SIMPLE MODEL FOR COMPACTION OF GRANULAR MATERIALS

Nebojša M. Ralević, Ljuba Budinski-Petković, Uranija Kozmidis-Luburić, Aleksandra Mihailović,
Faculty of Engineering, Trg D. Obradovića 6, 21 000 Novi Sad, Serbia and Montenegro

Abstract − *Compaction process in a vibrated granular material is studied by Monte Carlo simulations. The density relaxation of a given layer of the material, normal to the tapping force and parallel to the bottom of the container, is modeled by a simple adsorption-desorption model with diffusional relaxation. In the low desorption limit the system reaches the equilibrium state very slowly. The late stages of the process are governed by an inverse logarithmic behavior followed by an exponential approach to the equilibrium density.*

1. INTRODUCTION

Granular materials behave differently from any of the other standard forms of matter: solids, liquids or gases. In some cases, such as a sandpile at rest with a slope less than the angle of response, static friction produces solid-like behavior: the material remains at rest even though gravitational forces create macroscopic stresses on its surface. If the pile is tilted several degrees above the angle of response grains start to flow, like in fluid. However, this flow is not that of an ordinary fluid because it only exists in boundary layers at the pile's surface. Since gases are made up of discrete particles with negligible cohesive forces, we might view this flow, or any granular flow, as a flow of a dense gas. However, unlike in an ordinary gas, kT plays no role in a granular material. Instead, the relevant energy scale is the potential energy of a grain in the gravity of the Earth. Granular materials should therefore be considered an additional state of matter in its own right. The unusual dynamical behavior of granular materials has attracted much recent attention [1-11].

Transporting and storing granular materials is of a great importance for agriculture and the food processing industry, as well as for the pharmaceutical industry. Yet the technology for handling and controlling granular materials is poorly developed. Estimates show that up to 60% of the capacity of some industrial plants are wasted due to problems related to the transport of these materials. Hence even a small improvement in understanding of the behavior of granular media should be useful.

Granular material in a container can be assembled in many ways. In the case of spherical particles the packing fraction can vary from $\rho = 0.55$, for the mechanically least stable configurations, to $\rho \approx 0.64$ for the densest random close packing limit [2]. Cubes, for example, have maximum packing density of 1, but reach a density of only 0.68 on deposition.

By shaking or vibrating the container, the granular system can evolve from the less stable states to the more stable and densely packed states. The compaction process in granular materials was studied experimentally in [3] and an inverse logarithmic dependence on time was observed:

$$\rho(t) = \rho_f - \frac{\Delta\rho}{1 + B\ln(1 + t/\tau)} \tag{1}$$

where parameters ρ_f -the final equilibrium density, $\Delta\rho$, B and τ depend only on the vibration intensity.

A simple adsorption-desorption model, describing the kinetics of compaction of a given layer of the material, gives a good qualitative explanation of the process [12]. The layer is perpendicular to the tapping force and the particles leave the layer at random as a result of a tapping event. Compaction proceeds when particles fall back into the layer under the influence of gravity. The ratio of desorption to adsorption rates depends on the tapping strength. One-dimensional adsorption-desorption process of line segments adsorbing on a linear substrate was studied in [12]. In the small desorption limit the kinetics of the late stages of the process is an inverse logarithmic one, followed by a terminal exponential approach. Since the physical situation corresponds to a two-dimensional layer it would be interesting to study a two-dimensional case.

Desorption is not the only process that can lead to the rearrangement of the surface in the case of adsorption on substrates or to the compaction of a layer in a granular material. Exposed to a tapping event, particles in a layer of a granular material cannot only leave the layer at random and fall back into the layer under the influence of gravity, but they can also change their positions inside the layer. In that sense the adsorption-desorption model with diffusional relaxation provides more general picture of the compaction process. In this work, we present a Monte Carlo simulation model in which all three processes are present – adsorption, desorption and diffusion are proceeding simultaneously with different probabilities.

2. DEFINITION OF THE MODEL AND THE SIMULATION METHOD

In order to analyze the impact of diffusion on the compaction kinetics, we consider a simple model of adsorption, desorption and diffusion on a square lattice. In the case of the adsorption-desorption process the equilibrium coverage, as well as the relaxation time, depends on the adsorption/desorption probability ratio [13]. On the other hand, if the depositing objects are squares and if the only allowed processes are adsorption and diffusion, final coverage tends to unity [14]. Namely, at the late times of the process the additional adsorption events are possible only on the empty domains formed by the diffusion of the adsorbed objects. The diffusion leads to the formation of large clusters of covered sites and after long enough time, that depends on

the adsorption/diffusion probability ratio, a configuration is formed in which almost all sites are occupied.

