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Letter

Theory for size segregation in flowing granular mixtures based on computation of forces on a single large particle

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We measure the upward force acting on a single, unconstrained, large particle in a granular medium of small particles flowing over inclined plane using discrete element method (DEM) simulation. Based on the computed force, we obtain an expression for the flux of large particles in a binary mixture of large and small particles and predict the equilibrium concentration profile and the velocity profile of the flowing layer. The theoretical predictions are in very good agreement with the DEM simulation results for a wide range of concentrations of large particles and inclination angles.

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A granular mixture of different size particles flowing over an inclined surface is known to segregate with large particles concentrating near the free surface. Currently, the most promising approach for predicting segregation in flowing systems involves empirically relating the percolation velocity of the species to its concentration and the local shear rate [1,2]. This percolation velocity relation yields a segregation flux which is used in the convection-diffusion equation to predict the segregation. These empirical relations have enabled quantitative comparison of experiments and simulation results [3–5]. Different functional forms of the segregation flux have been proposed and comparison between these different forms have also been reported [6–8]. Despite their success in describing size segregation in several systems, these empirical relations do not relate directly to the particle scale processes.

A second approach involves measuring forces acting on the particles and using this information to predict segregation. Such an approach has been previously used to predict segregation of binary granular mixtures differing only in density [9,10]. The measurement of the upward force on large size particles in discrete element method (DEM) simulations have been reported by Guillard *et al.* [11] and van der Vaart *et al.* [12]. These studies were done by constraining the motion of the large size intruder particles in one direction by attaching it to a linear spring in order to measure the upward force which is given by the average spring force acting on the intruder. Concerns regarding the restricted motion of the large particles in one direction have been raised [13] and whether the restriction on the vertical motion of the large size particle affects the measurement of the force is not clear. The force measurement on an unrestricted intruder has been reported by Staron [13], which showed that the net upward force on the particle is equal to the weight of the particle, contradicting the results of Ref. [12].

In this Letter, we address this important gap in the current understanding of the size segregation phenomenon. Following the approach of Refs. [9,10], we measure the net upward force on a large size particle in a flowing granular medium without any restriction on the motion of the large particle and find it to be larger than the weight of the particle. We then present a theoretical formulation to use the upward force on the intruder particles to enable quantitative prediction of size segregation of a binary mixture flowing over an inclined surface under the influence of gravity. This theoretical formulation is able to account for the interdependence of the rheology and segregation on each other and enables prediction of various flow properties of interest from the momentum balance equations.

Consider a large size intruder particle of mass m_L rising upwards in a flowing granular layer. Force balance on a nonaccelerating intruder leads to

$$F_L - F_g - F_{\text{drag}} = 0, \tag{1}$$

where $F_g = m_L g \cos\theta$ is the gravity force and F_{drag} is the drag force opposing the upward motion of the large particle. F_L is the total upward force on the large size intruder that causes it to rise to the free surface and includes contributions from the buoyant force and the lift force [12,14]. We assume that the drag force on the intruder particle is given by a modified Stokes law [9,10], i.e., $F_{\text{drag}} = c\pi\eta d_L v_L$, where η is the local viscosity, d_L the diameter of the large particle, and the constant c depends on the local packing fraction [9,10]. Using this expression, we get

$$m_L g \cos\theta = F_L - c\pi\eta d_L v_L. \tag{2}$$

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Staron [13] accurately measured the net upward force on the large intruder particle and found it to be equal to the downward force due to gravity. This result is a reflection of the particle rising at a steady velocity with no acceleration. However, the measured upward force is due to the force pushing the particle upwards and the downward drag force resisting the motion of the particle [Eq. (2)]. Since the drag force is proportional to the velocity of the intruder, it can be easily separated from the upward force, which should be independent of velocity. Equation (2) shows that the upward force, F_L, is equal to the weight, $m_L g \cos\theta$, only for the limiting case of a neutrally buoyant large size intruder particle (i.e., when $v_L = 0$). We use this approach to obtain the force F_L on a large size intruder particle in a flowing granular medium.

DEM simulations of frictional ($\mu = 0.5$), slightly inelastic ($e_n = 0.88$), soft deformable spherical particles of diameter d_S and mass m_S flowing over an inclined bumpy surface are performed with few large particles of size d_L and mass m_L. The simulation box is $20d_S \times 20d_S$ long and wide in the x (flow) and z (vorticity) direction and is periodic in both x and z directions. The rough and bumpy chute base is made of a $1.2d_S$-thick slice of a randomly packed configuration of spheres of size d_S. The total number of particles are chosen to ensure that the height of the layer in the y direction at zero inclination is $20d_S$ for the intruder particle study and $25d_S$ for the mixture segregation study. All the quantities reported here are nondimensionalized using m_S, d_S, and $m_S g$ as the mass, length, and force units, respectively.

