Molecular dynamics studies of grain segregation in sheared flow

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Size segregation is a widely observed consequence of sheared flow in granular media, in which the larger grains rise to the upper surface of the bulk, despite the fact that all grains have the same material density. A two-dimensional molecular dynamics study of the phenomenon is described in this paper. The grains are represented by inelastic disks and the flow occurs down an inclined slope with a rough base. The simulations readily reproduce the segregation effect; the results of a series of measurements of various aspects of this so-called ''inverse grading'' are reported. [S1063-651X(97)14008-9]

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I. INTRODUCTION

The vertical segregation that occurs in granular flow down an inclined chute involving a mixture of particle sizes is a well-known effect that arises both in nature and in industrial material processing [1]. The simplest case to analyze is one in which all the grains are uniform in composition, but are of two or more distinct sizes. The larger grains are found to rise to the top of the flowing bulk, while the smaller grains sink downwards. In many processes this phenomenon is an important mechanism for separating grains of different sizes, but in other instances it can prove to be an undesirable effect since it destroys the compositional homogeneity of the mixture. In this class of system it is the gravitationally driven sheared flow that is responsible for the inverse size grading, but similar effects are observed under the influence of vertical vibration — the so-called ''Brazil nut'' effect [2].

This fascinating, almost counterintuitive behavior—which has no counterpart on the atomic scale—has attracted considerable attention from a numerical modeling point of view. Most of the emphasis has been on the vibration-driven segregation effect, with a variety of methods being employed, ranging from geometrical [3] and topological [4] analysis, through Monte Carlo simulation [2,5], to molecular dynamics studies [6,7]; the role of convection in this phenomenon has been studied experimentally [8], and detailed photographic analysis used to explore the actual particle trajectories [9]. Segregation under the influence of steady shear flow has attracted far less attention [10], and we are unaware of any detailed quantitative simulations of this particular class of phenomena. Yet another class of sheared flow that leads to size segregation occurs in a rotating drum [11].

In this paper we describe a series of simulations of the kind of shear-driven segregation that occurs during flow down an inclined chute. The simulations are based on a ''soft-disk'' model for two-dimensional grains, in which normal and transverse velocity-dependent forces are used to model the inelastic collisions and impede the shear motion. The study focuses on the behavior of a comparatively small number of large grains submerged in a ''sea'' of smaller grains of either fixed or randomly distributed sizes. Various factors affecting the rate at which size segregation occurs and the degree of completeness of the separation process are examined, including the chute inclination angle, the role of rotational motion and shear damping forces, and the relative sizes of the large and small disks.

II. BACKGROUND

The fact that the motion of individual grains under shear is extremely complex is evident from laboratory studies that permit full visualization of a system of identical spherical ''grains'' (actually small spheres) confined between vertical walls and flowing along an inclined rough bed, in what amounts to a two-dimensional experiment [12]. The material appears to divide into several zones parallel to the flow direction, with different kinds of behavior occurring in each zone. There are blocks of grains that move coherently over extended intervals of time, and blocks that are seen to deform and/or merge. Clearly, such collectively organized behavior could serve to complicate the mechanisms underlying shear segregation when mixed grain sizes are present.

Some aspects of this complex behavior were already apparent in a previous molecular dynamics study of chute flow [13], but this work was confined to grains of a single size. Direct comparison between experiment and simulation [14] suggests that the simulation results tend to be relatively insensitive to the interaction model and the resultant grain stiffness, but are sensitive to a feature not normally incorporated in simulations, namely, the drag force arising from the interstitial fluid (this is typically air). A brief account of a discrete particle study of irregularly shaped granular mixtures exists [10], but there are few details given, and the segregation appears to be only partial.

The most detailed experimental study of size segregation in chute flows to date [1] describes a series of measurements which are then tested against the predictions of a mechanism proposed to explain the effect. The mechanism actually involves two processes. The first is associated with size-dependent void filling, a form of random ''sieve'' that favors the smaller grains falling downwards into any short-lived gaps between larger grains. The second process is called ''squeeze expulsion''; it does not prefer a particular grain size or direction of movement, but is the result of an imbalance between the instantaneous forces acting on the grains, and so leads to transverse motion in either direction. One quantitative prediction of this analysis concerns the height h of the lowest large grain in the mixture as a function of the

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downstream distance from its starting point x,

$$h = \alpha\sqrt{x}, \tag{1}$$

where α depends on the ratio of grain sizes, the slope, and other parameters of the problem. This formula only applies until segregation is complete, after which h is of course constant.

