Numerical investigation of particle size segregation in saturated granular flows using CFD-DEM coupling approach

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Abstract

Particle size segregation is a common feature in debris-flow deposits and is assumed to develop in a similar way as in dry granular flows where fluid forces are neglected. Solid-fluid coupling however is a defining feature of debris flows and fluid forces must therefore be accounted for in modelling for the segregation that develops therein. This paper presents a numerical investigation of the mechanisms of segregation under the influence of fluid forces. For this, a segment of a fully submerged bi-disperse steady granular flow is simulated using the CFD-DEM method. The solid-fluid interactions come in the form of buoyancy and fluid drag force. It is found that the presence of the fluid generally retards the rate and quality of segregation primarily by promoting the formation of a plug flow in the stream-wise velocity profile. The plug flow region forms at the free surface where it significantly reduces or zeroes out the shear rates thus inhibiting the main mechanisms of segregation, i.e. kinetic sieving and squeeze expulsion, to take place. It is inferred that the rapid shearing that occurs near the base promotes segregation but is unable to proceed towards the free surface due to the presence of the plug flow region that serves as a barrier. The quality of submerged segregation improves at lower angles where the plug flow region is minimized and the usual parabolic shear profile develops.

Keywords: CFD-DEM; interstitial pore fluid; particle size segregation; debris flows; solid-fluid interaction

1. Introduction

Particle size segregation is a prominent physical feature observed in debris-flow deposits (Major 1997) and is believed to have significant effects on the flow’s overall dynamics (Johnson et al. 2012, Kokelaar et al. 2014). The head region and the lateral edges are primarily composed of larger and coarser grains while the tail region is mostly composed of fines. Cutting into the deposit, one can observe an inversely graded profile where the large particles rise to the free surface and the fine particles settle at the base. This phenomenon has been well observed in highly sheared dry granular mixtures (e.g. chute flows, rotating drums, heaps and silos) and has been found to be well accounted for by the theories of kinetic sieving and squeeze expulsion (Savage & Lun 1989, Vallance & Savage 2000, Gray & Thornton 2005, Gray & Chugunov 2006). Debris flows however are distinct from other granular and geophysical mass flows due to the active influence of the interstitial fluid on the particle dynamics (Cuossot & Meunier 1995, Iverson 1997).

Physical experiments on segregation (Vallance & Savage 2000, Zanuttigh & Ghilardi 2010, van der Vaart et al. 2015) have been invaluable in characterizing the mechanisms that drive the process and have been instrumental in the development of theories that are able to predict the degree of segregation for different initial conditions (Gray & Thornton 2005, Benjy & Marks 2011, Gajjar & Gray 2014). It is, however, only through computational and numerical simulations of particle interactions that the micro-mechanical origins (i.e. particle scale) of segregation can truly be investigated (Fan & Hill 2011, Hill & Tan 2014, Jing et al. 2017). Recently, particle dynamics simulations have been computationally ‘coupled’ with fluid dynamics solvers in order to model fluid effects on particle motion and vice
versa. Several works that employ these methods have already demonstrated their effectiveness in providing significant insight to the dynamics of coupled systems ranging from laboratory-scale granular transport (Tsuji et al. 1992), and saturated soil mechanics (Zhao et al. 2014), to landslides (Zhao & Shan 2013, Zhao et al. 2016) and debris flows (Leonardi et al. 2015, Zhao 2017, Li & Zhao 2018).

In this study, we report the results of a series of computational experiments that were aimed to study the development of particle size segregation under the influence of fluid forces. This is to further understand the driving mechanisms responsible for the size re-arrangement observed in natural debris flows. We use the coupled Discrete Element Method – Computational Fluid Dynamics (CFD-DEM) to simulate bi-disperse mixtures of particles ‘flowing’ at different angles of inclination in water. The segregation that develops in the saturated cases are compared with the segregation of dry particles.

