PHYSICAL REVIEW E **68**, 050301(R) (2003)

Numerical simulations of air-driven granular separation

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(Received 26 March 2003; revised manuscript received 31 July 2003; published 18 November 2003)

Recently it has been shown that binary mixtures of equal-sized fine granular materials exhibit spontaneous separation under vertical vibration in the presence of air [Science **295**, 1877 (2002)]. Here we describe a model of this behavior based on soft-sphere molecular dynamics coupled to the motion of the surrounding air. It exhibits many of the features observed experimentally including almost complete separation of the components into well defined regions with extremely sharp boundaries. The basic separation mechanism is robust and insensitive to many of the model parameters. Our results show that the forced flow of air through the bed, induced by vibration of the container, is responsible for this form of separation.

DOI: 10.1103/PhysRevE.68.050301 PACS number(s): 45.70.Mg, 02.70.Ns, 81.05.Rm

Granular systems are widespread in nature and the ability to understand and control their dynamical behavior is of central importance in many industrial processes [1]. The key feature that distinguishes granular systems from conventional solids, liquids, and gases is that the interactions between grains dissipate energy [2]. Consequently, nontrivial dynamical behavior requires the continuous injection of energy, frequently achieved by subjecting the system to vibrations.

In single-component systems, vertical vibrations are known to induce a variety of surface patterns [3] and complex convective flows in the bulk [4]. For fine particulates air effects are also important, resulting in Faraday piling [5] or surface tilting in confined geometries [6]. In multicomponent systems, a range of interesting behaviors has been observed including the Brazil nut effect [7] and separation or segregation in binary granular mixtures [8,9]. Recently Möbius *et al.* [10] have shown that the rise time of an intruder in a tapped fine granular bed depends in a nontrivial way on the surrounding air pressure. Moreover, for a mixture of fine particulates subjected to vertical vibration, Burtally *et al.* [11] have observed separation phenomena which are absent if the grains are vibrated in a vacuum. However, to date, there is no clear understanding of the role played by the air in fine granular mixtures subjected to vibration.

Computer simulations provide a powerful tool in the study of complex dynamical systems. Techniques based on molecular dynamics have been widely employed to study granular materials [12]. Simplified models for granular interactions and dynamics may often be used to identify the important physical mechanisms behind collective behavior, without including a detailed knowledge of many material properties [13]. Recently, simulations of binary mixtures have been carried out to investigate separation effects in multicomponent systems under vibration, in the absence of air [14].

There is a wide literature on the interaction between granular beds and flowing air [15]. Air effects have been incorporated into single-component granular simulations in approximate ways, by treating the granular bed as a porous medium [16], or by solving the Navier-Stokes equation coupled to the granular motion [17]. What has not been extensively considered in simulations are the effects of both air flow and vibration in fine multicomponent granular mixtures.

In this paper we describe numerical simulations carried out to investigate the effects of air on the behavior of fine granular mixtures under vibration. Specifically, we wish to identify the physical mechanisms responsible for the air-driven separation observed by Burtally *et al.* [11]. In our simulations, a binary mixture of particulates having equal sizes but different densities, spontaneous separates into two ''phases'' with extremely sharp separation boundaries, as is observed experimentally. We show that particle-particle and particle-wall friction can strongly influence the positioning of the phases. The dependence of the separation phenomena on the relative size and density of the components is also investigated. We have verified that the strong tendency to separate is insensitive to many details of the granular interactions and to the treatment of bed porosity. Our key finding is that this spontaneous separation is a robust phenomenon which results from the coupling between the granular motion and the air flow forced through the bed by vibration. Our simulations show that in the absence of air this form of separation does not occur, as has been observed experimentally [11].

Our simulation is based on soft-sphere molecular dynamics for mixtures of spherical particles of mean radii r_b and r_g, representing the bronze and glass components used in the experiments [11]. We have investigated a range of models for the grain-grain collisions based on either linear spring-dashpot interactions or Hertzian contact laws [18]. We find that the basic separation phenomena which we shall describe are insensitive to many details of these interactions. Consequently, for simplicity, we will present results for particles that interact through a Hookian repulsive force and a linear viscous damping force. Such a model has already been shown to provide an adequate description of granular dynamics in the absence of air [19].

