Journal of Electrostatics 71 (2013) 951–957

Contents lists available at ScienceDirect

Journal of Electrostatics

journal homepage: www.elsevier.com/locate/elstat

Discrete element modeling of triboelectric charging of insulating materials in vibrated granular beds

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ARTICLE INFO

Article history:
Received 26 March 2012
Received in revised form
26 July 2013
Accepted 4 August 2013
Available online 30 August 2013

Keywords:
Electrostatic processes
Triboelectric charge
Granular materials
Discrete Element Method (DEM)
Vibrated beds
Computational electrostatics

ABSTRACT

The triboelectric charging of granular insulating materials is very difficult to predict because of the complex physical mechanism involved in this process. The aim of this paper is to describe in detail the implementation of a numerical model of the tribocharging process taking place in vertically-vibrated beds of granular plastics. The charge exchanged in granule-to-granule and granule-to-wall collisions is computed by taking into account some electrical properties of the respective materials, their area of contact and the effect of the electric field generated by a system of high-voltage electrodes and by the charges of the granules themselves. The electrical model is coupled with the Discrete Element Method (DEM) which undertakes the whole granular dynamics and allows to compute accurately the contact surface of two colliding particles which is involved in the triboelectric charging model.

Beside the numerical simulations an experiment has been conducted with mixtures of mm-size polyamide and polycarbonate granules in a laboratory vibrated bed to validate the model. The numerical results have been found to be in good agreement with the experimental ones.

1. Introduction

Tribolelectrization of granular insulating materials is a complex physical phenomenon having both useful and hazardous effects [1,2]. The electrostatic separation of insulating materials [3,4] and the charging of toner particles for photo-copiers and laser-printers [5] are two of its major applications, which are perhaps less known than its disastrous effects: the explosions of flour mills, cereal silos and supertankers, due to electrical discharges occurring between charged granules [6,7]. Other effects of tribocharging are less spectacular, but may disturb the normal operation of industrial installations; for instance, the electrostatic adhesion forces between charged powders and the transport pipes in chemical or pharmaceutical industry may reduce the flow-rates at which such materials are processed [8].

Many physical models have been proposed to simulate the tribocharging effect [8–13], and most of them are based on the colliding surface area and surface state [9,10,14]. The aim of the present paper is to validate a model suitable for the simulation of tribocharging processes in vertically-vibrated granular beds, in relation to possible application to the electrostatic separation of plastics in the recycling industry.

Studies that have been carried out during the last decade at the University of Poitiers pointed out that various types of vibratory feeders [15] and fluidized beds [16–18] can be successfully employed as tribocharging devices for granular plastics. The tribocharged granules can be then passed through the electric field of an electrostatic separator, so that the Coulomb forces acting on them to achieve the selective sorting of the constituents of the processed granular mixtures [19].

This paper aims at modeling of triboelectric charging in vibrated granular beds. In order to simulate such a multi-physics problem, the global model should be able to estimate the charge exchange between two particles when they collide due to mechanical forces induced by the vibration of the bed. Therefore the authors elaborated an original electrostatic model for simulating the electric charge exchange, and made use of a well-established mechanical model for taking into account the particle collisions. These two models were coupled via the contact area between the colliding particles. The tribocharging model presented in this paper is mainly based on the works done by Ali et al. [10] and Schein et al. [11], while the granular dynamics through the contact forces is modeled by the Discrete Element Method (DEM) that is commonly utilized for such granular flows like those found for example in pneumatic conveyors or hopper emptying [20].

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http://dx.doi.org/10.1016/j.elstat.2013.08.001

The reminder of this paper is organized as follows. In the following section the charge exchange model is described and some theoretical principles are introduced. In the next section a detailed implementation of the Discrete Element Method is provided to facilitate the understanding of the coupling between the electrical and mechanical models. Some additional implementation details are given in Section 3 especially concerning an important feature of the model based on the work functions. In Section 4 the mean charge dynamic is experimentally measured and numerically computed for two types of insulating particles of Polycarbonate (PC) and Polyamide (PA). These results are compared and discussed. Finally, a conclusion is drawn in Section 5.