The kinetics of the adsorption-desorption process with diffusional relaxation is governed by the ratios of desorption to adsorption rate and diffusion to adsorption rate. In our model these ratios correspond to the ratios of desorption/adsorption probability and diffusion/adsorption probability, respectively. The time is rescaled to the adsorption process because the number of attempts per unit time is the quantity usually controlled in the experiments.

The Monte Carlo simulations of adsorption, desorption and diffusion are performed on a square lattice of size 100×100. The adsorbing objects are squares of size 2×2, covering four lattice sites. Periodic boundary conditions are used in both directions.

At each Monte Carlo step adsorption is attempted with probability P_a=1, desorption with probability P_{des} and diffusion with probability P_{dif}. For each of these processes a lattice site is selected at random. In the case of adsorption, we try to place the object with the fixed point (say the left upper corner of the object) at the selected site, i.e., we search weather all relevant sites are unoccupied. If the selected sites occupied by the fixed point of a previously adsorbed object and if the attempted process is desorption, the object is removed from the layer. On the other hand, when the attempted process is diffusion, we choose one of the four possible directions at random and try to move the object for a lattice constant in that direction. The object is moved if it does not overlap with any of the previously deposited objects; on the contrary, the attempt is abandoned.

The time t is counted by the number of adsorption attempts and scaled by the total number of lattice sites L^2. If we assume that one tap corresponds to one adsorption attempt per lattice site, the time is actually measured in the number of tapping events. The data are averaged over 100 independent runs for each combination of desorption and diffusion probabilities.

3. KINETICS OF THE COMPACTION PROCESS

In the context of the compaction process in granular materials we are interested in the cases with small desorption probabilities leading to coverages greater than the jamming coverage in the case of irreversible deposition $\rho(\infty)$. For an initially empty lattice the kinetics displays three different successive regimes. The first stage is dominated by adsorption events and the process displays an RSA-like behavior. For coverages greater than $\rho(\infty)$ the kinetics is dominated by $1/\ln(t)$ behavior. In the final stage an exponential approach to equilibrium is observed.

The simulations are performed for various combinations of desorption and diffusion probabilities such that $P_{des}/P_a \leq 0.1$ in order to obtain densities greater than the jamming density. Dependence of the coverage on time is shown in Figure 1. for the process with P_{des}/P_a =0.02 and P_{dif}/P_a =0; 0.1; 1. In all the cases the coverage reaches an equilibrium value after long enough time. Moreover, the equilibrium coverage depends only on the desorption/adsorption probability ratio and the presence of diffusion only fastens the approach to the equilibrium state. In Table 1. values of the equilibrium coverage ρ_{eq} are given for various ratios of desorption to adsorption probabilities. We can see that ρ_{eq} decreases when P_{des}/P_a increases.

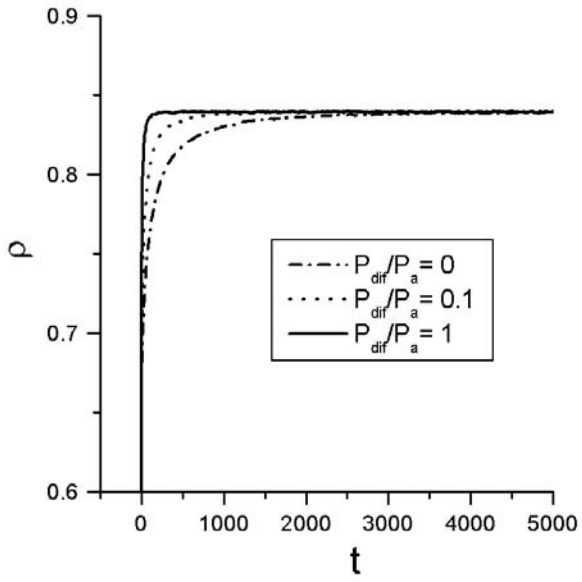

Figure 1: *Evolution of the coverage for P_{des}/P_a=0.02 and P_{dif}/P_a=0; 0.1; 1.*

Table 1. *Equilibrium coverage ρ_{eq} for various desorption probabilities.*

P_{des}/P_a	ρ_{eq}
0.001	0.9844
0.002	0.9758
0.004	0.9635
0.006	0.9531
0.008	0.9432
0.01	0.9321
0.02	0.8931
0.04	0.8497
0.06	0.8218
0.08	0.8007
0.1	0.7837

In the experiments concerning the density relaxation in vibrated granular materials [3], the vibration intensity is determined as $\Gamma=a/g$, where a is the peak acceleration of a tap and $g=9{,}81 m/s^2$ is the gravitational acceleration. In our model various combinations of desorption and diffusion probabilities correspond to various vibration intensities. The ratios of desorption to adsorption rates and diffusion to adsorption rates are increasing functions of the tapping strength.