2. Methodology

2.1. Definition of the system

The simulation consists of two separate but coupled domains. In the solid domain, the flow of a bi-disperse mixture of solid spheres is simulated using the open-source code ESyS-Particle (Weatherly et al. 2011). Periodic boundaries were set in the stream-wise direction to represent an infinitely long chute. The distance between the span-wise boundaries were set to be small enough for side-wall effects to be negligible (Jop et al. 2005). The floor was roughened by ‘gluing’ a randomized array of small particles to the base; the flow surface was free. The particles were initially set to be randomly mixed. The exact number of small and large particles were calculated according to a volume fraction of 0.5, a large to small particle size ratio of 1.5 and an initial packing volume of $0.3 \times 0.1 \times 0.4$ m ($L \times W \times H$). Flow was initiated by tilting the $xz$ plane of gravity to the desired inclination angle. It is to be noted that the chosen parameters are highly idealized and do not necessarily reflect natural debris flows which are known to have much wider size distributions and size ratios. The goals of this paper simply focus on the particle scale effects of fluid forces on the particle dynamics that lead to inverse grading and not on the effects of varying these parameters themselves. Hence they will be held constant throughout the study. In particular, the chosen size ratio is relatively small but is sufficient to induce size segregation within a short period of time.

The fluid domain was implemented using the open-source CFD code OpenFOAM. The whole domain was given the material properties of water at 20°C. The domain was uniformly discretized in such a way that at least 5 large particles would fit (Zhao et al. 2014). A free-atmosphere boundary condition (pressure is based on local velocity of adjacent mesh; velocity dynamically changes from zero gradient when there is outflow to having a flux dependence when there is inflow (OpenCFD 2004)) was set at the right, left and top walls, allowing the fluid to freely flow in and out of the domain. A no-slip condition (zero pressure gradient, fixed zero velocity) was set at the bottom wall. For the turbulence, the standard $k-\varepsilon$ model is implemented. The complete set of material and system parameters are summarized in Table 1.

The solid domain is positioned completely within the fluid domain. The fluid domain is set to be slightly longer stream-wise since setting both domains to exactly coincide would mathematically result to very sharp fluid pressure

Fig. 1. (a) The conceptual diagram of the system being simulated. Snapshots of the (b) velocity and (c) dynamic pressure distributions of the actual simulation which represents the segment bordered by the cube in (a).
gradients. Over-all one can imagine the whole simulation to be that of a segment of a submerged bi-disperse debris flow (Fig. 1a). A fully submerged case is chosen since, for now, we only wished to observe the effects of fluid forces on segregation, while avoiding the complications of solving for fluid free surface flows. The fluid is initially static and only flows as a reaction to the particle motion.

Snapshots of the velocity and dynamic pressure distributions are shown in Figs. 1b and c respectively. The highest velocities are observed at the top-right since particle velocities are highest near the free surface for a flow that moves from left to right. Relatively low velocities are measured at the left since that is where the ‘new’ particles enter whose velocities are impeded by the particles ahead of them. On average, granular flow and fluid velocities are approximately equal. Dynamic pressures fluctuate as a reaction to the random dilation and contraction of the particles within the mixture. The extremely low pressures at the boundaries of the solid domain are due to the velocity differences of the solids and the fluids (Zhao 2016).

2.2. The CFD-DEM method

The CFD-DEM method relies on a message passing algorithm that relays information from the DEM solver to the CFD solver after a pre-defined number of DEM time-steps. The algorithm proposed by Zhao et al. (2014) was used in this study.

The translational and rotational displacements resulting from particle-particle interactions are updated after each numerical time-step, determined after integrating the governing differential equations which are based on Newton’s second law of motion. The governing equations for the said trajectories can be written as:

\[
m_i \frac{d^2 x_i}{dt^2} = m_i g + \sum_c (f_{nc} + f_{tc}) + f_{fluid}
\]  

(1)

\[
I_i \frac{d \omega_i}{dt} = \sum_c r_c \times f_{tc}
\]

(2)

for linear and rotational motions respectively. Here \(m_i\) and \(x_i\) are the mass and position of a particle \(i\) at a single numerical time-step and \(g\) is the acceleration due to gravity. \(f_{nc}\) and \(f_{tc}\) are the normal and tangential forces defined at a contact point \(c\). A linear spring-dashpot contact model (Cundall & Strack 1979) is used to calculate for the contact forces. \(I_i\) is the moment of inertia of a sphere, \(\omega_i\) is the rotational acceleration, and \(r_c\) is the distance between the centers of two contacting spheres.