III. SIMULATION DETAILS

The model [10,15] for granular particles used in the present series of simulations is based on inelastically colliding soft disks. This kind of model, with minor variations of detail, is widely used in granular simulation work. The particular form used here is identical to that used in a recent study of discharge through a horizontal aperture (hopper flow) [16], but now generalized to allow for different grain sizes and masses.

The interaction that prevents overlap when grains collide is assumed (with some arbitrariness) to have the Lennard-Jones (LJ) form that is widely used in studies of fluids at the molecular level, with a cutoff at the point where the repulsive force is exactly zero:

$$\boldsymbol{f}^r_{ij} = \frac{48\epsilon}{r_{ij}}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \frac{1}{2}\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right]\hat{\boldsymbol{r}}_{ij} \tag{2}$$

for grains located at $\boldsymbol{r}_i$ and $\boldsymbol{r}_j$, where $\boldsymbol{r}_{ij} = \boldsymbol{r}_i - \boldsymbol{r}_j$, $r_{ij} = |\boldsymbol{r}_{ij}|$, and $\sigma_{ij} = (\sigma_i + \sigma_j)/2$. The interaction cutoff occurs at $r_{ij} = 2^{1/6}\sigma_{ij}$, so that $2^{1/6}\sigma_i$ is essentially the "diameter" of grain i, although since the grains possess a certain degree of softness this is not a precisely defined quantity. The LJ interaction is strongly repulsive at small r_{ij}, more so than the linear overlap or Hertzian-type repulsions used in other granular simulations. For convenience, we use reduced units in which the energy is expressed in terms of ϵ, length in terms of the value of the diameter of the smaller grains (or in the case of a mixture of small grain sizes, the largest of the small diameters), and mass is defined so that a grain with unit diameter (in reduced units) has unit mass as well.

Normal and transverse viscous damping forces [10,15] are introduced to produce inelastic collisions and inhibit sliding motion. The normal component is

$$\boldsymbol{f}^n_{ij} = -\gamma_n \dot{\boldsymbol{r}}_{ij}\cdot\hat{\boldsymbol{r}}_{ij}, \tag{3}$$

where γ_n is the normal damping coefficient. The transverse component is

$$\boldsymbol{f}^s_{ij} = -\mathrm{sgn}(v^s_{ij})\min(\mu|f^r_{ij} + f^n_{ij}|, \gamma_s|v^s_{ij}|)\hat{\boldsymbol{s}}_{ij}, \tag{4}$$

where

$$v^s_{ij} = \dot{\boldsymbol{r}}_{ij}\cdot\hat{\boldsymbol{s}}_{ij} + r_{ij}(\sigma_i\omega_i + \sigma_j\omega_j)/(\sigma_i + \sigma_j) \tag{5}$$

is the relative tangential velocity of the disks at their closest point, $\hat{\boldsymbol{s}}_{ij} = \hat{\boldsymbol{z}}\times\hat{\boldsymbol{r}}_{ij}$ is a unit vector tangential to the disks at this point ($\hat{\boldsymbol{z}}$ is the unit normal to the plane of the simulation), ω_i and ω_j are the angular velocities, and γ_s is the transverse damping coefficient. The static friction coefficient μ appears as part of an upper bound—based on the Coulomb criterion—imposed on the transverse force. Numerical values for the various parameters are the same as those used previously [16], namely, $\mu = 0.5$ and $\gamma_s = \gamma_n = 100$. The strength of the gravitational acceleration driving the flow, g, must be chosen so that the limiting flow speed is not too large, but at the same time it must be sufficient to ensure that the bottom layer of the material remains in close contact with the rough base of the chute for the range of inclination angles considered; the value $g = 10$ was found to satisfy both criteria.

The nature of the base of the chute is of particular importance, since it is responsible for ensuring that minimal or zero slip occurs in the bottom layer of grains. The base is constructed from a row of fixed disks with similar properties to those of the smaller grains, except that the diameter is reduced by 1/3; these disks are uniformly spaced sufficiently far apart (the separation is chosen to be 1.1 times the diameter) to achieve the effect of a corrugated boundary, but not so far apart that other grains are able to penetrate the wall. In the direction of flow periodic boundaries are used to recycle the grains. The upper boundary is remotely located so that the grains will not normally feel its presence; it serves (mainly at the start of the run) to elastically reflect the occasional high-flying grain back into the simulation region.

