Influence of geometry on stratification and segregation phenomena in bidimensional piles

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H I G H L I G H T S

- Simulation model considering only steric interactions.
- Systematic study of segregation patterns in piles with two different grain sizes.
- Definition and measurement of two suitable segregation indices.
- Qualitative agreement of the numerical results with experiments.
- Presence of striae although the grains only differ in their sizes.

A R T I C L E   I N F O

A B S T R A C T

We present a numerical study of the flow segregation problem in bidimensional piles. To simulate the pile formation, we employ a pseudo-dynamics method. The model allows us to vary the concentration of big and small grains present in the pile and the size ratio between them. The different segregation patterns arising after the pile is finished are studied by analyzing the spatial distribution of the grains. Two different segregation indices are defined and evaluated over the piles. The contact network of the final configuration of grains in the pile is also determined. The conditions under which the different segregation patterns show up are discussed. A comparison with a previous experimental study is performed for all the numerical results obtained in the present paper. The advantages and limitations of the simulation model are also discussed.

1. Introduction

Mixing and segregation processes are still topics of intensive research due to their technological importance and strong industrial applications. Many industries seek to improve the quality of their products through a better use of raw materials and optimizing the processing plants.

The segregation phenomena always occur when a mixture of grains of different sizes is simply poured onto a heap [1–10]. Typical segregation leads to the presence of large grains near the bottom of the pile, whereas small ones near the pouring point at the top of it. In recent works, a spontaneous stratification was observed for grains differing both in size and in shape [11–20]. Granular mixtures of small-rounded grains and large cubic grains stratify in alternating layers parallel to the surface of the pile as they are poured in the cell.

Makse et al. [12–16] have studied experimentally and analytically stratification and segregation phenomena. In their experiments they built piles inside a quasi bidimensional transparent cell throwing a mixture of two species of grains. They used grains of sand (cubic-shape with angle of repose equal to 35°) and glass beads. In the case that glass spheres have an angle of repose smaller than sand, they observed spontaneous stratification. In addition, when the angle of repose of glass spheres is greater than the sand angle, they found segregation. According to their experiments, the control parameter for stratification seemed to be the difference of the repose angles of the pure species, Θ. For $\Theta > 0$ (small rounded and large cubic grains) stratification was observed. On the other hand, strong segregation, but not stratification, occurred when $\Theta < 0$. They suggested that the resulting stratification derived from the competition between the size segregation and shape segregation. When $\Theta < 0$ and due to the size and shape segregation, the small cubic grains are located on the top of the pile and the spherical large ones are placed at the base of it, thus giving rise to a segregation phenomenon. In contrast, when $\Theta > 0$ large cubic grains segregate by size on the base of the pile and segregate by shape on the top of it. Simultaneously, spherical small grains size-segregate on the top of the pile and shape-segregate on the base of it. As a result of this competition, the resulting pile presents stratification. Additionally, to get stratification, grain flow below a certain limit value is required and the size ratio between large and small grains has to be greater than 1.5.

Grasselli and Herrmann have performed experiments with heaps of binary granular mixtures made of sand (rough) and glass spheres (smooth) that exhibited different internal structures [18]. They studied the pile morphology as a function of the size ratio of rough to smooth particles. For values of size ratio below 0.8, piles present typical segregation. Granular stratification is found to occur only for a size ratio greater than 1.5. They also observed that stratification depends on the separation between the walls of the cell where the pile is built and on the mass flux of the grain mixture.

There are in the literature few simulation models to address the stratification phenomenon. Continuous models [12,14,15] and cellular automata models [19] have been implemented to reproduce the stratification. However, the implementation of models that take into account the dynamic interactions between the grains has been hardly used in the stratification and segregation analysis [20]. Moreover, there are no models that take into account only the geometric aspects of the interaction between particles.

The aim of this work is to study the segregation phenomena using a simple bidimensional model to put into evidence the main aspects involved in the segregation–stratification mechanisms. We will use a pseudo-dynamic model to simulate granular piles of disks. This kind of models allows to show the relevant aspects related to the geometry of the problem. Indeed, our model does not take into account dynamical interactions and the main objective of our study is to pay special attention to the geometrical influence of interacting particles on stratification and segregation mechanisms. This simplification of the problem leads to computational costs being lower compared with other models currently used. Furthermore, these simulations were performed in order to reproduce the main aspects qualitatively obtained in our own earlier experimental results.

2. Experimental background

In a previous work, we have studied the segregation and mixture phenomena during the construction of granular piles [21]. The experimental device allowed us building piles of, at most, two different species of grains inside a quasi bidimensional transparent acrylic plexiglass cell. The piles could be constructed with a controlled vertical and horizontal relative motion between the grain injection point and the top of the pile in formation. It essentially consisted of a fixed grain feeding system and a cell where the pile is constructed. The grains are injected at the central top point of the acrylic cell and this cell can move vertically and horizontally as mentioned above. The feeding system consisted of two vibrating feeders and 3D and 2D static mixers in series to guarantee that the segregation in the piles is due to the build-up process and that the kinetic energy of the grains is the one gained along the vertical path between the injection point and the top of the pile.

