Why the Brazil Nuts Are on Top: Size Segregation of Particulate Matter by Shaking

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When a can containing one large ball and a number of smaller ones is shaken, the large ball rises to the top, even when the larger ball is more dense than the others. Similarly, a mixture of different sized particles will segregate by size when shaken. An adaptation of the Monte Carlo method is used to study this size segregation. The results show the local, geometric mechanism by which the segregation is produced. Segregation by size is to be distinguished from the more obvious sifting process which occurs when tiny grains filter down through the interstices between large particles.

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An important effect occurs in many industrial situations in which granular mixtures of particles of different sizes are used. When these particulate mixtures are shaken or jostled the larger particles rise to the top.[1-4] This size segregation occurs even if the large particles are significantly denser than the smaller ones and even when the size ratio is near 1. The resulting nonuniformity is usually an undesirable property, although there are some applications in which shaking is employed as a means of separating particles of differing sizes. Size segregation effects are important in powder metallurgy, pharmaceuticals, and the glass and paint industries.

If the discrepancy in size between the large and small particles is great, an obvious sifting mechanism, in which tiny grains filter down through the interstices between the large particles, is operative. In this case, the overall potential energy of the system is reduced by the shaking procedure. In this work we are concerned, instead, with the situation when the large and small particles are of comparable size, and thus sifting cannot occur. Indeed, most of our discussion will focus on the specific case of one large particle in a system of many smaller particles. This choice highlights the distinction between size segregation and sifting.

Because of its industrial importance, size segregation has been the subject of considerable study in the engineering community.[1-5] The emphasis in these studies has been on the segregation rate and its dependence on parameters such as particle size and weight ratio and shaking frequency. A basic phenomenological understanding of the segregation mechanism had remained elusive.

In this work, reported in greater detail elsewhere,[6] an adaptation of the Monte Carlo method commonly used in statistical mechanics was used to study the dynamics of size segregation. The results provide a clear view of the local, geometric mechanism by which the segregation is produced.

The segregation phenomenon is an example of a simple, mechanical system displaying nonequilibrium, counterintuitive behavior. At equilibrium, if a large particle is placed in a container filled with smaller particles of equal or lesser density the large particle will be on the bottom in order to minimize the potential energy. Generally, one thinks of shaking as a method of mixing. In particular, we expect shaking to dislodge metastable configurations and to aid the system in reaching equilibrium (as is the case, for example, with sifting). That the system would start from an equilibrium state and proceed upon shaking to a nonequilibrium metastable state is rather surprising.

In this paper we provide a dynamical picture of the segregation process. As the particles fall during a shake, small particles easily move in beneath a large particle whenever gaps open up. A large particle may move back down if many small particles simultaneously move from beneath it. This is an unlikely event, and therefore large particles move up relative to the small particles.

Our choice of model is governed by the observation that the phenomenon of segregation of granular mixtures by particle size is ubiquitous, occurring in widely differing experimental systems. One is led by this obser-

vation to infer that the segregation mechanism depends only weakly on system details such as shape distribution, or the precise nature of the frictional or electrostatic interactions between the particles.

The "shaking" simulation method may be described briefly as follows: (1) Because the creation of voids into which particles may move is the principal factor driving the segregation process we use, as mentioned above, hard spheres. (2) Shaking is modeled as a process in which all the particles are first lifted and then dropped to the bottom of the container. The dissipation of energy is essential to the segregation process in real systems. The precise mechanism of energy dissipation is unimportant. Conservation of energy is therefore not imposed by our simulation. Our Monte Carlo procedure allows particles to drop to the bottom of the container without bouncing back up again. (3) The effects of interparticle collisions, collisions with the walls, and slight horizontal jostlings of the container are modeled as random movements of the particles with respect to one another. This assumption allows us to simulate the many-body system without following the details of the collision dynamics. We hypothesize that the detailed particle interactions are not significant except in that they induce the random jostling mentioned above. (4) We simulate a two-dimensional system. This choice is made simply for computational efficiency and because we believe (and our results indicate) that the segregation mechanism is independent of dimensionality.

