Empty Site Models for Heap Formation in Vertically Vibrating Grains

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Heap formations of granular materials in a vertical vibrating bed are studied by a simulation model in which the effect of decrease in local density due to vibration is modeled by the creation of empty sites in the bulk. Dynamics of empty sites are introduced to simulate the bulk flow while the surface flow is modeled by rules similar to the sandpile model. Phenomena such as heap formation and downward and upward convection modes can be reproduced. Phase diagrams similar to experimental observations can be constructed. A continuum model based on the empty site dynamics is also proposed. Predictions from the continuum model compare favorably with experimental observations.

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The physics of granular materials has been the subject of great interest for over two centuries [1]. These granular materials cannot be easily classified as either solid or liquid since they can sustain shear like a solid up to a point and also flow like a liquid. A good example is the behavior of sand lying on a vertically vibrating bed. Similar to the Faraday waves [2] on liquid surfaces, many intriguing patterns can be generated. One of the most remarkable phenomena in such a system is the heap formation [3]. The relevant dimensionless parameter for this problem is the reduced acceleration amplitude, $\Gamma = A\omega^2/g$ of the bed where g, A, and ω are the gravitational acceleration, amplitude, and angular frequency of the vibrating bed, respectively. An originally flat layer of sand will turn into a heap with a well-defined structure if Γ is greater than some critical value Γ_c. The grains in the heap are not simply moving up and down vertically, but a convection roll with grains moving up along the wall and flows moving down the slope of the heap are also produced. The convective motion is qualitatively similar to the convection rolls formed when a fluid is heated from below [4]. There are many investigations both in theory [5–8] and experiment [9–11] as well as numerical simulation [12,13] to investigate the underlying mechanism in a vertically vibrating granular layer. One of the main issues is to understand the formation mechanism of heaps and to relate the granular properties with the observed dynamic behaviors such as the convection current. Friction between the grains and with the wall [14], driving mechanism, and boundary effects [15,16] all play important roles in the convection modes. To understand the origin of the convection there have been various theoretical attempts to include voids in the granular dynamics [5,8]. Vertical vibrations create voids which decrease the overall density and thus allow the rearrangement of grains in the bulk, providing a mechanism for convection. However, these models of voids are usually quite complicated and do not necessarily lead to the formation of heaps. Since bulk movement alone might not be sufficient to complete a convection cycle, presumably a surface flow is needed as observed in experiments. Also, it is found that interstitial gas is vital for the heap formation. Pak *et al.* have established in their experiments [10] that heaping and convection current disappear when there is no interstitial gas. This last finding suggests that the "voids" in the granular material are filled with air which might be compressed. Therefore, any successful heaping model should also include the effects of the interstitial gas. The sidewalls are also essential since they confine the grains to flow in a finite region and the frictional properties of the wall can affect the convection mode. In this Letter, we report the results of a new simulation model which is designed to study the mechanism of heap formations. The simulation model is based on the well-known sandpile model [17] which takes care of the surface flow of the granular materials and has been applied to granular segregation [18]. This simple model can reproduce many of the observed phenomena such as heap formation, downward, and upward modes of convection. The success of this model suggests that heap formation is mainly caused by interstitial gas and the sidewalls of the container. Finally, a continuum model based on the empty site dynamics is also constructed.

Our model is based on two important observations in vibrating bed experiments. The first is that density fluctuations are generated by vibration and convection can be induced. Second, surface flow is induced by grain topplings similar to a sandpile. To implement these ideas, we make use of a sandpile model [17] in which fluctuations in density can be realized by random creation of empty sites in the bulk. Since these empty sites will also generate fluctuations in heights, surface flow will be induced and taken care of automatically by the sandpile rules. However, in order to generate convection in the bulk, similar to the void models [5,8], these empty sites will need to follow some realistic dynamics. Therefore, our simulation consists of two essential steps. Vacant sites are first created in a sandpile, then the system is allowed to relax on the surface by sandpile rules and by the empty site dynamics in the bulk to be specified below. Grains of the pile are arranged in a

