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Charge dynamics in a model for grains electrization

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ABSTRACT

In this work we investigate a model for the dynamics of granular electrization using event-driven simulations and approximate calculations. The model is defined as a mixture of isolating grains of different species confined in a cubic box. During the collisions, the grains and the walls can acquire electric charge via tribocharging. We focus on the dynamics of charge exchange, and calculate the time evolution of the total charge in each species, that presents a double exponential behavior in the case of zero gravitational field. For non-zero field, a stretching of the curve is present, caused by the resulting density and velocity profiles.

1. Introduction

Triboelectrization is a complex phenomenon of charging that occurs when two different materials are put in contact [1,2]. It is a strictly surface process which depends on the density of states of superficial electrons and consequently the surface work function of the material. By the way, it is easy for granular matter to acquire electric charge even for almost homogeneous compounds, since small chemical defects on surface can change its work function [3–5]. The study of charged granular matter has large interest in areas as distinct as storage of grains, transport and separation of materials, painting and printing processes [5,6], astrophysics of lightning in cosmic dust [7,8] and generation of electric and magnetic fields in atmospheric dust devils [9]. Despite the importance of this subject, the dynamical processes involved in contact electrization and the role of the dissipative nature of collisions on the behavior of charged grains remain not well understood.

Contact electrization can lead to adhesion and deposition of opposite charged bodies, bringing difficulties in, for example, pharmacological manufacture, affecting uniformity of mixtures [10]. In extreme conditions, tribocharging causes discharges and consequently combustion and explosion of flammable substances [11]. Otherwise, charging is an efficient method for separating small particles of different compositions [12]. By colliding grains with a metallic plate, and by applying an external electric field, positively and negatively charged particles are deviated in opposite directions, and thus collected in separated containers. Recent experiments [13] on a mixture of colliding spheres of gold, Nylon and Teflon in a circular oscillating plate showed that the tribocharging and the electric interaction among particles lead to particles segregation that resembles the nucleation of ionic crystals from a polarizable liquid.

Some theoretical studies on the particles electrization were also performed. For example, in order to understand the role of particle size on charge distribution, Duff and Lacks [5] modeled particles as spheres with different sizes and with trapped high energy electrons on their surface. They observed that even equal composition grains can be tribocharged and that smaller particles charge negatively while larger ones become positive. On the other hand, the effect of the electrostatic forces on granular mixing of vibrating beds were also studied by Lu and Hsiau [14] which observed that the mixing rate constants increase as a power law of the electrostatic force.

In spite of the large literature concerning the microscopic aspects of electrization and on their leading macroscopic effects, much work must be done in order to acquire a complete understanding of the dynamics involved in granular charging. Thus, in this paper we study in detail the dynamical properties of a previously introduced model [15] for triboelectrization in granular media. Here, a mixture of two species of spherical grains is placed inside a cubic box with thermal walls in the presence of a gravitational field. The particles can exchange their charges during the collisions among themselves and with the container walls. They have the same mass and radius, and the only difference among them is in their surface properties, represented by their work functions, which lead to opposite sign charging. To obtain the system properties, we performed event-driven particle dynamics

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simulations [16–21] and mean-field like calculations for low density of grains. We analyzed the spatial density profile of particles, the dynamics of charge redistribution, and the relation of the characteristic times with the wall temperature and the fraction of particle species.

The remaining of this article is divided as follows: in the next section we introduce the model and the simulation method, in Section 3 we exhibit some approximate calculations for the time evolution of the system charge and in Section 4 we present our results and conclusions.

2. Model and simulations

The system model is defined by N non-conducting spherical particles divided in N_A grains of species A and N_B of species B, given that $N = N_A + N_B$. Every grain has mass m and radius R, and the only difference between A and B species resides on their surface composition, implying in further triboelectrization by contact. The particles are confined in a cubic box of linear size L, with thermal walls at temperature T_w, resembling high-frequency low-amplitude vibrating walls. This represents the external source of energy which prevents the system to reach an static equilibrium state. The volume fraction occupied by the grains is given by $\rho = 4N\pi R^3/3L^3$, and the simulations were carried out for $N = 1000$ particles in a system with linear size $L = 50R$. The enclosing box can also be charged when hit by the grains, and it is assumed to have the same composition of the A particles. External electric fields are not considered, as well as the electric forces between any two grains, and between walls and grains. However, we included the gravitational force which is given by $\vec{F} = m\vec{g}$ where $\vec{g}$ points to the $-z$ direction.

