Microscopic Model for Granular Stratification and Segregation

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(Europhys. Lett. **43**, 1-6 (1998))

We study segregation and stratification of mixtures of grains differing in size, shape and material properties poured in two-dimensional silos using a microscopic lattice model for surface flows of grains. The model incorporates the dissipation of energy in collisions between rolling and static grains and an energy barrier describing the geometrical asperities of the grains. We study the phase diagram of the different morphologies predicted by the model as a function of the two parameters. We find regions of segregation and stratification, in agreement with experimental finding, as well as a region of total mixing.

PACS Numbers: 05.40+j, 46.10+z, 64.75+g

When mixtures of grains [1–8] of different sizes are poured on a heap, a size segregation of the mixture is observed; the large grains are more likely to be found near the base, while the small grains are more likely to be near the top [9–14]. If the grains differ not only in size but also in shape and roughness, a spontaneous periodic pattern arises upon pouring the mixture in a two-dimensional cell. When a mixture of large-cubic grains and small-rounded grains is poured in a vertical Hele-Shaw cell (two vertical slabs separated by a gap of approximately 5 mm) the mixture spontaneously stratifies into alternating layers of small-rounded and large-cubic grains [15]. Otherwise, the mixture only segregates when the large grains are more rounded than the small grains [15] with the large-rounded grains being found near the bottom of the cell.

The dynamical process leading to stratification was recently studied numerically and theoretically [16], using the set of continuum equations for surface flows of granular mixtures developed in [17–20]. The physical quantities defined in this phenomenological formalism are to be understood as an average over a certain coarse grain length on the surface of the sandpile (larger than the size of the grains), where hydrodynamic equations are valid, and any quantity defined below this scale is not well-defined. Thus the relevant length scale appearing in this formalism is that of the coarse grain scale ($\approx 5d$) and not of the grain size (d). However fluctuations may also occurs at the level of the grains, so that a microscopic description of collisions and transport of grains may be needed to describe this situation. In this paper, we study the dynamical segregation process in two-dimensional silos by using a microscopic model of grain interactions.

We start by defining the model for the case of a single species pile [21,22], and then we discuss the generalization to two types of grains differing in size and shape. The microscopic model is defined on a square lattice. Each grain has width and height of one pixel. Since the experiments are done by pouring a fixed flux of grains, we deposit N grains at a given time step at the top of the first column of the pile. The grains start with a certain initial kinetic energy e_0, which will be lost in collisions with the static grains of the pile as the grains move down the slope. Only one rolling grain is in contact with the pile surface, and therefore interacts with the static grains of the pile. The remaining rolling grains are convected downward with unit velocity without loosing their energy, i.e., they move to the nearest-neighbor right column. The loss of energy of the rolling grain interacting with the surface pile is determined by the restitution coefficient, r, which gives the loss of energy per unit time. The interacting grain moves until its energy is smaller than a certain energy barrier u and stops. When the interacting rolling grain stops, one of the remaining rolling grains starts to interact with the surface pile until it losses its energy and stops. When all the N rolling grains stop, a new set of N grains is dropped at the first column of the pile, and the same rules are applied again.

The dynamics of a rolling grain with energy e interacting with a static grain located at height h_i are defined as follows:

- We test if the nearest neighbor position $i+1$ is energetically favorable, by first calculating the energy test e_{test}, defined as the energy the grain would have after moving to the new position $i+1$, according to

$$e_{test} = (e + \Delta h) * r, \quad (1)$$

  where $\Delta h = h_i - h_{i+1}$.

- Then, the energy test is compared with the energy barrier u. If $e_{test} > u$, the grain moves to the nearest neighbor position $i+1$, and the energy of the grains is updated: $e = e_{test}$. Then the procedure is applied to the interacting grain at column $i+1$, and so on. If $e_{test} \leq u$, the interacting grain stops at position i and increases the height of the pile at i by unity. The remaining rolling grains are always convected downward to the position $i+1$.

Simulations and analytical calculations [21] show that the angle of repose of the pile is an increasing function of the energy barrier u, and a decreasing function of the restitution coefficient r.

