Cellular-automaton model for segregation of a two-species granular flow

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A cellular-automaton model is presented for the segregation of a granular flow. The need for such a model arose originally from consideration of a problem related to the ferro-alloy industry. The flow consists of particles of two different sizes, which in this specific industrial application are lumps of ore and coal or coke. It is known from experiments [S. A. Halvorsen, S. E. Remnes, and P. Hyldmo (unpublished)] that these particles show different mobilities under different circumstances. This effect is incorporated in our model via the inclusion of a "hydrostatic pressure" term.

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I. INTRODUCTION

Recently there has been rapidly increasing interest in the phenomenon of "self-organized criticality," wherein large interactive systems exhibit a predisposition to evolve toward a critical state where even a minor event can initiate a "chain reaction" and lead to a major catastrophe [2–4].

The paradigm for studies of self-organized criticality is the simple process of creating a pile of a granular material, for example, sand, by dropping particles onto a solid surface. This problem has been the subject of several careful experimental studies. For example, Jaeger, Liu, and Nagel [5] investigated the unsteady motion of a sandpile when its surface angle was everywhere close to the limiting angle of friction. They confirmed the importance of dilatation, that is, the surface slope must exceed the angle of friction by a small but measurable amount before an avalanche can occur so that there is sufficient clearance on a local scale for the individual particles to move. Also of note is the work of Held *et al.* [6], who look for scale invariance in the distribution of avalanches. The subject area of granular flows has also seen the development of cellular-automaton models. These include the model of Baxter and Behringer [7], who endowed their sand particles with orientation. Although not strictly a cellular automaton, the model of Jullien and Meakin [8] simulated a two-species granular flow, as in the present work. The more general problem of the dynamics of a pile of granular material was also examined by Fauve, Douady, and Laroche [9], who noted that under the influence of vertical vibration, an initially planar layer of granular material formed a pile with a predictable surface angle.

In the present study, motivated by experimental observations, we pursue an alternative route and consider a granular flow that consist of two species of particles of different sizes. Our aim is to present a cellular-automaton model which shows the segregation of the two types of particles as seen in experiments [1,10]. Our model will assume that the flow is two dimensional, but can obviously be trivially extended to three dimensions.

The phenomenon of segregation has been studied with particular reference to the food industry by Barker and Grimson [11]. They noted the tendency of granular mixtures with two distinct grain sizes to segregate under vibration, the larger particles moving upward to form a distinct layer from the smaller particles. The context of the present model, however, arises from the ferro-alloy industry, where granular mixtures of ore and coke or coal are fed to an electric smelting furnace. Segregation patterns likely to occur within smelting furnaces have been studied by Halvorsen, Remnes, and Hyldmo [1], who have poured a mixture of quartz and coke into the top portion of an experimental rig consisting of an approximately rectangular hopper under gravity and drain through an exit hole in a bottom corner of the hopper.

Experiments show that, after the pile has developed in the hopper, a segregation phenomenon is observed where the larger particles form a diagonal layer on the outside of the pile above the exit hole. Further toward the center of the hopper, above the exit hole, a layer of small particles forms, so that the mixture that drains from the hopper is segregated. Under some circumstances, this effect can even be employed to provide an effective method of separating the two sorts of particles.

The previous model which is of the most relevance here is that of Jullien and Meakin [8]. They considered the buildup of a two-species sand pile with particles added one at a time and allowed to settle before the next particle is added. The particle falls vertically when not in contact with other particles or rolls in contact with other particles until it reaches a local minimum. Once a particle has come to rest it is not permitted to move again. In this model segregation was observed, with different characteristics from those shown here (principally because the large and small particles block the flow to different degrees). However, it is not clear how to generalize their model to unsteady motion and we shall pursue an alternative, unsteady, model here.