We analyzed the influence of the following control parameters: size ratio of grain species, injection flow, height of the injection point (which remained constant during all the construction process), and the magnitude of the longitudinal displacement for the case of experiments with horizontal motion. We worked with three different sizes of glass beads (3, 2 and 1 mm diameter) using two size ratios, 3:1 and 3:2.

Different final structural configurations for the piles were obtained, depending on the parameters used for their construction. For a size ratio 3:1, a small mass of coarse grains and a low injection height, piles presented stratification, as it can be seen in Fig. 1(a). As the injection height or the mass of coarse grains increased, stratification started to disappear.

For a size ratio 3:2, it was not possible to obtain stratified piles. For small mass of coarse grains, piles always showed typical segregation. Fig. 1(b) shows a pile obtained for this case. When the amount of coarse grains or the height of the injection point was increased, piles presented a higher degree of mixing. Finally, in experiments with horizontal motion, the top of the pile became more rounded, the stratification disappeared and the mixture of grains was improved, as shown in Fig. 1(c).

The experimental results were quantified using two segregation indices. These indices were defined in order to distinguish between the two kinds of segregation behaviors obtained in our experiments, i.e., typical segregation and stratification. For a given sample of volume V, one can evaluate the ratio of the volume occupied by the large particles to the total volume V. This is a measure of the local segregation in terms of the larger particles and this ratio will depend on
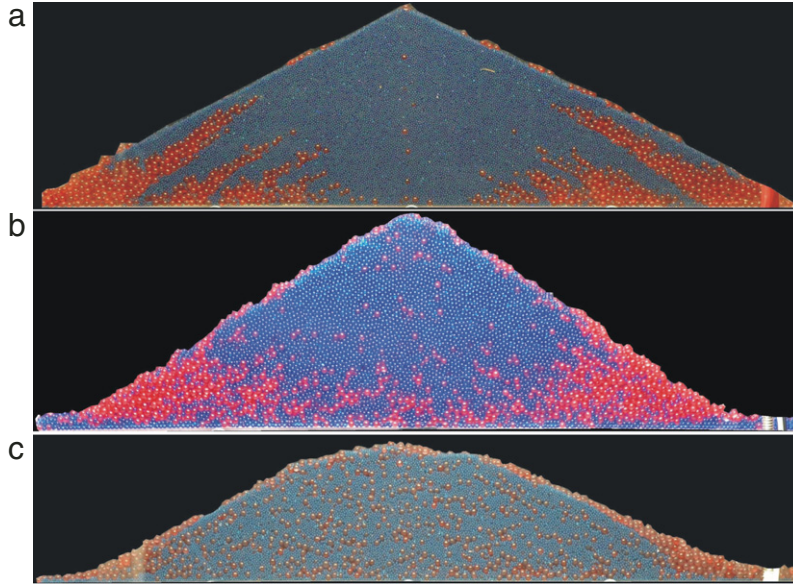
Fig. 1. Piles obtained with the experimental device for low height of the injection point, small mass of coarse grains and (a) size ratio 3:1; (b) size ratio 3:2; (c) size ratio 3:1 and horizontal motion [21].

how V is chosen in the pile. We defined the indices I_H and $I_\perp$ as [21]:

$$I_{H,\perp} = 2\frac{V_L}{V_L + V_S} - 1 = 2\frac{n_L}{a\frac{n_S}{27} + n_L} - 1 \quad \begin{cases} a = 1 \text{ for size ratio } 3:1 \\ a = 8 \text{ for size ratio } 3:2 \end{cases} \tag{1}$$

where V_L (V_S) is the total volume of the large (small) grains and n_L (n_S) is the number of large (small) grains present in the sample. In order to calculate I_H for a given pile, samples were taken over vertical strips all with the same volume. On the other hand, the corresponding samples to evaluate $I_\perp$ were taken over strips (all with the same volume) parallel to the free surface of the pile. As seen, the indices range from -1 ($n_L = 0$) to 1 ($n_S = 0$), where the extreme cases correspond to a complete segregation of the particles, i.e., $I_{H,\perp} = -1$ ($I_{H,\perp} = 1$) means no large (small) grains in the sample volume. A zero value corresponds to the presence of the same volume of large and small particles in the sample. The reason for using both indices simultaneously is due to the need to distinguish among the three possible final states for the piles: segregation, stratification and mixture. The index I_H varies linearly in the case of a pile presenting segregation, while it remains constant for piles presenting mixture or stratification states. Moreover, $I_\perp$ fluctuates for a stratified pile, while it does not vary in the case of segregation or mixture states. Thus, if one use a single index to characterize the results obtained, there will be two states indistinguishable.

