation, Large Eddy Simulation (LES) and Direct Numerical Simulation (DNS) codes. Point-particle models do not impose the exact boundary conditions corresponding to particle-fluid interaction, but rather they employ a particle acceleration model to represent the fluid-particle interaction. In two-way coupled problems the effect of the solid particles on fluid phase momentum balance is accomplished through an interphase coupling algorithm. Both the drag law and the interphase coupling algorithm affect the accuracy with which the coupled mean momentum and kinetic energy equations are solved. In this study we use particle-resolved direct numerical simulation (PR-DNS) in decaying isotropic turbulent flow to assess the accuracy of point-particle acceleration models, and also their implication for interphase energy transfer in point-particle direct numerical simulation (PP-DNS). Our results indicate that a steady drag model for particle acceleration underpredicts the true particle acceleration. In addition, the particle kinetic energy and viscous dissipation are also underpredicted. These discrepancies are traced to the simple form of the particle acceleration model, and motivate improvements.
4.1 Introduction

Interaction of solid particles with a turbulent flow is very common in nature and in industrial applications. Natural events include transport of volcanic ash in the atmosphere as well as sedimentation of solid particles in rivers. The industrial application that motivates this study is a solar receiver in which particles absorb solar energy by radiation, generating buoyant flow motions that lead to generation of a turbulent flow (Zamansky et al., 2014). Understanding particle-turbulence interaction is essential for better predictive modeling of particle-laden flows in natural events and of industrial applications.

Particle-laden flow problems are characterized by high-dimensional parameter space including particle-to-fluid density ratio $\rho^p/\rho^f$, mass loading, particle Stokes number $St_\eta = \tau_p/\tau_\eta$ with $\tau_p = \rho^p d_p^2/18 \rho^f \nu^f$ and $\tau_\eta$ being, respectively, the particle response time and Kolmogorov time scale, particle Reynolds number $Re_p = u'd_p/\nu^f$ with $u'$ being a fluid-phase velocity scale, and particle diameter to Kolmogorov length scale ratio $d_p/\eta$. The choice of numerical method depends on the region of the parameter space that is accessed by the particle-laden flow.

If particles are much smaller than the Kolmogorov length scale ($d_p < \eta$), the point-particle assumption is valid in the Lagrangian-Eulerian (LE) representation of particle-laden flow (Balachandar and Eaton, 2010), where particles are described in a Lagrangian frame and the carrier flow is described in an Eulerian frame. The effect of fluid-particle interaction in the form of the hydrodynamic force on a particle can be represented by a drag model. The Maxey-Riley-Gatignol equation provides a complete description of particle acceleration that accounts for contributions from various fluid-solid interaction mechanisms (Crowe et al., 2011). These contributions are from the (a) undisturbed carrier flow, (b) steady state drag, (c) virtual mass, (d) history term, (e) Saffman lift, and (f) Magnus lift. Depending on the regime of gas-solid flow, some of these contributions may or may not be important. For instance, when particle-to-fluid density ratio is high, the virtual mass force becomes negligible. Therefore, different terms in the Maxey-Riley-Gatignol equation may be significant depending on $\rho^p/\rho^f$ and flow time scales.
for particle acceleration model in LE simulations of gas-solid flows, although for simplicity the steady drag model is used in many applications.

In the current study we are interested in investigating the accuracy of using the steady drag model in predicting true particle acceleration in a turbulent particle-laden flow. It is also of interest to examine the implication of modeled particle acceleration on the kinetic energy of fluctuating velocities in the fluid phase $k^{(f)}$ and the solid phase $k^{(p)}$ as well as the viscous dissipation $\varepsilon^{(f)}$. For this assessment, we perform PR-DNS of turbulent particle-laden flow in a regime where the PP-DNS approach is valid and then compare the evolution of $k^{(f)}$, $k^{(p)}$ and $\varepsilon^{(f)}$ between the two approaches. Thus, we can isolate the effect of the particle acceleration model on the evolution of the aforementioned quantities. To the best of the our knowledge, this study involving the direct comparison between PR-DNS and PP-DNS is the first of its kind because the resolution requirement of PR-DNS makes it prohibitively expensive to simulate in a parameter regime also applicable to PP-DNS.

The rest of this report reads as follows. In Section 4.2, the kinetic energy equations of the gas-phase and the solid-phase and also the conservation of interphase TKE transfer principle are presented. In Section 4.3 PR-DNS and PP-DNS methods are described. In Section 4.4 simulation results are presented which are followed by discussions in Section 4.5. Finally, we summarize our findings and discuss future outlook for this work in Section 4.6.

### 4.2 Kinetic energy of fluctuating velocities

The evolution equation of gas-phase kinetic energy for a homogeneous gas-solid suspension is given by

$$\rho^{(f)}(1 - \phi) \frac{d k^{(f)}}{dt} = \Pi^{(f)} - \varepsilon^{(f)}$$  \hspace{1cm} (4.1)

(Xu and Subramaniam, 2007; Pai and Subramaniam, 2009), where $\rho^{(f)}$ is the gas-phase density, $\phi$ is the solid-phase volume fraction, $\Pi^{(f)}$ is the fluid-phase interphase turbulent kinetic energy (TKE) transfer, and $\varepsilon^{(f)}$ is the viscous dissipation. The evolution equation for the solid-phase kinetic energy $k^{(p)}$ in a homogeneous system is

$$\rho^{(p)} \phi \frac{d k^{(p)}}{dt} = \Pi^{(p)},$$  \hspace{1cm} (4.2)
where $\Pi^{(p)}$ is the solid-phase interphase TKE transfer. Note that in the above expression particle collisions are assumed to be elastic. Therefore, there is no energy loss owing to particle-particle interaction in the form of particle collisions. The mixture kinetic energy $e^{(m)}$ is defined as $\rho^{(f)}(1 - \phi)k^{(f)} + \rho^{(p)}\phi k^{(p)}$ which is the mass-weighted kinetic energy in the system. We can derive an evolution equation for the mixture energy by simply adding Eqs. 4.1 and 4.2. The principle of conservation of interphase TKE transfer first proposed by Xu and Subramaniam (2007) states that for a gas-solid system with zero mean slip velocity, the gas-phase and solid-phase interphase TKE transfer terms are conservative, i.e., $\Pi^{(f)} + \Pi^{(p)} = 0$. Applying this principle to the mixture energy equation reveals that

$$\frac{de^{(m)}}{dt} = \Pi^{(f)} + \Pi^{(p)} - \varepsilon^{(f)} = -\varepsilon^{(f)}.$$

(4.3)

Therefore, the mixture energy monotonically decays by only the viscous dissipation in the absence of any driving force.

In the PP-DNS approach, the evolution equations of $k^{(f)}$, $k^{(p)}$ and $e^{(m)}$ for a homogeneous gas-solid system with elastic particle collisions are given as

$$\rho^{(f)}(1 - \phi)\frac{dk^{(f)}}{dt} = \Pi_{pp}^{(f)} - \varepsilon_{pp}^{(f)},$$

$$\rho^{(p)}\phi\frac{dk^{(p)}}{dt} = \Pi_{pp}^{(p)},$$

$$\frac{de^{(m)}}{dt} = \Pi_{pp}^{(f)} + \Pi_{pp}^{(p)} - \varepsilon_{pp}^{(f)}.$$

(4.4)

In the above equations, the subscript $pp$ denotes point-particle approach quantities. Sundaram and Collins (1996) showed that if particle acceleration is modeled by a linear steady drag model of the form

$$\frac{d\mathbf{u}^{(p)}}{dt} = \frac{\mathbf{u}^{(f)}_{xp} - \mathbf{u}^{(p)}}{\tau_{p}},$$

(4.5)

with $\mathbf{u}^{(f)}_{xp}$ and $\mathbf{u}^{(p)}$ being, respectively, the fluid-phase velocity at the particle location and the particle velocity, then the summation of fluid-phase and solid-phase interphase TKE transfers is

$$\Pi_{pp}^{(f)} + \Pi_{pp}^{(p)} = -\rho^{(p)}\phi \left\langle \frac{(\mathbf{u}^{(f)}_{xp} - \mathbf{u}^{(p)}) \cdot (\mathbf{u}^{(f)}_{xp} - \mathbf{u}^{(p)})}{\tau_{p}} \right\rangle = -\varepsilon_{pp}^{*},$$

(4.6)
which is non-zero and violates the conservation principle of interphase TKE transfer (Xu and Subramaniam, 2007). This deviation from zero is interpreted as additional dissipation at particle surfaces and is denoted by \( \varepsilon_{pp}^* \). Therefore, the use of a particle acceleration model for fluid-solid interactions in the PP-DNS approach leads to a different form of the mixture energy equation, that is

\[
\frac{de^{(m)}}{dt} = -\varepsilon_{pp}^* - \varepsilon^{(f)}_{pp},
\]

which is now governed by the under-resolved viscous dissipation \( \varepsilon^{(f)}_{pp} \) and the model for additional dissipation at particle surfaces \( \varepsilon_{pp}^* \). We use our simulation data to assess the accuracy of the PP-DNS approach in predicting the evolution of \( k^{(f)} \) and \( k^{(p)} \), and also the true viscous dissipation \( \varepsilon^{(f)} \) by quantifying \( \varepsilon_{pp}^* \) and \( \varepsilon^{(f)}_{pp} \).

### 4.3 Numerical method

In the following sub-sections, we first introduce our PR-DNS approach followed by the PP-DNS methodology.

#### 4.3.1 Particle-resolved direct numerical simulation methodology

For the PR-DNS approach, we use the particle-resolved uncontaminated fluid reconcilable immersed boundary method (PUReIBM) that has been described in detail by Tenneti et al. (2010). In PUReIBM, particles are represented in a Lagrangian frame of reference at time \( t \) by \( \{ X^{(i)}(t), \ V^{(i)}(t) \ i = 1...N_p \} \) where \( X^{(i)}(t) \) and \( V^{(i)}(t) \) are the position and velocity of the \( i^{th} \) particle, respectively, and \( N_p \) is the total number of particles. The position and translational velocity of the \( i^{th} \) particle evolve according to Newton’s second law as

\[
\frac{dX^{(i)}(t)}{dt} = V^{(i)}(t),
\]

\[
m^{(i)} \frac{V^{(i)}(t)}{dt} = B + F_h^{(i)}(t) + \sum_{j=1 \atop j \neq i}^{N_p} F_{ij}^{(c)}(t),
\]

where \( B \) is any external body force, \( F_h^{(i)} \) is the hydrodynamic force arising from the stress tensor at the particle surface, and \( F_{ij}^{(c)} \) is the contact force on the \( i^{th} \) particle as a result of collision with \( j^{th} \) particle. Particle-particle interactions are treated by using a soft-sphere model originally
proposed by Cundall and Strack (1979). In the soft-sphere approach, the contact mechanics
between two overlapping particles is modeled by a system of springs and dashpots in both
normal and tangential directions. The particles considered in this study are assumed to be
frictionless and elastic. Thus, the tangential component of the contact force as well as the
normal dashpot damping coefficient are zero. Therefore, only the normal component of the
contact force $F_{nij}$ is considered at time $t$, and it is given by

$$F_{nij} = k_n \delta_{ij} \hat{r}_{ij},$$

where $k_n$ is the spring stiffness in the normal directions and $\hat{r}_{ij}$ is the unit vector along the line
of contact pointing from particle $i$ to particle $j$. In the above expression, $\delta_{ij} = d_p - |X^{(i)} - X^{(j)}|$ is the overlap of a colliding pair of particles. The hydrodynamic and contact forces computed at
each time step are used to evolve the position and translational velocity of particles by Eqs. 4.8
and 4.9, respectively.

In the fluid phase, the mass and momentum conservation equations solved by PUReIBM are

$$\nabla \cdot u = 0,$$

and

$$\rho^{(f)} \frac{\partial u}{\partial t} + \rho^{(f)} S = -g_{IB} + \mu^{(f)} \nabla^2 u + f,$$

where $u$ is the instantaneous velocity, $S = \nabla \cdot (uu)$ is the convective term in conservative
form, $g_{IB} = \nabla p$ is the pressure gradient, $f$ is the immersed boundary (IB) forcing that
accounts for the presence of particles by ensuring the no-slip and no-penetration boundary
conditions at the particle-fluid interface. The IB forcing in PUReIBM is non-zero only inside
the solid particle. Thus, the equations in the fluid phase are not contaminated by the IB
forcing. In our homogeneous and isotropic turbulence particle-laden flow setup, the governing
equations for the fluctuating velocity and pressure variables are solved using a tri-periodic
pseudo-spectral method, with the Crank-Nicolson scheme for the viscous terms, and an Adams-
Bashforth scheme for the convective terms. A fractional time-stepping method that is based
on Kim and Moin’s approach (Kim and Moin, 1985) is used to advance the fluctuating velocity
fields in time.
4.3.2 Point-particle direct numerical simulation methodology

For a dilute suspension ($\phi < 0.001$) with $d_p \leq \eta$, particles may be modeled as point sources of momentum and energy with respect to the fluid phase, and volume displacement effects in the fluid continuity and momentum equations can be neglected (Sundaram and Collins, 1996). Fluid-particle coupling then amounts to determination of the appropriate drag law and numerical implementation of that drag law. When the particle Reynolds number is of order unity or less, the Stokes drag is assumed to be the leading order contribution in the drag law. We adopt this assumption in the current work.

In the point-particle DNS algorithm, particle motions are governed by the same dynamic Eqs. 4.8 and 4.9. However, the hydrodynamic force is now estimated using a drag law. In addition, the collisional force is assumed to be negligible. The fluid-phase mass and momentum equations are, respectively, the same as Eqs. 4.11 and 4.12 with the term $f$ being replaced by $- \sum_{i=1}^{N_p} F^{(i)}_h \delta(x - x_p)/V$ which represents the transfer of momentum between the fluid phase and solid particles. The fluid equations are solved using a second order method on a staggered mesh. Fluid and particles equations are advanced in time using a fourth order Runge-Kutta scheme. To calculate the Stokes drag force, fluid velocities at cell faces are interpolated to particle locations. Once the Stokes drag has been calculated by forming the relative velocity between the $i^{th}$ particle and the interpolated fluid velocity, the force is projected back to the Eulerian grid using the same interpolation weights.

4.4 Results

We are interested in simulating a test case with $d_p = \eta$, where the PP-DNS approach holds, and that is also computationally feasible for the PR-DNS approach. Note that the computational resolution requirement for the PR-DNS approach increases inversely with the Table 4.1: Physical and numerical parameters of the turbulent gas-solid flow simulations. The grid resolution requirement across a particle is applicable only to the PR-DNS approach.

<table>
<thead>
<tr>
<th>$Re_\lambda$</th>
<th>$\phi$</th>
<th>$\rho^{(p)}/\rho^{(f)}$</th>
<th>$d_p/\eta$</th>
<th>$St$</th>
<th>$L/d_p$</th>
<th>$D_m$</th>
<th>$N_p$</th>
</tr>
</thead>
<tbody>
<tr>
<td>12</td>
<td>0.001</td>
<td>18</td>
<td>1</td>
<td>1</td>
<td>48</td>
<td>12</td>
<td>210</td>
</tr>
<tr>
<td>27</td>
<td>0.001</td>
<td>18</td>
<td>1</td>
<td>1</td>
<td>96</td>
<td>12</td>
<td>1690</td>
</tr>
</tbody>
</table>
Typical range of the particle Stokes number, Reynolds number and particle diameter in a solar power collector application are, respectively, $St_\eta = \mathcal{O}(1)$, $Re_p = \mathcal{O}(1)$, and $d_p < \eta$ (Horwitz, 2014). Although we match the non-dimensional parameters ($St_\eta = 1$ and $Re_p = 1$), we are now simulating larger particles that are less dense. This has consequences for the applicability of the steady drag model in the PP-DNS.

In the PR-DNS approach, the grid resolution across a particle should be sufficiently fine for the hydrodynamic boundary layer and velocity gradients at the particle surface to be accurately captured. In our problem, the grid resolution across each particle is $D_m = d_p/\Delta x = 12$. The large scales of isotropic turbulence are determined by the size of the computational box. In this study we considered two box sizes for our PR-DNS: A medium size box with a grid resolution $576^3$ and large size box with a grid resolution $1152^3$ that are, respectively, associated with turbulent Reynolds number $Re_\lambda = 12$ and $27$ based on the Taylor microscale length scale. Table 4.1 summarizes the physical and numerical parameters of the cases considered in this study. We choose the solid-phase volume fraction as $\phi = 0.001$ for solid particles that are uniformly distributed and initially at rest. We initialized the fluid-phase isotropic turbulence using the method of Rogallo (1981) with the energy spectrum function given by Pope (2000). Figure 4.1 shows a snapshot of the turbulent gas-solid flow in the large box.

Owing to the similarity of the results between $Re_\lambda = 12$ and $Re_\lambda = 27$ simulations, we present only the results for the case $Re_\lambda = 12$. Figure 4.2 shows a comparison of the evolution of kinetic energy in the gas-phase velocity fluctuations obtained from PR-DNS and PP-DNS. The PP-DNS result shows the same trend with a maximum difference of 3%. Note that the $k^{(f)}$ from PP-DNS is slightly overpredicted for $t\epsilon_0^{(f)}/k_0^{(f)} < 3$ compared with that of PR-DNS. The evolution of solid-phase velocity fluctuations in Figure 4.3 indicates that the maximum value of $k^{(p)}$ in PP-DNS is about 30% less than the maximum value in PR-DNS. In addition, the maximum value in the PR-DNS occurs at $t\epsilon_0^{(f)}/k_0^{(f)} = 0.5$, while it happens at $t\epsilon_0^{(f)}/k_0^{(f)} = 1.0$ in the PP-DNS.

Quantification of viscous dissipation shown in Figure 4.4 indicates an increase of about 30% in the PR-DNS, when compared with the initial viscous dissipation $\epsilon_0^{(f)}$ at the beginning of the simulation. Dissipation increases because particles that are initially at rest induce locally large
Figure 4.1: A snapshot of the large size turbulent gas-solid flow. The contour colors represent the intensity of the isotropic turbulence.

Figure 4.2: Comparison of the evolution $k^{(f)}$ between the PR-DNS and the PP-DNS approach.

Figure 4.3: Comparison of the evolution $k^{(p)}$ between the PR-DNS and the PP-DNS approach.

Figure 4.4: Comparison of the evolution of viscous dissipation between the PR-DNS and the PP-DNS approach.
Figure 4.5: Comparison of particle acceleration PDFs between the PR-DNS and PP-DNS at three different instances.

strain rates in the hydrodynamic boundary layers around each particle. The viscous dissipation from the PP-DNS approach $\varepsilon_{pp}$, however, does not show any increase from the dissipation in single-phase decaying isotropic turbulence (not shown here). If we also account for the additional viscous dissipation in Eq. 4.6 that arises from using a particle acceleration model in PP-DNS (Sundaram and Collins, 1996), only about one third of the additional dissipation at particle surface is recovered when compared with that of PR-DNS. After early stages of the simulations, particles relax to the local velocity of the flow field. Therefore, the strain rate at particle surfaces decreases and this leads to attenuation of viscous dissipation. Note that at $t\tau_0^{(f)}/k_0^{(f)} = 0.1$ there is no significant difference in viscous dissipation between PR-DNS and PP-DNS, although PR-DNS shows slightly lower dissipation. Higher value of $k^{(p)}$ and $\varepsilon^{(f)}$ in PR-DNS indicates that the mechanism of momentum and energy transfer between the fluid-phase and the solid-phase is different between the two simulation approaches.

4.5 Discussion

In this section, we first assess the ability of PP-DNS to predict the true particle acceleration, and then examine the mechanism of energy transfer between the fluid phase and the solid phase.

4.5.1 Particle acceleration PDF

We extract the magnitude of the hydrodynamic acceleration experienced by each particle and construct the corresponding probability density functions (PDF). Note that statistical error
due to a relatively low particle sample number yields relatively large confidence bounds on the data. The PDFs from the PR-DNS and the PP-DNS are compared at three times corresponding to increasing, maximum, and decreasing $k^{(p)}$, shown in Figures 4.5(a-c), respectively. The variance of PP-DNS and PR-DNS accelerations decreases in time as the particles equilibrate with the local fluid velocity. The PDFs are qualitatively similar between the PR-DNS and PP-DNS cases, although the PDF tails, corresponding to the maximum particle acceleration, do not match well at any of the times. In addition, as observed in Figure 4.5(b), the peak values of the PDFs in the PR-DNS and the PP-DNS as well as the corresponding accelerations where these peaks occur are different.

The deviation of PP-DNS particle accelerations from the PR-DNS true accelerations suggests that other types of hydrodynamic forces such as the virtual mass force, the history force, and the lift forces, may also be important and should be considered in LE simulation of a gas-solid flows (Crowe et al., 2011).

### 4.5.2 Interphase TKE transfer

Recall from Eq. 4.2 that the rate of change of solid-phase kinetic energy is governed by the interphase TKE transfer term. The interphase TKE transfer has the form

$$\Pi^{(p)} = \langle u^{(p)} \cdot A' \rangle,$$

which is the particle velocity-acceleration covariance. Tenneti et al. (2010) showed that the interphase TKE transfer acts as either a source or a sink of $k^{(p)}$ and can be quantified by a quadrant analysis. Figure 4.6(a) shows the fluctuating velocity-acceleration scatter plot of PR-DNS at $\varepsilon_\text{f}(f)/k_0^{(f)} = 0.2$. Those points that lie in quadrants 1 and 3 contribute to the source of $k^{(p)}$ whereas those in quadrants 2 and 4 contribute to the sink.

Figure 4.6 compares scatter plots of $u^{(p)} \cdot A'$ between the PR-DNS and PP-DNS during the increase, at maximum, and during the decrease of $k^{(p)}$. Figures 4.6(a) and 4.6(d) shows that in the region where $k^{(p)}$ increases, the contribution to the source is much more than the contribution to the sink. Therefore, the correlation on the right-hand side of Eq. 4.13 is positive that leads to the increase of $k^{(p)}$. When $k^{(p)}$ is at maximum, the scatter points are
Figure 4.6: Scatter plot of $u'(p) - A'$ that corresponds to the quantification of the source and the sink of solid-phase kinetic energy. The first row of figures with filled symbols corresponds to PR-DNS, and the second row of figures with hollow symbols belongs to PP-DNS. The first and last columns are extracted at a time when $k(p)$ is increasing and decreasing, respectively, while the middle column is extracted at the time when $k(p)$ reaches the maximum value. In these plots, the horizontal axes are normalized by the standard deviation of particle velocity fluctuations, and the vertical axes are normalized by the standard deviation of particle accelerations. The values of $\sigma_{u'}$ and $\sigma_{A'}$ are given in Table 4.2.
approximately uniformly distributed in all quadrants as shown in Figures 4.6(b) and 4.6(e), suggesting that the correlation is approximately zero. During the decay of $k^{(p)}$, the contribution to the sink is slightly more than the contribution to the source as shown in Figures 4.6(c) and 4.6(f), which leads to the attenuation of $k^{(p)}$. Although these normalized plots in each column comparing the PR-DNS with PP-DNS results are similar, the standard variations of $\sigma_{u'}$ and $\sigma_{A'}$ between the PR-DNS and PP-DNS are quite different at the first two time instances as shown in Table 4.2. These differences substantially change the mechanism of energy transfer from one phase to another which leads to a difference in the evolution of $k^{(p)}$ between the PR-DNS and PP-DNS.

Because particle acceleration plays a key role in the interphase transfer of energy to and from the solid phase, any inaccuracy in the prediction of particle acceleration affects the evolution of $k^{(p)}$ as well as the $k^{(f)}$ in the neighborhood of each particle. These effects are non-linear and feedback on each other. Therefore, accurate modeling of the particle acceleration term is crucial for accurate determination of both particle and fluid statistics.

### 4.6 Conclusion

In this study, we performed PR-DNS and PP-DNS of a turbulent particle-laden suspension in a regime identified by $St_\eta = 1$, $Re_p = 1$ and $d_p/\eta = 1$. Comparison of decaying isotropic turbulence shows similar trends for the fluid-phase kinetic energy between the PR-DNS and PP-DNS cases. However, $k^{(p)}$ is significantly different in terms of the maximum value and the time at which the maximum value occurs. This deviation is associated with the difference in the transfer of energy between the fluid phase and the solid phase in the two approaches. The

<table>
<thead>
<tr>
<th>$t\varepsilon_0^{(f)}/k_0^{(f)}$</th>
<th>0.2</th>
<th>At the peak of $k^{(p)}$</th>
<th>3.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\sigma_{u'}/u_\eta$</td>
<td>$\sigma_{A'}\tau_\eta/u_\eta$</td>
<td>$\sigma_{u'}/u_\eta$</td>
<td>$\sigma_{A'}\tau_\eta/u_\eta$</td>
</tr>
<tr>
<td>PR-DNS</td>
<td>1.13</td>
<td>0.25</td>
<td>0.79</td>
</tr>
<tr>
<td>PP-DNS</td>
<td>0.63</td>
<td>0.18</td>
<td>0.80</td>
</tr>
</tbody>
</table>

Table 4.2: Standard variation of particle velocity fluctuation and particle acceleration in the PR-DNS and the PP-DNS at three different times in accordance with Figure 4.6. These quantities are normalized by the initial Kolmogorov velocity scale $u_\eta$ and time scale $\tau_\eta$. 
covariance of particle acceleration-particle velocity acts as the source and sink of the solid-phase kinetic energy. Use of the Stokes drag law in the PP-DNS approach leads to inaccuracy in prediction of particle acceleration that in turn affects the solid-phase kinetic energy. The Stokes drag cannot solely represent the gas-solid interaction. Other contributions such as the virtual mass force or history force are also important at low $\rho^{(p)}/\rho^{(f)}$. This study will open the door for more simulations to be performed that directly compare PR-DNS and PP-DNS where the aforementioned hydrodynamic forces are also accounted for. As a validation tool, particle-resolved simulations will enable testing of theory established by point-particle simulations. Comparison of PR-DNS and PP-DNS will shed light on flow physics and lead to improvement of point-particle acceleration models.

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CHAPTER 5. IMPORTANCE OF THE FLUID-PARTICLE DRAG MODEL IN PREDICTING SEGREGATION IN BIDISPERSE GAS-SOLID FLOW

This chapter includes a manuscript titled “Importance of fluid-particle drag in predicting segregation in bidisperse gas-solid flow” and is under review in the International Journal of Multiphase Flow authored by M. Mehrabadi, S. Tenneti, and S. Subramaniam.

Abstract

The slip velocity between particle size classes in a homogeneous bidisperse gas-solid flow is quantified using particle-resolved direct numerical simulation (PR-DNS). This slip velocity is the key characteristic of size segregation in industrial devices. The ability of current gas-particle drag models to predict this slip velocity is examined by simultaneously solving the mean momentum equations for the gas phase and dispersed phases. PR-DNS of fixed particle assemblies is then used to validate and improve the bidisperse gas-particle drag model. The drag model inferred from bidisperse fixed beds is compared with the drag force measured from PR-DNS of freely evolving bidisperse suspensions. The ability of this new model to predict the slip velocity between particle size classes in a bidisperse gas-solid flow is also examined.

5.1 Introduction

Gas-solid flows are commonly found in industrial applications such as fluidized-bed combustion, fluid catalytic cracking, coal gasification, and biomass energy generation (Fan et al., 2004). In these flows, the dispersed phase is generally polydisperse, meaning that there is a distribution in the particle size and density. These distributions lead to a complex interplay of
various gas-particle and particle-particle interactions that in turn give rise to particle mass flux of one particle class with respect to the others (Holloway et al., 2011). This mass flux is the key signature of the segregation phenomenon observed in gas-solid suspensions (Nienow et al., 1987; Wu and Baeyens, 1998; Goldschmidt et al., 2003; Bokkers et al., 2004; Chew et al., 2011; Hoffmann et al., 1993; Fan and Fox, 2008; Holloway et al., 2011; Norouzi et al., 2012). Segregation is desirable in processes where separation of particle classes is required, while it may not be beneficial in processes where a homogeneous mixture of the dispersed phase is needed. Therefore, accurate modeling of the size and density-dependent particle mass flux in polydisperse suspensions sheds light on the segregation phenomenon and provides useful information for better engineering design.

In the gas-solid flow applications mentioned above, the material density ratio ranges from \( \rho^{(p)}/\rho^{(f)} \sim \mathcal{O}(100) \) to \( \mathcal{O}(1000) \) and the particle diameter varies from \( d_p \sim 50\mu m \) to \( 500\mu m \). The interaction of the gas phase with classes of particles in the form of gas-particle drag force depends on particle material density and particle diameter. This dependence leads to a net mean hydrodynamic force on each particle class that results in relative mean motion between particle classes. On the other hand, the hydrodynamic forces acting on each particle give rise to the growth of particle velocity fluctuations characterized by particle granular temperature (Tenneti et al., 2010). The random motion of particles increases the probability of a particle colliding either with other particles of the same class, or with particles belonging to other classes. Particle collisions in a polydisperse system leads to a transfer of mean momentum from one particle class to another that is referred to as the particle-particle drag force. This particle-particle drag hinders the increase of mean slip velocity between particle classes, and thus reduces segregation.

In a polydisperse suspension, the balance between gas-particle and particle-particle interactions governs the relative motion of particle classes. Bidisperse flows with two particle classes of differing size or density (or both size and density) are the simplest polydisperse flow. The interaction of two particle classes in a bidisperse flow also forms the basis for models of polydisperse flow that rely on a pairwise additive interaction between particle classes (Syamlal et al., 1993). Therefore, this work focuses on bidisperse flows.
The study of segregation in practical applications of polydisperse gas–solid flow is complicated by wall effects and statistical inhomogeneity, i.e. mean flow quantities such as average fluid velocity vary with spatial location. Therefore, it is difficult to isolate the effect of individual terms such as fluid–particle drag in such problems. In a statistically homogeneous flow the mean flow quantities are spatially uniform and wall effects are absent, which allows for easy evaluation of models for unclosed terms such as the fluid–particle drag, and their subsequent development. Therefore, in this work we focus on statistically homogeneous bidisperse gas–solid flow.

Although the kinetic theory of bidisperse granular flow predicts that non-zero particle mass flux arises only if there are gradients in particle number density, particle granular temperature, or external forces (Garzó et al., 2007), the interaction of particles with the ambient fluid provides another mechanism for segregation in gas–solid flow. At this point there is no comprehensive mapping of the regions in parameter space defined by particle class ratios of density, size and volume fraction \((\rho_2/\rho_1, d_2/d_1, \phi_2/\phi_1)\) which shows where segregation or mixing are expected.

Experimental investigations provide useful information about gas-solid flows (Bokkers et al., 2004; Chew and Hrenya, 2011) but experiments include wall effects and it is difficult to isolate the effects of individual terms in these studies. Furthermore, limited optical access into fluidized beds limits the applicability of experimental investigations to either dilute suspensions (Lee and Durst, 1982; Rogers and Eaton, 1991; Sato et al., 1996; Oakley et al., 1997; Kiger and Pan, 2000) or pseudo two-dimensional experimental setup (Goldschmidt et al., 2003; Bokkers et al., 2004).

Particle-resolved direct numerical simulation (PR-DNS) is an alternative approach that is well suited for discovering flow physics in particle-laden flow. The PR-DNS approach not only provides detailed information about the hydrodynamic velocity and pressure fields, it also provides particles trajectories along with their velocities and accelerations. Furthermore, properly designed PR-DNS studies can be used to either propose closure models used in CFD calculations of gas-solid flow, or to test the validity of these closure models.
The PR-DNS methodology has been successfully used to propose closure models for the average interphase momentum transfer, whose principal contribution is the average gas-solid drag. Early studies focused on monodisperse gas–solid flows and they are important because the bidisperse drag law is often proposed as a modification of the monodisperse drag law. Hill et al. (2001a) used the Lattice Boltzmann Method (LBM) to propose a drag model for monodisperse arrays of ordered and randomly distributed particles in the Stokes flow regime, and validated their results for low solid volume fraction with theoretical analysis. Hill et al. (2001b) extended their drag model to moderate Reynolds numbers. In a similar attempt, van der Hoef et al. (2005) also used LBM to a propose drag model for monodisperse gas-solid flow in the Stokes regime using fixed particle assemblies. Beetstra et al. (2007) used LBM to solve for flow past fixed particle assemblies to incorporate the effect of higher mean slip Reynolds number (up to 1000) into the low-Reynolds-number monodisperse drag model of van der Hoef et al. (2005).Tenneti et al. (2011) performed PR-DNS based on the Particle-resolved Reconcilable Immersed Boundary Method (PUReIBM) to solve the Navier–Stokes equations and reported the drag force in gas-solid flows using fixed particle assemblies over a wide range of flow parameters \(0.1 \leq \phi \leq 0.5\) and \(0.01 \leq Re_m \leq 300\). They also proposed a drag law as a function of the solid-phase volume fraction \(\phi\) and mean slip Reynolds number \(Re_m\).

