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NUMERICAL SIMULATION OF GRANULAR MATERIALS IN A ROTATING TUMBLER

HORACIO TAPIA-MCCLUNG

Using a simple numerical model based on particle dynamics, we perform two-dimensional simulations of granular materials inside a rotating tumbler. Still in its first stages of development, the model can quantitatively reproduce some of the general behavior observed in these systems, both for monodisperse and binary mixtures. Work is currently being done to validate the model and obtain results that are directly comparable to experiments.

1. Introduction

Until recently, two special cases of granular segregation have received the most attention: systems in which particles have the same size but differ in density (D-systems) and those in which particles have the same density but different size (S-systems). In both cases, the mechanisms that give rise to segregation are still not well understood. A more challenging case is that in which particles of different sizes and densities are present [Jain et al. 2005] . This last situation is of practical importance since many of the granular flows encountered in nature and industry involve particles of different sizes, shapes, and densities.

It is known that particles of higher density or smaller size segregate to the core of the granular bed while particles of lower density or larger size segregate to the outer edges and to the flowing layer. In mixed systems, it would be expected that the mechanisms that give rise to segregation compete to decrease or increase the final mixed state. Much of the experimental and numerical work already done to study segregation in a rotating tumbler has focused on bidisperse particle systems in which only one of the particle properties is varied (S and D systems), and only recently has a first step towards characterizing regimes of segregation for systems with mixed particles been done experimentally [Jain et al. 2005]. In this study it was found that when the different mechanisms all contribute to segregation, a *classical* behavior is observed, and when they oppose one another, a transition from a core composed of dense particles to a core composed of small particles occurs and mixing can be achieved if the denser particles are also bigger and if the ratio of particle size is greater that the ratio of particle density.

On the numerical side, granular flow has been approached by means of continuum-based models [Khakhar et al. 1997; Jain et al. 2005] and particle dynamics simulations [Dury and Ristow 1997], but in both cases, only the size or the density of the particles were different. In this work we present the preliminary results of a numerical study on granular materials placed in a two-dimensional rotating drum based on a particle dynamics simulation. Our final objective is to determine regimes of mixing and segregation and their dependence on system parameters such as particle properties, filling level of the

Keywords: granular materials, rotating drum, numerical simulations.

drum and angular velocity of rotation of the drum. Numerical simulations allow us to track the evolution of quantities that are not accessible in real experiments and to scan a wide range of system parameters in order to gain knowledge of the fundamental processes responsible for the complex collective behavior that is observed in granular materials.

2. The system

A rotating tumbler is probably one of the simplest and most common devices used to mix particles. In its most basic form, it is a cylindrical container that rotates about its axis of symmetry. Particles (or fluids) placed inside of it undergo different flow regimes that depend on many factors, the most evident one being the rotational velocity of the tumbler; but perhaps just as important as the angular velocity is the friction of the particles with the inside walls and with themselves.

In the case of granular materials, as the tumbler rotates, particles are transported inside the drum mostly by friction with the inner wall. For very small rotational velocities, the system of particles behaves as a rigid body. As the velocity is increased, individual avalanches begin to appear on the surface layer, carrying particles from one side of the rotating drum to the other. Further increase in the angular velocity above a critical value results in a continuous flow on the surface layer, and for even higher values of rotational velocity, the system reaches a centrifugal regime.

The choice of a rotating drum as a study case presents several advantages: rich behavior can be observed and, under appropriate conditions, the processes taking place in such a device can be considered almost two-dimensional. Industrial applications are wide and can provide a direct comparison between experimental and numerical work.