II. EXPERIMENTAL OBSERVATIONS AND THE CELLULAR-AUTOMATON RULES

In choosing the rules for our cellular-automaton model we draw heavily from experimental observations. The works of Halvorsen, Remnes, and Hyldmo [1] and Williams [10], in particular, give an indication of the physical mechanisms causing the segregation. They highlight three phenomena of particular importance, which are as follows.

(i) Flow occurs predominantly in a top layer near the surface of the growing pile. This layer is only a few particles deep and the particles within it experience large velocity gradients. The smaller, less flowable, particles separate downward and join the slower flow in the center of the heap while the larger particles flow rapidly along the surface.

(ii) In the internal flow there is a general percolation of the smaller particles through the relatively immobile larger particles.

(iii) Also in the internal flow the motion is governed more by the stresses experienced by the particles than by motion under gravity.

These phenomena create segregation patterns such as that shown in Fig. 1. Here we can see the segregation resulting in the larger particles lying at or near the surface. There are larger areas which contain mostly small particles and others in which the two sizes are of roughly equal proportion. A film of the filling of these hoppers also shows the rapid movement of the larger particles over the surface of the heap and the much slower flow of both sizes of particles in the interior.

Since our model is for a close-packed material, the stress at a point is evidently dependent upon properties of the flow (as for a continuum). At least two simple representations for this stress suggest themselves, both of them appealing because they make the problem more tractable. First, by analogy with hyperbolic models for plasticity we could assume that the stress at a point depends only on the mass of particles above that point and within the sector bounded by the angle of friction. (In the three-dimensional case the sector would become a cone.) It is not expected that this model would give significantly different results from our second proposition which is as follows.

FIG. 1. An experimental rig showing particle segregation (kindly supplied by S. Halvorsen, Elkem a/s Ltd., Norway).

In the present work we ignore the effects of internal stresses and concentrate on the effects of the different mobilities of the two types of particles under different conditions within the pile. By analogy with continuum models for fluid flows we introduce a "hydrostatic pressure," defined at each point in the flow, which we take to be the total weight of particles in the column immediately above that point. This pressure then determines which type of particle prefers to move down to a point below.

Our cellular-automaton model starts with a square grid (the "hopper") with n_r rows and n_c columns. Each of the squares in the grid (the "sites") have unit volume. There is a general motion downward (with rules to be described shortly), but there is no flow out of the sidewalls or out of the bottom except at designated exit holes. Particles are input over a given range of sites at the top of the array.

Definitions. Input details: i and j represent the labels of rows and columns; α represents the volume of large particles; β represents the volume of small particles ($0<\beta<\alpha<1$); and n_r and n_c represent the number of rows and columns in the hopper. Calculational details: M_{ij} and N_{ij} represent the number of large, small particles in box (i,j); $V_{ij}=1-\alpha M_{ij}-\beta N_{ij}$, the volume of the box (i,j) unfilled;

$$P_{ij}=(1/n_r)\sum_{k=j+1}^{n^*_{i,j}}(\alpha M_{ik}+\beta N_{ik})\,;$$

$$n^*_{i,j}=\min_{k\geq j+1}\{n_r\}\cup\{k:\ M_{ik}=N_{ik}=0\}\,,$$

R represents a uniformly distributed random variable in [0,1] (chosen afresh each call); S represents a random integer $-1,0,1$ with probabilities $\frac{1}{4},\frac{1}{2},\frac{1}{4}$ (chosen afresh each call); and $f(x)=\alpha^2[1-(\beta/\alpha)^{2x}]/(\alpha^2-\beta^2)$.

Rules. We begin with an empty hopper ($V_{ij}=1$).

(1) Add particles in prescribed number to the openings in the top row.

(2) Move to bottom row and remove all particles (if any) from each exit site.

(3) Move up one row and, unless this is now the top row [in which case return to (1)], order the sites in this row randomly.

(4) Following this random ordering for the sites, work along the row performing the following redistribution of particles, until the last site in this row has been dealt with in which case return to (3).