Fig. 2 shows the results for I_H and $I_\perp$ belonging to the piles in Fig. 1. For size ratio 3:1, the oscillatory behavior for $I_\perp$ indicates the presence of stratification, while I_H shows an increase of the segregation of large particles as one goes toward the tail of the piles. The analysis of the behavior of I_H alone would conclude in the presence of typical segregation: small particles in the center of the pile and large particles at the tails. However, the fluctuation in the values of $I_\perp$ is a demonstration of the presence of bands. For size ratio 3:2, $I_\perp$ remains practically constant with some fluctuations for the last points related to the sample volumes near the slope. This behavior reflects the fact that no stratification is found for a size ratio 3:2. On the other hand, I_H shows the presence of segregation at the end of the pile.

Finally, for the case of piles built up with lateral motion and size relation 3:1, I_H indicates no segregation tendency in most of the volume of the pile, in contrast with the behavior of I_H for piles built up with $A = 0$. $I_\perp$ is not shown here because stratification is never present with a lateral movement.

In addition to the experiments described above, Fan et al. [22] have studied experimentally the different final particle configurations of bidisperse granular mixtures obtained when filling a quasi bidimensional silo. As in our previous experimental results, they also found three possible final configurations: stratification, segregation and mixture. The experimental set up consisted of a quasi-2D silo which allows varying the gap thickness and the silo width. They used glass beads of different diameters, varying the size ratio R of the binary mixture from 1.3 to 6.0. The granular mixtures (composed of equal mass fraction of the two species) were dispensed into the silo using a small auger feeder, which controls the volumetric flow rate.

They found that the stratified state occurred at small flow rates and over a wide range of size ratios ($R > 1.4$). Stratification became weaker and eventually disappeared as the flow rate was increased toward a critical value. The transition from the stratified state to the non-stratified state was independent of the width of the silo and the size ratio R (with the exception of size ratio equal 6.0, which has a greater value of critical flow rate). Above this critical value, full
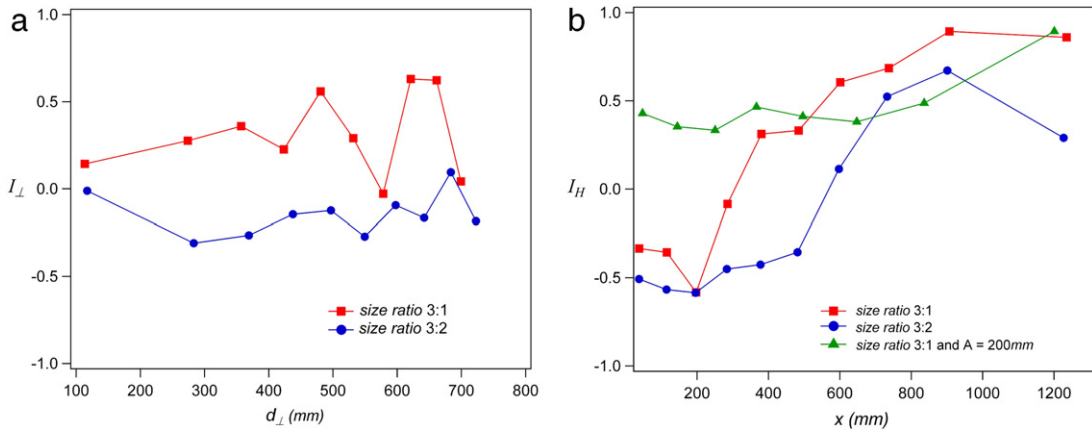
Fig. 2. Segregation indices I_H and $I_\perp$ for piles shown in Fig. 1. In all these cases, piles present a small mass of coarse grains [21].

segregation is observed and, at the highest achievable value of flow rate, a near mixed state was obtained. The transition from segregated to mixed state was controlled by the rise velocity of the heap. The critical rise velocity for the transition increased as the size ratio R was higher. In this way, the authors demonstrated that stratification of different sized-spherical particles was observed for a wide range of flow rates and size ratios. Besides, they suggested that the dynamics of stratification appear different from those for stratification of different size and shape particles observed by Makse et al. [12–16].

It is worth noting that in both experimental cases mentioned in this section [21,22], the stratification phenomenon occurs for size ratios greater than 1.4 and small flow rates.

3. Numerical model

Given the geometry of the experiments explained above, we decided that the built up of bidisperse piles be carried out using a two-dimensional pseudo-dynamic model [23,24].

This method does not require the solution of the classical motion equations for the grains of the system. In contrast, the motion of the particles is governed by the influence of gravity and local geometric constraints. This fact makes computing times lower than those for other simulation models like Molecular Dynamics (MD). For instance, a typical run for constructing a pile of 2000 particles is of the order of 10 h against the 3–7 days corresponding to an equivalent pile in MD, depending on the physical input parameters.

