

# Discrete element method modeling of the triboelectric charging of polyethylene particles: Can particle size distribution and segregation reduce the charging?

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**Abstract.** Polyethylene particles of various sizes are present in industrial gas-dispersion reactors and downstream processing units. The contact of the particles with a device wall as well as the mutual particle collisions cause electrons on the particle surface to redistribute in the system. The undesirable triboelectric charging results in several operational problems and safety risks in industrial systems, for example in the fluidized-bed polymerization reactor. We studied the charging of polyethylene particles caused by the particle-particle interactions in gas. Our model employs the Discrete Element Method (DEM) describing the particle dynamics and incorporates the ‘Trapped Electron Approach’ as the physical basis for the considered charging mechanism. The model predicts the particle charge distribution for systems with various particle size distributions and various level of segregation. Simulation results are in a qualitative agreement with experimental observations of similar particulate systems specifically in two aspects: 1) Big particles tend to gain positive charge and small particles the negative one. 2) The wider the particle size distribution is, the more pronounced is the charging process. Our results suggest that not only the size distribution, but also the effect of the spatial segregation of the polyethylene particles significantly influence the resulting charge distribution ‘generated’ in the system. The level of particle segregation as well as the particle size distribution of polyethylene particles can be in practice adjusted by the choice of supported catalysts, by the conditions in the fluidized-bed polymerization reactor and by the fluid dynamics. We also attempt to predict how the reactor temperature affects the triboelectric charging of particles.

## 1. Introduction

Triboelectrification is an undesired phenomenon in a vast majority of industrial processes, mainly in powder processing (polymers, drugs, flour). Although the triboelectric charging of dielectrics in natural and/or industrial systems has been observed for centuries, it is still inadequately understood and it lacks quantitative description. It is difficult to perform well-defined experiments with a good repeatability, since samples used for the measurements usually have random initial charge and the charging dynamics can be altered among other factors by a simple change of the particle surface. Thus mathematical modeling seems to be beneficial to aid in the better understanding of the electrostatic charge related problems.

## 2. Trapped electron approach

In this work, we follow the approach of Lowell and Truscott [1], who assume the existence of the insulator particle surface electrons that are trapped in the high energy levels of surface orbitals - even if equilibrium surface electron energy states distribution predicts them to be in a lower energy state. The non-equilibrium of surface electron energy states can last even for years, depending on the material of the insulator particle [2]. Due to the high surface resistivity of insulator materials (including polymers), the trapped high-energy (HE) electrons on the particle surface cannot be transferred to the state of lower energy on the same particle. However, the HE electrons trapped on the particle surface can be transported during the particle collision to a vacant low-energy (LE) level on



the surface of another particle. This theory was utilized for modeling of triboelectrification in granular systems by Lacks [3]. We shall call this approach the ‘Trapped Electron Approach’ (TEA) in this paper.

### 3. Model description

We have developed spatially 2D dynamic model of colliding polyethylene particles involving the contact charging (triboelectrification). The particle dynamics is computed using Discrete Element Method (DEM) incorporating Hertzian [4] description of solid particle contact mechanics and Coulomb’s law representing the electrostatic effects. Each particle is represented by a discrete element  $i$  in our model. The DEM utilizes Newton’s second law to track the motion of each particle  $i$  (equation (1)):

$$\frac{d^2 \mathbf{x}_i}{dt^2} = \frac{d\mathbf{v}_i}{dt} = \frac{\sum_j \mathbf{F}_{i,j}}{m_i}. \quad (1)$$

Here,  $\mathbf{x}_i$  and  $\mathbf{v}_i$  represent particle position and particle velocity, respectively, and  $m_i$  stands for the particle mass. The velocity and the position of each particle at each time step are thus computed, since the sum of forces  $\mathbf{F}_{i,j}$  acting between particle  $i$  and another particle  $j$  are precalculated for all the particle pairs. Considered forces are Hertzian elastic repulsive force and Coulomb electrostatic force. We utilize the principle of additivity in order to sum up the force effects of all particles acting on particle  $i$ .

