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Discrete element modeling of electrostatic charging of polyethylene powder particles

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ABSTRACT

The contacts of particles with a device wall as well as mutual particle collisions cause the redistribution of charge in systems with powder particles. This, usually undesirable phenomenon known as triboelectric charging, leads to operational problems and safety risks in industrial systems, e.g., in fluidized-bed polymerization reactors. We focus on the charging of polyethylene powder particles caused by the particle-particle interactions. Our model utilizes the Discrete Element Method (DEM) for the description of the particle motion and involves the balance of transferable charged species to quantify the triboelectric charging of particles in contact. The model predicts the charging dynamics of polyethylene powder particles in systems of various particle size distributions (PSD) and addresses the influence of segregation of particles on charging. Our simulation results are in agreement with two general trends in charging that are often observed in both industrial and naturally-occurring particulate systems: (i) Charging is most pronounced in systems with wide PSD and (ii) small particles charge mostly negatively, whereas big particles typically carry positive charge. Subsequently, our results suggest that particle segregation plays an important role in the charging dynamics of particulate systems, as segregation of particles of different sizes can alter PSD locally. It is important to include electrostatic forces in charging models, especially in systems that exhibit significant charging. Specifically, electrostatic attraction among unlike charged particles leads to the 'orbiting motion' of particles that is followed by the formation of particle aggregates.

1. Introduction

The friction contact between two objects is sufficient for the asymmetrical transfer of charged species and subsequent charging known as triboelectrification. While it is easy to generate such a charge, it is remarkably difficult to discharge objects, particularly those that are good insulators. Consequently, we are surrounded by an excess of electrostatic charge, concentrated mostly on surfaces of insulators. Although triboelectrification is advantageously exploited in some applications [1–4], the excess electrostatic charge is often viewed to possess a significant threat for industry in case that the products are dielectric powder particles (e.g. flour, drugs or polymers). These powder particles repeatedly undergo various particle-particle and particle-wall friction contacts during their production and transport, thereby resulting in a charge being generated on the particle surface. Both the repulsion of like-charged particles and the attraction of oppositely-charged particles severely complicate the manufacturing and storage of these powders. Since there is no simple way of discharging the particles, it is necessary to understand the charging process in order to reduce the undesirable charging. However, it is difficult to perform well-defined experiments with good repeatability, because the samples used for such measurements usually have a random initial charge and the charging dynamics can be altered by a simple change of the particle surface texture or composition (among other factors). Mathematical modeling is beneficial for the better understanding of electrostatic charge-related problems, because it enables detailed analysis of various phenomena and their mutual interactions.

Historical approach in this field is based on triboelectric series [5–7] for describing the charging process. The triboelectric series is a list of materials sorted according to experiments in such a way that a material from the upper part of the list 'earns' a positive charge after the friction contact with a material from the lower part of the list. However, triboelectric series predictions can quantify the

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charging process only in the limited cases in which the materials are always of the same friction type and geometry (e.g., rubbing of two parallel planes). Moreover, the triboelectric series inherently predicts no charging for the friction contact between objects of the same material, although the opposite has been observed both in natural and industrial systems [8–12]. To conclude, despite the mentioned limitations, the order of materials in triboelectric series suggests the trends in tribocharging especially for materials which lay far from each other in the series.

In order to quantify tribocharging, models utilizing the concept of work function were introduced first [13]. The driving mechanism of charging in these models is the difference of work functions for the various materials in contact. The concept states that for two metal bodies in contact the thermodynamic equilibrium is established and free electrons at the interface are shared and eventually transported proportionally to the difference in the work function of the two metals. The charge transferred during the collision of metals is then proportional to the contact potential difference and to the capacitance at separation distance of approximately 1 nm, where electron backflow tunneling no longer appears.

Aiming to describe the insulator-metal and insulator-insulator contact charging, the concept of effective (apparent) work function replaced the standard work function [14]. This effective work function was assigned to the insulator in the contact. However, the main criticism of effective work function model was that unlike in metals, there are no free charge carriers in insulators. Also to this point, none of the approaches was able to describe either the tribocharging of insulators made of the same material or the influence of asymmetric friction on charging.