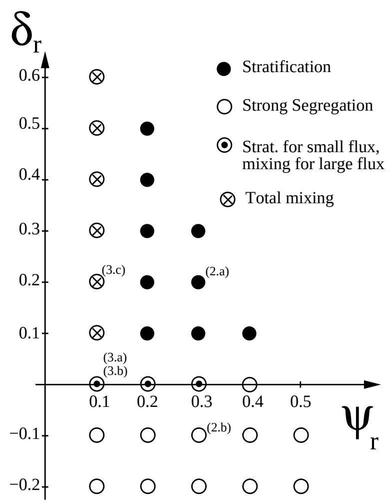

FIG. 1. Phase diagram for surface flows of granular mixtures predicted by the present model. In all simulations we deposit two grains of type 1 and two grains of type 2 ($N_1 = N_2 = 2$), and we set $e_0 = 1$, and $\psi_u = 0.3$. For the region where $\delta_r > 0$ we use $\delta_u = 0.3$, for the region where $\delta_r < 0$ we use $\delta_u = -0.3$, and for the intermediate region of $\delta_r = 0$ we use $\delta_u = 0$. The letters indicate the simulations shown in Figs. 2 and 3.

Next we generalize the model to the case of two types of grains. In [16] stratification was reproduced using a discrete model defining different critical angles between the grains. The critical angle is defined as the maximum angle at which a rolling grain will be converted into static grain. This angle depends on the type of rolling grain and the type of static grain which is interacting with. Thus, for two types of grains there are four different critical angles also called generalized angles of repose $\theta_{\alpha\beta}$, with $\alpha, \beta = 1, 2$. Stratification of grains differing in size and shape is the result of a competition between size segregation and shape segregation [23]. This competition was incorporated in the models of [16] at a macroscopic level, by considering certain relations between the generalized angles of repose. The angle of repose of the pure species depends on the shape of the grains: the rougher the grains the larger the angle of repose. Thus, for mixtures of cubic grains (type 2) and rounded grains (type 1) we have $\theta_{22} > \theta_{11}$. On the other hand, if the grains have different size, the cross-angles of repose $\theta_{\alpha\beta}$ are different. Since small grains roll down on top of large grains easier than large grains on top of small grains, this implies that $\theta_{12} > \theta_{21}$, if type 1 grains are smaller than type 2 grains. Thus we arrive to the relations for the case of a granular mixture composed of small-rounded grains (type 1), and large-cubic grains (type 2), which gives rise to stratification:

$$\theta_{21} < \theta_{11} < \theta_{22} < \theta_{12}. \quad (2)$$

On the other hand, if the large grains are more rounded than the small grains, one expects that $\theta_{22} < \theta_{11}$, and this type of mixture results only in segregation and not in stratification. The relation between the angles of repose is then

$$\theta_{21} < \theta_{22} < \theta_{11} < \theta_{12}, \quad (3)$$

which is valid for small-cubic grains (type 1), and large rounded grains (type 2).