(5) If $V_{ij}>\alpha$ (i.e., there is room for a large particle) and there are large or small particles available from the three sites above (immediately above and above diagonally) (or only two sites if the site is at the end of a row), then take one particle from site $(i+S,j+1)$ and place it in site (i,j), preferring to take a large particle if $f(P_{ij})<R$ and small otherwise. If the chosen site for removal does not

contain such a particle (either it only contains the other size or contains no particle at all), then choose another of the three sites above, again at random. Repeat from (5) until $V_{ij} < \alpha$, then go to (6). If there are no particles in any of the three sites above return to (4), choosing the new site to receive more particles.

(6) If $V_{ij} > \beta$ (i.e., there is room for a small particle) and there are small particles available from one or more of the three sites above, then take one small particle from site $(i+S, j+1)$ and place it in site (i,j). If the chosen site does not contain a small particle, then choose another of the three sites above. If there are no small particles available in any of the three sites above, then return to (4), choosing the new site to receive more particles.

These are the rules governing the behavior of the cellular automation. We note several points of importance. First, the rows are dealt with in order, starting at the bottom and working to the top. This mimics the action of gravity in only filling a site after particles have left that site. Second, the particles are more likely to move downward than diagonally, but cannot move sideways. Third, near the surface, where the pressure term P_{ij} is smallest, the large particles prefer to move, whereas in the interior, where the pressure is greater, the small particles are more mobile. Finally, unlike many cellular automata where the individual cells are updated simultaneously, the present model uses a sequential updating with randomness playing a major role.

The function $f(P_{ij})$ determines how the particle mobility depends upon the pressure. Observe that our chosen function has the properties (i) $0 \le f(x) \le 1$ for $0 \le x \le 1$ with (ii) $f(0)=0$, (iii) $f(1)=1$, and (iv) $f(\frac{1}{2})=\alpha/(\alpha+\beta)$. These signify that (i) $f(x)$ is a probability (for a small to move instead of a large), (ii) only large particles move at the surface, (iii) only small particles move deep inside, and (iv) at a typical depth the expected volume transfer is the same for large and small particles (i.e., the relative probabilities for the two sizes to move is the inverse ratio of their volumes).

We have referred to our model as a "cellular automaton." However, the strict use of this phrase would imply a totally deterministic model. That is, starting from the same initial conditions we would expect the same final outcome. It can be seen that randomness plays a large part in our model, in the decision about the order in which the cells are updated, the choice of site from which to remove particles, and the size of the particle to be moved. We can justify our approach by observing that ours is an attempt to model a genuinely unsteady phenomenon. We must either have a model for the order in which to update the sites (which will be numerically very expensive, but more satisfactory) up update all sites simultaneously (cheap numerically, but which would here bear too close a resemblance to a numerical scheme for equations of continuum mechanics, e.g., the equations for semiconductor device modeling). We would ideally like to present a totally deterministic model (and indeed such models can be readily conceived); however, for the time being we accept the faults of our model. The gross features of segregation are not expected to depend sensitively upon the initial conditions and thus the randomness within our model will not be a cause for concern.

The validity of the "trickle-down" model that we employ depends in reality on the relative size of the wave speed of disturbances propagating through the granular flow compared to a typical particle speed. Inherent in our model is the assumption that this ratio is large, and if this is so, then clearly systematic updating from the bottom of the hopper is equivalent to updating at all sites simultaneously. In this case the role (and direction) of gravity is clearly very important; gravity cannot operate to fill a site until particle removal has taken place in order to provide the necessary space. This, of course, is the key difference between the flow of a granular material such as ours and the flow of a fluid; although agreement is virtually universal that a continuum model is appropriate for both flows, it is evident that if the base of the hopper were to be instantaneously closed, flow would cease immediately in the hopper. For these reasons, we feel confident that the approach we have used is valid.

