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Simulations on Size Segregation: Geometrical Effects in the Absence of Convection

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Abstract. — Using a modification of an algorithm introduced by Rosato *et al.*, we study the segregation behaviour of a vibrated container filled with monodisperse discs and one large intruder disc. We observe size segregation on time scales comparable to experimental observations. The large disc rises with a size dependent velocity. For size ratios smaller than a critical value we find metastable positions during the ascent, in agreement with geometrical arguments by Duran *et al.* This confirms the importance of geometry as one of the possible causes for size segregation. We relate our results to recent experiments and discuss the mechanisms active in size segregation in the absence of convection.

1. Introduction

The investigation of the behaviour of noncohesive granular materials has received quite a lot of interest in the last years [1]. Powder processing is of great practical importance and furthermore, granular media show striking properties of both theoretical and experimental interest. One feature of the behaviour of granular materials which is usually considered annoying in industrial processes is size segregation [2–4]. The demixing of multidisperse powders, where the large particles rise to the top, occurs in shear flow as well as in vibrated powders. The latter is the effect we study in the present work.

Recently, there has been a vivid discussion on the question whether size segregation in vibrated powders might only be due to convection, another phenomenon widely observed in granular materials. This would imply that segregation should be regarded as being a secondary effect rather than a distinct phenomenon [5,6]. In systems where strong convective motion takes place, convection certainly is the dominating driving force for segregation [5]. In a vibrated container with rough vertical walls, large particles move to the top together with the small

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ones, due to the upward convective flux in the middle of the container. The small particles move down again, but the large particles stay at the top since they are not able to penetrate the rather dense array of small particles below them. In experimental setups, convection is initiated already for quite low values of the vibrational acceleration. For very small vibration intensities, convection is confined to a small region in the upper part of the container [7]. As has been shown experimentally [8,9], size segregation can be observed in this so-called quasi-static regime, too. We concentrate on it in the following.

It has been shown that geometric effects play an important role in size segregation in the quasi-static case [9]. Duran *et al.* [9] proposed a model for size segregation based on the evaluation of the positions that a large disc (or sphere) of radius R could take in a regular array of monodisperse small discs (or spheres) of radius r. In reference [9] a critical size ratio $\Phi_c = R/r$ ($\Phi_c = 12.9$ in 2D, $\Phi_c = 2.78$ in 3D) is deduced from these considerations. For size ratios below Φ_c the stable positions for the large disc are separated by some distance, whereas above this critical ratio they are continuous. From that one can conclude that the intruder should rise intermittently for small size ratios and continuously for size ratios $\Phi > \Phi_c$, a finding which is supported by experimental observations.

The existence of a critical size ratio below which no segregation is observed was discussed extensively [10,11]. Experiments by Duran *et al.* [8] show that a size ratio exists below which no ascent is observed within hours of experiment. The value of this critical size ratio was mentioned to depend on the shaking amplitude, the size of the container, and on the initial position of the particle. Size segregation was also related to the evidence of micro-fluctuations in the positions of the particles. Together with rough walls, that may lead to micro-cracks or long range block sliding in the bulk. A study of these phenomena in the 2D monodisperse case is presented in reference [12].

Quite a few computer simulations of shaken granular media exhibiting size segregation have been put forward, including Monte Carlo like simulation methods [13,14], molecular dynamics simulations [6,15] or sequential deposition models [16]. In this work we introduce an extension of the algorithm introduced by Rosato *et al.* [13] and discuss the physical relevance of the parameters used. The dependence of the ascent velocities of the large disc on the size ratio Φ is investigated and the mechanisms causing the ascent are discussed. We find good qualitative agreement with recent experiments [8], showing that size segregation occurs even without convection, only due to geometric effects.

2. Simulation Method

2.1. The Original Algorithm. — We first give a short description of the procedure as introduced in reference [13]. The algorithm is designed to model the motion of a 2-dimensional array of N hard discs in a vibrating container. Initially the discs are positioned at random inside the box and then they are allowed to relax by falling towards the bottom of the container, the details of which will be explained below. One period of the vibrational motion is modeled by first lifting all discs through some height A (called the shaking amplitude) without changing their horizontal positions. Secondly the discs are allowed to fall down. After relaxation has taken place the array is lifted again by A.