The simulations were carried out by applying the standard event-driven particle dynamics. In this case, the time evolution of the system is governed by the Newton's laws during intercollisional displacements of the particles. Instantaneous collisional events occur when the distance between the centers of the two given particles (i,j) is $|\vec{r}_j(t+\Delta t) - \vec{r}_i(t+\Delta t)| = 2R$ after a time interval Δt. No deformations are allowed despite the non-conservative nature of collisions. The loss of kinetic energy is a result of the non-unitary normal and tangential restitution coefficients (ε^n and ε^t respectively). We can write down the post-collisional linear and angular velocities [17] of the particles i and j as:

$$\vec{v}'_{i(j)} = \vec{v}_{i(j)} \mp \frac{1+\varepsilon^n}{2}\vec{f}^{\,n}_{ij} \mp \frac{\tilde{I}(\varepsilon^t - 1)}{2\left(\tilde{I}+1\right)}\vec{f}^{\,t}_{ij}, \tag{1}$$

$$\vec{\omega}'_{i(j)} = \vec{\omega}_{i(j)} - \frac{(\varepsilon^t - 1)}{2R\left(\tilde{I}+1\right)}\left(\vec{e}_{ij} \times \vec{f}^{\,t}_{ij}\right), \tag{2}$$

where

$$\begin{aligned} \vec{f}^{\,n}_{ij} &= \left(\vec{g}_{ij}\cdot\vec{e}_{ij}\right)\vec{e}_{ij}, \quad \vec{v}_{ij} = \vec{v}_i - \vec{v}_j \\ \vec{f}^{\,t}_{ij} &= -\vec{e}_{ij} \times \left(\vec{e}_{ij}\cdot\vec{f}_{ij}\right), \quad \vec{f}_{ij} = \vec{v}_{ij} - R(\vec{\omega}_i - \vec{\omega}_j). \end{aligned} \tag{3}$$

Here $\vec{e}_{ij}$ is the unit vector pointing from particle j to particle i, and $\vec{v}_i$ and $\vec{\omega}_i$ are the linear and angular velocities of particle i before the collision. $\tilde{I}$ is the reduced moment of inertia I/mR^2. In equation (1) the upper signs are for $\vec{v}_i$ and the lower ones are for $\vec{v}_j$. For simplicity, we assume that the grains are rigid spheres with moment of inertia $I = 2mR^2/5$. Note that due to the normal and tangential restitution coefficients, particles can loose kinetic energy as well as linear and angular momenta.

If a particle collides with the container walls, a new normal component of velocity is chosen accordingly to

$$v_i'^n = \sqrt{-\frac{2T_w}{m}\ln(1-r)}, \tag{4}$$

where r is randomly distributed in the interval (0,1).

After each particle–particle or particle–wall collision, both grains and the wall can become charged due to triboelectrization if they are of different species. If particles are of the same type, the charge is redistributed equally between the pair, otherwise, the relative velocity and surface potential govern the charge exchange. We divided each grain in 8 equal parts (quadrants) in order to mimic the contact surface during a collision. So, the charge exchanged between grains is homogeneously distributed in the quadrant where the collision occurred. In the same way, the container walls were divided in N_w squares of equal size, with side lengthz $L_w \cong \sqrt{\pi/2}R$.

The total charge in a given quadrant (or square) after a collision is then given by

$$q'_{i,l} = \frac{\left(q_{i,l} + q_{j,l}\right)}{2} \pm K_{ij}v^n_{ij}, \tag{5}$$

where $q_{i,l}$ is the initial charge in the quadrant l of particle i (in the case of container wall, $i = 1,\ldots, 6$ is the wall number, and l represents a given square), v^n_{ij} is the normal relative velocity modulus, and K_{ij} is a constant that depends on surface potentials of particles and walls. It is reasonable to assume $K_{ij} = -K_{ji}$ and $K_{ii} = 0$ since $K_{ij} \propto (\phi_i - \phi_j)$, the difference in surface potentials. The potentials are chosen in such a way that A particles loose negative charges to B particles. The walls have the same potential as A particles. Note that equation (5) is based on different experimental and theoretical results, been somewhat phenomenological [1,3,10,22,23]. If $K_{ij} = 0$ (equal particles collision) the charge is divided equally. For a collision with different particle species, the initial charge is equally divide and an amount of charge $K_{ij}v^n_{ij}$ is transferred from one particle to another, always conserving the total charge. The linear dependence of equation (5) on the normal relative velocity appears experimentally and is related to the increase of contact area due to deformation [23,24], which, in our case, is not considered explicitly in the simulations.

We can summarize the simulation algorithm as follows: 1) the system is initialized with a random distribution of particles and velocities. 2) An ordered list of collisions is created by calculating all possible particle–particle and particle–wall collisions. 3) The system is then evolved till the first collision, moving particles according to the equations of motion. 4) With the first pair in contact, we apply equations (1), (2) and (4), depending on the kind of collision (particle–particle or particle–wall). 5) We update the list of collisions and restart the process. 6) After the system has reached the stationary state we start collecting the quantities of interest.

The calculation of the characteristic times was performed after reaching the stationary state for a given set of the system parameters and by suddenly discharging all particles. We then monitored the time evolution of the total charge for each specie.

3. Mean-field calculations

A simple mean-field like calculation, similar to that one employed in the context of chemical reactions [25,26], can give an insight on the charge dynamics for the case of the zero gravitational field. We define the number of particles of the type A (B) with charge q as $A_q(B_q)$, and the number of squares in the wall with