III. RESULTS AND DISCUSSION

At this stage it is in order for us to mention the dimensionality of our model. Since the particles are constrained to move down or diagonally down we can adjust the "angle of friction" for the flow by adjusting the aspect ratio of the hopper. That is, although the actual ratio of hopper height to width might be 1, we would artificially rescale this aspect ratio by having more rows than columns, say. For a visual output the geometry would be returned to the correct aspect ratio, leaving an effective angle of friction of less than 45°. Once the aspect ratio has been fixed the position of the entry and exit holes determines the rest of the geometry. The number of rows (and columns) can then be increased (maintaining the same ratio) to improve detail. Next, the volumes of the large and small particles (α and β) can be adjusted. Lastly, the total volume of the input large and small particles can be chosen, but the effect of this on the end result is minor because of the buildup of the heap under the inlet holes and possible blockage for some geometries (nevertheless, these total volumes can be thought of as a way of varying the timescale of the motion). In all there are thus six degrees of freedom for a given geometry.

In Figs. 2 and 3 we see results of the cellular automaton.

Figure 2 shows a hopper of dimensions 100×100 with inlet over the top left 30 and outlet over the bottom right 20. The particles have sizes 0.1 and 0.05. Each mark represents a site at which the volume of large particles is greater than that of the small. Figures 2(a)–2(e) show the heap after 54, 100, 250, 500, and 1000 iterations, respectively. Note the uniformity of the size distribution during the initial transient period and the curvature of the surface. As time progresses and the distribution settles down we see the appearance of segregation and the straightening of the free surface. Note that after 1000 iterations the volume of small particles present in the hopper is 1375.25 and the volume of large particles is 943.4. The input ratio (of two small particles for every large) was maintained during the transient phase but

then, as segregation developed, settled down to a new steady state.

In Fig. 3 we show a slightly different geometry. Here dimensions are as before, but now the inlet is over sites 15–35 in the top and the outlets in sites 1–10 in the bottom row. Again the segregation can be seen very clearly. This geometry shows the combined effects of segregation at the free surface (at the right-hand side) and that emanating from the outlet (the left-hand side). The input volume ratio of large to small particles is 1:1, but the ratio retained in the hopper is, after 1000 iterations, 0.87. As well as the segregation near the two free surfaces one can see evidence of the dominance of large particles towards the bottom right corner.

Quantitative information concerning the process of segregation may also be determined using our model. A run was performed with a similar geometry to that of Fig. 2, but with inlets over the top left 80 sites. In Fig. 4 we see the total volume of each of the large and small particles leaving from the outlets 81–100. The volume of small particles is very nearly monotonic with most particles leaving from the outlet closest to the slope and away from the wall. The volume of large particles shows a pronounced peak at around exits 84–85. There is clearly some scope for design of the geometry to take advantage of this effect as a means of particle segregation. In Fig. 5