Given the form of the normal and tangential forces acting on each of the disks, formulating the remainder of the molecular dynamics computation is a straightforward matter [17]. The translational and rotational equations of motion are solved numerically using the leapfrog method, with an integration timestep $\Delta t = 10^{-3}$. The neighbor list technique is used to reduce the computational effort to a level proportional to the number of grains.

The initial positions of the grains are chosen randomly with the chute placed in a horizontal position. The grains are allowed to reach a steady state after falling under the influence of gravity over an interval of 2×10^4 timesteps. At the end of this relaxation period the entire system is rotated to the desired inclination angle—in practice by changing the direction of the gravitational field—and the flow measurements commence.

IV. RESULTS

A. Size segregation

We consider a two-dimensional system containing 2000 small circular grains, together with 20 larger grains made of material having the same density, but with double the diameter. The total chute length is 75 (in reduced units), and once the flow has settled into a relatively steady state the height of the upper surface is approximately 30 units.

Figure 1 shows how the average height of the large grains varies with time, for a series of different chute inclination angles β. It is immediately apparent that not only does size segregation occur, but that (except for the smallest β) the segregation process proceeds to completion. The large grains rise at a reasonably steady rate (on average) to what is essentially the maximum height possible, namely, the measured height of the material surface. The greater the inclination, the faster the segregation process.

To demonstrate that all large grains rise to the upper surface, or very close to it, Fig. 2 shows the time dependence of

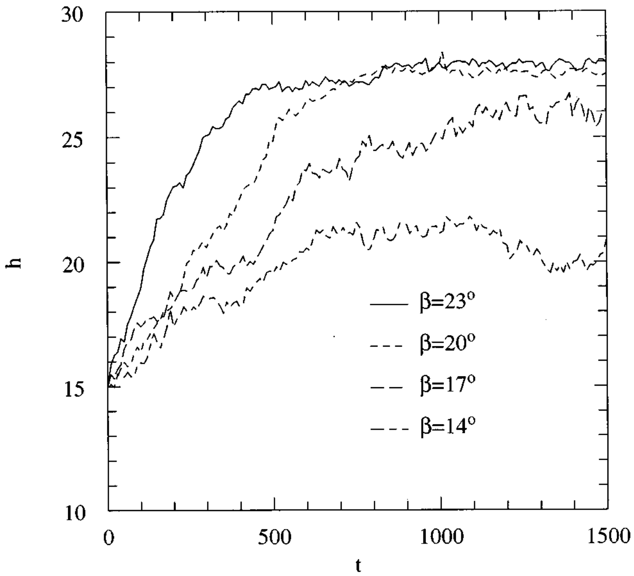

FIG. 1. Time dependence of the mean height of the large grains (in reduced units) for different chute inclinations β.

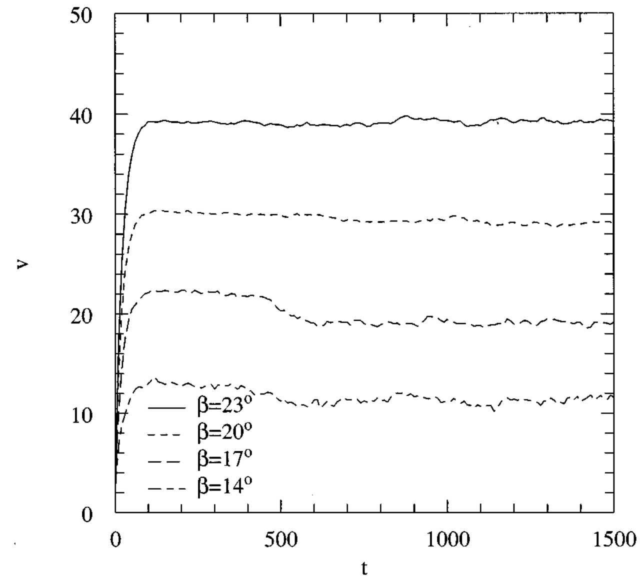

FIG. 3. Time dependence of the average flow speed (all grains are included).

the mean and minimum heights of the large grains for one particular value of β. From this result and from examination of snapshots of actual grain positions (see below), it is clear that while not all large grains ascend at the same rate (because of the way the initial state is constructed, not all large grains start at the same height), they all eventually climb to the top.

The majority of the segregation process takes place after the flow rate has reached its final steady value. Figure 3 shows the time dependence of the average flow speed— both large and small grains are included—for several chute inclinations: The flow is seen to reach its limiting value relatively quickly, well before segregation is complete. This leads to the conclusion that the faster the flow and, consequently, the larger the shear rate, the more rapid the segregation. (The need for periodic boundaries is also evident from these results; the flow rates imply that over the course of the run a typical grain will cycle through the system numerous times.)