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rectangular lattice with height h_i in the ith column. To create density fluctuations, empty sites are created randomly and uniformly in the pile with a probability α. Note that the empty site has the same size as a grain, as shown in Fig. 1. After the additions of empty sites, the heights of the pile will be increased and therefore α can be regarded as an expansion factor due to vibration. A realistic rule for these empty sites is to allow them to exchange their positions with their neighbors such that the empty sites are moving to regions of lower pressure. The pressure at an empty site is assumed to be proportional to the number of grains on top of that site. When the empty site gets to the top of the pile, it disappears. To be more specific, the probability of moving up for an empty site is always $\frac{1}{3}$ [19], while the probability of moving to the left or right depends on $\Delta h_L = h(i) - h(i-1)$ and $\Delta h_R = h(i) - h(i+1)$ as follows: If $\Delta h \le 0$ on both sides [Fig. 1(c)], the vacant site will not move horizontally. If $\Delta h > 0$ on one side and $\Delta h < 0$ on the other [Fig. 1(b)], then the void can move up or to the $\Delta h > 0$ side with equal probability of $\frac{1}{3}$. If both Δh are positive, then the probability of moving to the left or right are given by $(\frac{2}{3})\Delta h_L/(\Delta h_L + \Delta h_R)$ and $(\frac{2}{3})\Delta h_R/(\Delta h_L + \Delta h_R)$, respectively [Fig. 1(a)]. Hard wall boundary conditions such that no grain or vacant site is allowed to move into the walls are imposed.

The simulation cycle consists of one step of empty site generation followed by γ steps of relaxation. In each relaxation step, each empty site attempts to exchange with its neighbor once, and every surface site on the average is updated by the sandpile rule once. Thus γ can also be interpreted as the toppling rate for the grains. All the grains can finish their topples before the next vibration if γ is very large. The model has two time scales: one is the rate of expanding the piles due to vibration, and the other is the characteristic relaxation time governed by the toppling rate of the grains. The critical slope Δ in the sandpile rule is fixed to be 2 for convenience. Starting with a flat layer of N grains without any void in a system of width L, the steady state behavior of the system is monitored for various values of α and γ. We found that for small values of α, there is no instability in the layer configuration apart from small random fluctuations on the surface. However, when α is larger than some critical value, the originally flat layer becomes unstable and gives way to new steady state configurations. Figure 2 shows some representative steady state configurations of the simulation for different values of α with $\gamma = 10$, $L = 45$, and $N = 675$ [except $N = 225$ in Fig. 2(a)]. These values of parameters are chosen such that there are both sufficient surface and bulk flows. Therefore, in all the configurations, the slopes of the heaps are close to the critical slope, Δ. Figure 2(a) shows the formation of a one-sided heap in which a convection current with grains moving up the wall (upward mode) and slides moving down the slope can be easily observed by using tracer grains. Note that the heap does not extend to the other wall. The horizontal width of the one-sided heap is not controlled by the system size L, but rather by N and Δ such that the heap width $l \approx \sqrt{2N/\Delta}$. One might think that l will increase with N until $l = L$. However, as N is increased beyond some critical value well before $l = L$, the one-sided heap is no longer stable, and an initially thicker flat layer will turn into a steady downward heap [Fig. 2(b)] when α is larger than some critical value. With N fixed, side peaks will develop at the expenses of the central peak when α is increased as shown in Fig. 2(c). Further increase in α will result in a prominent upward heap [Fig. 2(d)]. The transition from downward to upward heap has also been observed in recent experiments [11] as Γ increases.

It is obvious that the two parameters γ and α produce competing effects. A large γ means faster relaxation of height fluctuations deviating from the critical slopes—more time for the empty site to escape and therefore suppress large fluctuations. Since fluctuations in our system are produced by the generation of empty sites, a large production rate α will enhance fluctuations. The competition between these two effects produces a phase diagram of different steady state configurations, as shown in Fig. 3.

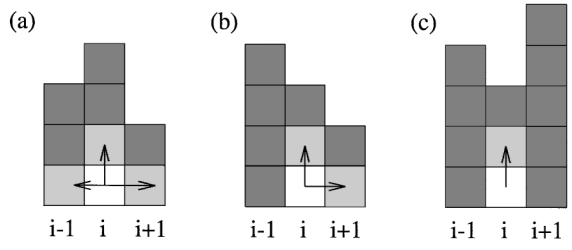

FIG. 1. Dynamic rules for the empty site. Grains are gray and voids are white. (a) The void can exchange in three directions; probability of the right exchange is higher than the left. (b) The void cannot exchange with the left since the left neighbor pile is taller. (c) The void has the only possibility for an upward exchange since both neighbor piles are taller.

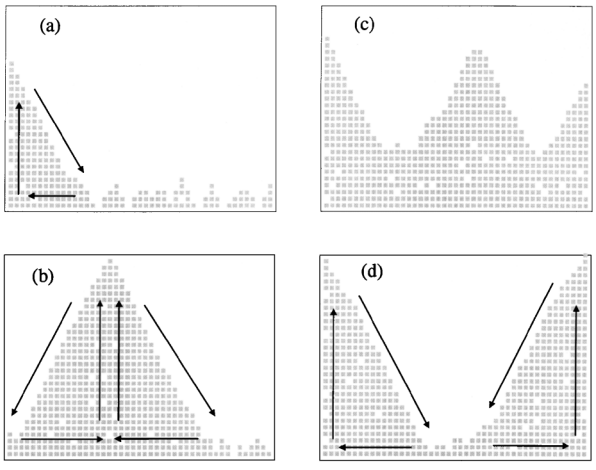

FIG. 2. Steady state configurations with an initially flat layer. $L = 45$ and $\gamma = 10$. Black arrows show the schematic convection directions. (a) $N = 225$ and $\alpha = 0.1$. $N = 675$ for (b), (c), and (d) with $\alpha = 0.05$, 0.1, and 0.3, respectively. Downward mode of heap in (b) and upward mode in (d).