The algorithm permits the construction of bidimensional piles using disks of two different sizes. Disks fall or roll a small distance in each iteration step and, after a number of iterations, they find stable positions.

First, we defined a rectangular box of width L, large enough in order that particles do not interact with lateral walls. Disks are injected from the middle of the top of the box. As in the experiments explained above, in simulations we injected a mixture of the two species (or sizes) of disks. We parameterize the mixture by defining the surface ratio RS as the ratio between the total surface of the two types of disks present in the final configuration, i.e., $RS = S_L/S_S$, where S_L (S_S) is the total area of the large (small) disks. Thus, given a value of RS for the construction of a pile, the probability of throwing a large or small disk into the box is automatically determined.

The particles are injected into the box following a pseudo-dynamics algorithm. This algorithm consists in picking up a disk in the system and performing a free fall of length δ if the disk has no supporting contacts with other particles, or a roll of arc-length δ over its supporting particle if the disk has one single supporting contact. The supporting contacts are those that constrain a disk movement. Disks with two supporting contacts are considered stable and left in their positions. Let us follow the procedure in more detail.

If during the course of a fall of length δ a disk collides with another one (or with the base), the falling disk is put just in contact and this is defined as its first supporting contact. Closely analogous, if during the course of a roll along a length δ a disk collides with another one, the rolling disk is set just in contact. If the first supporting contact and the second one are such that the disk is in a stable position, the second contact is defined as the second supporting contact; otherwise, the lower of the two contacting particles is taken as the first supporting contact of the rolling disk and the second supporting contact is left undefined. If, during a roll, a particle reaches to a lower position than the supporting particle over which it is rolling, its first supporting contact is left undefined. It is worth noting that a stable position for a disk is defined when its center of gravity is located between the two supporting contacts created during its fall or rotation movement. Once the disk has two supporting contacts, it is considered stable and is set down fixed in that position. With this definition of stability, a particle can have a supporting contact with other particle whose vertical position is higher than its corresponding one. This is precisely what happens when an arch is formed in granular media. To make it more clear, the two supporting contacts of a disk prevent it from falling down (first supporting contact) and from rolling (second supporting contact). In the same way, a grain belonging to an arch is stable because one supporting contact prevents the free fall and the second one prevents the
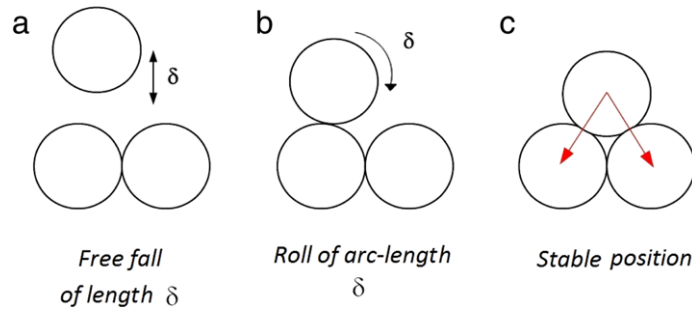
Fig. 3. Schematic representation of the three possible states of motion of a disk in the model: (a) free fall, (b) rolling and (c) stable position. Arrows indicate the supporting contacts.

rotation. Thus, for a disk forming an arch, the stable position would be achieved through two contacting neighbors among which, one is located below it.

In the case that a disk reaches the base of the box, it is left in that position, prevented to move (or roll). Here, a single supporting contact is sufficient for its stability.

In this way, particles can fall or roll in each iteration step, performing small movements. A schematic representation of the possible movements for a disk is sketched in Fig. 3. Iteration consists in moving every disk in the system by a distance δ or the amount allowed by the constraints imposed by neighboring disks. Notice that after one iteration step many disks may be left in unstable positions. A large number of iterations are needed before every disk finds its stable configuration. For very small values of δ ($\sim 7.5 \times 10^{-3}$), this method yields a realistic simultaneous deposition of grains with a zero restitution coefficient. More details on this algorithm can be found in Refs. [23,24].

4. Results and discussion

The numerical algorithm described above enabled us to build up piles with two different sizes of disks. In order to reproduce the experimental results explained early, we varied the parameters used for pile construction, i.e., the size ratio of grain species, the ratio of the injected mixture (RS) and the extent of the longitudinal displacement for the case of simulations with horizontal motion of the injection point. We worked with three different sizes of disks (0.8, 1.2 and 2.4 mm radii) using two size ratios 3:1 (a mixture of disks with 0.8 and 2.4 mm) and 2:1 (a mixture of disks with 1.2 and 2.4 mm). The values for RS were 0.5, 1.0 and 1.5. For simulations with horizontal motion, the amplitude for the movement were 100 and 200 mm, in accordance with experiments.