Thus the shaking of the container resembles distinct "taps" separated by long time intervals as used in reference [5]. Nevertheless, it should be possible to compare the simulations to experiments in which the vibration frequencies are higher, as long as the assembly of beads can relax sufficiently within one period.

In the simulation, the downward part of the vibration cycle is realized as follows. A disc is selected randomly and a trial position for this disc is generated. If this new position leads to an overlap with another disc, the motion is rejected and the old position is kept: otherwise the disc is moved to the new position. After this the next disc is chosen at random until a specified number of trials $n_{\max}$ are rejected ($n_{\max} = N$ in Ref. [13]). The assembly is then considered as relaxed and a new shaking cycle starts.

The trial position for a disc is chosen by generating two independent and equally distributed random numbers $\xi_x \in [-1, 1]$ and $\xi_y \in [-1, 0]$. The new position (x', y') of a disc is then given by

$$x' = x + \xi_x \delta \tag{1}$$

$$y' = y + \xi_y \delta \tag{2}$$

where x and y denote the old horizontal and vertical position respectively. Note that the choice for the new position corresponds to downward motion with fluctuations in the horizontal direction. The parameter δ, which corresponds to the maximum step width for a disc, was set to $\delta = r$ in reference [13].

2.2. MODIFICATIONS OF THE ALGORITHM. — We introduce two modifications to the original algorithm. The first and less important of the two consists of allowing small upward motions of the discs in the falling part of the shaking cycle. The reason for this modification is the following. The Rosato algorithm models the fluctuations in the system by random displacement. Because the fluctuations stem from interparticle collisions, the algorithm should also allow upward motion in some cases. For this reason, we take $\xi_y \in [-1, \delta_o]$, where δ_o is some small number larger than zero. The value of δ_o should not be too large, either, since in that case motion might never cease in the system. From another point of view, δ_o might also be considered as some measure of the elasticity of the discs. Large δ_o values correspond to large fluctuations and thus to weak dissipation. However, it is unclear how δ_o is related to physical quantities like the coefficient of restitution. We take $\delta_o = 0.05$ in our simulations, which corresponds to only very slight upward motion and mainly makes it easier for the system to relax into a final state.

The second modification of the algorithm consists of choosing a much smaller value for the maximum displacement δ than in the original work. This changes the behaviour of the system significantly. To illustrate this, we performed simulations with values of δ ranging from $0.05r$ to $0.5r$. In all simulations referred to in this paper, we use $N = 500$ discs of radius r with one large disc of radius R, i. e. the intruder. The assembly was considered as relaxed when no move could be accomplished for $n_{\max} = 5N$ trials. Clearly, this does not provide equally good relaxation for different values of δ, since the larger δ, the more moves will be rejected. We chose the abovementioned value for $n_{\max}$ by shaking an assembly of discs and checking for which value of $n_{\max}$ the density of the assembly could not be increased significantly by increasing $n_{\max}$. These tests also showed that including the possibility for the discs to move upwards substantially enhanced the relaxation of the assembly. The value $n_{\max}$ we finally adopted showed reasonable relaxation for the whole range of δ used here, although it was best for the smallest values. We should mention here that although the algorithm does not provide explicitly for rolling of discs on each other, discs on the surface always "roll" into a local minimum by a succession of Monte Carlo steps for our choice of parameters.

The initial configuration in these simulations was provided for as described above for the original algorithm, i. e. the large disc was placed at some height above the bottom of the container, then random positions were chosen for the background discs (see [13]) This configuration was then allowed to relax in the same way as in a normal shaking cycle, after which the shaking procedure started.