If particle i has radius r_i, the position of its center is $\mathbf{R_i}$ and it is moving with velocity $\mathbf{V_i}$, the normal repulsive force on particle j due to an overlap with particle i is

$$\mathbf{F_r} = -K[(\mathbf{R_j}-\mathbf{R_i})\cdot\hat{\mathbf{n}}-r_i-r_j]\hat{\mathbf{n}} \tag{1}$$

and the collisional damping force is

$$\mathbf{F_d} = -\mu_n[(\mathbf{V_j} - \mathbf{V_i}) \cdot \hat{\mathbf{n}}]\hat{\mathbf{n}}. \quad (2)$$

Here $\hat{\mathbf{n}}$ is a unit vector from $\mathbf{R_i}$ to $\mathbf{R_j}$ and K and μ_n are constants that determine the strength of the interaction and the damping. The particles are assumed to be contained within a rigid rectangular box and initially we will ignore tangential frictional forces between the particles themselves and between the particles and the walls of the container. The box is subjected to vertical vibration $A\sin(\omega t)$, of amplitude A and angular frequency $\omega = 2\pi f$. The maximum dimensionless acceleration $\Gamma = A\omega^2/g$.

The interaction between the particles and the surrounding air is included approximately by treating the bed as a porous medium [20] and the air as an incompressible fluid [11]. Conservation of fluid volume implies $\nabla \cdot [\phi \mathbf{V} + (1-\phi)\mathbf{U}] = 0$, where ϕ is the porosity of the bed, $\mathbf{U}$ is the local mean granular velocity, and $\mathbf{V}$ is the local mean fluid velocity [20]. Using Darcy's Law in the form $-(\kappa/\nu)\nabla P = \phi(\mathbf{V} - \mathbf{U})$, where κ is the permeability of the bed and ν is the air viscosity, one obtains the following equation for the air pressure P:

$$\nabla \cdot \left(-\frac{\kappa}{\nu}\nabla P + \mathbf{U} \right) = 0. \quad (3)$$

As the box moves under vibration, the dominant air flow is upwards and downwards through the bed; small sideways components will be ignored. At any instant, the air velocity $\mathbf{V_a}$ outside the bed will be equal to the velocity of the container, $A\omega\cos(\omega t)$. Equation (3) can be solved for the local pressure gradient subject to this boundary condition. The resulting average air-drag force on a grain j is then

$$\mathbf{F_a} = -\alpha r(\mathbf{V_j} - \mathbf{V_a}), \quad (4)$$

where $\alpha = 4\pi\nu r^2/3(1-\phi)\kappa$, a parameter which depends on the size of the particles, the local porosity of the bed and the viscosity of air. This force is an effective Stokes's drag on each particle, of a magnitude enhanced by the porosity of the bed. In all that follows, Eq. (4) is used to model the interaction of the grains with the surrounding air, initially under the assumption of constant porosity.

We will first consider a mixture of glass and bronze spheres of equal mean radii, $r_b = r_g = 50$ μm, with a 20% variation in the particles' size introduced to avoid crystallization. The densities of the two materials are $\rho_b = 8900$ kg/m^3 and $\rho_g = 2500$ kg/m^3. The model parameters are taken to be $K = 3000$ N m^{-1} and $\mu_n = 5 \times 10^{-5}$ N s m^{-1}. The corresponding coefficients of restitution lie in the range 0.95–0.97 and stability considerations require the use of a maximum time step of the order of 10^{-6} s. In all the simulations reported here we have used $\Delta t = 3 \times 10^{-7}$ s. The value of K is sufficiently large so that the maximum overlap of the spheres in our simulations is of the order of 0.1% of the radius [19]. We have also performed simulations with K values in the range 100–10 000 N m^{-1} and observed qualitatively the same separation behavior as described here. Similarly, the separation behavior is insensitive to the value of the coefficient of restitution, the losses being dominated by air damping. The parameter α can be calculated by assuming that the permeability of the bed depends upon the porosity through the Carman-Kozeny relation [21]. We have used $\alpha = 10^{-2}$ N s m^{-2}, which corresponds approximately to a bed of mean porosity of 50%.

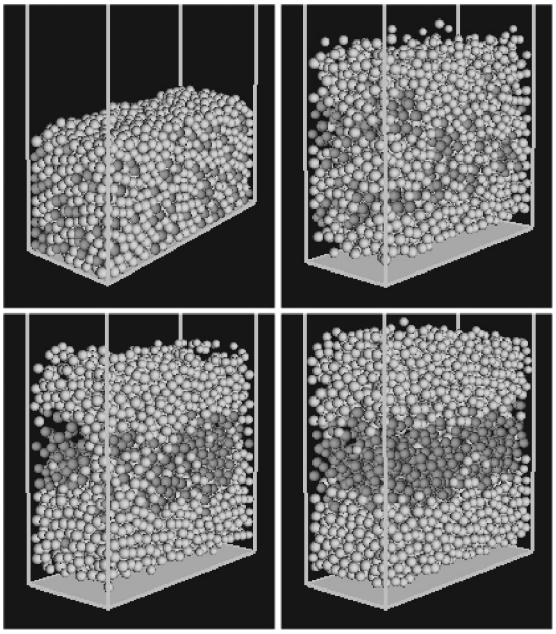

FIG. 1. A sequence of snapshots showing the time evolution of an equal-sized granular mixture vibrated at $\Gamma = 8$, $f = 60$ Hz starting from a well-mixed initial configuration. From top left to bottom right, the times correspond to $t = 0$, 0.1, 0.2, 0.4 s. The dark gray spheres represent the bronze component.