Four (nine) equidistant intruder particles of size ratio $r = d_L/d_S = 2\,(1.5)$ are sandwiched between two cubic lattice configuration of nontouching small particles at the beginning of the simulations. The particles are allowed to fall under the influence of gravity at an inclination of 30° for a brief time period after which the inclination is reduced to the desired angle of $\theta = 25°$ and the flow is continued until steady state. A small spring force centered at $y = 10.5$ (as in Refs. [11,12]) is used to ensure that the intruder particles remain nearly at the same height. In addition, a small repulsive force is used between the intruder particles to prevent them from coming close to each other during the evolution of the flow. Once the flow reaches steady state (characterized by a constant average kinetic energy of the flowing layer), the harmonic attraction force toward $y = 10.5$ and the repulsive force between the intruder particles are switched off. The mass of each intruder particles is set to be m_L and the simulation is continued. Using this protocol ensures that the large size intruder particles are at a nearly fixed height away from the base and are well separated from each other at the start of the simulation.

Figure 1(a) shows a schematic view of the system comprising of a large size intruder in layer of small size grains. Figure 1(b) shows a few examples of the y trajectory of the intruders of size ratio $r = d_L/d_S = 2$ for two different masses. Note that the particles begin at nearly same height ≈10.5 (shown by the broken horizontal line) and the trajectories for $m_L = 4$ and $m_L = 16$ have been shifted upwards and downwards by one length unit respectively for the sake of clarity. As expected, depending on their mass, the intruder particles may either rise ($m_L = 4$) or sink ($m_L = 16$) in the flowing layer. Their motion in the y direction is tracked for 50 time units. The individual trajectories of the intruders' y position with time show random fluctuations indicating that the motion of the intruder in the vertical direction is dominated by random collisions from the neighboring particles. For a given mass, m_L, of the intruder particle, we average over 4 sets of 90 (total 360) trajectories and obtain a linear variation of the average y position of the intruder particles with time as shown in Fig. 1(c). The average velocity v_L of the intruder is obtained as the slope of the average trajectory by means of a linear fit. In agreement with Eq. (2), we obtain a linear variation of m_L with $\eta d_L v_L$, as shown in Fig. 1(d). The mass of the neutrally buoyant intruder ($m_N = 11.57$) is obtained from the value of the intercept on m_L axis (shown as broken line). Similar results are obtained for intruder particles of size ratio $r = 1.5$ ($m_N = 4.85$). The upward force on a large size intruder is obtained from Eq. (2) as

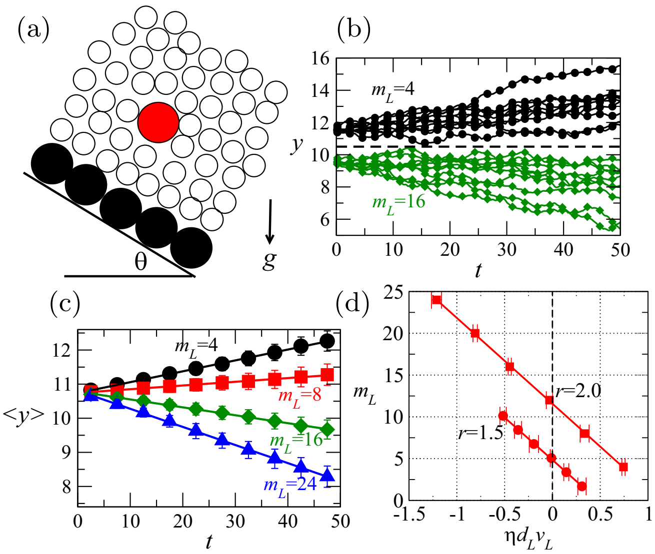

FIG. 1. (a) Two-dimensional schematic of the simulation setup for obtaining the force on the large size intruder particles. (b) Variation of y position of the intruder ($d_L = 2d_S$) with time for $m_L = 4$ (black) and $m_L = 16$ (green). (c) Variation of the average y position of the intruder with time for different masses. (d) Mass of the intruder shows a linear variation with $\eta d_L v_L$ for the two size ratios ($r = 2$ and $r = 1.5$) considered in this study. All the results are reported for $\theta = 25°$.

$$F_L = m_N g \cos\theta. \tag{3}$$

The upward force computed above ($1.45F_g$ for $r = 2$) is found to be slightly higher than that reported by van der Vaart *et al.* [12] ($1.28 \pm 0.10F_g$ for $r = 2$). This difference could be attributed to the absence of the restriction of the motion in the segregation direction in our study. However, in agreement with Ref. [12], the measured upward force is found to be higher than the weight of the large size intruder of same density as the small particles, resulting in an upward motion of the large particles.