3. The numerical model

We model single grains by idealized spherical particles (discs in two dimensions) of radius r_i^0 and mass m_i that interact only in pairs during collisions. The time evolution of each grain is obtained by numerically solving the coupled equations of motion using the velocity-explicit Verlet algorithm for temporal integration of second-order differential equations. This algorithm approximates the solution using a nonzero time step dt to update the positions at time $t_{n+1} = (n+1)dt$ from the knowledge of the position, the velocity and the forces acting on the particle at time $t_n = ndt$. The velocity is updated by using the information from the previous time step (at time t_n) and the forces acting on the particle at the current time. Further details can be seen in [Andersen 1983; Allen and Tildesley 1989; Tapia-McClung and Grønbech-Jensen 2005]. To use this numerical method, the forces acting on a particle have to be known in advance in order to update the positions and velocities. Because of the nature of granular materials and the complexity of their collective behavior, it is difficult to know what the forces acting on each individual grain are [Schaefer et al. 1996]. In a numerical simulation we need a model simple enough to be treated computationally, that is able to account for the observed behavior of the system. This is particularly true for granular materials which are highly dissipative systems. In this work we have chosen a simple and numerically tractable model that accounts for the basic interactions between particles in granular media and that has been successfully used to study granular flows in different configurations [Dury and Ristow 1997; Hirshfeld and Rapaport 1997]. According to Newton's second law, the equation

of motion for a single grain looks like

$$m_i\ddot{\bar{r}}_i + \alpha_i\dot{\bar{r}}_{ij} = -\nabla_i e(r_{ij}) - \sum_{i\neq j}\beta_{ij}u_{ij}(r_{ij})\dot{\bar{r}}_{ij} + \mu_{it}u_{it}(r_{it})(\Delta\bar{v}_R \times d\hat{r}) - m_i\bar{g},$$

where

$$e(r_{ij}) = \sum_{i>j} u_{ij}(r_{ij}),$$

$$u_{ij}(r_{ij}) = 4\epsilon_{ij}\left(\left(\frac{\sigma_{ij}}{r_{ij}^0 - r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}^0 - r_{ij}}\right)^{6}\right) + \epsilon_{ij}$$

is the potential energy between pairs of grains, given in terms of the parameters ϵ_{ij}, which is a measure of the strength of the interaction between grains and which provides a unit for the energy of the interaction, σ_{ij}, the *softness* of the grains, and r_{ij}, the relative separation of particles. The repulsive force in the normal direction along the line joining the centers of mass of the particles is thus given by $-\nabla_i e(r_{ij})$. This force depends only on the relative separation of the particles, r_{ij}, and prevents them from overlapping. The analytical expression for the potential energy is that of the common Lennard-Jones potential widely used in Molecular Dynamics simulations [Allen and Tildesley 1989]. This potential provides a smooth force function (required by the numerical method) with the desired physical properties for the system: strongly repulsive for small separations of the particles and zero for separation between particles that are larger than a cut-off, since the particles do not interact when they are far apart from each other.

The terms proportional to the relative velocity in the equations of motion, $\dot{\bar{r}}_{ij}$, correspond to a dissipative force that accounts for the inelastic collisions, and which is determined by the constant parameter β_{ij}. The force in the shear direction is connected to the normal force by the Coulomb laws of friction [Schaefer et al. 1996]. A diagram of the forces acting on a pair of grains is shown in Figure 1. It is worth noticing that, in three dimensions, the shear force in not uniquely defined and we must require that the tangential force lie in the plane of the relative velocity.

The last two terms in the equations of motion correspond to the interactions between the particles and the tumbler's wall. We use μ_{it} as the parameter for the frictional forces between the particles and the

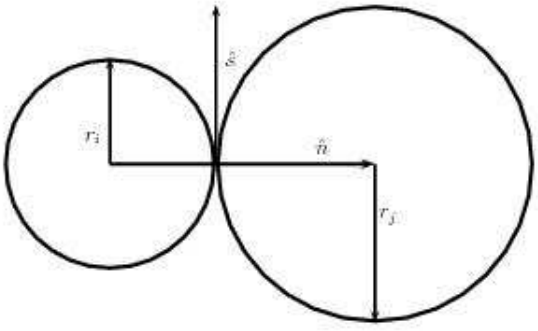

Figure 1. Normal and tangential directions during particle contacts.

interior wall, while the force resulting from the angular velocity is given by $\Delta\bar{v}_R \times d\hat{r}$, where $\Delta\bar{v}_R$ is the relative velocity between the particle and the tumbler, and where $d\hat{r} = \frac{\bar{r}_i - \bar{r}_t}{|\bar{r}_i - \bar{r}_t|}$ is a unit vector in the direction determined by the center of the particle and the center of the tumbler.

