Three-Dimensional Model for Particle-Size Segregation by Shaking

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A three-dimensional model for particle-size segregation by shaking has been developed and used to study the upward motion of a large sphere in a random packing of smaller spheres. In this model segregation occurs only for values of the diameter ratio (Φ) above a critical value $\Phi_c \simeq 2.8$. The ratio of the upward velocity of the large particles to their diameter is greatest for values of Φ just larger than Φ_c. The simulation results can be understood in terms of a simple theoretical model that becomes exact in the limit $\Phi \rightarrow \infty$.

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The segregation of particles with different properties is a ubiquitous process of major importance in areas as diverse as agriculture, geophysics, materials science, and almost all areas of engineering. Segregation can be brought about by many processes including pouring, shaking, vibration, shear, freeze-thaw cycling, and fluidization. In most cases the particle size is by far the most important property controlling segregation and size segregation is observed even in processes designed for particle mixing [1-3]. Because of its practical importance particle-size segregation has been studied extensively (see Refs. [4-10] for example) during the past few decades.

A growing interest in complex phenomena and disordered systems within the physics community has led to the recent development of simple two-dimensional models for size segregation by shaking [11-14] as well as both two-dimensional [15-18] and three-dimensional [17,18] models for size segregation by flow. Another segregation mechanism [19] that has been studied using computer models is the percolation of small particles through a random three-dimensional packing of larger particles [19,20].

In this Letter we describe results obtained using a model for size segregation by shaking that is simpler and more efficient than previous models. This model allows us to carry out simulations using a large number of particles (up to 10^5 or more) and to explore size segregation in three-dimensional systems.

Our model is based on the random-packing model of Visscher and Bolsterli [21] in which particles (spheres) are deposited, one at a time, via randomly located vertical trajectories onto a horizontal substrate. After first contacting the growing deposit the particles follow a path of steepest descent on the surface of the deposit until they reach either the substrate or a local minimum (a position at which the vertical projection of the center of the deposited particle lies within the triangle formed by the vertical projections of the centers of three contacting particles in the deposit). Immediately after reaching a local minimum or contacting the substrate the particles are incorporated irreversibly into the growing deposit. A more complete description of this model can be found in the literature [21-23]. Our size-segregation simulations are started by generating a random packing using this algorithm with spheres of two (or more) sizes. After the initial packing has been constructed the particles are placed in a list in order of ascending height (of their centers) and then redeposited in that order retaining their horizontal coordinates until contact is made with either the substrate or the growing deposit. The process of ordering according to height and deposition (with steepest descent to the local minima) is repeated many times to simulate the shaking process. Our model corresponds to a large-amplitude, low-frequency vertical shaking process with a large dilatation of the packing. It is assumed that the packing comes completely to rest after each shake. We neglect multiparticle effects such as arch formation and collective effects such as fluidization. Despite these approximations we believe our model captures the essential features of the segregation process.

Figure 1 illustrates a typical simulation with $\Phi = 4$ where 250 large spheres and 50000 small spheres were initially deposited randomly on a square base of size 16×16, in units of the large-sphere radius (with periodic

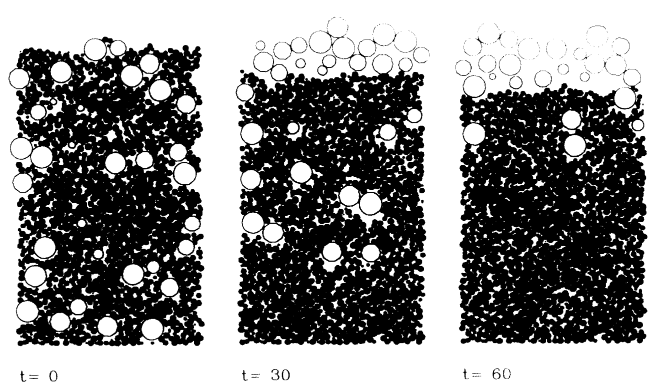

FIG. 1. A vertical cut through a packing made with 250 large spheres and 50000 small spheres with a diameter ratio $\Phi = 4$. From left to right the initial configuration and the packings after thirty shakes and after sixty shakes are shown.

boundary conditions in the lateral directions). Vertical cuts through the deposit are shown for the initial configuration and after thirty and sixty shakes. The upward motion of the large spheres can be clearly seen in this figure. In this Letter, we focus our attention on the case where one large sphere was initially deposited near the bottom of a packing of small spheres.