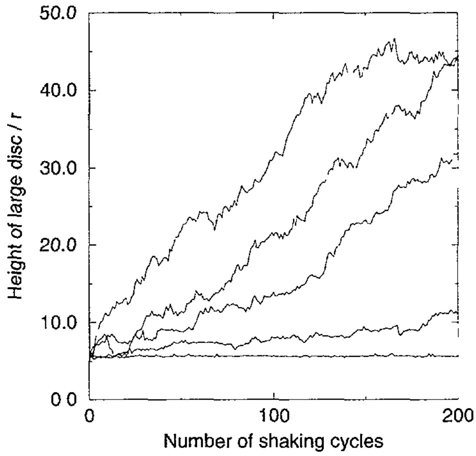

Fig. 1. — Influence of the choice of δ on the speed of ascent of a large disc of $\Phi = 2$ in simulations with $A = 2r$. The corresponding values of δ are (from top to bottom) $0.5, 0.3, 0.2, 0.1, 0.05$.

Figure 1 shows the strong dependence of the speed of ascent for an intruder of size ratio $\Phi = 2$ on δ. "Speed" is to be understood in terms of height per shaking period. The period is the only time scale defined in this kind of simulation. For small values of δ it even looks questionable if the large disc rises at all.

The parameter δ determines how much the whole assembly can expand during the falling part of the shaking cycle. The larger δ, the more it expands and thus larger relative motions of the discs are possible. In experiments it was observed that in the quasi-static situation the discs move nearly as a solid block with only small fluctuations around their mean position in the assembly [8]. Unfortunately, no data on these fluctuations are available. Thus, so far it is impossible to relate δ directly to physical quantities. However, it should be set to a small value still sufficiently larger than zero to provide observable fluctuations around the mean positions of the discs in falling. We investigated the segregation behaviour of the system for $\delta = 0.1r$, which gives quite good agreement of our simulations with experimental results.

Because small values of δ make the simulations more time-consuming there are some limitations to the size of the system and to the maximum number of shaking cycles. The maximum size ratio we used was $\Phi = 12$, because for larger size ratios the number of small discs would have to be increased, leading to longer computation times.

In the following simulations the starting configuration was obtained differently from the procedure described above, in order to be in close agreement with the experiments of [8]. Instead of using a random initial configuration of small discs, the box was filled with small discs in a triangular pattern as regularly as possible, after first having placed the intruder at some well-defined height. For the larger intruders (i. e. $\Phi \geq 8$) this was usually chosen as $(\Phi + 1)r$. We will discuss the implications of this choice in the following section, as they are related to the mechanism of size segregation.

3. Results

3.1. The Mechanism of Size Segregation in the Quasi-Static Case. — In this section we describe in detail the mechanisms by which size segregation takes place in our simulations.

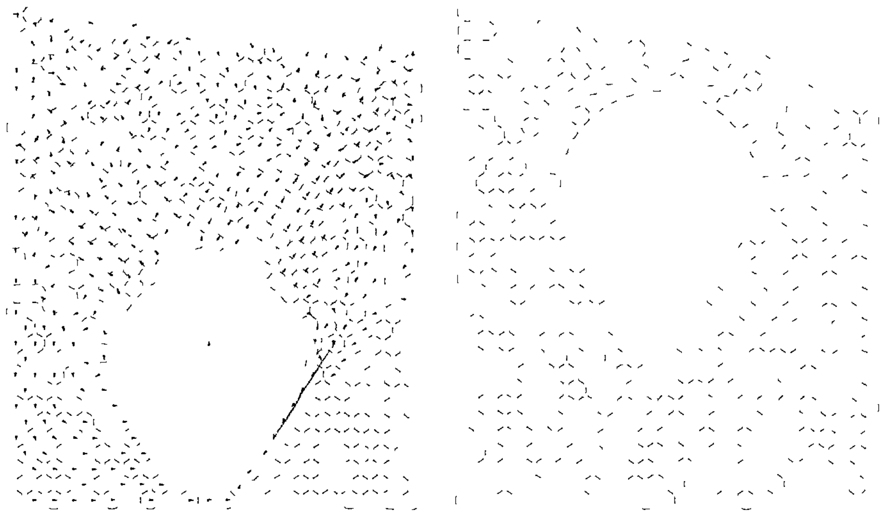

Fig. 2. — Snapshots of the ascent of an intruder ($\Phi = 10.5$, $A = 0.5r$). a) The circles denote the position of the discs after 445 shaking cycles, the arrows the final positions after 470 shaking cycles, always taken after complete relaxation of the assembly. b) Situation after 900 shaking cycles.