Because the segregation process may be explained solely by geometrical effects, all of the results scale with the ratio of the sizes of the particles and the ratio of the distance through which particles are lifted from the bottom during shaking to the size of the small particles. The critical factor is the creation of voids of the size of the small particles under large particles. Scaling with these ratios should be observable in experimental systems. Mass is not important for the segregation process.

In Sect. I we demonstrate that ordinary Monte Carlo equilibration leads to the expected equilibrium configuration with the large particles on the bottom and the small particles on top. In Sect. II a modified Monte Carlo procedure is used to model the shaking process. The results of these simulations provide an understanding of the mechanism by which the nonequilibrium state with the large particles on the top is produced.

I. *Equilibrium simulation.* — Hard disks are randomly placed in a cell having periodic boundary conditions in the horizontal direction [Fig. 1(a)]. The smaller disks have a diameter, d_s, half that of the others. The system is brought to equilibrium at a high temperature with the use of the Monte Carlo method and then slowly cooled as shown in Figs. 1(b)–1(d). In the lowest-temperature configuration, shown in Fig. 1(d), the larger disks are located near the bottom of the cell in order to minimize the height of the center of mass. Several different size systems were simulated.
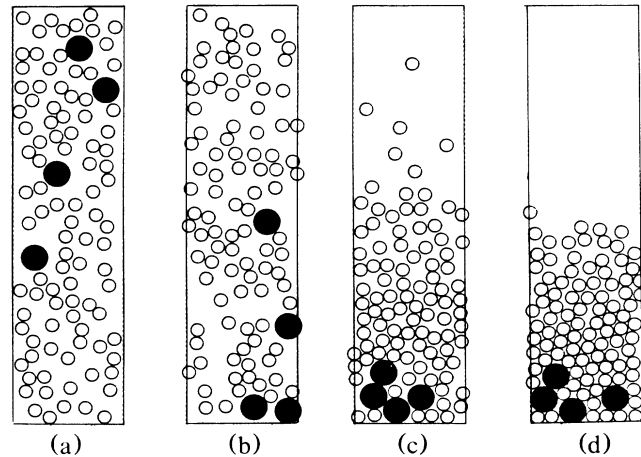

FIG. 1. A standard Monte Carlo cooling simulation tends to the global equilibrium configuration with the large particles on the bottom. (a) The initial random placement of the particles. (b)–(d) The configurations at $T^* = k_B T/m_s g d_s = 33.3$, 2.2, and 0.6, respectively.

In the shaking simulation the energy scales are such that room temperature is an extremely low temperature for both the large and small particles. In the equilibrium simulation, the initial temperature is high and the final temperature is low, relative to the gravitational potential energy of both large and small particles.

When a heavy ball is placed in a fluid, however, room temperature is high on the scale of the gravitational energy and the more important intermolecular forces of the fluid particles and low on the scale of the gravitational energy of the ball. In this case the fluid particles move relatively rapidly in all directions, allowing the heavy ball to sink to its equilibrium position on the bottom of the jar.

Shaking such a system induces random movements of the particles which might seem to be similar to those observed in the cooling simulation. In Sect. II, however, we present the results of a shaking simulation in which the larger particles rise to the top of the container.

II. *Shaking simulation.* — The Monte Carlo method is used to simulate pouring and then shaking of disks to achieve size segregation. The term "pouring" characterizes the first part of the simulation in which the disks simply fall under the influence of gravity.

Consider a particle-filled container fastened to a vibration table. When the container is dropped with an acceleration greater than g, the particles will separate from the container bottom. In our simulation shaking is accomplished by repeatedly lifting the assembly of fallen disks uniformly through a specific heat and then allowing them to fall again by use of the Monte Carlo method. This procedure is defined to be one cycle. A cycle models one "shake" of the container. A cycle is halted when the change in the average energy is less than 0.1%.