In an attempt to generalize the quantification of interphase momentum transfer to polydisperse systems, van der Hoef et al. (2005) performed PR-DNS of bidisperse gas-solid flow in the low Reynolds number regime. They proposed a bidisperse drag law that expresses the drag force experienced by each particle size class in terms of the drag experienced by an equivalent monodisperse suspension multiplied by a function of the particle size ratio. This function of the particle size ratio is referred to as VDH bidisperse drag model from hereon. The maximum particle size ratio of the bidisperse configurations used in their study was 1 : 4. Sarkar et al. (2009) then confirmed the applicability of VDH drag law even for extreme particle size ratios up to 1 : 10. Yin and coworkers (Yin and Sundaresan, 2009; Holloway et al., 2010) reasoned that the relative motion of particles in a suspension indirectly affects the hydrodynamic force experienced by neighboring particles through the lubrication force. They used frozen particle
configurations in the Stokes flow regime in their PR-DNS setup with assigned mean velocity to each particle class, which gives rise to evolution of flow motion through implementation of the no-slip and no-penetration boundary condition at particle surface. This methodology enabled them to explore the effect of indirect particle-particle interaction on the mean drag, and propose a new model for polydisperse suspensions in the Stokes flow regime. However, Tenneti et al. (2011) showed that this methodology is not Galilean–invariant, and may incur significant error in moderate Reynolds number flows. Rong et al. (2014) also used LBM to propose a drag model for the hydrodynamic force on each particle size class and is expressed in terms of a monodisperse drag law (Rong et al., 2013).

All of the aforementioned bidisperse PR-DNS exploited fixed or frozen particle assemblies as an approximation to real gas-solid suspensions with freely moving particles. In fixed particle assemblies, it is assumed that all particles have the same velocity. This assumption is useful for calculating the gas-particle drag in both monodisperse and polydisperse configurations, and is relatively inexpensive for parametric studies. Nevertheless, it is expected that the differences in hydrodynamic and collisional forces on particle classes result in the development of different mean velocities for each particle class. The significance of hydrodynamic and collisional forces on the development if the mean velocity difference between particle classes in freely evolving suspensions has not been reported, to the best of our knowledge.

Although the drag model proposed by van der Hoef and coworkers (van der Hoef et al., 2005; Beetsstra et al., 2007) solely depends on particle size ratio, models of Syamlal, M. and O’Brien, T. J. (1987), Yin and Sundaresan (2009), and Holloway et al. (2010) also consider the mean slip velocity between particle classes. It is not known a priori if the particle size ratio alone is adequate to characterize the mean gas-particle drag, and how well this holds in freely evolving suspensions.

In the current study we study the influence of the gas-particle drag model on the evolution of the mean slip velocity between two particle size classes in a bidisperse gas-solid flow. We start by deriving the mathematical description of a homogeneous bidisperse gas-solid flow in Section 5.2. We then provide details of our numerical approach to simulate gas-solid suspensions in Section 5.3. In Section 5.4, we perform PR-DNS of a homogeneous bidisperse freely evolving
gas-solid suspension at a moderate Reynolds number to measure the mean slip velocity between the two particle size classes that gives rise to particle mass flux. We also assess the ability of gas-particle drag models that are widely used in two-fluid model (TFM) CFD simulations to predict the slip velocity between the two particle size classes in Section 5.5. Also in an attempt to improve current bidisperse drag models, we report results from highly resolved PR-DNS of homogeneous bidisperse fixed particle assemblies and quantify the drag force on each particle size class in Section 5.6. We also discuss the remaining challenges in developing an accurate bidisperse gas-particle drag model, and possible directions for further improvement in Section 5.7. Finally, conclusions are summarized in Section 5.8.

### 5.2 Homogeneous bidisperse gas-solid suspension

Statistical representations of multiphase flow are widely used in macroscale descriptions based on the averaged conservation equations of mass, momentum, and energy (see Appendix B for more detail) that are used in device-scale computations. These averaged equations include unclosed terms that arise due to the statistical averaging procedure, and require modeling. A better understanding of the physics governing the microscale (at the scale of individual particles) and mesoscale (scale of clusters of hundreds of particles) dynamics of multiphase flow is needed for accurately modeling these unclosed terms. The PR–DNS approach is currently used to study the microscale dynamics because of the high computational cost involved in extending it to the mesoscale. Studying the microscale dynamics of gas-solid flows in canonical problems enables us to isolate the effect of specific unclosed terms, and thus quantify and characterize their behavior. For instance, in homogeneous gas-solid suspensions we can quantify the contribution of gas-particle drag and particle-particle drag to the mean momentum equations in the absence of transport terms, and thus improve the predictive capabilities of drag models in representing these unclosed terms.

In light of the homogeneity assumption all spatial variations of mean quantities disappear. Therefore, the conservation equation of mass (Eq. B.2) is trivially satisfied. In addition, in the conservation of mean momentum equation (Eq. B.3), the transport of second moment terms, such as the Reynolds stress tensor, and also the contribution from the divergence of viscous
stresses disappear. Thus, the mean momentum equation reduces to a balance between the rate of change of the mean momentum, mean pressure gradient (or other types of body force), mean interphase momentum transfer due to hydrodynamic and collisional interactions, which are presented in more detail in the following sub-section.

### 5.2.1 Mean momentum equations

The mean momentum equations of the fluid phase and a polydisperse solid phase are given in Appendix B. For homogeneous bidisperse suspensions with constant volume fractions and densities and in the absence of gravity, these equations simplify to:

\[
\begin{align*}
\rho^{(f)} \phi^{(f)} \frac{\partial}{\partial t} \langle u^{(f)} \rangle &= -\phi^{(f)} \langle g \rangle - \sum_{\alpha=1}^{2} \left\langle \tau \cdot n^{(\alpha)} \delta(x - x^{(f)}_{\alpha}) \right\rangle, \\
\rho^{(\alpha)} \phi^{(\alpha)} \frac{\partial}{\partial t} \langle u^{(\alpha)} \rangle &= -\phi^{(\alpha)} \langle g \rangle + \left\langle \tau \cdot n^{(\alpha)} \delta(x - x^{(f)}_{\alpha}) \right\rangle + \left\langle f^{(\beta \rightarrow \alpha)}_{\text{coll}} \right\rangle,
\end{align*}
\]

where \( \rho^{(f)} \) is the fluid-phase density, \( \phi^{(f)} \) is the corresponding volume fraction, \( \langle u^{(f)} \rangle \) is the mean fluid velocity, \( \langle g \rangle \) is the mean pressure gradient, \( \tau \) is the stress tensor at the fluid-solid interface that includes the fluctuating pressure and the viscous stress, \( n^{(\alpha)} \) is the normal vector at the surface of particles belonging to \( \alpha \)th class pointing into the fluid phase, \( \delta(x - x^{(f)}_{\alpha}) \) is a generalized delta function at the fluid-particle interface \( x^{(f)}_{\alpha} \), and \( N_c \) is the number of particle classes. Similarly, \( \rho^{(\alpha)} \) is the \( \alpha \)th particle class density, \( \phi^{(\alpha)} \) is the corresponding volume fraction, \( \langle u^{(\alpha)} \rangle \) is the particle class mean velocity, and \( \left\langle f^{(\beta \rightarrow \alpha)}_{\text{coll}} \right\rangle \) in Eq. 5.2 is the mean momentum transfer between particle classes \( \alpha \) and \( \beta \), identified as the particle-particle drag. The term \( \left\langle s^{(\alpha)}_{h} \right\rangle \) represents the transfer of mean momentum to the solid phase due to the hydrodynamic forces on particle class \( \alpha \). In gas–solid flows the hydrodynamic force is modeled as the drag force since that is the principal contribution, although in shear flows and with rotating particles (Kurose and Komori, 1999; Bagchi and Balachandar, 2002) the lift force can also be important. The sum of all hydrodynamic forces on the right-hand side of Eq. 5.1 represents the total hydrodynamic force experienced by solid particles, denoted by:

\[
\langle s_{h} \rangle = \sum_{\alpha=1}^{2} \left\langle s^{(\alpha)}_{h} \right\rangle.
\]
Again this is modeled as the average gas-particle drag, and the average gas-particle and particle-particle drag forces are not known a priori and need to be modeled in two-fluid model simulations.

5.2.2 Slip velocity between the two particle classes

It is worthwhile to examine the mean momentum equation governing the slip velocity between the two particle classes since this slip velocity determines the average particle mass flux. The slip velocity between the two particle classes \( \langle W^{(\beta,\alpha)} \rangle \) in a bidisperse suspension in the absence of gravity and driven by a mean pressure gradient is obtained by subtracting the conservation equation of mean momentum corresponding to particle class \( \alpha \) from that of particle class \( \beta \) in Eq. 5.2, resulting in

\[
\frac{d}{dt} \langle W^{(\beta,\alpha)} \rangle = - \langle g \rangle \left( \frac{1}{\rho(\beta)} - \frac{1}{\rho(\alpha)} \right) + \left( \frac{1}{\rho(\beta) \phi(\beta)} \langle s^{(\beta)}_h \rangle - \frac{1}{\rho(\alpha) \phi(\alpha)} \langle s^{(\alpha)}_h \rangle \right)
\]

\[
- \langle f^{(\beta \rightarrow \alpha)}_{\text{coll}} \rangle \left( \frac{1}{\rho(\alpha) \phi(\alpha)} + \frac{1}{\rho(\beta) \phi(\beta)} \right)
\]  

Equation 5.4 for the evolution of the mean slip velocity between particle classes shows that both gas-particle drag and particle-particle drag forces contribute to the rate of change of \( \langle W^{(\beta,\alpha)} \rangle \) that leads to particle mass flux in a homogeneous bidisperse suspension. Therefore, accurate modeling of both contributions is essential in particle-laden flow analysis.

5.2.3 Characterization of bidisperse gas-solid suspensions

The dynamics of a bidisperse gas-solid suspension depends on the regime of the flow in a high-dimensional parameter space that is characterized by:

1. total solid-phase volume fraction \( \phi^{(p)} \)

2. ratio of particle class volume fraction to the total solid-phase volume fraction \( x_\alpha = \phi^{(\alpha)}/\phi^{(p)} \)
3. ratio of particle class density to fluid-phase density \( \rho^{(\alpha)}/\rho^{(f)} \)

4. ratio of particle class diameter to Sauter mean diameter \( y_{\alpha} = d_{\alpha}/\langle d \rangle \)

5. mean slip Reynolds number \( Re_m \), and

6. particle class Stokes number \( St_{\alpha} \).

The mean slip Reynolds number based on the Sauter mean diameter \( \langle d \rangle = \left( \sum_{\alpha=1}^{N_c} \phi^{(\alpha)}/(\phi d_{\alpha}) \right)^{-1} \) is defined as

\[
Re_m = \frac{\phi^{(f)} | \langle W \rangle | \langle d \rangle}{\nu^{(f)}},
\]

(5.5)

where the mixture mean slip velocity is defined as the difference between the mass-weighted solid-phase velocity (see Eq. C.7) and the fluid-phase velocity, i.e.,

\[
\langle W \rangle = \langle \widetilde{u}^{(\rho)} \rangle - \langle u^{(f)} \rangle.
\]

(5.6)

The particle class Stokes number is defined as the particle response time to the characteristic fluid flow time scale that is given by

\[
St_{\alpha} = \frac{\tau^{(\alpha)}}{\tau^{(f)}} = \frac{1}{18} \frac{\rho^{(\alpha)}}{\rho^{(f)}} \left( \frac{d_{\alpha}}{\langle d \rangle} \right)^2 Re_m.
\]

(5.7)

These parameters are used to characterize the gas-solid flows considered in this study.

### 5.3 Numerical method

Several numerical methods have been developed for particle-resolved direct numerical simulation (PR-DNS) of fluid-solid flows, such as the finite element approach of Johnson and Tezduyar (1997), the immersed boundary method of Peskin (2002), the Lattice-Boltzmann method used by Chen and Doolen (1998), a combination of the two former methods implemented by Feng and Michaelides (2004), and the PHYSALIS method of Prosperetti and Oguz (2001). The Lattice-Boltzmann based PR-DNS solvers have been extensively used to study bidisperse gas-solid flows (van der Hoef et al., 2005; Beetstra et al., 2007; Sarkar et al., 2009; Yin and Sundaresan, 2009; Holloway et al., 2010). In this study, we use the particle-resolved uncontaminated-fluid reconcilable immersed boundary method (PUReIBM) of Tenneti et al.
The salient feature of PUReIBM is that the IB forcing in PUReIBM is non-zero only inside the solid phase, and the fluid-phase is uncontaminated by the IB forcing. Therefore, the velocity and pressure in the fluid phase satisfy the unmodified Navier-Stokes equations. In addition, 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. This feature enables us to directly compare the PR-DNS solution with any random-field theory of multiphase flow (Garg et al., 2010c; Tenneti et al., 2011), and in particular we can quantify the slip velocity between the two size classes $\langle W^{(\beta,\alpha)} \rangle$ in Eq. 5.4.

This method is shown to be accurate and numerically convergent (Garg et al., 2010c; Tenneti et al., 2011). In addition, PUReIBM has been successfully used to simulate fixed particle assemblies (Tenneti et al., 2010, 2011; Sun et al., 2015) and freely evolving suspensions of monodisperse gas-solid flows (Subramaniam et al., 2014; Mehrabadi et al., 2015; Tenneti et al., 2016). The extension of the PUReIBM formulation to account for polydisperse gas-solid suspensions is straightforward (see C).

In PUReIBM, the three dimensional Navier-Stokes equations are solved on a Cartesian grid for the whole computational domain in an accelerating frame that moves at the mean velocity of the particles. The instantaneous conservation equations of mass and momentum are

$$\nabla \cdot \mathbf{u} = 0, \quad (5.8)$$

and

$$\rho(f) \frac{\partial \mathbf{u}}{\partial t} + \rho(f) \mathbf{S} = -g_{\text{IBM}} + \mu(f) \nabla^2 \mathbf{u} + \mathbf{f} - \rho(f) \mathbf{A}_f, \quad (5.9)$$

respectively, where $\mathbf{u}$ is the instantaneous velocity, $\mathbf{S} = \nabla \cdot (\mathbf{u}\mathbf{u})$ is the convective term in conservative form, $g_{\text{IBM}} = \nabla p$ is the pressure gradient, $\mathbf{f}$ is the immersed boundary (IB) forcing that accounts for the presence of particles, and $\mathbf{A}_f$ accounts for the acceleration of the frame of reference (Tenneti et al., 2010) that moves with the mean velocity of particles in freely evolving suspensions. Simulation of freely evolving suspensions in an accelerating frame of reference (Tenneti et al., 2011) enables us to simulate suspensions at arbitrary Reynolds numbers while maintaining other parameters at fixed values. This accelerating frame resembles a sedimentation problem with a specified gravitational acceleration. This results in the particles settling
at a mean velocity corresponding to \(Re_m\) in a quiescent fluid (not necessarily corresponding to the terminal velocity with \(g = 9.81 \text{m/s}^2\)).

In PURReIBM the particles are represented in a Lagrangian frame of reference at time \(t\) by \(X^{(\alpha,i)}(t)\), \(V^{(\alpha,i)}(t)\), \(\alpha = 1 \text{ and } 2\), \(i = 1...N_\alpha\) with \(X^{(\alpha,n)}(t)\) and \(V^{(\alpha,n)}(t)\) being respectively the position and velocity of \(i^{th}\) particle in the \(\alpha^{th}\) size class. The position and translational velocity of each particle in class \(\alpha\) evolve according to Newton’s second law as

\[
\frac{dX^{(\alpha,i)}(t)}{dt} = V^{(\alpha,i)}(t), \tag{5.10}
\]

\[
m^{(\alpha,i)} \frac{dV^{(\alpha,i)}(t)}{dt} = -\langle g\text{IBM} \rangle V^{(\alpha,i)} + S_h^{(\alpha,i)}(t) + \sum_{j=1}^{N_\alpha} F_{\text{coll}}^{(\alpha,j \rightarrow i)}(t) + \sum_{\beta=1}^{2} \sum_{j=1}^{N_\beta} F_{\text{coll}}^{(\beta \rightarrow \alpha,j \rightarrow i)}(t) - m^{(\alpha,i)} A_f, \tag{5.11}
\]

where \(m^{(\alpha,i)}\) and \(V^{(\alpha,i)}\) are, respectively, the mass and volume of the \(i^{th}\) particle of class \(\alpha\), \(S_h^{(\alpha,i)}\) is the hydrodynamic force acting on the \(i^{th}\) particle with the form given in Eq. C.5, \(F_{\text{coll}}^{(\alpha,j \rightarrow i)}\) is the contact force on the \(i^{th}\) particle from collisions with the \(j^{th}\) particle in the same size class, and \(F_{\text{coll}}^{(\beta \rightarrow \alpha,j \rightarrow i)}\) is the contact force from collisions with the \(k^{th}\) particle belonging to the size class \(\beta^{th}\). Particle-particle interactions are treated using soft-sphere collisions based on a linear spring-dashpot contact mechanics model originally proposed by Cundall and Strack (1979). Further details of the particle-particle interaction are provided by Mehrabadi et al. (2015).

### 5.4 PR-DNS of Freely Evolving Suspensions

In this section, the PR-DNS of homogeneous bidisperse gas-solid flow considered in this study is presented. To generate a homogeneous particle configuration of a bidisperse suspension, non-overlapping spheres are first generated with particle centers on a cubic lattice. Particles are then assigned a Maxwellian velocity distribution and they undergo purely elastic collisions according to the soft-sphere model (Cundall and Strack, 1979) in the absence of the gas phase, establishing an equilibrium state with a homogeneous particle configuration (Tenneti et al., 2011). We consider two size class ratios with the details provided in Table 5.1. It should be
Table 5.1: Details of bidisperse configurations for PR-DNS of freely evolving suspensions for the particle size class diameter to Sauter mean diameter ratio \( y_\alpha = d_\alpha / \langle d \rangle \), size class volume fraction to total solid-phase volume fraction \( \phi^{(1)} / \phi^{(p)} \), number of particles in size classes \( N_\alpha \), and grid resolution per particle for each size class \( d_\alpha / \Delta x \). In both cases, \( \rho^{(p)} / \rho^{(f)} = 1000 \), \( \phi^{(p)} = 0.3 \), and \( Re_m = 50 \).

<table>
<thead>
<tr>
<th></th>
<th>( y_1 )</th>
<th>( y_2 )</th>
<th>( \phi^{(1)} / \phi^{(p)} )</th>
<th>( \phi^{(2)} / \phi^{(p)} )</th>
<th>( N_1 )</th>
<th>( N_2 )</th>
<th>( d_1 / \Delta x )</th>
<th>( d_2 / \Delta x )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Case I</td>
<td>0.75</td>
<td>1.125</td>
<td>0.25</td>
<td>0.75</td>
<td>73</td>
<td>65</td>
<td>23</td>
<td>34</td>
</tr>
<tr>
<td>Case II</td>
<td>0.5</td>
<td>1.5</td>
<td>0.25</td>
<td>0.75</td>
<td>247</td>
<td>27</td>
<td>15</td>
<td>45</td>
</tr>
</tbody>
</table>

noted that the particle size class diameter to Sauter mean diameter ratio is given by \( y_\alpha = d_\alpha / \langle d \rangle \). We limit our analysis to a fixed density ratio for all particle classes, i.e. \( \rho^{(1)} = \rho^{(2)} = \rho^{(p)} \), in order to only isolate the effect of particle size ratio. The solid-to-fluid density ratio is selected as \( \rho^{(p)} / \rho^{(f)} = 1000 \). The mean slip Reynolds number is chosen to be \( Re_m = 50 \) and the total solid-phase volume fraction is \( \phi^{(p)} = 0.3 \). In order to achieve a desired mean slip Reynolds number at steady steady state, a specific mean pressure gradient is required. The formulation of PUReIBM in an accelerating frame for polydisperse systems (see Appendix C for further detail) enables us to easily attain this mean pressure gradient.

The length of the computational box for these simulations is chosen as \( L = 6 \langle d \rangle \), which is long enough for convergence of the drag force (Tenneti et al., 2011), and for the decorrelation of gas-phase velocity fluctuations that is needed when using periodic boundary conditions (Mehrabadi et al., 2015). Note that the grid resolution requirement to capture the boundary layer around the smallest particle in the configuration limits the range of particle size ratio in our simulations. The grid resolution used for these simulations are \( \langle d \rangle = 30 \Delta x \) which is appropriate for grid-independent results. In order to account for the statistical variability in particle arrangements, we also perform three independent realizations for each case. We start our simulations with fixed particle assemblies until flow structures are formed and the relative error in the mean drag force reduces to less that \( 10^{-6} \). Then we release the particles and let them evolve under the influence of hydrodynamic and collisional forces they experience, as described by Eqs. 5.10 and 5.11.
5.4.1 Homogeneity of particle configuration

In order to ensure that the particle configurations in our simulations remain statistically homogeneous, we compute the particle number density along the mean flow coordinate in the computational box, which is the average number of particles per unit volume. To reduce statistical variability, the data have been averaged over six time intervals separated from each other by normalized time $t \langle d \rangle / |\langle W \rangle| = 5$, after the system reaches a steady state. The number density profiles in Fig. 5.1 indicate that both particle classes are uniformly distributed along the mean flow direction with no accumulation of particles. The radial distribution function (RDF) can also be used to identify preferential accumulation of neighbor particles. The RDF represents the probability of finding another particle at the vicinity of a test particle with separation $r$. RDF’s from our simulations (not shown here) did not indicate any deviation from the initial condition. This again confirms that the particle configurations in our freely evolving simulations remain homogeneous for flow conditions considered here ($\phi = 0.3$, $Re_m = 50$, $\rho(p)/\rho(f) = 1000$, with elastic particles).

At higher solid-phase volume fractions, the caging effect, in which particles are trapped by their neighbors, is initiated by formation of microscopic or mesoscopic particle clusters in the suspension. These structures cause the particle distribution to deviate from homogeneity. Experimental studies of an air-driven bidisperse configuration (Abate and Durian, 2006) and
Figure 5.2: Prediction of slip velocity between two particle size classes parallel to the mean flow obtained from PR-DNS.

also vertically vibrated monodisperse grains (Reis et al., 2007) indicate that the caging effect takes place near the solid-phase packing limit. In our cases, the configurations are much below the packing limit. Therefore, the caging phenomenon is not a matter of concern here, and particles are indeed homogeneously distributed.

5.4.2 Slip velocity between particle size classes

We can directly track the evolution of the axial component of the slip velocity between the two particle size classes that is governed by Eq. 5.4, as shown by symbols in Fig. 5.2 for Case I and Case II where the size ratios are $y_2/y_1 = 1.5$ and $3.0$, respectively. As time progresses, the axial component of the slip velocity between the two size classes grows in magnitude due to the differences between the gas-particle drag and particle-particle drag forces on each particle size class. This mean slip velocity between the two particle size classes indicates that there is a particle mass flux even in a homogeneous suspension in the absence of gradients in the number density or granular temperature, or external forces (Garzó et al., 2007). This shows how segregation in gas-solid flow is different from granular flows.
Figure 5.3: Evolution of normalized difference between axial component of particle size class
mean velocities and mass-weighted particles mean velocity $\langle u^{(p)} \rangle$. Normalization is by the
mean slip velocity $|\langle W \rangle| = |\langle u^{(p)} \rangle - \langle u^{(f)} \rangle|$.  

For Case II where $y_2/y_1 = 3.0$, the mean slip velocity between size classes $\langle W^{(2,1)} \rangle_{II}$ is
about 4 times that of Case I, where $y_2/y_1 = 1.5$. The relative magnitude of the steady mean slip
velocity between the two particle size classes can be characterized on the basis of the ratio of
their corresponding particle Stokes numbers. Since the particle Stokes number is proportional
to the square of particle size class diameter (cf. Eq. 5.7), the particle Stokes number ratio
$St_2/St_1$ in Case II compared to that of Case I is

$$\left(\frac{St_2}{St_1}\right)_{II} = \left(\frac{d_2/d_1}{d_2/d_1}\right)_{II} = \left(\frac{3}{1.5}\right)^2 = 4.$$  

The Stokes number ratio between size classes in a bidisperse suspension is close to the ratio of
the steady value of the slip velocity between the particle size classes parallel to the mean flow
direction, i.e. $\langle W^{(2,1)} \rangle_{II}/\langle W^{(2,1)} \rangle_{I}$. Therefore, in the general case where $\rho^{(2)} \neq \rho^{(1)}$ and
d_2 \neq d_1, it seems that rather than the relative particle size class ratio, it is the particle Stokes
number ratio that is relevant in determining the ratio of mean slip velocities between particle
size classes.
The transient region in the evolution of the mean slip velocity between two particle size classes in Fig. 5.2 indicates that there exists a peak value in the mean slip velocity difference followed by a reduction before the steady value is attained. This behavior can be better understood by analyzing the evolution of the mean momentum for each particle size class described by Eq. 5.2 since it is the difference in the mean velocities of each size class $\langle u^{(\alpha)} \rangle$ that results in $\langle W^{(\beta, \alpha)} \rangle$. The rate of change of $\langle u^{(\alpha)} \rangle$ is determined by the balance of terms on the right-hand side of Eq. 5.2 representing gas-particle drag and particle-particle drag forces. Since we start our freely evolving simulations after the hydrodynamic field characterized by a desired mean slip Reynolds number is developed, the mean gas-particle drag on each particle size class is already non-zero. Since the particle-particle drag force is negligible at the onset of freely moving suspension simulations that particles are initially at rest, the mean gas-particle drag force on each particle size class acts as a source of mean momentum on the right-hand side of Eq. 5.2. This source gives rise to the monotonic increase of the species diffusion velocity for each particle size class (difference between the mean velocity of particle size classes and the mass-weighted solid mixture velocity) as shown in Fig. 5.3 for Case II. This figure represents the evolution of the particle size class mean velocity with respect to the mass-weighted particle velocity $\langle \tilde{u}^{(p)} \rangle$. After the initial transition ($t |\langle W \rangle| / \langle d \rangle > 50$) during which each particle size class attains a finite species diffusion velocity, collisions between particles belonging to different size classes become more frequent. As a result of momentum transfer from one particle size class to another due to particle collisions, the particle-particle drag force becomes comparable to the gas-particle drag force and acts as a sink term in Eq. 5.2. This sink of mean momentum hinders further increase of $\langle u^{(\alpha)} \rangle$ (cf. Fig. 5.3), and once it balances the gas-particle drag force, the mean velocity of each particle size class reaches a steady value. The difference between the mean velocities of the two particle size classes then determines their corresponding mean relative motion. At the end of this section we find that both fluid-particle drag and particle-particle drag are responsible for particle mass flux that leads to segregation.
5.5 Assessment of bidisperse gas-particle drag models in predicting mean slip velocity between two particle size classes

We examine the capabilities of existing two-fluid closure models to capture the particle mass flux and mean slip velocity between particle size classes. The focus of the current study is mainly on the influence of the hydrodynamic force. Therefore, we use the gas-particle drag models proposed by Syamlal, M. and O’Brien, T. J. (1987), which is widely used in CFD packages such as MFIX, as well the drag models proposed by Kuipers’ group (van der Hoef et al., 2005; Beetstra et al., 2007; van der Hoef, 2007) and Rong et al. (2014) in the gas and solid-phase mean momentum equations 5.1 and 5.2. To close these set of equations, a particle-particle drag model is also needed to account for the mean momentum transfer between two particle size classes \( \langle f_{\text{coll}}^{(\beta \rightarrow \alpha)} \rangle \) due to particle collisions. Since the focus of the current study is on the contribution from the gas-particle drag to the mean slip velocity between two particle size classes, we use only the particle-particle drag model of Syamlal (1987), which is:

\[
\langle f_{\text{coll}}^{(\beta \rightarrow \alpha)} \rangle = \frac{3}{4} \left( 1 + \varepsilon_{\alpha\beta} \right) \frac{\phi^{(\alpha)} \rho^{(\alpha)} \phi^{(\beta)} \rho^{(\beta)}}{\rho^{(\alpha)} d_\alpha^3 + \rho^{(\beta)} d_\beta^3} (d_\alpha + d_\beta)^2 g_0 \left| \langle W^{(\beta,\alpha)} \rangle \right|, \tag{5.12}
\]

where \( \varepsilon_{\alpha\beta} \) is the coefficient of restitution in a collision between a colliding pair of particles belonging to classes \( \alpha \) and \( \beta \), and \( g_0 \) is the value of radial distribution function at contact represented by the model of Lebowitz (1964). It is worth mentioning that this gas-particle drag model has no dependence on the velocity distribution of each particle size class. This model assumes that the velocity distributions are delta-functions that correspond to non-zero mean velocities with zero variance. Other models like the one proposed by Jenkins (Louge et al., 1991) do not generalize to this case. However, for this study we do not change the particle-particle drag model and investigate the effect of gas-particle drag model.

For a better insight into the aforementioned gas-particle drag models, they are presented in Table 5.2. For the sake of convenience, we refer to these models, respectively, by SO, BVK, and RDY from hereon. These gas-particle drag models are presented based on the average drag force per particle normalized by the Stokes drag force on a particle in size class \( \alpha \), i.e. \( F_{St} = 3 \pi d_\alpha \mu^{(f)} (1 - \phi) \left| \langle W \rangle \right| \). It should be noted that the SO model is originally given based on the volumetric mean drag force. However, for ease of comparison with other drag models
Table 5.2: Bidisperse gas-particle drag models used in TFM-CFD simulations. These drag are
given for either the mean interphase transfer $S_h^{(α)}$ or the total gas-particle drag force that also
includes the contribution from the mean pressure gradient $F^{(α)} = S_h^{(α)} - \langle \nabla p \rangle \mathbf{V}^{(α)}$. These
drag models represent the mean drag force per particle normalized by the Stokes drag force,
that is $F_{St} = 3\pi d_\alpha \mu f (1 - \phi) |\langle \mathbf{W} \rangle|$. 

<table>
<thead>
<tr>
<th>Model</th>
<th>Source</th>
<th>Formulation</th>
</tr>
</thead>
<tbody>
<tr>
<td>SO</td>
<td>Syamlal and O’Brien (1987)</td>
<td>$\left\langle S_h^{(α)} \right\rangle = y_α \frac{Re_m}{24} \left[ \frac{C_{\text{mono}}^{(α)}}{(1 - \phi(p))^0.5} \left( \frac{\left</td>
</tr>
<tr>
<td>BVK</td>
<td>Beetstra et al. (2007)</td>
<td>$\left\langle F_h^{(α)} \right\rangle = \left\langle F_h^{\text{(mono)}} \right\rangle (y_α (1 - \phi(p)) + \phi^2(\phi(p)))$, $\left\langle F_h^{\text{(mono)}} \right\rangle = \frac{10.4}{(1 - \phi(p))^3} + (1 - \phi(p))(1 + 1.5\sqrt{\phi(p)})$ $+ \frac{0.413 Re_m}{24(1 - \phi(p))^3} (1 - \phi(p)) - 1.39(1 - \phi(p))(1 - 8.4 Re_m^0.343) \frac{1 + 108(1 - \phi(p))^3}{1 + 108(1 - \phi(p))^3}$</td>
</tr>
<tr>
<td>RDY</td>
<td>Rong et al. (2014)</td>
<td>$\left\langle S_h^{(α)} \right\rangle = y_α \left\langle S_h^{\text{(mono)}} \right\rangle$, $\left\langle S_h^{\text{(mono)}} \right\rangle = \frac{Re_m}{24} C_D 0(1 - \phi(p))^{-\beta}$, $\beta = 2.65 \left[ (1 - \phi(p)) + 1 \right] - 5.3 - 3.5(1 - \phi(p)$ $\times (1 - \phi(p))^2 \exp[-0.5(1.5 - \log(Re_m))^2]$,</td>
</tr>
<tr>
<td>MTS</td>
<td>Present study</td>
<td>$\left\langle F_h^{(α)} \right\rangle = \left\langle F_h^{\text{(mono)}} \right\rangle (y_α (1 - \phi(p)) + \phi^2(\phi(p)))$, $\left\langle F_h^{\text{(mono)}} \right\rangle = \frac{F_{\text{isol}}}{(1 - \phi(p))^2} + F_{\phi(p)} + F_{\phi(p),Re_m}$, $F_{\text{isol}} = 1 + 0.15 Re_m^0.867$, $F_{\phi(p)} = \frac{5.81\phi(p)}{(1 - \phi(p))^3} + 0.48 \phi^2(\phi(p))$, $F_{\phi(p),Re_m} = \phi(3,Re_m) \frac{0.95 + 0.918(1 - \phi(p))^3}{(1 - \phi(p))^2}$</td>
</tr>
</tbody>
</table>

In Table 5.2, it is shown here on a per particle basis (cf. Eq. 5.14). Similarly, the gas-particle
drag model of RDY for TFM simulation of freely evolving suspensions translates to the form
presented in Table 5.2.

It is evident that the SO model is based on purely inertial scaling, i.e. $F \sim \rho f |\langle \mathbf{W} \rangle|^2 / 2$. However, the BVK model relates the particle drag on each size class to that of an equivalent
monodisperse drag model by a quadratic expression in $y_α$. The equivalent monodisperse drag in
BVK model is a complex function of $\phi(p)$ and $Re_m$ obtained from Lattice-Boltzmann PR-DNS (Beetstra et al., 2007). The RDY drag model is similar to that of SO in its inertial scaling. Nevertheless, a different model is used for the monodisperse drag law (Rong et al., 2013).

It should be noted that the gas-particle drag models are presented either for the interphase
momentum transfer $\left\langle S_h^{(α)} \right\rangle$ or the total hydrodynamic drag force $\left\langle F_h^{(α)} \right\rangle$ which also includes
the contribution from the mean pressure gradient. Furthermore, these drag models are given
either based on mean per unit volume basis or mean per particle basis. In the current study,
the former are denoted with small letters ($\left\langle s_h^{(α)} \right\rangle$ and $\left\langle f_h^{(α)} \right\rangle$), while the latter are referred to
by capital letters ($S_h^{(\alpha)}$ and $F_h^{(\alpha)}$). These quantities are related to each other through the following expressions:

\[
\begin{align*}
\langle F_h^{(\alpha)} \rangle &= -\langle g \rangle V^{(\alpha)} + \langle S_h^{(\alpha)} \rangle, \\
\langle f_h^{(\alpha)} \rangle &= -\langle g \rangle \phi^{(\alpha)} + \langle s_h^{(\alpha)} \rangle, \\
\langle f^{(\alpha)}_h \rangle &= n^{(\alpha)} \langle F_h^{(\alpha)} \rangle, \\
\langle s^{(\alpha)}_h \rangle &= n^{(\alpha)} \langle S_h^{(\alpha)} \rangle
\end{align*}
\] (5.13)

where $V^{(\alpha)}$ is the volume of a particle in size class $\alpha$, and $n^{(\alpha)}$ is $\alpha^{th}$ size class particle number density.