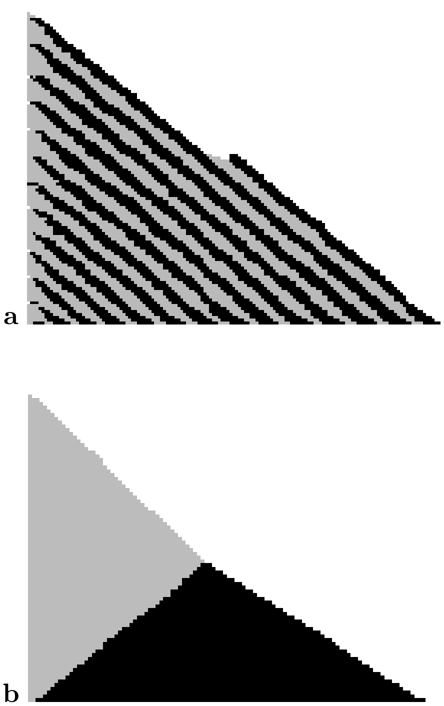

FIG. 2. Different morphologies predicted by the present model. **a,** Stratification ($\delta_r = 0.2$, $\psi_r = 0.3$, $\delta_u = 0.3$, $\psi_u = 0.3$, $u_{21} = 0.3$, and $r_{12} = 0.1$). Notice the "kink" formed by a pair of layers developed at the surface of the pile, similarly observed in [15,16]. **b**, Strong segregation ($\delta_r = -0.1$, $\psi_r = 0.3$, $\delta_u = -0.3$, $\psi_u = 0.6$, $u_{21} = 0.3$ and $r_{12} = 0.1$). Here the black grains are type 2, and grey grains are type 1. See Fig. 1 for the location of the morphologies in the phase space.

Next, we generalize the model to the case of two types of grains 1 and 2 with different size, shapes or material properties. We deposit N_1 and N_2 grains on the first column of the pile, and at a given time step, one rolling grain per species interacts with the sandpile surface, and the remaining rolling grains move downward to the nearest-neighbor column. We assume an overdamped situation where the rolling grains which do not interact with the surface achieve a constant convective velocity due to the collisions with other rolling grains. We define the generalized restitution coefficient and the generalized energy barrier as $r_{\alpha\beta}$, and $u_{\alpha\beta}$ with $\alpha, \beta = 1, 2$, for the four different possible collisions, i.e. r_{12} is used in Eq. (1) if a rolling grain of type 1 collides with a static grains of type 2. Since the angle of repose of the pure species is a monotonic increasing function of the energy barrier u, and a monotonic decreasing function of the restitution coefficient r, we can translate the relations (2) for stratification and (3) for segregation into relations for $r_{\alpha\beta}$ and $u_{\alpha\beta}$. Thus, we expect stratification for small-smooth grains (type 1), and large-rough grains (type 2) when

$$u_{21} < u_{11} < u_{22} < u_{12} \quad (4)$$

$$r_{12} < r_{22} < r_{11} < r_{21}, \quad (5)$$

and, we expect segregation for a mixture of small-rough (type 1) grains, and large-smooth (type 2) grains when

$$u_{21} < u_{22} < u_{11} < u_{12} \quad (6)$$

$$r_{12} < r_{11} < r_{22} < r_{21}. \quad (7)$$

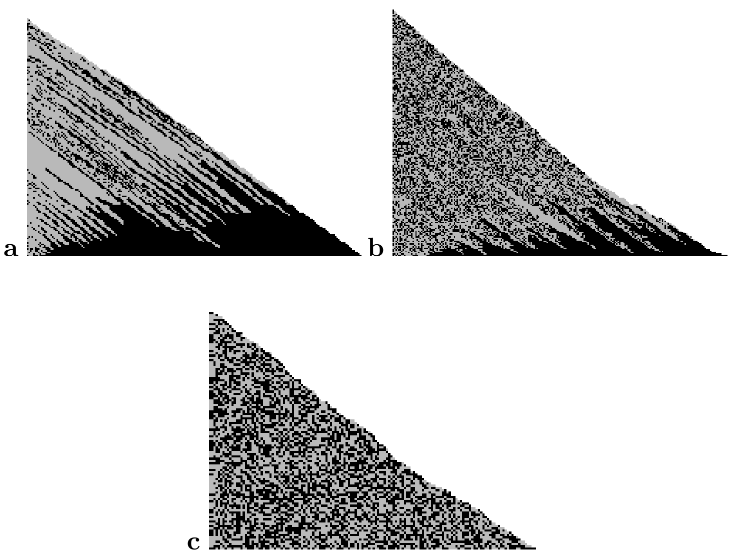

FIG. 3. Morphologies predicted by the present model when the grains are only slightly different. **a**, When $\delta_r = 0$ and $\psi_r \leq 0.3$ ($u_{21} = 0.1$, $r_{12} = 0.4$) we observe weak stratification with thin and irregular layers as observed in [26] for small flux rate $N_1 = N_2$=2, and **b**, mixing in almost all the pile plus weak segregation and some stratification with grains type 2 at the bottom of the pile for large flux rate $N_1 = N_2$=16. **c**, When $\delta_r > 0$ and $\psi_r = 0.1$ ($u_{21} = 0.3$, $r_{12} = 0.1$) we observe the total mixing of the species. See Fig. 1 for the location of the morphologies in the phase space.

