Granular Temperature and Segregation in Dense Sheared Particulate Mixtures†

Kimberly M. Hill1* and Yi Fan2

1 St. Anthony Falls Laboratory and the Department of Civil, Environmental, and Geo-Engineering, University of Minnesota, USA
2 The Dow Chemical Company, USA

Abstract

In gravity-driven flows of different-sized (same density) particles, it is well known that larger particles tend to segregate upward (toward the free surface), and the smaller particles downward in the direction of gravity. Alternatively, when the particles are of the same size but different density, lighter particles tend to segregate upward and heavier particles, downward. When particles differ in both size and density, true of most mixtures of interest in industry and nature, the details are complicated and no rule based on gravity alone has captured the segregation behaviours. Gradients of granular temperature and kinetic stress (i.e., energy and stress associated with velocity fluctuations) offer alternative segregation driving forces, but have, until recently, been discounted as these dynamics are relatively small in dense flows. Recently, gradients in kinetic stress have been shown to play a significant role in segregating densely sheared particle mixtures, even where the kinetic stress is a relatively small percentage of the total stress. We review recent modelling advances accounting for this effect and validation in computational experiments. We show how this framework may be useful in capturing the complicated segregation phenomenology that emerges for dense sheared flows of particles different in both size and density.

Keywords: segregation, mixing, DEM simulations, mixture model

1. Introduction

Sheared particulate mixtures of different sizes and/or densities segregate into a wide range of segregation patterns, important for a wide range of industrial processes (e.g., Mosby et al., 1996; Hogg, 2009), and complex even under simple boundary conditions. Examples include relatively simple experimental flows in a shear cell (Duffy and Puri, 2002; May et al., 2010a, 2010b), in an inclined plane flow (Savage and Lun, 1988; Gray and Thornton, 2005; Gray and Chugunov, 2006), and in a rotated drum (Hill et al., 1997; Khakhar et al., 1997; Hill et al., 1999b; Taberlet et al., 2004; Shinbrot and Muzzio, 2000), to relatively complex geophysical flows (e.g., Middleton, 1970), such as in a riverbed (Paola and Seal, 1995; Dietrich et al., 1989) and in a debris flow (Stock and Dietrich, 2006; Hsu et al., 2008; Yohannes et al., 2010).

The details of the segregation dynamics depend on several factors. Gravity has long been known to drive sorting of different types of particles (depending on relative size, density, etc) (Donald and Roseman, 1962; Bridgwater, 1976; Williams, 1976). For flow of very fine particles in air, the effect of air drag on particles likely is a cause of segregation (e.g., Williams, 1976; Schulze, 2008) just as in rivers, where drag from the moving water can lead to selective transport of smaller particles downstream, contributing to “downstream fining”. Under many conditions, particularly in collisional flows, interparticle interactions play a dominant role. Through these interactions, gradients in granular temperature (i.e., the random kinetic energy of the particles, as in Jenkins and Mancini, 1987; Xu et al., 2003; Galvin et al., 2005), similar to gradients in kinetic stress (Fan and Hill, 2011b), and solid fraction gradients (Hill and Fan, 2008) drive segregation. We focus here on the dynamics associated with the unmixing of particles in high-concentration (high solids volume fraction) sheared flows, applicable to a wide range of systems of variable boundary conditions and advective flow patterns. The focus of modeling efforts of segregation in high concentration gravity-driven flows has been largely associated with gravity as the driving force. In most cases, in mixtures of particles differing only in size, small particles sink in the direction of gravity, away from the free surface in gravity-driven flows, while large particles rise. In mixtures of particles differing only in density, the less
dense particles rise, and the denser particles sink. While granular temperature has been shown to play a role in segregating sparse mixtures (e.g., Jenkins and Mancini, 1987; Xu et al., 2003; Galvin et al., 2005), stresses related to velocity fluctuations in dense flows are significantly less than stresses associated with gravity, so they have largely been neglected in modeling segregation in dense flows.

The gravity-driven flow models have taken a few different forms (e.g., Duffy and Puri, 2003). Savage, S. and Lun, C. (1988) developed a model for size-dependent segregation based on two simultaneous mechanisms: geometrically-associated, gravity-driven sorting they described as a ‘random fluctuating sieve’, and a mass-balancing ‘squeeze expulsion’ mechanism. Essentially gravity pushes all particles in one direction, but the structure associated with the high packing fraction prevents most particles from responding. Statistically, in a mixture of different-sized particles it is more likely that small particles will find holes sufficiently large for them to enter. As the mixture is excited and the particles shift, holes of different sizes open and close, giving the small particles opportunities to drop downward via what they refer to as a ‘sieving’ mechanism. A higher shear rate results in a more frequent availability of holes and thus a higher segregation rate. Mass balance is achieved when the downward migrating smaller particles squeeze the larger particles upward via the ‘squeeze expulsion’ mechanism. Savage, S. and Lun, C. (1988) developed a detailed statistical model to predict segregation trends based on this process. However, gravity is not explicitly included in the model so the direction of segregation has to be determined implicitly.

Another model framework that is particularly useful for predicting evolution of a mixture is based on mixture theory. Specifically, there is a family of these models that can predict local segregation flux and constituent concentration evolution based on other details of the flow such as local and instantaneous concentrations of each constituent. We review a few such models for systems in simple shear flows, where the system is uniform in all directions except one, and the average flow is normal to that direction. In all cases here, we will adjust the coordinate system so that the direction of non-uniformity and the direction of segregation is the y-direction, though the other details of the coordinate system vary a bit with boundary conditions.

Khakhar, D. et al. (1997) proposed a ‘buoyancy’ mechanism for gravity-driven segregation according to particle density that took a form similar to pressure on a submerged object by a surrounding fluid. For example, for flow of such a mixture down a plane inclined by \( \zeta \) relative to the horizontal, where \( y \) is increasing away from the free surface (in the direction of gravity), the concentration flux of the less dense particles normal to the flow may be expressed according to:

\[
\phi_i^{ld}(y^d - v) = -C_K \left( 1 - \frac{\phi_i^{ld}}{\rho_m^{ld}} \right) \psi_i^{psi} (1 - \phi_i^{ld}) \rho \cos \zeta - D \frac{\partial \phi_i^{ld}}{\partial y} \tag{1.1}
\]

In the original form of this theoretical framework, \( C_K \) was an empirically determined parameter with dimensions of time that is inversely related to the resistance to local motion, what might be called an inverse drag function; \( D \) is the diffusivity. \( v^d \) is the local average velocity of species \( i \) in the segregation direction (normal to the average flow), \( \rho_m^{ld} \) is the material density of species \( i \), and \( \phi_i^{ld} \) is the local volume concentration of particles of species \( i \). \( \phi_i^{ld} = f_i^l / \Sigma f_i^l \), where \( f_i^l \) is the local solids fraction of constituent \( i \). The subscripts \( i = d, \text{ld} \) denote denser and less dense particles, respectively, and for the variables of the mixture no subscript is used (e.g., \( \Sigma f_i^l = f_i^ld + f_i^d \)). \( g \) refers to gravitational acceleration.

Gray, N. and Thornton, A. (2005) and Gray, N. and Chugunov, V. (2006) developed a continuum framework for segregation according to particle size for equal density particles based in part on mixture theory. Similar to the segregation model of Khakhar, D. et al. (1997), the focus of the segregation mechanism is on the gradient in ‘lithostatic pressure’ induced by gravity, \( p \). That is, for flow of a mixture down a plane inclined by \( \zeta \) relative to the horizontal, and, again, where \( y \) is increasing away from the free surface (in the direction of gravity), \( \partial p / \partial y = \rho g \cos \zeta \). The segregation mechanism is represented by the partitioning of that pressure among the different species. Specifically, each constituent \( i \) bears a fraction of the total pressure \( p = \psi_i^{psi} p \), where \( \psi_i^{psi} \) is a partial pressure coefficient, not necessarily equal to the local concentration of \( i \) in the mixture, \( \phi_i^{psi} \). The original argument posed by Gray, N. and Thornton, A. (2005) indicated that whichever constituent bears more of the stress relative to its local concentration moves to lower lithostatic pressures and the other constituent moves to higher pressures. For example, again, for \( y \) increasing away from the free surface (in the direction of gravity):

\[
\phi_i^{psi} (v^d - v) = \frac{1}{C_D} (\phi_i^{psi} - \psi_i^{psi}) \rho \cos \zeta - D \frac{\partial \phi_i^{psi}}{\partial y} \tag{1.2}
\]

In this Equation, \( C_D \) is a drag coefficient. They made some assumptions about the pressure partitioning coefficients, i.e., for the particles greater in size \( i = b \), \( \psi_i^{psi} = \phi_i^{psi} + B_{GT} \phi_i^{psi} (1 - \phi_i^{psi}) \), where \( B_{GT} \) is the magnitude of a non-dimensional perturbation of the partial pressure coefficients away from the solid volume fractions for each species. Then, for a flowing bidispersed mixture, Eqn. (1.2) takes a form not dissimilar from that in Eqn. (1.1):

\[
\phi_i^{psi} (v^b - v) = - \frac{B_{GT}}{C_D} (\phi_i^{psi} - \psi_i^{psi}) \rho \cos \zeta - D \frac{\partial \phi_i^{psi}}{\partial y} \tag{1.3}
\]
The function \( B/c_D \) in Eqn. (1.3) corresponds to the function \( C_K \times (\rho_{sl} - \rho_d) \) in Eqn. (1.1).