The layer remains flat when α is smaller than 0.01. For a given γ, when α increases gradually, the phenomena of heaping will occur. But if α is too large, the heaping state will disappear, which corresponds to the strongly fluidized phase in real experiments. In this aspect, α plays a very similar role to Γ in experiments. Furthermore, wall effects are also investigated by allowing the probability of creating voids for the two piles next to the walls (denoted by α_W) to be different from that of the bulk (α). A large wall friction suppresses the density fluctuations near the wall and corresponds to a small value of α_W. Our simulation results [20] show that for fixed α and γ the steady heap changes from the downward mode to the upward mode as α_W increases (wall friction decreases), which agrees with the experimental observation that the convection mode reverses its direction, from downward mode to upward mode, when the container wall is changed from a rough to a smooth one [21]. The effective wall friction can be changed experimentally by canting the vertical sidewalls outward. When the canting angle is increased, which corresponds to a decrease in effective wall friction, a similar reverse in convection modes is observed [16].

With the simple ideas contained in the simulation, we construct a continuum model for heap formation. Let $h(x,t)$ denote the height of the sandpile at position x and time t; the equation of motion of $h(x,t)$ is proposed to be

$$\partial h(x,t)/\partial t = D\nabla^2 h(x,t) + \Omega h(x,t) - \beta h(x,t)^2, \quad (1)$$

where D is a diffusion constant which approximates the surface relaxation of fluctuations in h, and Ωh is the effect of increase in height due to vibrations per unit time. In the simulation, the increase in height is αh per γ time step. One can think of Ω as being similar to α/γ. It is obvious that the $-\beta h^2$ term is the decrease in height per unit time which can be interpreted as the rate of dissipation of energy in the system. The two terms Ωh, $-\beta h^2$ can then be regarded as the first two terms of the Taylor expansion of some nonlinear interaction. The h^2 term signifies the nonlinear couplings of different modes in the system. Presumably higher order terms will enter for sufficiently strong nonlinear effects. However, for simplicity, we will use the form in Eq. (1). With the form given above, the steady state continuum equation can be solved with appropriate boundary conditions. To solve for the steady state solution, it is convenient to rewrite the equation as

$$\nabla^2 h(x) + k^2 h(x) - \mu k^3 h(x)^2 = 0, \quad (2)$$

where $k = \sqrt{\Omega/D}$ and μ is a dimensionless parameter controlling the strength of the leading nonlinear effect. We have taken β/D to be μk^3 for dimensional reasons. Details of the solution of the above equation will be given elsewhere [20].

One of the remarkable predictions of such a simple model is that both downward (mountain) and upward (valley) modes of steady heap can be obtained as k is varied. Similar to the result of our discrete model, it can be shown that a downward mode of heaps will be formed for low values of k while upward mode heaps result for larger values of k. If one identifies $k \propto \sqrt{\alpha/\gamma}$, one can even compare the results from simulation with this continuum model. A characteristic measure of heaping is the ratio $h(0)/H$, where H and $h(0)$ are the height of the originally flat grains and the height in the center of the system, respectively. Hence $h(0)/H > 1$ and $h(0)/H < 1$ correspond to the downward and upward heaps, respectively. Figure 4 displays the dependence of $h(0)/H$ on the scaled variable $\sqrt{\alpha/\gamma}$ obtained from the simulation for various values of γ. The data roughly collapse, suggesting α/γ is an appropriate scaling parameter. The continuum model also predicts a peak in $h(0)/H$ (solid curve) which is in qualitative agreement with the simulation data. The continuum model even fits the simulation data quantitatively for low values of k. Deviations at large values of k are expected since higher order nonlinearities are important at strong vibrations. With this continuum equation, one can also solve for steady state heaping profiles to compare with real experiments. Figure 5 shows the steady profile obtained from a quasi-2D heaping experiment [22] with $\Gamma = 1.5$ together with the calculated profile from the continuum model. It can be seen that the theoretical prediction agrees well with the experimental profile.