We corroborate these predictions by investigating the different morphologies predicted by the model for the different internal parameters. Since the general model has eight parameter, we reduce the number of them to be able to investigate the resulting phase diagram. We assume some relations between the parameters and define [16]

$$\psi_u \equiv u_{11} - u_{21} = u_{12} - u_{22} \quad (8)$$

$$\psi_r \equiv r_{11} - r_{21} = r_{12} - r_{22}, \quad (9)$$

and

$$\delta_u \equiv u_{22} - u_{11} \quad (10)$$

$$\delta_r \equiv r_{11} - r_{22}. \quad (11)$$

Further, we assume some values for δ_u and ψ_u (see Fig. 1). We notice that ψ_u describes the difference in size of the grains, δ_u and δ_r are determined by the different shapes of the grains, and the material properties and asperities are described by ψ_r and δ_r. If grains 2 are rougher that grains 1, we have $\delta_r > 0$, and if grains 2 are more smoother than grains 1, we have $\delta_r < 0$.

Figure 1 shows the resulting phase diagram and Figs. 2 and 3 show the resulting morphologies. We find a region of stratification when $\delta_r > 0$ (Fig. 2a), and a region of strong segregation for $\delta_r < 0$ (Fig. 2b), as found in the experiments performed in [15,24,25].

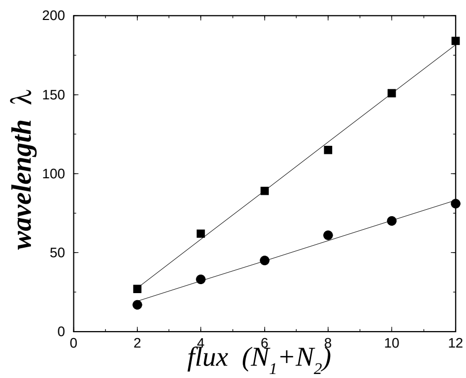

FIG. 4. Wavelength of the layers (measured in pixel units) as a function of the flux of incoming grains ($N_1 + N_2$) for two different sets of parameters in the region of stratification. We find a linear dependence in agreement with conservation arguments [16], the coefficient of the linear relation depends on the internal parameters. The circles correspond to $u_{21} = 0.1$, $u_{11} = 0.2$, $u_{22} = 0.6$, $u_{12} = 0.9$, while the squares correspond to $u_{21} = 0.5$, $u_{11} = 0.9$, $u_{22} = 1.5$, $u_{12} = 1.9$. We take all the restitution coefficients equal to 0.2, and we use an equal volume mixture ($N_1 = N_2$).

When some of the properties of the grains are very similar we find the additional morphologies shown in Fig. 3. When $\delta_r = 0$ and $\psi_r \leq 0.3$ we observe a weak stratification pattern (Fig. 3a) but only for small flux rate $N_1 = N_2 = 2$. The resulting layers are very thin and irregular, as can be seen in Fig. 3a. The negligible difference in grain properties gives rise to identical angles of repose of the pure species, so that the kink, which is observed to give rise to the layers by stopping the rolling grains [16], is very small. As a consequence, when we increase the flux of grains, the small kink is not able to stop the arriving rolling grains; the grains ride over the kink so that not segregation at the kink is observed. Therefore, for these particular parameters, the stratification pattern dissapears upon increasing the flux. In Fig. 3b we show the results of our simulations where the same calculations of Fig. 3a are done, but for a larger flux of grains $N_1 = N_2 = 16$. We see that at the 2/3 upper part of the pile the grains are mixed, and that at the 1/3 lower part of the pile there is some reminiscence of stratification plus the segregation of the large grains at the bottom. In general we find that when $N_1 = N_2 \gtrsim 8$, the stratification disappears for these kind of parameters, a prediction that was recently confirmed by experiments [26]. Finally, when $\delta_r > 0$ and $\psi_r = 0.1$ we observe the total mixing of the species for any value of the flux of grains (Fig. 3c). As in the previous case, the mixing might be due to the existence of a weak kink that is not able to stop and segregate the grains.

