Particle segregation and diffusion in fluid-saturated granular shear flows

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Differently sized particles in sheared granular mixtures undergo size segregation and diffusive remixing, the relative magnitude of which controls the degree to which distinct particle layers form. The presence of viscous interstitial fluids affects individual particle dynamics, resulting in complex segregation and diffusion behaviors. In this study, the effects of different types of fluids (characterized by fluid density and viscosity) on these two processes are investigated, for various flow conditions and material parameters, via coupled numerical simulations of immersed granular shear flows. We observe that both the segregation velocity and the diffusion strength decrease with the fluid viscosity, but these effects occur only when the viscosity exceeds certain threshold values, indicating a transition from viscous to inertial regimes. In the low-viscosity limit where fluid and grain inertia dominate, both segregation and diffusion processes depend on flow conditions and material properties in a manner that is similar to those in dry inertial granular flows. On the other hand, decreasing the relative density between the particles and the fluid slows down segregation but does not significantly affect diffusion. Based on scaling analysis of the simulation data, empirical relationships for the segregation velocity and diffusion coefficient are developed as functions of a modified Stokes number, and are then used to extend an existing segregation-diffusion continuum equation for granular mixtures immersed in different types of fluids.

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I. INTRODUCTION

Particle size difference in sheared granular mixtures leads to particle segregation, where larger particles rise to the top while finer particles settle to the base [1,2]. Modeling particle size segregation is relevant to many industrial [3,4] and geophysical [5,6] processes due to its impacts on flow rheology [7–9] and deposit morphology [10,11]. Granular flows occurring in nature are usually mixed with fluids at different proportions, ranging from dry to wet to completely immersed or fully saturated [12]. Interactions between the solid and fluid components of the mixture influence individual particle dynamics [13] and result in complex segregation behaviors. The effects of fluid in dry granular flows is negligible and the efficiency of particle segregation depends mainly on the coupled yet asymmetric motion of constituent size species [14]: Constant rearrangement of particles due to shear tends to generate voids, through which small particles preferentially percolate.

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downward under gravity [15,16], whereas enduring frictional-collisional interactions between particles moving across adjacent flowing layers slowly roll the large particles upward [17,18]. Competing with segregation is diffusive remixing which results from random collisions and shearing among particles; this instead drives the mixture to become evenly mixed. The relative magnitude of size segregation and diffusive remixing determines the sharpness at which particle layers separate [19].

In the presence of denser interstitial fluids, such as water, size segregation becomes less evident since buoyancy weakens the contact force magnitudes that drive the large particles up [20,21] and possibly slow down the descent of the small particles through voids as they travel downward [22]. Segregation weakens as the difference in the particle and fluid densities is decreased and is no longer evident when they are isodense. Earlier studies involving fluid-saturated bidisperse chute flows further demonstrated that the effects of viscosity (varied over a narrow range of values) on segregation are negligible compared to the influence of the relative density [23]. This result formed the basis for a granular-fluid segregation theory in which fluid viscous effects are ignored [18].

However, it has also been shown that highly viscous fluids, with viscosities that are hundreds to thousands times greater than water, further diminish the extent at which differently sized particles form distinct layers [24]. Such high values of the interstitial fluid viscosity are common in nature, such as muddy slurries in debris flows and lahar flows [25,26], and may be responsible for the reduced particle size segregation observed in debris deposits [27]. In our recent work, using computer simulations of sheared granular flows immersed in fluids, we found that viscous effects are evident only when the fluid viscosity is beyond certain threshold values, while below these thresholds, segregation is independent of viscosity and is controlled only by buoyancy and the inertial effects in the granular flow [28]. Viscous fluids may also slow down segregation by inducing the formation of plug zone regions [21,29], where shear-rate-dependent segregation mechanisms [30] are inhibited.

The enhanced understanding of fluid effects on segregation are derived based on the assumption that fluids directly influence segregation driving mechanisms, and in most cases the contribution of diffusion in diminishing segregation is ignored [20,28]. Indeed, although the diffusion of particles in dense granular flows has been extensively studied for different flow configurations [31], flow regimes [32,33], and size distributions [34], our knowledge of the fluid effects on diffusion remains incomplete. It is also interesting to see whether fluid buoyant and viscous forces affect diffusion in the same manner as segregation. Improved understanding of both segregation and diffusive remixing in the presence of different interstitial fluids will enable continuum modeling of particle size segregation across a wide range of granular-fluid flows.

The objective of this work is to investigate the influence of different types of fluids, characterized by their density and viscosity, on the size segregation and diffusive remixing in immersed granular shear flows through extensive two-phase granular-fluid simulations. In the following we present results on the effects of varying the fluid density and viscosity on the segregation velocity magnitude and on the diffusion coefficient across different flow conditions. Empirical relationships developed from the simulation results are then used to extend a previous continuum segregation model [19] for cases where viscous interstitial fluids are present. We further show that using this extended framework, the spatial-temporal evolution of particle size distributions of immersed bidisperse mixtures can be adequately modeled.

**II. BACKGROUND: CONTINUUM SEGREGATION-DIFFUSION EQUATION FOR DRY GRANULAR FLOWS**

Based on the mixture theory, Gray and Chugunov [19] derived a continuum framework for particle size segregation in dry bidisperse mixtures in the form of an advection-diffusion equation with an additional dependence on a species-dependent segregation flux. In a coordinate system where the $x$ axis is along the flow direction, the $y$ axis is along the lateral direction, and the $z$ axis is...
along the flow height, the continuum equation is written as

\[ \frac{\partial C_i}{\partial t} + \nabla \cdot (U_G C_i) + \frac{\partial}{\partial z} (w_{p,i} C_i) = \nabla \cdot (D \nabla C_i), \]  

(1)

where \( U_G = (u, v, w) \) is the velocity vector and \( C_i \) is the concentration of a particle belonging to a size species \( i \) (\( i = L \) and \( S \) represent large and small particles, respectively). The segregation velocity \( w_{p,i} \) determines the velocity at which large (small) particles rise (sink) and the diffusion coefficient \( D \) controls the tendency of particle migration from high to low concentrations. The first two terms on the left-hand side define the change of particle concentrations in time and space. The third term defines the transport of particles along the flow height due to segregation at an average rate \( w_{p,i} \). The final term on the right-hand side represents diffusion which serves to generate evenly distributed mixtures by driving \( C_i \) toward lower concentrations at a magnitude \( D \). Note that \( C_i \) is calculated from the ratio of the species volume fraction \( \phi_i \) with the total granular volume fraction, i.e., \( C_i = \frac{\phi_i}{\phi_L + \phi_S} \), and the total concentration for all size species sums to unity \( \sum_{L,S} C_i = 1 \). Details on the calculation of \( \phi_i \) from discrete element method (DEM) data is provided in the Appendix.