4. LOW VIBRATION INTENSITIES

For sufficiently low values of diffusion and desorption probabilities the exponential approach is not reached in the times of interest and the kinetics is governed by an inverse logarithmic function. As an example of this behavior the dependence of the coverage on time is shown in Figure 2. for P_{des}/P_a=0.002 and P_{dif}/P_a=0.05. The results of the simulations are shown as open circles and the solid lines represent the fit of the form:

$$\rho(t) = \rho_f - \frac{\Delta\rho}{1 + B\ln(1 + t/\tau_1)}, \qquad (2)$$

observed experimentally. In this regime the relaxation time τ_1 is a decreasing function of the ratios of desorption to adsorption and diffusion to adsorption probability.

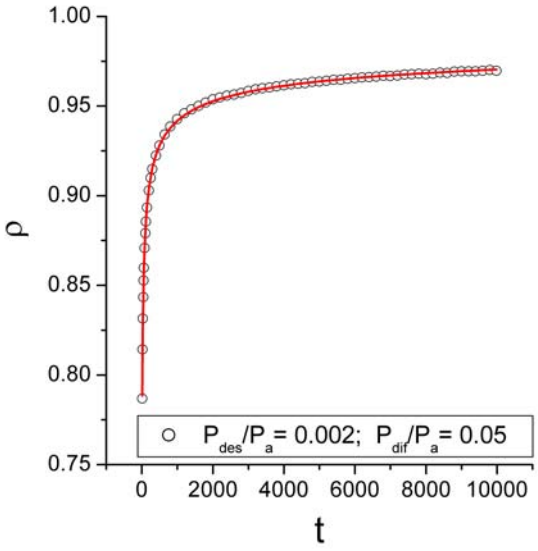

Figure 2. *Coverage vs. time for* P_{des}/P_a=0.002 *and* P_{dif}/P_a=0.05. *The solid line represents the fit of the form:*

$$\rho(t) = \rho_f - \frac{\Delta\rho}{1 + B\ln(1 + t/\tau_1)}$$

5. HIGH VIBRATION INTENSITIES

In very late times of the process, the plots of $\ln(\rho_{eq} - \rho(t))$ are straight lines for all desorption and diffusion probabilities, suggesting that the final approach to the equilibrium state is exponential, of the form:

$$\rho_{eq} - \rho(t) \propto e^{-t/\tau_2}. \qquad (3)$$

Such plot is shown on Figure 3. for P_{des}/P_a=0.01 and P_{dif}/P_a=0.1. The values of the relaxation time τ_2 can be obtained from the slopes of the lines.

When P_{des}/P_a increases, the relaxation time decreases. This decrease is most prominent for low desorption probabilities. For a fixed value of P_{des}/P_a, τ_2 decreases when diffusion probability increases. A complex time-evolution observed in [3] could be explained as a consequence of the variation of desorption and diffusion rates during the process.

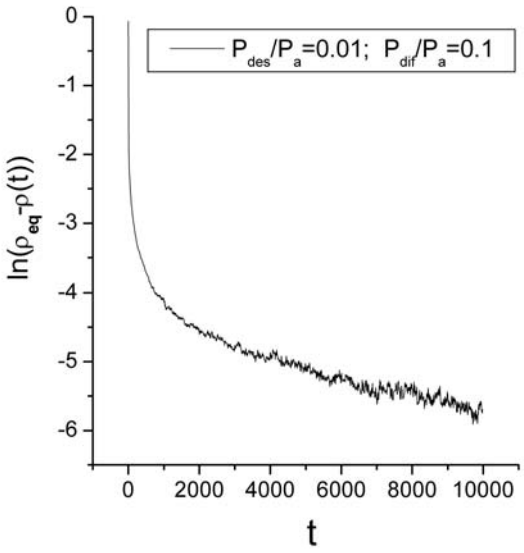

Figure 3. *Plot of* $\ln(\rho_{eq} - \rho(t))$ *for* P_{des}/P_a=0.01 *and* P_{dif}/P_a=0.1.

6. CONCLUSION

The values of desorption and diffusion probabilities that correspond to the relaxation processes in granular material are often very small, so the model gives the experimentally observed inverse logarithmic behavior in the times of interest. However, in the case of large vibration intensities it is possible to exceed the logarithmic regime and the complex time-evolution of the coverage observed in [3] could be explained as a consequence of the variation of the diffusion rate during the process.

In the addition to the slow density relaxation, the adsorption-desorption model also exhibits some other features of real granular materials, such as memory effects [15]. Our model is a lattice based model, but it does reproduce the complex phenomenology of granular media governed by the geometric exclusion effects. The simplicity of the model enables simulations of systems containing large numbers of particles.