4. Preliminary results

We are currently performing simulations for monodisperse systems of particles in order to establish an appropriate correspondence between the model and the experimental measurements. For these simulations, we fix the tumbler's radius and the total number of particles used. It should be noticed that with this choice, varying the size of the grains also changes the filling level of the tumbler and therefore the dynamics since, clearly, a tumbler that is 10% filled will show different behavior than one that is 90% filled. We also fix the model parameters α_i, β_{ij} and μ_{it} and study the system as the rotational velocity of the tumbler is varied. Figure 2 shows the results of simulations using 1500 particles of size $r_i^0 = 1.0$ (in arbitrary units) inside a tumbler of radius $R = 52.5$ with $\alpha_i = \beta_{ij} = \mu_{it} = 1.0$ for rotational velocities between 2.0 rpm and 2.4 rpm. The s-shape that can be seen in the surface layer has been observed experimentally, and is commonly seen before a transition in the flow regime occurs [Ding et al. 2002].

A first step towards successfully applying the model discussed here to the study of mixing and segregation in granular materials is shown in Figure 3. In this case, the simulation is done with 850 particles of size $r_i^0 = r^0 = 0.1$ in a drum of radius $R = 35$. Both types of particles have the same mass density and the rotational speed is $\Omega = 2.0$ rpm. The figure at the left is a snapshot of the simulation at the initial stage and the one at the right shows a snapshot taken after only a few rotations of the tumbler. The images show that the system is reaching a segregation state in which the smallest particles are accumulating around the cores, as should be expected.

5. Discussion

Although this work is in a development stage, the simple model presented here is enough to observe some of the general features of granular particles inside a rotating tumbler, not only for monodisperse systems but also for the classical cases of D- and S-systems. Even in the simplest cases of monodisperse

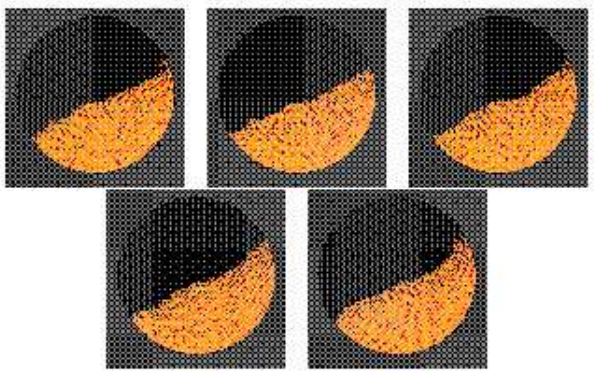

Figure 2. Numerical simulations for mono disperse particles. Rotational speeds from left to right are: $\Omega = 2.0$, 2.1, 2.2, 2.3 and 2.4 rpm.

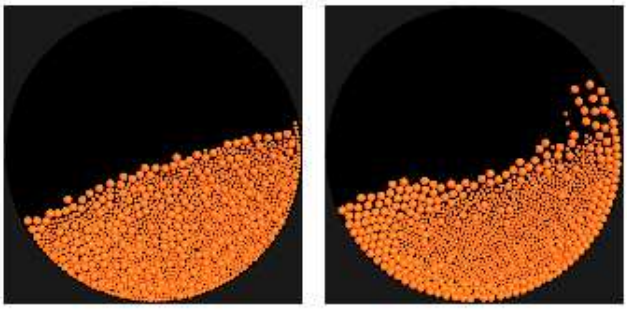

Figure 3. Snapshot of a numerical simulation of a binary mixture. The final segregated state can be observed on the right.

systems, our simulations have shown features and behavior that are richer than the originally expected ones. A phase diagram of the flow transitions as the rotational speed increases is being constructed while monitoring physical quantities like the average energy, the average torque on the tumbler due to the particles, etc.

Another work currently in progress is the study of the dynamics of elongated grains inside the rotating tumbler. In [Tapia-McClung and Grønbech-Jensen 2005] an efficient numerical algorithm was developed to constrain particles in a linear geometry. This allows us to numerically construct elongated grains that are composed of several individual particles and no longer have to be considered ideal grains represented by spherical particles, since we are able to construct grains with irregular shapes.

Even where we have not mentioned it, three-dimensional simulations are also being considered. The computational effort required to extend the calculations from two to three dimensions is relatively simple, and so it is contemplated as a future goal of this research.

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