Equation (1) was originally developed for gravity-driven free surface flows [19] but similar models have been successfully developed to model segregation in different flow geometries [35,36].

The application of the continuum framework in Eq. (1) predicts the spatial-temporal evolution of \( C_i \) when appropriate expressions for the percolation velocity \( w_{p,i} \) and diffusion coefficient \( D \) are provided. At steady state, the absence of diffusion implies the formation of pure layers of large and small particles separated by an abrupt concentration jump [37]. The diffusion term ensures a smoother transition between particle concentrations, which is more consistent with experimental observations [38].

In dry granular flows, segregation of a particular particle size species is often considered to be a local phenomenon, and the segregation velocity depends on the concentration of the opponent size species \( (1-C_i) \). This concentration dependence can be generally expressed as

\[ w_{p,i} = \pm Q(1-C_i), \]

(2)

where \( Q \) is the segregation velocity magnitude [37] that has nontrivial dependencies on the flow material properties [36], and inertial conditions [35,39]. These dependencies will be evaluated in detail in the succeeding sections. The positive and negative symbols denote the direction of the segregation for different size species, i.e., positive for large particles since they go up and negative for the downward moving small particles. Equation (2) also implies that \( w_{p,i} \) of the large and small particles are linear and have similar magnitudes. It should be mentioned that several previous studies have already shown that differently sized particles segregate at different rates [15,17,40] and segregation flux models have already been proposed that capture this asymmetric behavior [14,41,42]. In this study, however, we adopt the simplest linear symmetric model for convenience and since it is found to be sufficiently accurate for shallow granular flows having approximately equal large and small particle volume fractions [43]. We also note that Thornton \textit{et al.} [20] have previously proposed an expression for \( w_{p,i} \) for granular-fluid flows incorporating the effects of buoyancy, wherein segregation weakens as the fluid density approaches the solid density, but the fluid viscosity effects are neglected.

SubJECTED to random collisions and shearing, particles tend to migrate randomly within the granular mixture, which is analogous to the way Brownian particles diffuse in dilute suspensions. Previous experiments [44,45] and numerical simulations [46] on diffusion reveal that for dry granular flows, \( D \) linearly increases with the flow shear rate \( \dot{\gamma} \) and with the square of the averaged particle diameter \( d \) [44]. This is formally expressed as

\[ D = k_d \dot{\gamma} d^2, \]

(3)

where \( k_d \) is a dimensionless constant, which has been shown to depend on the mixture volume fraction [34]. Appropriate functional relationships for \( w_{p,i} \) and \( D \) can extend the application of the continuum model in Eq. (1) for the case of granular-fluid flows across a wide range of
interstitial fluids, which are developed below based on scaling analysis of well-controlled granular flow simulations and incorporate the dependence of the segregation and diffusion processes on the buoyant and viscous effects.

III. METHODOLOGY

A. Simulation setup

The influence of fluids on segregation and diffusion is investigated through three-dimensional numerical simulations of immersed granular shear flows using coupled computational fluid dynamics (CFD) and the discrete element method (DEM). The CFD and DEM are implemented using two independent open-source solvers, OPENFOAM [47] and LIGGGHTS [48], respectively. The CFD-DEM coupling is implemented using the CFDEMproject open-source library [49]. The DEM solves for the trajectory and interactions of cohesionless spherical particles while CFD solves for the fluid velocity and pressure. Fluid and particle data obtained from each solver are communicated with each other using a message passing algorithm after a fixed number of DEM time steps in which solid-fluid interaction forces are calculated. In this study, these interaction forces come in the form of buoyancy and fluid drag. The CFDDEM is already widely used in studying real-world granular-fluid systems [49–55], and validation of the numerical model’s efficacy will no longer be discussed here. Details on the governing equations of the CFD-DEM implementation are provided in the Appendix.

Figure 1 shows an illustration of the simulation setup. The DEM phase is a bidisperse granular bed of large and small particles, with average diameters $d_L$ and $d_S$, respectively, bounded by rough top and bottom walls in the vertical direction ($z$ axis) and by periodic boundaries along the streamwise ($x$ axis) and spanwise ($y$ axis) directions. The DEM domain has a constant initial length, $L = 60d_S$, width, $W = 15d_S$, and height, $H = 20d_S$, respectively. The top and bottom walls are roughened by gluing a layer of small particles. The Hertz contact model is used to simulate particle interactions with a Young’s modulus of $5 \times 10^7$ Pa, Poisson’s ratio 0.4, friction coefficient 0.5, and the coefficient of restitution 0.8. The above-mentioned contact parameters are adopted from commonly used values in the literature of size segregation [39,56] and granular flows [57,58]. The top wall imposes a constant confining pressure $P_0$ and drives the particles to flow by translating at a constant velocity according to $u_{\text{wall}} = \dot{\gamma} H_{\text{wall}}$, where $\dot{\gamma}$ is the imposed shear rate and $H_{\text{wall}}$ is the vertical position of the wall which varies slightly with time in response to the compaction and dilation of the granular bed. The confining pressure is imposed by applying a constant downward force on the top wall particles.

The fluid phase is modeled as an incompressible Newtonian fluid. The CFD domain is discretized into uniformly sized cells with dimensions of $2d_L$ in all directions [51]. In each cell, the Navier-Stokes equation (detailed in the Appendix) is solved to calculate for fluid properties such as the velocity and pressure. Consistent with the DEM, periodic boundaries are set along the streamwise and spanwise directions of the CFD domain. Fluid is not allowed to exit through the bottom wall, while the upper wall is set to be the atmosphere where the fluid is allowed to freely enter and exit. The CFD domain is higher than the DEM and the granular flow is completely immersed in the fluid domain. The sheared particles drag the fluid into motion whereas the fluid constantly exerts drag and buoyant forces on the particles. The top wall is set to be unaffected by the fluid forces: Buoyant forces do not reduce the confining pressure while drag forces do not impede its streamwise translation. The fluid is also allowed to freely pass through the top wall preventing the buildup of pore pressures due to confinement [59]. The $P_0$ values used here are low and do not result in discontinuous shear thickening [60,61] that is observed in dense sheared granular-fluid mixtures when the confining pressure is high. In this work, we focus on the fluid effects of buoyancy and drag force using a coarse-grid CFD-DEM approach, but we note that other mechanisms of fluid-particle interaction may also affect segregation. An example is contact lubrication in which a layer of compressed viscous fluid dampens the contacts of incident particles approaching each other [59], which can be tackled using fully resolved CFD-DEM methods in future work.
Confining pressures and viscous ambient fluids might result in formation of spatially varying streamwise velocity profiles which induce localized segregation behaviors [21,62,63]. Examples of this would be plug zone regions which may form due to the apparent yield stress of the interstitial fluids [29] or from viscous drag forces, acting opposite to the flow direction, resulting from relative motion of fluid and particle phases [21,64]. To ensure that a constant $\dot{\gamma}$ is maintained along the flow height, a small stabilizing force, $F_{st} = A_{st}[\dot{\gamma}(z) - u(z)]$, is applied to each particle at a height $z$ having a streamwise velocity $u$ at each time step [39]. Nonlinear velocity profiles tend to persist in more viscous fluids due to the stronger drag forces opposing the flow along the streamwise direction; hence the values of the control parameter $A_{st}$ used here are varied accordingly between 0.7 and 0.9 kg/s. This stabilizing algorithm has recently been used to study granular rheology [65] and particle size segregation [39, 56, 66]. Note that $F_{st}$ does not affect the segregation behavior because the added forces are small enough that the rheological flows are not affected and since it is applied perpendicular to the direction of segregation. Particle trajectories change only slightly within a single computational iteration ($\Delta t = 1 \times 10^{-5}$ s); hence fluid-interaction forces are computed only after every 10 DEM time steps.

