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Effect of humidity on triboelectric charging in a vertically vibrated granular bed: Experiments and modeling

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HIGHLIGHTS

- Humidity effect is modeled for triboelectrification of insulating granular materials.
- Triboelectrification is accounted by humidity dependent effective work function between the materials.
- The proposed model is validated by vertical vibrated bed experiments with different mass loadings.
- The proposed model is used to predict qualitatively fluidized bed behavior compared with small experimental fluidized bed.

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ABSTRACT

Polyethylene particles were tribocharged in a glass container subjected to vertical vibration and the resulting charge per unit mass was measured. The experimental data in conjunction with discrete element method simulations coupled with a tribocharging model were used to deduce effective work function differences between the particles and the glass container at different humidity levels. In addition, we investigated the effect of different mass loadings on the particle charge, and found that the charge increased non-linearly when the mass loading was decreased. The proposed phenomenological model was found to capture this effect. Based on the estimated effective work function difference, it was predicted that a glass-walled fluidized bed of these particles would manifest vastly different hydrodynamics at 20% and 60% relative humidity levels. These predictions were confirmed experimentally.

1. Introduction

Triboelectric charging of granular matter has been studied for decades (Matsusaka et al., 2010; Lacks and Mohan, 2011). It has been observed in multiple experimental studies that triboelectric charging can cause particle agglomeration and wall-particle adhesion in granular (Lim et al., 2006; LaMarche et al., 2010) and gas-solid flows (Rokkam et al., 2013; Jalalinejad et al., 2012, 2015; Fotovat et al., 2016). These effects are typically unwanted and may result in sparking and ultimately even in dust explosions (Jones and King, 1991) or sheeting of the walls with particles in polymerization reactors (Hendrickson, 2006). However, there exist applications, such as triboelectric separators (Mehrotra et al., 2007; Bendimerad et al., 2014) and triboelectric generators (Nguyen and Yang, 2013; Kim et al., 2016), which rely on contact charging of granular matter.

Many aspects of triboelectric charging still remain unknown (Lacks and Mohan, 2011). For instance, what species is transferred during contact charging is under debate. The oldest and most widely known theory suggested by Harper (1967) in his influential thesis is that electrons transfer from surface to surface during mechanical contact of materials. The charge transfer is dictated by work function value, defined as the energy needed to remove an electron from the surface of the material in a vacuum. Contact charging occurs when two surfaces with different work functions come into contact. While this electron transfer model seem to hold reasonably well for conductive materials, it is commonly known fact that work function values correlate poorly with the triboelectric charging behavior of insulators (Lowell and Rose-Innes, 1980; Lacks and Mohan, 2011). As a result, *effective work function* values, which are essentially phenomenological properties, are often used

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instead to describe the contact charging characteristics (Matsusaka et al., 2010).

Whitesides and co-workers (Wiles et al., 2004; McCarty et al., 2007; McCarty and Whitesides, 2008) proposed a different theory in which triboelectric charging occurs through transfer of mobile ions as opposed to electrons. It was hypothesized that the mobile ions might come from ambient humidity (Gouveia and Galembeck, 2009), that would help to explain well-known dependency of triboelectric charging on the relative humidity (Guardiola et al., 1996; Pence et al., 1994; Park et al., 2002; Németh et al., 2003; Schella et al., 2017). McCarty and Whitesides (2008) explained this dependency by the formation of electrical double layer where mobile ions are attached on the surface ions of the material. When the relative humidity is sufficiently small the mobile ions originating from ambient humidity are distributed in isolated patches across the material surface and cannot move freely on the surface. Once two patches come in contact during a collision or rubbing, a water bridge forms between the patches that allow ions to move between the two contacting patches. Increasing relative humidity leads to build up of mobile ions on the surface that causes the patches become interconnected leading to increased surface conductivity. It is thought that the increase in electrical conductivity at the surface layer causes a decrease in triboelectrification (Pence et al., 1994; McCarty and Whitesides, 2008; Choi et al., 2017). Furthermore, a recent article by Waitukaitis et al. (2014) showed that the electrons alone cannot account for the full extent of charge transfer, hence supporting the idea that transfer of another charged species is also involved.

Most of the attempts to model triboelectric charging are based on the concept of effective work function values (Harper, 1967; Matsuyama and Yamamoto, 1995; Laurentie et al., 2013). Models based on particle polarization (Shinbrot and Herrmann, 2008; Siu et al., 2014; Yoshimatsu et al., 2017; Yoshimatsu et al., 2016); particle electron surface density (Duff and Lacks, 2008); high and low energy electrons (Kok and Lacks, 2009); and saturation charge surface density limited by dielectric break-down (Korevaar et al., 2014) have also been examined in the literature, primarily to probe how charge transfer occurs between seemingly similar materials. However, effective work function based models appear to be the primary vehicle to examine charge transfer between two different materials. The present study focuses on analysis of tribocharging based on effective work function.

Laurentie et al. (2013) proposed a triboelectric charging model based on effective work function concept, and calibrated the effective work function by comparing discrete element method (DEM) simulations of tribocharging in a vibrated bed with experimental data. Essentially the same model was used in recent papers by Naik et al. (2015, 2016) to model tribocharging of pharmaceutical powders flowing in a chute; in these recent studies, effective work function values were based on quantum chemical calculations, instead of calibration through experiments as in Laurentie et al. (2013), and the charging predictions agreed fairly well with experimental measurements.

