Segregation in Moderately Dense Granular Binary Mixtures

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Abstract. A solution of the inelastic Enskog kinetic equation that applies to a wide range of values of the coefficients of restitution and densities is used to determine the thermal diffusion factor of an intruder immersed in a granular fluid under gravity. Thermal diffusion gives a criterion for segregation in terms of the parameters of the system (masses, sizes, density and dissipation). In contrast to previous theoretical attempts our model retains the complete nonlinear dependence of the transport coefficients on dissipation, takes into account the influence of both thermal gradients and gravity on segregation and applies for moderate densities. The present analysis extends previous results derived in the dilute limit case and is consistent with the findings of some recent experimental results.

Although segregation and mixing of dissimilar grains in agitated granular mixtures is one of the most important problems in granular matter, the physical mechanisms involved in this problem are still not completely understood [1]. Among the different competing mechanisms, thermal diffusion becomes the most relevant one at large shaking amplitude where the system resembles a granular fluid and kinetic theory tools can be quite useful to analyze segregation. Thermal diffusion is caused by the relative motion of the components of a mixture due to the presence of both gravity and temperature gradients. Due to this motion, a steady state is achieved in which the separation effect arising from thermal diffusion is balanced by the remixing effect of ordinary diffusion.

The thermal diffusion factor has been recently evaluated for a *dilute* granular binary mixture [2] from a solution of the inelastic Boltzmann equation that applies for strong dissipation and takes into account non-equipartition of energy. The segregation criterion found in Ref. [2] is consistent with previous experimental results [3] and also in agreement with molecular dynamics (MD) simulations reported in the intruder limit case [4]. The objective here is to extend the analysis made in Ref. [2] at higher densities by considering the revised inelastic Enskog kinetic theory. By extending the Boltzmann analysis to high densities comparisons with MD simulations become practical and allows one to quantitatively test the use of a hydrodynamic description for describing segregation in granular vibrated mixtures. In addition, at higher densities, it is possible that other segregation mechanisms different from the one identified in the dilute limit become relevant at those densities.

Some previous theoretical attempts based on kinetic theory for *dense* granular mixtures have been reported in the literature. Thus, Jenkins and Yoon [5] developed a hydrodynamic theory for the segregation of *elastic* particles, finding a criterion for segregation relatively close to the numerical results obtained by Hong *et al.* [6]. Given that the criterion derived in Refs. [5] and [6] only applies for elastic particles, more recently Trujillo *et al.* [7] have obtained an evolution equation for the relative velocity of the intruder for *nearly* elastic particles. Interestingly, they considered the non-equipartition of granular energy through the constitutive relations for the partial pressures. To the best of my knowledge, this is the only theory in the dense case where the breakdown of energy equipartition has been taken into account. However, the results reported by Trujillo *et al.* [7] have been derived by neglecting the presence of temperature gradients in the bulk region so that, the segregation dynamics of intruders is only driven by the gravitational force. The present work covers some of the aspects not accounted for in the theory of Trujillo *et al.* [7] since it is based on a kinetic theory [8] that goes beyond the weak dissipation limit and consider the combined effect of thermal gradients and gravity on segregation.

The model system considered is a moderately dense granular fluid of inelastic hard disks ($d = 2$) or spheres ($d = 3$) of mass m and diameter σ, plus one intruder or impurity of mass m_0 and diameter $\sigma_0 > \sigma$. This is formally equivalent to a binary mixture in the tracer limit for the impurity component. Collisions among fluid–fluid and intruder-fluid particles are inelastic and are characterized by two independent (constant) coefficients of normal restitution α and α_0, respectively. The system is in presence of the gravitational field $\mathbf{g} = -g\hat{\mathbf{e}}_z$, where g is a positive constant and $\hat{\mathbf{e}}_z$ is the unit vector in the positive direction of the z axis. To fluidize the system, here particles are assumed to be heated by a

CP1027, *The XVth International Congress on Rheology, The Society of Rheology 80th Annual Meeting*
edited by A. Co, L. G. Leal, R. H. Colby and A. J. Giacomin

stochastic-driving force which mimics a thermal bath. Although the relation between the use of this driven idealized method with the use of vibrating walls is not completely clear, it must be stressed that the results derived in Ref. [2] for the temperature ratio T_0/T from this stochastic driving method compare quite well with MD simulations of agitated mixtures [3].