For the purpose of the mathematical development in these original papers (Khakhar et al., 1997; Gray and Thornton, 2005; Gray and Chugunov, 2006), coefficients related to drag and diffusion (e.g., \( C_K \), \( c_D \), and \( D \)) were initially approximated as constant. These frameworks have been shown to be effective in reproducing segregation trends in a range of granular flows, e.g., in the case of the original model by Khakhar et al. (1997), segregation in cylindrical and spherical drums (e.g., Hill et al., 1999a, 1999b; Gilchrist and Ottino, 2003) and in the case of the Gray-Thornton-Chugunov framework in other simple and complex granular flows by, for example, Wiederseiner et al. (2011); Thornton et al. (2012); Weinhart et al. (2013); Fan et al. (2014). However, these studies have also provided evidence that some details are not fully captured by the model.

Subsequent work has suggested specific modifications to this general framework to better capture the discrepancies between model and experimental and computational data. For example, more recent work by Khakhar, and colleagues (Sarkar and Khakhar, 2008; Tripathi and Khakhar, 2011, 2013) derived a more physical form of the inverse drag function \( C_K \) by considering movement of particles differing in density through an effective medium and showed the drag increased with an effective temperature. May, L. et al. (2010a, 2010b) was the first who considered the effects of a non-constant shear rate on the Gray-Thornton-Chugunov model in the form of a shear-rate dependent maximal segregation rate, though a quantitative comparison between theory and experiments has not yet been performed. Weinhart, T. et al. (2013) demonstrated that the linear drag law contained within the original Gray-Thornton-Chugunov framework may not be sufficient for capturing the drag in the system, which appeared to vary with time in their system. Gray, J. and Ancey, C. (2011) expanded the framework into a theory incorporating multiple discrete particle sizes. Marks, B. et al. (2012) partitioned the stresses explicitly according to particle size ratio; they derived a shear-rate-dependent segregation velocity, and they extended the model for continuously varying particle size distributions. They demonstrated that their new model captured segregation dynamics in a simulated polydisperse mixture. Most recently, Fan, et al. (2014) considered both shear-rate-dependent coefficients of segregation, velocity, and diffusion in the framework and showed a more quantitative agreement with experiments and DEM simulations. Tunuguntla et al. (2014) extended this framework to mixtures of particles varying in density and size and, with a shear rate dependent drag coefficient, achieved good agreement with data from computational simulations of a broad range of mixtures.

As flexible as these frameworks are, they do not have the capacity to represent how shear rate gradients and associated effects such as granular temperature gradients might affect the direction and degree of segregation. Recent work has shown that dynamics associated with shear rate gradients not only may segregate particles in cases where gravity does not play a role in segregating the particles (Hill and Fan, 2008; Fan and Hill, 2010, 2011a, 2011b), as illustrated in Fig. 1 but they also appear to play a significant role comparable to that of gravity (Hill and Tan, 2014).

A model developed by Fan, Y. and Hill, K. (2011b) showed how the basic development used for the original Gray-Thornton-Chugunov model (Gray and Thornton, 2005; Gray and Chugunov, 2006) for different sized particles could be expanded to include consideration of shear rate gradients, also in the context of a gravitational field (Hill and Tan, 2014) and for particles differing in density (Fan and Hill, 2015). As explained in more detail in the next section, the model considered the local stress to be the sum of contact and kinetic stresses, \( \sigma^c \) and \( \sigma^k \), respectively, so that \( \sigma = \sigma^c + \sigma^k \) (similar to others, such as Chikkadi, V. and Alam, M. 2009). The contact and kinetic stresses are separately partitioned between the mixture components according to partial stress coefficients \( \psi^{c/c} \) and \( \psi^{k/c} \), e.g., \( \sigma_{ij}^{c/c} = \psi^{c/c} \sigma_{ij}^{c/c} \) and \( \sigma_{ij}^{k/c} = \psi^{k/c} \sigma_{ij}^{k/c} \). For the flow of a mixture down a plane inclined by \( \zeta \) and \( y \) normal to the average flow direction as for Eqns. (1.1–1.3): \( \Sigma_{j=c,k}(\partial \sigma_{ij}/\partial x + \sigma_{ij}/\partial y + \sigma_{ij}/\partial z) = \rho \cos \zeta \), for particles differing in size and density:

\[
\rho'(v' - v) = \frac{(\psi^{c} - \psi^{k})}{c_D} \frac{\partial \sigma_y^k}{\partial y}
\]

\[
+ \left(\frac{\phi_i - \psi_d}{c_D} \right) \rho \cos \zeta - D \frac{\partial \rho'}{\partial y} \tag{1.4}
\]

All variables are as previously defined, and \( \rho' \) is the local bulk density of constituent \( i \), related to the material density of constituent \( i \) and its local solids fraction \( f \) according to \( \rho' = f' \rho_{li} \). While Equation (1.4) is of similar form to Eqns. (1.1–1.3), there are some key difference, most notably the new term dependent on the gradient in kinetic stress \( \partial \sigma_{ij}^k / \partial y \).

In the following sections, we show how Eqn. (1.4) can be derived and the similarities to Eqns. (1.1–1.3) under analogous conditions where the gradient in kinetic stress is negligible. Then, we provide a few examples validating this framework for dense flows. We conclude with some discussion of both the potential generalizability and also limitations of this model in its current form and some next steps that are needed for further improving the model.
2. Mixture theory with effects of velocity fluctuations

Generalizing the work by Fan, Y. and Hill, K., (2011b, 2015) and Hill, K. and Tan, D. (2014) we consider a mixture of particles differing in size and/or density in high solids fraction sheared flows. For simplicity, we present the model in terms of binary mixtures of two constituents $i=1, 2$ which may differ in material density $\rho_i$ and diameter $d_i$, though the model is generalizable to multiple constituents. We denote bulk Eulerian properties of each species with superscripts and those of the mixture of both species together as variables without superscript.

As is true of standard mixture theory, the local bulk mixture density $\rho$ is the sum of the densities of each of the constituents $\rho_i$, i.e., $\rho = \sum_i \rho_i = \sum_i f_i \rho_i^m$. We recall the volume concentration of species $i$ is $\phi_i = f_i / f$ and define the mass concentration of species $i$ as $\phi_i^m = \rho_i / \rho$, both of which satisfy $\sum_i \phi_i^m = 1$. We approximate the solid fraction $f = \sum_i f_i$ as constant, but, if the particles of the two constituents differ in material density, $\rho_i^m$, the average local density $\rho = \sum_i \rho_i$ varies with the local concentrations of the constituents. The velocity of the constituents is allowed to differ from the average mixture velocity, and we define it in terms of the volume concentrations of the species: $u = \sum_i u_i \phi_i$.

2.1 Conservation equations for gravity-driven mixtures

We first consider conservation of mass and momentum for the mixture when subjected to gravity:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \quad (2.1a)$$

$$\frac{\partial (\rho u)}{\partial t} + (\rho u \otimes u) = \nabla \cdot \sigma + F \quad (2.1b)$$

Here, $\sigma$ represents the stress tensor, and $F$ represents body forces per volume. Since our mixture is subjected to gravity, $F = \rho g$, where $g$ is the gravitational acceleration vector.

The conservation equations are similar for the individual constituents:

$$\frac{\partial \rho_i}{\partial t} + \nabla \cdot (\rho_i u_i) = 0 \quad (2.2a)$$

$$\frac{\partial (\rho_i u_i)}{\partial t} + (\rho_i u_i \otimes u_i) = \nabla \cdot \sigma_i + F_i + \beta_i \quad (2.2b)$$

Here, all of the terms used for constituent $i$ are identical in form to those used for the mixture in Equation (2.1b), with the exception of the new term $\beta_i$. $\beta_i$ represents the interaction force exerted on constituent $i$ by the other species. $\sigma_i$ is the total local stress borne by species $i$, where the total stress $\sigma = \sum_i \sigma_i$.
We consider these equations in the context of flows of relatively high concentration where the mixture kinematics reach steady state long before segregation reaches steady state, as demonstrated for simulations of flows of \( f \approx 0.6 \) in a vertical chute (Fan and Hill, 2011b, 2015) and in a rotated drum (Hill and Tan, 2014). Then, we can set \( \partial q / \partial t = \partial (\mu u) / \partial t = 0 \) in Eqns. (2.1a) and (2.1b). We then follow operations similar to Reynolds decomposition (Schlichting, 1979) and set each variable \( q \) at position \( r \) equal to a sum of the local temporal average \( \bar{q}(r) \) and the difference between its instantaneous and average values \( q'(r, t) = q(r, t) - \bar{q}(r) \). This mathematical manipulation allows for the explicit representation of the effect of fluctuating velocities on flow dynamics. In particular, the second term on the left side of Eqn. (2.1b) \( \nabla \cdot (\mu u \otimes u) \) may be written as \( \nabla \cdot [(\bar{p} + \rho') \times (\bar{u} + u') \otimes (\bar{u} + u')] \). Taking the average of this expression, assuming temporal correlations between velocity fluctuations and densities are negligible (detailed in Fan and Hill, 2011b), yields terms like \( \partial (\bar{p} v v + \bar{\rho} v v' v') / \partial y \). Assuming the simple flows that are non-uniform in only the \( y \)-direction and the average flow direction is in a direction normal to that direction, Eqn. (2.1b), the conservation of momentum equation normal to the flow for the mixture may be simply expressed according to:

\[
\frac{\partial \sigma_{yy}^c}{\partial y} + \frac{\partial \sigma_{yy}^k}{\partial y} = \bar{p} \cos \zeta
\]  

(2.3)

This indicates that the sum of the gradients in contact stresses and kinetic stresses balance the lithostatic pressure generated by the weight of the particles. Here, \( \sigma_{yy}^c = \rho v v' \) is a normal component of the kinetic stress tensor (Chikkadi and Alam, 2009) and \( \sigma_{yy}^k \) represents a component of the normal contact stresses generated by repulsive contacts between particles. We note that granular temperature scales as the trace of the kinetic stress tensor \( T = \rho (v v' + v v' + v v') \), and has a similar form to \( \sigma_{yy}^k \) (e.g., Fan and Hill, 2011).