Triboelectric charging of polyethylene particles in our model is implemented as TEA. Inspired by the work of Lacks [3], we simply assume that electrons on a particle surface can be present only in two energy levels; that is a high-energy (HE) state and a low-energy (LE) state. In the beginning of our simulations, all particles are considered to have neutral charge and the same surface density of HE electrons (since it is a material property). We set the initial value of LE surface density to be zero, since LE electrons cannot be transferred. The HE electrons are transferred from a particle to another (or in both ways) during their mutual collisions. We assume that during such collision all the HE electrons present on the contact area of the two colliding particles are transferred according to equations (2) and (3):

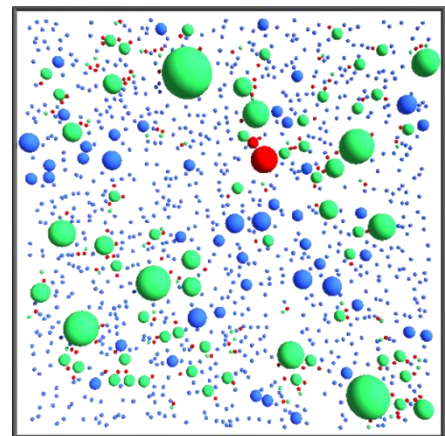
$$n_{i,j}^e = \rho_i^{HE} A_c \quad (2)$$

$$n_{j,i}^e = \rho_j^{HE} A_c, \quad (3)$$

where  $n_{i,j}^e$  and  $n_{j,i}^e$  stand for the number of electrons transferred from the surface of particle  $i$  onto particle  $j$  and vice versa, respectively,  $\rho^{HE}$  refers to the number of HE electrons present on the surface of given particle.  $A_c$  represents the maximum collision contact area, i.e., contact area at the moment, when the distance between the colliding particles centroids reaches its minimum value. The numbers of HE and LE electrons on each particle are recorded in each time step, thus the particle charge at each time step can be calculated using equation (4):

$$Q_{i,t} = [(n_{i,0}^{HE} - n_{i,t}^{HE}) - (n_{i,t}^{LE} - n_{i,0}^{LE})]q, \quad (4)$$

where  $Q_{i,t}$  is the charge of particle  $i$  in time  $t$ ,  $n_{i,0}^{HE}$  and  $n_{i,t}^{HE}$  denotes the number of HE electrons present on the particle in the beginning of the simulation and in time  $t$ , respectively; and  $n_{i,0}^{LE}$  and  $n_{i,t}^{LE}$  are analogical variables related to LE electrons. In equation (4),  $q$  represents the charge of an electron. It is convenient to think of equation (4) as of a simple electron balance:



**Figure 1.** An example of the colliding particles snapshot from the DEM model simulations.

$$[charge] = [electrons\ donated] - [electrons\ accepted]. \quad (5)$$

Once all HE electrons initially present on the particle surface are depleted (transferred), the charging process and thus also the simulation is finished.

### 3.1. Model assumptions

In terms of contact mechanics, we assume perfectly elastic, perfectly spherical solid particles with negligible adhesion and no permanent particle deformation. We further assume that the electrons are uniformly distributed on the particle surface.

The charge transfer is considered to be much faster than the collision time of particles. We thus consider the charge accumulation to be in quasi-stationary state, i.e., we treat the charge affecting the Coulomb force in the sum of forces in Equation 1 as a constant. The charge transfer is instant (it takes one time step) and the absolute value of the charge transferred is only a little value, since only a little fraction of the HE electrons is transferred during one collision.

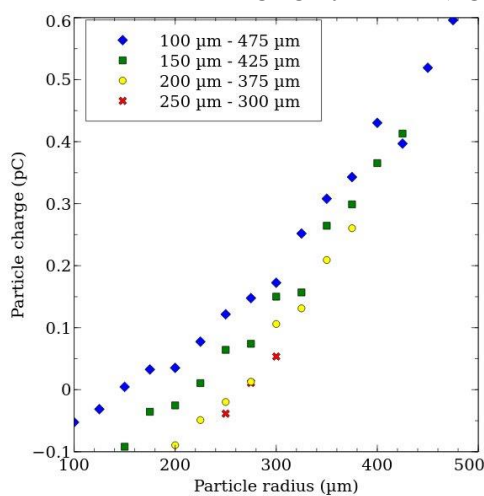
## 4. Results and discussion

### 4.1. The effect of particle size distribution on charging

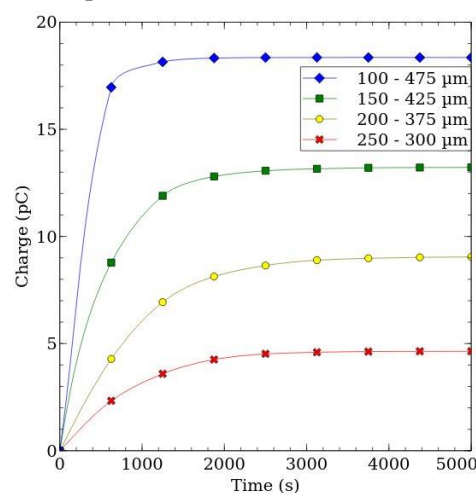
We investigated the charging of spherical polyethylene particles in a spatially 2D box with implemented periodic boundary conditions instead of solid walls. We simulated collisions of particles of various particle size distributions. Although the width of the particle size distribution varied among the simulations, the total mass of the particles and the particle fraction remained constant. The particles were formally divided into several categories according to particle radius and each category contained the same mass of particles. Such a division allows us to deduce on the behavior of real systems like fluidized-bed polymerization reactors, where a constant mass of polyethylene particles is present. For the sake of simplicity, we present results obtained without HE electrons regeneration and without discharge mechanism.