Using this measure of the net force acting on the large size intruder particle, we next formulate a theory to predict the segregation due to size difference. The convection diffusion equation for the steady, fully developed chute flow without sidewalls and end effects (so that the properties vary only along y direction) for the case of size disperse binary mixtures, reduces to balance of segregation flux $j_{\text{seg}} = f_L(v_L - v_m)$ that acts to completely separate the large and small particles and diffusion flux $j_{\text{diff}} = -D df_L/dy$ which contributes to the mixing of the species. Since the mean mixture velocity in the y direction $v_m = 0$ due to mass conservation, using the flux balance $j_{\text{seg}} + j_{\text{diff}} = 0$ dictates

$$f_L v_L = D\frac{df_L}{dy}, \tag{4}$$

where f_L is the volume concentration of large particles and D is the diffusivity. The segregation velocity is obtained from Eqs. (2) and (3) as

$$v_L = \frac{\alpha_0 m_L g \cos\theta}{c\pi\eta d_L}, \tag{5}$$

where $\alpha_0 = (m_N/m_L - 1)$. The effective viscosity of the granular medium $\eta = |\tau_{yx}|/\dot{\gamma}$ is obtained using the shear stress from the momentum balance equation for steady, fully developed, chute flow case as $\rho g(h-y)\sin\theta/\dot{\gamma}$, where h is the height of the flowing layer and $\rho = \phi\rho_P$ is the bulk density of the granular medium with $\rho_P = \rho_L = \rho_S$ being the density of the particles. In the dense regime, the diffusivity scales as $D = bd_{\text{mix}}^2\dot{\gamma}$ where $d_{\text{mix}} = f_L d_L + (1-f_L)d_S$ is the local volume averaged diameter [3,10,15].

As the concentration of the large particle increases, the net upward force on a single large particle should reduce and must approach to zero as $f_L \to 1$ since all the particles will be identical in this case. Substituting Eq. (5) in Eq. (4) with the expression for η along with a concentration dependent $\alpha(f_L)$, we get

$$\frac{\alpha(f_L)m_L\cot\theta f_L\dot{\gamma}}{c\pi\phi\rho_P(h-y)d_L} = D\frac{df_L}{dy}. \tag{6}$$

The concentration dependence of $\alpha(f_L)$ must ensure that $\alpha(f_L) \to \alpha_0$ in the limit $f_L \to 0$ and $\alpha(f_L) \to 0$ as $f_L \to 1$. Dotted line in Fig. 2(a) shows that theoretical prediction using a linear variation $\alpha(f_L) = \alpha_0(1-f_L)$ consistent with these limits fails to capture the concentration variation with y. Hence we choose $\alpha(f_L) = \alpha_0(1-f_L)(1+kf_L)$, with k being a fitting parameter. When this quadratic form of $\alpha(f_L)$ is used in Eq. (6), we obtain

$$\frac{y}{h} = 1 - \exp\left\{\frac{1}{Ar^2}\left[\frac{r^2}{k+1}\ln\frac{(1-f_L)}{(1-f_{0L})} + \frac{(k+1-r)^2}{k(k+1)}\ln\frac{(1+kf_L)}{(1+kf_{0L})} - \ln\frac{(f_L)}{(f_{0L})}\right]\right\}, \tag{7}$$