By performing Reynolds decomposition and then averaging the conservation of momentum equation for the constituents, Eqn. (2.2b), we may write:

\[
\frac{\partial \sigma_{yy}^c}{\partial y} + \frac{\partial \sigma_{yy}^k}{\partial y} = \rho' \cos \zeta + \bar{p}_y
\]  

(2.4)

Since all terms in Eqns. (2.3) and (2.4) are averaged, from this point on, we drop the overbar, so that unless noted for each variable \( q \) alone refers to the average \( \bar{q} \).

### 2.2 Stress partitioning and interaction forces

To account for stress partitioning, this theory follows the suggestion of Gray, N. and Thornton, A. (2005) and Gray, N. and Chugunov, V. (2006) to allow for the partitioning of stresses between the constituents, but differs somewhat in the separate partitioning of the kinetic and contact. Specifically:

\[
\sigma_{yy}^{\text{co}} = \psi^{\text{c}} \sigma_{yy}^{\text{c}}, \quad \text{and} \quad \sigma_{yy}^{\text{ki}} = \psi^{\text{k}} \sigma_{yy}^{\text{k}}
\]  

(2.5)

where we explicitly define the normal contact and kinetic stress partition coefficients for these stress components as \( \psi^{\text{c}} \) and \( \psi^{\text{k}} \), respectively. Neither stress partition coefficient is required to follow the concentrations of the constituents, for example, \( \psi^{\text{c}}, \psi^{\text{k}} \neq q_i \). To assure that \( \Sigma \sigma_{yy}^{\text{co}} = \sigma_{yy}^{\text{c}}, \Sigma \sigma_{yy}^{\text{ki}} = \sigma_{yy}^{\text{k}} \) two constraints must be satisfied: (1) that \( \Sigma \psi^{\text{c}} = 1 \) and \( \Sigma \psi^{\text{k}} = 1 \), and (2) wherever only one species is present (i.e., when \( q_i = 1 \)) \( \psi^{\text{c}}, \psi^{\text{k}} = q_i \), where \( \delta_{ij} \) is the Kronecker Delta function. Otherwise, no functional form is specified for either.

For the interaction term \( \beta'_y \), we can use a similar form to that proposed by Gray, N. and Chugunov, V. (2006) for granular mixtures and for flow through porous media provided by Morland, L. (1992):

\[
\beta'_y = \sigma_{yy}^{\text{c}} \frac{\partial \psi^{\text{c}}}{\partial y} + \sigma_{yy}^{\text{k}} \frac{\partial \psi^{\text{k}}}{\partial y} - \rho c_D (v_i - v) - d \frac{\partial \rho_i}{\partial y}
\]  

(2.6)

The first two terms on the right side of the equation ensure that the segregation processes are driven by intrinsic rather than partial stress gradients. The third term is effectively a linear drag law, where \( c_D \) is the linear drag coefficient. The fourth term acts as a ‘remixing force’ along gradients in the concentration of each species, where the coefficient \( d \) is similar to a linear diffusion coefficient.

### 2.3 General segregation flux expression

Combining Eqn. (2.4)–(2.6) with Eqn. (2.3), we can express the theoretical net flux of species \( i \), \( \Phi_i = [\rho' (v_i - v)]_1 \), as:

\[
\Phi_i = \Phi^{\text{ci}}_t + \Phi^{\text{ki}}_t + \Phi^{\text{di}}_t
\]  

(2.7)

where:

\[
\Phi^{\text{ci}}_t = \left(\psi^{\text{c}} - \psi^{\text{k}}\right) \frac{\partial \sigma_{yy}^{\text{k}}}{\partial y}
\]  

(2.8a)

\[
\Phi^{\text{ki}}_t = \left(\psi^{\text{k}} - \psi^{\text{c}}\right) \frac{\partial \sigma_{yy}^{\text{c}}}{\partial y}
\]  

(2.8b)

\[
\Phi^{\text{di}}_t = \frac{d}{c_D} \frac{\partial \rho_i}{\partial y}
\]  

(2.8c)

This expression is identical to that in Eqn. 1.4, with the substitution \( D = d/c_D \), and suggests that there are three ‘forces’ dictating the segregation behavior. The first, \( \Phi^{\text{ci}}_t \),
is controlled by the gradient in the kinetic stress of the mixture and the difference between the two stress partition coefficients. If a constituent bears a higher contact stress than kinetic stress then it moves in the direction of an increasing kinetic stress. The other two terms are similar to other models where the effects of kinetic stresses are not included. The second term in Eqn. (2.7), $\Phi_{\text{g}}$, is the segregation associated with gravity, specifically, the pressure gradient induced by gravity. If a species supports a higher fraction of the contact stress than its local concentration, the species moves opposite the direction of gravity, toward the free surface. The third term in Eqn. (2.7), $\Phi_{\text{d}}$, is akin to a diffusion force. Like normal Fickian diffusion with diffusion coefficient $D = d/cD$, this term results in a flux in the direction opposite to that of the concentration gradient of a particular species, and thus serves to limit the degree of local segregation.

In the next section, we show how the general flux expression in Eqn. (2.7) can be simplified to one of two scenarios: (1) where there is no kinetic stress or temperature gradient (as one would expect where fields such as the velocity and velocity fluctuations are uniform), and (2) to situations where there is a gradient in velocity fluctuations but no gravity. In these cases, the models are similar to those previously published. We demonstrate this in the next section.

3. Segregation flux in special cases

As noted above, Eqn. 2.7 is meant to be a general expression for high concentration sheared flows. For more insight about this expression, in this section we first investigate the implications of this expression for systems where the kinetic stress gradient is negligible and gravity dominates. Then we investigate this for systems where the effect of gravity on segregation is negligible, and kinetic stress gradients dominate.

3.1 Segregation flux for a negligible kinetic stress gradient

We mentioned in Section 1 that the general flux expression in Eqn. (2.7) is similar to those derived for mixtures of particles differing only in size or density (Eqn. (1.1) and (1.2), respectively) for cases where these is a negligible kinetic stress gradient. To demonstrate that, we first eliminate the kinetic stress gradient in Eqn. (1.4):

$$\rho' (v' - v) = \rho (\frac{\partial \bar{v}}{\partial \rho}) \frac{\partial \rho'}{\partial y}$$

In the case of particles of the same material density, if $f$ is uniform, $\rho$ is uniform and constant as well. Additionally, the mass and volumetric concentration of constituent $i$ are the same, so one can substitute $\bar{v}' = \phi_{\text{m}} \bar{v}'$. Then one may divide both sides of Eqn. (3.1) by $\rho$ to get a segregation prediction similar to the one from Gray, N. and Chugunov, V. (2006) expressed by Eqn. (1.2):

$$\phi_{i}' (v' - v) = \frac{1}{cD} (\phi_{i}' - \psi_{i}' \rho) g \cos \zeta - D \frac{\partial \phi_{i}'}{\partial y}$$

(3.2)

For the expressions in Eqns. (1.2) and (3.2) to be identical, the contact stress must be partitioned between the constituents identically to the pressure and the kinetic stress. Then, for the large particles to rise to the top, the large particles must have more of the contact stress partitioned relative to their concentration ($\phi_{i}'$) than the small particles. In particular, for Eqns. (1.2) and (3.2) to be identical, we would require $\psi_{i} = \phi_{i}' = B \phi_{i} \phi_{i}'$. We explore this in the next section using computational simulations of sheared flows.

In the case of particles of the same size, different material density, we cannot simply divide by $\rho$. We recall that $\rho' = f' \rho_{\text{m}} = f \rho_{\text{m}}$, and divide Eqn. (3.1) by $f \rho_{\text{m}}$:

$$\phi_{i}' (v' - v) = \frac{\rho}{cD f \rho_{\text{m}}} (\phi_{i}' - \psi_{i}' \rho) g \cos \zeta - D \frac{\partial \phi_{i}'}{\partial y}$$

(3.3)

The model summarized by Eqn. (1.1) does not seem equivalent, at first glance. However, with a bit of algebra, one can show that if $\psi_{i} = \phi_{i}'$, Eqns. (1.1) and (3.3) are actually equivalent. We will discuss this in more detail in Section 5 in the context of computational measurements of $\psi_{i}'$ for special cases in Section 4.