Besides, we discuss qualitatively the dependence of the rising behaviour of the intruder on the size ratio. A quantitative discussion will be presented in the following section. Figure 2 shows two snapshots of the ascent of an intruder of $\Phi = 10.5$. The mechanism by which this ascent is accomplished can be seen clearly from Figure 2a. Due to the fluctuations in the falling part of the motion of the whole assembly, a small disc is able to squeeze in beneath the large disc and rolls down into the hole below it, followed by an avalanche of other small discs. The intruder is then stabilized in this new (higher) position. In the motion of the small discs no convection was observed. Usually, an avalanche as the one in Figure 2a is followed by another one on the other side of the intruder as to make up for the asymmetry induced by the first one.

The small discs whose arrangement above the intruder was disturbed before arrange themselves in an orderly fashion below the large disc as it rises. Besides, a triangular hole forms below the intruder as can be seen from Figure 2b. This hole is very stable and persists throughout the further rise of the intruder. We will discuss the relevance of this effect in the following subsection.

In Figure 3, we plot the vertical position of a rather small intruder ($\Phi = 2$) *versus* the number of shakes and observe the intermittent ascent as also reported experimentally [9]. Figure 3 shows that ascent takes place, but very slowly. The plateaus on which the intruder rests for very long times correspond to the stable positions calculated in reference [9]. The speed of rise is approximately 4 layers of small discs during 10 000 shakes. In experiments, see Figure 4 of reference [9], the speed is 7 layers during 54 000 shakes (1h with a frequency of 15 Hz). This is a very crude evaluation, but it shows that the time scales observed in our simulation are of the same order of magnitude as those observed experimentally. The positions from which the intruder falls down again once in a while correspond to the less stable of the two positions an intruder of $\Phi = 2$ can take on the triangular lattice formed by the small discs (see Ref. [9])

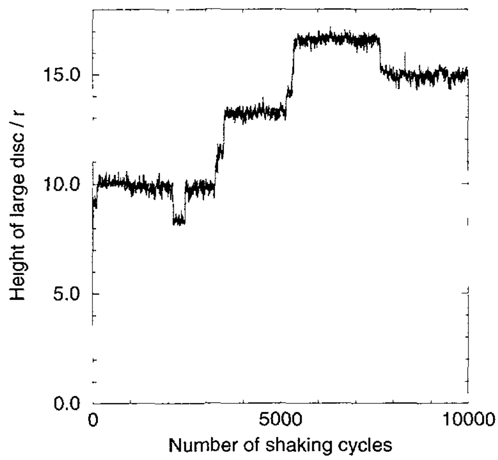

Fig. 3. — Ascent diagram for an intruder of size ratio $\Phi = 2$ at $A = r$ and $\delta = 0.1r$.

Intermittent ascent of an intruder with $\Phi = 3$ already was reported in reference [13] for small vibration amplitudes A, but on much shorter time scales. For larger intruders. intermittent ascent can still be observed in our simulations, as well as continuous ascent for $\Phi = 12$ (see Fig. 4). We investigated the influence of Φ on the segregation speed for $\Phi \leq 12$ in some detail which led to surprising results that will be discussed in the following subsection.

3.2. INFLUENCE OF THE DIAMETER RATIO ON SEGREGATION SPEED. — The influence of the diameter ratio on the segregation speed of a large intruder in the non-convective regime has been investigated experimentally [8]. A linear dependence of the speed of ascent on the diameter ratio has been found, as well as a critical diameter ratio $\Phi_c \approx 3.5$ for the given experimental situation.