The present study examines whether an effective work function difference based tribocharging model can be used in a phenomenological sense to capture the effect of humidity. Clearly, in such a model the effective work function difference between the particles and the container wall would have to be a function of humidity level. We have performed vibrated bed experiments at different mass loadings of polyethylene particles held in a glass container and different humidity levels, and determined the average charge acquired by the particles. These experiments were then supplemented by a simulation study based on the effective work function approach presented in Laurentie et al. (2013) to determine the dependence of the effective work function difference on humidity level. As discussed in the experimental section, the charge per unit mass acquired by the particles at a fixed humidity level was found to vary with the mass loading of particles in the vibrated bed. To verify the triboelectrification model we performed a simulation campaign with a fixed effective work function difference obtained from our phenomenological model for a given humidity level and variable mass loadings. The specific charge predicted by the simulations is in good agreement with the experimental results. Based on the results, it is then argued that these polyethylene particles would stick to the glass wall of a fluidized bed under low humidity conditions, but not at higher humidity levels. This qualitative prediction was then confirmed experimentally.

2. Mathematical modeling

2.1. Discrete element method

In the Discrete Element Method (Cundall and Strack, 1979), particle motion is tracked by solving Newton's equations of motion:

$$m_i \frac{d\boldsymbol{v}_i}{dt} = \sum_j (\boldsymbol{f}^n_{c,ij} + \boldsymbol{f}^t_{c,ij}) + \boldsymbol{f}_{e,i} + m_i \boldsymbol{g} + m_i \boldsymbol{a} \quad (1)$$

$$I_i \frac{d\boldsymbol{\omega}_i}{dt} = \sum_j \boldsymbol{T}_{t,ij} \quad (2)$$

In the equations, particle i has mass m_i, moment of inertia I_i, translational and angular velocities $\boldsymbol{v}_i$ and $\boldsymbol{\omega}_i$. The forces acting on the particle i are: $\boldsymbol{f}^n_{c,ij}$ and $\boldsymbol{f}^t_{c,ij}$ which are the normal and tangential contact forces between two particles i and j; $\boldsymbol{f}_{e,i}$ which is the electrostatic force on particle i; $m_i\boldsymbol{g}$ is the gravitational force contribution; and $m_i\boldsymbol{a}$ presents external force contribution. The torque acting on particle i due to particle j is $\boldsymbol{T}_{t,ij}$. $\boldsymbol{T}_{t,ij} = \boldsymbol{R}_{ij} \times \boldsymbol{f}^t_{c,ij}$, where $\boldsymbol{R}_{ij}$ is the vector from the center of particle i to the contact point. Rolling friction is not accounted for in this study.

The particle contact forces $\boldsymbol{f}^n_{c,ij}$ and $\boldsymbol{f}^t_{c,ij}$ are calculated using (Johnson, 1987; Renzo and Paolo Di Maio, 2004):

$$\boldsymbol{f}^n_{c,ij} = \frac{4}{3} Y^* \sqrt{r^*} \delta_n^{3/2} \boldsymbol{n}_{ij} + 2\sqrt{\frac{5}{6}} \beta \sqrt{S_n m^*} \boldsymbol{v}^n_{ij}, \quad (3)$$

$$\boldsymbol{f}^t_{c,ij} = \begin{cases} -8G^* \sqrt{r^* \delta_n} \boldsymbol{t}_{ij} - 2\sqrt{\frac{5}{6}} \beta \sqrt{S_t m^*} \boldsymbol{v}^t_{ij} & \text{for } \left|\boldsymbol{f}^t_{c,ij}\right| < \mu_s \left|\boldsymbol{f}^n_{c,ij}\right| \\ -\mu_s \left|\boldsymbol{f}^n_{c,ij}\right| \frac{\boldsymbol{t}_{ij}}{|\boldsymbol{t}_{ij}|} & \text{for } \left|\boldsymbol{f}^t_{c,ij}\right| \geqslant \mu_s \left|\boldsymbol{f}^n_{c,ij}\right|, \end{cases} \quad (4)$$

where

$$\frac{1}{Y^*} = \frac{1-\nu_i^2}{Y_i} + \frac{1-\nu_j^2}{Y_j}, \quad \frac{1}{r^*} = \frac{1}{r_i} + \frac{1}{r_j}, \quad (5)$$

$$\beta = \frac{\ln(e)}{\sqrt{\ln^2(e) + \pi^2}}, \quad S_n = 2Y^* \sqrt{r^* \delta_n}, \quad (6)$$

$$\frac{1}{G^*} = \frac{2(2+\nu_i)(1-\nu_i)}{Y_i} + \frac{2(2+\nu_j)(1-\nu_j)}{Y_j}, \quad S_t = 8G^* \sqrt{r^* \delta_n}. \quad (7)$$

The subscripts i, j denote spherical particle i or j, and the superscript $*$ denotes the effective particle property of those two particles. The effective particle mass m^* is calculated as $m^* = m_i m_j/(m_i + m_j)$; e is the restitution coefficient; δ_n is normal overlap distance; $\boldsymbol{n}_{ij}$ represents the unit normal vector pointing from particle j to particle i; $\boldsymbol{v}^n_{ij}$ represents the normal velocity of particle j relative to particle i; $\boldsymbol{t}_{ij}$ represents the tangential displacement obtained from the integration of the relative tangential velocity at the contact point $\boldsymbol{v}^t_{ij}$ during the collision; and μ_s is the particle sliding friction coefficient. Here, Y is Young's modulus, G is shear modulus, ν is Poisson's ratio, r is particle radius, and variables S_n and S_t are related to tangential and normal damping terms as shown in Eqs. (6) and (7).