3.2 Segregation flux for a negligible gravitational effect

There have also been situations where a gradient in velocity fluctuations have been shown capable of segregating particles without help from gravity. Examples include: microgravity experiments (Xu et al., 2003); experiments using thin layers (Conway et al., 2006) or internal shear bands (Hill and Fan, 2008), and simulations of vertical chutes (Fan and Hill, 2011a). These cases may be modeled using the general flux expression in Eqn. (2.7) by eliminating the term associated with gravity:

$$\rho' (v' - v) = \frac{(\psi_{i}' - \psi_{\perp}) \frac{\partial \sigma_{y}}{\partial y}}{cD} - D \frac{\partial \phi_{i}'}{\partial y}$$

(3.4)

For a qualitative picture of the segregation process dictated by this term, we consider that the kinetic stress scales similarly to the granular temperature (e.g., Fan and Hill, 2011b). A constituent that bears more kinetic stress might be considered more mobile and more likely to find spaces or vacancies to move away from the high temperature region, somewhat like ‘kinetic sieving’ of the particles to the ‘cooler’ region. On the other hand, a constituent that bears more contact stress is physically pushed by in-
that particle contacts to a region of lower contact stress and higher temperature, somewhat like ‘squeeze expulsion’ in the qualitative balance of movement induced by kinetic sieving suggested by Savage, S. and Lun, C. (1988). For mixtures of particles differing only in size, the mixture density $\rho$ is nearly constant, so we can rewrite Eqn. (3.4) for a form identical to that originally proposed by Fan, Y. and Hill, K. (2011b):

$$\phi_i'(v' - v) = \frac{(\psi^{ij} - \psi^{kk})}{c_D} \frac{1}{\rho} \frac{\partial \sigma_{ij}^n}{\partial y} - D \frac{\partial \phi_i'_{ij}}{\partial y}$$

(3.5)

While it is rare to have a situation where granular temperature works alone to segregate a particulate mixture, understanding its effect is important as in most cases gravity and granular temperature gradients coexist.

In the next section we review two examples of segregation associated with shear rate gradients and associated kinetic stress gradients in dense flows, one where gravitational effects do not contribute in the direction of segregation, and one where both kinetic stress gradients and gravity are both important.

4. Examples of shear-induced segregation

Examples supporting the framework described above have mainly been obtained from Discrete Element Method (DEM) Simulations first introduced by Cundall, P. and Strack, O. (1979). This simulation framework is powerful as it allows the user to input mechanistically representative interparticle forces and then essentially perform a computational experiment. The user may track all particles and associated forces throughout the simulations so all quantities in the model such as contact stresses and kinetic stresses can be calculated and used to test the theory. On the other hand, there can be significant limitations to the model. Even though contact forces can be represented reasonably well, they still have limitations in their representations for real dissipative materials. Additionally, variability of the surface such as roughness elements and asperities cannot be represented well. Ultimately, experiments are the best test of models. To this point, since we do not have access to experimental contact stresses, we limit our review to simulation results.

The simulations we review here use a nonlinear soft sphere contact force model. As is common, the particle deformations resulting from particle-particle contacts are represented by small overlaps between particles and related to interparticle forces. The model representing the relationship between deformations (overlaps) and interparticle forces follows Hertz-Mindlin contact theory with damping components related to the coefficient of restitution as developed by Tsuji et al. (1992) and Coulomb sliding friction:

$$F_n = -k_n \delta_n^{3/2} - \eta_n \delta_n^{1/4} \dot{\delta}_n$$

(4.1a)

$$F_i = \text{min}\{-k_i \delta_i^{1/2} - \eta_i \delta_i^{1/4} \dot{\delta}_i, \mu F_n\}$$

(4.1b)

where $F_n$ and $F_i$ are the contact forces in the directions normal and tangential to the contact plane between two contacting particles, $\delta_i$ and $\delta_i$ are the corresponding deformations, and $\dot{\delta}_i = \partial \delta_i / \partial t$ and $\dot{\delta}_i = \partial \delta_i / \partial t$ are the local time derivatives of these fluctuations. The coefficients in the force model ($k_n$, $k_i$, $\eta_n$, and $\eta_i$) are related to material properties of the two contacting particles such as elastic moduli, mass, and diameter as suggested in the original papers (e.g., Hertz, 1882; Mindlin and Deresiewicz, 1953; Johnson, 1985; Tsuji et al., 1992) and detailed in the relevant recent papers cited below (i.e., Fan and Hill, 2011; Hill and Tan, 2014).

4.1 Vertical chute flows

To isolate the effect of shear rate gradients from the effect of gravity, Fan, Y. and Hill, K. (2011a, 2011b; 2015) used DEM simulations of mixtures of particles differing only in size (Fan and Hill, 2011a) and only in density (Fan and Hill, 2015) sheared in a vertical chute [Fig. 1(a)]. The vertical chute is ideal for studying the effect of shear rate gradients and associated granular temperature gradients on segregation because of its simple geometry but inhomogeneous flow structure [Fig. 1].

Fig. 1 presents some kinematics and segregation snapshots for a mixture of 2 mm and 3 mm particles of different average system solids fractions, $\langle f \rangle = 0.2$ to 0.6. Here, we use angular brackets to indicate that these values represent the solid fraction of the whole mixture. For the high concentration system, $\langle f \rangle = 0.6$ Fan, Y. and Hill, K. (2011b) calculated partial stress coefficients throughout the simulations to test the applicability of the theory presented in Eqn. (3.4) for cases where the flow was dense and kinetic stress gradients dominated in the direction of segregation.

The results for the normalized coefficients $R^{cij} = \psi^{cij} / \phi_i'$, and $R^{kij} = \psi^{kij} / \phi_i'$ from the simulations for $\langle f \rangle = 0.6$ are plotted in Fig. 2. As shown, $R^{cij} = 1$ everywhere except adjacent to solid boundaries, so that $\psi^{cij} \approx \phi_i'$ for these systems. In other words, the contact stress is partitioned between species exactly according to the volumetric concentration in the mixture. In contrast, $R^{kij} > 1$ and $R^{kij} < 1$ everywhere, so that $\psi^{kij} > \phi_i'$, and $\psi^{kij} < \phi_i'$, except where either $\phi_i' = 1$ or $\phi_i' = 1$. In other words, except in locations completely segregated where there are only large or small particles, the smaller particles carry a greater share of the kinetic stress than their concentration, while the larger particles carry less of the kinetic stress than their concentration. Considering this and the observation that the kinetic stress is greatest near the walls and
decreases inward, that is, $\frac{\partial \sigma^k}{\partial y} > 0$ for $y < 0$ and $\frac{\partial \sigma^k}{\partial y} < 0$ for $y > 0$ (similar to temperature in Fig. 1(a)), Eqn. (3.5) predicts that small particles segregate to the center of the chute, consistent with observation (Fig. 1).

For a more quantitative prediction, Fan, Y. and Hill, K., (2011b) adapted a simplifying form of the kinetic stress partition coefficient from the partial pressure coefficient from Gray, N. and Thornton, A. (2005). Specifically, they approximated $k_{FH,1} = \frac{c_{sb}}{\sigma_c}$, and $k_{FH,1} = -\frac{D}{c} \frac{\partial \phi^s}{\partial y}$, where $B_{FH,1}$ is the magnitude of a non-dimensional perturbation of the kinetic stress partition coefficients away from the solid volume fractions for each species. This form satisfies some basic restrictions on the partial pressure coefficients, namely, that they must sum to 1 so that stresses of the constituents sum to the stress of the mixture, regardless of the concentration of the individual constituents. Using this form for the partial kinetic stress coefficients and the previously mentioned finding that $c_i \approx c_s$, we can write $\psi^{CI} - \psi^{KH} = B_{FH,1} \phi^s$. Then, we can write Eqn. (3.5) for large particles as:

$$\phi^s_v = \frac{B_{FH,1} \phi^s}{c_0} - \frac{1}{\rho} \frac{\partial \sigma^k}{\partial y} - D_0 \frac{\partial \phi^s}{\partial y}$$

Upon substituting Eqn. (4.2) into Eqn. (2.2a), we find the time dependence of the local concentration of larger particles:

$$0 = \frac{\partial \phi^s}{\partial t} +$$

$$\frac{B_{FH,1}}{c_0} \frac{\partial}{\partial y} \left( \phi^s (1 - \phi^s) \right) - \frac{1}{\rho} \frac{\partial \sigma^k}{\partial y} \left( \frac{\partial \phi^s}{\partial y} \right)$$

The tempo-spatial profiles of concentration of large particles can then be obtained by solving Eqn. (4.3) numerically provided that $\rho$, $\frac{\partial \sigma^k}{\partial y}$, $\frac{1}{\rho} \frac{\partial \sigma^k}{\partial y}$, and $\frac{\partial \phi^s}{\partial y}$ are known. The comparison between simulation and theoretical predictions is shown in Fig. 3.