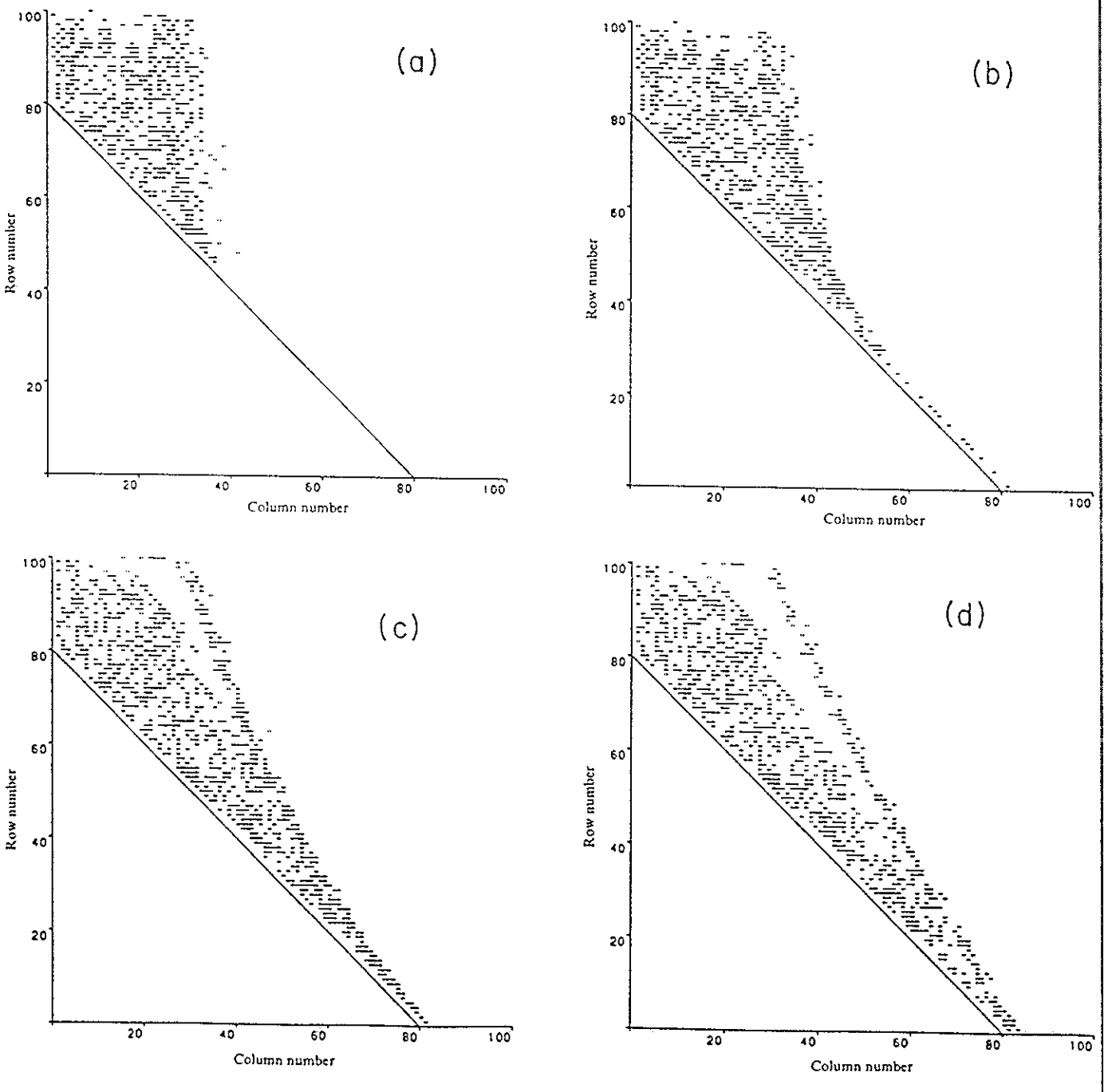

FIG. 2. Results of the automaton for a 100×100 hopper with inlets over the left-hand 30 sites and exits at the right-hand 20 sites. There is a fixed slope from top left to bottom right. Volume of the large particles is 0.1 and of the small particles it is 0.05. (a)–(d) show results after 54, 100, 250, 500, and 1000 iterations.