In Fig. 4 we show the average height of the large grains as a function of the average downstream distance traversed by the grains, for different values of β; larger β leads to earlier separation, although there is little difference between the results for the two smaller β values. The large-β results include a fit to Eq. (1), although this is not a particularly convincing result; improved statistics from repeated runs—especially at the smaller β values where the ascent rate is more gradual—would be required to establish whether this

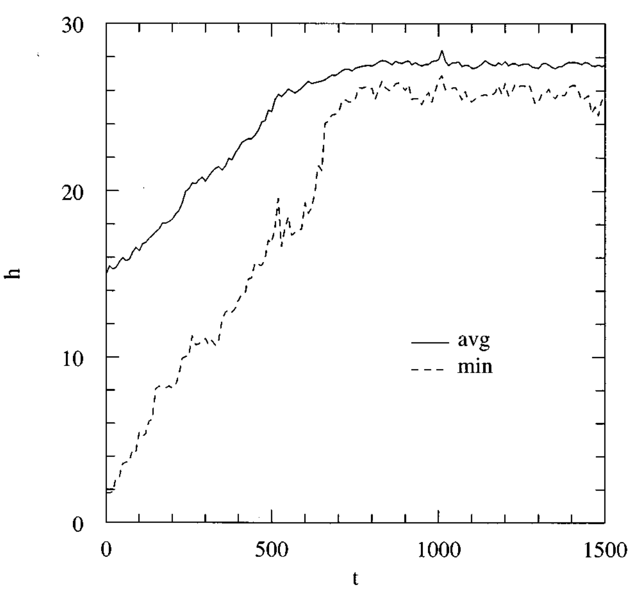

FIG. 2. Time dependence of the mean and minimum heights of the large grains for $\beta = 20°$.

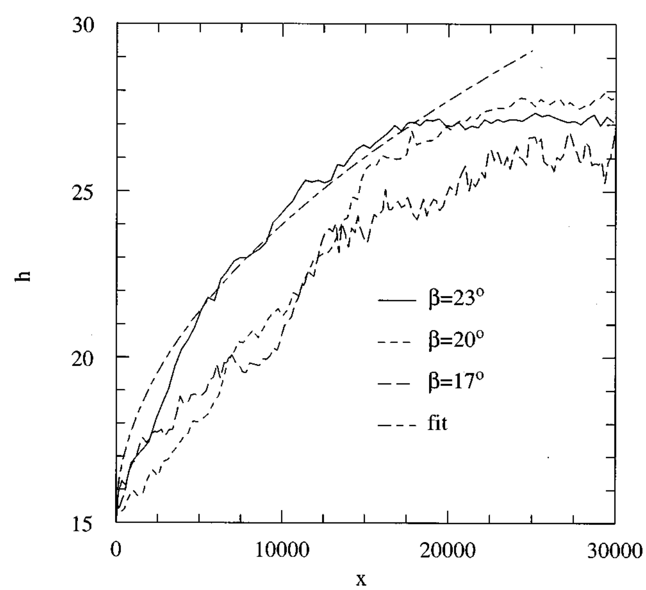

FIG. 4. Dependence of the mean height of the large grains on the average downstream distance moved by the material (the fit is discussed in the text).

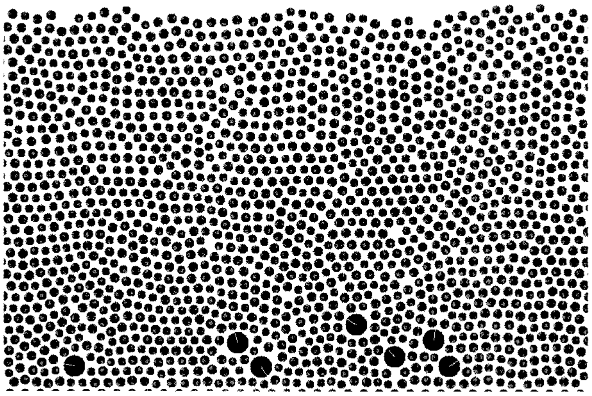

FIG. 5. Snapshot showing system during the early stage of a run (in this case the large grains start close to the bottom and the smaller grains have mixed sizes); gravitational acceleration is directed towards the lower-right corner ($\beta = 17°$).

formula correctly represents the behavior. The dependence on inclination angle predicted in [1] is not observed here, although the experimental system on which this theoretical prediction was tested consisted mainly of large grains— exactly the opposite of the case here—and this could explain the difference.