Figure 1 shows the time evolution of a mixture of 3000 particles confined within a box of horizontal cross section 2.3×10^{-3} m by 1×10^{-3} m [22]. The ratio of bronze to glass is 25%:75% by volume. The system is vibrated vertically at 60 Hz with $\Gamma = 8$ starting from a randomly mixed configuration. As the system evolves, bronze-rich and glass-rich regions form and develop into a single bronze layer sandwiched between glass. Eventually, the interface between the regions becomes extremely sharp, being only a single particle wide. The glass regions are then almost completely free of bronze, whereas there are a few glass particles within the bronze layer. This configuration is stable within the time scales accessible to simulation. Under vibration, the bronze particles are extremely kinetically active, whereas the glass particles are largely inactive. The motion of the upper surface is thus substantially damped by the presence of the trapped bronze layer. All of these features, including the spontaneous separation into bronze-rich and glass-rich ''phases'' forming a sandwich configuration, the sharpness of the interfaces and the composition of the phases have been observed experimentally for similar particle sizes and vibratory conditions [11].

There is some variation in porosity throughout the glass and bronze regions following separation. However, this variation is small, typically of the order of a few percent. We have performed some simulations in which the parameter α is calculated locally over cells containing a few particles and

have employed both the Carman-Kozeny [21] and the Di Felice [23] relations between permeability and local porosity. Separation with sharp boundaries still occurs. However, the position of the bronze layer is somewhat sensitive to model parameters.

To understand the role played by air in this model and in experiments, we have carried out simulations in which the mean external air velocity $\mathbf{V_a}$ is zero, i.e., the air external to the bed does not move in the laboratory frame. We find that the mixture does not then separate under vibration, as observed experimentally using a porous-bottomed box [24]. There is only a slight tendency for the heavier component to collect at the bottom of the system, and there are no sharp boundaries between distinct phases. Similar behavior is also observed if the air-drag term is removed completely from the simulations, or particles larger than 500 μm are used. These behaviors demonstrate that the strong separation described here is intimately related to the action of the air as it is driven through the bed by the vibration of the container. It is distinct from the conventional Brazil nut effect which is not driven by air [9].

The model described above appears to capture many of the features which are observed experimentally and clearly demonstrates the air-driven separation mechanism. However, for all the frequencies and Γ values we have investigated, the bronze always forms a sandwich configuration, whereas it is known experimentally that at low frequencies the bronze goes to the top [11]. An effect that is missing from the simulations which we have described above is granular convection induced by the frictional forces between the particles and the container walls. In many systems, convection acts to mix the components and it is thus important to understand how convective mixing competes with the separation mechanism described above. Convective flows can also influence the dynamics of an intruder, as in the Brazil nut effect [25].

To induce convection, we have introduced a tangential frictional force between grains and between the grains and the walls. The shear force on particle j due to an interaction with particle i is assumed to have the form

$$\mathbf{F_f} = -\mu_t |\mathbf{F_n}| \hat{\mathbf{t}}, \tag{5}$$

where $\mathbf{F_n}$ is the normal force, $\hat{\mathbf{t}}$ is a unit vector perpendicular to $\hat{\mathbf{n}}$ in the direction of relative motion, and μ_t is the coefficient of sliding friction. Here we take $\mu_t = 0.2$ between particles and $\mu_t = 0.3$ between particles and the walls [19]. All the other model parameters are as above.

At high frequencies, the mixture initially separates into a sandwich configuration as in the case without friction. There is then a tendency for the bronze layer to drift very slowly upwards, the rate of rise being strongly dependent on the value of μ_t. Increasing μ_t increases the tendency to rise. As the frequency is lowered, the tendency for the bronze to rise to the top is greatly enhanced. This low-frequency behavior is shown in Fig. 2. Note that it is the heavier bronze-rich component that rises to the top, as has been observed experimentally under low-frequency vibration [11]. Also as observed in experiment [11], the model exhibits convection currents in the bed which are confined to the individual