We solve the mean momentum equations 5.1 and 5.2 with the use of gas-particle drag models in Table 5.2 and the particle-particle drag model in Eq. 5.12 for the cases I and II presented in Section 5.2. The driving force in the mean momentum equations is the mean pressure gradient $\langle g \rangle$. We set the mean pressure gradient such that the mean slip Reynolds number at the steady state matches that of the PR-DNS. The predicted mean slip velocity between the two particle size classes are then compared with our PR-DNS results. It is evident from Fig. 5.4 that the steady values significantly deviate from 100% for BVK model to 200% for RDY and SO models compared to PR-DNS data. In addition, the evolution of the mean slip velocity obtained from
the closure models is not able to correctly capture the transient behavior when compared to the PR-DNS results. The difference in the steady value of the mean slip velocity between two size classes, and also the inability of correctly predicting the transient evolution may indicate that either the gas-particle drag or the particle-particle drag model is not accurately predictive in this particular gas-solid flow problem. To validate this assumption, in the following section we analyze the gas-particle drag force in bidisperse suspensions in more detail. The analysis of particle-particle drag force, however, is not covered in the present study.

5.6 Gas-particle drag in a bidisperse gas-solid suspension

We use fixed bidisperse particle assemblies in PR-DNS of homogeneous gas-solid flows to extract the average mean drag force on each particle size class. Kuipers’ group (van der Hoef et al., 2005; Beetstra et al., 2007; Sarkar et al., 2009) and Rong et al. (2014) also used fixed particle assemblies to propose their gas-particle drag models for monodisperse and bidisperse suspensions. Xu and Subramaniam (2010), Tenneti et al. (2011) and Mehrabadi et al. (2015) argued that the use of fixed particle assemblies is legitimate in suspensions containing massive particles with high particle Stokes number because the time it takes for changes in the particle spatial configuration is much greater that the momentum relaxation time. Tenneti et al. (2011) and Mehrabadi et al. (2015), respectively, showed that drag and the level of gas-phase velocity fluctuations are similar between fixed particle assemblies and freely evolving suspensions. Fixed particle assemblies are less computationally expensive compared to simulations of freely evolving suspensions. In addition, the dimensionality of the parameter space is now reduced because the density ratio is no longer a parameter. We perform PR-DNS of these particle assemblies until a steady state is obtained. Then the average drag force per particle for each size class is computed and normalized by the Stokes drag force.

Our PR-DNS data set includes simulations with \(Re_m\) values of 50, 65, 75, and 100 at total volume fractions 0.1, 0.2, 0.3, and 0.4. At each volume fraction, the volume fraction ratio \((\phi^{(2)}/\phi^{(1)})\) is varied from 1 to 6 and the diameter ratio \((d^{(2)}/d^{(1)})\) from 1.5 to 4. In order to account for the statistical variability in particle configurations, four different realizations are considered for each case. It should be noted that although our simulation data set covers a
range of solid-phase volume fractions and mean slip Reynolds numbers, due to the similarity of results we only present those for \( Re_m = 50 \) and 75, and \( \phi^{(p)} = 0.3 \) and 0.4.

We first compare the gas-particle drag force obtained from our PR-DNS of fixed particle assemblies corresponding to particle size classes used in freely evolving suspensions of cases I and II with the predictions obtained from SO, BVK and RDY at the same flow parameter in Fig. 5.5. Note that the \( y_\alpha \) values used in the freely evolving suspensions are 0.5 and 1.5 for Case I, and 0.75 and 1.125 for Case II at \( \phi^{(p)} = 0.3 \) and \( Re_m = 50 \).

The comparison in Fig. 5.5 reveals that the SO drag model significantly over-predicts the drag force on smaller particle size classes with the maximum difference being about 45%, whereas the prediction improves with increasing \( y_\alpha \). Over-prediction of the gas-particle drag force on smaller particles gives rise to higher mean acceleration that leads to higher mean velocity for the smaller size class. This in turn appears as higher slip velocity between the two particle size classes observed in Fig. 5.4. The RDY drag model over-predicts the drag force over the entire range of \( y_\alpha \) with the difference ranging from 20% to 50% in Fig. 5.5. These over-predictions of the drag force, consequently, do give rise to inaccurate slip velocity between two particle size classes in Fig. 5.4. The BVK model provides closer drag prediction compared
with the PR-DNS data with the maximum difference being about 15% in Fig. 5.5. Therefore, it provides a better mean slip velocity prediction between the two particle size classes in Fig. 5.4 as compared to the SO and RDY drag models.

Inaccuracy of existing gas-particle drag models in predicting the mean slip velocity difference motivates us to propose an improved gas-particle drag model based on the PR-DNS data of fixed particle assemblies. We use the normalized gas-particle drag correlation of BVK for bidisperse suspension which has the following form:

\[
\frac{\left\langle F_{h}^{(\alpha)} \right\rangle}{\left\langle F_{h}^{(\text{mono})} \right\rangle} = y_{\alpha} (1 - \phi^{(p)}) + y_{\alpha}^2 \phi^{(p)},
\]

(5.15)

where \(\left\langle F_{h}^{(\text{mono})} \right\rangle\) is the equivalent monodisperse drag model at the same total solid-phase volume fraction and mean slip Reynolds number. This expression indicates that the bidisperse drag and the equivalent monodisperse drag forces can be related to each other through a simple function of total solid-phase volume fraction and size class diameter to Sauter mean diameter ratio. van der Hoef et al. (2005) proposed the above correlation based on the condition that in Stokes flow, the total volumetric drag force in a bidisperse suspension should be equal to
the volumetric drag force of a monodisperse system with particle diameter as \( \langle d \rangle \). The above correlation has also been tested for intermediate and high Reynolds number suspensions.

The above correlation accompanied by the monodisperse drag model of Beetstra et al. (2007) provides the basis for the BVK bidisperse drag model given in Table 5.2. As observed in Fig. 5.6, the BVK model (represented by dashed lines) is not able to quantitatively predict our PR-DNS data. The maximum difference between the two data sets is more than 15% for particle size classes \( y_{\alpha} < \langle d \rangle \). The monodisperse drag model of Beetstra et al. (2007) relies on drag force obtained from a grid resolution of \( d/\Delta x = 17.5 \) for \( \phi^{(p)} \leq 0.3 \), and grid resolutions \( d/\Delta x = 17.5 \) and 25 for \( \phi^{(p)} > 0.3 \), to simulate Reynolds numbers ranging from 21 to 1000. However, other studies indicate that the grid resolution requirement increases with both mean slip Reynolds number and solid volume fraction (Tenneti et al., 2011). As the mean slip Reynolds number increases, the thickness of particle boundary layers decrease (\( \delta \sim 1/\sqrt{Re_{m}} \)) and higher resolution is needed to resolve these adequately and to accurately compute the drag force. As the solid volume fraction increases, the distance between particle surfaces decreases and again higher resolution is needed to resolve the flow in the interstices adequately.

Here, we use Eq. 5.15 jointly with the monodisperse drag model of Tenneti et al. (2011), which has the following form:

\[
\langle F_{h}^{(\text{mono})} \rangle = \frac{F_{\text{isol}}(Re_{m})}{(1 - \phi)^3} + F_{\phi}(\phi) + F_{\phi,Re_{m}}(\phi, Re_{m}) \tag{5.16}
\]

where, \( F_{\text{isol}} \) is the drag force acting on an isolated sphere moving in an unbounded medium. The drag on an isolated sphere is taken to be the correlation proposed by Schiller and Naumann (1935). The remaining two terms in Eq. 5.16 are given by

\[
F_{\phi}(\phi) = \frac{5.81\phi}{(1 - \phi)^3} + 0.48\frac{\phi^{1/3}}{(1 - \phi)^4},
\]

\[
F_{\phi,Re_{m}}(\phi, Re_{m}) = \phi^3 Re_{m} \left( 0.95 + \frac{0.61\phi^3}{(1 - \phi)^2} \right).
\]

If we use Eqs. 5.15 and 5.16, the prediction of gas-particle drag force on each particle size class over the entire range of \( y_{\alpha} \) improves. This improvement in predicting bidisperse gas-particle drag model in Fig. 5.6 arises from the fact that the monodisperse drag model of Tenneti et al. (2011) is based on highly resolved PR-DNS of gas-solid flow over the range of solid-phase
volume fraction $0.1 \leq \phi^{(p)} \leq 0.5$ and the mean slip Reynolds number $0.01 \leq Re_m \leq 300$. Therefore, we recommend using Eq. 5.15 jointly with the monodisperse drag model of Tenneti et al. (2011) for bidisperse gas-particle drag in CFD calculations. We refer to this model as the MTS bidisperse gas-particle model.

### 5.6.1 Comparison of drag force from closure models with PR-DNS of freely evolving suspensions

It is of interest to compare the evolution of the gas-particle drag force obtained from PR-DNS of freely evolving suspension for Cases I and II in Section 5.4 with predictions of the closure models in Table 5.2. It should be noted that the drag models assume that both size classes move with the same mean velocity, implying that the mean slip velocity between particle size classes is neglected. This is due to the fact that BVK and MTS models do not incorporate the slip velocity between particle size classes. However, since the steady size class diffusion velocity is about 2% of the mean slip velocity $|\langle W \rangle|$ in these cases (cf. Fig. 5.3), the influence on the drag force is at most about 4% at steady state. Nevertheless, this may not always be true for cases where particle size classes have different material densities. The comparison of the drag force from freely evolving PR-DNS with the drag models in Fig. 5.7 reveals that the difference in the drag force on smaller particle size classes ($y_\alpha = 0.5$ and 0.75) predicted by MTS and BVK compared to PR-DNS results is about 5% to 8%, while the difference ranges from 15% to 40% for SO and RDY models. However, BVK and SO models predict the drag for larger particles ($y_\alpha = 1.125$ and 3.0) at steady state with less than 5% difference when compared with PR-DNS data, while this difference is about 8% for the MTS model and about 20% for the RDY model. This comparison indicates that the MTS and BVK drag models are more reliable for computing the gas-particle drag force in a freely evolving bidisperse suspension for the range of particle size classes considered in the current study (for size class density ratio of unity).
Figure 5.7: Comparison of the mean gas-particle drag force per particle in each particle size class obtained from PR-DNS of freely evolving suspensions and those obtained from drag models described in Table 5.2. The symbols show the evolution of the drag with respect to normalized time, while the solid lines represent the drag for fixed assemblies. Note that line are colored with respect to the corresponding symbols. (a) Case I with size class diameters $y_\alpha = 0.75$ and 1.125, (b) Case II with size class diameters $y_\alpha = 0.5$ and 1.5.

We now examine the ability of the MTS drag model to predict the mean slip velocity between two particle classes, similar to the assessment we performed in Section 5.5 for other drag models. Therefore, we solve the mean momentum equations 5.1 and 5.2 with the MTS gas-particle drag model jointly with the particle-particle drag model of Syamlal (1987) for Cases I and II, and then compute the parallel component of $\langle W^{(2,1)} \rangle$ along the mean flow direction. The comparison of the result with PR-DNS data as in Fig. 5.4 indicates that the MTS drag model has slightly improved the prediction of the mean slip velocity between two particle size classes (about 10% improvement compared to BVK drag model).

5.7 Discussion

The development of drag models for bidisperse and polydisperse systems poses certain unique challenges that are not encountered in monodisperse systems. For a bidisperse suspension the drag force on each particle size class in general depends on the size ratio, density ratio, and also the mean particle class slip velocity with respect to the mean fluid velocity.

In the previous section, we used fixed bidisperse particle configurations to quantify the drag force on each particle size class. We then used the BVK bidisperse expression to relate the drag force on each particle class to the equivalent monodisperse suspension having the same total
solid-phase volume fraction and mean slip Reynolds number based on Sauter mean diameter. This relation is solely a function of the particle size ratio \( y_\alpha \) and solid-phase volume fraction \( \phi^{(p)} \) that includes only geometrical information. No information about the size class inertia or dynamics of the bidisperse mixture is considered. In reality, particles are free to move and the difference between the mean velocities between particle size classes gives rise to the mean slip velocity between two particle size classes. However, Eq. 5.15 does not reflect any dependence the drag force may have on the mean slip velocity of each particle size class. Fixed particle assembly simulations have been used to study the effect of different mean slip velocity between particle size classes (Yin and Sundaresan, 2009). However, Tenneti et al. (2011) showed that such simulations are not Galilean invariant, and could lead to significant error if performed at high mean slip Reynolds numbers.

It should be noted that for a given particle configuration and flow parameters \((\phi^{(p)}, \phi^{(2)}/\phi^{(1)}, d_2/d_1, \rho^{(2)}/\rho^{(1)}, Re_m)\), a specified particle size class mean slip velocity develops that is unknown a priori. Therefore, for a particular bidisperse gas-solid suspension there is no easy way to setup a suite of numerical simulations for populating the accessed values of \( |\langle W^{(\alpha)} \rangle| / |\langle W \rangle| \) in the parameter space.

If the mean slip velocity between two particle size classes is negligible, then it is expected that the MTS or BVK drag models predict the gas-particle drag force of each particle size class accurately. However, if in problems with notable difference in material densities of the particle size classes, the mean slip velocity between two particle size classes would be significant. Under these circumstances, the larger or heavier particles may experience an inertial flow regime, while the smaller or lighter particles may be in the Stokes flow regime. For such systems, the MTS or BVK drag models may not be able to correctly predict the drag force on each particle size class since they are solely based on \( y_\alpha \) and \( \phi^{(p)} \) relative to the equivalent monodisperse system. This is the condition where these models may break down. The SO drag model, on the other hand, includes the effect of the particle size class slip velocity through the term \( (|\langle W^{(\alpha)} \rangle|/|\langle W \rangle|)^2 \). Although there are differences in these two approaches in expressing the drag force on each particle size class, the appropriate form of a bidisperse drag model that can represent both geometrical and dynamical characteristics of a bidisperse suspension is still an open question.
It may be inferred from the SO and either MTS or BVK drag models that a tentative form of a bidisperse drag model that includes both geometrical and inertial dynamics effects could have the form

\[
\langle F_h^{(a)} \rangle = f \left( y_\alpha, \frac{\langle |W^{(a)}| \rangle}{\langle |W| \rangle} \right) \langle F_h^{(mono)} \rangle. \tag{5.17}
\]

As a starting point, one path could be to take the SO drag model and modify the \( C_D_{0} \) coefficient for a better match with the PR-DNS data from freely moving bidisperse gas-solid flow. The other path could be to start with MTS/BVK drag model and modify those by analogy to the SO drag model with the term \( \left( \frac{\langle |W^{(a)}| \rangle}{\langle |W| \rangle} \right)^2 \). However, currently we did not follow these paths because they do not seem to be a completely rational approach that can be expected to result in a physics-based bidisperse drag model that covers a wide range of parameters.

### 5.8 Conclusions

The slip velocity between two particle classes in a bidisperse gas-solid flow is the key signature of particle mass flux that in turn leads to segregation phenomena observed in fluidized beds. In this work, we used the PR-DNS methodology to quantify the slip velocity between particle classes in a homogeneous bidisperse gas-solid suspension at finite mean slip Reynolds number. Our simulations indicate that even in the absence of a body force, or gradients in particle number density or granular temperature, there exists a non-zero slip velocity between the two particle classes in a bidisperse suspension. This slip velocity arises from the difference in gas-particle drag and particle-particle drag forces on each particle class. We compared different bidisperse gas-particle drag models that are in use. While all of them reproduce the general trends, there are quantitative differences with PR-DNS data. In order to obtain a more accurate gas-particle drag model, we used fixed particle assemblies to perform PR-DNS of homogeneous bidisperse gas-solid flow over a range of total solid-phase volume fractions (0.1 ≤ \( \phi \) ≤ 0.4) and mean slip Reynolds number (50 ≤ \( Re_m \) ≤ 100) with different particle size ratio (0.5 ≤ \( y_\alpha \) ≤ 2.0) and volume fraction ratio (1 ≤ \( \phi^{(2)}/\phi^{(1)} \) ≤ 6). Measurement of the mean drag force for each particle size class from our fixed PR-DNS results validates the correlation of Beetstra et al. (2007) in Eq. 5.15 for polydisperse gas-solid flow when used in conjunction with the equivalent
monodisperse drag model of Tenneti et al. (2011). Comparison of the gas-particle drag force predicted from the MTS model with those obtained from PR-DNS of freely moving particles shows a good agreement for the range of particle size ratios provided in the current study. Using the MTS gas-particle drag model to solve the mean momentum equations of a bidisperse suspension also improves the prediction of the slip velocity between the two particle classes when compared to the predictions obtained using other gas-particle drag models. The unique challenges in developing physics-based bidisperse gas-particle drag model that is capable of predicting the drag force in a freely evolving bidisperse gas-solid suspension for a wide range of parameters are discussed. This discussion highlights the need for further investigation into the bidisperse gas-particle drag model.

Acknowledgments

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CHAPTER 6. MECHANISM OF TRANSFER OF KINETIC ENERGY IN HOMOGENEOUS BIDisperse FLUID-SOLID FLOW

This chapter includes a manuscript titled “Mechanism of transfer of kinetic energy in homogeneous bidisperse gas-solid flow” in preparation for submission to *Physics of Fluids* journal authored by M. Mehrabadi and S. Subramaniam.

Abstract

The coupling between the mean momentum and kinetic energy equations due to interphase interactions is explained by extending the conservation of interphase turbulent kinetic energy transfer principle originally proposed for monodisperse gas-solid flows to bidisperse suspensions. This analysis is performed by deriving the phasic and mixture conservation equations governing the flow dynamics for the mean flow and velocity fluctuations. This coupling arises from the momentum balance obtained from the driving force of the suspension, gas-particle drag and particle-particle drag forces. This balance gives rise to transfer of kinetic energy from the mean flow to velocity fluctuations. These velocity fluctuations affect the particle-particle drag that plays a key role in determining the particle mass flux, which is the signature of particle segregation. A better understanding of the source of kinetic energy and quantification of the partitioning of kinetic energy in velocity fluctuations between particle classes through the use of the proposed kinetic energy transfer principle provides a regime map to predict segregation and mixing of particle classes in industrial devices.
6.1 Introduction

Interaction of solid particles with a carrier fluid is very common in nature and industry. Transport of volcanic ashes and pollutants in atmosphere, sandstorms and sedimentation of solid grains and organic remnants at the bottom of rivers and oceans are examples of fluid-solid interaction in nature that significantly affect different aspects of human life. This interaction is also important in industrial processes and devices, such as chemical reactors where catalyst particles are used to break down heavy molecules of crude oil into more useful products, or in fluidized bed burners where coal particles are burned to produce steam which is then used to generate electricity, or in fast pyrolosis process where organic materials undergo a thermal process to produce biofuel and syngas. Therefore, understanding the coupling between the fluid and particles in these applications and the corresponding interphase interactions is very important because this coupling determines the overall efficiency of these devices and processes.

In the industrial gas-solid flow applications mentioned above, the particle diameter varies from $d_p \sim 50\mu m$ to $500\mu m$ and the material density ratio ranges from $\rho(p)/\rho(f) \sim \mathcal{O}(100)$ to $\mathcal{O}(1000)$. Therefore, there are particle size and density distributions in these applications that can be approximated with discrete distributions consisting of several particle size and mass classes. Due to the different gas-particle and particle-particle interactions experienced by particle classes, they acquire different velocity distributions with distinct mean values and variances. These differences give rise to a mean slip velocity between any of two particle classes that is the key signature of segregation of particle classes in gas-solid flow (Nienow et al., 1987; Wu and Baeyens, 1998; Goldschmidt et al., 2003; Bokkers et al., 2004; Chew et al., 2011; Hoffmann et al., 1993; Fan and Fox, 2008; Holloway et al., 2011; Norouzi et al., 2012). Prediction of segregation in devices utilizing gas-solid flow is important because this phenomenon may have substantial effect on the performance of the device device. Therefore, understanding the mechanisms that govern this phenomenon is important in prediction and control of segregation.

Mehrabadi et al. (2016) have shown that in a homogeneous gas-solid suspension, both gas-particle drag and particle-particle drag contribute to the segregation of particle classes. On one
hand, the gas-particle drag on each particle class leads to a net mean motion of the class along the flow direction which is different from the other particle classes. The difference between the net mean velocity of the two particle classes contributes to the relative particle mass flux that is the signature of particle segregation. On the other hand, the interaction of particles with flow structures gives rise to generation of particle velocity fluctuations (Tenneti et al., 2016) that are characterized by a non-zero level of kinetic energy. If the particle suspension is dense, then the probability of particle collisions increases with increase of particle velocity fluctuations. Particle collisions not only redistribute kinetic energy in particle velocity fluctuations from one particle class to another, they also affect mean momentum transfer between particle classes. This momentum transfer is called particle-particle drag which opposes the particle segregation and promotes mixing of particles. As a result, particle segregation is the outcome of a balance between the gas-particle drag which enhances separation of particle classes and the particle-particle drag that enhances mixing of particles. This implies that the control of segregation is closely tied to understanding and quantification of these two drag forces. Gas-particle drag which solely originates from interaction of solid particles with the carrier flow has been studied for bidisperse and polydisperse gas-solid suspensions (van der Hoef et al., 2005; Beetstra et al., 2007; Sarkar et al., 2009; Yin and Sundaresan, 2009; Holloway et al., 2010; Rong et al., 2014; Mehrabadi et al., 2016) and various drag models have been proposed with respect to flow parameters. Particle-particle drag has also been studied in the context of kinetic theory of granular gases in the absence of interstitial fluid, and closure models have been proposed to represent this drag as well (Syamlal, 1987; Jenkins and Mancini, 1989; Gao et al., 2006). However, since the level of particle velocity fluctuations affect the particle-particle drag, a better understanding the mechanism of partitioning of kinetic energy between the energies in the mean flow and velocity fluctuations leads to a better analysis of particle segregation and mixing.

The mechanism of transfer of kinetic energy between the fluid phase and solid particles in a homogeneous monodisperse gas-solid suspension has been explained by the conservation of interphase turbulent kinetic energy (TKE) transfer principle (Xu and Subramaniam, 2007), and is validated by particle-resolved direct numerical simulation (PR-DNS) (Mehrabadi et al.,
Figure 6.1: Schematic representation of transfer of kinetic energy from the mean flow to velocity fluctuations in the fluid phase and the solid phase due to interphase interactions in monodisperse gas-solid flow. The mixture interphase TKE transfer subtracts energy $\Pi^{(m)}$ from the mean flow and distributes it between fluid-phase and solid-phase velocity fluctuations through their corresponding interphase transfer terms, i.e. $\Pi^{(f)}$ and $\Pi^{(p)}$. The energy in the system is dissipated by viscous dissipation $\varepsilon^{(f)}$.

This mechanism of transfer of energy is schematically shown in Fig. 6.1. In homogeneous monodisperse suspension, a body force or mean pressure gradient is used to provide the driving force for sustaining the mean slip velocity between fluid and particles in the suspension. This driving force causes development of a relative mean motion or mean slip velocity between the two phases denoted by $\langle \mathbf{W} \rangle = \langle \mathbf{u}^{(p)} \rangle - \langle \mathbf{u}^{(f)} \rangle$, where $\langle \mathbf{u}^{(p)} \rangle$ and $\langle \mathbf{u}^{(f)} \rangle$ are, respectively, the mean velocity of the solid phase and the fluid phase. The driving force eventually balances the mean drag force on particles, and a steady mean slip velocity is achieved. The power required to sustain this mean slip velocity and overcome the drag force on particles is equal to the product of the mean pressure gradient times the mean slip velocity. This amount of power given to the suspension is subtracted from the mean flow by the mixture interphase turbulent kinetic energy (TKE) transfer $\Pi^{(m)} = \langle \mathbf{W} \rangle \cdot \langle \nabla p \rangle$, and then partitioned between the fluid phase and the solid phase as the sources of velocity fluctuations through the fluid-phase and solid-phase interphase TKE transfer terms, denoted respectively by $\Pi^{(f)}$ and $\Pi^{(p)}$. The energy of the system is finally dissipated through the fluid-phase viscous dissipation $\varepsilon^{(f)}$. This mechanism also reveals that the transfer of kinetic energy due to the interphase interactions is conservative, which is analogous to the transfer of kinetic energy from the mean flow to velocity fluctuations through the production term in single-phase turbulent flow.
Although the mechanism of TKE transfer from the mean flow to velocity fluctuations due to interphase interaction in homogeneous monodisperse gas-solid flow has been explained (Xu and Subramaniam, 2007; Mehrabadi et al., 2015), this transfer mechanism for bidisperse and polydisperse suspensions, to the best of our knowledge, is unknown. In a bidisperse suspension (as the simplest form of polydisperse gas-solid flow) not only does each particle class experience a different mean slip velocity with respect to the carrier flow, there also exists a mean slip velocity between the two particle classes. Based on our findings from the monodisperse suspension, we can expect that mean slip velocities between the carrier fluid and each of particle classes lead to energy transfer from the mean flow to velocity fluctuations. However, the influence of the mean slip velocity between the two particle classes on transfer of the kinetic energy as well as the particle-particle drag needs to be explained.

In the current study, we first provide statistical representations of governing equations in the mean flow and velocity fluctuations for bidisperse gas-solid suspensions. We then use these equations to extend the conservation of interphase TKE transfer principle to bidisperse suspensions. This extended principle is a first step towards providing a regime map for segregation and mixing phenomena in engineering design and optimization processes for given particle properties and flow parameters.

6.2 Statistical representation of conservation equations

Computational fluid dynamics (CFD) simulations of gas-solid flow utilizing the averaged mass, momentum and energy conservation equations are widely used for device-scale calculations as a feasible approach for engineering purposes. These conservation equations are derived from statistical approaches applicable to multiphase flow. The statistical equations are derived in gas-solid flow are mainly the stochastic point process approach\(^1\) and the random field approach (Tenneti and Subramaniam, 2014; Subramaniam, 2013). In the stochastic point process approach (Subramaniam, 2000, 2001) the dispersed phase is represented in a Lagrangian frame, while the carrier phase is described in an Eulerian frame. In the random field approach, however, an Eulerian description is used to represent both phases.

\(^1\)Note that stochastic point process approach is not the same as the point particle approximation.
The stochastic point process approach (Daley and Vere-Jones, 1988; Stoyan and Stoyan, 1995) can be used to provide the statistical information corresponding to the state of particles in a gas-solid suspension. The Liouville probability density function (pdf) provides a complete description of the multi-particle event in the suspension. This detailed multi-particle description of dispersed phase is not directly usable in engineering applications. Instead, in practice the one-particle distribution function as a function of the sample space position, velocity and radius at each instant of time is used to represent the state of solid particles (Subramaniam, 2001). The transport of zeroth, first, and second moments of the one-particle distribution function are then used to obtain the conservation equations of the mean mass, mean momentum, and mean energy of the dispersed phase in a gas-solid flow (Jenkins and Savage, 1983; Liboff, 2003; Garzó et al., 2007).

In the random field approach, the velocity field is defined at each point in the suspension including the gas phase as well as the solid phase. This velocity field is considered to be a random field defined everywhere for each flow realization. Phasic indicator fields are used to distinguish phases from each other. For example the solid phase indicator field is zero, unless the spatial position is located inside the solid phase which leads to the indicator field being unity. In this approach the indicator fields are also random variables that change from one realization to another. Although a complete description of the flow field based on multi-point joint pdfs provides more information than needed for engineering applications, the simplest statistical description based on single-point representation is more useful for practical analysis. This single-point description leads to the two-fluid theory in which both phases are considered as inter-penetrating continua represented in Eulerian-Eulerian frames (Drew, 1983; Drew and Passman, 1998).

In the current study, we focus on understanding the mechanism of transfer of kinetic energy from the mean flow to velocity fluctuations as well as from one phase to another due to interphase interactions. Therefore, we need to derive the evolution equations of kinetic energy for each of the phases in the suspension. The derivation of conservation equations for polydisperse gas-solid flow from the one-particle distribution function in the Lagrangian-Eulerian (LE) frame as well as the two-fluid theory in the Eulerian-Eulerian (EE) frame have been provided,
respectively, in Appendices D and E. It is observed that the transport equations obtained from both approaches for the dispersed phase are the same. Therefore, we use the equations provided in Appendix E for the rest of our analysis.

In order to isolate the role of interphase interactions in segregation of particle size classes from other effects (such as presence of walls, inflow/outflow boundary conditions, and mean shear rate), we consider a homogeneous gas-solid flow in which the mean flow quantities remain invariant with respect to spatial position. Therefore, the spatial gradient of all mean flow quantities is zero. In spite of the homogeneity assumption, analyzing the mechanism of transfer of energy in a polydisperse suspension is still very complicated. In order to reduce the complexity of our analysis, we consider a bidisperse gas-solid flow since it has essential elements to represent the interaction of the fluid-phase with different particle classes, as well as the interaction of the two particle classes with each other. In addition, usually multifluid models (Syamlal et al., 1993; Yin and Sundaresan, 2009; Sarkar et al., 2009) are based on pairwise additivity of bidisperse interactions. Also, we assume that all particle collisions are elastic. Therefore, there is no energy loss during particle collisions.

Considering the above assumptions, the evolution equation of the mean slip velocity between two particle size classes \( \langle W^{(\beta,\alpha)} \rangle \) is obtained by subtracting the mean momentum equation of particle size class \( \alpha \) (cf. Eq. D.20) from that of size class \( \beta \), that is:

\[
\frac{d}{dt} \langle W^{(\beta,\alpha)} \rangle = \left( \frac{\langle f^{(f \rightarrow \beta)}_h \rangle}{\rho^{(\beta)} \phi^{(\beta)}} - \frac{\langle f^{(f \rightarrow \alpha)}_h \rangle}{\rho^{(\alpha)} \phi^{(\alpha)}} \right) - \frac{\langle f^{(\beta \rightarrow \alpha)}_c \rangle}{\rho^{(\alpha)} \phi^{(\alpha)}} - \frac{1}{\rho^{(\beta)} \phi^{(\beta)}} + \frac{1}{\rho^{(\alpha)} \phi^{(\alpha)}} ,
\]

where \( \rho^{(\chi)} \) and \( \phi^{(\chi)} \) are, respectively, the mass density and solid-phase volume fraction of particle class \( \chi \in (\alpha, \beta) \). In the above equation, the symbol \( \langle \cdot \rangle \) represents the ensemble-average. Consequently, the term \( \langle f^{(f \rightarrow \chi)}_h \rangle \) is the mean gas-particle drag force from the fluid phase on particle class \( \chi \in (\alpha, \beta) \), and \( \langle f^{(\beta \rightarrow \alpha)}_c \rangle \) is the mean particle-particle drag force acting on particle class \( \alpha \) as a result of collisions with the particles belonging to class \( \beta \). This equation clearly indicates that the mean slip velocity between the two classes is influenced by the mean gas-particle drag on each particle class as well as the mean particle-particle drag between the two
particle classes. The dependence of particle-particle drag on the level of kinetic energy in each class (Jenkins and Mancini, 1989; Gao et al., 2006), which in turn influences the evolution of \( \langle W^{(\beta,\alpha)} \rangle \), necessitates a better understanding of the mechanisms by which the kinetic energy is transferred from either the fluid phase to solid particles, or one particle class to another. This understanding is tied to the analysis of kinetic energy transport equations. Therefore, in the following sections, we first present the kinetic energy in the mean flow followed by the kinetic energy in velocity fluctuations. Then, the coupling between the two sets of equations is described, and the mechanism of transfer of kinetic energy among these phases is explained.