It is worth noting that the height of the injection point is not relevant in our simulations since the method does not take into account the dynamics of the movement of the disks and any interaction force between grains is calculated. Thereby, the spirit of our simulations is to put into evidence the effect that the geometrical restrictions have on the movement of the particles and the resulting effect on the segregation phenomena.

Fig. 4 shows the resulting piles using size ratio 3:1 and two different RS values. When the value of RS is small, piles present striae, i.e., large disks lie parallel to the free surface of the pile giving rise to the formation of chains (see Fig. 4(a)). As the value of RS is increased, typical segregation effects become also visible, leading to a greater amount of grains located at the base of the pile, as seen in Fig. 4(b).

It is important to note from the figures that the slope of the simulated piles is greater than the one corresponding to experiments. This is due to the particular simulation model we used, where any equation is solved to establish the equilibrium state of a particle. The stability of the disks is just obtained through geometric conditions for the supporting contacts. However, the results obtained through this numerical model reveal the importance of the geometry on the stratification phenomenon.

For piles built up with size ratio 2:1, the chains of large grains completely disappear and piles show a slight tendency to typical segregation. Examples of piles with this size ratio can be seen in Fig. 5. It is important to note that typical segregation effects obtained in simulations are not as visible as in experiments. This is due to the absence of dynamic effects in our model: here particles find stable positions more easily than in experiments. Consequently, disks would not always roll until the base of the pile and, also, no avalanche processes are to be expected.

Finally, simulations were carried out for piles with horizontal movement of the injection point. Fig. 6 shows the resulting piles with size ratio 3:1, $RS = 1.0$ and different amplitudes for the horizontal movement. Comparing these piles with those shown in Fig. 4 (constructed with the same parameters, but with no horizontal motion), it can be seen that striae (or chains of larger grains) tend to disappear. In turn, a higher degree of mixing is observed. When the amplitude is increased, the top of the pile becomes more flat and the mixture of grains is improved, as seen in Fig. 6(b). These results are in complete qualitative accordance with our experiments (Fig. 1(c)) [21].

The different final structures of the simulated piles were characterized through the two indices of segregation I_H and $I_\perp$ already defined above, but adapted to the present 2D case. For a given sample of area M, one can evaluate the ratio of the
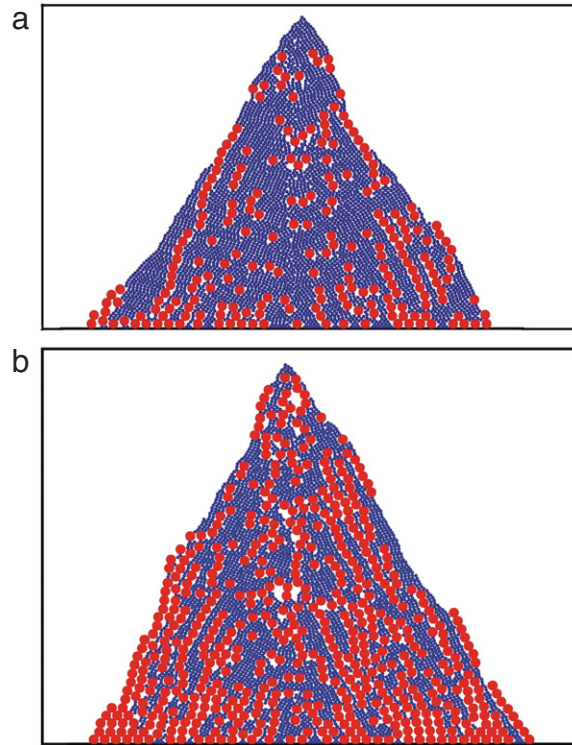
Fig. 4. Piles obtained with simulations, using size ratio 3:1 and (a) $RS = 0.5$; (b) $RS = 1.5$.
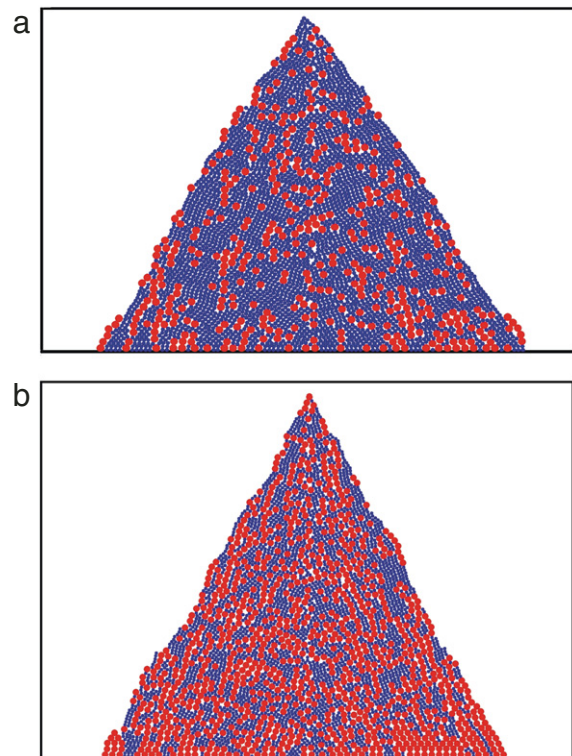