**B. Test plan and flow characterization**

Granular shear flows immersed in different types of fluid are simulated by varying the fluid viscosity and density over ranges of $0.001 \text{ Pa s} \lesssim \eta_F \lesssim 1 \text{ Pa s}$, and $1000 \text{ kg/m}^3 \lesssim \rho_F \lesssim$
TABLE I. Fluid parameters and the corresponding symbols.

<table>
<thead>
<tr>
<th>ρ_F (kg/m³)</th>
<th>̂ρ</th>
<th>η_F (Pa s)</th>
<th>Symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>1000</td>
<td>0.60</td>
<td>0.001 ≤ η_F ≤ 1</td>
<td>○</td>
</tr>
<tr>
<td>1300</td>
<td>0.48</td>
<td></td>
<td>△</td>
</tr>
<tr>
<td>1600</td>
<td>0.36</td>
<td></td>
<td>□</td>
</tr>
<tr>
<td>1900</td>
<td>0.24</td>
<td></td>
<td>◊</td>
</tr>
<tr>
<td>2200</td>
<td>0.12</td>
<td></td>
<td>▼</td>
</tr>
<tr>
<td>1.29a</td>
<td>0.99</td>
<td>1.85 × 10⁻⁵</td>
<td>+</td>
</tr>
</tbody>
</table>

2200 kg/m³, respectively. The effects of fluid density are taken into account via a dimensionless density, ̂ρ = (ρ_G − ρ_F)/ρ_G, where ρ_G and ρ_F are the solid and fluid material densities, respectively, following the results of Thornton et al. [20] on the buoyant effects on size segregation. With this definition, ̂ρ = 1 indicates that the fluid density is negligible, while ̂ρ = 0 means that the fluid and particles have equal densities. The η_F and ̂ρ values used in this study are summarized in Table I.

Fluid effects on segregation are studied for a wide range of flow conditions and material parameters, including confining pressure P₀, shear rate ̇γ, gravity g, solid density ρ_G, and the mean diameter ̄d = (φ_Ld_L + φ_Sd_S)/ (φ_L + φ_S), where φ_L and φ_S are volume fractions of the large and small particles, respectively. Material and flow parameters used in the simulations are listed in Table II, including a base case from which different parameters are varied. Note that ρ_G is varied while ̂ρ is kept constant according to Table I, while ̄d is varied by changing both the large and small diameters while maintaining a size ratio of 2. Dry flows having pressures and shear rates of P₀ = [100, 300, 500] Pa and ̇γ = [1, 1.5, 2.5, 5, 10] s⁻¹, respectively, are also simulated using DEM for reference. In the following, test cases having different ̂ρ are represented by different symbols (Table I), while varying material properties and flow conditions are represented by different colors (Table II). Unless otherwise specified, this manner of representation will be adopted in the subsequent figures for consistency.

Figure 1(b) shows that the velocity profiles of the immersed granular flows with different η_F and ̂ρ are nearly linear along the height owing to the stabilizing algorithm (see Sec. III A), which eliminates segregation effects resulting from fluid-induced inhomogeneous shear gradients [21,66] from the subsequent analysis. Figures 1(c) and 1(d) further show that the rheology of all simulated flows, characterized by their effective friction μ and volume fractions φ_G, scales with a dimensionless viscousinertial number K = √I² + 4J which is a function of the inertial I = ̇γd√ρ_G/P_G and viscous number J = ̇γη_F/P_G, where P_G = P₀ + φ_G(ρ_G − ρ_F)gH is the total granular pressure [67].

TABLE II. Test cases and corresponding symbol colors.

<table>
<thead>
<tr>
<th>̇γ (s⁻¹)</th>
<th>P₀ (Pa)</th>
<th>g (m/s²)</th>
<th>ρ_G (kg/m³)</th>
<th>d_S (m)</th>
<th>d_L (m)</th>
<th>Color</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>100</td>
<td>9.8</td>
<td>2500</td>
<td>0.005</td>
<td>0.01</td>
<td>Blacka</td>
</tr>
<tr>
<td>1</td>
<td>500</td>
<td>9.8</td>
<td>2500</td>
<td>0.005</td>
<td>0.01</td>
<td>Red</td>
</tr>
<tr>
<td>1.5</td>
<td>100</td>
<td>9.8</td>
<td>2500</td>
<td>0.005</td>
<td>0.01</td>
<td>Green</td>
</tr>
<tr>
<td>5</td>
<td>100</td>
<td>9.8</td>
<td>2500</td>
<td>0.005</td>
<td>0.01</td>
<td>Blue</td>
</tr>
<tr>
<td>10</td>
<td>100</td>
<td>9.8</td>
<td>2500</td>
<td>0.005</td>
<td>0.01</td>
<td>Purple</td>
</tr>
<tr>
<td>1</td>
<td>100</td>
<td>19.6</td>
<td>2500</td>
<td>0.005</td>
<td>0.01</td>
<td>Turquoise</td>
</tr>
<tr>
<td>1</td>
<td>100</td>
<td>9.8</td>
<td>3000</td>
<td>0.005</td>
<td>0.01</td>
<td>Orange</td>
</tr>
<tr>
<td>1</td>
<td>100</td>
<td>9.8</td>
<td>2500</td>
<td>0.003</td>
<td>0.006</td>
<td>Gray</td>
</tr>
</tbody>
</table>

aThe base case.
FIG. 2. The progress of segregation measured from the trajectory of the large particles’ center of mass when (a) the relative density difference \( \hat{\rho} \) (with constant \( \eta_F \)) and (b) the fluid viscosity \( \eta_F \) (with constant \( \hat{\rho} \)) are varied. These profiles are measured for the base case (refer to Table II). (c) The segregation velocity \( w_{p,i} \), as a function of \( 1 - C_i \), of a representative case. Solid lines represent the best fit of Eq. (2) for large particles where the slope is the segregation velocity magnitude \( Q \).