### 6.3 Transport equation of kinetic energy in the mean flow

The transport equation of the mean kinetic energy \( \bar{E}^{(\chi)} = \langle u^{(\chi)} \rangle \cdot \langle u^{(\chi)} \rangle /2 \) for a homogeneous bidisperse gas-solid suspension with elastic particles in the fluid phase and the solid phase can be obtained by simplifying Eqs. E.15 and E.16. Here, superscript \( \chi \) takes the values \( f, \alpha, \text{or} \beta \) representing, respectively, the fluid phase, particle class \( \alpha \), and particle class \( \beta \). Also \( \langle u^{(\chi)} \rangle \) is the mean velocity of phase \( \chi \). The simplified equations for the mean kinetic energy are obtained as

\[
\frac{d}{dt} \rho^{(f)} \phi^{(f)} \bar{E}^{(f)} = \left\langle u^{(f)}_i \right\rangle \left\langle f^{(\alpha \rightarrow f)}_{h,i} \right\rangle + \left\langle u^{(f)}_i \right\rangle \left\langle f^{(\beta \rightarrow f)}_{h,i} \right\rangle + \rho^{(f)} \phi^{(f)} \left\langle u^{(f)}_i \right\rangle g_i, \quad (6.2)
\]

\[
\frac{d}{dt} \rho^{(\alpha)} \phi^{(\alpha)} \bar{E}^{(\alpha)} = \left\langle u^{(\alpha)}_i \right\rangle \left\langle f^{(f \rightarrow \alpha)}_{h,i} \right\rangle + \left\langle u^{(\alpha)}_i \right\rangle \left\langle f^{(\beta \rightarrow \alpha)}_{c,i} \right\rangle + \rho^{(\alpha)} \phi^{(\alpha)} \left\langle u^{(\alpha)}_i \right\rangle g_i, \quad (6.3)
\]

\[
\frac{d}{dt} \rho^{(\beta)} \phi^{(\beta)} \bar{E}^{(\beta)} = \left\langle u^{(\beta)}_i \right\rangle \left\langle f^{(f \rightarrow \beta)}_{h,i} \right\rangle + \left\langle u^{(\beta)}_i \right\rangle \left\langle f^{(\alpha \rightarrow \beta)}_{c,i} \right\rangle + \rho^{(\beta)} \phi^{(\beta)} \left\langle u^{(\beta)}_i \right\rangle g_i. \quad (6.4)
\]

In the above equations, the term \( \left\langle f^{(f \rightarrow \chi)}_h \right\rangle \) with \( \chi \in (\alpha, \beta) \) satisfies \( \left\langle f^{(f \rightarrow \chi)}_h \right\rangle = - \left\langle f^{(\chi \rightarrow f)}_h \right\rangle \) due to the conservation of interphase mean momentum transfer. Also the term \( \left\langle f^{(\psi \rightarrow \chi)}_c \right\rangle \) is the mean particle-particle drag from the particle class \( \psi \in (\alpha, \beta) \) on class \( \chi \in (\alpha, \beta) \) with \( \chi \neq \psi \) which satisfies \( \left\langle f^{(\psi \rightarrow \chi)}_c \right\rangle = - \left\langle f^{(\chi \rightarrow \psi)}_c \right\rangle \) due to the conservation of mean interphase momentum transfer. It should be noted that \( \left\langle f^{(\chi \rightarrow \chi)}_c \right\rangle = 0 \) due to the conservation of momentum transfer in collisions between pairs of particles belonging to class \( \chi \).
Now we define the mixture mean energy that is the mass-weighted sum of the mean kinetic energies in the system:

\[ \tilde{E}^{(m)} = \rho(f)\phi(f)\bar{E}(f) + \rho^{(\alpha)}\phi^{(\alpha)}\bar{E}^{(\alpha)} + \rho^{(\beta)}\phi^{(\beta)}\bar{E}^{(\beta)}. \]  

(6.5)

The evolution equation for the mixture mean energy is then obtained by summing the Eqs. 6.2 to 6.4 which yields:

\[
\frac{d\tilde{E}^{(m)}}{dt} = \left(\langle u_i^{(\alpha)} \rangle - \langle u_i^{(f)} \rangle\right)\left\langle f^{(f \rightarrow \alpha)}_{h,i} \right\rangle + \left(\langle u_i^{(\beta)} \rangle - \langle u_i^{(f)} \rangle\right)\left\langle f^{(f \rightarrow \beta)}_{h,i} \right\rangle \\
+ \left(\langle u_i^{(\beta)} \rangle - \langle u_i^{(\alpha)} \rangle\right)\left\langle f^{(\alpha \rightarrow \beta)}_{c,i} \right\rangle + \rho^{(m)}\langle u_i^{(m)} \rangle g_i, \tag{6.6}
\]

where \(\rho^{(m)}\) is the mixture density defined as \(\rho^{(f)}\phi^{(f)} + \rho^{(\alpha)}\phi^{(\alpha)} + \rho^{(\beta)}\phi^{(\beta)},\) and \(\langle u^{(m)} \rangle\) is the mixture mean velocity given by:

\[
\langle u^{(m)} \rangle = \frac{\rho^{(f)}\phi^{(f)}\langle u^{(f)} \rangle + \rho^{(\alpha)}\phi^{(\alpha)}\langle u^{(\alpha)} \rangle + \rho^{(\beta)}\phi^{(\beta)}\langle u^{(\beta)} \rangle}{\rho^{(f)}\phi^{(f)} + \rho^{(\alpha)}\phi^{(\alpha)} + \rho^{(\beta)}\phi^{(\beta)}}. \tag{6.7}
\]

The mean slip velocity is defined as the relative mean velocity difference between any of the two phases. Therefore, the mean slip velocity between the fluid phase and particle class \(\chi\) as well as the mean slip velocity between the two particle class are defined as:

\[
\langle u^{(\chi)} \rangle - \langle u^{(f)} \rangle = \langle W^{(\chi,f)} \rangle, \quad \{\chi = \alpha, \beta\},
\]

\[
\langle u^{(\beta)} \rangle - \langle u^{(\alpha)} \rangle = \langle W^{(\beta,\alpha)} \rangle. \tag{6.8}
\]

It is interesting to observe that Eq. 6.6 can be rewritten in terms of these mean slip velocities. Therefore, Eq. 6.6 simplifies to:

\[
\frac{d\tilde{E}^{(m)}}{dt} = \left\langle W^{(\alpha,f)} \right\rangle \cdot \left\langle f^{(f \rightarrow \alpha)}_{h} \right\rangle + \left\langle W^{(\beta,f)} \right\rangle \cdot \left\langle f^{(f \rightarrow \beta)}_{h} \right\rangle + \left\langle W^{(\beta,\alpha)} \right\rangle \left\langle f^{(\alpha \rightarrow \beta)}_{c} \right\rangle \\
+ \rho^{(m)}\langle u^{(m)} \rangle \cdot g. \tag{6.9}
\]

In the above equation, \(\Pi^{(m,\alpha)}\) and \(\Pi^{(m,\beta)}\) are the mixture turbulent kinetic energy (TKE) transfer terms due the interphase interactions between the fluid phase and each of the two particle classes. These terms arise due to the hydrodynamic interactions in the mixture. The term \(\Theta^{(m)}\) corresponds to the mixture TKE transfer between the two particle classes originating
from particle-particle interactions. These mixture interphase TKE transfer terms appear with negative sign in the mixture mean kinetic energy equation since the gas-particle and particle-particle drag forces in Eq. 6.9 are acting in the direction opposite to their corresponding mean slip velocities. Therefore, the above equation indicates that the rate of change of mixture mean kinetic energy is balanced by the energy source from the body forces and the mixture interphase TKE transfers.

### 6.4 Transport equation of kinetic energy in velocity fluctuations

Transport equations of the kinetic energy in velocity fluctuations of the gas phase and particle classes are obtained by simplifying Eqs. E.19 and E.20 which have the following forms:

\[
\rho^{(f)} \phi^{(f)} \frac{dk^{(f)}}{dt} = \left( \frac{u_i}{\Pi^{(\alpha \rightarrow f)}} \right)^{n^{(f)}} \left( \frac{u_i}{\Pi^{(\beta \rightarrow f)}} \right)^{n^{(f)}} - 2\mu^{(f)} \left( s_{ij} \right),
\]

\[6.10\]

\[
\rho^{(\alpha)} \phi^{(\alpha)} \frac{dk^{(\alpha)}}{dt} = \left( \frac{u_i}{\Pi^{(f \rightarrow \alpha)}} \right)^{n^{(\alpha)}} \left( \frac{u_i}{\Theta^{(\beta \rightarrow \alpha)}} \right),
\]

\[6.11\]

\[
\rho^{(\beta)} \phi^{(\beta)} \frac{dk^{(\beta)}}{dt} = \left( \frac{u_i}{\Pi^{(f \rightarrow \beta)}} \right)^{n^{(\beta)}} \left( \frac{u_i}{\Theta^{(\alpha \rightarrow \beta)}} \right).
\]

\[6.12\]

In Eq. 6.10, the term \( \Pi^{(\chi \rightarrow f)} \) with \( \chi \in (\alpha, \beta) \) represents fluid-phase interphase TKE transfers due to interphase interactions with particle class \( \chi \), which originates from the covariance of fluid-phase velocity fluctuations and gas-particle drag force of class \( \chi \) at fluid-particle interface. In addition, the term \( \varepsilon^{(f)} \) is the viscous dissipation (Mehrabadi et al., 2015) that provides a mechanism for transform of kinetic energy into internal energy. In Eqs. 6.11 and 6.12, the term \( \Pi^{(f \rightarrow \chi)} \) with \( \chi \in (= \alpha, \beta) \) is the interphase TKE transfer to particle class \( \chi \) due to interphase interactions with the fluid phase that that arises from the covariance of particle velocity fluctuations in class \( \chi \) and their corresponding gas-particle drag at fluid-particle interface. The term \( \Theta^{(\psi \rightarrow \chi)} \) is the interclass TKE transfer to particle class \( \chi \in (\alpha, \beta) \) due to interphase interaction with particles belonging to class \( \psi \in (\alpha, \beta) \) with \( \psi \neq \chi \). Similarly, this term arises from the covariance of particle velocity fluctuations and particle-particle drag at the interparticle interface. Now we can define the mixture energy in the velocity fluctuations as the sum of kinetic
energies in velocity fluctuations of all phases in the mixture weighted by their corresponding mass densities

\[ \tilde{e}^{(m)} = \rho^{(f)} \phi^{(f)} k^{(f)} + \rho^{(\alpha)} \phi^{(\alpha)} k^{(\alpha)} + \rho^{(\beta)} \phi^{(\beta)} k^{(\beta)}. \]  

(6.13)

The evolution equation for the mixture energy in velocity fluctuations is then obtained by summing Eqs. 6.10 to 6.12, which yields:

\[
\frac{d\tilde{e}^{(m)}}{dt} = \left\langle \left( u_i^{n(\alpha)} - u_i^{n(f)} \right)^2 f_{h,i}^{(f\rightarrow\alpha)} h,i \right\rangle + \left\langle \left( u_i^{n(\beta)} - u_i^{n(f)} \right)^2 f_{h,i}^{(f\rightarrow\beta)} h,i \right\rangle \\
+ \left\langle \left( u_i^{n(\beta)} - u_i^{n(\alpha)} \right)^2 f_{c,i}^{(\alpha\rightarrow\beta)} + \left( u_i^{n(\alpha)} f_{c,i}^{(\alpha\rightarrow\alpha)} \right) + \left( u_i^{n(\beta)} f_{c,i}^{(\beta\rightarrow\beta)} \right) \right\rangle.
\]  

(6.14)

We can use the kinematic condition at the mutual interface between the fluid and solid phases to relate the difference in their velocity fluctuations to the corresponding mean slip velocity (Xu and Subramaniam, 2007). The kinematic condition at particle surface guarantees that the instantaneous velocity of the fluid phase and solid particles at the fluid-solid interface is equal. Also in the soft-sphere representation, the two particles in a pair of colliding particles share the same instantaneous velocity in their mutual contact region. We can use these properties to show that the difference between velocity fluctuations of any of the two phases is equal to their corresponding mean slip velocity, that is:

\[
\begin{align*}
  u^{n(\chi)} - u^{n(f)} &= -\left\langle \text{W}(\chi,f) \right\rangle, \quad \chi \in (\alpha, \beta), \\
  u^{n(\beta)} - u^{n(\alpha)} &= -\left\langle \text{W}(\beta,\alpha) \right\rangle.
\end{align*}
\]  

(6.15)

Substituting the above expressions into Eq. 6.14 provides the final expression for the mixture energy in the velocity fluctuations, which is

\[
\frac{d\tilde{e}^{(m)}}{dt} = -\left\langle \text{W}(\alpha,f) \cdot f_{h}^{(f\rightarrow\alpha)} \right\rangle_{\Pi^{(m,\alpha)}} - \left\langle \text{W}(\beta,f) \cdot f_{h}^{(f\rightarrow\beta)} \right\rangle_{\Pi^{(m,\beta)}} - \left\langle \text{W}(\beta,\alpha) \cdot f_{c}^{(\alpha\rightarrow\beta)} \right\rangle_{\Theta^{(m)}} \\
+ \left\langle u^{n(\alpha)} \cdot f_{c}^{(\alpha\rightarrow\alpha)} \right\rangle_{\Theta^{(\alpha\rightarrow\alpha)}} + \left\langle u^{n(\beta)} \cdot f_{c}^{(\beta\rightarrow\beta)} \right\rangle_{\Theta^{(\beta\rightarrow\beta)}} - \varepsilon(f).
\]  

(6.16)

Therefore, it is understood that the mixture interphase TKE transfer terms associated with fluid-solid interactions \( \Pi^{(m,\chi)} \) with \( \chi \in (\alpha, \beta) \) are equal to sum of their corresponding fluid-phase and solid-phase interphase TKE transfer terms \( \Pi^{(f\rightarrow\chi)} \) and \( \Pi^{(\chi\rightarrow f)} \) arising from hydrodynamic
interactions. Also the mixture interphase transfer term associated with particle-particle interactions $\theta^{(m)}$ is equal to the sum of corresponding particle class interphase transfer terms $\theta^{(\beta\rightarrow\alpha)}$ and $\theta^{(\alpha\rightarrow\beta)}$. In other words, the following expressions hold for interphase interactions in a bidisperse gas-solid flow:

\[
\begin{align*}
\Pi^{(m,\alpha)} &= \Pi^{(\alpha\rightarrow f)} + \Pi^{(f\rightarrow\alpha)} \\
\Pi^{(m,\beta)} &= \Pi^{(\beta\rightarrow f)} + \Pi^{(f\rightarrow\beta)} \\
\Theta^{(m)} &= \Theta^{(\beta\rightarrow\alpha)} + \Theta^{(\alpha\rightarrow\beta)}
\end{align*}
\]  

(6.17)

which means that the transfer of kinetic energy due to interphase interactions in a bidisperse gas-solid flow is indeed conservative.

Comparison of the mixture mean kinetic energy equation in Eq.6.9 with those for velocity fluctuations in Eqs. 6.10 to 6.12, and also considering the mean momentum equations E.12 and E.14 reveals a complex coupling between the mean momentum and kinetic energy equations in addition to the conservation of interphase TKE transfer terms. In a bidisperse suspension, the driving force $\nabla p$ in the suspension leads to the development of a mean slip velocity between the fluid phase and each of the particle classes $\langle W^{(\chi,f)} \rangle$ with $\chi \in (\alpha, \beta)$. These slip velocities give rise to the development of mean gas-particle drag forces $\langle f^{(f\rightarrow\chi)} \rangle$ on each particle class. Also because of the difference in the gas-particle drag experienced by each particle class, a mean slip velocity between the two classes $\langle W^{(\beta,\alpha)} \rangle$ develops in time as well. This relative mean motion between the two particle classes leads to the particle mass flux which is the signature of particle segregation. The power required to overcome the mean drag between the gas phase and any of the two particle classes is subtracted from the mean flow by the corresponding mixture interphase TKE transfer term $\Pi^{(m,\chi)}$ in Eq. 6.9 and is fed into the velocity fluctuations in the fluid phase and the corresponding particle class by means of the interphase transfer terms $\Pi^{(\chi\rightarrow f)}$ and $\Pi^{(f\rightarrow\chi)}$ in Eqs. 6.10 to 6.12. Also the amount of power required to sustain the mean slip velocity between the two particle classes and overcome the particle-particle drag is subtracted from the mean flow by the term $\Theta^{(m)}$ in Eq. 6.9, and then distributed between velocity fluctuations in the two particle classes through the interphase TKE transfer terms $\Theta^{(\beta\rightarrow\alpha)}$ and $\Theta^{(\alpha\rightarrow\beta)}$ in Eqs. 6.11 and 6.12. This transfer of energy from
the mean flow to velocity fluctuations is called extended conservation of interphase TKE transfer principle and is schematically shown in Fig. 6.2. This energy redistribution leads to increase of velocity fluctuations in the solid phase, which in turn increases the probability of particle collisions belonging to different particle classes. This also leads to the enhancement of the particle-particle drag. This interplay of the momentum and energy transfer continues until the system reaches a steady state.

Figure 6.2: Schematic representation of transfer of kinetic energy from the mean flow to velocity fluctuations in the fluid phase and the solid phase due to interphase interactions. The mixture interphase TKE transfers required to sustain the mean slip velocity between the fluid phase and any of the two particle classes and overcome the gas-particle drag forces subtract energy from the mean flow and distribute the energy between the velocity fluctuations in the fluid phase and particle classes through their corresponding interphase transfer terms. Also the power required to sustain the mean slip velocity between the two particle classes and overcome the particle-particle drag is subtracted from the mean flow and then distributed between the velocity fluctuations in the two particle classes through their corresponding interphase transfer terms. The energy in the system is finally dissipated by viscous dissipation $\varepsilon^{(f)}$.

Since the mechanism of transfer of kinetic energy in a bidisperse gas-solid flow is described by the above extended conservation of interphase TKE transfer principle, the role of mean slip velocity between the two particle classes and also the particle-particle drag in prediction of segregation is clearly highlighted. If we are allowed to change particle properties, such as
particle class volume fractions, diameters and densities, as well as flow parameters, such as the body force or mean pressure gradient, these changes lead to steady mean slip velocities (either between the fluid phase and any of the particle classes, or between the two particle classes) in a homogeneous suspension. Nevertheless, the steady value of these mean slip velocities are not know a priori. Quantification of these mean slip velocities over the range particle properties and flow conditions is important because in the extended interphase TKE transfer principle, they affect the transfer of kinetic energy from the mean flow to velocity fluctuations. It should also be noted that from the mean momentum equations for a homogeneous bidisperse suspension, the mean slip velocities also depend on the gas-particle drag and particle-particle drag forces (Mehrabadi et al., 2016). Because of the dependence of the particle-particle drag on particle velocity fluctuations, it is important to study the source of velocity fluctuations in the dispersed phase, which is explained by the extended interphase TKE transfer principle. Therefore, this study is the first step towards providing a regime map for segregation and mixing of particle classes that can be used for a parametric study of the level of gas-particle and particle-particle drag forces, the mean slip velocities, the particle class kinetic energies and their corresponding sources with respect to particle properties and flow parameters. This regime map will then be useful for the design and optimization of industrial devices and processes where segregation and mixing are important.

6.5 Conclusion

In this study, we explain the coupling between the momentum and kinetic energy equations in a bidisperse gas-solid flow by introducing the extended conservation of interphase TKE transfer principle. In a homogeneous bidisperse suspension driven by a body force or a mean pressure gradient, each particle class experiences a different mean gas-particle drag. This difference causes the development of different mean slip velocities between the fluid phase and each of the particle classes. In addition, this difference leads to a mean slip velocity between the two particle classes, which is associated with the particle mass flux that is the signature of particle segregation. Nevertheless, the mean slip velocity between the two particle classes does not increase monotonically. Instead, this mean slip is hindered by the particle-particle drag
arising from particle collisions which leads to redistribution of momentum and energy between the two particle classes. Therefore, the mean slip velocity between the two particle classes reaches a steady value. This interplay of momentum and energy transfer reveals a complex coupling that can be analyzed by deriving the conservation equations for the mixture kinetic energy in the mean and velocity fluctuations. These equations indicate that the interphase TKE transfer due to interphase interactions in a homogeneous bidisperse suspension is conservative. Also the amount of power required to sustain the mean slip velocity between the fluid phase and each of the two particle classes is subtracted from the mean flow and distributed between the velocity fluctuations of the fluid phase and the corresponding solid phase. Similarly, the power required to sustain the slip velocity between the two particle classes is subtracted from the mean flow and distributed between the velocity fluctuations of the two particle classes. The particle velocity fluctuations directly influence the particle-particle drag which in turn affects the mean slip velocity between the two particle classes. Therefore, quantifying the amount of partitioning of kinetic energy between the particle classes due to interphase interactions with respect to particle class properties and flow parameters helps us gain a better understanding of segregation and mixing regime map for engineering applications.
CHAPTER 7. DEVELOPMENT OF A GAS-SOLID DRAG LAW FOR CLUSTERED PARTICLES USING PARTICLE-RESOLVED DIRECT NUMERICAL SIMULATION

This chapter includes a manuscript titled “Development of gas-solid drag law for clustered particles using particle-resolved direct numerical simulation” and is under review in the Chemical Engineering Science journal authored by M. Mehrabadi, E. Murphy, and S. Subramaniam.

Abstract

Particle-resolved direct numerical simulation (PR-DNS) is used to quantify the drag force on clustered particle configurations over the solid phase volume fraction range $0.1 \leq \phi \leq 0.35$ and the mean slip Reynolds number range of $0.01 \leq Re_m \leq 50$. The particle configurations and flow parameters correspond to gas-solid suspensions of Geldart A particles in which formation of clusters have been reported. In our PR-DNS, we use clustered particle configurations that match cluster statistics observed in experimental studies. To generate the particle configurations, we perform discrete element method (DEM) simulations of homogeneous cooling gas (HCG) systems with cohesive and inelastic particles in the absence interstitial fluid. Clustered particle sub-ensembles are then extracted from HCG simulations to match the statistics of cluster size distributions observed in experiments. These sub-ensembles are used for PR-DNS. It is found that the mean drag on clustered configurations decreases when compared to the drag laws for uniform particle configurations. The maximum drag reduction belongs to the configuration with low solid-phase volume fraction $\phi = 0.1$ in Stokes flow, and is about 35%. The drag reduction reduces with increase in both $\phi$ and $Re_m$. A clustering metric is introduced to explain the behavior of the drag reduction with respect to solid-phase volume fraction. Also
the behavior of the drag reduction with mean slip Reynolds number is related to the Brinkman screening length. PR-DNS results are then used to propose a clustered drag model for the range of flow parameters considered in this study. Also a generalized drag law that represents the mean drag for both uniform and clustered configurations is proposed. This general drag model provides a smooth transition between the uniform and clustered states by means of a weighting function with two model parameters.

7.1 Introduction

Gas-solid flows are commonly found in industrial applications such as fluidized-bed combustion, fluid catalytic cracking, coal gasification, and biomass energy generation (Fan et al., 2004). In these applications, there are several mechanisms that tend to bring individual particles close to each other. These particles then form locally denser regions of particles compared to ambient that surrounds them. These structures are known as particle clusters that dynamically form and break up in response to gas-particle and particle-particle interactions in gas-solid flows. The presence of particle clusters significantly influences interphase transfer of mass, momentum and energy in a suspension. For instance, interphase heat and mass transfer in suspensions with particle clusters is significantly reduced when compared to those flows where particles are uniformly distributed in the suspension. Also in fluidized bed risers once particle clusters form the pressure drop along the riser decreases. This indicates a reduction of gas-particle drag when clusters exist in the riser. Therefore, it is essential to account for the presence of these structures when analyzing engineering applications that utilize gas-solid suspensions.

In the gas-solid flow applications mentioned above, the material density ratio ranges from $\rho^{(p)}/\rho^{(f)} \sim \mathcal{O}(100)$ to $\mathcal{O}(1000)$ and the particle diameter varies from $d_p \sim 50\mu\text{m}$ to $500\mu\text{m}$. In the Geldart classification, gas-solid suspensions are characterized based on particle diameter and the density difference between the two phases. From the Geldart chart shown in Fig. 7.1 it can be understood that the aforementioned ranges for density ratio and particle diameter belong to Geldart A and Geldart B particles. For Geldart A particles that are associated with smaller and lighter particles, the dominant clustering mechanism is particle-particle interaction arising from electrostatics, cohesion, van der Waals forces, or liquid bridging (Gao et al., 2008;
van Wachem and Sasic, 2008; Royer et al., 2009), while for Geldart B particles with larger and heavier particles, the effect of hydrodynamic interactions is more dominant.

It is evident from homogeneous cooling gases (HCG) of granular materials that the level of particle velocity fluctuations, also known as particle granular temperature, plays a significant role in the formation of particle clusters. In homogeneous cooling gases as the suspension cools down, locally concentrated regions of particles form is the suspension. In these concentrated regions, the particle collision frequency is higher than in the less concentrated regions. Therefore, the particles in the concentrated regions loose more energy due to higher frequency of inelastic collisions which accelerates the cooling of these locally concentrated regions. Since the granular temperature is associated with particle pressure, these highly concentrated cool regions appear as low pressure zones which lead to attraction of more particles and enhancement of particle clustering.

In spite of the importance of particle granular temperature in clustering of particles, the generation of particle clusters in gas-solid flows arises from a complex dynamic interplay between fluid-particle and particle-particle interactions. In a gas-solid suspension, formation of these particle clusters arises from the balance between the attractive forces (hydrodynamics, electrostatics, or cohesion) bringing the particles together and the repulsive forces (hydrod-
Particle-particle and fluid-particle interactions in a gas-solid flow. The presence of clusters then gives rise to a reduction in the drag force. We have learned from PR-DNS of freely evolving gas-solid suspensions that the rate of work done in maintaining a flow with constant mean slip between the gas and solid phases by means of a constant mean pressure gradient results in the production of velocity fluctuations in both gas and solid phases (Mehrabadi et al., 2015). Therefore, reduction in the local drag force acting on particle clusters leads to local reduction of the amount of power input to the granular temperature. This reduction in granular temperature enhances the formation of clusters. The carrier flow can also directly influence particle clusters by reorienting and restructuring of the clusters. These interconnected phenomena dynamically affect the interphase transfer of momentum and energy between the gas phase and solid particles. The outcome of this complex dynamic interplay is growth of particle clusters and formation of mesoscale structures as observed in experiments (Shaffer et al., 2013). Figure 7.2 schematically describes this interplay in which the mean flow indirectly influences particle clustering by tuning the supply of kinetic energy to the granular temperature. The interplay between dissipation, of hydrodynamic or collisional origin, the granular temperature, and cohesive potentials then determines the formation of clusters. Once the clusters form, they are directly influenced by the carrier flow, in a way that differs from dispersed particles. In addition to this complex mechanism arising from interphase interactions, wall effects, inflow
and outflow boundaries, and inhomogeneities in the carrier flow can influence the formation of particle clusters as well, which make the clustering analysis more complicated.

In computational fluid dynamics (CFD) calculations of gas-solid flow, the momentum exchange between the gas phase and the solid phase is modeled by drag closure models. In this regard, empirical correlations based on experiments (Wen and Yu, 1966; Ergun, 1952), or those proposed from particle-resolved direct numerical simulation (Hill et al., 2001a,b; van der Hoef et al., 2005; Beetstra et al., 2007; Tenneti et al., 2011) are widely used to account for the average drag force on particles in gas-solid flows. These drag laws are generally applicable to suspensions with particles uniformly distributed in the suspension. However, the use of these drag laws for cases where particle clusters are likely to form, such as Geldart A suspensions, shows inconsistency between the CFD simulations and experimental data (Zimmermann and Taghipour, 2005; Mazzei and Lettieri, 2008; Garg et al., 2010b). This inconsistency indicates that the closure models proposed for uniformly distributed particle configurations are not capable of correctly predicting the unresolved interphase interactions for suspensions where particle clusters form.

The current state-of-the-art drag model that accounts for the effect of particle clusters in CFD calculations is a class of energy minimization multi-scale (EMMS) models (Li et al., 1999; Yang et al., 2004; Wang and Li, 2007) that are extensions to conventional drag models, and is based on the minimum required energy for suspending and transporting dense particle regions in a gas-solid suspension. While the EMMS model is useful, there is scope to develop a physics-based model of drag in clusters particle suspensions.

Experimental investigations provide invaluable insight into formation, distribution, interaction and more importantly characterization of particle clusters in gas-solid flows. For instance, Harris et al. (2002) compiled a wide range of experimental and industrial data corresponding to near-wall particle clusters in risers and provided correlations for cluster properties such as cluster volume fractions, cluster diameter, cluster roundness factor, etc. Cocco et al. (2010) used a fiber optical probe to provide cluster size distribution in and above fluidized beds. Also Chew et al. (2012) investigated the formation, duration and frequency of appearance of particle clusters at different operating conditions along a riser for different materials. Gokaltun et al.
(2012) used shadow-sizing technique to measure cluster size and velocity distribution in a circulating fluidized bed. Also, McMillan et al. (2013) reported that in a riser although short-range particle-particle forces initiate small clusters, it is the fluctuations and gradients in gas-particle forces that promote cluster formation.

In spite of the useful information provided by the experiment, detailed spatio-temporal analysis of the flow hydrodynamics and transfer of mass, momentum and energy due to interphase interactions cannot be obtained from experiment. In an experiment it is not easily possible to exclude the wall effects in the flow setup, making it difficult to differentiate the role of wall effects from other mechanisms that contribute to formation of particle clusters.

Particle-resolved direct numerical simulation (PR-DNS) is an alternative approach that is well suited for discovering flow physics in particle-laden flow (Tenneti and Subramaniam, 2014). The PR-DNS approach not only provides detailed information about the hydrodynamic velocity and pressure fields, it also provides particles trajectories along with their velocities and accelerations. Furthermore, properly designed PR-DNS studies can be used to either propose closure models used in CFD calculations of gas-solid flow, or to test the validity of these closure models.

The PR-DNS methodology has been successfully used to propose closure models for the average gas-particle drag. Hill et al. (2001a) used the Lattice Boltzmann Method (LBM) to propose a drag model for monodisperse arrays of ordered and randomly distributed particles in the Stokes flow regime, and validated their results for low solid volume fraction with theoretical analysis. Later, Hill et al. (2001b) extended their drag model to moderate Reynolds numbers. van der Hoef et al. (2005) also used LBM to a propose drag model for monodisperse gas-solid flow in the Stokes regime using fixed particle assemblies. Beetstra et al. (2007) used LBM to solve for flow past fixed particle assemblies to incorporate the effect of higher mean slip Reynolds number (up to 1000) into the low-Reynolds-number monodisperse drag model of van der Hoef et al. (2005). Similarly, Rong et al. (2013) used LBM simulations to propose a drag in the range of the solid-phase volume fraction $0.1 \leq \phi \leq 0.6$ and mean slip Reynolds number $0.002 \leq Re_m \leq 3000$. Tenneti et al. (2011) performed well-resolved PR-DNS based on the particle-resolved Reconcilable Immersed Boundary Method (PUReIBM) continuum solver to
simulate the Navier-Stokes equations and reported the drag force in gas-solid flows using fixed particle assemblies over a wide range of flow parameters \((0.1 \leq \phi \leq 0.5\) and \(0.01 \leq Re_m \leq 300\)). They also proposed a drag law as a function of \(\phi\) and \(Re_m\).

In an attempt to generalize the quantification of interphase momentum transfer to clustered particle configurations using PR-DNS, Beetstra et al. (2006) performed simulations for four types of particle clusters which were originally constructed by Tran-Cong et al. (2004) for experimental analysis. Based on their PR-DNS results, Beetstra et al. (2006) reported that the interstitial distance among particles in a cluster has significant effect on the drag force, and neglecting this parameter leads to inaccurate drag prediction. Shah et al. (2013) also used LBM to study the effect of clusters on the drag force. They successfully demonstrated the dependence of the drag on flow Reynolds number and solid-phase volume fraction. However, in their configurations they used a stand-alone cluster in the middle of the computational box surrounded by individual particles. Again this type of particle configuration with a limited degree of freedom may not accurately represent the configurations observed in real applications, because the clustered configurations obtained from this deterministic approach may not represent the statistics of clustered observed in experiment.

In spite of the initial insight about the effect of clustering on the drag force, the aforementioned PR-DNS works neglected the simultaneous co-existence of different cluster types that lead to a cluster size distribution in a gas-solid flow. Experimental analysis of Cocco et al. (2010) in fluidized bed shows that a significant percentage of particles participate in formation of clusters ranging from a few to hundreds of particles in each cluster. The shape of the distribution may depend on particle materials, operating conditions and flow location. Also particle clusters appearing as a result of hydrodynamic interactions may have geometrical characteristics that have not yet been extensively addressed. Therefore, those analysis that do not account for clustering metrics may have limited applicability.

In the current study we first describe different types of PR-DNS for clustered configurations, and analyze their numerical feasibility by performing a time scale analysis. Then, in order to have clustered configurations that better match real applications, we perform homogeneous cooling gas simulation of inelastic and cohesive particles using discrete element method (DEM)
Figure 7.3: Depiction of the functional form of particle-particle interaction potentials. The Harmonic potential representing the particle-particle interaction due to elastic collision is shown in long dashed lines. The van der Waals potential representing the cohesive force is shown in short dashed lines. The total interaction potential obtained from superposition of the Harmonic and van der waals potentials in shown in solid line.

and extract particle configurations that are statistically equivalent to the distribution provided by the experiment of Cocco et al. (2010). In order to identify the level of clustering at different solid-phase volume fractions, we propose a clustering metric that expresses the deviation of particle configuration from a uniformly distributed state. These clustered configurations are then used for PR-DNS of gas-solid flow over a rage of flow parameters and the results are used to provide a drag model for clustered configurations.

