PHYSICAL REVIEW E **78**, 020301(R) (2008)

Brazil-nut effect versus reverse Brazil-nut effect in a moderately dense granular fluid

Vicente Garzó*
Departamento de Física, Universidad de Extremadura, E-06071 Badajoz, Spain
(Received 20 March 2008; revised manuscript received 11 June 2008; published 20 August 2008)

A segregation criterion based on the inelastic Enskog kinetic equation is derived to show the transition between the Brazil-nut effect (BNE) and the reverse Brazil-nut effect (RBNE) by varying the different parameters of the system. In contrast to previous theoretical attempts, the approach is not limited to the near-elastic case, takes into account the influence of both thermal gradients and gravity, and applies for moderate densities. The form of the phase diagrams for the BNE-RBNE transition depends sensitively on the value of gravity relative to the thermal gradient, so that it is possible to switch between both states for given values of the mass and size ratios, the coefficients of restitution, and the solid volume fraction. In particular, the influence of collisional dissipation on segregation becomes more important when the thermal gradient dominates over gravity than in the opposite limit. The present analysis extends previous results derived in the dilute limit case and is consistent with the findings of some recent experimental results.

DOI: 10.1103/PhysRevE.78.020301 PACS number(s): 45.70.Mg, 05.20.Dd, 05.60.−k, 51.10.+y

Segregation and mixing of dissimilar grains in agitated granular binary mixtures is one of the most important problems in granular matter from both fundamental and practical points of view. In some cases it is a desired and useful effect to separate particles of different types, while in other processes it is undesirable and can be difficult to control. Usually, the larger intruder particles tend to climb to the top of the sample against gravity [Brazil-nut effect (BNE)], but under certain conditions they can also accumulate at the bottom [reverse Brazil-nut effect (RBNE)]. However, although there is extensive observational evidence of these phenomena, much less is known about the physical mechanisms involved in this problem [1]. Among the different competing mechanisms proposed to explain the transition BNE⇔RBNE [2–5], thermal (Soret) diffusion becomes the most relevant one at large shaking amplitude where the system resembles a granular gas and kinetic theory becomes useful to study segregation. Some previous theoretical attempts have been reported in the literature analyzing thermal diffusion effects on segregation in bidisperse granular systems. Nevertheless, these early contributions have been restricted to elastic [6] and quasielastic particles [7], have considered thermalized systems (and so the segregation dynamics of intruders is only driven by the gravitational force) [6,7], and/or have been limited to dilute gases [8–10]. The main goal of this paper is to propose a theory based on a recent solution of the inelastic Enskog equation [11] that covers some of the aspects not accounted for in previous works. The theory subsumes all previous analyses [6–9], which are recovered in the appropriate limits. Furthermore, the theoretical predictions are in qualitative agreement with some molecular dynamics (MD) simulation results [5,8,12] and are also consistent with previous experimental works [4,5].

We consider a binary mixture of inelastic hard disks ($d=2$) or spheres ($d=3$) where one of the components (of mass m_0 and diameter σ_0) is present in tracer concentration. In this limit case, one can assume that (i) the state of the dense gas (excess component of mass m and diameter $\sigma<\sigma_0$) is not affected by the presence of tracer particles and (ii) one can also neglect collisions among tracer particles in their kinetic equation. This is formally equivalent to study an intruder in a dense granular gas, and this will be the terminology used here. Collisions among gas-gas and intruder-gas particles are inelastic and are characterized by two independent (constant) coefficients of normal restitution α and α_0, respectively. The system is in the 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 mixture and reach a steady state, in most of the experiments energy is injected into the system through vibrating horizontal walls. Here, in order to avoid the use of vibrating boundary conditions, particles are assumed to be heated by a stochastic-driving force which mimics a thermal bath. Although previous experiments [14] have shown a less significant dependence of the temperature ratio T_0/T on inelasticity than the one obtained in driven steady states [13], the results derived in Ref. [9] for T_0/T from this stochastic driving method compare quite well with MD simulations of agitated mixtures [5]. This agreement suggests that this driving method can be seen as a plausible approximation for comparison with experimental results. A sketch of the geometry of the problem is given in Fig. 1.