Finally, since actual images of the segregation process provide the most satisfying evidence of what is occurring, Figs. 5 and 6 show snapshots of two stages in a particular simulation run with $\beta = 17°$. Unlike the runs described so far, where the small grains are monodisperse, here the smaller grains have a range of randomly distributed sizes; a system of this type will be examined later in the paper. Furthermore, this run involves a different means of constructing the initial state in which the large grains are all positioned close to the base of the chute. The first of the two images (Fig. 5) shows the situation early in the run. The second (Fig. 6) shows how the large grains have all risen; some have succeeded in traveling all the way to the top, while the others have completed most of the ascent and continue to rise as the simulation proceeds further.

B. Factors affecting segregation rate

Shear rate is just one of the elements influencing the rate at which segregation occurs. The details of the model, as well as the other parameters defining the physical problem, can also affect the separation rate. The first of these factors we investigate here is the role of rotational motion and the transverse viscous damping force that accompanies it. The actual question is whether segregation can occur at all in the absence of transverse damping, if the only dissipation that occurs in the system is due to the normal damping force. If the transverse force is absent, there is no coupling between the translational and rotational motion, and so the latter degrees of freedom can be omitted from the calculation.

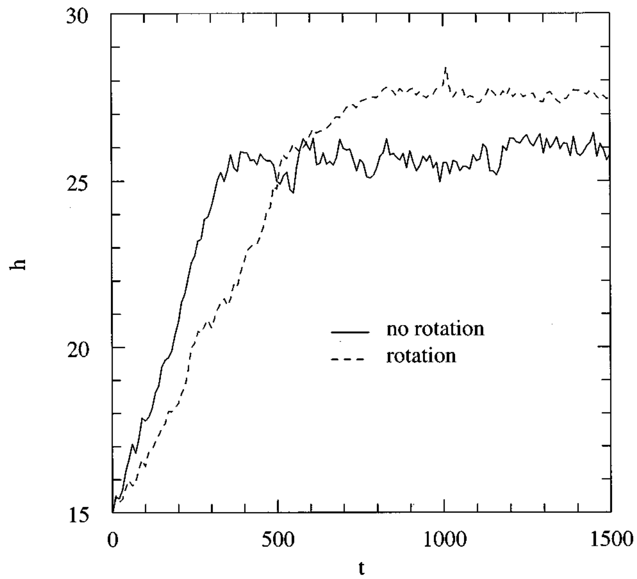

FIG. 7. Time dependence of the large grain mean height, with and without rotation ($\beta = 20°$).

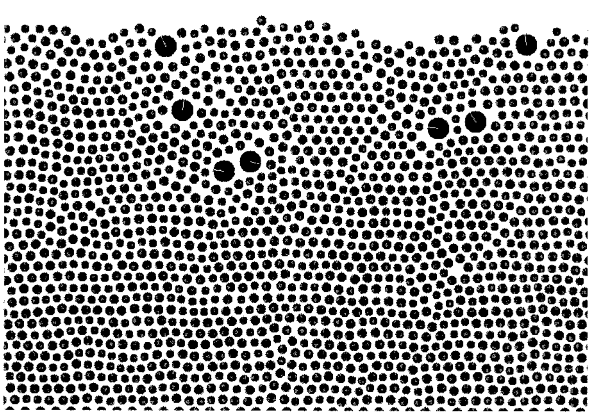

FIG. 6. The same system at a later time showing how the large grains have either reached the upper surface or are approaching it.

Figure 7 provides at least a part of the answer. Complete size segregation occurs in both cases and, at least at first sight, it even appears to occur more rapidly in the absence of rotational motion. Thus the need for grains to roll over one another turns out not to be an essential part of the segregation mechanism.

However, in determining the speed of the segregation process it is important to ensure a fair basis for the comparison. So while it might appear from Fig. 7 that segregation is retarded by the presence of rotation in the dynamics, this is not the entire story. In Fig. 8 we show the time dependence of the overall mean flow velocity, with and without the inclusion of grain rotation. As might be expected, the final flow speed is substantially higher without rotation and the concomitant transverse damping force.