7.2 Analysis of numerical constraints

In PR-DNS of freely evolving suspensions, particle collisions are treated with the soft-sphere model that allows finite overlap of particles during the collision process. This model typically employs a linear spring-dashpot to represent the contact force that results in elastic or inelastic restitution on contact (Cundall and Strack, 1978), though more physics based contact force model alternatives are also used (Kuwabara and Kono, 1987). The attractive potential that we consider between a pair of particles not yet in contact is modeled by the van der Waals (VDW) potential given by

$$U_{coh}(r) = -\frac{A d_p}{12 (r + d_0 - d_p)}, \quad (7.1)$$
where \( A \) is the Hamaker constant, \( d_p \) is the particle diameter, \( d_0 \) is the interatomic distance, and \( r \) is the particle center to center distance. The attractive force saturates once particles are in contact. Figure 7.3 shows the spring \( U_{\text{Harmonic}} \) and cohesion potentials \( U_{\text{VDW}} \) for a pair of cohesive particles undergoing an elastic collision, and the resulting total potential \( U_{\text{total}} \). Note that the cohesive force at contact, \( r < 0 \), is constant. In order to resolve the motion of a pair of particles going through this pair potential in a discrete element method (DEM) simulation, two time scales should be resolved. The first one is the collision time scale defined as

\[
t_{\text{coll}} = \pi \sqrt{\frac{m}{k}},
\]

(7.2)

where \( m \) is the effective mass of the particle pair and \( k \) is the spring stiffness. We can derive an expression for this time scale normalized by the characteristic time scale of the fluid \( t_{\text{fluid}} = \frac{d_p}{|\langle W \rangle|} \) by writing the energy balance between the spring potential energy and the particle kinetic energy

\[
\frac{1}{2} k \delta^2 = \frac{1}{2} mv^2
\]

(7.3)

where \( v \) is the characteristic velocity of colliding particles. In a gas-solid flow this characteristic velocity can be considered as the second root of solid-phase granular temperature \( v = \sqrt{T} \), where \( T = \langle v'' \cdot v'' \rangle / 3 \) with \( v'' \) being particles velocity fluctuations, i.e., \( v'' = v - \langle v \rangle \). Now if the velocity in Eq. 7.3 is replaced with \( \sqrt{T} \) and both sides of the equations are multiplied by \((|\langle W \rangle|/d_p)^2\), Eq. 7.3 becomes

\[
\frac{m}{k} \left( \frac{|\langle W \rangle|}{d_p} \right)^2 = \frac{|\langle W \rangle|^2}{T} \left( \frac{\delta}{d_p} \right)^2.
\]

(7.4)

If one divides the left-hand side by the right-hand side, it is evident the ratio of contact to fluid time scale scales with the non-dimensional overlap \( t_{\text{coll}}/t_{\text{fluid}} \propto \delta/d_p \). The model presented herein assumes nearly rigid particles \( \delta/d_0 < O(1) \) (Derjaguin et al., 1975) and hence very small overlaps. Additionally, it has been found that physically accurate simulations require large spring stiffness, on the order of the stiffness of actual particles (Murphy and Subramaniam, a). As a result very little speed-up can be achieved through softening of the interaction without affecting the physics.
While the limiting time scale for these simulations is the collision time-step, we can still gain an appreciation of the cost of such numerical simulations by looking at the cohesive time-scale. The cohesive time scale is the time-scale that must be resolved in order to enforce energy conservation between particles as they move through the attractive potential well as shown in Fig. 7.3. Now if we assume that in Eq. 7.4 the maximum overlap $\delta$ is 1% of the particle diameter $d_p$ and also assume that the granular temperature in gas-solid flow scales as $T/|\langle W \rangle|^2 \sim 10^{-2}$ (Tenneti et al., 2016), it can be concluded from Eq. 7.4 that the contact to fluid time scales ratio is

$$\frac{t_{\text{coll}}}{t_{\text{fluid}}} \sim 0.1. \quad (7.5)$$

The second important time scale in systems with attractive forces, particularly with cohesive forces in the current analysis, is the cohesion time scale that should also be resolved to capture the motion of a colliding pair through the particle-particle well potential as shown in Fig. 7.3. The cohesion time scale relative to the fluid time scale is defined as (Murphy and Subramaniam, a)

$$\frac{t_{\text{coh}}}{t_{\text{fluid}}} = \frac{d_0}{d_p} \frac{|\langle W \rangle|}{T^{1/2}} \sqrt{\frac{2000}{Ha + 40}}, \quad (7.6)$$

where the non-dimensional $Ha$ parameter describes the ratio of the energy associated with the cohesive forces to the characteristic kinetic energy in a pair of colliding particles, which is given as

$$Ha = \frac{A}{\rho_p \pi d_0^2 d_0 T}, \quad (7.7)$$

where $\rho_p$ is the particle mass density. For a given cohesive and colliding system with $A = 10^{-19} J$, $d_0/d_p = 10^{-4}$, $T = 0.0085$ and $\rho_p = 1000$, the $Ha$ parameter appears to be 0.8. For this system, the cohesion to fluid time scales ratio in Eq. 7.6 is

$$\frac{t_{\text{coh}}}{t_{\text{fluid}}} \sim 0.007. \quad (7.8)$$

The above time scale ratio indicates that the cohesion time scale is about two orders of magnitude smaller than the collision time scale for the softened systems normally simulated in gas-solid flows, $\delta/d_p$, as calculated by Eq. 7.5. From this analysis the simulation time for PR-DNS of gas-solid systems with cohesive particles is at least two orders of magnitude longer than a similar system in the absence of cohesive forces.
Based on the preceding time scale analysis provided, we identify three simulation approaches for PR-DNS of flow past particle clusters:

1. PR-DNS of homogeneous freely evolving gas-solid suspensions of cohesive particles from an initially unclustered state where the cohesion time scale given by Eq. 7.8 is resolved.

2. PR-DNS of homogeneous freely evolving suspensions of initially clustered particles that still resolves the cohesion time scale but eliminates cluster formation time.

3. PR-DNS of homogeneous fixed assemblies of particle clusters where the cohesion and collision time scales are irrelevant because the particles do not move.

The first approach that involves the formation of clusters from a uniform initial state accounting for both cohesive and hydrodynamic forces is computationally expensive owing to the range of time and length scales needed to be resolved. Note that we have found from DEM of HCG that the formation time is long (of the order of weeks based on CPU time). The second approach is useful for studying the restructuring and reorientation of clusters in a gas-solid flow, but although it avoids the simulation of the time to form clusters, it is still expensive for parametric studies using PR-DNS. The third approach is the most inexpensive and expedient one to investigate the effect of particle clusters on flow hydrodynamics. The use of rigid clusters or fixed particle assemblies implies that the cohesive forces among particles in a cluster overcome the hydrodynamic forces experienced by particles that tend to break clusters apart; the particles are effectively ‘sintered’ into clusters. Therefore, the focus of this study is on the third approach. It has been shown that fixed particle assemblies of high Stokes number particles in PR-DNS are a good approximation to freely evolving suspensions (Xu and Subramaniam, 2010; Tenneti et al., 2011; Mehrabadi et al., 2015), because the time required for the particle configuration to change significantly is much larger than the fluid relaxation time scale.

Therefore, in this work we use the third approach to study the effect of particle clustering on gas-particle drag over a range of mean slip Reynolds number and solid-phase volume fraction. These clusters are associated with Plascoat polyethylene particles based on previously established analysis (Cocco et al., 2010) that predicts the maximum size of clusters under the influence of interparticle attractions and flow hydrodynamics. The computational generation
of particle clusters with statistics that match experimental findings is discussed in the following section.

### 7.3 Initialization of clustered particle configuration

Characterization of particle clusters and relating this characterization to flow parameters as well as particle properties is a challenging task. The dynamic formation and breakup of particle clusters usually leads to the existence of a range of particle cluster sizes in the system. Although some correlations for the size, concentration and shape of particle clusters have been proposed for some specific flow conditions such as core-annular flow (Harris et al., 2002), the dynamics of clusters as well as their corresponding size and shape distributions in engineering applications is an open question. In this regard, the experimental work of Cocco et al. (2010) provides detailed information about the cluster size distribution of Plascoat polyethylene and FCC catalyst particles in a fluidized bed. They used a specially designed borescope connected to a high speed camera that was inserted into the fluidized bed. Images from the fluidized bed were post-processed to provide information about particles and clusters. Their analysis for polyethylene particles indicates that there exists a cluster size distribution in the bed. Although there are clusters with hundreds of particles, the mean number of particles in a cluster is about 26. In addition, about 75% of particles form clusters, while the rest appear isolated particles. Their measurement for FCC particles showed similar findings. However, the mean number of particles in a FCC cluster was reported as 13. The experimental findings of Cocco et al. (2010) indicate that those studies in which the interaction of the carrier flow with a single particle cluster (Beetstra et al., 2006) or a single particle cluster with surrounding individual particles (Shah et al., 2013) may have limited applicability in interphase interactions in a practical situation where there is a cluster size distribution in the system.

In this study we use PR-DNS of clustered configurations that match the statistics of particle clusters represented in experimental findings. PR-DNS of gas-solid flow for the entire range of cluster size distribution provided by Cocco et al. (2010) requires huge computational resources. Instead, in the current study we quantify the drag force on sub-ensembles of particle clusters that have been extracted from DEM simulation of a HCG with both inelastic and cohesive
particles in the absence of interstitial fluid. We select the extracted sub-ensembles to be consistent with the results of Cocco et al. (2010) for polyethylene particles as the baseline for the particle configurations in our PR-DNS. We expect these sub-ensembles to meet the following constraints:

1. The particle volume fraction in the sub-ensembles should be close to that of the HCG system
2. Particle structures in the sub-ensembles have the same statistics as those in the whole HCG system
3. The maximum number of particles in the largest cluster of the sub-ensemble be around 26
4. Approximately 75% of particles in the sub-ensemble are in clusters

HCG simulations are performed using the LAMMPS code (Plimpton, 1995) developed in Sandia National Lab. These simulations are performed in a periodic computational box in the same way as documented in (Murphy and Subramaniam, 2015). The simulations are performed in a domain size with $L/d_p = 50$ for solid-phase volume fractions in the range $0.1 \leq \phi \leq 0.4$. The number of particles can be determined by the following expression:

$$N_p = \frac{6\phi}{\pi} \left( \frac{L}{d_p} \right)^3.$$

Particles are initially uniformly distributed in the domain with a given Maxwellian velocity distribution that is characterized by granular temperature $T$. The short-range interaction forces among particles are represented by the van der Waals force arising from the well potential given by Eq. 7.1. Also the particle collisions in these HCG simulations are modeled by a soft-sphere method using the nonlinear spring-dashpot model of Kuwabara and Kono (1987). In the absence of any external forces, particles lose energy as they undergo inelastic particle collisions. Once the kinetic energy of a pair of colliding particles is not enough to overcome the energy in the well potential described by Eq. 7.1, these particles become bound, eventually sticking together and forming clusters. This process progressively leads to formation of larger particle
clusters in the domain since there is no mechanism to compensate the energy loss in inelastic particle collisions, and therefore, eventually all particles fall into a giant cluster that spans through the computational box.

All various time instants during the HCG simulation, the systems are searched during the cooling process for particle sub-ensembles that meet the constraints mentioned above and have the box length as $\mathcal{L}/d_p = 10$. Due to the periodic image of particle configurations in sub-ensembles, there may be overlap of particles near the boundaries. For those particle pairs that overlap more than 5% of a particle diameter, one of the particles in the pair is removed. It should be noted that this process leads to sub-ensembles that have slightly smaller volume fractions (1 to 10%) compared to the original HCG systems. Figure 7.4 shows the comparison between the radial distribution function $g(r)$ of the HCG system with the averaged $g(r)$ obtained from the sub-ensembles for the cases with solid-phase volume fractions $\phi = 0.1$ and 0.3. The radial distribution function represents the probability of finding a particle in the neighborhood of a test particle with separation $r$ between particles centers compared to that of a completely random Poisson process. The comparison of $g(r)$ in Fig. 7.4 indicates that the structures in the sub-ensembles have the same characteristics as those in the HCG system. It should be noted that it is more practical to compare the radial distribution functions of clusters in sub-ensembles with those obtained from experiments of gas-solid flow. However, in the absence of
Figure 7.5: Examples of the sub-ensemble configurations for (a, b) $\phi = 0.1$, and (c, d) $\phi = 0.3$. The contour colors represent the number of particles in a cluster.
such experimental results, we check that the distributions of particles in sub-ensembles are as close as to the ones in the HCG systems.

Figure 7.5 represents two particle sub-ensembles for $\phi = 0.1$ as well as for $\phi = 0.3$ where color contours indicate the number of particles in a cluster. These sub-ensembles clearly show that there exist different cluster sizes in the selected configurations. These sub-ensembles are used as particle configurations in our PR-DNS.

### 7.4 Numerical method

Several numerical methods have been developed for particle-resolved direct numerical simulation (PR-DNS) of fluid-solid flows (Johnson and Tezduyar, 1997; Peskin, 2002; Chen and Doolen, 1998; Prosperetti and Oguz, 2001; Feng and Michaelides, 2004). In this study, we use the particle-resolved uncontaminated-fluid reconcilable immersed boundary method (PUReIBM) of Tenneti et al. (2010). This method is shown to be accurate and numerically convergent (Garg et al., 2010c; Tenneti et al., 2011). In addition, PUReIBM has been successfully used to simulate flow over uniformly distributed particles in fixed assemblies (Tenneti et al., 2011, 2013; Mehrabadi et al., 2015) and propose a gas-particle drag law for uniform particle configurations (Tenneti et al., 2011).

In PUReIBM, the Navier-Stokes equations are solved on a three dimensional Cartesian grid for the whole computational domain. The instantaneous conservation equations of mass and momentum are

$$\nabla \cdot \mathbf{u} = 0,$$

(7.9)

and

$$\rho^{(f)} \frac{\partial \mathbf{u}}{\partial t} + \rho^{(f)} \mathbf{S} = -\mathbf{g}_{\text{IBM}} + \mu^{(f)} \nabla^2 \mathbf{u} + \mathbf{f},$$

(7.10)

respectively, where $\mathbf{u}$ is the instantaneous velocity, $\mathbf{S} = \nabla \cdot (\mathbf{u} \mathbf{u})$ is the convective term in conservative form, and $\mathbf{g}_{\text{IBM}} = \nabla p$ is the pressure gradient. The no-slip and no-penetration conditions on the fluid velocity at the particle surfaces is imposed via the additional immersed boundary (IB) force term $\mathbf{f}$ in Eq. (7.10).
To compute the IB force, the surface of the sphere is represented by a discrete number of points called boundary points that are parametrized in spherical coordinates. Two additional sets of points, termed as exterior and interior points are generated by projecting the boundary points onto spheres of radii $r + \Delta r$ and $r - \Delta r$ respectively, with $\Delta r$ chosen to be equal to the grid spacing. In PUReIBM, the IB force is computed at the interior points so that a desired velocity $u^{(k,d)}$ is obtained at the $k^{th}$ interior point. Following the direct forcing method proposed by Mohd-Yusof (1996) the IB force $f^{(k)}$ at the $k^{th}$ interior point is specified to cancel the remaining terms in the momentum conservation, and to force the velocity to its desired value $u^{(k,d)}$:

$$f^{(k)} = \rho^{(f)} \frac{u^{(k,d)} - u^{(k,n)}}{\Delta t} + \rho^{(f)} S^{(k,n)} + g_{\text{IBM}}^{(k,n)} - \mu^{(f)} \nabla^2 u^{(k,n)}.$$  \hspace{1cm} (7.11)

Note that all the terms in the above equation are evaluated at the $k^{th}$ interior point. The desired velocity $u^{(k,d)}$ depends on the velocity of the particle. For instance, for a fixed particle the desired velocity at the interior point is equal in magnitude but opposite in direction of the fluid velocity at the corresponding exterior point so that the velocity at the boundary point is zero. The IB force so computed at all the interior points is interpolated to the neighboring grid nodes that do not include those lying in the fluid phase to get $f$.

The governing equations in PUReIBM are decomposed into time-varying volumetric mean and spatio-temporal fluctuations. These quantities are simultaneously solved at each time step. The fluctuating fields are solved using a pseudo-spectral method, with the Crank-Nicolson scheme for the viscous terms, and an Adams-Bashforth scheme for the convective terms. A fractional time-stepping method that is based on Kim and Moin’s approach (Kim and Moin, 1985) is used to advance the fluctuating velocity fields in time. The salient feature of PUReIBM is that the IB forcing in PUReIBM is non-zero only inside the solid phase, and the fluid-phase is uncontaminated by the IB forcing. Therefore, the velocity and pressure in the fluid phase satisfy the unmodified Navier-Stokes equations. In addition, 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. This feature enables us to directly compare the DNS solution with any random-field theory of multiphase flow (Garg et al., 2010c; Tenneti et al., 2011), and in particular we can quantify the drag force of particles in clustered configurations.
Before measuring the clustered particle drag force over a range of flow parameters, we need to check the grid convergence behavior of the drag force with respect to particle grid resolution. For each solid-phase volume fraction, we choose a representative particle configuration. We then perform PR-DNS of flow passing through this configuration with different grid resolutions that are defined as the number of grid points across each particle, i.e. \( D_m = d_p / \Delta x \). We perform these convergence tests for the mean slip Reynolds number \( Re_m = 50 \) that is expected to be the upper limit for Geldart A particles. The grid convergence study at this \( Re_m \) ensures that the drag force is also grid independent. The convergence behavior of the drag force for a specified particle sub-ensemble for different solid-phase volume fractions is given in Fig. 7.6(a), while the relative error in the drag is shown in Fig. 7.6. It should be noted that the relative error is the difference between the mean drag force for a given grid resolution and that obtained from the highest grid resolution normalized by the drag force of the highest grid resolution, i.e. \( |F - F_{fine}| / F_{fine} \). Based on this analysis, we use a particle grid resolution of \( D_m = 30 \) for \( \phi = 0.1 \) and 0.2, and \( D_m = 40 \) for \( \phi = 0.3 \) and 0.4.

Simulations are performed with different mean slip Reynolds numbers ranging from \( Re_m = 0.01 \) to 50 and solid-phase volume fraction in the range \( 0.1 \leq \phi \leq 0.4 \) with five realizations, each corresponding to a different particle configuration, for each case (\( \langle \phi \rangle = 0.1, 0.27 \) and 0.35 with \( \langle \phi \rangle \) being the mean volume fraction of the five realizations). Quantification of the mean
drag force per particle normalized by the Stokes drag is shown in Fig. 7.7. The comparison of the PR-DNS results from the clustered cases with the uniform drag model of Tenneti et al. (2011) indicates that the mean drag reduces in clustered configurations for the range of $\langle \phi \rangle$ and $Re_m$ considered in the current study. The relative amount of drag reduction compared with the uniform drag model of Tenneti et al. (2011) is shown in Fig. 7.8. This figure indicates the maximum reduction up to about 35% for $\langle \phi \rangle = 0.1$ in Stokes flow when compared to the uniform drag model of Tenneti et al. (2011).

It is observed in Fig. 7.8 that the amount of drag reduction decreases with increase of mean slip Reynolds number. The attenuation of drag reduction with Reynolds number is associated with the reduction of the Brinkman screening length as the Reynolds number increases. The Brinkman screening length is equivalent to the integral length scale associated with the Eulerian two-point covariance of velocity fluctuations (Koch et al., 1998). Mehrabadi et al. (2015) showed that the integral length scale decreases with increasing mean slip Reynolds number. Therefore, increase of the Reynolds number causes the fluid loses its spatial correlation over shorter length scales that leads to smaller drag reduction.

Figure 7.8 reveals that the amount of drag reduction is higher for low solid-phase volume fraction $\langle \phi \rangle = 0.1$ compared with higher volume fractions. It also shows that the level of drag
Figure 7.8: Symbols show the relative amount of drag reduction from PR-DNS of clustered configurations when compared with the uniform drag model of Tenneti et al (2011). The error bars show the 95% confidence intervals obtained from five independent sub-ensembles. The solid lines represent the drag reduction model given by Eq. 7.16.

reduction for the cases with volume fraction $\langle \phi \rangle = 0.27$ and 0.35 are the same. This leveling off of the drag reduction behavior with respect to solid-phase volume fraction can be explained by a closer look at clustering metrics.

Several methods for characterizing the level of clustering have been proposed. One approach is to obtain the probability density function (PDF) of Voronoi cell volumes (Monchaux et al., 2010). In this method, Voronoi cells are constructed around the center of each particle such that they contain only a single particle. This construction of Voronoi cells leads to appearance of small volume cells in regions where particles are very close to each other, in contrast to the void regions where the volume of Voronoi cells is relatively large. Comparison of the PDF of these Voronoi cell volumes when compared to that obtained from the case with uniformly distributed particles indicates the level of clustering. The disadvantage with using Voronoi cell volumes as a metric of clustering is that it is difficult to construct a transport equation for this quantity for use in two–fluid multiphase CFD simulations.

Another approach is excess two-body entropy which is based on the radial distribution function of particle configuration (Baranyai and Evans, 1989). Recall that the radial distribution function $g(r)$ provides a two-point statistics about the location of particles with respect to each
other. Therefore, configurational information of a particle assembly is embedded in the radial distribution function. The excess entropy is computed from the following expression:

\[
S_{\text{excess}}^{(2)} = -\frac{1}{2} \rho \int 4\pi r^2 g(r) \ln (g(r)) \, dr + \frac{1}{2} \rho \int 4\pi r^2 (g(r) - 1) \, dr.
\] (7.12)

If a particle configuration has a Poisson distribution, then the corresponding radial distribution function is unity for all separations. It can be easily shown that for such a \( g(r) \), the excess two-body entropy from Eq. 7.12 is zero. However, if particle clusters exist, the \( g(r) \) deviates from unity, as shown in Fig. 7.4, which in turn leads to a non-zero excess two-body entropy. In this case, the value of \( S_{\text{excess}}^{(2)} \) determines how far a configuration is from the uniformly distributed state.

Although the above method is provides an appropriate metric for characterizing the level of particle clustering when particle locations are changed, it cannot be generalized to a case where the number of particle change from one realization to another. Usually, the mean volume fraction for a homogeneous configuration is defined from averaging \( \phi \) over different realizations. Therefore, volume fraction which is related to the number of particles in a volume may change from one realization to another. In other words, the number of particles is itself a random variable that may be different between two realizations. This randomness in the number of particles is not considered in Eq. 7.12. However, a more general approach that allows randomness in the number of particles in addition to the randomness in particle configuration is the configuration entropy of a point process method (Murphy and Subramaniam, b).

In this method an entropy for the configuration can be computed by reconstructing the probability distribution function of particle number density in sub-volumes taken from a simulation. If we consider the one-particle density function, constructed from a measurement volume, for a grand canonical ensemble, that is with a variable number of particles, we obtain the following expression:

\[
f (x, v, t; V_m) = \sum_k P(k; V_m) f^{(k)} (x, v, t; V_m).
\] (7.13)

The probability mass function \( P(k; V_m) \) denotes the probability that there are \( k \) particles in a realization of the point process in sub-volume. In the above expression \( f^{(k)} (x, v, t; V_m) \) is the
one-particle distribution function of a particle assembly defined over the position and velocity sample space for a given sub-volume $V_m$ that includes $k$ particles (Subramaniam, 2000). We want to find the entropy of this probability mass function, constructed from a simulation. It has been shown that the entropy of a particle configuration has the following form (Subramaniam, 2014):

\[
S_n = - \sum_{k=0}^{\infty} P(k; V_m) \ln (P(k; V_m)).
\]

(7.14)

The salient feature of this method is although it may require more computational time compare to the PDF of Voronoi cells method, it is derived from a mathematical perspective explaining a physical observation. Therefore, it is possible to derive a transport equation for the configurational entropy compared to the PDF of Voronoi cells method. In addition, the configurational entropy method is more general compared to the excess two-body entropy method explained earlier since configurational entropy method allows variation in the number of particles as well.

We select the configuration entropy approach to compare the configuration entropy of the grand canonical ensemble at two different states, for instance at uniformly distributed and clustered states, in order to measure the level of clustering in the configuration. Quantification of the configurational entropy given by Eq. 7.14 has been performed for the HCG systems at (i) the initial state where particle are uniformly distributed, (ii) the time the cluster-containing sub-ensembles have been extracted for the PR-DNS in this study, (iii) and also at the final time of HCG simulation when all particles in the computational box form a giant cluster. Figure 7.9 shows that the difference in configurations entropy between the initial state and the time when PR-SNS sub-ensembles are extracted is significant for $\langle \phi \rangle = 0.1$. However, the difference in the configuration entropy between the two states for higher volume fractions is not noticeable. This indicates that the configurational changes due to the presence of particle clusters are higher for low solid-phase volume fraction since particles are allowed to rearrange more in microscate, and form simultaneous clustered and void regions. Presence of these regions in configurations at low solid-phase volume fraction influences the flow hydrodynamics and therefore higher drag reduction is achieved when compared with high solid-phase volume fraction cases. This point can also be confirmed by comparing the amount of entropy difference between the initial and
Figure 7.9: Configuration entropy quantification for homogeneous cooling gas simulations as a function of measurement volume $V_m$ normalized by the volume of the system $V$. These quantifications have been performed for the initial condition where particles are uniformly distributed (presented with solid lines), when sub-ensemble clustered configurations are extracted for PR-DNS (shown in dashed lines), and the final state of HCG when all particles form a single giant cluster in the computational box (shown with dash-dot lines).
final states which seems to be relatively greater for $\langle \phi \rangle = 0.1$, when compared with higher volume fractions for which the difference between the initial and selected states are very close.

### 7.6 Clustered drag model

For the purpose of formulating a clustered drag law, we assume that once particle clusters are formed, they match the distribution provided by Cocco et al. (2010). In the absence of further evidence for the evolution of cluster formation and breakup and also cluster metrics at different operating conditions, we assume that the distribution provided by Cocco et al. (2010) is a valid representation for particle clusters in a fluidized bed. This allows us to provide a drag model from our PR-DNS results of homogeneous gas-solid flow when the cluster size distribution in PR-DNS approximately matches the one reported by Cocco et al. (2010). Therefore, this clustered drag model would represent the interphase mean momentum transfer when the maximum clustering state exists in the suspension.

Figure 7.8 indicates that the correlation $g(\phi, Re_m)$ for drag reduction can be a function of the solid-phase volume fraction and the mean slip Reynolds number:

$$\frac{F_U(\phi, Re_m) - F_C(\phi, Re_m)}{F_U(\phi, Re_m)} = g(\phi, Re_m),$$

(7.15)

where $F_C$ and $F_U$ are, respectively, the clustered and uniform drag models. Based of the drag reduction quantification in Fig. 7.8 and physical considerations, the following constraints should be imposed on $g(\phi, Re_m)$:

1. The function should be finite in Stokes flow ($Re_m \to 0$) because the maximum drag reduction appears at Stokes flow

2. The function should tend to zero at high Reynolds number flow ($Re_m \to \infty$) due to the fact that the Brinkman screening length monotonically decreases with Reynolds number and the flow seems to feel the particles as isolated sphere rather than as in clusters

3. The function should monotonically increase with the decrease of volume fraction, reaching an upper limit of unity, i.e. $\lim_{\phi \to 0} g(\phi, Re_m) = 1$
Considering the above constraints, we propose a model for drag reduction with the following form

\[
g(\phi, \text{Re}_m) = \left( \frac{a}{1 + b \text{Re}_m} \right) \left( 1 - \exp \left( -c \phi^d \right) \right),
\]

which provides a good match to our PR-DNS results as shown in Fig. 7.8 for the range of flow parameters considered in this study. The model constants in the above expression are

\[
a = 1.16 \times 10^{1}, \quad b = 3.52 \times 10^{-2}, \quad c = 8.25 \times 10^{-3}, \quad d = -5.19 \times 10^{-1}.
\]

It is possible to rearrange the terms in Eq. 7.15 to obtain the clustered drag model with respect to the uniform drag law and the drag reduction model, given as

\[
F_C(\phi, \text{Re}_m) = \{1 - g(\phi, \text{Re}_m)\} F_U(\phi, \text{Re}_m),
\]

where the drag model of Tenneti et al. (2011) for \( F_U \) and Eq. 7.16 for \( g \) are used. This clustered drag model has been compared with PR-DNS results of cluster-containing sub-ensembles in Fig. 7.7, and indicates a good agreement between the model and simulations for the range of parameters considered in this study. As mentioned earlier, it is assumed that this drag model represents the mean momentum transfer when the system is at the maximum state of clustering. The transition between the uniform and clustered drag models is discussed in the next section.

### 7.7 General drag model: transition between uniform and clustered drag laws

In general, the drag force on a clustered particle configuration, depends on cluster dynamics as well as clustering metrics. It is known that the cluster dynamics depend on gas-particle and particle-particle interactions. However, details of the dynamics that lead to formation and breakup of particle clusters is not yet well understood. Characterization of clusters at microscopic scales requires detailed information about particle locations that may not be available in coarse grained or two-fluid theory approaches. The solution to this discrepancy is either to develop a transport equation for clustering metrics that are closed with respect to flow-transported quantities, or to consider particle clusters with pre-assumed characteristics and corresponding metrics.
As a starting point, we assume that the balance of processes determining the formation and break-up of clusters is at a steady state. Therefore, no significant changes in the state of clustering in a particle configuration occur. Also in the absence of adequate knowledge about the mechanism of hydrodynamic interactions that lead to formation of particle clusters as of those observed by Capecelatro et al. (2014a), we assume that for Geldart A particle, the major driving mechanism for formation of clusters in particle cohesion. The balance between production of kinetic energy from the mean flow, and dissipation of energy would then produce a unique granular temperature and distribution of cluster sizes for a given attractive interparticle potential (such as cohesion, electrostatic, van der Waals forces). As mentioned earlier, the ratio between the potential energy and fluctuating kinetic energy is characterized by the $Ha$ parameter given by Eq. 7.7. Therefore, the tentative form of the general drag model can be described as:

$$F = f(\phi, Re_m, Ha).$$  \hspace{1cm} (7.18)

The $Ha$ parameter can be dynamically computed in each computational cell of CFD simulation using the two-fluid approach or CFD-DEM approach. The $Ha$ parameter is obtained by knowing the energy associated with the attractive forces between the particles (characterized by Hamaker constant particle diameter, minimum allowed particle separation) and the granular temperature in each cell. Once $Ha$ exceeds a critical value, then particle clusters form, otherwise the configuration remains uniform.

The limit $Ha \to 0$ is reached when either the particle granular temperature is infinite or there is no attraction among particles, and in that limit the particles are uniformly distributed inside of a CFD cell. Therefore, a uniform drag law should be used in this limit. In contrast, the limit $Ha \to \infty$ is achieved when the particles are strongly attracted towards each other, or the granular temperature tends to zero. In these circumstances, a clustered drag model should be used.

Switching back and forth between the uniform and clustered drag laws in a simulation may lead to numerical instabilities. Therefore, it is preferable to use a smooth transition between the two states. Although this transition can depend on several flow parameters as well as particle properties, currently we only consider the transition dependence on the $Ha$. The mean
Figure 7.10: The shape of $Ha$ function given by Eq. 7.20.

drag force on a configuration is specified as a weighted sum of the two limiting drag laws in the following form:

$$F = f(\phi, \text{Re}_m, Ha) = F_U(\phi, \text{Re}_m) \{1 - h(Ha)\} + h(Ha)F_C(\phi, \text{Re}_m),$$  \hspace{1cm} (7.19)$$

where $h(Ha)$ is the smooth function used to switch between the uniform and clustered drag models. Since particle clusters dynamically form and break up, $h$ should be determined based on the dynamics of the system. However, because of the lack of any information about the behavior of the transition between the uniform and clustered drag forces, we limit ourselves to a monotonically increasing function with respect to $Ha$ with the following form:

$$h(Ha) = \frac{1}{2} + \frac{1}{\pi} \arctan^{-1} \left( \frac{Ha - Ha_0}{\varepsilon} \right).$$  \hspace{1cm} (7.20)$$

In the above expression, $Ha_0$ determines the critical value of $Ha$ when the switching between the uniform and clustered drag models takes place. Additionally, the parameter $\varepsilon$ determines the slope of switching between the two states. This family of curves asymptotes to a Heaviside function in the limit of $\varepsilon \to 0$. The parameter $\varepsilon$ is a model constant that should be specified based on model testing.
The $h$ function given in Eq. 7.20 is anti-symmetric about $Ha_0$. The value for this parameter can be either determined by experimental analysis, or the Type 1 PR-DNS of gas-solid flow explained in Section 7.2, or model testing in CFD simulations. However, we can estimate based on our PR-DNS results. Our data show that for a case with solid-phase volume fraction $\phi = 0.1$ and particle diameter $d_p = 50\mu m$ suspended by a mean flow with mean slip Reynolds number up to 100 the particle granular temperature is in the range of $0.064 m^2/s^2$ to $2.728 m^2/s^2$ by uniform estimates (Tenneti et al., 2016). If we assume that the Hamaker constant is $A = 10^{-19} J$, the solid-to-fluid density ratio is 1000, and the minimum particle separation is $d_0 = 10^{-4}d_p$, then the minimum and maximum values of $Ha$ for the particles suspended in an air flow would be $Ha_{\text{min}} = 6.3 \times 10^{-4}$ and $Ha_{\text{max}} = 3.77 \times 10^{-2}$, respectively. The $Ha_0$ is then defined as the average value of these two limits, that is

$$Ha_0 = \frac{Ha_{\text{max}} + Ha_{\text{min}}}{2} = 1.92 \times 10^{-2}.$$  

(7.21)

This $Ha_0$ value is chosen for representing the $h(Ha)$ function in Fig. 7.10. Nevertheless, this is a model constant and could be used to tune the model for CFD simulations. The tuning process can be performed by simulating a fluidized bed for which the experimental data are also available. In the simulations, the tuning variables $Ha_0$ and $\varepsilon$ should be such that the numerical results match the experimental findings, such as the pressure drop or solid-phase volume fraction profile along the bed. In order to accelerate the tuning process, an appropriate optimization algorithm can also be employed. Once the model parameters are tuned, the model can be CFD simulation of other geometries and applications.

It should be highlighted that in this work we chose the $Ha$ parameter based on the energy associated in the particle attractive forces and characteristic kinetic energy of a pair of particles as a metric to determine existence of particle clusters in the proposed model. Although this parameter does not account for the formation of clusters due to solely hydrodynamics interactions, it is a good candidate for cluster detection in Geldart A gas-solid flows where the main mechanism of clustering is cohesive forces. In addition, in the absence of experimental results for realizations of particle clusters in gas-solid flow, we used HCG simulations to produce clusters that match in size to those reported by (Cocco et al., 2010). Once experimental results
for clusters of particles in gas-solid flows for difference flow parameters and particle properties become available, then the clustered drag model proposed by Eq. 7.17 may be revisited for better predictions in CFD applications.