Figs. 3(a) and (b) show tempo-spatial profiles of concentration of large particles from simulation data and theoretical predictions, respectively. In both the simulation results and theoretical predictions, the large particles segregate to the side walls, and small particles segregate toward the center of the chute. For physical intuition about how this process is related to kinetic stresses, we can consider that particles tend to be pushed away from regions of high granular temperature associated with high collisional interactions. This is especially true for systems of lower solids fraction when all particles can move away from regions of high granular temperature (e.g., as in Fig. 1(e)–(f) and in other sheared systems, as those reported in this paper).
Kimberly M. Hill et al. / KONA Powder and Particle Journal No. 33 (2016) 150–168

In high solid fraction sheared flows, where particles cannot “escape” en masse from the higher temperature regions, the smaller particles, with their higher kinetic stress or higher granular temperature but the same material density have more variability in their displacements (direction and magnitude). Thus have a higher likelihood of finding a way around other particles away from the region of higher granular temperature. In the center of the chute, where the gradient of normal kinetic stress is very small, the segregation process is much slower than other regions. All of these indicate a good qualitative agreement between theoretical predictions and simulation results, though they do not reach a perfect quantitative agreement.

Hill, K. and Fan, Y. (2015) performed analogous chute flow simulations of mixtures of particles differing only in density (2mm particles of densities 2520 kg/m$^3$ and 7800 kg/m$^3$). In contrast with the mixtures of particles of different size, in this case, the heavier (denser) particles segregated to regions of low kinetic stress, low granular temperatures in the center of the chute.

The results for the normalized coefficients $R^{k,i} = \psi^{k,i} / \phi$, and $R^{k,i} = \psi^{k,i} / \phi$, from the simulations for $\langle f \rangle = 0.6$ are plotted in Fig. 4. As shown, $R^{k,i} \approx 1$ everywhere except adjacent to solid boundaries, so that $\psi^{k,i} \approx \psi$ for these systems. In other words, the contact stress is partitioned between species exactly according to the volumetric concentration in the mixture. In contrast, $R^{k,d} > 1$, and $R^{k,d} < 1$ everywhere, so that $\psi^{k,d} > \psi^d$, and $\psi^{k,d} < \psi^d$, except where either $\phi^d = 1$ or $\phi^d = 1$. In other words, except in locations completely segregated where there are only denser or less dense particles, the denser particles carry a greater share of the kinetic stress than their concentration, while the less dense particles carry less of the kinetic stress than their concentration. Considering this and the observation that the kinetic stress is greatest near the walls and decreases inward, that is, $\partial \sigma_{yy} / \partial y > 0$ for $y < 0$ and $\partial \sigma_{yy} / \partial y < 0$ for $y > 0$, Eqn. 3.4 predicts that denser particles segregate to the center of the chute, consistent with observation.

For a more quantitative prediction, similar to the case for different sized particles, Fan, Y. and Hill, K., (2015) approximated the variation of the kinetic stress partition functions as: $\psi^{k,d} = \phi^d \phi^d + B_{HF,2}^d \phi^d \phi^d$, and $\psi^{k,d} = \phi^d - B_{HF,2}^d \phi^d \phi^d$, where $B_{HF,2}$ is the magnitude of a non-dimensional perturbation of the kinetic stress partition coefficients away from the solid volume fractions for each species. This form satisfies some basic restrictions on the partial pressure coefficients, namely, that they must sum to 1 so that that stresses of the constituents sum to the stress of the mixture, regardless of the concentration of the individual constituents. Using this form for the partial kinetic stress coefficients and the previously mentioned finding that $\psi^{k,d} \approx \phi$, we can write $\psi^{k,d} - \psi^{k,d} = B_{HF,2} \phi^d \phi^d$. Then

$$\text{Eqn. 3.4 may be rewritten for less dense particles as:}$$

$$\rho^{k,d} (v^{k,d} - v) = \frac{B_{HF,2} \phi^d \phi^d}{c_D} \frac{\partial \sigma_{yy}^k}{\partial y} - D \frac{\partial \rho^{k,d}}{\partial y}$$

Upon substituting Eqn. (4.4) into Eqn. (2.2a), we find the time dependence of the local concentration of less dense particles:

$$0 = \frac{\partial \rho^{k,d}}{\partial t} + \frac{B_{HF,2}}{c_D} \frac{\partial}{\partial y} \left( \phi^d (1 - \phi^d) \frac{1}{\rho} \frac{\partial \sigma_{yy}^k}{\partial y} - D \frac{\partial \phi^d}{\partial y} \right)$$

Again, noting that, $\rho^l = f \rho^l_m = f \phi^l \rho^l_m$, we divide by $f \rho^l_m$ for the following expression for the evolution of the concentration:

$$\frac{\partial \phi^d}{\partial t} = \frac{B_{HF,2}}{c_D f \rho^l_m} \frac{\partial}{\partial y} \left( \phi^d (1 - \phi^d) \frac{1}{\rho} \frac{\partial \sigma_{yy}^k}{\partial y} \right) + \frac{\partial}{\partial y} \left( D \frac{\partial \phi^d}{\partial y} \right)$$

The tempo-spatial profiles of concentration of less dense particles can be obtained by solving Eqn. (4.6) numeri-
calculated provided that $\rho, \partial \sigma_{\parallel} / \partial y, D = d/c_D$, and a segregation coefficient defined according to $q_s = B/c_D$ can be obtained. For this case, Fan, Y. and Hill, K. (2015) found the best empirically determined values: $q_s = 1 \times 10^{-3}$, and $D = 0.2 \text{ mm}^2/s$. $q_s$ is approximately half that found for the mixture differing only in size, and $D$ for this mixture is approximately four times that found for the mixture differing only in size. This is consistent with the observation that segregation is slower for these systems. However, it is not clear whether or not this difference is significant, particularly given that it is likely that both $c_D$ and $D$ vary spatially with shear rate or other quantity so the difference in these variables is only a qualitative indicator. The comparison between simulation and theoretical prediction for the mixture differing in density is in Fig. 5.

Fig. 5(a) and (b) show tempo-spatial profiles of concentration of denser particles from simulation data and theoretical predictions, respectively. In both the simulation results and theoretical predictions, the less dense particles segregate to the side walls, and denser particles segregate toward the center of the chute. For physical intuition about this process, we note first that, unlike the case of the different sized same density particles, for this case of the particle differing only in density, the particles have the same magnitude of velocity fluctuations. Thus the greater magnitude of the kinetic stresses in the dense particle constituent arises from the higher material density of particles alone. In this context, we can still consider that particles tend to be pushed away from regions of high granular temperature associated with high collisional interactions. In high solid fraction sheared flows, we posit that the denser particles are able to push through a relatively tight mass of particles toward the “cooler” regions, whereas the lighter particles cannot “escape” as easily. As is the case for the mixture of particles differing only in size, in the middle slow creeping region, where the gradient of normal kinetic stress is very small, the segregation process is much slower than other regions. There is evidence of the discrete nature of the particles in the segregation trends in Fig. 5(a) not realizable in the continuum model results shown in Fig. 5(b). Nevertheless, the average trends are similar in both.

4.2 Rotating drum flows

In contrast with the simulations described in Section 4.1, in many sheared flows (such as inclined chute flows and rotated drums, e.g., Fig. 6), gravity, velocity gradients, and corresponding gradients in kinetic stress and temperature coexist in the direction of segregation. Hill, K. and Tan, D. (2014) investigated the effectiveness of the segregation expression in Eqn. (2.7) for the segregation in the thin flowing layer in a rotated drum (Fig. 6). In particular, they investigated whether the segregating effect of the kinetic stress gradient shown in vertical chute flows where the gravity had negligible segregating effect was significant in the presence of gravity.

Their simulated circular drum had periodic boundaries in the axial direction (e.g., no front and back walls in Fig. 6(a)) to eliminate side wall segregation effects (e.g. Hill and Zhang, 2008). The drum diameter is 72 mm; the thickness (periodic length in axial direction) is 30 mm. They ‘filled’ the drum partway with binary mixtures of particles of the same density and two different diameters, 2 mm and 3 mm, with a 10 % variability in particle size of each constituent. The particles were initially well-mixed when drum rotation was commenced at a speed of $\omega = 16$ rotations per minute (rpm). They studied the segregation dynamics for five different concentrations of large particles (by volume) in the mixture: $\phi_s = 10 \%, 25 \%, 50 \%, 75 \%,$ and $90 \%$. In all cases, the flow in the radial center of the drum (i.e., the center of the flowing layer) was nearly uniform in the streamwise ($x$-) and transverse ($y$-) directions, so the basic assumptions under which Eqn. (2.7) was developed hold, even though the entirety of the flow is relatively non-uniform.

The segregation dynamics vary somewhat from one
mixture to the next, as shown in Fig. 7. Specifically, for each, Fig. 7 row 1 shows snapshots of the near steady-state segregation patterns in the first row, the corresponding plot for the solid fractions $f_i$ in the second row, and the early-time segregation fluxes $f_i \Delta v_i$ in the third row. In all cases, the large particles segregated upward in the flowing layer and toward the outside of the drum. However, the segregation flux magnitudes and steady state relative concentrations of the two constituents varied from one mixture to the next.