The final term on the right hand side of Eqn. (1) represents the force exerted by the fluid on particle \(i\). This is called the solid-fluid interaction force (Zhao 2016) and is calculated as the sum of 2 types of fluid forces: the hydrostatic and the hydrodynamic. The hydrostatic forces are represented by buoyancy \(f^b = -\rho_i V p\), which is basically a function of the particle volume and the pressure gradient that develops between two adjacent fluid cells. The hydrodynamic forces are born from the relative motion of the solid and the fluid phases and usually come in the form of the drag force which is quantified as:

\[
F_{di} = \frac{1}{2} C_d \rho_f \frac{\pi D^2}{4} |U - V| (U - V) n^{-\alpha + 1}
\]

(3)

<table>
<thead>
<tr>
<th>DEM Parameters</th>
<th>CFD Parameters</th>
<th>Simulation Parameters</th>
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<tbody>
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<td>Small particle diameter (mm)</td>
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<td>Large particle diameter (mm)</td>
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<td>Gravity (m/s²)</td>
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<td>Young’s modulus (N/m)</td>
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<td>DEM time-step (s)</td>
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<tr>
<td>Poisson’s ratio</td>
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<td>CFD time-step (s)</td>
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<tr>
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<td>Coupling frequency*</td>
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<tr>
<td>Linear Damper Coefficient</td>
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<tr>
<td>Inclination angle (°)</td>
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*Coupling frequency pertains to the number of DEM time steps that have to elapse before a single CFD time step.
where:

\[
C_D = \frac{24}{Re} \left(1 + 0.15 Re^{0.681}\right) + \frac{0.407}{1 + \frac{8710}{Re}}
\]

\[
Re = \rho_f d |U - V|/\mu
\]

are the drag coefficient and Reynold’s number defined at the particle scale respectively. \(U\) and \(V\) are the fluid and particle velocities, \(\rho_f\) is the fluid density, and \(\mu\) is the dynamic viscosity. \(n\) is the local porosity while \(\chi\) is the empirical porosity correction factor calculated as \(\chi = 3.7 - 0.65 \exp\left[-\frac{1.5 - \log_{10} Re}{2}\right]\).

The fluid domain is discretized into 3-dimensional cells where the Navier-Stokes equations are solved using the Finite Volume Method (FVM) (OpenCFD 2004). The mass and momentum continuum equations are written as:

\[
\frac{\partial(\rho_f n)}{\partial t} + \nabla \cdot (\rho_f n \mathbf{U}) = 0
\]

\[
\frac{\partial(\rho_f n \mathbf{U})}{\partial t} + \nabla \cdot (\rho_f n \mathbf{UU}) - n \nabla \cdot \mathbf{t} = -n \nabla p + n \rho_f \mathbf{g} + \mathbf{f_d}
\]

where \(\mathbf{t}\) fluid stress tensor calculated via the standard \(k - \varepsilon\) turbulent model (Zhao 2016), and \(p\) is the fluid pressure. The term \(\mathbf{f_d} = \sum_{i=1}^{N} \mathbf{F_{di}}/V_{cell}\) is the drag force per unit fluid volume. The fluid pressures and velocities that are calculated in each cell are used, in turn, to calculate for the interaction forces.

3. Results and discussions

3.1. Post-processing

To calculate for the relevant kinematics of the system, the whole granular flow was divided into bins of fixed dimensions along the flow depth (\(y\)-direction). The kinematic properties will be calculated considering the contribution of the part of each particle that falls within a certain bin with height \(\Delta y\) centered at \(y\). The bin height is arbitrarily set to be 1/5 of the small particle diameter. Dry and submerged mixtures flowing at 26° were simulated to provide comparison between the segregation that develops with and without buoyant forces. Submerged mixtures at different angles of inclination were simulated to show how the segregation process varies under different flow conditions.

3.2. Measuring segregation

Segregation is measured as the deviation of the local volume concentration \(\phi^n\) of a certain size species \(n\) from the global volume concentration (which is 0.5 at all times) at a height \(y\) for a certain time \(t\). This is calculated using the equation proposed by Hill & Tan (2014):

\[
S^n(y) = \sqrt{\frac{\sum_{j=1}^{N_{bin}} \left(\phi^n_j(t) - \phi\right)^2}{(N_{bin} - 1)}}
\]

where \(S^n\) is the segregation of a species and \(N_{bin}\) is the number of bins along the \(y\)-direction respectively. The higher the value of \(S^n\) the better the ‘quality’ of segregation, where the best case involves a complete separation of small and large particles into two homogeneous layers.