IV. RESULTS

A. Influence of fluid on segregation

The segregation process is measured from the trajectory of the large particles’ center of mass \( \bar{z}_L \) relative to that of the mixture \( \bar{z}_M \), i.e., \( z_L = \bar{z}_L - \bar{z}_M \), and \( \bar{z}_M \) changes mainly due to shear dilation. In our simulations, mixtures are initially normally graded, which is reflected by a negative \( z_L \) at the onset (\( z_L < 0 \)). As seen in Figs. 2(a) and 2(b), \( z_L \) subsequently becomes approximately zero (\( z_L \approx 0 \)) when large and small particles are well mixed and positive when large particles segregate to the surface (\( z_L > 0 \)). Although \( z_L = 0 \) might also represent a situation where small particles are sandwiched between large particle layers, this situation is not observed in our simulations.

Figures 2(a) and 2(b) show the change of \( z_L \) with time for different \( \hat{\rho} \) (constant \( \eta_F = 0.001 \) Pa s) and \( \eta_F \) (constant \( \hat{\rho} = 0.6 \)) values, respectively. At the onset of shearing, \( z_L \) rapidly increases, corresponding to the rise of large particles upward. The process slows down as more large particles accumulate near the top lid and eventually achieves a steady state where there is only minimal net change in the large particles’ position. Decreasing \( \hat{\rho} \) results in slower segregation and its effects on the final segregation height are minimal when \( \hat{\rho} \geq 0.12 \). Mixtures where the particle density is only slightly larger than the fluid (\( \hat{\rho} = 0.02 \)) show that as long as the particles are denser, segregation is possible despite significantly reduced segregation rate and final segregation height. When the
particles and the fluid are equally dense ($\hat{\rho} = 0$), segregation is no longer observed and the mixture appears to approach a mixed state due to the rearrangement of particles under random collisions. In the following, we focus on the situations where particles are significantly denser than the fluid ($\hat{\rho} > 0.12$). On the other hand, increasing $\eta_F$ slows down the segregation process, noticeable only when $\eta_F > 0.1$ Pa s but does not significantly affect the maximum segregation height [Fig. 2(b)].

The segregation velocity is calculated as

$$w_{p,i} = w - w_i,$$  \hspace{2cm} (4)

where $w$ is the bulk vertical velocity, which is close to zero but with some fluctuations resulting from the dilation and contraction of the mixture, while $w_i$ is the averaged velocity of a size species $i$. Both $w_{p,i}$ and $C_i$ are measured locally along the flow height, which is divided into discrete measurement layers with a thickness equal to $d_S$, over a 5-s time window during which segregation is the most rapid. Figure 2(c) shows $w_{p,i}$ plotted against $(1 - C_i)$ for a typical simulation. Note that fitting the data of both particle sizes separately using Eq. (2) yields different values of $Q$. The solid lines in Fig. 2(c) represent the best fit for the large particle data applied for both particle sizes. It can be seen that $Q$ for large particles can sufficiently approximate the segregation for both particle constituents except for the sudden increase of small particle segregation velocities at large $1 - C_L$. This nonlinear behavior is related to the fact that small particles percolate faster when they are surrounded by larger particles owing to the existence of larger void spaces.

Figure 3(a) shows the change of $Q$ with $\eta_F$ for different $\hat{\rho}$ (refer to Table I for symbols) and (b) different flow conditions (refer to Table II for meaning of each color).
mixture conditions; i.e., segregation rates derived from the trajectory of the centers of mass would be different for initially well-mixed and normally graded granular mixtures. Therefore, the subsequent analysis in Sec. IV B is similar to the results of our recent study [28], but with a different definition of the segregation velocity, and is more applicable to different initial conditions, which is tested in Sec. IV D.

**B. Scaling relationship for the segregation velocity**

As mentioned in Sec. II, $Q$ encodes the dependence of the segregation process on the various material properties and flow conditions. To collapse the data in Fig. 3, we consider the $\eta_F$-independent limit where the segregation velocity approaches a nearly constant maximum value $Q^*$ for each simulation condition. $Q^*$ is expected to depend only on the relative density and fluid-inertial effects. Figure 4(a) shows that plotting $Q/Q^*$ against $\eta_F$ satisfactorily collapses the data points for the inertial flows but fails to fully account for the segregation behaviors for high fluid viscosities. We attempt to enhance the scaling of segregation at high fluid viscosities by using the Stokes number:

$$St = \frac{\rho_G d^2}{18\eta_F} \sqrt{\frac{\hat{\rho} g}{2d}},$$

(5)

which quantifies the relative influence of viscous and inertial stresses on the motion of immersed spherical particles [13,68,69]. Figure 4(b) shows that scaling by $St$ instead of $\eta_F$ indeed results in an improved collapse of the data points. However, relatively poor collapse of $Q$ is still observed for high shear rates possibly due to the lack of dependence of Eq. (5) on $\dot{\gamma}$. It should be mentioned that we also have alternative forms of the Stokes number [18–20,70,71] and the viscoinertial number $K$ to improve the scaling with $\dot{\gamma}$, but none of these result in a better collapse of the data.

It is illustrated in Fig. 4(b) that the change of $Q/Q^*$ with $St$ can be expressed as (solid lines)

$$\frac{Q}{Q^*} = \frac{St}{\lambda_1 + St},$$

(6)
FIG. 5. The (a) change of the normalized maximum segregation rate in inertial flows $Q^*$ with $I^\alpha$. (b) The change of $Q^*$, normalized by its dependence on the inertial number, with $\hat{\rho}$. The solid line represents a power law with an exponent $\beta = 0.65$. (c) The change of $Q^*/\sqrt{g\bar{d}}$ with $BI^\alpha \hat{\rho}^\beta$. The trend line follows a power law with a slope of 1.

where $\lambda_1$ is a dimensionless constant with a value of 0.44. A transition in the $St$ dependence can be observed for $St = 1–10$ (shaded areas), below which segregation is significantly influenced by $\eta_F$ whereas the segregation velocity is independent of it when $St$ is beyond the transition regime.