The information in these two figures can now be combined to produce Fig. 9; this shows the flow speed in terms of the mean height of the large grains (note that time advances at an uneven rate along the curves themselves). The two curves overlap until the system with rotation reaches its final flow speed. This provides an indication that the rate of climb of the large grains is associated with the prevailing shear rate; the presence or absence of rotational motion has only an indirect influence through its control of the shear rate. A large grain attempting to ''climb'' over a smaller neighbor just ahead of it does not appear to be aided by the ability to roll (although in real, irregularly shaped granular materials this will be unavoidable).

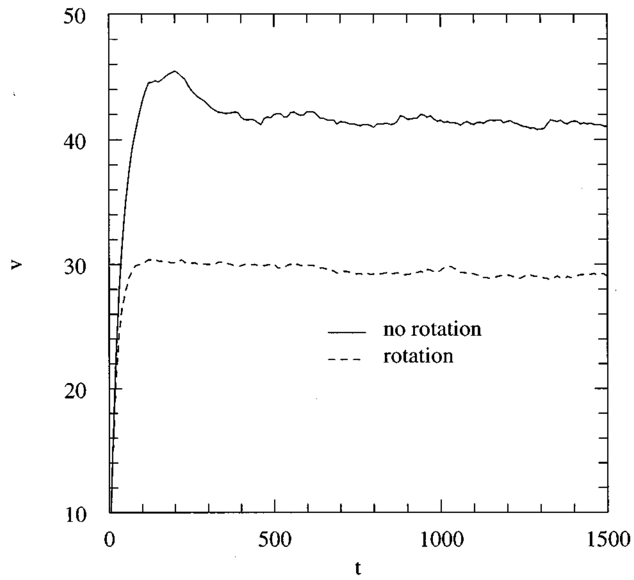

FIG. 8. Time dependence of the flow velocity, with and without rotation.

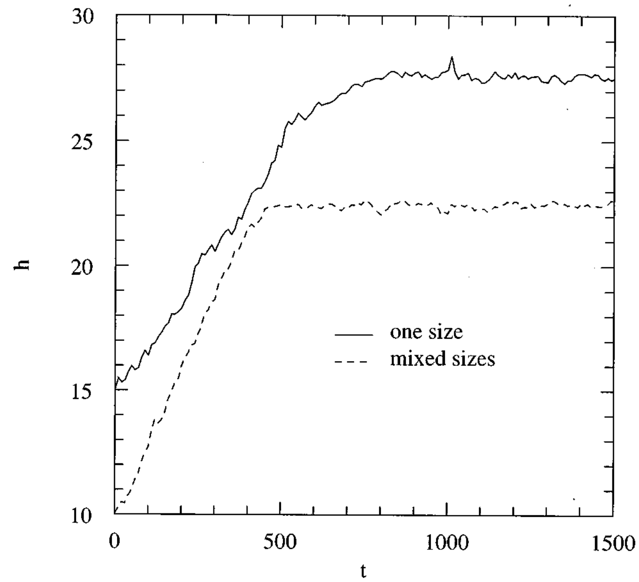

FIG. 10. Time dependence of the large grain mean height for constant and mixed small grain sizes ($\beta=20°$).

A somewhat more realistic system is one in which the small grains are of mixed sizes (as shown in the snapshots earlier); such polydispersity also helps avoid any tendency for the grains to pack into ordered layers, which could influence the segregation process in some unexpected manner. Figure 10 shows an example of measurements made in a system where the small grains have a random range of diameters uniformly distributed between 0.75 and 1 (reduced units). The results are essentially the same as before. The segregation occurs slightly more rapidly (as measured by the initial gradients of the curves) because of the increased relative size of the large grains with respect to the average size of the small grains; the fact that the surface height is reduced because the overall mean grain size is smaller also aids in more rapid completion of the process.

Since the relative grain size D influences the segregation rate, the manner in which the rate depends on this ratio can also be studied. We have carried out a preliminary examination of the effect of increasing the large grain size in a system containing identical small grains. Figure 11 shows the rate at which a single large grain rises as a function of D. For $D=2$ (the diameter ratio employed in the preceding results) the behavior is subject to large fluctuations, but as the size disparity increases the climb rate becomes more rapid and practically linear with time. Study of a single large grain, as