Fig. 2a shows the segregation trends of the large particles of both dry and submerged mixtures. The segregation of the dry mixture (at 26°) shows a rapid increase at the beginning which evens out to a nearly constant value at around 120 seconds. Beyond this point, there is no longer a clear change in the local large particle concentration deviations.
implying that there is no longer a net flux of large (small) particles to the free surface (base) and segregation has achieved a steady state.

The segregation of submerged mixtures are significantly different. The levels of segregation are lower and slower compared to the dry case. Instead of a parabolic trend, segregation rapidly increases in a linear manner initially for a short period of time before abruptly slowing down. The slow increase continues until the end of the simulation. Segregation steady-state was not achieved except for the mixture flowing down at a 30° angle. This flow was very diffuse – random particle motion dominated – and hence no net upward nor downward flux was able to develop, maintaining a constant concentration deviation until the end.

Segregation is a shear driven process. At higher velocities shear rates are high, more random voids appear for small particles to percolate down to and more inter-particle contacts to hoist large particles up. High velocities will increase random particle motion and create voids that even large particles can fall into, preventing them from segregating up. Flows that are relatively slow result to lower shear rates which also effectively reduce segregation. Simply put, the presence of the fluid slows down the granular flow, reducing local shear rates and consequently slows down segregation. The difference that the presence of fluid makes can be seen when comparing Figs. 2b and c – snapshots of dry and submerged mixtures respectively, both simulated at an inclination angle of 26°; taken at 160 seconds.

3.3. Particle distribution

For a more qualitative assessment of the spatio-temporal development of segregation, phase diagrams representing the solid volume concentrations of large particles \(\phi^l\) for the dry case at 26° (Fig. 3a) and the submerged cases (Figs. 3b–e) at different angles of inclination are presented in the first column of Fig. 3. As in section 3.1, the dry case is simply included for comparison. For the dry case, a thick layer composed of purely large particles is observed at the free surface. One that is dominated by small particles develops at the bottom. The black dashed line near the floor marks the height of the base particles. A blurred transition line develops between these two regions. This area is where both size species co-exist and mix under dynamic equilibrium (cf. Jing et al. 2017). This is usually attributed to diffusivity which prevents the perfect segregation of the two particle species (cf. Vallance & Savage 2000, Gray & Chugunov 2006).

For the submerged case, the large particle layers are noticeably much thinner and take much longer times to develop. Immediately under this layer is a region which, although dominated by large particles, is also sufficiently populated with small particles. This layer continues to thicken over time indicating that large particles still continue to rise from the bottom. Most of these large particles, however, do not continue all the way upwards but instead remain suspended there. This can be seen from the granularity that develops in this region where a certain degree of striation is observed. This indicates that the solid concentrations at a certain height remain constant for prolonged periods of time. All throughout the rest of the flowing body, the mixture is more or less homogenous and a more ‘diffuse’ granularity is observed. This suggests that there is a difference between the flow properties along the height of the flow that, in effect, causes particles to behave differently.

Comparing the phase diagrams of the flows at different angles, it can be seen that the lower the slope angles the better the segregation, and the more the distribution resembles that of the dry case. At low angles (i.e. low velocities; 22° and 24°) the large particles in the stagnant layer accumulate at the beginning but then slowly rise up to be a part of the pure large particle layer. This is accompanied by the continued increase in the thickness of the small particle
layer. This means that although slow, segregation and its primary mechanisms (e.g., kinetic sieving, squeeze expulsion) are still in progress and the inhomogeneities in the flow profile are less pronounced. At higher angles (i.e., higher velocities; 26° and 30°), the striation in the stagnant regions are more pronounced, indicating that almost no relative change in the solid concentration has occurred for long periods of time. The same is also true for the fine particle layer near the base whose thickness has ceased to increase indicating that even the gravity-driven downward percolation of small particles is also inhibited. In addition (especially at an inclination of 30°), distinct layers start to form at the lower regions indicating more pronounced differences in the flow profile along the depth.