Since $Q^*$ is different for each case, it is convenient to derive a functional relationship expressing its dependence on the various flow parameters. From Figs. 3(a) and 3(b) we observe that $Q^*$ is proportional to $\dot{\gamma}$, $\rho_G$, $\bar{d}$, and $g$ but inversely proportional to $P_0$. Previously, the work of Fry et al. [39] showed that the dependence of the averaged segregation rate on various flow conditions can be summarized into a functional form through the inertial number $I$. Since $Q^*$ is a measure of the segregation rate, we assume that

$$Q^*/\sqrt{g\bar{d}} = BI^\alpha,$$

where $\alpha$ is a tuning parameter and $B$ is a proportionality constant. Figure 5(a) shows that plotting the dimensionless segregation rate against $I^\alpha$ for dry granular flows (cross marks) results in the collapse of all data points when $\alpha = 0.88$ and $B = 0.22$. In the presence of fluid, an additional dependence on $\hat{\rho}$ is needed. Figure 5(b) shows that by normalizing $Q^*$ with its inertial dependencies, through $BI^\alpha \sqrt{g\bar{d}}$, the influence of $\hat{\rho}$ is isolated from which a power-law relationship, with an exponent $\beta = 0.65$, can be obtained (solid lines). Combining the relationships determined in Figs. 5(a) and 5(b), Eq. (7) is rewritten as

$$Q^*/\sqrt{g\bar{d}} = BI^\alpha \hat{\rho}^\beta$$

where $\hat{\rho}$ is a dimensionless density ratio with a value of 0.88 and $B = 0.22$. In the presence of fluid, an additional dependence on $\hat{\rho}$ is needed. Figure 5(b) shows that by normalizing $Q^*$ with its inertial dependencies, through $BI^\alpha \sqrt{g\bar{d}}$, the influence of $\hat{\rho}$ is isolated from which a power-law relationship, with an exponent $\beta = 0.65$, can be obtained (solid lines). Combining the relationships determined in Figs. 5(a) and 5(b), Eq. (7) is rewritten as

$$Q^*/\sqrt{g\bar{d}} = BI^\alpha \hat{\rho}^\beta.$$
where, as seen in Fig. 5(c), a good collapse is observed for both dry and immersed granular mixtures. The solid line is a power law with an exponent of 1. It should be mentioned that in immersed flows, $P_G$ (encoded in $I$) also depends on the density difference between the particles and fluid although using the total granular pressure instead of $P_0$ in Eqs. (7) and (8) results in a better collapse of the data points. Recent experiments of Trehwela et al. [40] studying the segregation of single large or small intruders immersed in a granular bed with a low-viscosity fluid ($\sim 0.005$ Pa s) revealed a similar dependence on these inertial parameters, although with different considerations for $\hat{\rho}$ and $P_G$. These distinctions may stem from the difference in the flow geometries: Here we use nearly equal volume mixtures while they use single intruder particles [40]. The value of the tuning parameter $\alpha$ in $I$ obtained here is also comparable with those obtained in other studies ($\alpha = 0.84$ [39] and $\alpha = 0.85$ [72]) despite subtle differences in the way the segregation velocity is measured.

Combining Eqs. (6) and (8) into (3), we obtain an expression that incorporates both the inertial and viscous effects on the percolation velocity:

$$w_{p,i} = \pm BI^\alpha \hat{\rho}^\beta \sqrt{\frac{g d}{(\lambda_1 + \text{St})^2}} (1 - C_i).$$  \hfill (9)

The viscous term $\frac{\text{St}}{(\lambda_1 + \text{St})^2}$ reduces to approximately 1 in the absence of a viscous fluid, which resembles the dependence of $w_{p,i}$ dry granular flow inertia [39,40]. Moreover, the equation above predicts that no segregation would occur when the fluid and the particles have an equal density.

### C. Influence of fluids on diffusion

Collisions among particles in sheared mixtures drive them to randomly diffuse throughout the granular body [44], which effectively results in a homogeneous mixture. The diffusion of particles counteracts their tendency to segregate [19] and leads to poorer separation of size species. Diffusion is quantified by the diffusion coefficient:

$$D = \langle \Delta y(\Delta t)^2 \rangle / 2\Delta t,$$  \hfill (10)

which is a function of the mean squared displacement of particles measured along the y direction over a time interval $\Delta t$, and $\langle \cdots \rangle$ denotes an ensemble average. Although diffusion occurs in all three dimensions, here we consider the lateral diffusion ($y$ axis) for better statistics, because particle motion is independent of other driving forces along this direction. On the contrary, advection drives particle motion along the streamwise direction ($x$ axis), and segregation influences the particle trajectories along the vertical direction ($z$ axis) [73], both of which would affect the measurement of diffusivity. For simplicity, we assume that diffusion is isotropic [73] and the diffusion parameter that we measure is representative of those in other directions, although situations where diffusion is anisotropic have been reported in the literature [44]. Particle displacement is calculated as [34,45]

$$\Delta y(\Delta t) = y(t + \Delta t) - y(t) - \Delta Y(\Delta t),$$  \hfill (11)

where $y$ is the position of a particle along the $y$ axis, and $\Delta t$ is varied over $0.1 \leq \Delta t \leq 3$ s. The range of $\Delta t$ is set arbitrarily, although it is also found that the change of $\langle \Delta y(\Delta t)^2 \rangle$ is no longer linear when $\Delta t$ is greater than 4 s which may be attributed to finite size effects. The net lateral displacement of all particles $\Delta Y(\Delta t)$ is approximately equal to zero with small random fluctuations in its value. To minimize the effects of the confining walls, $D$ is only measured for particles within $0.2 \leq z/H \leq 0.8$.

Figures 6(a) and 6(b) show that $\langle \Delta y(\Delta t)^2 \rangle$ is linear with $\Delta t$ for flows where $\hat{\rho}$ and $\eta_F$ are varied, respectively, demonstrating that the particles are indeed diffusive and, based on Eq. (10), $D$ can be derived as half the slope of the best-fit line. It can be observed that the slopes (dashed lines) are largely invariant for different $\hat{\rho}$ but decrease with $\eta_F$. Figure 7(a) illustrates that $D$, similar to $Q$, exhibits a transition in its dependence on the fluid viscosity. In contrast, $D$ shows no systematic change with $\hat{\rho}$, which implies that the effects of buoyancy on diffusion are less significant compared to other factors.
FIG. 6. The change of the mean squared displacement with the time interval $\Delta t$ for different (a) $\hat{\rho}$ and (b) $\eta_F$ for flows belonging to the base case. Dashed lines are best fits provided by Eq. (10).