where $A = \alpha_0\cot\theta/6bc\phi$ and $f_{0L} = f_L(0)$. The Stokes' drag coefficient c can be obtained from the slope of the line in Fig. 1(d). To explore the appropriateness of the proposed theory over a wide range of inclinations, the values reported in Tripathi and Khakhar [10] are used. Constants b and ϕ are taken from the simulation data and f_{0L} is obtained using mass balance of the large particles in the layer from $f_T = (1/h)\int_0^h f_L dy$, where f_T is the known total volume fraction of large particles in the binary mixture. Due to the nonlinear nature of the Eq. (7), a trial and error method is used to obtain the value of f_{0L}. Profiles computed using Eq. (7) for different values of k were compared to the profiles from DEM simulations for different compositions. Based on the mean-square error between the two, value of $k = 1.5$ for $r = 1.5$ and $k = 2$ for $r = 2$ was found appropriate. Predictions from Eq. (7) are shown by thick solid line in Fig. 2 for $k = 1.5$. Excellent quantitative agreement between the theory and DEM simulation results is obtained. The predictions using a constant $\alpha(f_L) = \alpha_0$ are shown using dashed line. While the predictions agree well with simulation results for most of the bulk layer, they fail to capture the segregation behavior near the free surface. The quadratic variation of $\alpha(f_L)$, shown as a solid line in Fig. 2(b) inset for $k = 1.5$, is necessary to capture behavior near the free surface. This quadratic variation shows that the net upward force on the large particles up to an intermediate volume concentrations is higher than its value in extremely dilute limit and suggests a cooperative collective motion of large particles at intermediate concentrations as mentioned in Refs. [6,16].

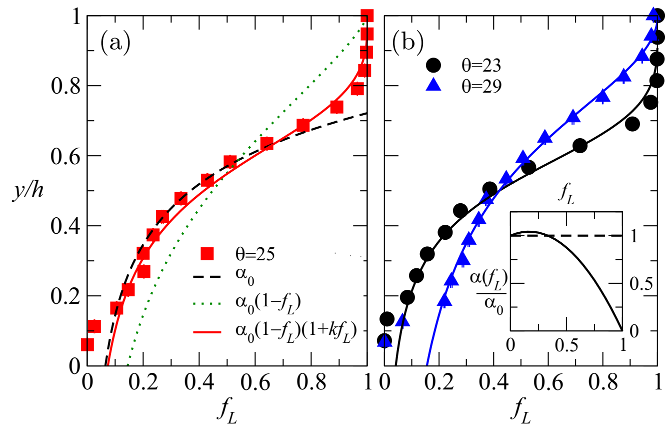

FIG. 2. Concentration (f_L) of large particles for a 50% large (size ratio 1.5) binary mixture for chute flow. Symbols represent DEM simulations results and lines represent predictions from theory. (a) Results for chute inclination $\theta = 25^\circ$. Dashed, dotted, and solid lines show predictions for a constant, linear and quadratic variation of $\alpha(f_L)$. (b) Results for $\theta = 23^\circ$ and $\theta = 29^\circ$. Solid line in the inset shows the quadratic variation of $\alpha(f_L)/\alpha_0$.

Following the results reported by van der Vaart *et al.* [12], we assume that the F_L/F_g is independent of the inclination angle. In other words, the mass of the neutrally buoyant particle m_N and the parameter α_0 are assumed to be independent of θ. Figure 2(b) shows concentration profiles for 50%–50% mixture at $\theta = 23^\circ$ and $\theta = 29^\circ$ obtained from theory using $\alpha(f_L)$ are in excellent agreement with DEM simulations. These results validate the assumption of inclination independent α_0 and confirm that the predictions from Eq. (7) are able to capture the influence of the inclination angle on the segregation. This influence of the inclination θ is accounted explicitly by $\cot\theta$ and implicitly by parameters c and ϕ in Eq. (7) via parameter A. This influence of the inclination angle (hence packing fraction) on the segregation is difficult to capture by percolation velocity relations that use the linear dependence of the species percolation velocity on the local

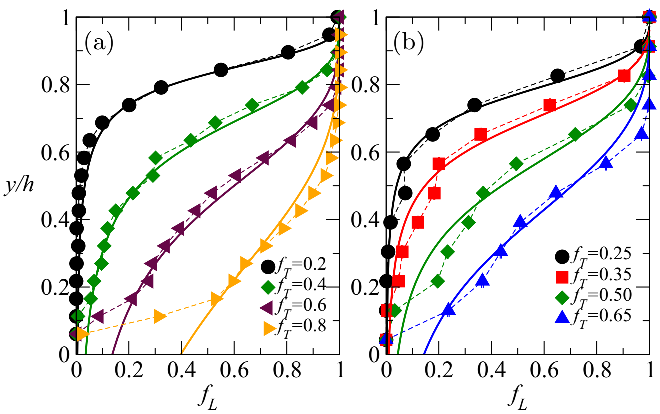

FIG. 3. Concentration (f_L) of large particles for different total concentration (f_T) of large particles for a binary mixture at inclination $\theta = 25^\circ$. Symbols (connected with broken line) represent DEM simulations results and solid lines represent predictions from Eq. (7). (a) Results for size ratio $r = 1.5$ and (b) $r = 2$.