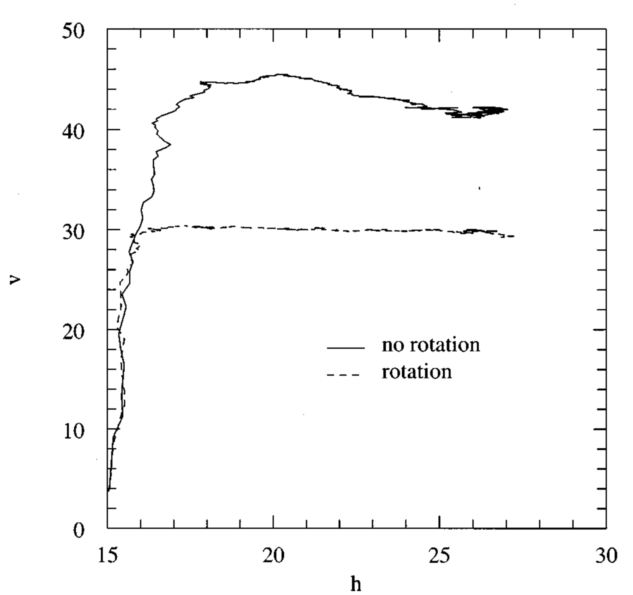

FIG. 9. Flow velocity as a function of the large grain mean height, with and without rotation; note that time advances at an uneven rate along each curve.

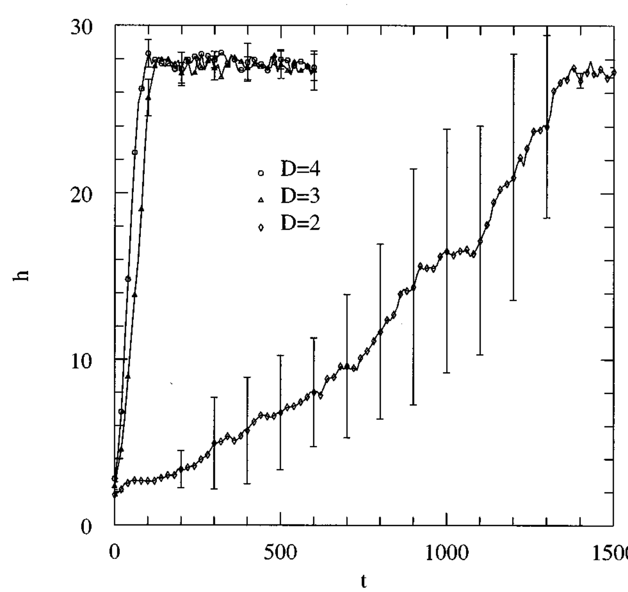

FIG. 11. Time dependence of the height of a single large grain for different size ratios D; the error bars reflect the spread of values over separate runs.

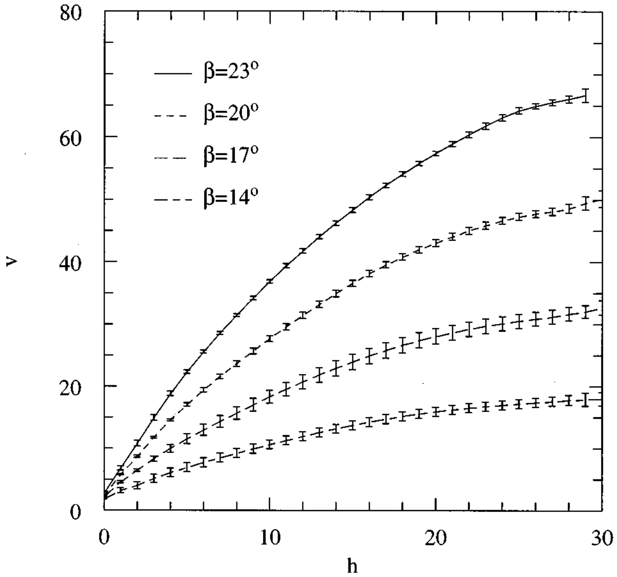

FIG. 12. Height dependence of the layer-averaged flow speed for different chute slopes β.

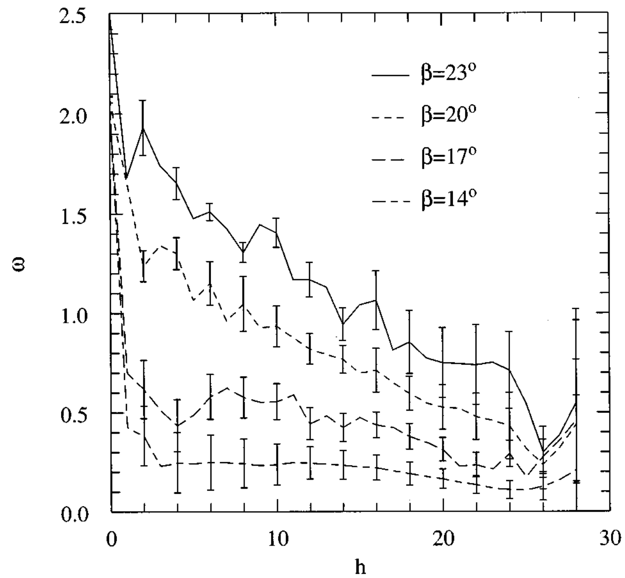

FIG. 13. Height dependence of the layer-averaged angular velocity for different slopes.