FIG. 7. The change of the diffusion coefficient $D$ with $\eta_F$ for (a) different $\hat{\rho}$ (refer to Table I for list of symbols) and (b) different flow conditions (refer to Table II for meaning of each color).
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FIG. 8. The change of the normalized diffusion coefficient $D/D^*$ with (a) $\eta_F$ and (b) St for all simulation setups. The solid lines represent the best fit provided by Eq. (10). The gray band represents the limits over which the dependence of diffusion on the viscosity changes. The dashed line is the ideal limit over which granular-fluid flows transition from fluid inertial to viscous regimes. The diagonal bands are empirical limits determined by [13] on the phase transition. (c) The change of $D^*$ with $\dot{\gamma}d^2$ for different flow conditions and relative densities. The dashed line is the best fit provided by Eq. (3) where $k_d = 0.047$.

Figure 7(b) shows that diffusion is most sensitive to changes in $\dot{\gamma}$ and $d$, but is less dependent on $P_0$, $g$, and $\rho_G$. To systematically derive an empirical function for the diffusion coefficient, we first normalize it with the plateau value of $D$ in the $\eta_F$-independent limit [Fig. 7(a)], denoted as $D^*$, which isolates the dependence of $D$ on the shear rate and mean diameter. Figure 8(a) shows that although plotting $D/D^*$ versus $\eta_F$ results in a general collapse of the data points when viscous effects are negligible, the scaling at high viscosities can still be improved. Similar to $Q$, we find that scaling with St slightly improves the collapse of the data points, although some scatter is still evident especially for data at high shear rates. Nevertheless, as shown in Fig. 8(b), the curve over which the data collapse into can be defined by an asymptotic function having a similar form as Eq. (6):

$$\frac{D}{D^*} = \frac{St}{(\lambda_2 + St)}.$$  \hspace{1cm} (12)

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where the fitting parameter $\lambda_2$ has a value of 0.17. Kharel and Rognon [75] showed that diffusion in dry granular flows, particularly those having very low inertial numbers ($I \leq 0.01$), depends on the formation of partially jammed clusters of grains, referred to as granular vortices [74,75]. Specifically, they show that a better scaling of $D$ is achieved when the size of the vortices is incorporated into the diffusion length scale, instead of only $\bar{d}$. The size of these vortices is limited by the system size. Although the range of inertial number we explore here is above the value in which vortex length scales are relevant, the dampening of particle motion by viscous fluids may also promote the formation of these vortices. The size of our simulation domain allows us to achieve segregation steady states at relatively short times but may truncate vortex formation, even with the use of periodic boundaries, possibly affecting our measurements of $D$. A more dedicated study to understand diffusion in the context of granular vortices is needed to obtain a deeper understanding of diffusion in the presence of viscous fluids, which may enhance the scaling in Fig. 8(b).

Figure 8(c) shows that when viscous effects are negligible, the diffusion coefficient $D^*$ scales linearly with $\dot{\gamma}\bar{d}^2$ where the slope of the best-fit line provided by Eq. (3) is $k_d = 0.047$. Note that our immersed granular flow results agree with our dry granular flow results (cross marks) in the low-viscosity limit, and that the value of $k_d$ obtained here is comparable to those reported in previous dry granular shear flow simulations ($k_d = 0.042$–0.049) [34,73] and experiments ($k_d = 0.051$–0.057) [76]. By combining Eqs. (3) and (10), we obtain an empirical expression for the diffusion coefficient over the full range of parameters that we explore here, which can be written as

$$D = \frac{\text{St}}{(\lambda_2 + \text{St})} k_d \dot{\gamma} \bar{d}^2. \quad (13)$$

Equation (13) states that when St is large, the viscous term approaches the value of 1 and diffusion behaves similarly as in dry flows. At high viscosities, diffusion decreases as St tends toward zero.

D. Continuum modeling of segregation in immersed shear flows

Up to this point we have determined empirical expressions for the segregation velocity $w_{p,i}$ [Eq. (7)] and the diffusion coefficient $D$ [Eq. (13)] in immersed sheared flows. Applying these formulas to Eq. (1) allows one to model size segregation in the presence of different types of fluid. We test such theoretical predictions by comparing them with the segregation data obtained from the CFD-DEM simulations.

As previously shown in Fig. 2, the presence of fluids slows down segregation but does not significantly affect the final segregation height when the relative density difference is large ($\geq 0.12$). Therefore, here we are first interested in the temporal evolution of $C_i$. Since segregation only occurs along the vertical direction and no concentration gradients occur along the streamwise and lateral directions (where periodic boundaries are applied in our CFD-DEM simulations), i.e., $\frac{\partial C_i}{\partial x} = 0$ and $\frac{\partial C_i}{\partial y} = 0$, Eq. (1) can be simplified as

$$\frac{\partial C_i}{\partial t} + \frac{\partial}{\partial z}(w_{p,i} C_i) = D \frac{\partial^2 C_i}{\partial z^2}. \quad (14)$$

Note that Eq. (14) ignores the effect of the flow velocity profiles on the vertical segregation of particles. However, since the velocity profiles of the generated flows are linear along the height and are consistent for all simulated cases, their influence can be ignored. Equation (14) is numerically solved using the pdepe routine of MATLAB subject to an initially normally graded concentration profile:

$$C_L(0, z) = \begin{cases} 1, & 0 \leq z/H \leq 0.55 \\ 0, & 0.55 < z/H \leq 1. \end{cases} \quad (15)$$
FIG. 9. Spatial-temporal distribution of $C_L$ measured (a) from the simulation and (b) from the numerical model in Eq. (1) of a representative base case (refer to Table II) with $\eta_F = 0.1$ Pa s for an initially normally graded mixture. (c) Spatial distribution of $C_L$ along the height measured from the simulations (solid black line) and from the theory (solid red line) for different times corresponding to different stages in the segregation process.

and no-flux boundary conditions at the top and bottom walls:

$$w_{p,i}C_i + D\frac{\partial C_i}{\partial z} = 0 \quad \text{at} \quad \frac{z}{H} = 0, 1. \quad (16)$$

Figures 9(a) and 9(b) compare the evolution of the large particle concentration $C_L$ with time measured from the simulation of a base case (refer to Table II) with $\eta_F = 0.1$ Pa s with a numerical solution obtained from Eq. (1), respectively. Good agreement can be observed between the simulation and the theory, although the model tends to predict a sharper transition between particle layers. This can be explained by plotting the simulated and theoretical $C_L$ profiles at different times corresponding to three different stages (marked with three vertical dashed lines) of segregation [Fig. 9(c)], showing that as segregation approaches a steady state, some large particles remain in the lower layers of the flow ($z/H = 0.2–0.4$). Experiments of van der Vaart et al. [15] also reveal that it becomes increasingly difficult for large particles to rise when they are surrounded by more small particles, which is a signature of the underlying asymmetry between particle size species [15]. Jing et al. [17] also explain that the large particles that remain trapped in the sea of small particles
FIG. 10. Spatial-temporal distribution of $C_L$ measured (a) from the simulation and (b) from the numerical model in Eq. (1) of a representative base case (refer to Table II) with $\eta_F = 0.1$ Pa s for an initially well-mixed mixture. (c) Spatial distribution of $C_L$ along the height measured from the simulations (solid black line) and from the theory (solid red line) for different times corresponding to different stages in the segregation process.

are not stagnant but are constantly being exchanged between particle layers in a state of dynamic equilibrium. Figure 10 shows results from additional simulations where the mixture is initially well mixed, illustrating that our model remains accurate for different initial mixture conditions.