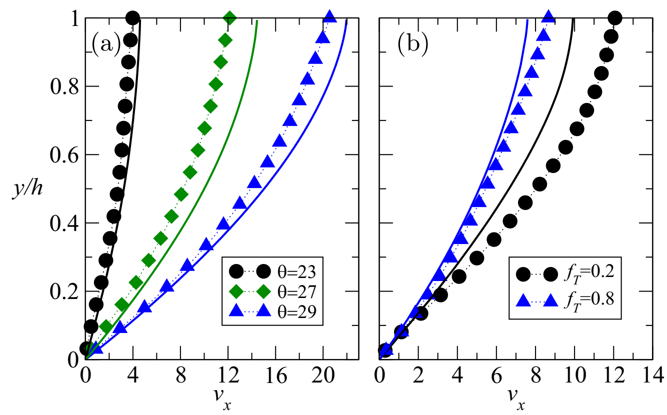

FIG. 4. Velocity (v_x) variation of a binary mixture (a) at different inclinations with 50% large ($r = 1.5$) particles and (b) at two different overall compositions (f_T) at $\theta = 25^\circ$. Solid lines are theoretical predictions from momentum balance equations.

shear rate, i.e., $v_L \propto \dot{\gamma}$ [2]. Since the diffusivity D varies linearly with the local shear rate, Eq. (4) leads to a shear rate (and hence inclination) independent concentration profile in this case.

Next we report the results for different compositions of the mixture at an inclination of $\theta = 25^\circ$. Figure 3(a) shows that the theory is able to accurately predict the concentration profile for all the mixture compositions considered. The theory predicts the segregation behavior in excellent agreement with simulation results for mixtures rich in small particles ($f_T = 0.2$) as well as mixtures rich in large particles ($f_T = 0.8$) using the same value of $k = 1.5$ for size ratio $r = 1.5$. Figure 3(b) shows the results for size ratio $r = 2$ using $k = 2.0$ for different mixture compositions. Again, the theoretical predictions for this size ratio are also found to be in good agreement with DEM simulation results.

A few words about the deviation of theoretical predictions from the simulation results near the base are in order here. DEM simulations show that nearly complete segregation is observed at the base with $f_L = 0$. However, the theoretical formulation predicts a finite value of f_L at the base, f_{0L}. Simulation results [10] show that the value of the diffusion coefficient D is smaller near the base. Equation (6) suggests that to compensate for this decreased value of D, the slope df_L/dy should be higher near the base and the DEM results shown in Figs. 2 and 3 confirm this hypothesis. The constant b that relates the diffusion coefficient with shear rate and volume average diameter in the theory does not account for this decrease in the diffusion coefficient near the base, and hence predicts a lower value of the slope df_L/dy near the base, leading to the difference in the concentration profile near the base.

The present theory accounts for the intercoupling of the rheology and segregation by means of viscosity η in Eq. (6). It is thus possible to predict various flow properties of interest from the momentum balance equations. Using the predicted concentration profiles shown in Fig. 3 and following the approach and rheological model parameters mentioned in Ref. [17], we predict the velocity profile for three different inclinations and two different total concentrations of large size particles for $r = 1.5$ in Fig. 4. The symbols represent the results obtained from DEM simulations and solid lines are the theoretical predictions. It is evident that theory is able to predict the effect of inclination angle and mixture composition on the velocity profile of the mixture reasonably well. The existing approaches of size segregation, on the other hand, rely on the *a priori* knowledge of the velocity field (determined either experimentally or through simulations) in order to be able to predict segregation.

In this work, the upward force acting on large size intruder particles in a flowing granular medium was measured in terms of the mass of the freely flowing neutrally buoyant intruder (m_N) for dilute concentrations of the large intruder particles. By accounting for the drag force acting on the large size intruder particles, we accurately measure the net upward force causing the segregation of large particles of same density. This measured net upward force, when corrected for the large particle concentration dependence, yields a segregation flux with cubic dependence on the large particle concentration and linear dependence on shear rate as in Refs. [2,6,7] along with a dependence on the inclination angle which is not captured in the empirical segregation flux-based approaches. Accurate predictions of the concentration and the velocity filed are done using this approach for steady, fully developed chute flow of binary mixtures for a wide range of compositions and inclinations for two different size ratios. The theoretical formulation in this letter suggests a simple, yet quantitative, way of predicting size segregation in size bidisperse mixtures and paves way for predicting segregation of mixtures differing in both size and density.

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