The thermal (Soret) 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 [9]

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

where n_0 and n are the number densities of the intruder and fluid particles, respectively. Let us assume that gravity and the thermal gradient point in parallel directions (i.e., the bottom plate is hotter than the top plate, $\partial_z \ln T<0$) (see Fig. 1). Obviously, when $\Lambda>0$, the intruder rises with respect to the fluid particles [BNE, i.e., $\partial_z \ln(n_0/n)>0$], while if $\Lambda<0$, the

*vicenteg@unex.es

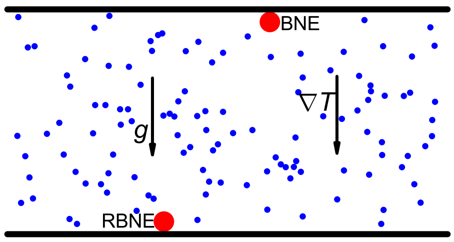

FIG. 1. (Color online) Sketch of the problem studied here. The small circles represent the particles of the granular fluid, while the large circles are the intruders. The BNE (RBNE) effect corresponds to the situation in which the intruder rises (falls) to the top (bottom) plate.

intruder falls with respect to the fluid particles [RBNE, i.e., $\partial_z \ln(n_0/n)<0$].

In order to determine the dependence of the coefficient Λ on the parameters of the system, we focus our attention on an *inhomogeneous* steady state with gradients along the z direction. Since the flow velocity vanishes, the mass flux of the intruder $j_z=0$. In addition, the momentum balance equation yields

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

where p is the pressure and $\rho=mn$ is the mass density of the fluid particles. Upon writing Eq. (2), we have taken into account that p depends on z through its dependence on n and T [11]. To first order in the spatial gradients (Navier-Stokes description), the constitutive equation for the mass flux of the intruder is [11]

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

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 [11]. The extension of these results to the driven case is straightforward. The condition $j_z=0$ along with the balance equation (2) allows one to get the thermal diffusion factor Λ in terms of the parameters of the mixture as

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

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

$$D_0^*=\frac{\gamma}{\nu_D}, \tag{5}$$

$$D^{T*}=-\frac{M}{\nu_D}\left(p^*-\frac{\gamma}{M}\right)+\frac{(1+\omega)^d}{2\nu_D}\frac{M}{1+M}\chi_0\phi(1+\alpha_0), \tag{6}$$

$$D^*=-\frac{M}{\nu_D}\beta+\frac{1}{2\nu_D}\frac{\gamma+M}{1+M}\frac{\phi}{T}\left(\frac{\partial\mu_0}{\partial\phi}\right)_{T,n_0}(1+\alpha_0). \tag{7}$$

Here, $\gamma\equiv T_0/T$ is the temperature ratio, $M\equiv m_0/m$ is the mass ratio, $\omega\equiv\sigma_0/\sigma$ is the size ratio, and

$$\nu_D=\frac{\sqrt{2}\pi^{(d-1)/2}}{d\Gamma\left(\frac{d}{2}\right)}\chi_0\sqrt{\frac{\gamma+M}{M(1+M)}}(1+\alpha_0). \tag{8}$$

In addition, χ_0 is the intruder-gas pair correlation function and μ_0 is the chemical potential of the intruder. When the granular gas is driven by means of a stochastic thermostat, the temperature ratio γ is determined [9] from the requirement $\gamma\zeta_0=M\zeta$, where the expressions for the cooling rates ζ_0 and ζ in the local equilibrium approximation can be found in Ref. [11].

The condition $\Lambda=0$ provides the segregation criterion for the transition BNE$\Leftrightarrow$RBNE. Since β and D_0^* are both positive, then according to (4), $\text{sgn}(\Lambda)=\text{sgn}[\beta D^{T*}-(p^*+g^*)(D_0^*+D^*)]$. Consequently, taking into account Eqs. (5)–(7), the segregation criterion can be written as

$$g^*(\gamma-M\beta)-\gamma\phi\frac{\partial p^*}{\partial\phi}+\frac{(1+\omega)^d}{2}\frac{M}{1+M}\chi_0\phi(1+\alpha_0)\times\left[(p^*+g^*)\frac{M+\gamma}{M}\Delta-\beta\right]=0, \tag{9}$$