After verifying that the extended continuum model can adequately predict the evolution of particle size concentrations, we further test the application of the empirical models in predicting the trajectory of the large particles’ center of mass for different interstitial fluids. Figures 11(a) and 11(b) show the trajectory of the large particle centers of mass obtained from the simulations (dotted lines) and as predicted by the model (solid lines) for flows in the base case with different $\hat{\rho}$ and $\eta_F$, respectively. Although good quantitative agreement is achieved for the segregation rates, the segregation heights predicted by the model are noticeably greater and are possibly related to the fact that the model disregards the large particles that remain near the base shown in Figs. 9 and 10. Discrepancies between the model predictions and the simulation results may also be resolved by using asymmetric segregation flux models. Despite these shortcomings it is demonstrated here that the application of the simple empirical relationships incorporating the various fluid effects can adequately capture the segregation and diffusive behaviors in immersed flows.
FIG. 11. The measured (dotted lines) and simulated (solid lines) change of the large particles’ center of mass with time for flows in the base case with different (a) $\hat{\rho}$ for a constant $\eta_F$ and (b) $\eta_F$ for constant $\hat{\rho}$.

V. CONCLUDING REMARKS

We use fluid-granular numerical simulations to study the effects of different types of fluids on the particle size segregation and diffusive remixing in immersed sheared granular flows, over a wide range of densities and viscosities. The use of a simple plane shear geometry complemented by a feedback scheme for the streamwise velocity ensures that the segregation and diffusion behaviors observed here are not influenced by spatially varying shear profiles that were previously found to influence segregation behaviors in immersed granular flows.

The presence of fluids primarily slows down segregation but has minimal effect on the final segregation height as long as the relative density of the particle and the fluid is large ($\hat{\rho} \geq 0.12$). At small fluid viscosities, the segregation rate is independent of viscosity, while beyond a certain threshold viscosity, the segregation rate decreases with viscosity. The segregation rate also decreases as the density difference between the particles and the fluid is reduced. Moreover, in the viscosity-independent limit, size segregation depends also on the flow conditions (e.g., gravity, shear rates, confining pressure) and the particle material properties (e.g., mean diameter), which can be accounted for collectively by the inertial number.

In dry granular shear flows, the random motion of particles under shear results in homogeneous mixtures and effectively counteracts their tendency to segregate [19]. Results here show that particle diffusion exhibits a transitional tendency with the viscosity and depends only on the shear rate and the mean particle diameter in the $\eta_F$-independent limit; diffusion is less affected by changes in the relative density.

Through scaling analysis, the viscous dependence of both the segregation velocity and the diffusion across all the parameters considered here can be expressed in terms of the Stokes number. In the study of granular-fluid rheology, critical values of $St$, along with the density number $r_\rho = \sqrt{\rho_G/\rho_F}$ and Reynolds number $Re = St/r_\rho$, define different flow regimes which are characterized by distinct solid-fluid interactions [13]. These limits are ideally defined at $St = r_\rho = Re = 1$ while studies on wet granular avalanches have determined these limits to lie at $St = 10$, $r_\rho = 4$, and $Re = 2.5$ [35]. Two of these flow regimes, applicable for cases where the interstitial fluid is dense, are the fluid-inertial and viscous regimes. In the fluid-inertial regime, a dense fluid is present but the granular flow is still controlled by the inertial interactions between particles. In the viscous regime, the fluid viscosity significantly hampers and controls the motion of the particles.

The boundaries separating the fluid-inertial and viscous regimes for the range of $r_\rho$ (1.06 $< r_\rho < 1.58$) corresponding to the values of $\hat{\rho}$ considered here are plotted in Figs. 4(a) and 7(a). It
can be seen that the ideal (dashed lines) and empirical limits (region in dashed lines) fall within the estimated transition boundaries (gray shaded region). This shows that the transition in the segregation and diffusion of particles is closely related to the transition of the flow rheology. This implies that the reduction of the segregation rate and diffusion with the viscosity is related to the tendency of viscous fluids to reduce the characteristic time over which particles migrate from one position to the other due to shear induced rearrangement [13,68]. Specifically, segregation is independent of the viscosity in the fluid-inertial regime where inertial mechanisms dominate and is dependent on it in the viscous regime. This is consistent with the results of our recent works investigating the mechanical origin of this viscous dependence wherein we find that segregation rates decrease due to the reduction of the kinetic stress gradients, which is a function of particle velocity fluctuations, by viscosity [21,28]. It should be mentioned, however, that although the Stokes number provides a convenient and intuitive way to account for viscous effects on segregation and diffusion, it cannot adequately model their behaviors at high shear rates resulting in the scatter of scaled data points observed here. A closer look into how the viscous effects can be better modeled at high shear rates is consigned to future work.

The wide range of simulated cases allows us to develop empirical relations that define segregation and diffusion in different types of fluids. Using these relations as input in a segregation-diffusion equation previously developed for shallow free-surface flows, we are able to model the spatial-temporal evolution of particle size concentrations for bidisperse granular mixtures immersed in different types of fluids. Theoretical predictions are validated against measurements from the simulations where reasonable agreement is obtained. The model depends on five dimensionless constants ($B, \alpha, \beta, \lambda_1,$ and $\lambda_2$) whose physical meanings are yet to be determined. Existing three-phase segregation theories [20] assume that fluids weaken segregation only through buoyancy. Results here show that in addition to buoyancy, viscosity also influences segregation in the same way that it affects the flow rheology and flow regimes. With this enhanced understanding of how fluids affect segregating particles it is now possible to derive an improved granular-fluid segregation theory that accommodates the effects of viscous stresses.