Therefore, the Surface States theory was developed, assigning the effective work function only to the surface of insulators in a particular way. Specifically, Surface States theory assumes the existence of number of electrons with high energy within the forbidden gap present at the nonhomogeneous surface of insulators [9,15]. These electrons can be exchanged between mating insulator surfaces proportionally to the difference between the effective work function associated with the two materials. This theory has two limits – high and low density limit. For the high density limit, the charging is limited by electric field generated due to the charge transfer across the interface. Such an approach was successfully utilized mainly in models of bipolar toner particle charging [16]. In the case of low density limit, finite number of high energy electrons that can be transferred is present on the surface of insulators [17,18]. The existence of such high energy trapped electrons is supported by experiments utilizing photoluminescence and thermoluminescence [19].

The low density limit of Surface States theory was recently utilized in models of Lacks et al. [17] aiming to explain the charging of granular particles made of the same material. Specifically, Lacks and co-workers suggested that the electrons trapped in high energy states on particle surface are transferred during particle collisions from one particle to another (and also in the opposite direction) until they are depleted. Both their probabilistic model [18] and also the event driven particle dynamics model [17] predicted the charging of granular materials due to the particle-particle contact in a qualitative agreement with observations of both natural and industrial granular particles tribocharging behavior in air [8–12]. That is, the bigger particles in the powder mixture tended to gain positive charge and the smaller ones the negative one. Such bipolarity in charging by particle size was first experimentally demonstrated by Castle/Incullet research group [10,20] and is further supported by other researchers [21–23]. It is still unclear, what charged species are transferred (ions, electrons) and also what is the exact mechanism of charge transfer. However, recent experiments suggest that trapped electrons are not necessary ingredient for same-material tribocharging [24]. It is important to note that although Lacks et al. attribute the charging to trapped electron transfer, there is nothing special in their models specific to electrons and thus analogous model predictions would be obtained with negative ions instead of trapped electrons as transferable charged species [25].

The models of Lacks et al. [17] don't include a connection to some particular real system through appropriate particle dynamics description. Their probabilistic model was based on the assumption that big particles are more likely to collide than the small ones due to the particle radius. The models also involved hard-sphere approximation, thus the radius of particle contact area during a collision was involved as a fitting parameter and neither the mechanical properties in the form of parameters associated with the granular material, nor the forces acting among the particles were involved. On the other hand, their models provided a valuable insight into particle-particle charging, showing that geometric asymmetry may be sufficient for bipolar charging in granular systems, thus providing a solid base for further development of particulate models of charging.

Although our model was inspired by the idea of trapped electrons, we formally use more general term transferable charged species (TCS) instead of trapped electrons, in order to reflect recent experimental results that question the role of trapped electrons in charging [24]. In order to make a step towards the practical application of the approach of Lacks et al., we pair the balance of TCS with the Discrete Element Method (DEM) involving Hertzian model of contact [26] and Coulomb's law (Fig. 1). This enables us to include both material properties and forces acting among particles. Subsequently, we compute contact area of colliding granular particles and thus also the number of transferred TCS during each collision. We apply our model to the prediction of the charging of spherical polyethylene particles caused by particle-particle collisions, not only as a function of particle size distribution and particle segregation, but we also address the effect of electrostatic forces on charging. We compare the influence of these parameters on the charging of polyethylene particles in order to contribute to a better understanding of the complex phenomenon of triboelectric charging.

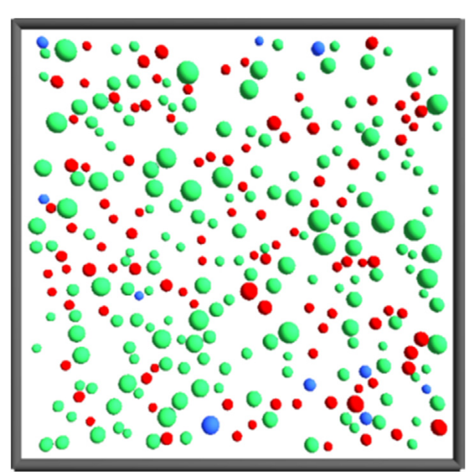

Fig. 1. A snapshot from our model simulation depicting polyethylene particles enclosed in a periodic box. Blue color - particles with no charge, red color – negative charge, green color – positive charge. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)