An analysis of the dependence of the segregation speed on the diameter ratio by means of the original algorithm of Rosato *et al.* has been conducted before [14], but mainly to derive an amplitude dependence for amplitudes much larger than the typical values we use. The time scales on which segregation occurred in their work were of the order of time scales in the original work, both of which are much shorter than in the experimental work of reference [8] and in our simulations. For further comparison of our simulation to experiments. we performed simulations for intruders of size ratios $8 \leq \Phi \leq 12$ to measure the segregation speed.

In Figure 4, we plot the position of the intruder as a function of the number of shakes for different size ratios for $A = 0.5r$ and $\delta = 0.1r$. As can be seen from Figure 4, it is almost impossible to deduce some exact ascent speed from these diagrams. We calculate the velocity by averaging it over the whole simulation run (except in cases where the intruder reaches the surface earlier). Due to the long computation time each simulation took we performed only a few runs for each Φ value. Figure 5 shows the dependence of segregation speed on Φ as extracted from simulations of the type of those shown in Figure 4. Averages are taken from 2 to 3 simulation runs. However, the values for different realization for fixed parameters are consistent.

We checked that the initial position of the intruder did not affect the simulation results. When placed as described at the end of Section 2, the intruder would in all cases rise quickly on a first layer of particles. During this time, the whole assembly of small discs relaxed into the typical configuration that can be seen in Figure 2, with the intruder still resting on the first

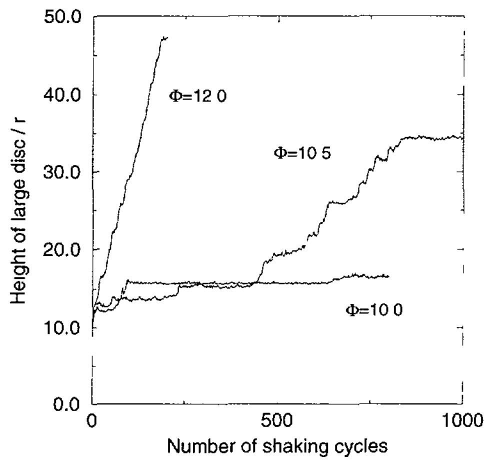

Fig. 4. — Ascent diagrams of an intruder for various values of Φ at $A = 0.5r$ and $\delta = 0.1r$.

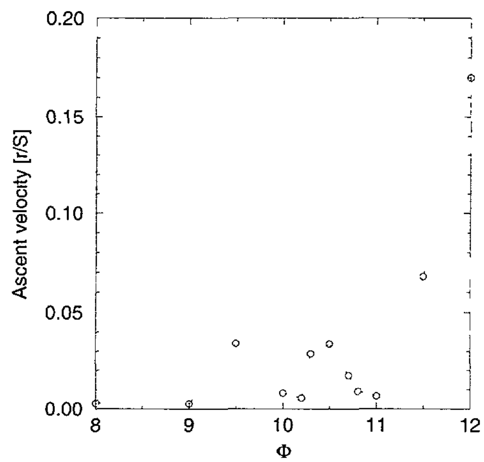

Fig. 5. — Dependence of ascent velocity on Φ. S denotes the number of shaking cycles.

layer of small discs. Thus, all intruders started from stable and well-defined initial positions, which can be recognized as small plateaus in the beginning of the simulation at height $(\Phi + 2)r$. The intruder was considered to start its ascent when it left this plateau. Starting the intruder not in the middle of the box, or on more than one complete layer did not change the simulation results.