where $\Delta\equiv[(1+\omega)^{-d}/T\chi_0](\partial_\phi\mu_0)_{T,n_0}$. Equation (9) gives the phase diagram for the BNE-RBNE transition due to Soret diffusion of an intruder in a moderately dense granular gas. This is the most relevant result of this paper. The parameter space of the problem is sixfold: 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. (9). As expected, when $m_0=m$, $\sigma_0=\sigma$, and $\alpha=\alpha_0$, the system (intruder plus gas) is monodisperse and the two species do not segregate. This is consistent with Eq. (9) since in this limit case $D^{T*}=D_0^*+D^*=0$, and so the condition (9) holds for any value of α and ϕ. In the dilute limit case ($\phi\to 0$), $\beta=p^*=1$ so that Eq. (9) reads

$$g^*(\gamma-M)=0. \tag{10}$$

Note that in the absence of gravity ($g^*=0$), Eq. (10) applies for any value of the parameters of the system and so the intruder does not segregate in a dilute gas. When $g^*\neq 0$, the solution to (10) is $\gamma=M$. This result agrees with the recent segregation condition derived from the Boltzmann equation [8,9].

In general, segregation is driven and sustained by both gravity and temperature gradients. The combined effect of both parameters on Soret diffusion is through the reduced parameter g^*. This parameter measures the competition between these two mechanisms on segregation. In previous theoretical studies on dense gases [6,7], the temperature was assumed to be uniform in the bulk of the system ($\partial_z T=0$) so that segregation of intruders was essentially driven by gravity. This is quite an interesting limit since most of the experiments [3,4,15] have been carried out under these conditions. In this limit ($|g^*|\to\infty$), Eq. (9) becomes

$$\frac{1+\frac{(1+\omega)^d}{2}\chi_0\phi(1+\alpha_0)\frac{\gamma+M}{1+M}\frac{\Delta}{\gamma}}{1+2^{d-2}\chi\phi(1+\alpha)[1+\phi\partial_\phi \ln(\phi\chi)]}\frac{T_0}{T}-\frac{m_0}{m}=0, \quad (11)$$

while the segregation criterion found independently by Jenkins and Yoon [6] (for an elastic system) and by Trujillo *et al.* [7] is

$$\frac{1+\frac{(1+\omega)^d}{2}\chi_0\phi}{1+2^{d-1}\chi\phi}\frac{T_0}{T}-\frac{m_0}{m}=0. \quad (12)$$

Equation (11) reduces to Eq. (12) when one (i) neglects the dependence on inelasticity and assumes equipartition in certain terms, (ii) takes the approximation $\Delta=1$ (which only applies for a dilute gas of mechanically equivalent particles), and (iii) neglects high-density corrections [last term in the denominator of (11)]. Thus, even in the particular limit $|g^*|\to\infty$, the criterion (11) is much more general than the one previously derived [7] since it covers the complete range of the parameter space of the problem.

Henceforth and for the sake of concreteness, we assume a three-dimensional system with $\alpha=\alpha_0$. In this case [16], $\chi=(1-\frac{1}{2}\phi)/(1-\phi)^3$ and

$$\chi_0=\frac{1}{1-\phi}+3\frac{\omega}{1+\omega}\frac{\phi}{(1-\phi)^2}+2\frac{\omega^2}{(1+\omega)^2}\frac{\phi^2}{(1-\phi)^3}. \quad (13)$$