It is clear that in both the discrete and continuum models, there are two main effects, namely the input and the dissipation of energy. In both models, energy is put into the system by the increase in height of the system. For the simulation model, the sandpile and void dynamics relax the height fluctuations and dissipate the

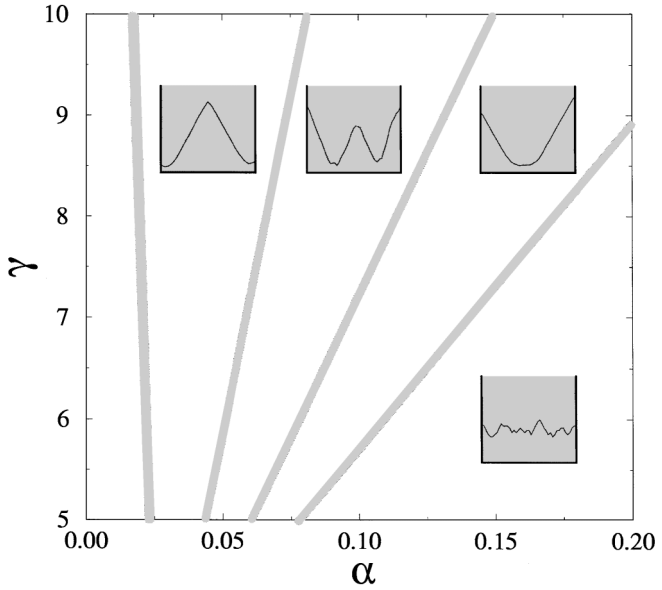

FIG. 3. Phase diagram of steady heaps for a system with $N = 675$ and $L = 45$. The insets show the characteristic steady structures.

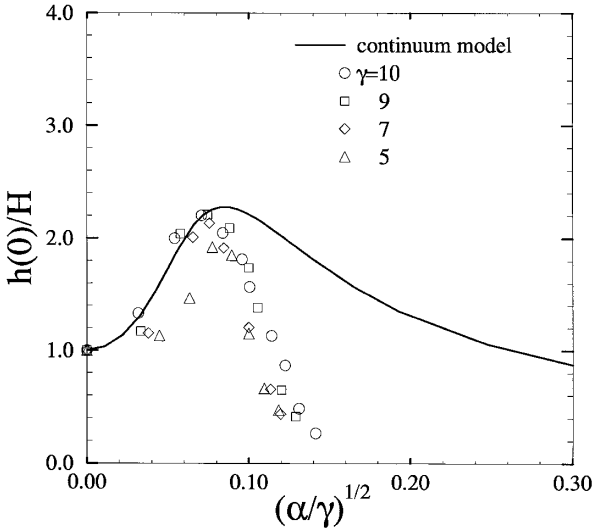

FIG. 4. Reduced height of the central pile, $h(0)/H$ vs $(\alpha/\gamma)^{1/2}$. The result of the continuum model is from solving Eq. (2) with $k \propto (\alpha/\gamma)^{1/2}$ for some fixed proportional constant and $\mu = 0.14$.

input energy, while in the continuum model, the $-\beta h^2$ term removes the potential energy. Steady states can be reached when the system balances these two effects. It can also be seen from our models that vibration is treated as a mean field with its effect averaged over one vibration cycle. Its mere effect is to produce fluctuations in local densities (input of energy). In response to these increases in fluctuations, the empty site dynamics and the sandpile rules interact to relax the fluctuations. Therefore, our model is more or less a pure relaxation model. There is no direct interaction of the granular flow with the vibration, and the heap formation is just a steady state which happens to be a stable state to dissipate the input energy. It is obvious that our model will fail if the dissipation is not strong enough to produce a compact sandpile. In real experiments, when $\Gamma \gg 1$, the heap will disappear and the system becomes gaslike, which means the dissipation rate of the granular material is not fast enough. In this case, the system is characterized by how the granular flow interacts with the external drive rather than how energy is being dissipated. Such situations occur in the oscillon

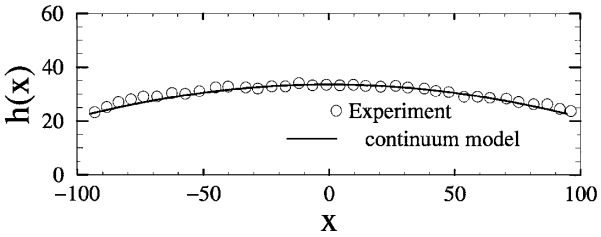

FIG. 5. Profile of downward heap from experiment and the continuum model. h and x are in units of mm. Data from the experiment in Ref. [22] in a quasi-two-dimensional rectangular vertical vibrating bed at $\Gamma = 1.5$. (Glass beads of diameter $a = 3$ mm, initially flat layer of height 30 mm, and width 190 mm.)

and wave patterns in experiments of a thin layer under vibration [23], where direct interaction of the granular flow with the vibrating bed is strong.

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