Fig. 5. Piles obtained with simulations, using the size relation 2:1 and (a) $RS = 0.5$; (b) $RS = 1.5$.
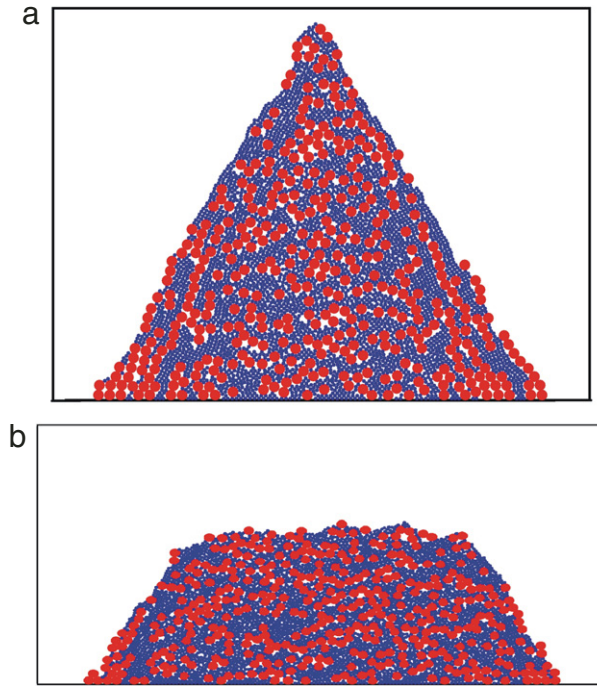
Fig. 6. Piles obtained with simulations, using the size relation 3:1, $RS = 1.0$ and horizontal displacement of the injection point with amplitude (a) 100 mm and (b) 200 mm. Note that scales for figures (a) and (b) are not the same.
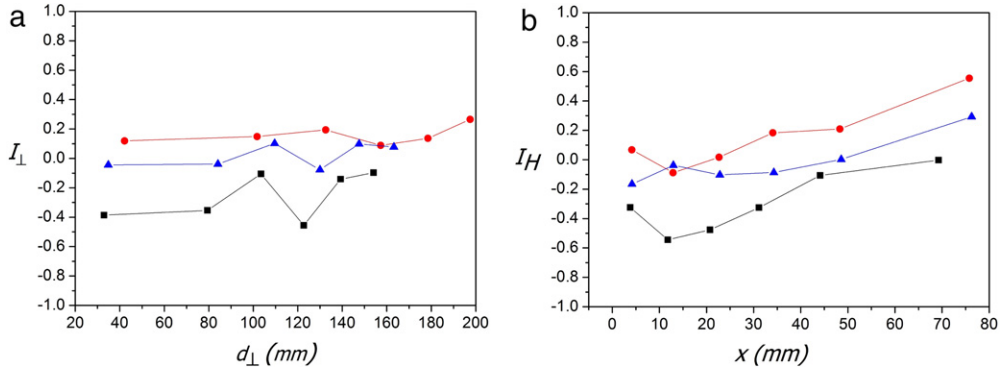

Fig. 7. Segregation indices $I_\perp$ (a) and I_H (b) for size relation 3:1 and (■) $RS = 0.5$, (▲) $RS = 1.0$ and (●) $RS = 1.5$.

area occupied by the large particles to the total area M. In this way, we defined the indices I_H and $I_\perp$ as:

$$I_{H,\perp} = 2\frac{S_L}{S_L + S_S} - 1 = 2\frac{n_L}{a\,n_S + n_L} - 1 \qquad (2)$$

where S_L (S_S) is the total area of the large (small) disks; n_L (n_S) is the number of large (small) disks present in the sample and a is a constant which depends on the size relation used for the pile construction. For the case of 3:1, $a = 9$ and for ratio 2:1, $a = 4$. As previously explained, the indices range from -1 ($S_L = 0$) to 1 ($S_S = 0$), i.e., $I_{H,\perp} = -1$ ($I_{H,\perp} = 1$) means no large (small) particles are present in the sample area. A value of zero corresponds to the same area of large and small disks in the sample. In Eq. (2), the samples to evaluate I_H for a given pile are taken over vertical strips all with the same area. On the other hand, the corresponding samples to evaluate $I_\perp$ are taken over strips (all with the same area) parallel to the free surface of the pile.