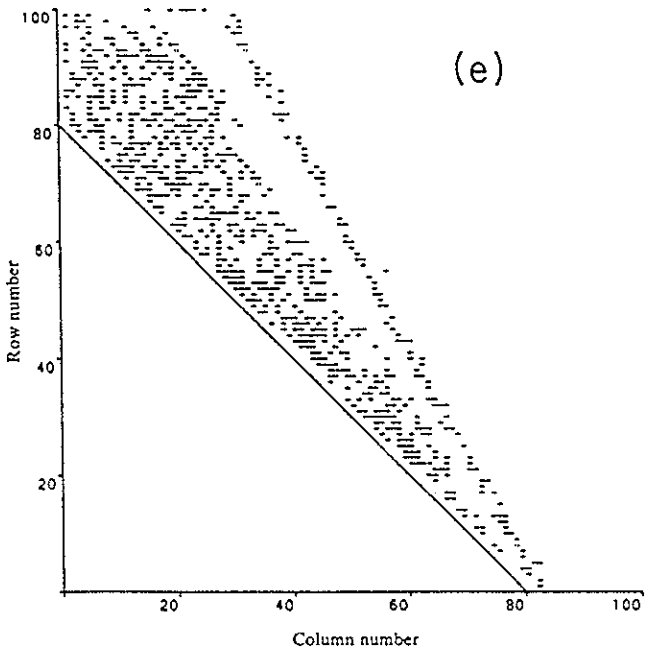

FIG. 2 (*Continued*).

we see the (moving five-iteration average of the) total volume of particles leaving the exit area against time. This average is consistently around the value 10, showing that only half of the exit area is being fully utilized.

As a test of the sensitivity of the results to our chosen rules of motion we made the following changes. First, we altered the pressure rule. Several alternatives were employed including $f(x)=\frac{1}{2}$, $\alpha/(\alpha+\beta)$, and x. The second of these corresponds to equal expected volume transport regardless of pressure and the third contains a simple pressure dependence. It was found that rules that incorporated a pressure dependence [that is, $f(x)$ not constant] were better at achieving segregation. Second, we changed the absolute values of α and β while maintaining their ratio constant. This was found not to make any qualitative difference until α became greater than about 0.5. At this point segregation began to appear virtually regardless of the pressure rule. The explanation of this is that only one large particle could be at a site at one time. These large particles formed a "lattice" through which

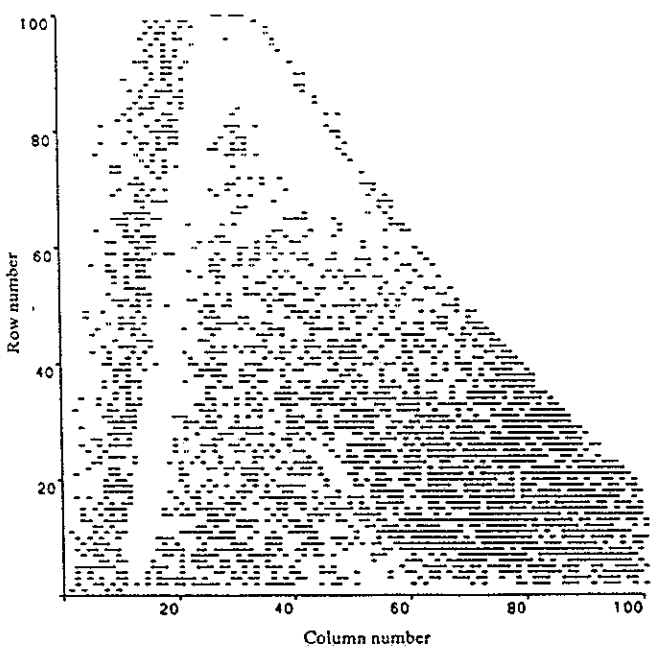

FIG. 3. Results of the automaton for a 100×100 hopper with inlets over the top 15–35 and exits over the left-hand ten. Volume of the large particles is 0.1 and of the small particles it is 0.05. Results after 1000 iterations.