In order to investigate the influence of shape on compaction of granular materials, depositing objects of various shapes can for example be formed by self-avoiding walks on the lattice. On a square lattice shapes with a symmetry axis of first, second a fourth order can be formed. Simulations for various objects would show how the kinetics of the process depends on the shape of the object, on the object dimension and on the symmetry properties of the object.

ACKNOWLEDGEMENT

This work was supported by the Serbian Ministry of Science and Technology under the project “Dynamical and Thermodynamical Properties of Strongly Correlated Systems

with Complex Structures" (No 1895) and the project "Mathematical Models of Nonlinearity, Uncertainty and Decision" (No 1866).

REFERENCES

[1] L.A. Pugnaloni and G.C. Barker, "Structure and distribution of arches in shaken hard sphere deposits," *Physica A*, vol. 337, pp. 428-442, February 2004.

[2] K. To, Pik-Yin Lai and H.K. Pak, "Jamming of granular flow in a two dimensional hopper," *Physical Review Letters*, vol. 86, pp. 71-74, January 2001

[3] J.B. Knight, C.G. Fandrich, C.N. Lau, H.M. Jaeger and S.R. Nagel, "Density relaxation in a vibrated granular material," *Physical Review E***,** vol. 51, pp. 3957-3963, May 1995.

[4] E.R. Nowak, J.B. Knight, E. Ben-Naim, H.M. Jaeger and S.R. Nagel, "Density fluctuations in vibrated granular materials," *Physical Review. E*, vol. 57, pp. 1971-1982, February 1998.

[5] I.C. Rankenburg and R.J. Zieve, "Influence of shape on ordering of granular systems in two dimensions," *Physical Review E*, vol. 63, 061303 1-9, May 2001.

[6] C. Josserand, A Tkachenko, D.M. Mueth and H.M. Jaeger, "Memory effects in granular materials," *Physical Review Letters*, vol. 85, pp. 3632-3635, October 2000.

[7] D.A. Head, "Phenomenological glass model for vibratory granular compaction," *Physical Review E***,** vol. 62, pp. 2439-2449, August 2000.

[8] P. Phillipe and D. Bideau, "Numerical model for granular compaction under vertical tapping," *Physical Review E***,** vol. 63, pp. 051304 1-9, April 2001.

[9] F.X. Villarruel, B.E. Lauderdale, D.M. Mueth and H.M. Jaeger, "Compaction of roods: Relaxation and ordering in vibrated anisotropic granular material," *Physical Review E***,** vol. 61, pp. 6914-6921, Jun 2000.

[10] R.Y. Yang, R.P. Zou and A.P. Yu, "Computer simulation of pacing of fine particles," *Physical Review E*, vol. 62, pp. 3900-3908, September 2000.

[11] M.V. Sapozhnikov, A, Peleg, B. Meerson, I.S. Aranson and K.L. Kohlstedt, "Far-from equilibrium Ostwald ripening in electrostatically driven granular powders," *Physical Review E*, vol. 71, pp. 011307 1-5, January 2005.

[12] J. Talbot, G. Tarjus and P. Viot, "Adsorption-desorption process of extended objects on a square lattice," *Physical Review E*, vol. 61, pp. 5429-5438, May 2000.

[13] Lj. Budinski-Petković and U. Kozmidis-Luburić, "Adsorption-desorption process of extended objects on a square lattice," *Physica A***,** vol. 301, pp. 174-180, June 2001.

[14] Lj. Budinski-Petković, U. Kozmidis-Luburić and A. Mihailović, "Random sequential adsorption with diffusional relaxation on a square lattice," *Physica A*, vol. 293, pp. 339-344, April 2001.

[15] Lj. Budinski-Petković, S.B. Vrhovac, "Memory effects in vibrated granular systems: Response properties in the generalized random sequential adsorption model," *The European Physical Journal E*, vol. 16, pp. 89-96, January 2005.

Sadržaj: Proces sabijanja u granularnim materijalima podvrgnutim vibracijama proučavan je pomoću Monte Carlo simulacija. Relaksacija gustine u datom sloju granularnog materijala, normalnom na silu udara i paralelnom dnu suda, modelovana je jednostavnim adsorpciono-desorpcionim procesom sa difuzionom relaksacijom. U graničnom slučaju malih verovatnoća desorpcije sistem veoma sporo dostiže ravnotežno stanje. Za kasne etape procesa karakteristična je obrnuta logaritamska zavisnost prekrivenosti od vremena i krajnji eksponencijalni prilaz ravnotežnoj prekrivenosti.

JEDNOSTAVNI MODEL ZA SABIJANJE GRANULARNIH MATERIJALA

Nebojša M. Ralević, Ljuba Budinski-Petković,
Uranija Kozmidis-Luburić, Aleksandra Mihailović