We also study the wavelength λ of the layers as a function of the flux of grains (i.e., as a function of the total number $N_1 + N_2$ of deposited grains per unit time). We find a linear increase of λ (Fig. 4) as a function of the flux as is expected from a conservation argument [15,16,24]:

$$\lambda \propto N_1 + N_2. \tag{12}$$

We find that the coefficient of the linear relation depends on the internal parameters of the model (Fig. 4). In general, we find that the larger the difference in energy barrier of the two species, the larger the wavelength of the layers, since the kink becomes steepest as the difference in angle of repose of the pure species increases.

[1] R. A. Bagnold, *The physics of blown sand and desert dunes* (Chapman and Hall, London, 1941).

[2] J. L. Borges, *The book of sand* (Emece, Buenos Aires, 1977).

[3] H. M. Jaeger and S. R. Nagel, Science **255**, 1523 (1992).

[4] H. J. Herrmann, in *Disorder and Granular Media*, (eds. D. Bideau and A. Hansen) (North-Holland, Amsterdam, 1993).

[5] S. F. Edwards, in *Granular matter: an interdisciplinary approach*, (ed. A. Mehta) 121 (Springer-Verlag, New York, 1994).

[6] H. M. Jaeger, S. R. Nagel, and R. P. Behringer, Rev. Mod. Phys. **68**, 1259 (1996).

[7] J. Duran, *Sables, poudres et grains* (Ed. Eyrolles, 1997).

[8] D. E. Wolf and P. Grassberger (eds), *Friction, Arching, Contacts Dynamics* (World Scientific, Singapore, 1997).

[9] R. L. Brown, J. Inst. Fuel **13**, 15 (1939);

[10] R. A. Bagnold, Proc. R. Soc. London A **225**, 49 (1954).

[11] J. C. Williams, Univ. Sheffield Fuel Soc. J. **14**, 29 (1963).

[12] J. A. Drahun and J. Bridgwater, Powder Technol. **36**, 39 (1983).

[13] S. Savage, C. K. K. Lun, J. Fluid Mech. **189**, 311 (1988).

[14] P. Meakin, Physica A **163**, 733 (1990).

[15] H. A. Makse, S. Havlin, P. R. King, and H. E. Stanley, Nature **386**, 379 (1997).

[16] H. A. Makse, P. Cizeau, and H. E. Stanley, Phys. Rev. Lett. **78**, 3298 (1997).

[17] J.-P. Bouchaud, M. E. Cates, J. R. Prakash, and S. F. Edwards, Phys. Rev. Lett. **74**, 1982 (1995).

[18] J.-P. Bouchaud, M. E. Cates, J. R. Prakash, and S. F. Edwards, J. Phys. I France **4**, 1383 (1994).

[19] P.-G. de Gennes, C. R. Acad. Sci. (Paris) **321** II, 501 (1995); P.-G. de Gennes, *Granular matter*, Varenna Lectures (1996).

[20] T. Boutreux and P.-G. de Gennes, J. Phys. I France **6**, 1295 (1996).

[21] J.-P. Hovi, J. J. Alonso, and H. J. Herrmann (preprint).

[22] M. Rimmele, Diplomarbeit (Stuttgart, 1997).

[23] H. A. Makse, Phys. Rev. E **56**, 7008 (1997).

[24] Y. Grasselli and H. J. Herrmann, Granular Matter, **1** (1998).

[25] J. Koeppe, M. Enz, and J. Kakalios, in *Powders and Grains*, (eds R. Behringer, and J. Jenkins), p.443 (1997).

[26] J. Baxter, U Tüzün, D. Heyes, I. Hayati, and P. Fredlund, Nature **391**, 136 (1998).

ACKNOWLEDGEMENTS. We thank J.J. Alonso, T. Boutreux, S. Luding, M. Rimmele, and H. E. Stanley for stimulating discussions. H.A.M. acknowledges BP and CPS for financial support.