Figure 2(a) shows the time dependence of the height, $z(t)$, of a single large sphere divided by its radius R for different Φ values. Here, the time t is the number of "shakes" and $z(0)=0$. We found a clear change of behavior at a threshold value $\Phi_c \simeq 2.8$. While for $\Phi < \Phi_c$ the maximum upward displacement, z_m, remains finite, for $\Phi > \Phi_c$, there is a monotonic upward motion $z = vt$ characterized by a well-defined velocity v. The change of behavior at Φ_c is like that at a second-order phase transition where z_m plays the role of a correlation length that diverges when Φ approaches Φ_c. However, we found that z_m depends strongly on the initial packing configuration. Consequently we would need to make an average over many runs to obtain a continuous curve for $z_m(\Phi)$ and

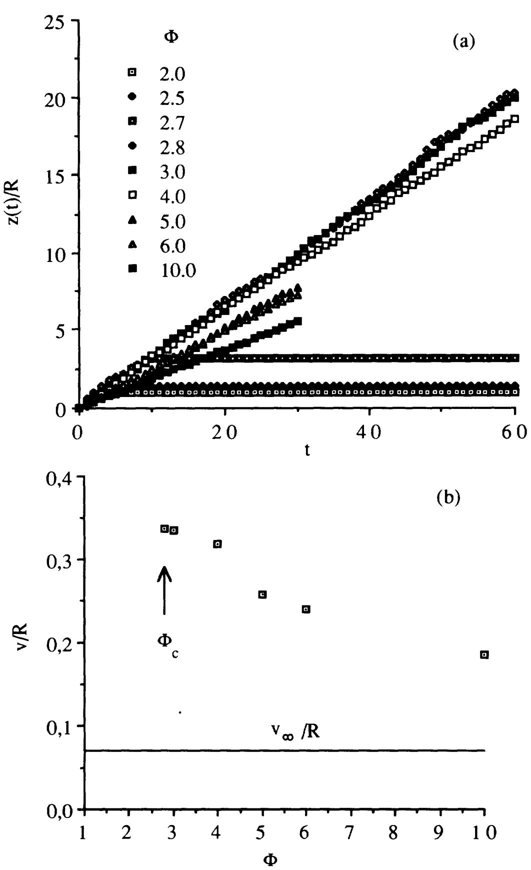

FIG. 2. (a) Dependence of the large-particle altitude $z(t)$ on the number of shakes t for simulations with one large particle and various diameter ratios. (b) The velocity $v(\Phi)$ as a function of the diameter ratio Φ for $\Phi > \Phi_c$. The location of Φ_c and the asymptotic value v_∞ obtained from the theoretical model are indicated by vertical and horizontal arrows, respectively.

estimate an exponent. The ratio v/R is largest at the threshold ($v_c/R \simeq 0.35$). Above Φ_c the ratio v/R seems to decrease towards an asymptotic value v_∞/R as $\Phi \rightarrow \infty$ [Fig. 2(b)]. We have not obtained an accurate value for this asymptotic ratio from our simulations since much more computer time is required for large values of Φ.

The monotonic upward motion above Φ_c can be understood by using a simple analytical model which becomes exact in the limit $\Phi \rightarrow \infty$. Here we make use of the "angle of the repose" α as an input parameter. As is clearly suggested by the simulations at large Φ values (see Fig. 3) we suppose that in the steady-state regime a conical hole, tangent to the sphere, lies beneath the large sphere. The velocity is determined by the upward displacement δ after one shake. Since all small particles that are located below the large-sphere center will be deposited before the large sphere, this cone will be partially filled prior to the large-sphere deposition. During each shake, the small spheres that are in the annular region (1) [whose cross section is indicated in black in Fig. 4(a)] will slide into region (2) [whose cross section is indicated in black in Fig. 4(b)]. After some simple algebra we can express the volume V_1 of region (1) as a function of α and R (the radius of the large sphere),

$$V_1 = \frac{\pi R^3}{3} \frac{\cos^3\alpha}{\sin^2\alpha}, \tag{1}$$

and, after equating this volume to the volume $V_2(\delta)$ of region (2),

$$V_2(\delta) = \frac{\pi}{3} \frac{\delta}{\sin^2\alpha} (\delta^2 \cos^2\alpha - 3\delta R \cos\alpha + 3R^2), \tag{2}$$

we find

$$\delta = v_\infty = \frac{1-(1-\cos^4\alpha)^{1/3}}{\cos\alpha} R. \tag{3}$$

According to this formula, v_∞ should decrease monotonically from R to 0 when α increases from 0 to $\pi/2$. We

