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Contact electrification and charge distribution on elongated particles in a vibrating container

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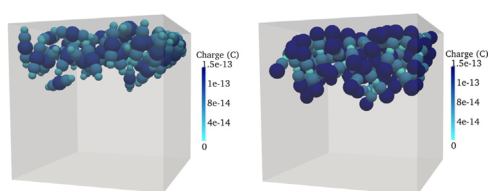
HIGHLIGHTS

- A contact electrification model is applied to analyze the charge transfer process.
- A multi-sphere method is used to model the elongated particles.
- Higher net charge is obtained on the larger primary sphere.
- The maximum surface charge increases with the shape factor.

GRAPHICAL ABSTRACT

Charge distributions for particles with different shape factors during the container vibration.



(a) $\delta = -0.65$ (d) $\delta = 0.65$

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ABSTRACT

The electrostatic charge can be transferred between particles during collisions. The particle shape plays an important role and, in the current study, the charge accumulation and distribution on elongated particles in a vibrating container are investigated using a discrete element method, in which a contact electrification model is implemented. The elongated particle geometry is modelled using a multi-sphere approach. Five different shapes are considered and characterized using a shape factor, δ, which is defined as the ratio of the difference of the radii between the distal sphere and central sphere to the mean radius of the particle. It is found that the net charge on the central sphere is greater than that on the distal sphere when $\delta < 0$. For a particle with $\delta > 0$, greater net charge is accumulated on the larger distal sphere. The maximum surface charge difference between the distal and central sphere increases as the shape factor increases. The net charge of the granular system with different particle shapes achieves an equilibrium state during the vibrating process. This accumulating process follows an exponential trend.

1. Introduction

Contact electrification is a charge transfer process between objects during collisions in powder handling processes. The contact potential difference, which is considered as the difference in electron affinities, is the driving force during contact electrification so that the charge is transferred from one surface to another during contact (Matsusaka et al., 2000, 2010). However, for highly insulating materials, the transferred charge can be retained on particle surfaces due to slow electrostatic relaxation and redistribution (Haenen, 1976; Kornfeld, 1976), which will lead to a non-uniform charge distribution on particles. With the accumulated charge, the induced electrostatic force can become dominant and lead to undesirable phenomena, such as particle aggregation and segregation (Grzybowski et al., 2003; Pei et al., 2010; Nwose et al., 2012). Therefore, the study of charge accumulation and

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distribution on particles is important for a more detailed understanding of particle dynamics in powder handling processes.

Surface charge distribution on insulating materials was examined experimentally by Liu and Bard (2009) and Rezende et al. (2009). Liu and Bard (2009) used a corner of a piece of poly(methylmethacrylate) (PAMM) as a pen to rub on the surface of polytetrafluoroethylene (PTFE) with a predefined pattern (Chinese characters). Then graphite powder was used to decorate the surface of the PTFE. It was observed that the powder was only attracted and located in the rubbed area and made the predefined pattern visible. This indicates a non-uniform distribution of charge on the surface of the insulating material. The transferred charge on the surface of the PTFE can be stable in the contact area over many minutes. Rezende et al. (2009) reviewed several experimental measurement methods, especially for charge detection on insulator surfaces and found that the charge distribution on the surface of insulators can have complex and different patterns. For example, Kelvin force microscopy (KFM) was used to obtain the electric potential distribution (image) of poly (styrene-co-acrylamide) (PS-AAM) latex particles dried on the mica. It is found that, due to the anisotropic electrical polarity of the particle, the electric potential on the surface of the particle was not uniformly distributed and there was excess concentrated charge on the particle. However, if the charge concentration is relatively small (*e.g.* $<10^{-10}$ mol/l), it is still difficult to quantify and analyze the charge density and distribution even with some sensitive methods, such as the analytic transmission electron microscopy method (Rezende et al., 2009).

Particle shape plays an important role in charge transfer during contact. Watanabe et al. (2007) investigated the contact electrification of various pharmaceutical particles impacting a tilted steel surface and found that, assuming the particle is spherical, the transferred charge is generally linearly proportional to the estimated contact area. However, ethylcellulose particles developed a different transferred charge from that calculated by assuming a spherical particle shape. It was concluded that the irregular shape of an ethylcellulose particle might result in sliding or rolling after impact, which would change the contact area and the charge transfer process. Ireland (2010a,b) observed different modes of contact, including sliding (contact), rolling and bouncing when particles were dropped on a titled surface. Ireland (2010b, 2012) argued that the irregular shape of a particle could affect the modes of contact and the contact area and subsequently the charge transfer and distribution during contact.