To facilitate a more systematic analysis of fluid effects on the segregation process, here we only consider bidisperse mixtures having a size ratio of 2. Recent research on the mechanisms of segregation of single particle intruders reveal that when size differences are large (much greater than 2), contact forces experienced by a large intruder from its surroundings may not be sufficient to support its weight nor will it be sufficient to push it upward [66,77]. On the other hand, segregation is also less efficient when the size ratio is close to 1 since the rising particles depend on interlocking mechanisms that rely on the formation of transient force chains [78]. These mechanisms may be affected by the presence of viscous fluids possibly resulting in complex segregation behaviors that depend on both the size ratio and fluid viscosity. Moreover, real granular flows are polydisperse according to power-law or lognormal distributions [79] and segregation equations for such mixture conditions have already been developed for dry cases. Segregation in polydisperse mixtures is modeled by summing over the concentration gradients of a wider range of particle sizes that are subjected to segregation rates defined for pairs of size constituents [80,81]. With this said, the segregation mechanisms in immersed shear flows presented here are expected to hold true for polydisperse mixtures and Eq. (9) can be generalized for more continuous size distributions, although a characteristic length scale, similar to that introduced in [36], may have to be determined to accommodate the effects of varying size ratios. Therefore, detailed investigations on the coupled effects of fluid with the size ratio and particle size distribution are an interesting direction for future research.

Modeling size segregation and diffusive remixing in immersed scenarios is relevant to several real-world granular flows including hazardous geophysical flows where it may influence the local rheology, run-out distance, and deposit morphology. Results here may also be relevant to research on bedload transport and river bed armoring which is also considered as a granular system [82]. This work aims to aid the prediction of segregation behaviors and patterns over a wide range of fluid material parameters and flow conditions. In future work, it would be instructive to validate
the segregation behaviors observed here with physical experiments, although replicating a highly controlled setup would be challenging. To improve its relevance, the empirical relationships derived here should be extended to accommodate the asymmetry in particle motion. It is also interesting to consider the evolution of excess pore water pressures which develop with the granular microstructure in confined sheared flows [83] as well as the effects of lubricating fluid layers between interacting particles immersed in highly viscous fluids [24].

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APPENDIX: GOVERNING EQUATIONS OF THE CFD DEM AND CALCULATION OF KINEMATIC PROPERTIES FROM DEM

The discrete element method (DEM) calculates the translational and rotational motion of spherical particles, resulting from their respective interactions, from Newton’s second law of motion whose governing equations can be written as

\begin{equation}
m_j \frac{d^2 x_j}{dt^2} = \sum_{k=1}^{N_c} (F_{\text{norm}}^c + F_{\text{tan}}^c)_{jk} + m_j g + F_{FP}^j,
\end{equation}

\begin{equation}
I_j \frac{d\omega_j}{dt} = \sum_{k=1}^{N_c} M_{jk}^c,
\end{equation}

where $m_j$ and $x_j$ are the mass and position of a particle $j$, $F_{\text{norm}}^c$ and $F_{\text{tan}}^c$ are the normal and tangential forces defined at a contact point $c$ wherein there are $N_c$ number of contacts experienced by a single particle. These two particle contact forces are calculated using the Hertz model which is dependent on the Young’s modulus, Poisson’s ratio, restitution, and friction coefficients, and balanced by the particle weight $m_j g$ and the solid-fluid interaction force $F_{FP}^j$ [50]. Particle rotation is calculated from the moment of inertia of a sphere $I_j$, the particles’ rotational acceleration $\omega_j$, and the moment exerted by a particle $k$ on $j$ or a boundary $M_{jk}^c$.

The solid-fluid interaction term in Eq. (A1), $F_{FP}^j$, is the sum of hydrostatic and hydrodynamic forces represented by the buoyant $F_{F}^b$ and drag $F_{F}^d$ forces, respectively, acting on a particle:

\begin{equation}
F_{FP}^j = F_{F}^b + F_{F}^d = -V_j(\nabla P_F + \nabla \tau_F) + \frac{1}{8}C_d \rho_F \pi d_j^2 |U_F - U_{G,j}|(1 - \phi_G)^{1-\chi},
\end{equation}

where $V_j$ is the volume of a particle $j$ and $\nabla P_F$ is the fluid pressure gradient. $U_F$ and $U_{G,j}$ are the averaged fluid and solid velocities, respectively, measured within a single computational domain. The drag coefficient $C_d$ is calculated using the relation proposed by Di Felice [84] formally written as

\begin{equation}
C_d = \left( 0.63 + \frac{4.8}{\sqrt{Re}} \right)^2.
\end{equation}

The term $(1 - \phi_G)^{1-\chi}$, where $\chi = 3.7 - 0.65 \exp[-0.5(15 - \log_{10} Re)^2]$, expresses the influence of particle concentration on the drag coefficient.

The CFD calculates relevant fluid fields by solving the mass and momentum continuum equations:

\begin{equation}
\frac{\partial(\phi_F)}{\partial t} + \nabla \cdot (\phi_F U_F) = 0,
\end{equation}
\[
\frac{\partial (\phi_F \rho_F \mathbf{U}_F)}{\partial t} + \nabla \cdot (\phi_F \rho_F \mathbf{U}_F \otimes \mathbf{U}_F) = -\phi_F \nabla P_F + \phi_F \nabla \tau_F + \phi_F \rho_F \mathbf{g} - f_{FP}, \quad (A6)
\]

using the finite volume method (FVM) within each three-dimensional computational domain. \( \tau_F \) is the fluid stress tensor. The term \( f_{FP} \) expresses the force experienced by the fluid phase due to the particle motion and is calculated as

\[
f_{FP} = \Omega(\mathbf{U}_F - \langle \mathbf{U}_G \rangle). \quad (A7)
\]

\( \Omega \) is a momentum transfer term computed as

\[
\Omega = \frac{\sum_j F_j^d}{V_F |\mathbf{U}_F - \langle \mathbf{U}_G \rangle|}, \quad (A8)
\]

where \( V_F \) is the volume of a computational fluid cell.

Kinematic and rheological quantities relevant to this study are calculated from DEM data by dividing the granular flow domain into sampling volumes with fixed dimensions \( V_M = L \times W \times d_s \).

The volume fraction \( \phi_i \) and streamwise velocities \( U_i \) of particles belonging to a size species \( i \) are calculated as [30,85]

\[
\phi_i(z) = \frac{\sum_j V_{ij}}{V_M}, \quad (A9)
\]

\[
U_i(z) = \frac{\sum_j U_{ij} V_{ij}}{\sum_j V_{ij}}, \quad (A10)
\]

respectively. \( V_{ij} \) and \( u_{ij} \) are the fractional volumes and velocities of a particle \( j \) of size species \( i \).

The bulk mixture velocity is calculated as \( \mathbf{U}_G(z) = \sum_i [\phi_i(z) \mathbf{U}_i(z)] / \sum_i \phi_i(z) \).

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