is the case here, eliminates any potential interference between large grains that might affect the conclusions; consequently, the statistics are significantly poorer and multiple runs are needed to produce results of a similar quality to those shown earlier (which were based on systems containing 20 large grains). At some value of D between 2 and 3 there is a crossover from a fluctuating to an essentially monotonic ascent rate. A more detailed study of the relationship between segregation rate and relative grain size is in progress; however, the fact that the shear rate varies with depth (see below) complicates the analysis.

C. Cross-flow profiles

Further details of the nature of the flow emerge from the cross-flow profiles of the linear and angular velocities, and the dependence of these results on the chute angle β. The flow velocity profiles shown in Fig. 12 reveal the way flow varies between horizontal (more precisely, parallel to the flow direction) layers; the measurements are based on averages over 1000 samples of 2000 time steps each. The flow speed close to the base of the chute is practically zero, and the shear rate (the gradient of the curve) falls off monotonically with height in each case. The form of the curves tends to suggest that when each is divided by the corresponding limiting flow speed that can be obtained from Fig. 3 the profiles might all collapse onto a single universal curve; unfortunately, the actual results reveal systematic deviations that preclude such behavior. As alluded to above, the fact that the shear rate varies with height makes it difficult to relate the ascent rate (Fig. 1) to the flow rate.

The angular velocity profiles shown in Fig. 13 are subject to considerable noise, despite the length of the runs (2×10^6 time steps) used for the measurements. The overall trend is for a relatively large angular velocity close to the corrugated base, an indication that rolling is an important contributor to the motion in the lowest layer of material. The value then drops — although the nature of the height dependence seems to depend on chute inclination (and thus on the flow speed) — and finally there is a sudden increase associated with the motion of grains that are at or very near the upper surface.

Comparison of Figs. 12 and 13 provides further information about trends in behavior. For a given h between 10 and 20 (approximately) the layer-averaged speed v and the angular velocity ω appear to grow at about the same rate with β. Furthermore, for each β, both the gradient dv/dh and ω exhibit a similar h dependence, although the former is seen to be larger. These results are consistent with the observed particle motion, which is a combination of rotation and sliding; both of these components increase in value as the overall flow rate increases. The behavior observed here has nothing to do with mixed grain sizes, but is an example of the complex nature of the collective dynamics (which turns out to be considerably more complicated than implied by these graphs) noted previously in both experimental [12,18] and simulational [13] studies of sheared granular flow.

V. SUMMARY AND CONCLUSIONS

The simulations described in this paper focus on the phenomenon of size segregation that occurs in sheared granular flow. The principal result is that the effect can be readily observed in a relatively simple granular model. Various aspects of the behavior have been examined in the course of a series of simulations, including the dependence of the segregation rate on the flow speed (which depends, in turn, on the chute inclination) and on the relative grain size, as well as on the presence or absence of the transverse frictional damping force (and the accompanying rotational motion). The fact that transverse damping is not required to achieve segregation is unexpected, although since such a situation does not occur in nature it is of little practical consequence; apparently, only the normal damping force is required to suppress the random local (‘‘thermal’’) velocities that would otherwise develop as a result of the gravitationally generated shearing, and the transverse force is incidental to the process.

The quantitative aspects of segregation have only been probed in a preliminary fashion, with more extensive simulations being required to establish the precise dependence of the behavior on the flow parameters. The results clearly show that segregation is faster for larger differences in grain size, as well as for greater shear rates. Determining the dependence in a more accurate manner is made difficult by (a) the fact that over the range of grain sizes of interest the behavior switches from a slow intermittent ascent mode to one that is monotonic and fast and (b) the varying local shear rates (as well as the more complicated local flow patterns) encountered by a large grain during its ascent. Both these observations imply that the task of quantifying the relationship between the segregation rate and the characteristics of the flow will not be a simple one; hopefully, more extensive simulational studies of this system will help clarify these issues.

ACKNOWLEDGMENT

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