For typical experimental conditions $mg\Delta z/kT \sim 10^{16}$
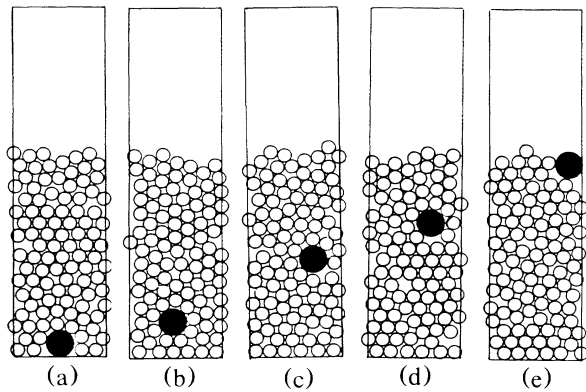
(a)   (b)   (c)   (d)   (e)

FIG. 2. In the shaking simulation the large particles rise to the top. (a) The initial configuration. (b)–(e) The configurations obtained after 10, 30, 40, and 60 "shakes," respectively. Approximately 3000 Monte Carlo steps per particle were performed during each shake. The maximum displacement in a single step was $\frac{1}{2} d_s$. In the pictured simulation the particles were lifted a distance d_s for each "shake."

(a)   (b)   (c)

FIG. 3. Segregation of a 50/50 binary mixture with size ratio 1.5. (a) The initial random placement. (b) The configuration obtained by "pouring" and (c) the configuration obtained after 300 shakes.

which is essentially $T = 0$. This extremely large value effectively results in preventing upward movements during the "falling" portion of the cycle. Horizontal and downward movements are always accepted, providing they do not cause an overlap of the particles. Thus each accepted move results in a decrease of the system's potential energy. This leads to a situation in which local energy minima, rather than global equilibrium, will be reached. Such local minima are exactly the type of states generated in the physical shaking process. Indeed, the segregated state is itself a metastable state.

A system of hard disks, one of which has a diameter twice that of the others, is randomly placed into a cell with periodic boundary conditions in the horizontal direction. The large disk is placed on the cell bottom. The small disks are allowed to fall to a stable configuration as shown in Fig. 2(a). The shaking simulation is then carried out for 70 "shakes" during which we find that the large disk rises to the top of the bed. Figures 2(b)–2(e) depict this process. These configurations clearly demonstrate that our model contains the essential features necessary for size segregation to occur. Again, several size systems were investigated.

During the shaking of a granular mass, relative motion between the particles occurs. A void which opens beneath a large particle may be filled by a smaller one. From the size difference alone, it is clear that a small particle possesses a higher probability of filling this void than does the larger. During the segregation process the larger particle is moved upward as smaller particles fill voids created beneath it.

In order for a large particle to move back down, however, a large void must open beneath it. Because several small particles must move simultaneously in order to create such a large void, the appearance of such a large void is relatively unlikely, and thus the larger particles
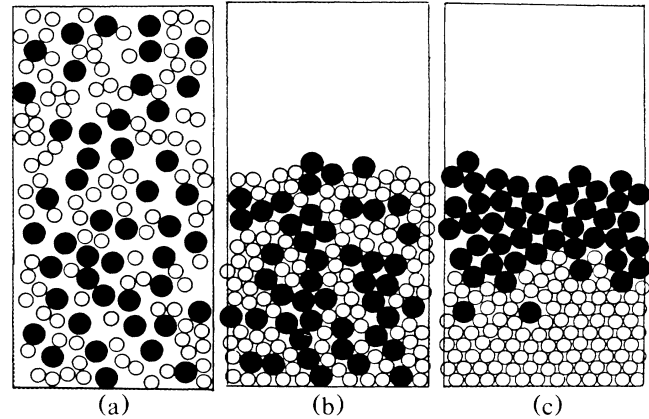
experience a net upward motion. This process is illustrated in the simulation results shown in Fig. 2. Figure 3 shows the results of a shaking simulation for a 50/50 mixture of large and small disks.

Our simulations have several conclusions which should be experimentally observable. The scaling of segregation behavior with the particle sizes and the distance through which they are lifted is easily tested. Also, our results indicate that lateral shaking should be relatively ineffective in promoting segregation. We also find an apparent threshold value for the lift distance below which segregation does not occur.

The method developed here is trivially expandable to three-dimensional systems. More detailed information concerning the dependence of segregation rate on size ratio, lift distance, and size distribution is easily obtainable. Information obtained from these simulations should be useful in developing an analytical description of the size segregation process. In addition, the method could be used to examine the behavior under shaking of anisotropic particles and the effects of the container walls on the shaking process.

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