### 7.8 Conclusion

In this work, we used PR-DNS to quantify the mean gas-particle drag in gas-solid suspensions where the particle configurations contain particle clusters. These simulations are performed in homogeneous flow setup in order to isolate the effect interphase interaction on particle clusters. In our PR-DNS, we used clustered configurations that approximately matched the statistics of experiments, while earlier works used deterministic approaches to generate particle configurations for PR-DNS. We extracted the clustered particle configurations from DEM simulation of a HCG with inelastic and cohesive particles in the absence of interstitial fluid. The selected cluster-containing sub-ensembles were selected to match the cluster distribution provided by the experiment (Cocco et al., 2010). PR-DNS of flow over these sub-ensembles indicates that existence of particle clusters lead to drag reduction compared with configurations that contain uniformly distributed particles at the same flow condition. Our PR-DNS results indicate that the maximum drag reduction appears at Stokes flow. The attenuation of drag reduction with Reynolds number is associated with reduction of the Brinkman screening length. Therefore, an increase in the mean slip Reynolds number reduces the spatial extent of the flow disturbance caused by particles. This makes the flow see particles as individual entities rather than a cluster, which leads to attenuation of drag reduction. Our results also indicate that the drag reduction attenuates with increase of solid phase volume fraction. In order to understand the reason for this attenuation, we introduced a cluster metric to measure configurational entropy for a particle assembly. Our analysis indicates that the changes in configurational entropy of particles in dilute regimes is higher compared with dense suspensions. Therefore, particle configurations in the dilute regimes change significantly when particles form clusters as compared to dense suspensions. Clustering in turn leads to higher drag reduction for dilute regimes.
We have used our PR-DNS data to propose a drag law for clustered configurations for the range of flow parameters considered in this study, that is $0.1 \leq \langle \phi \rangle \leq 0.35$ and $0.01 \leq Re_m \leq 50$. This drag model has been proposed based on the amount of drag reduction when compared with the uniform drag model of Tenneti et al. (2011). We have also provided a smooth transition between the uniform and clustered drag models for stability of CFD simulations by means of using a weighting function. This function has two adjusting parameters that can be determined by comparing CFD predictions with experimental results of for instance solid-phase volume fraction profile or pressure drop along a fluidized bed riser. The tuned model then can be used for CFD simulations of complex geometries and engineering applications.

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CHAPTER 8. IMPORTANCE OF MICROSCALE HYDRODYNAMICS IN INSTABILITY ANALYSIS OF GAS-SOLID FLOW

8.1 Introduction

Both experiments (Cocco et al., 2010; McMillan et al., 2013) and simulations (Agrawal et al., 2001; Capecelatro et al., 2014a; Yin et al., 2013) report instabilities in gas-solid flow. Understanding the underlying mechanisms that give rise to instabilities in gas-solid flow is essential to building a predictive model for gas-solid flow. In the study of gas-solid flow instabilities, it has become evident that instabilities in velocity and density fields can arise from a number of distinct candidate mechanisms, for instance: (i) instabilities that could arise in homogeneous gas-solid flow (Koch, 1990; Glasser et al., 1998; Agrawal et al., 2001), (ii) coupled Kelvin-Helmholtz and Rayleigh-Taylor instabilities that arise in particle-laden shear layers (Narayanan et al., 2002; Lakehal and Narayanan, 2003), and (iii) instabilities triggered due to the presence of walls (Capecelatro et al., 2014b). Numerical simulation is a suitable approach to study these mechanisms since we can easily isolate the effect of each of these mechanisms on flow instability. Due to the multiscale nature of phenomena in gas-solid flows, a physics-based numerical simulation capturing the entire range of interactions is needed. PR-DNS is shown to be the most appropriate numerical approach for physics discovery in gas-solid flow (Tenneti and Subramaniam, 2014) because in this model-free method flow dynamics are not affected by numerical and modeling errors. In PR-DNS of gas-solid flows, the fluid-phase velocity and pressure fields are well resolved by using a fine grid across each particle. As a result, the interaction of the fluid phase and solid particles through interphase transfer of momentum and energy can be accurately quantified. Most PR-DNS studies are limited to homogeneous gas-solid flows in small domain sizes ($L/d_p \approx 300$) (Uhlmann and Doychev, 2014).
LES/CFD simulations of particle-laden flows are useful in simulating bigger computational domains. In LES/CFD simulations, the conservation equations are filtered/averaged in order to leverage the use of coarser grid compared to PR-DNS. This allows one to perform simulations that include larger mesoscopic/macroscopic gas-solid interactions extending to several particle diameters/geometric scales (Capecelatro et al., 2014a; Agrawal et al., 2001). In LES/CFD simulations of particle-laden flows, the grid resolution is not fine enough to capture microscopic gas-solid interactions, such as momentum and energy transfers at gas-solid interface, that occur at the scale of a single particle. These microscopic interactions are referred to as sub-grid scale interactions and their effect should be incorporated into the filtered/averaged equations. Since it is likely that mesoscopic/macroscopic flow structures such as instabilities in fluid-phase structures as well as the resulting particle spatial distribution originate from interactions at the sub-grid scale, it is important to examine their role in cluster formation. Several drag models have been proposed to represent the steady transfer of momentum between the fluid phase and the solid phase. These models are based on experimental data (Wen and Yu, 1966; Ergun, 1952) or on computational studies (Hill et al., 2001a,b; van der Hoef et al., 2005; Beetstra et al., 2007; Tenneti et al., 2011). Use of these steady drag models in LES/CFD simulations, not only affects the momentum transfer between the gas phase and solid particles at microscale, but they also directly influence the evolution of kinetic energy in particle velocity fluctuations. The level of particle velocity fluctuations is one of the key mechanisms in attenuation or enhancement of instabilities in homogeneous gas-solid flows. Therefore, in this chapter we examine the implication of using a steady drag model on the evolution of particle velocity fluctuations in LES/CFD applications.

8.2 Evolution equation of kinetic energy in solid-phase velocity fluctuations

The evolution equation of kinetic energy in solid-phase fluctuating velocities $k^{(p)}$ for a homogeneous gas-solid suspension with elastic particles is given by

$$\frac{d k^{(p)}}{dt} = \Pi^{(p)} = \langle \mathbf{A}'' \cdot \mathbf{v}'' \rangle,$$

(8.1)
Figure 8.1: The scatter plot of $A'' - v''$ for the case $\phi = 0.1$, $Re_m = 20$ and $\rho^{(p)}/\rho^{(f)} = 100$ at steady state obtained from PR-DNS. Only the component along the mean slip velocity is plotted. Each axis is normalized by the corresponding standard deviation.

where $\Pi^{(p)}$ is the interphase TKE transfer of the solid phase that represents the covariance of particle fluctuating acceleration $A''$ and fluctuating velocity $v''$. Tenneti et al. (2010) showed that the source and the sink associated with the rate of change of $k^{(p)}$ are both included in the particle fluctuating acceleration-fluctuating velocity covariance on the right-hand-side of Eq. 8.1, i.e. $\langle A'' \cdot v'' \rangle = \langle A'' \cdot v'' \rangle^+ + \langle A'' \cdot v'' \rangle^-$ that can be quantified using a quadrant analysis of acceleration-velocity scatter plot. Figure 8.1 shows such a scatter plot obtained from PR-DNS of a homogeneous gas-solid flows with $\phi = 0.1$, mean slip Reynolds number $Re_m = 20$, solid to fluid density ratio $\rho^{(p)}/\rho^{(f)} = 100$, and particle coefficient of restitution $\varepsilon = 1.0$ at steady state. This scatter plot shows that the points in quadrants 1 and 3 contribute to the source in the rate of change of $k^{(p)}$, while those in quadrants 2 and 4 contribute to the sink. This is because the product of $A''$ and $v''$ is positive in the former case, while it is negative in the latter case. In addition, all scatter points are relatively uniformly distributed in all four quadrants in Fig. 8.1 indicating that $A''$ and $v''$ are uncorrelated and thus the system is at steady state.
Any deviation from accurately predicting particle acceleration leads to inaccuracy in predicting the source and the sink in Eq. 8.1 that affects the evolution of particle kinetic energy. In LES/RANS simulations of gas-solid flows, the particle acceleration is modeled using a steady drag law that is a function of local volume fraction and mean Reynolds number based on the local slip velocity. It is of interest to carefully analyze the implication of such modeling on the source and the sink corresponding to the rate of change of $k^{(b)}$.

### 8.3 Implication of using a drag model on particle velocity fluctuations

Although use of drag models ensures that the conservation of mean momentum between the fluid phase and the solid phase is satisfied, the kinetic energy in velocity fluctuations between the two phases is not conserved. This inconsistency arises due to the fact that drag models depend on the slip velocity between the fluid phase and the solid phase, i.e. $v - \langle u^{(f)} \rangle$. The fluid-phase mean velocity is interpolated from the Eulerian grid points that surround a solid particle at the particle location. This interpolated velocity is not the same as the instantaneous velocity of the particle. This is unlike the PR-DNS approach that guarantees the fluid phase and the solid particle share a mutual velocity at fluid-solid interface due to the kinematic boundary condition. The artifact of using a steady drag law is that the interphase TKE transfer between the fluid phase and the solid phase is not conservative (Sundaram and Collins, 1999), while Xu and Subramaniam (2007) showed that the conservation of interphase TKE transfer principle is a physical constraint for modeling of gas-solid flows. The deviation from the conservation of interphase TKE transfer in modeling approaches that use a drag model is ascribed to an additional viscous dissipation arising from the flow interacting with particle surfaces (cf. Chapter 4).

The use of a drag law in modeling particle acceleration also influences the evolution of particle kinetic energy $k^{(b)}$, since the particle fluctuating acceleration-fluctuating velocity covariance contributes to the rate of change of $k^{(b)}$. To analyze this influence, we use the aforementioned PR-DNS case at steady state and replace the true particle acceleration by an acceleration model recently proposed by Tenneti et al. (2011) that is derived from PR-DNS of gas-solid flow over a wide range of mean slip Reynolds number ($0.01 \leq Re_m \leq 300$) and solid-phase volume fraction...
We first construct a measurement volume around each particle with a given box length \( l_m \) that is larger than the particle diameter. The solid-phase volume fraction contained in this measurement volume is

\[
\phi_m = \frac{1}{V_m} \int_{V_m} I^{(p)} d\mathbf{v},
\]

where \( I^{(p)} \) is the solid-phase indicator function, and \( V_m \) is the total volume occupied by the region \( V_m \). The volume-averaged fluid velocity in this region is defined as

\[
\langle \mathbf{u}^{(f)} \rangle_m = \frac{1}{V_m^{(f)}} \int_{V_m} I^{(f)} \mathbf{u}^{(f)} d\mathbf{v},
\]

where \( I^{(f)} \) is the fluid-phase indicator function, and \( V_m^{(f)} \) is the volume occupied by the fluid phase in region \( V_m \). Knowing the volume-averaged fluid-phase velocity in the proximity of a particle, we can now define the particle slip velocity as

\[
\langle \mathbf{W} \rangle_m^{(p)} = \mathbf{v} - \langle \mathbf{u}^{(f)} \rangle_m
\]

that corresponds to the slip Reynolds number given by

\[
Re_m^{(p)} = \frac{(1 - \phi_m) \left| \langle \mathbf{W} \rangle_m^{(p)} \right|}{\nu^{(f)}},
\]

with \( \nu^{(f)} \) being the fluid-phase kinematic viscosity. Calculating the local solid-phase volume fraction and slip Reynolds number that correspond to each particle in this manner allows us to use the steady drag model proposed by Tenneti et al. (2011) for particle acceleration. We use this steady drag model to replace the true hydrodynamic force obtained from integration of stress tensor at each particle surface and apply it to the PR-DNS result of the gas-solid flow for the case \( \phi = 0.1 \), \( Re_m = 20 \) and \( \rho^{(p)}/\rho^{(f)} = 100 \) at steady state. The corresponding \( A'' - v'' \) scatter plot in Fig. 8.2 indicates that the replacement of the true particle acceleration with a model leads to an imbalance in the distribution of scatter points in the scatter plot, and the redistribution of the scatter points contributes more to the sink term when compared to the PR-DNS result at steady state in Fig. 8.1. This implies that the use of a particle acceleration model for a PR-DNS solution at steady state leads to a new steady value of \( k^{(p)} \) that is different from that of the PR-DNS. Figure 8.2 also illustrates the same scatter plot for different sizes of the measurement volume. As the measurement volume size increases, the estimated particle acceleration deviates from the true acceleration predicted by PR-DNS, and the scatter points redistribute increasingly towards the sink quadrants 2 and 4. This increase in the sink term
leads to an enhancement of the sink term in the particle kinetic energy evolution equation. Therefore, it is expected that the modeled $k^{(p)}$ at steady state will be smaller than the one obtained from PR-DNS.

In order to examine the implication of using a drag model for particle acceleration on the evolution of $k^{(p)}$, we continue the simulation obtained from the aforementioned PR-DNS with the true particle acceleration replaced by the model proposed by Tenneti et al. (2011) using the procedure explained above with a measurement volume size $l_m = 6dp$. Figure 8.3 shows the evolution of the particle kinetic energy normalized by the kinetic energy in the mean flow $E^{(f)} = \langle \mathbf{W} \rangle \cdot \langle \mathbf{W} \rangle / 2$ for the entire course of simulation (including the PR-DNS phase as well as the phase with the particle acceleration model). The vertical line in Fig. 8.3 at $t \mid \langle \mathbf{W} \rangle \mid / dp = 147$
Figure 8.3: The evolution of $k^{(p)}$ for the case $\phi = 0.1$, $Re_m = 20$ and $\rho^{(p)}/\rho^{(f)} = 100$ with PR-DNS approach (left side of the vertical line) and particle drag model (right side of the vertical line).

indicates the time at which the acceleration model is turned on. This shows that as the particle drag model is activated, $k^{(p)}$ drops significantly with a high slope until it reduces about 75% of its original value and is the new steady value. This reduction in $k^{(p)}$ is associated with the enhanced sink term.

Figure 8.4 shows the evolution of the source and sink that correspond to the rate of change of $k^{(p)}$ after the particle drag model is activated. This plot confirms that at the onset of using the particle acceleration model, the sink term is significantly larger than the source, and thus $k^{(p)}$ reduces at early stages of the simulation using the particle acceleration model. The source term, which is negligible at the beginning, increases until it balances the sink at the new steady state. This process leads to a lower level of particle velocity fluctuations when using a particle acceleration model as compared to the PR-DNS approach.

### 8.4 Summary

We performed PR-DNS of freely evolving suspensions and extracted the kinetic energy associated with particle velocity fluctuations. We demonstrated the influence of the particle acceleration model on the kinetic energy associated with particle velocity fluctuations by comparing the PR-DNS data with that obtained from identical simulations performed with an
assumed steady drag law. The use of a steady drag model for particle acceleration in LES/CFD applications of gas-solid flow affects the level of particle velocity fluctuations and results in significant reduction of $k^{(p)}$ compared to PR-DNS. In large-scale simulation of gas-solid flows, regions with low value of $k^{(p)}$ and high particle number density are associated with particle clusters that represent instabilities in gas-solid flows. The use of a steady drag model for particle acceleration may artificially enhance the formation low $k^{(p)}$ regions, which in turn enhances formation of particle clusters that dynamically exchange momentum and energy with the fluid phase. Therefore, the instabilities reported in big scale calculations of gas-solid flows using LEA (Capecelatro et al., 2014a) or RANS approaches (Agrawal et al., 2001) could be strongly dependent on the particle acceleration model. The dependence of $k^{(p)}$ on the particle acceleration model strongly suggests that large scale PR-DNS of gas-solid simulations are needed in order to rigorously identify the mechanisms associated with generation of instabilities in such flows.
CHAPTER 9. PARTICLE-LADEN MIXING LAYER

9.1 Introduction

There is experimental evidence showing that once particle clusters form, these particle structures become unstable due to their interactions with the flow hydrodynamics and finally break up. These instabilities generally happen at the edge of a particle cluster where it is exposed to the flow in the voidage that surrounds the cluster. The presence of a particle cluster in a voidage in conjunction with the difference in the gas-phase velocity between these two adjacent regions gives rise to formation of a local particle-laden mixing layer. The particle-laden mixing layer is also analogous to the near air jet regions at the bottom of a fluidized bed (Halvorsen and Mathiesen, 2002). This particle laden mixing layer enhances growth of instability in the cluster which finally leads to breakup the cluster.

Particle-laden mixing layers have been numerically studied using point-particle Lagrangian-Eulerian simulations with both one-way coupled (Narayanan and Lakehal, 2006a) and two-way coupled (Narayanan and Lakehal, 2006b) interactions. These studies have generally focused on small particle diameters (compared to Kolmogorov length scale), low particle Stokes number and very dilute suspensions. However, the regime of our interest corresponds to much larger particles, high particle Stokes numbers and moderate to dense suspensions. In this regime PR-DNS is the most appropriate methodology to study the particle-laden mixing layer.

9.2 PR-DNS of particle-laden mixing layer

In order to understand the growth of perturbations in the average particle number density, we initialize a particle-laden mixing layer in which the particle number density profile has the form of a step function as shown in Fig. 9.1(b). The particle configuration corresponding to
this number density profile is shown in Fig. 9.1(a) with a solid-phase volume fraction $\phi = 0.2$ uniformly distribution in the dense region. The dense region amounts to a quarter of the computational box, while the rest of the domain is free of particles. The computational box size is selected as $L/d_p = 50$ based on available computational resources and it includes about 12,000 particles. This particle configuration provides high number density gradients as well as drag force gradients at the edges of the step function. It is useful to study the evolution of particle-voidage interface due to density and velocity differences in the particle and fluid phases.

This particle configuration explained above is used for PR-DNS of freely evolving gas-solid suspension. In this simulation, both phases are initially at rest. The configuration is then exposed to a gravitational acceleration along the $x$-axis. The flow is characterized by the Archimedes number $Ar = 800$ that represents the ratio of buoyancy to viscous forces. This configuration setup implies that the flow is homogeneous in $xz$-plane, while it is inhomogeneous along $y$-axis. As the simulation evolves, both particle velocity and the fluid-phase velocity as well as the particles granular temperature gradually increase. This gives rise to entrainment of particles into the voidage and thus the particle number density profile also evolves in time. Fig. 9.2 shows particle number density and particle velocity profiles at different time instants. The simulation continues until particles moving into the void region from both fronts meet.
The evolution of particle number density profile in Fig. 9.2(a) and mean particle velocity profile in Fig. 9.2(b) suggests the existence of similarity solutions for these quantities. By analogy with the single-phase free shear mixing layer (Pope, 2000), we can define the variables \( n_h \) and \( n_l \) that correspond to the 90% and 10% of the maximum particle number density. We also define the mean value of the particle number density as \( n_c = (n_h + n_l)/2 \) and difference between the maximum and minimum number densities as \( n_s = n_h - n_l \). The locations associated with \( n_h \) and \( n_l \) are defined as \( y_h \) and \( y_l \). Similarly, the mean of and the distance between these two locations are defined by \( \bar{y}(t) = (y_h + y_l)/2 \) and \( \delta(t) = n_h - n_l \), respectively. Using these variables, we can define a self-similar variable as

\[
\eta = \frac{y - \bar{y}(t)}{\delta(t)},
\]  

(9.1)

and the self-similar number density profile as

\[
f(\eta) = \frac{n(y, t) - n_c}{n_s}.
\]

(9.2)

Similarly, the self-similar particles mean velocity profile can be defined as

\[
g(\eta) = \frac{\langle V^{(p)} \rangle_x(y, t) - \langle V^{(p)} \rangle_{x,c}}{\langle V^{(p)} \rangle_{x,c}}.
\]

(9.3)

It is evident in Figs. 9.3(a) and 9.3(b) that these profiles are self-similar since they all collapse on a single curve.
It is of interest to observe the development of the mixing length $\delta(t)$ in time as shown in Fig. 9.4 in red color, and determine the mechanism responsible for this development. By assuming that the mixing phenomenon is diffusive, the mixing length scales as $\delta \sim \sqrt{D t}$ with $D$ being the diffusion coefficient. The diffusion coefficient should scale as $D \sim d_p \sqrt{T}$ where $T$ is particle granular temperature. By combining these expressions together, the final scaling expression is obtained as

$$\frac{\delta}{d_p} \sim \sqrt{\frac{t}{d_p \sqrt{T}}}.$$  \hfill (9.4)
When this expression is compared with the mixing length development, they are qualitatively in good agreement indicating that the diffusive mechanism assumption in particle-laden mixing layer is valid.

9.4 Summary

In this study, the particle-laden mixing layer is analyzed by PR-DNS for the first time, to the best of our knowledge. The simulation indicates that particle distribution function initialized with a step function evolves to a monotonic profile as particles are entrained into the voidage. It is shown that the particle number density and particle mean velocity profiles are self-similar, provided that appropriate quantities are used for self-similar variables and profiles. In addition, the mechanism of the mixing phenomenon is observed to be diffusive that is characterized by particle granular temperature.
CHAPTER 10. FUTURE WORK

In this chapter, possible future directions associated with the main objectives of this research are mentioned. Some of these future tasks are currently supported by preliminary results, and are required to be pursued for comprehensive conclusions.

10.1 PUReIBM code development for mesoscale PR-DNS

Two-fluid CFD calculations (Agrawal et al., 2001) and LES (Capecelatro et al., 2014a) of gas-solid flows indicate that in order to observe instabilities and clusters in numerical simulations of homogeneous gas-solid flows, a mesoscopic length must be captured. This length scale required for formation of mesoscale clusters in a computational domain is given as $L = \tau_p^2 g$ (Agrawal et al., 2001; Capecelatro et al., 2014a; Ozel et al., 2013; Igci et al., 2008), where $\tau_p$ is the particle response time, and $g$ is the magnitude of gravitational acceleration. Contour levels in Fig. 10.1 determine the ratio of the length scale $L$ to particle diameter in the Geldart classification map. For a gas-solid system with Geldart B particles, this length scale lies in a range from 700-2000 particle diameters. PR-DNS of a gas-solid suspension with an appropriate computational domain size that resolves such a length scale requires huge computational resources ($3 \times 10^{12}$ to $6 \times 10^{13}$ grid points with $7 \times 10^6$ to $1.5 \times 10^8$ particles for $\phi = 0.01$). These resources are currently feasible only through petascale/exascale computational resources provided by, for instance, the Blue Waters computer cluster. This large computational problem also requires a massively scalable and efficient PR-DNS code to handle such a simulation. A PR-DNS code that is suitable for simulating freely evolving suspensions has two main modules: 1) the hydrodynamic solver for the hydrodynamic field, 2) the discrete element method (DEM) solver for tracking individual particles. In Chapter 2, the parallelization of the hydrodynamic solver
Figure 10.1: Geldart classification map of gas-solid suspensions. Contour levels represent the ratio of the mesoscale length $L = \tau^2 g$ to particle diameter $d_p$. The hollow circle identifies the problem of our interest in this study.

and its scalability was addressed. However, the DEM solver that is responsible for handling the particle motions and particle-particle collisions should also be scalable.

In mesoscale PR-DNS of gas-solid flow, the number of solid particles is of the order of $O(10^6)$. To have a better estimate of the number of particles in such a suspension, we can use the following expression

$$N_p = \frac{6\phi}{\pi} \left( \frac{L}{d_p} \right)^3$$

that relates the number of particles to the solid-phase volume fraction and the particle diameter to box length ratio. For a gas-solid flow with solid-phase volume fraction of $\phi = 0.01$ and box length of $L/d_p = 700–2000$, the total number of particles in the system is 7,000,000 to 150,000,000. The current DEM solver of our PR-DNS is able to efficiently handle only thousands of particles. Our tests indicate that the DEM solver is not scalable and needs to be significantly improved.

A better route to improving our DEM solver is replacing it with a well-developed code that is widely used in academia and industry for simulating interaction of millions of particles. One of the most appropriate packages for this purpose is LAMMPS that is distributed by Sandia National Labs. LAMMPS is a classical molecular dynamics simulation code that models atomic, polymeric, biological, metallic, granular, and coarse-grained systems using a variety of force fields and boundary conditions. This package can easily handle systems with few particles up to
millions or billions of particles. To handle the computational load of large systems on parallel machines, LAMMPS uses a domain decomposition technique to partition the computational domain. The current DEM solver in our PR-DNS code can be replaced with the LAMMPS package, and to check its performance and accuracy through a set of tests. After testing the new coupled hydrodynamic-DEM code, it will then be ready for mesoscale PR-DNS of gas-solid flow for analyzing the effect of microscale interactions on mesoscale structures.

### 10.2 Particle-laden turbulent flow modulation

In Chapter 4 the modulation of isotropic turbulence with the presence of low Stokes number solid particles initialized with zero velocity was presented. This modulation was analyzed from both PR-DNS and PP-DNS approaches in a regime that is feasible by PR-DNS, and that is also in the range of validity for PP-DNS. The comparison between the two data sets indicated that for low Stokes number particles, in the interval wherein the particles have not equilibrated with the local fluid, there is a significant difference in flow quantities such as the solid-phase kinetic energy $k^{(p)}$ and the viscous dissipation $\varepsilon^{(f)}$ between the two approaches. Once a local equilibrium is reached, both calculations yield almost the same results for flow quantities for $k^{(p)}$ and $\varepsilon^{(f)}$. The mismatch between the two approaches at early times is associated with the inaccuracy of the PP-DNS Stokes drag model in predicting particle acceleration in conditions where particles experience a significant change in momentum.

The results from these simulations suggest that if particles are initialized with the local fluid-phase velocity, the effect of these low Stokes number particles on the turbulence will be negligible. In addition, the PP-DNS data might quantitatively and qualitatively match those of PR-DNS. To check these assumptions, we repeat our simulations presented in Chapter 4 with particles initialized with the local fluid velocity.

Furthermore, it is also expected that a significant difference between the PR-DNS and PP-DNS results might arise over the entire duration of the simulation when the particle Stokes number is high. In this scenario, the particle response time is much larger than the flow time scale, and thus particles respond to the interphase transfer of momentum at a rate that is much slower than the relaxation time of the surrounding fluid. Therefore, it is expected that
the Stokes drag model may not accurately represent particle acceleration for high Stokes number particles. Thus, there would be a significant difference between the results from PP-DNS and PP-DNS of particle-laden isotropic turbulence. To check this assumption, one could repeat the simulations with a higher particle Stokes number.

10.3 Dynamic interaction of particle clusters with flow hydrodynamics

In Chapter 7 we used fixed clustered particle configurations to perform Type III PR-DNS. The results were used to propose a drag model for clustered particle configurations in gas-solid flow. Although these results are useful, the dynamic fluid-particle interactions that lead to formation and breakup of particle clusters are missing. Also the reorientation of clusters due to interaction with the carrier flow as well as cluster-cluster interactions are not present in static particle clusters. One possible future route to better understand the physics underlying cluster dynamics is to perform Type I and II PR-DNS of gas-solid flow with cohesive particles. The use of cohesive particles, which is reconcilable with Geldart A particles interacting with a carrier flow, enhances formation of particle clusters. Since the particle clusters generated in these simulations have originated from the first-principles dynamics, the results are better candidates for physics discovery and model development.

10.4 Importance of microscale hydrodynamics in instability analysis of gas-solid flow

In Chapter 8, we presented the effect of LES filtering of flow hydrodynamics. It was shown that the use of gas-particle drag models to represent particle acceleration in DEM-LES/CFD analysis of gas-solid flows may lead to a different particle granular temperature when compared with PR-DNS. Since the granular temperature plays a key role in formation of particle clusters, it is concluded that the clusters observed in DEM-LES/CFD simulations may not be comparable with those observed in PR-DNS of suspensions at the same flow conditions.

To further pursue this analysis, one could choose flow parameters as those reported by Capecelatro et al. (2014a) since they used LES method to show formation of mesoscale particle
structures in a homogeneous gas-solid flow with a finite mean slip velocity. In addition, for consistency in terms of the gas-particle drag model, it is needed to replace the drag model of Tenneti et al. (2011) used in our analysis with the Stokes drag which is used by Capecelatro et al. (2014a) for gas-particle drag model.

10.5 Particle-laden mixing layer

The particle-laden mixing phenomenon presented in Chapter 9 is expected to be coupled with the hydrodynamic instabilities in the gas-phase as well. Further analysis is required to shed light on the coupling between the instabilities in the fluid phase and the diffusion of particles in a particle-laden mixing layer. Once this analysis becomes available, it would complement the materials presented in Chapter 9.
APPENDIX A. SIMPLIFICATION OF THE COVARIANCE OF FLUCTUATING VELOCITY AND GRADIENT OF STRESS TENSOR TO DISSIPATION IN STATISTICALLY HOMOGENEOUS GAS-SOLID FLOW

The conservation equation for $k^{(f)}$ in statistically homogeneous flows is written as

$$
\rho^{(f)}(1-\phi) \frac{\partial k^{(f)}}{\partial t} = - \left\langle u_i^{\prime\prime(f)} \tau_{ji} n_j^{(p)} \delta(x - x^{(I)}) \right\rangle + \left\langle u_i^{\prime\prime(f)} \frac{\partial (I^{(f)} \tau_{ji})}{\partial x_j} \right\rangle \tag{A.1}
$$

In this equation $\tau_{ji}$ is the fluid phase stress tensor given by

$$
\tau_{ji} = -p\delta_{ji} + \mu^{(f)} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)
$$

where $p$ and $u$ are the instantaneous pressure and velocity fields respectively. The second term on the right-hand side is the covariance of the fluctuating fluid velocity field and the gradient of the stress tensor in the fluid phase. Using the product rule this term can be written as

$$
\left\langle u_i^{\prime\prime(f)} \frac{\partial (I^{(f)} \tau_{ji})}{\partial x_j} \right\rangle = \left\langle \frac{\partial}{\partial x_j} \left( u_i^{\prime\prime(f)} I^{(f)} \tau_{ji} \right) \right\rangle - \left\langle I^{(f)} \tau_{ji} \frac{\partial u_i^{\prime\prime(f)}}{\partial x_j} \right\rangle \tag{A.2}
$$

Commuting the gradient and averaging operators and invoking the assumption of statistical homogeneity, the first term on the right hand side of the above equation simplifies to zero. The second term on the right-hand side can be further simplified by considering the definition of the stress tensor:

$$
\tau_{ji} \frac{\partial u_i^{\prime\prime(f)}}{\partial x_j} = \left( -p\delta_{ji} + \mu^{(f)} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right) \frac{\partial u_i^{\prime\prime(f)}}{\partial x_j} \tag{A.3}
$$

Since the fluctuating velocity field is divergence free, the pressure term is zero. So the above equation reduces to:

$$
\tau_{ji} \frac{\partial u_i^{\prime\prime(f)}}{\partial x_j} = \mu^{(f)} \left( \frac{\partial u_i^{\prime\prime(f)}}{\partial x_j} \frac{\partial u_i^{\prime\prime(f)}}{\partial x_j} + \frac{\partial^2}{\partial x_i \partial x_j} \left( u_i^{\prime\prime(f)} u_j^{\prime\prime(f)} \right) \right) = 2\mu^{(f)} s_{ij} s_{ij}, \tag{A.4}
$$
where $s_{ij} = \left( \frac{\partial u_i^{n(f)}}{\partial x_j} + \frac{\partial u_j^{n(f)}}{\partial x_i} \right)/2$. Therefore, the second term on the right-hand side of Eqs. (A.1) and (3.34) simplifies to

$$
\left\langle u_i^{n(f)} \frac{\partial (f^{(f)} \tau_{ji})}{\partial x_j} \right\rangle = -2\mu^{(f)} \left\langle f^{(f)} s_{ij} s_{ij} \right\rangle.
$$

(A.5)

which is strictly negative and can be identified as the dissipation rate of $k^{(f)}$ in statistically homogeneous gas-solid flow.
APPENDIX B. STATISTICAL REPRESENTATION OF MEAN MOMENTUM EQUATION FOR GAS-SOLID FLOW

Statistical models of multiphase flow are widely used to describe averaged conservation equations of mass, momentum, and energy of carrier and dispersed phases due to the statistical variability in multiphase flows. The two principal statistical approaches are: (i) The random field approach in which both carrier and dispersed phases are represented as random fields in the Eulerian frame, (ii) The point process approach in which the dispersed phase is represented as a stochastic point process in the Lagrangian frame while the carrier phase is represented as a random field in the Eulerian frame. In this section, the first approach is briefly reviewed because it is widely used in CFD of industrial applications.