The thermal diffusion factor Λ is defined at the steady state with zero flow velocity and gradients only along the vertical direction (z axis). Under these conditions, the factor Λ is defined by [2]

$$-\Lambda \partial_z \ln T = \partial_z \ln\left(\frac{n_0}{n}\right), \tag{1}$$

where n_0 and n are the number densities of the intruder and the fluid particles, respectively. Let us assume that gravity and thermal gradient point in parallel directions (i.e., the bottom plate is hotter than the top plate, $\partial_z \ln T < 0$). Obviously, when $\Lambda > 0$, the intruder rises with respect to the fluid particles while if $\Lambda < 0$, the intruder falls with respect to the fluid particles. The former situation is referred to as the Brazil-nut effect (BNE) while the latter is called the reverse Brazil-nut effect (RBNE). Under the above conditions, the momentum conservation equation leads to

$$\frac{\partial p}{\partial z} = \frac{\partial p}{\partial T}\partial_z T + \frac{\partial p}{\partial n}\partial_z n = -\rho g, \tag{2}$$

where p is the pressure and $\rho = mn$ is the mass density of the fluid particles. Moreover, since the flow velocity vanishes, then the mass flux of the intruder $j_z = 0$. The constitutive equation for the mass flux j_z is [8]

$$j_z = -\frac{m_0^2}{\rho} D_0 \partial_z n_0 - \frac{m_0 m}{\rho} D \partial_z n - \frac{\rho}{T} D^T \partial_z T, \tag{3}$$

where D_0, D, and D^T are the relevant transport coefficients. Expressions for the pressure p and the transport coefficients D_0, D, and D^T have been recently obtained in the undriven case by solving the Enskog kinetic equation by means of the Chapman-Enskog method in the first Sonine approximation [8]. The extension of these results to the driven case is straightforward. The condition $j_z = 0$ along with the balance equation (2) allow one to get the thermal diffusion factor Λ in terms of the parameters of the mixture as

$$\Lambda = \frac{\beta D^{T*} - (p^* + g^*)(D_0^* + D^*)}{\beta D_0^*}, \tag{4}$$

where D^*, D_0^*, and D^{T*} are the reduced forms of the transport coefficients. Moreover, $\beta = p^* + \phi \partial_\phi p^*$, $g^* = \rho g / n \partial_z T < 0$ is a dimensionless parameter measuring the gravity relative to the thermal gradient, $p^* = p/nT = 1 + 2^{d-2}\chi\phi(1+\alpha)$, $\chi(\phi)$ is the pair correlation function for the granular fluid, and $\phi = [\pi^{d/2}/2^{d-1}d\Gamma(d/2)]n\sigma^d$ is the solid volume fraction.

The condition $\Lambda = 0$ provides the segregation criterion for the transition BNE $\Leftrightarrow$ RBNE. Taking into account the expressions of the transport coefficients, one gets the criterion [9]

$$g^*(\gamma - M\beta) - \gamma\phi \frac{\partial p^*}{\partial \phi} + \frac{\omega^d}{2}\frac{M}{1+M}\chi_0 \phi (1+\alpha_0)\left[(p^* + g^*)\frac{M+\gamma}{M}\Delta - \beta\right] = 0, \tag{5}$$