The expression for the chemical potential consistent with the above approximations can be found in Ref. [17]. A phase diagram delineating the regimes between BNE and RBNE is shown in Fig. 2 for $\phi=0.1$, $g^*=0$, and two values of the (common) coefficient of restitution α. We observe that, in the absence of gravity, the main effect of dissipation is to reduce the size of the BNE. It is also apparent that the RBNE is dominant at both small mass ratio and/or large diameter ratio. In addition, comparison with the results obtained for $\alpha=0.8$ assuming that $T_0=T$ shows that the nonequipartition of granular energy has an important influence on segregation in the absence of gravity. This is consistent with MD-based findings of Galvin *et al.* [12]. Moreover, the results obtained from Eq. (9) show that the form of the phase diagrams depends significantly on the value of the reduced gravity $|g^*|$ (namely, reverse buoyancy relative to the effect of Soret diffusion). Thus, in general for given values of m_0/m, σ_0/σ, α_0, α, and ϕ, a transition between both states BNE and RBNE is possible by changing $|g^*|$. To illustrate the influence of the reduced gravity, a phase diagram is plotted in Fig. 3 when $|g^*|=1$ (gravity comparable to the thermal gradient) for different values of the volume fraction ϕ. In contrast to Fig. 2, it is apparent that the RBNE regime appears essentially now for both large mass ratio and/or small size ratio. With respect to the dependence on density, Fig. 3 shows that in general the role played by density is quite important since the regime of the RBNE decreases significantly with increasing density. Following Trujillo *et al.* [7], since the effect of shaking strength of vibration on the BNE-RBNE phase diagram can be tied to the effect of varying the volume fraction ϕ, it is apparent from Fig. 3 that the possibility of the RBNE will increase with increasing shaking strength. This feature agrees with the experimental findings of Breu *et al.* [4] since their results show similar behavior with the external excitation. The form of the phase diagram in the limit $|g^*|\to\infty$ is shown in Fig. 4 for $\phi=0.5$ and two values of the coefficient of restitution $\alpha=1$ and 0.9. Our results indicate that, in contrast to the case of Fig. 2, the main effect of inelasticity is to reduce the size of the RBNE region, which qualitatively agrees again with experiments [4]. On the other hand, our predictions disagree with the theoretical results derived by Trujillo *et al.* [7] since the latter found that the mass ratio is a two-valued function of the size ratio and so the main effect of dissipation is to introduce a threshold value of the size ratio above which there is no RBNE. The results also indicate (not shown in Fig. 4) that nonequipartition has a weaker influence on segregation when $|g^*|\to\infty$ than in the opposite

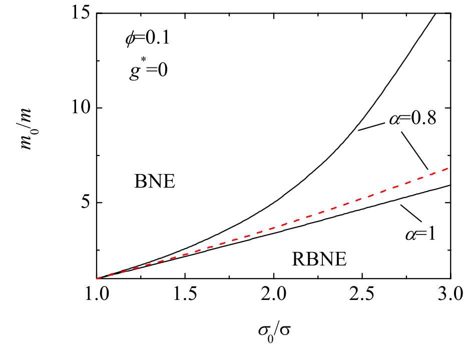

FIG. 2. (Color online) Phase diagram for the BNE-RBNE transition for $\phi=0.1$ in the absence of gravity for two values of the (common) coefficient of restitution α. Points above the curve correspond to $\Lambda>0$ (BNE), while points below the curve correspond to $\Lambda<0$ (RBNE). The dashed line is the result obtained for $\alpha=0.8$ assuming energy equipartition ($T_0=T$).

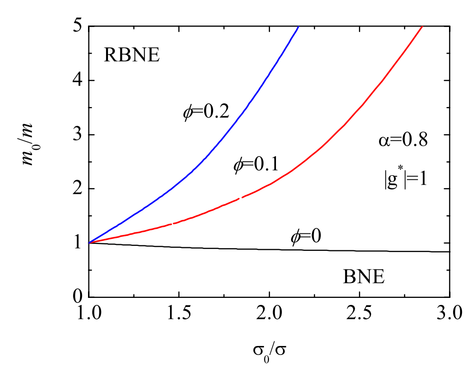

FIG. 3. (Color online) Phase diagram for the BNE-RBNE transition for $\alpha=0.8$, $|g^*|=1$, and three different values of the solid volume fraction ϕ.

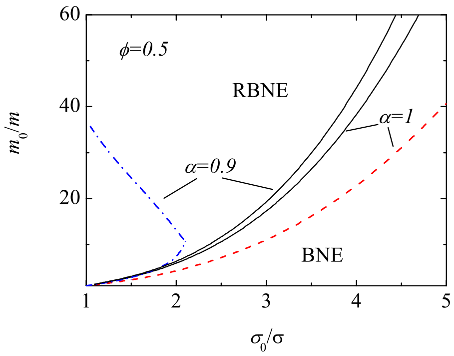

FIG. 4. (Color online) Phase diagram for the BNE-RBNE transition for ϕ=0.5 in the absence of a thermal gradient ($|g^*|\to\infty$) for two values of α. The dashed and dash-dotted lines refer to the results obtained by Jenkins and Yoon [6] and Trujillo *et al.* [7], respectively.

limit ($|g^*|$=0). This behavior qualitatively agrees with the experiments carried out by Schröter *et al.* [5] for vibrated mixtures since they find energy nonequipartition to have no discernible influence on their results.