In the Eulerian-Eulerian (EE) two-fluid theory approach, it is assumed that the conservation equations of mass, momentum and energy are valid for the entire system. The fluid-phase and the dispersed-phase cannot coexist at the same space location in a given time. Thus, an indicator field $I^{(\beta)}(x,t)$ is used to represent the existence of phase $\beta$ at $(x,t)$, that is (Drew and Passman, 1998)

$$I^{(\beta)}(x,t) = \begin{cases} 
1 & \text{if } x \text{ is in phase } \beta \\
0 & \text{if } x \text{ is not in phase } \beta,
\end{cases}$$

(B.1)

Multiplying the conservation equations with the indicator field $I^{(\beta)}$ and using the corresponding topological equation (Drew and Passman, 1998) followed by the density-weighted phasic averaging yields the EE representation of the fluid phase and the solid phase. The fluid-phase conservation equations of mass and momentum in an isothermal non-reacting flow are given by

$$\frac{\partial}{\partial t} \left( \rho^{(f)} \phi^{(f)} \right) + \nabla \cdot \left( \rho^{(f)} \phi^{(f)} \langle u^{(f)} \rangle \right) = 0,$$

(B.2)
\[
\frac{\partial}{\partial t} \left( \rho^{(f)} \phi^{(f)} \left\langle u^{(f)} \right\rangle \right) + \nabla \cdot \left( \rho^{(f)} \phi^{(f)} \left\langle u^{(f)} \right\rangle \left\langle u^{(f)} \right\rangle \right) = \phi^{(f)} \langle g \rangle - \nabla \cdot \left( \rho^{(f)} \left\langle f^{(f)} u^{(f)} u^{(f)} \right\rangle \right) + \nabla \cdot \left\langle f^{(f)} \tau \right\rangle - \sum_{\alpha=1}^{N_c} \left\langle \tau \cdot n^{(a)} \delta(x - x^{(I)}_{\alpha}) \right\rangle,
\]
(B.3)

where \( \phi^{(f)} = \langle I^{(f)} \rangle \) is the mean fluid volume fraction, \( \left\langle u^{(f)} \right\rangle \) is the mean fluid velocity, \( u^{(f)} = u^{(f)} - \left\langle u^{(f)} \right\rangle \) is the fluid-phase velocity fluctuation, \( \langle g \rangle \) is any body force, \( \tau \) is the stress tensor, \( n^{(a)} \) is the normal vector pointing outward from particle surface belonging to \( \alpha \)th class into the fluid phase, and \( \delta(x - x^{(I)}_{\alpha}) \) is a generalized delta function at the fluid-particle interface \( x^{(I)}_{\alpha} \), and \( N_c \) is the number of particle classes. The last term represents the mean momentum transfer between the fluid-phase and the particle class \( \alpha \), known as gas-particle drag.

The corresponding conservation equations of mass and momentum for the particle class \( \alpha \) are respectively:

\[
\frac{\partial}{\partial t} \left( \rho^{(a)} \phi^{(a)} \left\langle u^{(a)} \right\rangle \right) + \nabla \cdot \left( \rho^{(a)} \phi^{(a)} \left\langle u^{(a)} \right\rangle \left\langle u^{(a)} \right\rangle \right) = 0,
\]
(B.4)

\[
\frac{\partial}{\partial t} \left( \rho^{(a)} \phi^{(a)} \left\langle u^{(a)} \right\rangle \right) + \nabla \cdot \left( \rho^{(a)} \phi^{(a)} \left\langle u^{(a)} \right\rangle \left\langle u^{(a)} \right\rangle \right) = \phi^{(a)} \langle g \rangle - \nabla \cdot \left( \rho^{(a)} \left\langle f^{(a)} u^{(a)} u^{(a)} \right\rangle \right) + \nabla \cdot \left\langle \tau^{(a)} \right\rangle + \left\langle \tau \cdot n^{(a)} \delta(x - x^{(I)}_{\alpha}) \right\rangle + \sum_{\beta=1}^{N_c} \left\langle f^{(\beta \rightarrow \alpha)}_{\text{coll}} \right\rangle,
\]
(B.5)

where the last term in the Eq. B.5 is the mean momentum transfer, known as particle-particle drag, due to collisions with particle from other classes.
APPENDIX C. FORMULATION OF PUReIBM FOR A HOMOGENEOUS BIDISPERSE GAS-SOLID SUSPENSION

The IB force is non-zero only inside the particle to generate a fictitious flow. This fictitious flow imposes the no-slip and no-penetration boundary conditions at the particle surface which is represented by discrete points in spherical coordinates. The computation of IB forcing at the \((n+1)^{th}\) time-step is specified as (Tenneti et al., 2010; Mehrabadi et al., 2015)

\[
f^{n+1} = \rho^{(f)} \frac{u^d - u^n}{\Delta t} + \rho^{(f)} S^n + g^{n}_{\text{IBM}} - \mu^{(f)} \nabla^2 u^n + \rho^{(f)} A_f. \tag{C.1}
\]

where \(u^d\) is the desired velocity at a computational grid point inside the particle that is used to impose the appropriate boundary condition.

In PUReIBM any instantaneous field \(Q(x, t)\) is decomposed into a mean and a fluctuating part as \(\langle Q \rangle_V(t) + Q'(x, t)\), where the operator \(\langle \cdot \rangle\) represent the ensemble averaging. In a homogeneous suspension, the mean quantity is independent of the spacial coordinate. Additionally, it is legitimate to replace the ensemble averaging with volume averaging (Tenneti et al., 2010, 2011; Mehrabadi et al., 2015) given by

\[
\langle Q \rangle_V(t) = \frac{1}{V} \int_V Q(x, t) dv, \tag{C.2}
\]

where \(V\) is the volume of the region \(V\). Applying the above volume averaging on the conservation equations of mass (Eq. 5.8) and momentum (Eq. 5.9) gives us the volume-averaged mass and momentum conservation equations. Because the volumetric means are independent of spatial location, the conservation equation of the mean mass is trivially satisfied. The mean momentum conservation equations is then obtained as

\[
\rho^{(f)} \frac{d \langle u \rangle_V}{dt} = -\langle g_{\text{IBM}} \rangle_V + \langle f \rangle_V - \rho^{(f)} A_f. \tag{C.3}
\]
The mean IB forcing term $\langle f \rangle$ is computed by volume-averaging the IB force specified in Eq. C.1 over the region $V$.

The phasic averaged momentum equation of the fluid phase is obtained by multiplying the Eq. 5.9 with the fluid-phase indicator function $I^{(f)}(x, t)$ followed by averaging over the fluid region $V^{(f)}$. The fluid-phase mean momentum equation then reads as

$$
\frac{d}{dt} \langle u^{(f)} \rangle = -\frac{1}{\rho^{(f)}} \langle g_{\text{IBM}} \rangle_V - \frac{1}{\rho^{(f)}} \sum_{\alpha=1}^{N_c} \langle s^{(\alpha)}_M \rangle - A_f,
$$

where

$$
\langle s^{(\alpha)}_h \rangle = \frac{1}{V} \sum_{i=1}^{N_\alpha} \int_{\partial V^{(p)}} (-\psi I + \mu^{(f)} \nabla u) \cdot n^{(\alpha,i)} dA,
$$

represents the sum of hydrodynamic forces acting on all particles in size class $\alpha$. In the above equations $N_c$ is the number of size classes, $N_\alpha$ is the number of particles in $\alpha$th size class, $\psi$ is the fluctuating pressure, $V$ is the total volume of the system, and $n^{(\alpha,i)}$ is the normal vector on the $i$th particle of $\alpha$th size class.

The phasic mean velocity of particle size class $\alpha$ is determined by averaging the dynamic equation of motion given in Eq. 5.11 using $\langle u^{(\alpha)} \rangle = 1/N_\alpha \sum_{i=1}^{N_\alpha} V^{(\alpha,i)}$. Thus, the evolution equation of the mean momentum for $\alpha$th particle size class is

$$
\frac{d}{dt} \langle u^{(\alpha)} \rangle = -\frac{1}{\rho^{(\alpha)}} \langle g_{\text{IBM}} \rangle_V + \frac{1}{\rho^{(\alpha)} \phi^{(\alpha)}} \left[ \langle s^{(\alpha)}_h \rangle + \sum_{\beta=1}^{N_c} \left( \langle f^{(\beta \rightarrow \alpha)}_{\text{coll}} \rangle \right) \right] - A_f,
$$

where $\rho^{(\alpha)}$ and $\phi^{(\alpha)}$ are respectively the mass density and solid-phase volume fraction of $\alpha$th size class, and $\langle f^{(\beta \rightarrow \alpha)}_{\text{coll}} \rangle$ represents the contact force per unit volume acting on $i$th size class due to particle collisions from particles in the $\beta$th size class. Due to the conservation of momentum in particle collisions, the average of the collision term $\langle f^{(\alpha,j \rightarrow i)}_{\text{coll}} \rangle$ in Eq. 5.11 is zero.

The phasic mean momentum equation (Eq. C.6) is used to derive the mass-weighted mean momentum of the solid phase. The mass-weighted velocity of the solid phase is defined as

$$
\langle \tilde{u}^{(p)} \rangle = \frac{\sum_{\alpha=1}^{N_c} \rho^{(\alpha)} \phi^{(\alpha)} \langle u^{(\alpha)} \rangle}{\sum_{\alpha=1}^{N_c} \rho^{(\alpha)} \phi^{(\alpha)}}.
$$

The mass-weighted conservation equation of the solid phase is then revealed as

$$
\frac{d}{dt} \langle \tilde{u}^{(p)} \rangle = -\frac{\phi^{(p)} \langle g_{\text{IBM}} \rangle_V}{\sum_{\alpha=1}^{N_c} \rho^{(\alpha)} \phi^{(\alpha)}} + \frac{\sum_{\alpha=1}^{N_c} \langle s^{(\alpha)}_h \rangle}{\sum_{\alpha=1}^{N_c} \rho^{(\alpha)} \phi^{(\alpha)}} - A_f,
$$

(C.8)
where $\phi$ is the total solid-phase volume fraction. Note that the collision term $\langle f^{(\beta \rightarrow \alpha)}_{\text{coll}} \rangle$ in Eq. C.6 is zero due to the conservation of momentum in particle collisions among all classes. By assuming all size classes have the same mass density ratio $\rho^{(\alpha)} = \rho^{(p)}$, an expression for the mean pressure gradient is obtained by subtracting Eq. C.4 from Eq. C.8 that has the following form:

$$
\frac{d}{dt} \langle \tilde{u}^{(p)} \rangle - \frac{d}{dt} \langle u^{(f)} \rangle = \left( \frac{1}{\rho^{(f)}} - \frac{1}{\rho^{(p)}} \right) \langle g_{\text{IBM}} \rangle \nu + \left( \frac{1}{\phi \rho^{(p)}} + \frac{1}{(1 - \phi) \rho^{(f)}} \right) \sum_{\alpha=1}^{N_c} \langle s^{(\alpha)}_M \rangle. \tag{C.9}
$$

The above equation is used to determine the mean pressure gradient corresponding to a pre-determined mean slip Reynolds number. In PURelIBM, the accelerating frame moves at the mean velocity of the particles. Therefore, the mean particle velocity $\langle \tilde{u}^{(p)} \rangle$ and the corresponding mean acceleration $d \langle \tilde{u}^{(p)} \rangle / dt$ is zero in this accelerating frame. Additionally, the mean acceleration of the fluid phase $d \langle u^{(f)} \rangle / dt$ in Eq. C.9 is discretized as $\left( \langle u^{(f)} \rangle^d - \langle u^{(f)} \rangle \right) / \Delta t$ where $\langle u^{(f)} \rangle^d$ denotes the desired fluid-phase mean velocity. This velocity is set such that the desired mean slip Reynolds number is satisfied. The mean slip Reynolds number is defined based on the mean slip velocity between the gas and the solid phase, i.e., $\langle W \rangle = \langle \tilde{u}^{(p)} \rangle - \langle u^{(f)} \rangle$, and the Sauter mean diameter $\langle d \rangle = \left( \sum_{\alpha=1}^{N_c} \phi^{(\alpha)} / (\phi d^{(\alpha)}) \right)^{-1}$ given by

$$
Re_m = \frac{(1 - \phi) |\langle W \rangle|}{\nu^{(f)}} \langle d \rangle, \tag{C.10}
$$

where $\nu^{(f)}$ is the gas-phase viscosity. Once the mean pressure gradient is established, the reference frame acceleration is determined from Eq. C.8. The mean pressure gradient and the reference frame acceleration are then used to solve the mean momentum equation given in Eq. C.3.

On the other hand, the momentum conservation equation for the fluctuating pressure and velocities is obtained by subtracting the mean momentum equation (Eq.C.3) from the instantaneous momentum equation (Eq.5.9). Periodic boundary conditions are imposed on fluctuating variables due to the homogeneity of the flow. A pseudo-spectral method is used with Crank-Nicolson scheme for the viscous terms and an Adams-Bashforth scheme for the convective terms. A fractional time-stepping method based on Kim and Moin’s approach (Kim and Moin,
1985) is used to advance the fluctuating velocities in time. Further details of PUReIBM are also reported by Tenneti et al. (2010).
APPENDIX D. ONE-PARTICLE DISTRIBUTION FUNCTION APPROACH FOR DERIVING GOVERNING EQUATIONS

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 (Koch, 1990; Subramaniam, 2000, 2001; Liboff, 2003; Pai and Subramaniam, 2009; Tenneti et al., 2010). For a polydisperse system the distribution function $f(x, v, r; t)$ is defined in a position-velocity-radius space, and evolves by the following transport equation:

$$
\frac{\partial}{\partial t} f(x, v, r; t) + \nabla_x \cdot (v f(x, v, r; t)) + \nabla_v \cdot (\langle A_h | x, v, r; t \rangle f(x, v, r; t)) \\
+ \nabla_v \cdot (\langle A_c | x, v, r; t \rangle f(x, v, r; t)) = 0,
$$

(D.1)

where $\nabla_x$ and $\nabla_v$ denote the gradient operators on the position and velocity space, respectively. The term $\langle A_h | x, v, r; t \rangle$ is the particle acceleration conditional on position and velocity, and can be interpreted as the average acceleration experienced by a particle with radius $r$ and velocity $v$ at position $x$ due to external forces. Also the term $\langle A_c | x, v, r; t \rangle$ represents the acceleration on particle due to collision with other particles. In the above transport equation, particle collisions are assumed to obey a soft-sphere model with a finite overlap during the course of collision. Therefore, this equation is valid for any instance of time.

Note that in the kinetic theory description of gas-solid flow using the one-particle distribution function, the conditional accelerations are obtained by integrating out their dependence on the two-particle density (pair correlation function). In other words, the conditional accelerations are not completely determined by the particle velocity, but may be affected by the presence of neighbor particles. The statistical description of multiparticle interactions is not contained in the one-particle distribution function.
The distribution function $f(x, v, r; t)$ for a polydisperse suspension can be obtained from the Kilimontovic approach from the first principles (Subramaniam, 2001). In this approach, a fine-grained density function $f'$ for the ensemble of particles is given as:

$$f'(x, v, r; t) \equiv \sum_{i=1}^{N_p} \delta(x - X_i(t)) \delta(v - V_i(t)) \delta(r - R_i)$$  \hspace{1cm} (D.2)

where $N_p$ is the total number of particles, and $X_i$, $V_i$, $R_i$ are position, velocity and radius of $i^{th}$ particle in Lagrangian coordinates. We assume that particles are rigid, and they do not break up or coalesce during collisions. Hence, the total number of particles and their radii are constant. Now the droplet distribution function (ddf) can be used to describe the average property the suspension which is defined as the ensemble average of the fine-grained density function as

$$f(x, v, r; t) \equiv \langle f'(x, v, r; t) \rangle.$$  \hspace{1cm} (D.3)

In a polydisperse particle system where the particle size distribution is discrete, the ddf can be rewritten as

$$f(x, v, r; t) = \sum_{\alpha=1}^{N_{\alpha}} f_{\alpha}(x, v; t) \delta(r - R_{\alpha}),$$  \hspace{1cm} (D.4)

where $N_{\alpha}$ is the total number of species, and $f_{\alpha}(x, v; t)$ is the ddf corresponding to the size class with radius $R_{\alpha}$. If the expected number of particles in any region $B$ in $[x, v, r; t]$ space is denoted by $\langle N(t) \rangle_B$, it is obtained by integrating $f$ over the region $B$ such that

$$\langle N(t) \rangle_B = \int_{B} f(x, v, r; t) \, dx \, dv \, dr$$

$$= \int_{B} \left( \sum_{\alpha=1}^{N_{\alpha}} f_{\alpha}(x, v; t) \delta(r - R_{\alpha}) \right) \, dx \, dv \, dr$$

$$= \sum_{\alpha=1}^{N_{\alpha}} \langle N^{(\alpha)}(t) \rangle_B,$$  \hspace{1cm} (D.5)

with $\langle N^{(\alpha)}(t) \rangle_B$ being the expected number of particles from $\alpha^{th}$ size class in region $B$. The ddf does not show the normalization property of a pdf, which is the integration to unity over the phase space it is defined over. If the ddf is integrated only on $[v, r]$ space, the expected number density of particles $n(x; t)$ is obtained as

$$n(x; t) = \int_{[v,r]} f(x, v, r; t) \, dv \, dr$$

$$= \int_{[v,r]} \left( \sum_{\alpha=1}^{N_{\alpha}} f_{\alpha}(x, v; t) \delta(r - R_{\alpha}) \right) \, dv \, dr$$

$$= \sum_{\alpha=1}^{N_{\alpha}} n^{(\alpha)}(x; t),$$  \hspace{1cm} (D.6)
where \( n^{(\alpha)}(x; t) \) is the number density of \( \alpha \)th size class. It is shown by Subramaniam (2001) that the ddf can be written as the product of the number density in physical space and the joint probability distribution function (jpdf) of velocity and radius conditional on physical location as

\[
f(x, v, r) = n(x; t) \, f_{VR}^c(v, r | x; t) = \sum_{\alpha=1}^{N_{\alpha}} n^{(\alpha)}(x; t) \, f_{VR,\alpha}^c(v | x; t),
\]

(D.7)

with \( f_{VR}^c(v, r | x; t) \) and \( f_{VR,\alpha}^c(v | x; t) \) being probability density functions that satisfy the normalization condition. By substituting the one-particle density function in Eq. D.1 with the last term in the above expression, the transport equation for a one-particle density function of a polydisperse system reads as

\[
\frac{\partial}{\partial t} \left( \sum_{\alpha=1}^{N_{\alpha}} n^{(\alpha)}(x; t) \, f_{VR,\alpha}^c(v | x; t) \right) + \nabla_x \cdot \left\{ v \left( \sum_{\alpha=1}^{N_{\alpha}} n^{(\alpha)}(x; t) \, f_{VR,\alpha}^c(v | x; t) \right) \right\} + \nabla_v \cdot \left( \sum_{\alpha=1}^{N_{\alpha}} \langle A_h^{(\alpha)} | x, v; t \rangle \, n^{(\alpha)}(x; t) \, f_{VR,\alpha}^c(v | x; t) \right) + \nabla_v \cdot \left( \sum_{\alpha=1}^{N_{\alpha}} \langle A_c^{(\alpha \rightarrow \alpha)} | x, v; t \rangle \, n^{(\alpha)}(x; t) \, f_{VR,\alpha}^c(v | x; t) \right) = 0,
\]

(D.8)

where \( \langle A_h^{(\alpha)} | x, v; t \rangle \) and \( \langle A_c^{(\alpha \rightarrow \alpha)} | x, v; t \rangle \) are the conditional acceleration on \( \alpha \)th particle size class due to, respectively, hydrodynamic and collisional forces. The collisional acceleration due to collisional forces can be further partitioned into the contributions from particles colliding with other particles in the same size class, \( \langle A_c^{(\alpha \rightarrow \alpha)} | x, v; t \rangle \), as well as contributions from colliding with particles belonging to other size classes, \( \langle A_c^{(\beta \rightarrow \alpha)} | x, v; t \rangle \). Applying this decomposition, the final form of the transport equation for a polydisperse mixture will be:
\[
\frac{\partial}{\partial t} \left( \sum_{\alpha=1}^{N_\alpha} n^{(\alpha)}(x; t) f^c_{V,\alpha}(v | x; t) \right) \\
+ \nabla_x \cdot \left( v \left( \sum_{\alpha=1}^{N_\alpha} n^{(\alpha)}(x; t) f^c_{V,\alpha}(v | x; t) \right) \right) \\
+ \nabla_v \cdot \left( \sum_{\alpha=1}^{N_\alpha} \left< \mathbf{A}^{(f\rightarrow\alpha)}_h | x, v; t \right| n^{(\alpha)}(x; t) f^c_{V,\alpha}(v | x; t) \right) \\
+ \nabla_v \cdot \left( \sum_{\alpha=1}^{N_\alpha} \left< \mathbf{A}^{(\alpha\rightarrow\alpha)}_c | x, v; t \right| n^{(\alpha)}(x; t) f^c_{V,\alpha}(v | x; t) \right) \\
+ \nabla_v \cdot \left( \sum_{\alpha=1}^{N_\alpha} \sum_{\beta=1}^{N_\alpha} \mathbf{A}^{(\beta\rightarrow\alpha)}_c | x, v; t \right| n^{(\alpha)}(x; t) f^c_{V,\alpha}(v | x; t) \right) = 0. \quad (D.9)
\]

It is now possible to derive hydrodynamics equations of motion from the kinetic equation of the one-particle density function for a polydisperse system given by Eq. D.9. In order to simplify the notation, the independent variables \([x, v, r; t]\) are excluded from the equations from hereon. Based on Eq. D.9, the evolution of particle number density for each particle size class is governed by:

\[
\frac{\partial}{\partial t} \left( n^{(\alpha)} f^c_{V,\alpha} \right) + \nabla_x \cdot \left( v n^{(\alpha)} f^c_{V,\alpha} \right) + \nabla_v \cdot \left( \left< \mathbf{A}^{(f\rightarrow\alpha)}_h \right| n^{(\alpha)} f^c_{V,\alpha} \right) \\
+ \nabla_v \cdot \left( \left< \mathbf{A}^{(\alpha\rightarrow\alpha)}_c \right| n^{(\alpha)} f^c_{V,\alpha} \right) + \nabla_v \cdot \left( \sum_{\beta=1}^{N_\alpha} \mathbf{A}^{(\beta\rightarrow\alpha)}_c \right| n^{(\alpha)} f^c_{V,\alpha} \right) = 0. \quad (D.10)
\]

In the rest of this Appendix, derivation of hydrodynamic conservation equations of mass, momentum, and energy are presented which are respectively correspond to zeroth, first, and second moments of the above kinetic equation.
D.1 Number Density

The number density evolution equation is derived by integrating Eq. D.10 over the velocity phase space, i.e.

\[ \int_v \frac{\partial}{\partial t} \left( n^{(\alpha)} f_{V,\alpha}^{c} \right) dV + \int_v \nabla \cdot \left( v n^{(\alpha)} f_{V,\alpha}^{c} \right) dV + \int_v \nabla \cdot \left( \langle A_{h}^{(f \rightarrow \alpha)} \rangle n^{(\alpha)} f_{V,\alpha}^{c} \right) dV \\
+ \int_v \nabla \cdot \left( \langle A_{c}^{(a \rightarrow \alpha)} \rangle n_{\alpha} f_{V,\alpha}^{c} \right) dV + \int_v \nabla \cdot \left( \sum_{\beta=1}^{N_{\alpha}} \langle A_{c}^{(\beta \rightarrow \alpha)} \rangle n^{(\alpha)} f_{V,\alpha}^{c} \right) dV = 0. \]  

(D.11)

Since the independent variables are not correlated, integral and derivative operators commute. Also, gas-particle and particle-particle interactions do not lead to any changes in the number of particle (neither source nor sink of particles). Therefore, the following terms including accelerations become zero, i.e.

\[ \nabla \cdot \int_v \left( \langle A_{c}^{(f \rightarrow \alpha)} \rangle n^{(\alpha)} f_{V,\alpha}^{c} \right) dV = 0 \]

\[ \nabla \cdot \int_v \left( \langle A_{c}^{(a \rightarrow \alpha)} \rangle n^{(\alpha)} f_{V,\alpha}^{c} \right) dV = 0 \]

\[ \nabla \cdot \int_v \left( \sum_{\beta=1}^{N_{\alpha}} \langle A_{c}^{(\beta \rightarrow \alpha)} \rangle n^{(\alpha)} f_{V,\alpha}^{c} \right) dV = 0. \]

Therefore, Eq. D.11 simplifies to

\[ \frac{\partial}{\partial t} \left( n^{(\alpha)} \int_v f_{V,\alpha}^{c} dV \right) + \nabla \cdot \left( n^{(\alpha)} \int_v v f_{V,\alpha}^{c} dV \right) = 0. \]

The first integral in the above equation reduces to unity due to the normalization condition, and the second integral represents the mean velocity of \( \alpha \)th size class \( \langle u^{(\text{alpha})} \rangle \) over the phase space \([x; t]\). Therefore, the particle size class number density is governed by the following expression:

\[ \frac{\partial n^{(\alpha)}}{\partial t} + \nabla \cdot \left( n^{(\alpha)} \langle u^{(\alpha)} \rangle \right) = 0. \]  

(D.12)
D.2 Mean Momentum

The mean momentum equation is obtained by multiplying Eq. D.10 with velocity and integrating the result over the velocity space, i.e.

\[
\int v \frac{\partial}{\partial t} \left( n^{(\alpha)} f_{V,\alpha}^c \right) dv + \int_v v \nabla_x \cdot \left( v n^{(\alpha)} f_{V,\alpha}^c \right) dv + \int_v v \nabla_v \cdot \left( \left\langle A^{(f\rightarrow\alpha)}_h \right\rangle n^{(\alpha)} f_{V,\alpha}^c \right) dv \\
+ \int_v \nabla_v \cdot \left( \sum_{\beta \neq \alpha} \left\langle A^{(\alpha\rightarrow\beta)}_c \right\rangle n^{(\alpha)} f_{V,\alpha}^c \right) dv + \int_v \nabla_v \cdot \left( \left\langle A^{(\alpha\rightarrow\alpha)}_c \right\rangle n^{(\alpha)} f_{V,\alpha}^c \right) dv = 0.
\]

(D.13)

The terms in the above equation are investigated separately. Following the math used in Section D.1, terms I and II of the above expression are simplified as

\[
\frac{\partial}{\partial t} \left( \int_v v f_{V,\alpha}^c \right) dv = \frac{\partial}{\partial t} \left( \int_v \langle u^{(\alpha)} \rangle \right),
\]

(D.14)

and

\[
\nabla_v \cdot \left( \int_v v f_{V,\alpha}^c dv \right) = \nabla_v \cdot \left( \int_v \langle u^{(\alpha)} \rangle \langle u^{(\alpha)} \rangle \right) + \nabla_v \cdot \left( \int_v \langle u^{(\alpha)} u^{(\alpha)} \rangle \right),
\]

(D.15)

respectively. Note that in the above expression, the second term on the right-hand side appears due to the covariance of velocity fluctuations \( u^{(\alpha)} = u^{(\alpha)} - \langle u^{(\alpha)} \rangle \), and is recognized as the transport of the Reynolds stress tensor.

Term III in (D.13) that includes the conditional acceleration is evaluated by Green's theorem, i.e.

\[
\int_v v \nabla_v \cdot \left( \left\langle A^{(f\rightarrow\alpha)}_h \right\rangle n^{(\alpha)} f_{V,\alpha}^c \right) dv = \oint_v \nabla_v \cdot \left( \left\langle A^{(f\rightarrow\alpha)}_h \right\rangle n^{(\alpha)} f_{V,\alpha}^c \right) dv - \int_v \nabla_v \cdot \left( \left\langle A^{(f\rightarrow\alpha)}_h \right\rangle n^{(\alpha)} f_{V,\alpha}^c \right) dv,
\]

(D.16)

where \( n \) is the normal vector on the boundary of velocity phase space. The first term on the right-hand side of the above equation is zero since \( f_{V,\alpha}^c \) is zero on the boundary of velocity phase space. Now the second term on the right-hand side of the above equation can be written as

\[
\int_v I \cdot \left( \left\langle A^{(f\rightarrow\alpha)}_h \right\rangle n^{(\alpha)} f_{V,\alpha}^c \right) dv = n^{(\alpha)} \left\langle A^{(f\rightarrow\alpha)}_h \right| x; t \right\rangle,
\]

(D.17)
where \( I \) is the identity tensor. The term \( \langle A_{h}^{(f \rightarrow \alpha)} | x; t \rangle \) on the right-hand side of the above equation is hydrodynamic acceleration conditional on spatial position arising from the fluid-particle interaction. When multiplied by the mass of a particle in size class \( \alpha \), this term represents the hydrodynamic drag that is denoted by \( \langle f_{h}^{(f \rightarrow \alpha)} \rangle \).

Term \( IV \) in Eq. D.13 corresponds to the mean change of rate of momentum due to the collision among particles of the same size class, and leads to a term similar to the one given in Eq. D.17. Nevertheless, because the accelerations acting on a pair of colliding particles are equal and opposite, the ensemble average of this term for the whole colliding pairs in size class \( \alpha \) is zero, i.e.

\[
\int_{V} v \nabla \cdot \left( \left( \langle A_{c}^{(\alpha \rightarrow \alpha)} \rangle \right) n^{(\alpha)} f_{V,\alpha}^{c} \right) dv = 0.
\]

Term \( V \) represents the mean momentum transfer between particles of different size classes due to particle collision which is non-zero. Similar to the hydrodynamic acceleration term in Eq. D.13, it can be shown that term \( V \) simplifies to

\[
\int_{V} v \nabla \cdot \left( \left( \langle A_{c}^{(\beta \rightarrow \alpha)} \rangle \right) n^{(\alpha)} f_{V,\beta}^{c} \right) dv = n^{(\alpha)} \left\langle A_{c}^{(\beta \rightarrow \alpha)} \right\rangle.
\]  \hspace{1cm} (D.18)

The above expression when multiplied by the mass of a particle in size class \( \alpha \) represents the mean momentum transfer from size class \( \beta \) to \( \alpha \) due to particle-particle collision. This mean momentum transfer between the two particle size classes is called the particle-particle drag force and is denoted by \( \langle f_{c}^{(\beta \rightarrow \alpha)} \rangle \). The conservation of momentum transfer between size classes \( \alpha \) and \( \beta \) necessitates that

\[
\left\langle f_{c}^{(\beta \rightarrow \alpha)} \right\rangle = - \left\langle f_{c}^{(\alpha \rightarrow \beta)} \right\rangle.
\]

It can be easily shown that the transfer of momentum due to particle collision among all particle size classes is conservative, i.e. \( \sum_{\alpha=1}^{N_{p}} \sum_{\beta=1}^{N_{p}} \left\langle f_{c}^{(\beta \rightarrow \alpha)} \right\rangle = 0 \). Now we can rewrite the final moment equation of the particle number density for class \( \alpha \) as
\[
\frac{\partial}{\partial t} \left( n^{(\alpha)} \langle u^{(\alpha)} \rangle \right) + \nabla_x \cdot \left( n^{(\alpha)} \langle u^{(\alpha)} \rangle \langle u^{(\alpha)} \rangle \rangle \right) + \nabla_x \cdot \left( n^{(\alpha)} \langle u^{(\alpha)} u^{(\alpha)} \rangle \right) \]
\[
= n^{(\alpha)} \langle A_{h}^{(f \rightarrow \alpha)} \rangle + n^{(\alpha)} \sum_{\beta=1}^{N_{\alpha}} \langle A_{c}^{(\beta \rightarrow \alpha)} \rangle , \tag{D.19}
\]

or the equivalent mass-weighted mean momentum equation as
\[
\frac{\partial}{\partial t} \left( \rho^{(\alpha)} \phi^{(\alpha)} \langle u^{(\alpha)} \rangle \right) + \nabla_x \cdot \left( \rho^{(\alpha)} \phi^{(\alpha)} \langle u^{(\alpha)} \rangle \langle u^{(\alpha)} \rangle \right) + \nabla_x \cdot \left( \rho^{(\alpha)} \phi^{(\alpha)} \langle u^{(\alpha)} u^{(\alpha)} \rangle \right) \]
\[
= \langle f_{h}^{(f \rightarrow \alpha)} \rangle + \sum_{\beta=1}^{N_{\alpha}} \langle f_{c}^{(\beta \rightarrow \alpha)} \rangle . \tag{D.20}
\]

In the above equation, the covariance of velocity fluctuations \( \langle u^{(\alpha)} u^{(\alpha)} \rangle \) as well as the hydrodynamic and collision drag terms are not closed at the level of first moment equations that necessitates the use of appropriate models.

**D.3 Transport equation of the total kinetic energy**

The transport equation for the evolution of the total energy in a particle size class is obtained by multiplying equation D.10 with \( v_i v_i \) and integrating it over the velocity phase space, i.e.
\[
\int_{V} v_i v_i \frac{\partial}{\partial t} \left( n^{(\alpha)} f_{V,\alpha}^c \right) dv + \int_{V} v_i v_i \nabla_v \cdot \left( v n^{(\alpha)} f_{V,\alpha}^c \right) dv + \int_{V} v_i v_i \nabla_v \cdot \left( \left\langle A_{h}^{(f \rightarrow \alpha)} \right\rangle n^{(\alpha)} f_{V,\alpha}^c \right) dv + \int_{V} v_i v_i \nabla_v \cdot \left( \left\langle A_{c}^{(\alpha \rightarrow \alpha)} \right\rangle n^{(\alpha)} f_{V,\alpha}^c \right) dv + \int_{V} v_i v_i \nabla_v \cdot \left( \sum_{\beta=1}^{N_{\alpha}} \left\langle A_{c}^{(\beta \rightarrow \alpha)} \right\rangle n^{(\alpha)} f_{V,\alpha}^c \right) dv = 0. \tag{D.21}
\]

Similar to the mean momentum equation, the terms in the above expression are considered separately. Term \( I \) which represents the rate of change of energy in time can be written as
\[
\int v_i v_i \frac{\partial}{\partial t} \left( n^{(a)} f_{V,\alpha}^c \right) dV = \frac{\partial}{\partial t} \left( n^{(a)} \left\langle u_i^{(a)} \right\rangle \left\langle u_i^{(a)} \right\rangle \right) + \frac{\partial}{\partial t} \left( n^{(a)} \left\langle u_i^{n(\alpha)} u_i^{n(\alpha)} \right\rangle \right) . \tag{D.22}
\]

Term II also yields
\[
\int v_i v_i \frac{\partial}{\partial x_k} \left( v_k n^{(a)} f_{V,\alpha}^c \right) dV = \frac{\partial}{\partial x_k} \left( n^{(a)} \left\langle u_i^{(a)} \right\rangle \left\langle u_i^{(a)} \right\rangle \right) + \frac{\partial}{\partial x_k} \left( n^{(a)} \left\langle u_i^{n(\alpha)} u_i^{n(\alpha)} \right\rangle \right) + \frac{\partial}{\partial x_k} \left( 2n^{(a)} \left\langle u_i^{n(\alpha)} u_i^{n(\alpha)} \right\rangle \right) . \tag{D.23}
\]

In the above expression, the first and second terms on the right-hand side represent, respectively, the convection of energy in the mean flow and in velocity fluctuations. The third and forth terms are associated with the flux of energy due to the mean and velocity fluctuations. It should be noted that the triple velocity covariance in not closed at the level of second order moment, and requires higher order moment for closure.