While the segregation dynamics varied from one system to the next, the stress partition coefficients did not. Similar to the vertical chute flows, $R^{c,i} \approx 1$ everywhere except adjacent to solid boundaries, so that $\psi_{c,i} \approx \phi^c_i$ for all mixtures. In other words, the contact stress is partitioned between species exactly according to the volumetric concentration in the mixture. That is, Eqn. (2.7) reduces to Eqn. (3.5) in this circumstance, as with the additional substitution that $\psi_{c,j} \approx \phi^c_j$, this yields:

$$
\Phi^c_i = \frac{(\phi^c_i - \psi_{c,j})}{\epsilon_D} \rho g \cos \zeta = 0
$$  \hspace{1cm} (4.7a)

$$
\phi^c_i (v^i - v) = \left( \phi^c_i - \psi_{c,j} \right) \frac{1}{\epsilon_D} \frac{\partial \sigma_{c,j}^k}{\partial y} - D \frac{\partial \phi^c_j}{\partial y}
$$  \hspace{1cm} (4.7b)

In contrast, but, again, similar to the chute flows, $R^{k,s} > 1$ and $R^{k,b} < 1$ everywhere, so that $\psi_{k,s} > \phi^k_i$, and $\psi_{k,b} < \phi^k_i$, except where either $\phi^k_i = 0$ or $\phi^b = 1$. In other words, except in locations completely segregated where there are only large or small particles, the smaller particles carry a greater share of the kinetic stress than their concentration, while the larger particles carry less of the kinetic stress than their concentration. In fact, the relationship between $\psi_{k,b}$ and $\phi^k_i$ was essentially the same for all mixtures at all times (Fig. 8):

$$
\psi_{k,b} = 0.39 \times (\phi^k_i)^2 + 0.61 \times \phi^k_i
$$  \hspace{1cm} (4.8)

These results are similar in form to the pressure coefficient suggested by Gray and colleagues note in Section 1, though here we would write:

$$
\psi_{c,b} = \phi^c_i + B^c \phi^c_i 
$$  \hspace{1cm} (4.9a)

$$
\psi_{k,b} = \phi^k_i + B^k \phi^k_i
$$  \hspace{1cm} (4.9b)

where based on the simulations results, $B^c = 0$, and $B^k = -0.39$. Unlike the positive value of $B$ for the analogous total pressure partition coefficient suggested by Gray and colleagues, these two values, $B^c$ and $B^k$ are distinct,
and both less than or equal to zero because the large particles actually carry less than (or equal to) the portion of the stress compared to their concentration in the mixture. These results are not inconsistent with the results from the chute flows described in Section 4.1, for which Fan, Y. and Hill, K. (2011b, 2015) assumed, $\phi^c_b - \phi^k_b = B_{\phi} \phi^c_b$.

In these drum flows, $\psi^{b} - \psi^{k} = (B^c - B^k)\phi^c_b$, so that $B = B^c - B^k = 0.39$.

Finally, a predictive form for these gravity-driven flows, including effects of kinetic stress gradients associated with the shear rate gradients, can be written:

$$\phi^c_b (\psi^b - \psi) = \frac{B^k \phi^c_b (1 - \phi^c_b)}{c_D \rho} \frac{\partial \sigma_{y_b}}{\partial y} - D \frac{\partial \phi^c_b}{\partial y} \quad (4.10a)$$

$$\phi^k_b (\psi^b - \psi) = - \frac{B^k \phi^c_b (1 - \phi^c_b)}{c_D \rho} \frac{\partial \sigma_{y_b}}{\partial y} - D \frac{\partial \phi^k_b}{\partial y} \quad (4.10b)$$

for the large or big (b) and small (s) particle constituents, respectively.

For any particular mixture, a reasonable functional form for the drag and diffusion coefficients $c_D$ and $D$ may be found empirically using simulations of the mixtures. At early times, $c_D$ may be empirically derived by noting

---

**Fig. 7** Segregation of mixtures of different sized particles (2 mm and 3 mm) of equal material densities, where the system-averaged large (3 mm) particle concentration, $(\phi^c_b)$, varies from one column to the next. Specifically, $(\phi^c_b)$ increases from left to right from system-averaged large-particle concentrations $(\phi^c_b)$ from 0.1 to 0.9 as noted above each column. Row 1: Snapshots of the segregated mixtures from the time at which mixtures were under statistically steady state conditions (after $\approx 30$ s of rotation). Rows 2 and 3: Solid fraction and segregation flux data from the region of the drum indicated by the box in the first snapshot in row 1. In both rows, the $y$-direction is positive downward and normal to the free surface as indicated in the first snapshot in row 1. Row 2: Solid fraction profile for each species and for the mixture in the region corresponding to the simulation represented by each snapshot in the first row. The data are taken after $\approx 30$ s of rotation once each system has reached a statistically steady segregated state. Row 3: The segregation flux at the beginning of the simulation for each mixture. In each case the mixture started relatively well-mixed, and the data shown in Row 3 was taken from $\approx 0.5$ s after beginning rotation while the system was still relatively well-mixed. Negative values of the segregation flux indicate segregation upward toward the free surface, and positive values of the flux indicate segregation downward. The data shown in Rows 2 and 3 were obtained by averaging over a 500 ms period. From Hill, K. and Tan, D. (2014).

---

**Fig. 8** Kinetic stress partition coefficient as a function of concentration in the flowing layer of the drum simulations: (a) For the mixture with 50% large particles, at different times during segregation. (b) For mixtures of different global concentration, at steady state ($t \approx 29.5$ to 30 s). The fitted lines in both (a) and (b) are Eqns. 4.5a, 4.5b, $B^k = -0.39$. 
the gradient in concentration $\partial \phi / \partial y = 0$, so the total flux in Eqn. (4.8) reduces to that determined by the kinetic stress gradient alone:

$$\phi^i (v^i - v) = \frac{B^k \phi^i (1 - \phi^i)}{c_D \rho} \frac{\partial \sigma^k}{\partial y}$$

(4.11a)

$$\phi^v (v^v - v) = - \frac{B^k \phi^v (1 - \phi^v)}{c_D \rho} \frac{\partial \sigma^v}{\partial y}$$

(4.11b)

Once the functional form for $B^k$ is determined as described above (e.g., Eqn. 4.8), all other variables in Eqns. (4.9a–4.9b) can be measured directly from the simulations, to determine the functional form for $c_D$. While it is likely that $c_D$ is not constant, for a first order model, Hill and Tan (2014) first approximated $c_D$ as constant for each mixture. Then they used the calculated values for each of the variables at early times to separately determine $\phi^i (v^i - v)$ and $B^k (\phi^i (1 - \phi^i) / \rho) (\partial \sigma^k / \partial y)$ throughout the flowing layer. By using the method of least squares fitting, they determined the best value for $c_D$ for each mixture. An example of these data for a 50/50 mixture is shown in Fig. 9, row 1.

The diffusion coefficient $D$ can be similarly empirically determined. Hill and Tan (2014) used conditions at later times under steady segregated conditions, where the segregation flux $\phi^v (v^v - v) \approx 0$. In this case, Eqns. (4.10a–4.10b) may be rewritten:

$$\frac{B^k \phi^v (1 - \phi^v)}{\rho} \frac{\partial \sigma^v}{\partial y} = c_D \frac{\partial \phi^v}{\partial y}$$

(4.12a)

Once $B^k$ and $c_D$ are determined as described above, all other variables can be determined for the simulations, except $D$. Again, Hill and Tan (2014) approximated $D$ as constant for each mixture. Then, they used the values for each variable computed from the simulations under later times at steady state conditions to independently determine $B^k (\phi^i (1 - \phi^i) / \rho) (\partial \sigma^k / \partial y)$ and $c_D \partial \phi^v / \partial y$ throughout the flowing layer. Then they used the method of least squares fitting to determine the best value for $D$ for each mixture. An example for a 50/50 mixture is shown in Fig. 9, row 2.

They found that there was some variability from one mixture to the next, but not a systematic variation of either $c_D$ or $D$ with $\phi^i$. While this is likely an artifact of performing these calculations assuming values for $c_D$ and $D$ this still provides a manner for validating the model more quantitatively and a first order estimate for these parameters. For a predictive form for all mixtures in their simulations they used the average value they obtained for each mixture:

$c_D = 6.3$ s$^{-1}$ and $D = 0.20$ mm$^2$/s. When they used the results for different mixtures at different time steps (e.g., Fig. 10), they found reasonable agreement. While not a rigorous test, these data indicate that, indeed, the gradient kinetic stress is a dominant segregation driver, even in the presence of a gravitational field.
5. Outlook for generalizability

For this model to be easily applicable to other systems, a mechanistic understanding and general expressions are needed for parameters such as the partition coefficients and the drag and diffusion coefficients. As mentioned in the introduction, there has been much work recently on developing these expressions for various types of particle mixtures. Additionally, some expressions are derivable from kinetic theory, e.g., Jenkins, J. and Mancini, F. (1987) and Larcher, M. and Jenkins, J. (2013). On the other hand, relatively little work has been done investigating how contact and kinetic stress are partitioned between the constituents. To investigate the generalizability of the simulation results for the stress partition coefficients described for certain mixtures in Section 4, we borrow insight from previous related work.