where $\gamma = T_0/T$ is the temperature ratio, $M = m_0/m$, $\omega = (\sigma + \sigma_0)/\sigma$, χ_0 is the intruder-fluid pair correlation function and $\Delta \equiv [\omega^{-d}/T\chi_0](\partial_\phi \mu_0)_{T,n}$, μ_0 being the chemical potential of the intruder. The temperature ratio γ is determined from the condition $mT_0\zeta_0 = m_0 T\zeta$, where ζ_0 and ζ are the cooling rates for T_0 and T, respectively. Equation (5) gives the phase-diagram for the BNE/RBNE transition due to thermal diffusion of an intruder in a moderately dense granular fluid. The parameter space of the problem is six-fold: the dimensionless gravity g^*, the mass ratio m_0/m, the ratio of diameters σ_0/σ, the solid volume fraction ϕ, and the coefficients of restitution α and α_0. The influence of density on segregation is accounted for by the second and third terms in Eq. (5). In particular, when $\phi = 0$ (dilute limit case), the solution to Eq. (5) is $\gamma = M$, which is consistent with previous results [4, 2]. This means that, while in a dilute molecular gas segregation is predicted for particles that differ in mass (no matter what their radii may be), for a granular gas the segregation criterion involves all the mechanical parameters of the system because of the lack of equipartition ($\gamma \neq 1$). According to Eq. (5) the combined effect of gravity and thermal gradients on segregation is

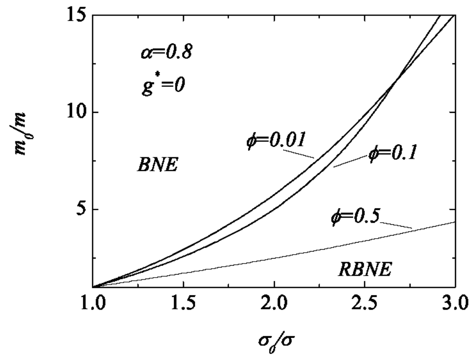

FIGURE 1. Phase diagram for BNE/RBNE for $\alpha = 0.8$ in the absence of gravity for three different values of the solid volume fraction ϕ. Points above the curve correspond to $\Lambda > 0$ (BNE) while points below the curve correspond to $\Lambda < 0$ (RBNE).

through the dimensionless parameter g^*. An interesting limit corresponds to $|g^*| \to \infty$ (gravity dominates over thermal gradient) since many experiments have been performed under these conditions. In this case, Eq. (5) becomes

$$\frac{1+\frac{\omega^d}{2}\chi_0\phi(1+\alpha_0)\frac{\gamma+M}{1+M}\frac{\Delta}{\gamma}}{1+2^{d-2}\chi\phi(1+\alpha)\left[1+\phi\partial_\phi \ln(\phi\chi)\right]}\frac{\gamma}{M}-1=0, \tag{6}$$

while the segregation criterion found independently by Jenkins and Yoon [5] (for an elastic system) and by Trujillo *et al.* [7] is

$$\frac{1+\frac{\omega^d}{2}\chi_0\phi}{1+2^{d-1}\chi\phi}\frac{\gamma}{M}-1=0. \tag{7}$$

Equation (6) reduces to Eq. (7) after some approximations. Thus, even in the particular limit $|g^*| \to \infty$, the criterion (6) is much more general than the one previously derived [5, 7] since it covers the complete range of the parameter space of the problem.

To draw the phase-diagram in the $(\sigma_0/\sigma, m_0/m)$–plane, one needs to solve the criterion (5) in conjunction with the expression for T_0/T. As an illustration, in Fig. 1 I plot the phase diagram for the BNE/RBNE transition for a three-dimensional system with $\alpha = \alpha_0 = 0.8$ in the absence of gravity. Three different values of the solid volume fraction have been considered. It is apparent that the influence of density is quite important since the regime of RBNE decreases significantly with increasing density. Since the effect of shaking strength of vibration on the diagram BNE/RBNE can be tied to the effect of changing the density ϕ, it is evident from Fig. 1 that the possibility of BNE will decrease with increasing shaking acceleration. This behavior is consistent with the experimental results obtained by Breu *et al* [10]. A more complete discussion on the form of the phase diagrams BNE/RBNE for different values of the parameter space of the problem can be found in Ref. [9].

This work has been supported by the Ministerio de Educación y Ciencia (Spain) through Grant No. FIS2007-60977, partially financed by FEDER funds and by the Junta de Extremadura (Spain) through Grant No. GRU07046.

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