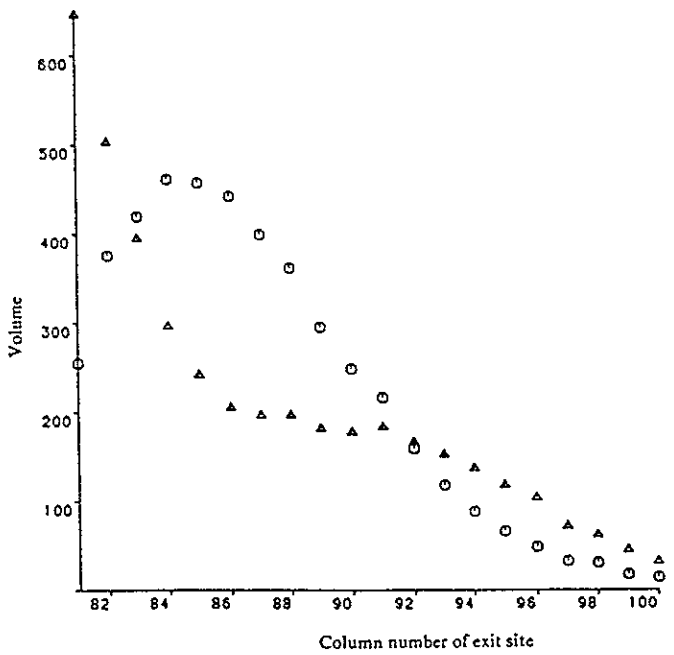

FIG. 4. Total volume of each of the large (○) and small (△) particles that have left each exit site after 1000 iterations. The particle sizes are the same as in other examples, the geometry is as in Fig. 2 but with input over the left-hand 80.

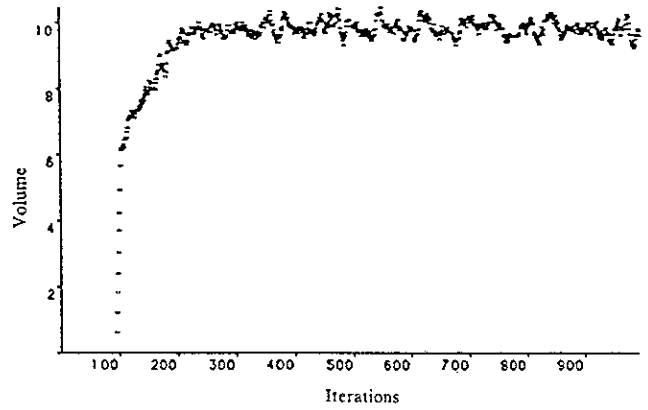

FIG. 5. Five iteration moving average of the volume of particles leaving the exit area at each iteration. The geometry is the same as in Fig. 4.

the small particles could move. The large particles could only move to a site off the free surface and very rapidly the flow segregated into three regions: interior lattice, with motion of small particles; interior compact, with slow motion of small particles and no large particles; and near surface, with rapid motion of large and small particles. This itself models an interesting phenomenon, but not one in which we are presently interested. Third, we dropped the rule that each site must be as full as possible before we move to the next site. This rule was changed so that the site must be at least half, three-quarters, and, finally, seven-eighths full on the odd iteration and then fully filled on the even iteration. This was an attempt to move closer to an "all-at-once" updating. No qualitative difference was found with this rule.

The above results, which show qualitative agreement with experiment, suggest that segregation is initiated in two ways. The first is obviously the free-surface effect which has been built into the model; large particles are more mobile when close to the surface. Second, it appears that the exit boundaries can mark the edge of regions of segregation. This is because, in the neighborhood of the exit, although the individual particles still obey the mobility-pressure rules, there is a much greater motion in general than higher up the pile. The segregation thus has a greater chance of being set up and maintained. An obvious design criterion that can be deduced from the present model is that, in order to segregate particles effectively, a number of small hoppers arranged in a cascade will be more efficient than a single hopper of the same size.

One of the motivations for creating a cellular-automaton model of the segregation process is to be able to test new hopper geometries prior to their construction. This will clearly be more cost effective than performing many experiments, especially if the hoppers are large and must be operated at high temperatures, as is often the case. If the model can be shown to be reliable and robust in test cases with simple geometries, then there will be confidence in designing more sophisticated hoppers. Future work will be aimed at comparison with test cases in order to determine the parameters in the model and make improvements to its underlying structure.

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