5.1 Contact stress partition coefficients—insight from density segregation model

The systems in Section 4 are relatively special in that the particles differ only in size or density. However, there are some considerations we can use to test the generalizability for other systems where the particles differ in both size and density.

First, we recall that the simulation data obtained by Fan, Y. and Hill, K. (2011b, 2015) and Hill, K. and Tan, D. (2014) indicate that for mixtures of particles differing modestly in density or size, the constituents bear a portion of the contact stress equal to their volumetric concentration in the mixture, i.e., $\psi c \approx \phi_i$. For a working definition of “modest” for here and for the rest of the paper, we consider those where a different mechanism is not obviously in play, so we limit our immediate consideration to size differences in bimodal mixtures that do not exceed that for which the smaller particles can passively sieve through the larger particles and to density differences that range up to a factor of 7, approximately that of a mixture of steel and plastic particles. We revisit the general expression in Eqs. (2.7–2.8) and note this impacts the gravitational temperature and velocity fluctuations. In particular, Hill, K. and Zhang, J. (2008) investigated the variation of granular temperature of particle mixtures of different sizes and densities in the dense flows using experiments and simulations of drum flows similar to that in Section 4.2. In particular, they noted how the granular temperature and velocity fluctuations varied for different constituents in a mixture. While not exactly equal to the kinetic stress, they are related. In particular, Zhang, K. and Hill, J. (2008) reported on results for what they called a “kinematic temperature” (in 2d):

$$T_{kj} = \overline{uu}^b + \overline{vv}^b.$$  \hspace{1cm} (5.4)

Here, $u$ corresponds to the streamwise velocity, and $\overline{uu}$

$$[\rho'(v' - v)]_{T,g} = \frac{f'_i f'_j (\rho_{m}^i - \rho_{m}^j)}{f'_D} \rho \cos \zeta. \hspace{1cm} (5.2)$$

This is similar to what one might predict qualitatively from simple expectations that denser particles should sink relative to lighter particles, and the magnitude of the segregation flux associated with this should depend on their relative concentration in the mixture.

Moreover, we can compare by the model proposed by Khakhar, D. et al. (1997) by setting $i = ld$ and recalling that $\rho' = \rho_{m}^i f'_i = \rho_{m}^i \phi_i f$. Then with a little rearranging of Eqn. (5.2), we can write:

$$[\phi_i (v' - v)]_{T,g} = -\frac{\rho_{m}^i}{\rho_{m}^j} \phi_i \phi_j \left(1 - \frac{\rho_{m}^j}{\rho_{m}^i}\right) \rho \cos \zeta \hspace{1cm} (5.3)$$

This is nearly identical to the model originally proposed by Khakhar, D. et al. (1997) in Eqn. (1.1), with $C_K = \rho_{m}^i / (\rho_{m}^j)$). This consistency between the general model predictions of Eqsns. (2.7–2.8), with the more mechanistic derivation of the model in Eqn. (1.1) (e.g., Sarkar, S. and Khakhar, D., 2008; Tripathi A. and Khakhar, D., 2013), lends credence to the results from the general theoretical framework and the further generalizability that $\psi c \approx \phi_i$ for a wider range of mixtures. These results have not been tested extensively, but one might hypothesize that this is likely limited to cases where size and density are only modestly different.

5.2 Kinetic stress partition coefficients—insight from granular temperature

While similarly little work has been done investigating how kinetic stress is partitioned among constituents in a mixture, there has been some related work on granular temperatures, that is, kinetic energy associated with velocity fluctuations. In particular, Hill, K. and Zhang, J. (2008) investigated how granular temperature varies for particles in a mixture. We now consider the generalizability of the kinetic stress coefficient derived here based on their work. Then, we consider similar issues regarding the segregation flux associated with kinetic stress gradients.

Hill, K. and Zhang, J. (2008) investigated the variation of granular temperature of particle mixtures of different sizes and densities in the dense flows using experiments and simulations of drum flows similar to that in Section 4.2. In particular, they noted how the granular temperature and velocity fluctuations varied for different constituents in a mixture. While not exactly equal to the kinetic stress, they are related. In particular, Zhang, K. and Hill, J.(2008) reported on results for what they called a “kinematic temperature” (in 2d):
ic variance of the velocity fluctuations of constituent \( i \) in the streamwise direction, analogous to \( \nu'_{i} \) in the direction normal to flow. Hill, K. and Zhang, J. (2008) noted that the fluctuations in the different directions scale similarly, that is, \( \bar{u}_{ii} \) is roughly proportional to \( \nu'_{i} \) for mixtures of 2 mm and 3 mm particles differing in densities up to a factor of 3. While there are likely limits to this approximate relationship, we do not explore these limits here. Rather we use this as a method to explore the implication for how this theoretical framework may be further extended for similar systems. Based on this simplifying assumption, we can approximate:

\[
T^{k,b}_{k,s} \approx \frac{T^{b}_{b,s}}{\bar{v}'_{v}}
\]

(5.5)

We can compare this to the results for the mixtures described in Section 4 by noting

\[
\frac{\psi^{k,b}_{b,k}}{\psi^{k,s}_{b,k}} \approx \frac{\rho^{b}_{b}}{\rho^{k,s}_{b,k}} \approx \frac{T^{k,b}_{k,s}}{T^{b}_{b,s}}.
\]

(5.6)

For a 50/50 mixture of equal density particles, \( \rho^{b}_{b} = \rho^{s}_{s} \), and so for this special case \( \psi^{k,b}_{b,k} = \psi^{k,s}_{b,k} \approx T^{k,b}_{k,s} \). We return to this analogy in a moment, but first explore these previous results for how relative kinematic temperature varies according to relative particle size and density in a mixture.

Hill, K. and Zhang, J. (2008) reported that in the dense region of the flowing layer in physical experiments, the velocity fluctuations scale primarily with relative size of particles in the mixture (increasing as relative particle size decreases) and have very little dependence on density. In other words, in mixtures of particles differing only in density the less dense particles have velocity fluctuations of similar magnitude to the dense particles, i.e., \( T^{k,b}_{k,s} \approx T^{b}_{b,s} \). In mixtures of particles differing only in size, small particles have higher average velocity fluctuations than large particles \( T^{k,b}_{k,s} < T^{k,s}_{k,s} \). Moreover, they used simulations to investigate the effect of systematic variations of the relative particle density of particles of two different (fixed) sizes and found that \( T^{k,b}_{k,s} \) did not change. In other words, they found that \( T^{k,b}_{k,s} \) for particles differing in both size and density only depended on the relative sizes of particles in the mixture, not their relative densities.

To explain their results, Hill and Zhang reasoned that, in contrast with sparser regions of the flow, this scaling is associated with geometric considerations. They developed a simple model, the essence of which is as follows. Particle movement in sheared dense flow is primarily laminar in nature, where particles move in enduring contact over neighboring layers of particles. Velocity fluctuations are generated when beads must slide around neighbors below or when the neighbors below push them as they themselves slide around their neighbors. One can extend this qualitatively to particles of different properties by noting that smaller particles sliding over larger neighbors will be jostled more than larger particles sliding over smaller neighbors (e.g., Fig. 11). On the other hand, density should have relatively little effect on this primarily geometric problem. The model, presented in more detail in the paper, fit the data well and the results are consistent with the kinetic stress partition coefficients described in Section 4.

The overlap between the measured temperature data from Hill, K. and Zhang, J. (2008) and the mixture results described in Section 4 are in the 50/50 mixtures of particles of 2 mm and 3 mm. Hill, K. and Zhang, J. (2008) found the relative kinematic temperatures for a 50/50 mixture of 3 mm and 2 mm particles was approximately \( \frac{(\bar{u}'_{u} + \bar{v}'_{v})}{(\bar{u}'_{u} + \bar{v}'_{v})} \approx 0.7 \). Again, using the simplifying assumption that \( \bar{u}'_{i} \approx \bar{v}'_{i} \), we use this to approximate \( \frac{\bar{v}'_{v}}{\bar{v}'_{v}} \approx 0.7 \). As noted above, for a 50/50 mixture of equal density particles, \( \rho^{b} = \rho^{s} \). Thus, the results from Hill, K. and Zhang, J. (2008) indicate that for a 50/50 mixture of 2 mm and 3 mm particles \( \psi^{k,b}_{b,k} = \psi^{k,s}_{b,k} \approx 0.7 \).

Using this with the requirement \( \psi^{k,b}_{b,k} + \psi^{k,s}_{b,k} = 1 \), these results imply \( \psi^{k,b}_{b,k} \approx 0.41 \), and \( \psi^{k,s}_{b,k} \approx 0.59 \). The results from Hill, K. and Tan, D. (2014) in Eqs. (4.9b) with \( B^{k} = -0.39 \) and \( \phi_{0}^{k} = 0.5 \) indicate that \( \psi^{k,b}_{b,k} \approx 0.40 \), and \( \psi^{k,s}_{b,k} \approx 0.60 \), very similar.