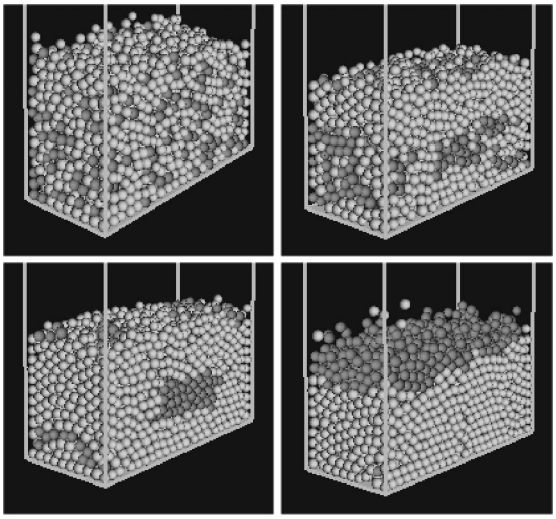

FIG. 2. A sequence of snapshots showing the time evolution of an equal-sized granular mixture vibrated at $\Gamma = 4$, $f = 35$ Hz starting from a well-mixed initial configuration. From top left to bottom right, the times correspond to $t = 0$, 0.4, 2.5, 6.7 s.

phases and do not act to cause mixing. However, the positioning and relative motion of the two phases are sensitive to the values of the frictional parameters we have used. Due to the limited time scales accessible to simulation, it is not clear whether the high-frequency sandwich configuration is stable, or if ultimately the bronze will always go to the top. These simulations also suggest that friction may play an important role in the conventional Brazil nut effect [7,9].

If the air-driven effect described above is the dominant separation mechanism, it should still be active to some extent in mixtures of particles having different sizes as well as different densities. The coupling between the air flow and the particle motion is described approximately by an effective

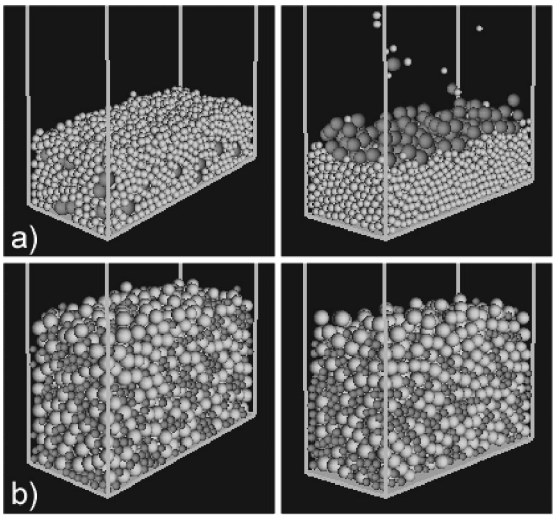

FIG. 3. Snapshots of the time evolution of mixtures with ratios $S \approx 12$ (a) and $S \approx 1$ (b) vibrated at 60 Hz with $\Gamma = 8$. The times correspond to 0 and 1.1 s, from left to right, respectively. The particle radii are (a) $r_b = 69$ μm and $r_g = 38$ μm, (b) $r_b = 38$ μm and $r_g = 69$ μm.

Stokes's drag in the frame of reference of the container, Eq. (4). Consequently, the relative acceleration of the two components generated by such a force can be characterized by the ratio $S=\rho_b r_b^2/\rho_g r_g^2$. For mixtures in which $S\approx 1$ there will be little difference between the effects of air on the two components, whereas for S sufficiently different from 1, there will be strong differentiation between the components. Figure 3 shows snapshots of the time evolution for mixtures with $S\approx 12$ (a), and $S\approx 1$ (b), both started from a well-mixed configuration. It is clear that the mixture with $S\approx 12$ separates easily whereas the mixture with $S\approx 1$ remains mixed. The time scale for separation and the positioning of the phases depend quite strongly on the value of μ_t. We have also investigated mixtures with $S<1$ and find that there is a slight tendency for the system to separate, with the roles played by the bronze and the glass reversed. However, the separation effect is not as strong as for $S>1$. Thus the simulations suggest that S is a useful quantity in predicting whether or not a fine powder mixture will separate under vibration, in cases where the particles are sufficiently small that air-effects are strong. This has now been confirmed by experiment [24].

Visual inspection of our simulations clearly shows the basic physical mechanism for the air-driven separation. During bed flight, the glass and bronze components are influenced differently by the air forced through the bed by vibration, and have a tendency to move with respect to one another. However, if a number of glass grains come together, they tend to stay together since they experience similar air drag. The same is true for any group of adjacent bronze particles. Over many cycles this process repeats, resulting in the almost complete separation which is observed both in our simulations and in experiment.

We have shown that the simple air-driven model with friction reproduces very many of the features that have been observed experimentally. However, a more detailed quantitative comparison would require far larger system sizes and a more microscopic treatment of the air flow. Nevertheless, the model contains the essential ingredients needed to describe air-driven separation in binary granular mixtures. In particular, it highlights the importance of forced air-flow through the bed as the mechanism that is responsible for separation. This mechanism is found to be robust and independent of many of the model parameters.

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