Fig. 7 resumes the results obtained for I_H and $I_\perp$ for the simulated piles with size ratio 3:1 and different values of RS. In each case, the right side of each pile was divided into 6 equal samples of constant area M. As observed, when RS is small, $I_\perp$ shows an oscillatory behavior (Fig. 7(a)). This indicates the presence of striae (or chains of large disks). The oscillations disappear when RS increases, in qualitative agreement with experimental results. Besides, I_H increases, showing a segregation effect, i.e., more large particles are present when going toward the tail of the piles in all cases (Fig. 7(b)).
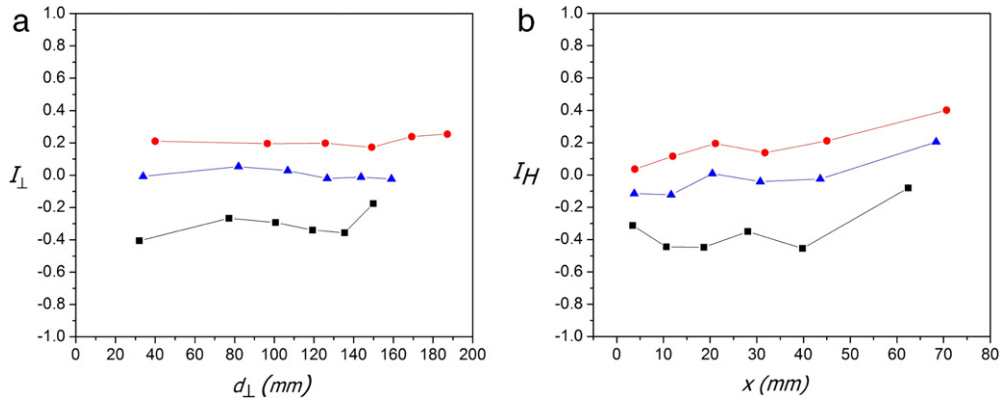
Fig. 8. Segregation indices $I_\perp$ (a) and I_H (b) for size relation 2:1 and (■) $RS = 0.5$, (▲) $RS = 1.0$ and (●) $RS = 1.5$.
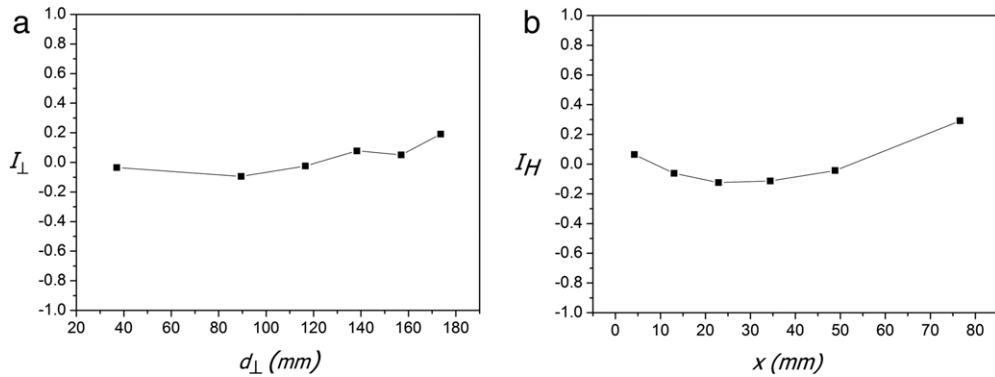

Fig. 9. Segregation indices $I_\perp$ (a) and I_H (b) for size relation 3:1, $RS = 1.0$ and $A = 100$ mm.

On the other hand, Fig. 8 shows the segregation indices for size ratio 2:1 and different values of RS. $I_\perp$ does not oscillate (Fig. 8(a)), indicating the absence of chains or striae, in accordance with the experimental results. Furthermore, I_H indicates the presence of segregation, which is moderately reduced when increasing the value of RS (Fig. 8(b)). This effect has already been discussed above. The absence of a strong segregation (which is expected according to experiments) is due to the simplicity of the implemented numerical model.

Finally, Fig. 9 shows the results for I_H and $I_\perp$ for simulated piles with a horizontal movement of the injection point with $A = 100$ mm. The striae almost disappear in contrast with the cases studied with no horizontal movement, as it can be seen in Fig. 9(a). I_H (Fig. 9(b)) remains constant indicating no tendency to segregate.

In order to add a complementary characterization of the structural organization of the segregation patterns, we have an analysis of the distribution of contact angles for different simulated piles. The implemented algorithm allows having information about the coordinates of the centers of all disks forming a pile. Through this information, it was possible to obtain the contact network of the final configuration. We have to say that in the case of experiments, this is a practically impossible task given that the visualization of the contacts is very difficult due to the depth (perspective) in three-dimensional photographs.