Figure 5 illustrates the strange behaviour we found and should be taken as a qualitative rather than a quantitative result. The dashed line is merely meant to guide the eye. The speed of ascent exhibits an irregular behaviour where certain size ratios seem to rise preferentially which can be explained by purely geometrical arguments. To our knowledge, no experiments in 2D have covered this range of size ratios in such detail. We observe no size segregation for $\Phi < 9$ on these time scales, i. e. for 1000 shaking cycles. Naturally, it is possible and even probable that smaller intruders might rise as well in longer simulation runs. In experimental situations as described in [8], for $\Phi = 5.3$ waiting times of several minutes occurred, after which

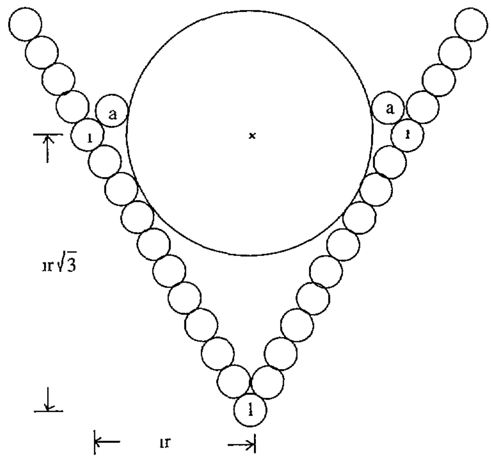

Fig. 6. — Schematic drawing of the situation encountered by the large disc after having risen through some distance in the simulations.

the intruder resumed its ascent. This corresponds to a few thousand shaking cycles, which is already longer than the simulation runs presented in Figures 4 and 5.

To explain the irregular behaviour we observed in our simulations in the ascent speed of the intruder, one has to look into the mechanism by which the ascent takes place. As mentioned before, a small disc has to squeeze in between the intruder and the supporting discs in order to stabilize it in a higher position. After some time, a triangular hole has formed below the intruder. Figure 6 shows a schematic drawing of the situation. The walls of this hole are geometrically very stable, so that the only discs likely to promote the ascent of the intruder are the discs labeled a in Figure 6. As we now proceed to show, the size of the small hole between the intruder and the disc labeled i is a non-monotonous function of Φ. Since the disc a has to fit into this hole, the typical size of the hole strongly affects the speed of ascent.

We now calculate the position of the disc i in a geometry as shown in Figure 6. When this position is known, the distance between the disc i and the intruder can be calculated. One can assume that the center of the intruder is at height $2(R+r)$ with respect to the center of the disc labeled 1 in Figure 6. The center of the disc i is at height

$$y_i = ir\sqrt{3}, \tag{3}$$

because it is the i-th disc in the wall. The value of i can be expressed as

$$i = \left[\frac{2}{\sqrt{3}r}(R+r)\right]. \tag{4}$$

The square brackets denote the integer part, i e. the largest natural number smaller or equal to the argument. This corresponds to the disc i being the highest of the discs in the walls of the triangular hole whose center is still below the center of the intruder. The corresponding value of the x-coordinate of the position of the disc i is $x_i = ir$ (always with respect to the center of the disc 1). For the distance d between the disc i and the intruder we get

$$d = \sqrt{\left(2(R+r) - ir\sqrt{3})^2 + (ir)^2\right)} \tag{5}$$

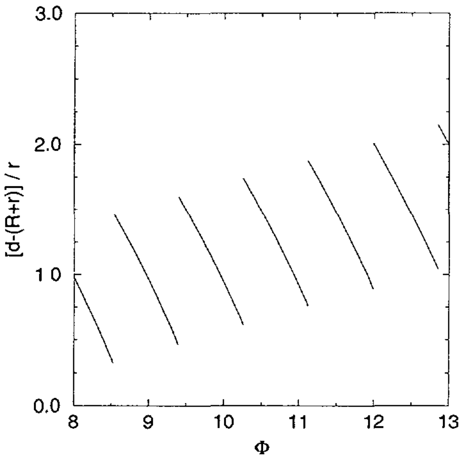

Fig. 7. — Distance between the disc i and the large disc. $(R + r)$ was subtracted from d to draw attention to the size of the hole between the two discs.