2. Electrical and mechanical models

The purpose of this study is to determine the charge exchanged between colliding particles and estimate the final charge hold by each of them. The particles considered in this study make up a granular bed which is subjected to mechanical constraints such vibrations. The first step of the numerical algorithm consists in the computation of the contact forces between colliding particles. The location of each particle is determined by twice integrating the second's Newton's law. From these new positions, contact detection can be processed and new contact forces can be computed. The computation of the contact forces has been done using the Discrete Element Method (DEM), which is a soft sphere model based on the concept of overlapping particles. Indeed, during the collision, the deformation of the two particles is represented by an overlap that allows computing of the contact forces in a next step. The electrostatic model employed for the computation of the charge exchanged during the collision is based on the contact area between the two impacting particles (see Fig. 1). The whole computation process is integrated in a transient time loop which involves the mechanical model and the electrostatic one which are coupled together via the contact area. The numerical integration of the second Newton's law requires the simulation time to be discretized into small time steps and the purpose is to determine the charge exchanged between two particles during to consecutive time steps n and n + 1.

2.1. Electrostatic model

The starting point of the model is derived from equation (1) which expresses, in the high density limit of surface state theory, the charge exchanged per unit area between two insulating surfaces [11]. Furthermore this theory has been extended to model charge exchange between insulating particles involved in electrophotographic processes [11–13].

This model links the charge σ_{ij} exchanged per unit area during the collision process between two particles i and j with surface work functions Φ_i and Φ_j needed to extract an electron from their surfaces. It also depends on some physical properties of the materials in contact.

$$\sigma_{ij} = \frac{\varepsilon_0}{\delta.e}\left(\Phi_i - \Phi_j - \vec{E}_{ij}.\frac{\vec{d}_{ij}}{\left\|\vec{d}_{ij}\right\|}\delta.e\right) \tag{1}$$

where: ε_0 is the permittivity of free space; δ is the cutoff distance of the charge transfer (typically 500 nm); e, the electron charge; $\vec{E}_{ij}$ is the electric field. $\vec{d}_{i,j} = \vec{X}_i - \vec{X}_j$ is the position vector between the two particles.

Therefore, when a collision occurs between the ith and jth particles, it can be deduced from (1) that the variation of the total charge exchanged between two consecutive time steps n and n + 1 can be expressed as follows:

$$\Delta q_{ij}^{n\to n+1} = \Delta A_{ij}^{n\to n+1}\frac{\varepsilon_0}{\delta.e}\left(\Phi_i - \Phi_j - \vec{E}_{ij}^{n}.\frac{\vec{d}_{ij}}{\left\|\vec{d}_{ij}\right\|}\delta.e\right) \tag{2}$$

where $\Delta A_{ij}^{n\to n+1} = A_{ij}^{n+1} - A_{ij}^{n}$ represents the contact surface variation between particles i and j during one time step and $\vec{E}_{ij}^{n}$ is the electric field located at the point of impact between the two particles at previous time step n.

The determination of the surface contact variation ΔA_{ij} is not straightforward and depends greatly on the contact force between the particles. To tackle this problem, some authors [12] have proposed to specify an averaged contact area $\langle \Delta A_{ij} \rangle$ for all collisions in the domain which would depend on the size and on the total number of particles. This option might be satisfactory if the spatial distribution of the particles were uniform. In our case, the model is meant to be applied to fluidized and vibrated beds of granular materials, which are characterized by a wide disparity in term of particle size and volume concentration. Ali et al. [11] have related the contact surface to an assumed contact force F^C between the particles but without computing it.

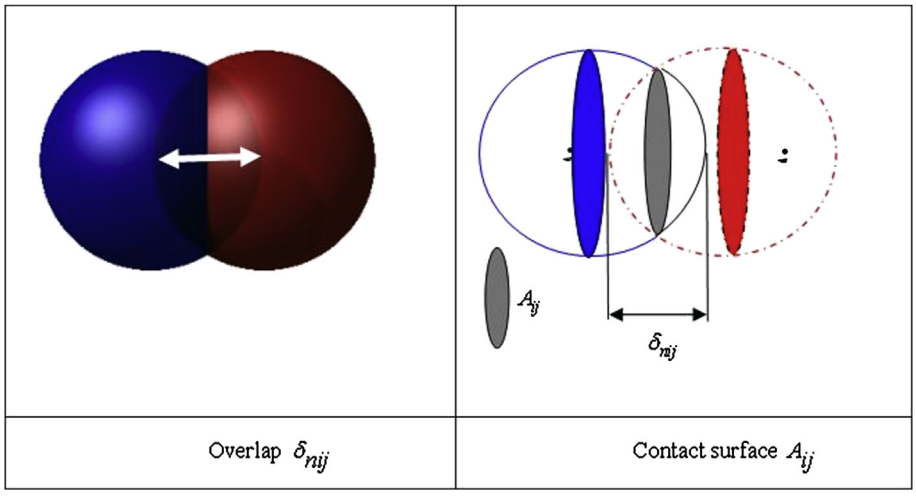

Fig. 1. Definition of the contact surface and the overlap between two particles.