It is still difficult to apply the above experimental methods during powder handing processes to determine the surface charge distribution concurrently. Therefore, numerical methods have also been employed to understand the electrostatic charge distribution on a particle surface in a granular system during collisions (Duff and Lacks, 2008; Liu et al., 2010; Ireland, 2012). Duff and Lacks (2008) randomly generated points on the surface of spherical particles and assumed that high energy electrons were trapped at these points. A hard-sphere model was then used to simulate the motion of the particles with initial random velocities. When the points on a given particle were within the contact region, the trapped electrons would be transferred to the region with the lowest energy state on the contacting particle. Although the initial surface charge density was identical for particles with different sizes, it was shown that larger particles were charged positively while smaller particles became negatively charged. Although this method utilised the randomly generated points with high energy electrons to represent the charge distribution on the surface of a particle, it was not able to accurately analyse the charge transfer and the charge distribution during collisions.

In order to determine the charge distribution, the particle surface is usually divided into meshes or elements so that the charge concentration in each element could be determined and subsequently the charge distribution could be obtained. Liu et al. (2010) discretized the surfaces of spherical particles and a cylindrical electrode into meshes and used a boundary element method (BEM) to simulate the charge distribution on the surface of the particles induced by an electric field. A discrete element method (DEM) was applied to simulate the dynamics of the particles in the electric field. The induced electrostatic interactions forced particles to deposit on the cylindrical electrode and form straight particle chains. This method can be used to calculate the electrostatic interactions and model the surface charge distribution for conductors and dielectrics. However, in order to determine the surface charge generated by contact electrification within a collisional system, this method can be extremely computationally intensive as finer meshes are required to detect the contact region especially when 3D irregularly shaped particles are considered. Ireland (2012) modelled the charge transfer between a 2D elliptical particle and a tilted surface during impact using DEM. The surface of the particle was discretized into segments and the charge was only transferred onto the segments inside the contact region because of the insulting nature of the particle. It was shown that, when the particle made contact with the surface, a smaller roundness ratio, which was defined as the ratio of radii between the major and the minor axis, lead to a larger contact area. And also the transferred charge was greater with a larger contact area, which meant that the charge transfer process could be affected by the particle shape.

In the current study, a 3D discrete element model for contact electrification of irregular shaped particles is developed. The charging process and charge distribution on particles in a vertically vibrating container are modelled. The contact frequency at different parts of the particle is further examined to explore its relationship with the charge distribution on the particles.

2. The DEM model

Using a current DEM computer programme (Kafui et al., 2002), elongated particle shapes were approximated using the symmetric multi-sphere model (Favier et al., 1999) in which a particle is assembled by a row of primary spheres of various sizes with negligible overlaps (*i.e.* $<5\%$ of the sphere radius). For each particle, the primary spheres are rigidly connected without relative movement. Thus, the mass and moment of inertia of the particle can be calculated as a summation of all the primary spheres. Contact detection and contact force calculation are based on the primary spheres. The contact of particles is detected between constituent primary spheres as shown in Fig. 1.

Contact forces and moments between primary spheres of different particles are calculated once the contacts between these primary spheres are determined, as illustrated in Fig. 2. For elastic particles, the normal contact is modelled using Hertz theory (Johnson, 1985), and that of Mindlin and Deresiewicz (1953) is employed for the tangential interaction. The contact forces and moments are first summed on each primary sphere, s, as

$$\mathbf{f}_s = \sum_{c=1}^{c_n} (\mathbf{f}_{nc}^s + \mathbf{f}_{tc}^s) \tag{1}$$

$$\mathbf{M}_s = \sum_{c=1}^{c_n} (\mathbf{r}_{sc} \times \mathbf{f}_{tc}^s) \tag{2}$$

where $\mathbf{f}_{nc}^s$ and $\mathbf{f}_{tc}^s$ are the normal and tangential contact force at the contact point c, respectively; $\mathbf{r}_{sc}$ is the vector from the centre of the primary sphere to the contact point c; c_n is the total number of contacts on the primary sphere; $\mathbf{f}_s$ and $\mathbf{M}_s$ are the resultant force and moment, respectively.

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