Fig. 3. The solid volume concentration distributions of large particles $\phi_l$ of (a) a dry bi-disperse mixture at 26° and submerged mixtures for angles (b) 22°, (c) 24°, (d) 26°, and (e) 30°. The stream-wise velocity and shear profiles of the (f) dry and (g-j) submerged mixtures at 160 seconds. The kinetic stress profiles of the (f) dry and (g-j) submerged mixtures at 160 seconds.
3.4. Kinetic properties

To further shed light on the flow properties that are believed to affect the manner of segregation, the kinetic properties of the simulated granular mixtures are evaluated according to their velocity, shear rate and kinetic stress profiles. The kinetic stress is a measure of the degree of individual particle mobility, expressed in terms of their relative velocities to the average velocity of the surrounding particles at the height where they are located. This value is analogous to the granular temperature. Here we calculate the kinetic stress through (Fan & Hill 2011):

\[
\sigma_{yy}^{k,n}(y) = \rho_m \phi^n \left( \frac{1}{N} \sum_{i=1}^{N} \frac{\sum_j (v_{ij}^n - v(y))^2 v_{ij}^n}{\sum_j v_{ij}^n} \right)
\]

where \(v_{ij}^n\) is the velocity of the volume portion of a certain particle and \(v(y)\) is the average velocity of both size species at bin center \(y\). \(i\) is the time-step number, of which there are \(N\) at which the velocity per bin is averaged, \(v_{ij}^n\) is the total volume of a particle specie at \(y\), and \(\rho_m\) is the material density.

Figs. 3f and k show the relevant kinetic properties of the dry flow respectively. The measured stream-wise velocity and shear rate profile of the dry case is typical for dry granular flows (cf. Jop et al. 2004). In dry mixtures, the kinetic stress is mostly borne by the small particles and is highest near the base where the shear rate is highest. Large particle kinetic stress is significantly lower and more or less even throughout the flow height.

The flow profiles of the submerged mixture (Figs. 3g-j) exhibit a plug flow near the free surface and a rapid shear at the base. This profile is consistent with the stream-wise flow profiles of submerged (Istad et al. 2004) and even free-surface debris flows (Mainali & Rajaratnam 1994). The kinetic stress magnitudes (Figs. 3l-o) of both small and large particles are lower in the submerged case and are also notably less distinct – both of them show near zero values at the plug flow region and both peak near the base. This implies that the presence of fluid reduces individual particle mobility and does this to the point that individual particle motion for both species are nearly equalized. Relating the inhomogeneity of the kinetic profiles to the concentration profiles in 3.2, one can infer that the particles in the plug flow region almost move as a single block where due to the lack of shearing find it hard to segregate up or down.

Comparing the velocity profiles at different angles, the plug flow region is more pronounced and is wider for higher velocities. The larger the relative velocities of the particles and the surrounding fluid, the greater the opposing drag force and hence when the particles move faster, the greater the drag force they experience from an initially static fluid. When the granular flow is slow, the fluid resistance is less and hence a velocity and shear profile resembling a dry flow can be achieved.

4. Conclusions and outlook

A simple case of a submerged bi-disperse mixture is simulated using the CFD-DEM method to investigate the effects of fluid forces on the development of particle size segregation. From the initial results, it can be seen that the fluid generally retards the degree and rate of segregation. It is inferred that the resistive forces of the fluid create a plug flow region near the free surface wherein the shearing of the particles are greatly reduced to the point that the particles seemingly move as a single block. The reduction of the shearing inhibits the generation of random voids which are essential for small particle percolation downwards and reduces the relative inter-particle motion which necessary for the ‘squeezing’ of the large particles upwards. The shearing that exists in the lower regions continues to promote the aforementioned mechanisms, however, it is supposed that further segregation from this region is suppressed due to the plug flow that develops at the upper regions.

The aforementioned mechanism however still requires a more stringent evaluation which would involve knowing the fluid effects on particle contacts and how the shear profile that develops actually affects the particle trajectory. Further insight can also be gained through the variation of particle parameters such as the size ratio and the density ratio between the solid and the fluid.

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