In summary, a kinetic theory based on a solution of the inelastic Enskog equation has been used to analyze thermal (Soret) diffusion effects on segregation for an intruder in a driven moderately dense granular gas under gravity. The present study goes beyond the weak dissipation limit, takes into account the influence of both thermal gradient and gravity on thermal diffusion, and applies for moderate densities. Although the theory is consistent with previous numerical and experimental results, a more quantitative comparison with the latter would be desirable. As a first test, kinetic theory predictions in the Boltzmann limit [9] compare well with MD simulations of agitated dilute mixtures [8]. Given that the results derived here extend the description made in Ref. [9] to moderate densities, it can be reasonably expected that such a good agreement is also kept at finite densities. In this context, it is hoped that this paper stimulates the performance of such simulations. On the other hand, it must be stressed that the present work only deals with the tracer or intruder limit. This precludes the possibility of comparing our theory with the results reported by Schröter *et al.* [5] in agitated mixtures constituted by particles of the same density and equal total volumes of large and small particles. When convection is practically suppressed, they studied the influence of dissipation on Soret diffusion. I plan to extend the present theory to finite concentration to carry out a comparison with the above computer simulation results [5] in the near future.

I am grateful to C. M. Hrenya, J. W. Dufty, and A. Santos for useful comments on an early version of this paper. 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. GRU08069.

[1] A. Kudrolli, Rep. Prog. Phys. **67**, 209 (2004).
[2] J. Duran, J. Rajchenbach, and E. Clément, Phys. Rev. Lett. **70**, 2431 (1993).
[3] D. C. Hong, P. V. Quinn, and S. Luding, Phys. Rev. Lett. **86**, 3423 (2001).
[4] A. P. J. Breu, H. M. Ensner, C. A. Kruelle, and I. Rehberg, Phys. Rev. Lett. **90**, 014302 (2003).
[5] M. Schröter, S. Ulrich, J. Kreft, J. B. Swift, and H. L. Swinney, Phys. Rev. E **74**, 011307 (2006).
[6] J. T. Jenkins and D. K. Yoon, Phys. Rev. Lett. **88**, 194301 (2002).
[7] L. Trujillo, M. Alam, and H. J. Herrmann, Europhys. Lett. **64**, 190 (2003); M. Alam, L. Trujillo, and H. J. Herrmann, J. Stat. Phys. **124**, 587 (2006).
[8] J. J. Brey, M. J. Ruiz-Montero, and F. Moreno, Phys. Rev. Lett. **95**, 098001 (2005).
[9] V. Garzó, Europhys. Lett. **75**, 521 (2006).
[10] D. Serero, I. Goldhirsch, S. H. Noskowicz, and M.-L. Tan, J. Fluid Mech. **554**, 237 (2006).
[11] V. Garzó, J. W. Dufty, and C. M. Hrenya, Phys. Rev. E **76**, 031303 (2007); V. Garzó, C. M. Hrenya, and J. W. Dufty, *ibid.* **76**, 031304 (2007).
[12] J. E. Galvin, S. R. Dahl, and C. M. Hrenya, J. Fluid Mech. **528**, 207 (2005).
[13] S. R. Dahl, C. M. Hrenya, V. Garzó, and J. W. Dufty, Phys. Rev. E **66**, 041301 (2002).
[14] R. D. Wildman and D. J. Parker, Phys. Rev. Lett. **88**, 064301 (2002); K. Feitosa and N. Menon, *ibid.* **88**, 198301 (2002).
[15] T. Schnautz, R. Brito, C. A. Kruelle, and I. Rehberg, Phys. Rev. Lett. **95**, 028001 (2005).
[16] N. F. Carnahan and K. E. Starling, J. Chem. Phys. **51**, 635 (1969); T. Boublik, *ibid.* **53**, 471 (1970); E. W. Grundke and D. Henderson, Mol. Phys. **24**, 269 (1972).
[17] T. M. Reed and K. E. Gubbins, *Applied Statistical Mechanics* (McGraw-Hill, New York, 1973), Chap. 6.