In Figure 7, we plot the distance between the surfaces of the disc i and the intruder in units of r for certain values of Φ according to equation (5). The jumps correspond to a change of the supporting disc (and thus of the value of i) due to an increase in the size of the intruder. It occurs whenever $2(\Phi + 1)/\sqrt{3}$ is an integer (see Eq. (4)). The irregular behaviour of the ascent speed of the intruder as a function of Φ can now be explained as follows. For size ratios slightly below such a jump value, the size of the hole is too small for the disc a to squeeze in. Above the jump value, the hole is much larger, thus promoting a fast ascent of the intruder. As the size of the intruder is increased further, the size of the hole decreases again. That way the probability for a hole that is large enough to accommodate the disc a to open up decreases and therefore the speed of ascent decreases. Simulations performed for diameter ratios slightly below and above these jump values show the expected behaviour (see Fig. 8), implying that

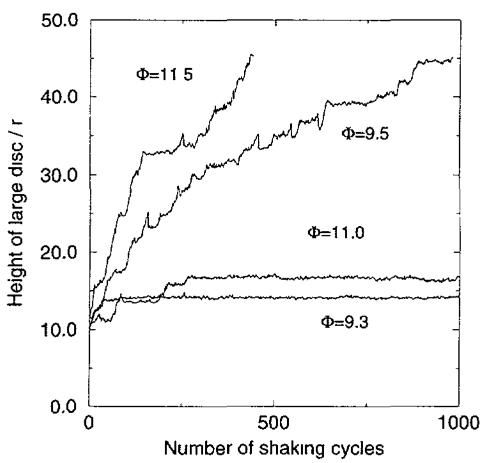

Fig. 8. — Ascent diagrams for $A = 0.5r$ and $\delta = 0.1r$. The corresponding jump values for the size d of the hole are at $\Phi = 9.39$ and $\Phi = 11.12$, respectively.

this is the reason for the irregularities in the speed of ascent. In experiments, no such behaviour could be observed because the development of a triangular hole below the intruder does not take place in the experimental situation. Therefore, we assume that fluctuations will wash out this purely geometric effect in most experiments. Small holes do develop, but larger ones are too instable not to be filled eventually, mainly by horizontal block motions of the small beads. The walls of such a hole are too feeble to resist the forces exerted on them by the other discs from the sides, forces which are absent from our simulation.

One should be able to reduce this "locking" behaviour of the intruder by introducing a size distribution of relatively narrow width on the small particles to disturb the regular arrangement observed in monodisperse packings. Another possibility might be to use a different probability distribution for the choice of the displacement of the single discs. Experiments evidence fluctuations of the discs around their mean position [8]. If more about these fluctuations were known, they might be incorporated in the simulations to render them more realistic.

4. Summary

We studied a periodically tapped system of discs with one large intruder disc in a background of monodisperse smaller discs by means of a Monte Carlo like simulation method which emphasizes geometric effects. By using a much smaller value for the maximum displacement in one Monte Carlo step than in previous work [13], the agreement with experiments could be enhanced substantially. We observed size segregation without accompanying convective motion of the background discs. The typical ascent velocities are similar to the ones observed in experiments conducted in this quasi-static regime [8], due to a suitable choice of the maximum step width δ in the simulations.

The ascent of the intruder takes place in an intermittent or continuous fashion, depending on the size ratio $\Phi = R/r$. In the case of intermittent ascent we find well defined stable positions of the intruder. In simulations with a very small intruder, the system may stay in such a stable configuration for a very long time as observed in experiments [9]. For very large values of Φ, close to the theoretical threshold for continuous ascent of $\Phi = 12.9$, the Φ-dependence of the stability of these positions affects the ascent velocity significantly. We give a purely geometrical explanation for this, based on the mechanism by which the ascent of the intruder is accomplished in our simulations. In experiments, other mechanisms besides this are active. As recent experiments show, large scale horizontal block motions are likely to untrap the intruder [17]. These do not occur in our simulations, which emphasize the local influence of geometry instead of long-range interactions. Their absence may be an explanation for the irregularity of the ascent velocity even for large intruders. Thus, the simulation can contribute to the understanding of the mechanisms active in size segregation by clearly showing which effects are due to the geometry of the problem and which are not.

Acknowledgments

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