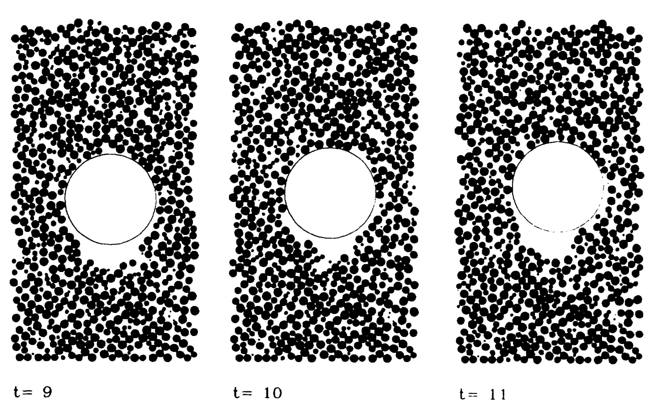

FIG. 3. Vertical cut through a packing containing one large sphere in the steady-state regime from a simulation with a large diameter ratio $\Phi = 10$. The configurations after three successive shakes are shown.

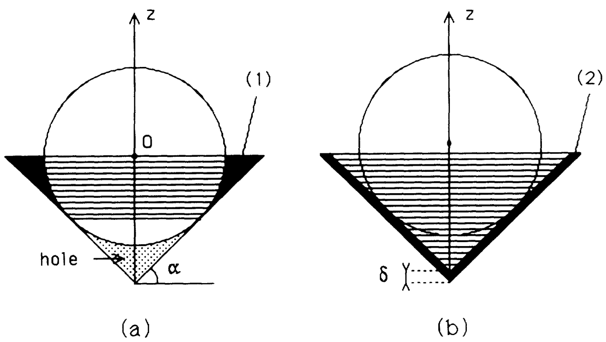

FIG. 4. The model for an infinite diameter ratio ($\Phi \rightarrow \infty$). (a) and (b) correspond to configurations before and after one shake, respectively.

have estimated the angle of repose for our model in a separate simulation in which equal-sized particles were deposited uniformly outside of a circular region, leaving a conical hole in the surface of the deposit. We have found $\alpha \simeq 54°$ (the same value that was obtained earlier for a heap [17]). This gives the estimate $v_\infty/R \simeq 0.07$ which is shown in Fig. 2 and which is consistent with the data obtained for finite Φ values. Here the value of the angle of repose is imposed by our algorithm. In most real systems it is smaller than 54° because of avalanches and other multiparticle effects.

This calculation allows us to better understand the geometrical mechanism involved in the upward motion of the large sphere. The presence of the hole beneath the sphere is essential to its upward motion. Moreover the larger values of the velocity for finite Φ and the existence of the threshold can be qualitatively understood by including finite-size effects. The mean shape of the hole should deviate from a cone for finite Φ and the angle α should be replaced by an effective (smaller) angle in Eq. (3), giving a larger value for v/R. The threshold Φ_c occurs when the small spheres are too large for their centers to have a chance to lie in volume (1).

A rich phenomenology is associated with particle-size-segregation processes but it appears that the ability of small particles to fill voids that develop beneath large particles (and to remain beneath the large particles preventing their fall) plays a key role in many systems. In the Monte Carlo model of Rosato *et al.* [12–14] this mechanism has a stochastic origin. In our model only the construction of the initial packing is stochastic. The segregation process is completely deterministic. It is clear that a simple model such as that described in this Letter cannot represent all the complex processes that occur in real systems (inelastic collisions, friction between particles, multiparticle interactions, etc.). However, this model does appear to capture the essential features of many size-segregation phenomena and leads to interesting predictions that could be compared with experiments. Our results are consistent with some experiments [6] in which the segregation rate was found to increase when the size of the large particles was increased. It would be interesting to test experimentally the linear dependence of the upward velocity on the radius of the large spheres in the limit of large Φ values.

The existence of a critical diameter ratio (Φ_c) below which segregation does not occur, with a maximum of the ratio v/R for $\Phi \simeq \Phi_c$, is a distinctive characteristic of this model that could also be tested experimentally. However, the critical ratio decreases as the angle of repose decreases (to a value of about 1.5 at 35°). Preliminary results show that a corresponding two-dimensional model leads to a much larger (4 times greater) critical ratio so that it might be easier to observe the segregation threshold in pseudo-two-dimensional experiments. A critical diameter ratio is also a characteristic of the quite different percolation [19,20] model for size segregation. Most other size-segregation models are too complex for theoretical analysis and do not permit extensive enough simulations to determine numerically if a size ratio threshold exists.

The most important advantage of our model is that it leads to a simple geometrical explanation of the rising mechanism and of the existence of a critical diameter ratio. We have also used this model to study the compaction of both monodisperse and polydisperse packings and to simulate the relaxation of heaps induced by shaking. Very similar models can be used to study the effective interactions between large particles and their motion near container walls.

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