Based on these results, Eqs. (5.6) and the results expressed by Eqs. (4.9b), we would suggest that for particles of modest size and density differences, the kinetic stress partition coefficients can be found using material densities of the two constituent particles, local volumetric concentrations, and one parameter \( B^{k} \), according to:

\[
\frac{\psi^{k,b}_{b,k}}{\psi^{k,s}_{b,k}} = \frac{\rho^{b}_{b}}{\rho^{s}_{b,k}} \times \frac{\phi_{0}^{k}}{\phi_{0}^{b}} \times \frac{\phi_{0}^{b} + B^{k}\phi_{0}^{k}\phi_{0}^{b}}{\phi_{0}^{b} - B^{k}\phi_{0}^{k}\phi_{0}^{b}}
\]

(5.7)

Based on the results by Hill, K. and Zhang, J. (2008), the parameter \( B^{k} \) may likely be a function only of relative particle size in a mixture, but their theoretical expression for the relative temperatures is not easily expressed in this way. This might be better approximated by a polynomial fit to the experimental data.
form. While it is beyond the scope of this review, it provides some indication that the framework is generalizable to a range of mixtures modestly differing in both size and density.

6. Summary and outlook

In this paper, we reviewed recent developments indicating the importance of velocity fluctuations, such as that manifested in a “granular temperature” and “kinetic stress gradients” in segregating mixtures of particles of different sizes and densities. Simulations support recent model development. The model captures the segregation by considering two different types of stresses, the kinetic and contact stress, and allowing for independent partitioning of stresses between constituents that is different than their concentration in the mixture. In this way, the model illustrates that segregation can be driven solely by dynamics associated with gradients in kinetic stresses, or temperatures, such as those produced by a shear rate gradient.

Comparing predictions with computational experiments based on DEM simulations indicates that the model framework is reasonable for capturing shear-induced segregation in dense flows. Further, comparing with other model efforts and recent complimentary simulations, there is indication that the model is generalizable for a wide range of mixtures.

However, for a predictive model a deeper understanding of the rheology and other kinetics of dense sheared mixtures is needed. First, we need a predictive relationship between \( \psi^k \) and flow properties such as particle concentrations, relative particle sizes and flow velocities to close the governing equations. Similarly, it is not clear that the drag force on the particles should be linear with relative velocity, or, even if it is linear, what the coefficient of drag should be. Further, it is unlikely that diffusivity \( D \) and the drag coefficient \( c_D \) are constant for any particular mixture. As mentioned by Wiederseiner, S. et al. (2011) and Natarajan, V. et al. (1995) and demonstrated by Hill et al. (2003) and others, \( D \) may depend on the local shear rate as well as other factors. A more mechanistic way to obtain relationships for \( D \) and \( c_D \) as they depend on kinematics on the flow is necessary for a predictive model for shear-induced segregation.

We conclude by briefly noting the potential importance of interstitial fluids in some segregating mixtures, not discussed in this review. Indeed, in many industrial and natural segregating systems, interstitial fluid (e.g., air in industrial powder or grains or water and mud in geophysical flows) is unavoidable and may alter or even drive (e.g., water over a riverbed) the system dynamics. For example, Burtally et al. (2002) demonstrated that the presence of an interstitial fluid can have a strong influence on a segregation pattern in a granular system, particularly for smaller particles. They showed that for mixtures composed of micron-sized glass and brass spheres, in the presence of air at atmospheric pressures, the segregation was markedly different compared to that where the air pressure was significantly reduced. On the other hand, in sediment transport in riverbeds, the particle transport itself is not only influenced by, but also, driven by fluid stresses; there is evidence that particle-particle dynamics can still play a significant role in driving segregation (e.g., Recking et al., 2009; Frey and Church, 2011). Thus, while the work reviewed in this paper takes a significant step toward a more complete representation of the importance of granular temperature in influencing segregation dynamics, for a more complete picture of segregation in a wide range of systems, the influence of fluid-particle interactions needs to be incorporated into this framework.

Acknowledgements

We gratefully acknowledge helpful discussions with Prof. Jenkins and funding that supported the original research described here from NSF Grant No. CBET-0932735 and Proctor & Gamble Co.

Nomenclature

- \( B \) magnitude of a non-dimensional perturbation of the contact stress partition coefficients away from the solid volume fractions for each species
- \( B^k \) magnitude of a non-dimensional perturbation of the kinetic stress partition coefficients away from the solid volume fractions for each species
- \( C_K \) a parameter in the model originally proposed by Khakhar, D. et al. (1997) related to an inverse drag coefficient (s)
- \( c_D \) a drag coefficient (1/s)
- \( d \) particle diameter (m)
- \( D \) the diffusivity (m²/s)
- \( B_{GT} \) the magnitude of a non-dimensional perturbation of the partial pressure coefficients away from the solid volume fractions for each species in the model proposed by Gray, N. and Thornton, A. (2005). Specifically, for constituent \( i \) (consisting of larger or smaller particles) in a bimodal mixture of large and small particles of equal material density, \( B_{GT} = \phi^i (\phi(1 - \phi) \) )
- \( f^i \) local solids fraction of constituent \( i \)
- \( f \) local solids fraction of the mixture
- \( \langle f \rangle \) system-averaged solid fraction of the mixture
- \( F_n \) interparticle normal force (N)
\( \eta_n \) damping coefficient associated with compressive deformation of a particle (Ns/m\(^{5/4} \))

\( \mu \) interparticle friction coefficient

\( \rho \) local bulk density of the mixture: \( \rho = \Sigma \rho_{\text{m}} \) (kg/m\(^3 \))

\( \rho^i \) local bulk density of constituent \( i \), related to the material density of the particles of which constituent \( i \) is comprised (kg/m\(^3 \))

\( \rho_{\text{m}} \) the material density of the particles of which constituent \( i \) is comprised (kg/m\(^3 \))

\( \sigma^e \) local contact stress tensor of the mixture \( \sigma^e = \Sigma \sigma^e \) (N/m\(^2 \))

\( \sigma^k \) local contact stress tensor of the mixture \( \sigma^k = \Sigma \sigma^k \) (N/m\(^2 \))

\( \sigma^{ij} \) local contact stress tensor of species \( i \) (N/m\(^2 \))

\( \sigma^{ij} \) local kinetic stress tensor of species \( i \), where the components are stresses associated with velocity fluctuation correlations, e.g., \( \sigma^{ij} = \rho u_i u_j \); \( \sigma^{ij} = \rho u_i v_j \); \( \sigma^{ij} = \rho v_i v_j \) (N/m\(^2 \))

\( \phi_{\text{in}} \) the local volume concentration of particles of species \( i \): \( \phi_{\text{in}} = f/\rho_{\text{in}}/\Sigma f/\rho_{\text{m}} = f/\rho \)

\( \phi_{\text{ic}} \) the local volume concentration of particles of species \( i \), related to Eqn. 2.8a: \( \phi_{\text{ic}} = f/\Sigma f \)

\( \Phi^i \) the segregation flux of species \( i \): \( \Phi^i = \rho (v^i - v) \)

\( \Phi_{\text{i}} \) the theoretical net segregation flux of species \( i \) derived in Section 2, according to Eqn. (2.7): \( \Phi_{\text{i}} = \Phi_{\text{ik}} + \Phi_{\text{ik}} + \Phi_{\text{id}} \)

\( \Phi_{\text{ik}} \) the kinetic stress segregation flux of species \( i \); according to Eqn. 2.8a: \( \Phi_{\text{ik}} = (\partial \sigma_{\text{ik}} / \partial y) \times (\nu_{\text{ik}} - \nu_{\text{ik}}) / \zeta \)

\( \Phi_{\text{id}} \) the diffusion flux of species \( i \); according to Eqn. 2.8c: \( \Phi_{\text{id}} = (\rho d / c_{\text{id}}) \times (\partial \rho / \partial y) \)

\( \psi^{ij} \) the partial contact stress coefficient of species \( i \)

\( \psi^{ij} \) the partial kinetic stress coefficient of species \( i \)

\( \psi^{ij} \) the partial pressure coefficient of species \( i \)

References


Donald M.B., Roseman B., Mixing and de-mixing of solid par-


Kimberly M. Hill et al. / KONA Powder and Particle Journal No. 33 (2016) 150–168


Author’s short biography

Kimberly Hill
Kimberly Hill is an Associate Professor in the Department of Civil, Environmental, and Geo-Engineering at the University of Minnesota, Twin Cities. Prior to this she held faculty positions in the Department of Theoretical and Applied Mechanics, University of Illinois, Champaign-Urbana and in the Department of Physics, University of Wisconsin, Whitewater and Postdoctoral Research positions in the Department of Chemical Engineering at Northwestern University and in Sandia National Laboratory, Albuquerque. Her research interests and experience are related to fundamental and applied particulate flows. They include segregation and rheology of granular mixtures including applications in geophysical and industrial flows.

Yi Fan
Yi Fan is currently a senior R&D engineer at the Solids Processing group in the Corporate R&D of The Dow Chemical Company. Prior to this, he was a Postdoctoral Fellow in the Department of Mechanical Engineering at Northwestern University. He received his Bachelor (2003) and Mater (2006) degrees in Thermal and Power Engineering from Tsinghua University of China and received his PhD (2011) in Civil engineering from the University of Minnesota – Twin Cities. His research interests and experience focus on understanding the fundamental physics of particulate flows including granular flows and granular-fluid flows, as well as their applications in chemical industry.