In figure 2 we show the average particle charge at the end of the simulation as the function of particle radius. We can observe a clear trend – big particles tend to gain a positive charge and small particles the negative one. The low absolute value of the average charge for small particles (in comparison to the average charge value for big particles) is expected, because small particles outnumber big particles and the sum of all charges in the system must be inherently zero.

The evolution of the total absolute charge was studied in order to deduce the effect of particle size distribution on the charging dynamics (figure 3). The wider the particle size distribution is the more



**Figure 2.** Average resultant particle charge dependency on the particle size for various particle size distributions.

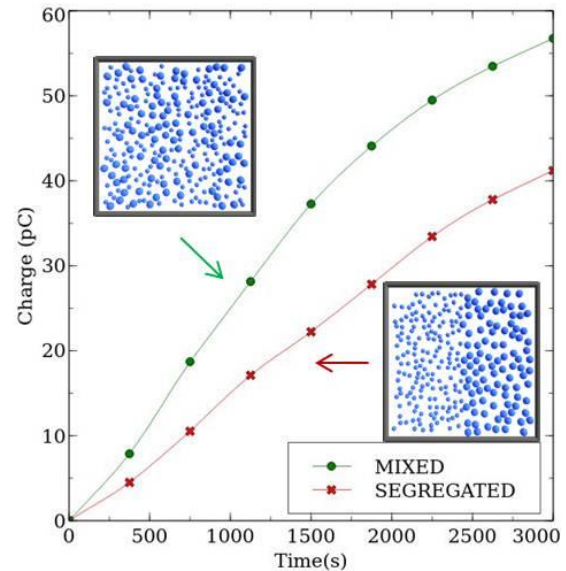


**Figure 3.** The evolution of the total absolute charge for various particle size distributions.

pronounced and faster is the charging. Also the absolute charge value related to the total surface area of particles in the system (surface charge density) increased if the particle size distribution was wider.

#### 4.2. The effect of particle segregation on charging

In this section we discuss the influence of particle mixing/segregation on the triboelectric charging, since in fluidized-bed polymerization reactor, the particle segregation varies and depends mainly on the flow regime. Our simulations involved polyethylene particles of two particle sizes (1.0 mm and 0.6 mm in diameter) in 2D periodic box. The mass, particle number of each size and particle fraction of the system were constant, however, the level of segregation varied (figure 4). We again follow the time evolution of the sum of absolute particle charges. In figure 4 we show that in the system filled with initially well-mixed particles the charging process was roughly about 30% more pronounced. To explain this behavior, we can think of the system with segregated particles as of the combination of two quasi-isolated systems with a narrow particle size distribution. In case of well-mixed particles, we see the system of wider particle size distribution. Since we know that the charging is intensified in systems with a wide particle-size distribution (figure 3), we expect the system of well mixed particles to charge more than the one of segregated particles – which is observed.



**Figure 4.** The evolution of the total absolute charge in the segregated and the mixed system, respectively.

## 5. Conclusions

Although triboelectric charging of polymer powder particles is a significant industrial problem, the phenomenon is regrettably only poorly understood. It is difficult to perform well-defined charging experiments with a good repeatability due to practical complications. As a consequence, mathematical models are unlikely to be quantitatively validated in a short-time perspective, however, such models can provide us with valuable trends and predictions. We present dynamic model of colliding polyethylene particles employing the Discrete Element Method (DEM) approach to describe the particle dynamics. We incorporate the ‘Trapped Electron Approach’ (TEA) as the physical basis for the charging mechanism. Our results indicate that the wider is the particle size distribution, the more pronounced is the charging process. This observation resonates well with the work of Lacks [3] and with the observation of some natural granular particles charging behavior [5]. We further predict that polymer particles significantly segregated in the system charge less than well mixed particles. We note that both the level of the particle segregation and the particle size distribution of polyethylene particles can be in practice adjusted by the choice of supported catalysts, by the conditions in the fluidized-bed polymerization reactor and by the present flow regime.

## References

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