To evaluate term III in Eq. D.21, the Green’s theorem is used for simplification as follows:
\[
\int v_i v_i \frac{\partial}{\partial v_k} \left( \left\langle A_{h,k}^{(f-\alpha)} \right\rangle n^{(a)} f_{V,\alpha}^c \right) dV = \int v_i v_i \left( \left\langle A_{h,k}^{(f-\alpha)} \right\rangle n^{(a)} f_{V,\alpha}^c v_k \right) dA - \int v_i v_i \left( \left\langle A_{h,k}^{(f-\alpha)} \right\rangle n^{(a)} f_{V,\alpha}^c \right) dV = 0 - 2 \int v_i \frac{\partial v_i}{\partial v_k} \left( \left\langle A_{h,k}^{(f-\alpha)} \right\rangle n^{(a)} f_{V,\alpha}^c v_k \right) dV = -2 \int v_i \delta_{h,k} \left( \left\langle A_{h,k}^{(f-\alpha)} \right\rangle n^{(a)} f_{V,\alpha}^c \right) dV = -2 \int v_i \left( \left\langle A_{h,i}^{(f-\alpha)} \right\rangle n^{(a)} f_{V,i}^c \right) dV = -2n^{(a)} \left\langle u_i^{(a)} A_{h,i}^{(f-\alpha)} \right\rangle \tag{D.24}
\]

In a similar way, Term IV in Eq. D.21 can be integrated over the velocity space that yields:
\[
\int v_i v_i \frac{\partial}{\partial v_k} \left( \left\langle A_{c,k}^{(\alpha-\alpha)} \right\rangle n^{(a)} f_{V,\alpha}^c \right) dV = -2n^{(a)} \left\langle u_i^{(a)} A_{c,i}^{(\alpha-\alpha)} \right\rangle \tag{D.25}
\]

The term on the right-hand side of the above expression represents the transfer of energy among particles of size class \( \alpha \) due to collisions other particles in the same size class. Similarly, Term V in Eq. D.21 can be simplified as:
\[
\int v_i v_i \nabla \cdot \left( \sum_{\beta=1}^{N_\alpha} \left\langle A_{c}^{(\beta-\alpha)} \right\rangle n^{(a)} f_{V,\alpha}^c \right) dV = -2n^{(a)} \sum_{\beta=1}^{N_\alpha} \left\langle u_i^{(a)} A_{c,i}^{(\beta-\alpha)} \right\rangle \tag{D.26}
\]
The term on the right-hand side of the above equation represents the rate of change of kinetic energy in particle size class $\alpha$ due to the collisions with particles of other size classes.

Since all terms in Eq. D.21 have been evaluated in Eqs. D.22 to D.26, the transport equation for the total energy in particle size class $\alpha$ can be presented as

$$\frac{\partial}{\partial t} \left( n^{(\alpha)} \left( \langle u_i^{(\alpha)} \rangle \langle u_i^{(\alpha)} \rangle \right) \right) + \frac{\partial}{\partial x_k} \left( n^{(\alpha)} \langle u_i^{(\alpha)} u_k^{(\alpha)} \rangle \right) + \frac{\partial}{\partial x_k} \left( n^{(\alpha)} \langle u_i^{(\alpha)} u_i^{(\alpha)} u_k^{(\alpha)} \rangle \right) = 2n^{(\alpha)} \left( \langle u_i^{(\alpha)} A_{h,i}^{(f\rightarrow\alpha)} \rangle \right) + 2n^{(\alpha)} \left( \langle u_i^{(\alpha)} A_{c,i}^{(\alpha\rightarrow\alpha)} \rangle \right) + 2n^{(\alpha)} \sum_{\beta=1}^{N_{\alpha}} \langle u_i^{(\alpha)} A_{c,i}^{(\beta\rightarrow\alpha)} \rangle. \quad (D.27)$$

If we define the kinetic energy in the mean with $\bar{E}^{(\alpha)} = \langle u_i^{(\alpha)} \rangle \langle u_i^{(\alpha)} \rangle / 2$ and the kinetic energy in the velocity fluctuations as $k^{(\alpha)} = \langle u_i^{(\alpha)} u_i^{(\alpha)} \rangle / 2$, then the above equation is further simplified as

$$\frac{\bar{D}}{\bar{D}t} (n^{(\alpha)} \bar{E}^{(\alpha)}) + \frac{\overline{D}}{\overline{D}t} (n^{(\alpha)} k^{(\alpha)}) + \frac{1}{2} \frac{\partial}{\partial x_k} \left( n^{(\alpha)} \langle u_i^{(\alpha)} u_i^{(\alpha)} u_k^{(\alpha)} \rangle \right) = n^{(\alpha)} \langle u_i^{(\alpha)} A_{h,i}^{(f\rightarrow\alpha)} \rangle + n^{(\alpha)} \langle u_i^{(\alpha)} A_{c,i}^{(\alpha\rightarrow\alpha)} \rangle + n^{(\alpha)} \sum_{\beta=1, \beta \neq \alpha}^{N_{\alpha}} \langle u_i^{(\alpha)} A_{c,i}^{(\beta\rightarrow\alpha)} \rangle, \quad (D.28)$$

where $\bar{D} (\cdot) / \bar{D}t$ is the material derivative of a presumed quantity in the following form:

$$\frac{\bar{D}}{\bar{D}t} (\cdot) = \frac{\partial}{\partial t} (\cdot) + \frac{\partial}{\partial x_k} \left( \langle u_k^{(\alpha)} \rangle (\cdot) \right).$$

It is also useful to rewrite Eq. D.28 mass-weighted kinetic energy by multiplying it with the mass of a particle in size class $\alpha$, that is

$$\frac{\bar{D}}{\bar{D}t} \left( \rho^{(\alpha)} \phi^{(\alpha)} \bar{E}^{(\alpha)} \right) + \frac{\overline{D}}{\overline{D}t} \left( \rho^{(\alpha)} \phi^{(\alpha)} k^{(\alpha)} \right) + \frac{1}{2} \frac{\partial}{\partial x_k} \left( \rho^{(\alpha)} \phi^{(\alpha)} \langle u_i^{(\alpha)} u_i^{(\alpha)} u_k^{(\alpha)} \rangle \right) = \rho^{(\alpha)} \langle u_i^{(\alpha)} f_{h,i}^{(f\rightarrow\alpha)} \rangle + \rho^{(\alpha)} \langle u_i^{(\alpha)} f_{c,i}^{(\alpha\rightarrow\alpha)} \rangle$$

$$+ \sum_{\beta=1, \beta \neq \alpha}^{N_{\alpha}} \rho^{(\alpha)} \langle u_i^{(\alpha)} f_{c,i}^{(\beta\rightarrow\alpha)} \rangle. \quad (D.29)$$
D.4 Transport equation for the kinetic energy in velocity fluctuations

Since the transport equation in D.28 corresponds to the total energy in the system, it is useful to separate contributions of energy from the mean flow and velocity fluctuations to the total energy. To do so, first we focus on the transport equation of kinetic energy in velocity fluctuations. We multiply the kinetic equation D.10 with \( v''_i v''_i \) and integrate the equation over the velocity phase space. Here, \( v'' \) is the sample-space variable corresponding to velocity fluctuations. The steps to perform integration are similar to those presented in D.3. The final expression for the transport equation of kinetic energy in fluctuating velocity will have the following form:

\[
\bar{D} \frac{\partial}{\partial t} (\bar{n}^{(\alpha)} \bar{u}^{(\alpha)} \bar{k}^{(\alpha)}) + \frac{1}{2} \frac{\partial}{\partial x_k} (\bar{n}^{(\alpha)} \langle u_k^{(\alpha)} u_i^{(\alpha)} u_i^{(\alpha)} \rangle) = -\bar{n}^{(\alpha)} \langle u_k^{(\alpha)} u_i^{(\alpha)} \rangle \frac{\partial}{\partial x_k} \langle u_i^{(\alpha)} \rangle + \bar{n}^{(\alpha)} \langle u_i^{(\alpha)} A^{(f\rightarrow\alpha)} \rangle + \bar{n}^{(\alpha)} \langle u_i^{(\alpha)} A^{(\alpha\rightarrow\alpha)} \rangle + \bar{n}^{(\alpha)} \sum_{\beta=1}^{N_\alpha} \beta \neq \alpha \langle u_i^{(\beta)} A^{(\beta\rightarrow\alpha)} \rangle. \tag{D.30}
\]

Also the transport equation for the mass-weighted kinetic energy in velocity fluctuations is obtained by multiplying the above equations with \( m^{(\alpha)} \), which reads as

\[
\bar{D} \frac{\partial}{\partial t} (\bar{\rho}^{(\alpha)} \bar{\phi}^{(\alpha)} \bar{k}^{(\alpha)}) + \frac{1}{2} \frac{\partial}{\partial x_k} (\bar{\rho}^{(\alpha)} \phi^{(\alpha)} \langle u_k^{(\alpha)} u_i^{(\alpha)} u_i^{(\alpha)} \rangle) = -\rho^{(\alpha)} \phi^{(\alpha)} \langle u_k^{(\alpha)} u_i^{(\alpha)} \rangle \frac{\partial}{\partial x_k} \langle u_i^{(\alpha)} \rangle + \langle u_i^{(\alpha)} f^{(f\rightarrow\alpha)} \rangle + \langle u_i^{(\alpha)} f^{(\alpha\rightarrow\alpha)} \rangle + \sum_{\beta=1}^{N_\alpha} \beta \neq \alpha \langle u_i^{(\beta)} f^{(\beta\rightarrow\alpha)} \rangle. \tag{D.31}
\]

In the above equation, the third term on the right-hand side represents the mean rate of transfer of energy between two colliding particles belonging to the same class. Since the particle collisions are instantaneous, this term is always non-zero during the collision time. However, when this term is time-averaged over the collision time, then if the colliding particles are elastic this term is zero. Otherwise, the time-averaged value is always negative and is associated with the collisional dissipation for collisions among particles of class \( \alpha \). The same argument is also true about the last term, meaning that if the colliding particles belonging to classes \( \alpha \) and \( \beta \) are elastic, then the time-averaged energy transfer between the two particles during collision is conservative. Otherwise, there exist a non-zero energy loss that is associated with collisional dissipation for particle collisions taking place between classes \( \alpha \) and \( \beta \).
D.5 Transport equation for the kinetic energy in the mean flow

The transport equation for the kinetic energy in the mean flow can be obtained by subtracting Eq. D.30 from Eq. D.28 that has the following form:

\[
\frac{\bar{D}}{Dt} \left( n^{(\alpha)} \bar{E}^{(\alpha)} \right) + \frac{\partial}{\partial x_k} \left( n^{(\alpha)} \left< u_i^{(\alpha)} n^{(\alpha)} u_k^{(\alpha)} \right> u_i^{(\alpha)} \right) = n^{(\alpha)} \left< u_k^{(\alpha)} u_i^{(\alpha)} \right> \frac{\partial}{\partial x_k} \left< u_i^{(\alpha)} \right> + n^{(\alpha)} \left< u_i^{(\alpha)} \right> \left< A_{h,i}^{(f\rightarrow\alpha)} \right> \\
+ n^{(\alpha)} \left< u_i^{(\alpha)} \right> \sum_{\beta=1}^{N_\alpha} \sum_{\beta \neq \alpha} A_{c,i}^{(\beta \rightarrow \alpha)} (D.32)
\]

A similar equation for the mass-weighted kinetic energy in the mean flow can be obtained that has the following form

\[
\frac{\bar{D}}{Dt} \left( \rho^{(\alpha)} \phi^{(\alpha)} \bar{E}^{(\alpha)} \right) + \frac{\partial}{\partial x_k} \left( \rho^{(\alpha)} \phi^{(\alpha)} \left< u_i^{(\alpha)} n^{(\alpha)} u_k^{(\alpha)} \right> u_i^{(\alpha)} \right) = \rho^{(\alpha)} \phi^{(\alpha)} \left< u_k^{(\alpha)} u_i^{(\alpha)} \right> \frac{\partial}{\partial x_k} \left< u_i^{(\alpha)} \right> + \left< u_i^{(\alpha)} \right> \left< f_{h,i}^{(f\rightarrow\alpha)} \right> \\
+ \left< u_i^{(\alpha)} \right> \sum_{\beta=1}^{N_\alpha} \sum_{\beta \neq \alpha} f_{c,i}^{(\beta \rightarrow \alpha)} (D.33)
\]
APPENDIX E. TWO-FLUID THEORY APPROACH FOR DERIVING GOVERNING EQUATIONS

In the Eulerian-Eulerian (EE) two-fluid theory approach, it is assumed that the conservation equations of mass, momentum and energy are valid for the entire system. In fact, flow properties and quantities such as density, velocity and pressure fields are continuous since the fluid phase and the dispersed phase are inter-penetrating media. The conservation of mass and momentum that govern the flow motion are, respectively, given as

\[
\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0, \tag{E.1}
\]

and

\[
\frac{\partial (\rho u_i)}{\partial t} + \frac{\partial (\rho u_j u_i)}{\partial x_j} = \frac{\partial \sigma_{ji}}{\partial x_j} + \rho g_i, \tag{E.2}
\]

where \(\rho\) is the material density, \(u\) is the velocity, \(\sigma = -p\delta + \tau\) is the total stress with \(p, \delta, \) and \(\tau\) being, respectively, the pressure, the Kronecker delta and the viscous stress, and \(g\) is the gravitational acceleration.

The fluid-phase and the dispersed-phase cannot coexist at the same space location in a given time. Thus, an indicator field (Drew and Passman, 1998) is used to distinguish phase \(\alpha\) at \((x,t)\) from other phases in the domain, that is

\[
I^{(\alpha)}(x,t) = \begin{cases} 
1 & \text{if } x \text{ is in phase } \alpha \\
0 & \text{if } x \text{ is not in phase } \alpha,
\end{cases}
\]

Therefore, the gas phase is identified by the indicator function \(I^{(f)}\). In polydisperse gas-solid suspensions, particles can be classified as discrete classes with different particle diameters or mass densities. This implies that there are \(N_\alpha\) particle classes in the suspension that are distinguished from others by using the indicator function \(I^{(\alpha)}\) with \(\alpha = 1..N_\alpha\).
It should also be noted that similar to the assumptions in D, interphase interactions are assumed to be instantaneous. Therefore, particle-particle collisions are expected to occur over a finite collision time with infinitesimal reversible deformation. In this general case, surface of a particle that belongs to class $\alpha$ is represented by the normal vector at the surface of the particle pointing outward $\mathbf{n}^{(\alpha)}$. This particle may have interphase interactions with the carrier fluid, with other particles in the same size class, and particles from other particle size classes. Therefore, the surface of the particle can be decomposed into three regions: (1) particle-fluid interface that is represented by the normal vector $\mathbf{n}^{(\alpha \rightarrow f)}$, (2) particle-particle interface when colliding with another particle from the same particle class that is indicated by the normal vector $\mathbf{n}^{(\alpha \rightarrow \alpha)}$, (3) particle-particle interface when colliding with a particle from a different particle class that is shown by the normal vector $\mathbf{n}^{(\alpha \rightarrow \beta)}$. Note that the geometrical property of the interface necessitates that

$$\begin{align*}
\mathbf{n}^{(\alpha \rightarrow f)} &= -\mathbf{n}^{(f \rightarrow \alpha)} \\
\mathbf{n}^{(\alpha \rightarrow \beta)} &= -\mathbf{n}^{(\alpha \rightarrow \beta)}
\end{align*}$$

(E.3)

Now the mean phasic conservation equations of mass, momentum and energy can be obtained by multiplying the phase indicator function with Eqs. E.1 and E.2 and use the above surface decomposition to represent interphase interactions. These equations are derived in detail for the two-fluid approach in the rest of this Appendix.

### E.1 Averaging process

In Eulerian-Eulerian two-fluid approach, the phasic average is a conditional ensemble average which is conditioned on the presence of phase $\alpha$. For flow quantity $Q$, the mass-weighted phasic average for phase $\alpha$ is defined as

$$\left\langle \tilde{Q}^{(\alpha)} \right\rangle = \frac{\left\langle I^{(\alpha)} \rho Q \right\rangle}{\left\langle I^{(\alpha)} \rho \right\rangle},$$

(E.4)

where the symbol $\langle \cdot \rangle$ represents the ensemble-averaging. Now if the density in phase $\alpha$ conditional on the presence of phase $\alpha$ is constant, ie. $\left\langle \rho \mid I^{(\alpha)} = 1 \right\rangle = \rho^{(\alpha)}$, the mass-weighted phasic average simplifies to the phasic average as

$$\left\langle Q^{(\alpha)} \right\rangle = \frac{\left\langle I^{(\alpha)}Q \right\rangle}{\left\langle I^{(\alpha)} \right\rangle},$$

(E.5)
with $\langle I^{(\alpha)} \rangle = \phi^{(\alpha)}$ being the mean volume fraction of the phase \( \alpha \). The fluctuation of \( Q \) can now be defined as \( Q'' = Q - \langle Q \rangle \).

### E.2 Conservation of mass

The product of the phase \( \alpha \) indicator function and Eq. E.1 yields

$$ I^{(\alpha)} \frac{\partial \rho}{\partial t} + I^{(\alpha)} \frac{\partial (\rho u_i)}{\partial x_i} = 0. \quad (E.6) $$

Using the chain rule, the above expression can be rewritten as

$$ \frac{\partial (\rho I^{(\alpha)})}{\partial t} + \frac{\partial (\rho I^{(\alpha)} u_i)}{\partial x_i} = \rho \left( \frac{\partial I^{(\alpha)}}{\partial t} + u_i \frac{\partial I^{(\alpha)}}{\partial x_i} \right). $$

Pai and Subramaniam (2009) showed that the right-hand side of the above expression is the interphase mass transfer at tow-phase interface, arising from the difference between the interphase velocity and the instantaneous two-phase velocity,

$$ \frac{\partial I^{(\alpha)}}{\partial t} + u_i \frac{\partial I^{(\alpha)}}{\partial x_i} = \left( u_i - u_i^{(I)} \right) \frac{\partial I^{(\alpha)}}{\partial x_i}. \quad (E.7) $$

In gas-solid flows with no reaction at particle surface, the above term is zero. Therefore, the mass conservation equation becomes

$$ \frac{\partial (\rho I^{(\alpha)})}{\partial t} + \frac{\partial (\rho I^{(\alpha)} u_i)}{\partial x_i} = 0. \quad (E.8) $$

By averaging the above equation, the conservation equation for the mean mass is derived, as then obtained, that is:

$$ \frac{\partial}{\partial t} \left\langle \rho I^{(\alpha)} \right\rangle + \frac{\partial}{\partial x_i} \left\{ \left\langle \rho I^{(\alpha)} \right\rangle \left\langle u_i^{(\alpha)} \right\rangle \right\} = 0. \quad (E.9) $$

### E.3 Conservation of momentum

Phasic conservation equation of momentum is obtained by multiplying Eq. E.2 with the phase indicator function, and then use the chain rule. By assuming that there is no momentum transfer due to mass transfer at the interphase, the momentum equation is obtained as follows:

$$ \frac{\partial (I^{(\alpha)} \rho u_i)}{\partial t} + \frac{\partial (I^{(\alpha)} \rho u_j u_i)}{\partial x_j} = \frac{\partial (I^{(\alpha)} \sigma_{ji})}{\partial x_j} - \sigma_{ji} \frac{\partial I^{(\alpha)}}{\partial x_j} - I^{(\alpha)} \rho g_i. \quad (E.10) $$
In the above equation, the term $\partial I^{(\alpha)}/\partial x$ is equivalent to $-n^{(\alpha)}\delta(x - x^{(I)})$, where $n^{(\alpha)}$ is the surface normal vector as explained earlier in this Appendix, and $\delta(x - x^{(I)})$ is the generalized delta function that is non-zero only at the surface of particles. This interface surface for the fluid phase representing the fluid-solid interactions can be decomposed into fluid-phase interaction with each of the solid phases in the suspension. Therefore, from Eq. E.10 the fluid-phase momentum equation is obtained as

$$\frac{\partial}{\partial t} \left( I^{(f)\rho u_i} \right) + \frac{\partial}{\partial x_j} \left( I^{(f)\rho u_j u_i} \right) = \frac{\partial}{\partial x_j} \left( I^{(f)\sigma_{ji}} \right) + \sum_{\alpha=1}^{N_{\alpha}} \sigma_{ji} n^{(f-\rightarrow \alpha)} \delta(x - x^{(I)}) + I^{(f)}\rho g_i, \quad (E.11)$$

where $n^{(f-\rightarrow \alpha)}$ indicates the interface between the fluid phase and particle size class $\alpha$. Now ensemble-averaging of the above equation proves the mean momentum equation for the fluid phase which is

$$\bar{D} \left\{ \left\langle I^{(f)\rho} \right\rangle \left\langle u_i^{(f)} \right\rangle \right\} + \frac{\partial}{\partial x_j} \left\{ \left\langle I^{(f)\rho u_j u_i^{(f)}} \right\rangle \right\} = \frac{\partial}{\partial x_j} \left\langle I^{(f)\sigma_{ji}} \right\rangle - \sum_{\alpha=1}^{N_{\alpha}} \left\langle \sigma_{ji} n^{(f-\rightarrow \alpha)} \delta(x - x^{(I)}) \right\rangle + \left\langle I^{(f)\rho} \right\rangle g_i. \quad (E.12)$$

In the above equation, $\bar{D} \left\langle \cdot \right\rangle /\bar{D}t$ is the material derivative of a presumed quantity in the following form:

$$\frac{\bar{D}}{\bar{D}t} \left\langle \cdot \right\rangle = \frac{\partial}{\partial t} \left\langle \cdot \right\rangle + \frac{\partial}{\partial x_k} \left\langle \left\langle u_k^{(\alpha)} \right\rangle \left\langle \cdot \right\rangle \right\rangle.$$

Also the term $\left\langle \sigma_{ji} n^{(f-\rightarrow \alpha)} \delta(x - x^{(I)}) \right\rangle$ is the mean fluid-particle drag acting on the particle size class $\alpha$ and is denoted by $\left\langle f_h^{(f-\rightarrow \alpha)} \right\rangle$, and is reconcilable with the gas-particle drag force in Eq. D.20 obtained from the Lagrangian approach.

In a similar fashion, the momentum equation for particle size class $\alpha$ can be derived by considering the fact that particles in this size class can have interphase interactions simultaneously with the fluid phase, particles in the same size class, and particles in other size classes. Therefore, from Eq. E.10 the momentum equation for size class $\alpha$ is as follows:

$$\frac{\partial}{\partial t} \left( I^{(\alpha)\rho u_i} \right) + \frac{\partial}{\partial x_j} \left( I^{(\alpha)\rho u_j u_i} \right) = \frac{\partial}{\partial x_j} \left( I^{(\alpha)\sigma_{ji}} \right) + \sigma_{ji} n^{(\alpha-\rightarrow f)} \delta(x - x^{(I)}) + \sigma_{ji} n^{(\alpha-\rightarrow \beta)} \delta(x - x^{(I)}) + \sum_{\beta=1}^{N_{\beta}} \sigma_{ji} n^{(\alpha-\rightarrow \beta)} \delta(x - x^{(I)}) + I^{(\alpha)}\rho g_i. \quad (E.13)$$
Now if we perform ensemble-averaging on the above equation, the mean momentum equation for particle class $\alpha$ is

$$\frac{D}{Dt} \left\{ \left\langle I^{(\alpha)} \rho \right\rangle \left\langle u_i^{(\alpha)} \right\rangle \right\} + \frac{\partial}{\partial x_j} \left\{ \left\langle I^{(\alpha)} \rho u_j^n u_i^n \right\rangle \right\}
= \frac{\partial \langle I^{(\alpha)} \sigma_{ji} \rangle}{\partial x_j} + \frac{\langle \sigma_{ji} n_{j}^{(\alpha\rightarrow\beta)} \delta(x - x^{(I)}) \rangle}{\langle f_{c}^{(\betaightarrow\alpha)} \rangle}
+ \frac{1}{2} \frac{\partial}{\partial x_j} \left\{ \left\langle I^{(\alpha)} \rho u_i^n u_j^n \right\rangle \right\}
= \frac{\langle u_i \rho \sigma_{ji} \rangle}{\langle f_{c}^{(\betaightarrow\alpha)} \rangle} + \left\langle u_i \right\rangle \left\langle g_i \right\rangle, \quad (E.14)$$

In the above equation, the term $\left\langle \sigma_{ji} n_{j}^{(\alpha\rightarrow\beta)} \delta(x - x^{(I)}) \right\rangle$ represents the mean momentum transfer from class $\beta$ to $\alpha$ due to particle-particle collision and is referred to as particle-particle drag. This term is denoted by $\langle \text{mathbf{f}}^{(\betaightarrow\alpha)} \rangle$ and is reconcilable with the particle-particle drag obtained from the Lagrangian approach in Eq. D.20. Note that the ensemble average of the term $\sigma_{ji} n_{j}^{(\alpha\rightarrow\alpha)} \delta(x - x^{(I)})$ in Eq. E.13 is zero because the net of momentum exchange arising from all colliding pairs of particles that belong to the class $\alpha$ is zero.

### E.4 Conservation of total kinetic energy

The conservation equation for the total kinetic energy from is obtained by first multiplying Eq. E.10 with velocity $u_i$. Then, the interphase interactions with distinct phases can be identified, followed by ensemble averaging of the equations. This process leads to the total energy equations in the fluid phase and particle class $\alpha$ with the forms respectively given by

$$\frac{D}{Dt} \left\{ \left\langle I^{(f)} \rho \right\rangle \bar{E}^{(f)} \right\} + \frac{D}{Dt} \left\{ \left\langle I^{(f)} \rho \right\rangle k^{(f)} \right\} \frac{\partial}{\partial x_j} \left\{ \left\langle u_i^{(f)} \right\rangle \left\langle I^{(f)} \rho u_j^n u_i^n \right\rangle \right\}
+ \frac{1}{2} \frac{\partial}{\partial x_j} \left\{ \left\langle I^{(f)} \rho u_i^n u_j^n \right\rangle \right\} = \left\langle u_i^{(f)} \frac{\partial \langle I^{(f)} \sigma_{ji} \rangle}{\partial x_j} \right\rangle
+ \left\langle u_i^{(f)} \sum_{\alpha=1}^{N_a} f_{h,i}^{(\alpha\rightarrow f)} \right\rangle + \left\langle u_i^{(f)} \right\rangle \left\langle g_i \right\rangle, \quad (E.15)$$
\[
\frac{D}{Dt} \left\{ \langle I^{(a)} \rangle \bar{E}^{(a)} \right\} + \frac{D}{Dt} \left\{ \langle I^{(a)} \rho \rangle k^{(a)} \right\} + \frac{\partial}{\partial x_j} \left\{ \langle u_i^{(a)} \rangle \langle I^{(a)} \rho u_i^{n(a)} u_j^{n(a)} \rangle \right\} \\
+ \frac{1}{2} \frac{\partial}{\partial x_j} \left\{ \langle I^{(a)} \rho u_i^{n(a)} u_j^{n(a)} \rangle \right\} = \left\{ \langle u_i^{(a)} \rangle \partial \langle I^{(a)} \rangle \sigma_{ji} \right\} + \left\{ \langle u_i^{(a)} \rangle f_{h,i}^{(\alpha \rightarrow \alpha)} \right\} \\
+ \left\{ \langle u_i^{(a)} \rangle f_{c,i}^{(\alpha \rightarrow \alpha)} \right\} + \left\{ \langle u_i^{(a)} \rangle \sum_{\beta=1}^{N_{\alpha}} f_{c,i}^{(\beta \rightarrow \alpha)} \right\} + \left\{ \langle u_i^{(a)} \rangle \langle I^{(a)} \rho \rangle g_i \right\} 
\]

(E.16)

### E.5 Conservation of kinetic energy in the mean

In the Eulerian-Eulerian approach, the evolution equations for the mean energy in the fluid phase and each of particle classes are obtained by multiplying the mean momentum equations in E.3 with their corresponding mean velocities, and then appropriately using the chain rule and conservation of mass. The results for the fluid phase and particle class \( \alpha \) are respectively obtained as

\[
\frac{D}{Dt} \left\{ \langle I^{(f)} \rangle \bar{E}^{(f)} \right\} + \frac{\partial}{\partial x_j} \left\{ \langle u_i^{(f)} \rangle \langle I^{(f)} \rho u_j^{n(f)} u_i^{n(f)} \rangle \right\} = \left\{ \langle I^{(f)} \rho u_j^{n(f)} u_i^{n(f)} \rangle \partial \langle u_i^{(f)} \rangle \right\} \\
\]

(E.17)

\[
\frac{D}{Dt} \left\{ \langle I^{(a)} \rangle \bar{E}^{(a)} \right\} + \frac{\partial}{\partial x_j} \left\{ \langle u_i^{(a)} \rangle \langle I^{(a)} \rho u_j^{n(a)} u_i^{n(a)} \rangle \right\} = \left\{ \langle I^{(a)} \rho u_j^{n(a)} u_i^{n(a)} \rangle \partial \langle u_i^{(a)} \rangle \right\} \\
\]

(E.18)

### E.6 Conservation of kinetic energy in velocity fluctuations

The evolution equations associated with velocity fluctuations in the fluid phase as well particle size class \( \alpha \) can be derived by subtracting the mean energy equations obtained in E.5 from those obtained for the total kinetic energy in E.4. This process leads to the kinetic energy equations for velocity fluctuations in the fluid-phase and for particle class \( \alpha \), which are
\[
\frac{D}{Dt} \left\{ \left\langle I(f) \rho \right\rangle k(f) \right\} + \frac{1}{2} \frac{\partial}{\partial x_j} \left\langle I(f) \rho u_j^{n(f)} u_i^{n(f)} u_i^{n(f)} \right\rangle = \\
- \left\langle I(f) \rho u_j^{n(f)} u_i^{n(f)} \right\rangle \frac{\partial}{\partial x_j} \left\langle u_i^{n(f)} \right\rangle + \left\langle u_i^{n(f)} \sum_{\alpha=1}^{N_a} f_{h,i}^{(\alpha \rightarrow f)} \right\rangle + \left\langle u_i^{n(f)} \frac{\partial}{\partial x_j} (I(f) \sigma_{ji}) \right\rangle,
\]
(E.19)

\[
\frac{\tilde{D}}{Dt} \left\{ \left\langle I(\alpha) \rho \right\rangle k(\alpha) \right\} + \frac{1}{2} \frac{\partial}{\partial x_j} \left\langle I(\alpha) \rho u_j^{n(\alpha)} u_i^{n(\alpha)} u_i^{n(\alpha)} \right\rangle = - \left\langle I(\alpha) \rho u_j^{n(\alpha)} u_i^{n(\alpha)} \right\rangle \frac{\partial}{\partial x_j} \left\langle u_i^{(\alpha)} \right\rangle \\
+ \left\langle u_i^{n(\alpha)} f_{h,i}^{(f \rightarrow \alpha)} \right\rangle + \left\langle u_i^{n(\alpha)} f_{h,i}^{(a \rightarrow \alpha)} \right\rangle + \left\langle u_i^{n(\alpha)} \sum_{\beta=1}^{N_{\alpha}} f_{c,i}^{(\beta \rightarrow \alpha)} \right\rangle + \left\langle u_i^{n(\alpha)} \frac{\partial}{\partial x_j} (I(\alpha) \sigma_{ji}) \right\rangle.
\]
(E.20)

It should be noted that the terms in the above equation are reconcilable with Eq. D.31 which was obtained from the Lagrangian approach. The only difference in the above equation is the last term which does not appear in the equation from the Lagrangian approach. To explain the implication of this term, first it should be noted that the third term in the above equation represents the instantaneous rate of change of kinetic energy between a pair of colliding particles belonging to class \( \alpha \). When particles are allowed to reversibly deform during a collision (soft-sphere collision assumption), a collision stress is formed inside the two colliding particles. Formation of this stress causes conversion of the kinetic energy into potential energy during the collision, which reach the maximum value when the separation between the centers of the colliding particles become minimum. When the two particles start to bounce back this potential energy converts back to the kinetic energy. The last term in the above equation represents this potential energy for the colliding particle belonging to particle class \( \alpha \). If particle collisions are elastic, then the rate of conversion of energy between the potential and kinetic energies is conservative, otherwise the difference between the the two represents the instantaneous collisional dissipation.
Bibliography


Murphy, E. and Subramaniam, S. Binary collision outcomes for inelastic soft-sphere models with cohesion. In preparation.