Each contact between two disks can be represented by a segment connecting their centers, and forming an angle α with the vertical axis. Thereby, we decided to build the contact angle distribution, i.e., a polar diagram indicating the number of contacts oriented in a range $(\alpha; \alpha + \Delta\alpha)$.

Fig. 10 shows the results of the contact angles distribution for two different piles built up with size ratio 3:1, but different RS values. As it can be seen, for a small surface ratio RS (Fig. 10(a)), the contact angle distribution has two pronounced peaks in 30° and 330°. This indicates the presence of a large amount of contacts aligned parallel to the free surface of the pile. It is important to recall that the slopes of the simulated piles are larger than those for the experimental case. Thus, the two peaks found in the polar diagram correspond to pile angles 60° and 120° (measured from the horizontal axis). These peaks account for presence of chains of large disks (or striae) observed in the simulated piles (Fig. 4(a)).

When increasing the surface ratio RS, the polar diagram (Fig. 10(b)) shows the presence of two less pronounced peaks at 30° and 330°, and a more uniform distribution of the contacts. This behavior indicates that striae are still present, but coexisting with a large grain segregation at the base and at the tails of the pile (Fig. 4(b)). Thus, the contact angle distribution changes depending on the surface ratio RS used for the simulation.
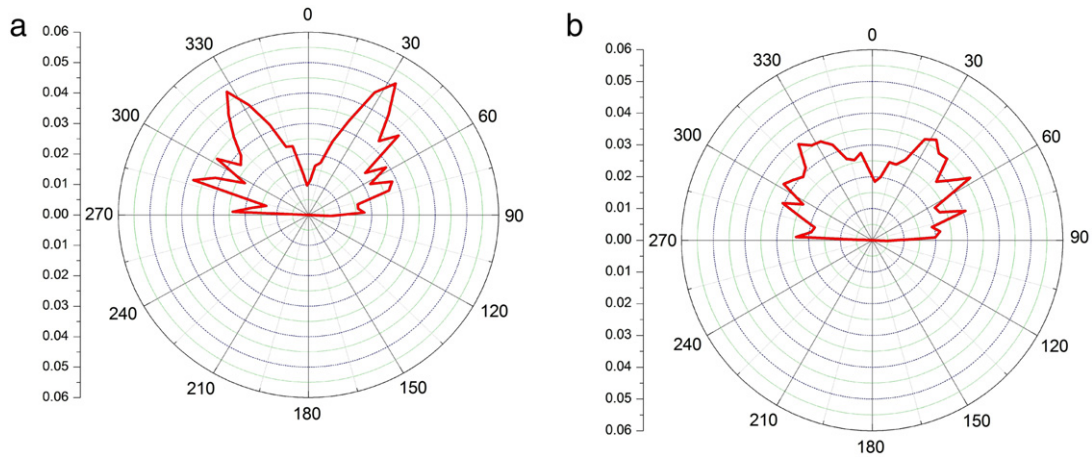
Fig. 10. Contact angle distributions for piles simulated with size ratio 3:1 and (a) $RS = 0.5$ and (b) $RS = 1.5$.

5. Conclusions

We have carried out simulations of bidimensional piles using a simple model. The implemented algorithm has enabled us to understand the general features of stratification and segregation phenomena that are driven by geometrical constraints. Our numerical model does not take into account the dynamics of the disks, nor are movement equations solved. Thereby, the aim of our simulations was to put into evidence the effect that geometrical restrictions have on particle interactions and on the resulting effect on segregation and stratification phenomena. A virtue of the model is that computing times are lower than those required by the other models.

Our numerical results have shown the existence of striae for piles formed with disks of size ratio 3:1 and small values of RS. The visualization of these chains suggests that geometric effects are relevant to the stratification phenomena. Besides, as the value of RS increases, we have found that piles also exhibit typical segregation phenomena.

For piles built up with size ratio 2:1, simulated piles show that chains or striae completely disappear. Instead, piles present a slight tendency to typical segregation. We have observed that this typical segregation effects obtained in simulations are less pronounced than in experiments. This is related to the absence of dynamic effects in our model.

When piles are built up with horizontal movement of the injection point the stratification also tends to disappear and the mixture of grains is improved.

Despite the simplicity of our model, numerical results are in all cases in qualitative agreement with the corresponding experimental results.

As it was mentioned in previous works, the defined segregation indices explain properly the different segregation patterns found in the simulations.

Finally, we have performed a complementary characterization of the structural organization of the simulated piles. The analysis of the contacts between disks was found to be a useful tool to distinguish between different segregation–mixing patterns. Thereby, according to the type of segregation present in a pile, polar diagrams help to determine the internal structure and to evaluate the eventual response of this structure to an external excitation.

Our results demonstrate that, taking into account steric effects alone, one can find typical segregation or stratification in a pile of disks.

Future efforts will be driven to implement avalanches during the formation of the pile to verify if the typical segregation phenomena increase.

Acknowledgments

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