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Monte Carlo simulation of pneumatic tribocharging in two-phase flow for high-inertia particles

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Abstract

Pneumatic transport, triboelectrostatic experimentation studying the removal of carbon from fly ash has shown the importance of particle charging on process performance. To further elucidate the influence of particle charging, a tribo-electrification model for charging spherical particles in vertical pipes is proposed. Unlike previous numerical approaches, the charging mechanism is studied in the framework of a charge relaxation process in which the equilibrium charge for uniform and localized charge distributions on the particle surfaces are determined. A recently proposed statistical model was also adopted to evaluate particle–wall collisions for wall-bounded flows, taking into account the influence of particle–particle collisions. Effects of particle concentrations, along with particle size and turbulence intensity, are also investigated. Model predictions are compared with experimental results, with good agreement found if the charge is assumed to be distributed on small surface sector of the particles. After defining suitable probability density functions for the variables considered, a Monte Carlo analysis is employed for simulating particle charge distributions and compared with published measurements to identify the important parameters during particle tribocharging.

Keywords: Monte Carlo simulation; Tribocharging; Gas−solid two-phase flow

1. Introduction

The introduction of low-NO_x burners in the utility industry, and the concomitant increased loss-on-ignition (LOI) contents of ash, has been one factor hindering the use of coal combustion fly ash as an admixture for cement and concrete worldwide. Ash must meet ASTM C618 and C311-902 specifications in the US and the EN-450 specification in Europe if it is to be used as a concrete admixture. Dry separation of unburned carbon from ash eliminates major drawbacks of wet processing, including high water demands, process water cleanup, and ash dewatering.

Pneumatic transport, triboelectrostatic separation is a two-step process in which a mixture of particles is bipolar charged and then separated by using an electric field [1,2]. From a qualitative point of view, it is widely accepted that the mechanism of tribocharging is driven to some extent by the difference in work functions between the particles [3,4]: when a particle collides with a material having a different work function, the Fermi level at the contact point tends to be equalized through electron transfer. Fly ash and silica normally become negatively charged whereas carbon particles normally become positively charged when they are transported within a copper tube [5]. The influence particle charge has on separation efficiency has been highlighted [6], yet a theoretical approach for particle tribocharging in turbulent pipe flows and its relationship to process performance has not been adopted.

Although frictional electrification between insulators is a well known phenomenon, the pneumatic transport of particles in pipes is complicated because of two-phase fluid dynamics, particle–wall and particle–particle collisions. Nevertheless, pneumatic transport tribocharging parameters can be grouped into “single impact” and “fluid dynamics” variables. The former ones are variables determining the charge acquired by a particle with an initial charge q_0, impacting a single time on a metal surface with a

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specified velocity. Fluid dynamics variables define the number of impacts and the impact velocities.

Tanoue et al. [7] developed the first fully predictive tribo-charging model in which single impact charging was based on the condenser model theory and the number of collisions was determined using Lagrangian particle tracking in the fluid field by a $k-\varepsilon$ closure model from Navier-Stokes equations. Two main drawbacks arise from this approach. First, recent studies [8] showed that the condenser model is not completely appropriate for describing single impact charging and Lagrangian particle tracking is computationally too expensive to model the behaviour of non-dilute systems of primary interests in industrial applications. Second, the Lagrangian approach proposed did not consider particle–particle collisions which dissipate particle fluctuating velocities in the case of inelastic collisions even for dilute systems. In the present paper, different approaches are presented both for a single impact model and for particle–wall collisions with high-inertia particles in vertical pipe flow. They are used to elucidate previous results for the particle charge distribution on silica beads [6].

2. Single impact tribo-electrification

As suggested in tribo-electrification experiments using particles having dimensions of millimeters [8] and a few hundred micrometers [9], a linear dependency between the initial charge on a colliding particle and the charge acquired after impact on a metal surface can be expressed as:

$$\Delta q = \frac{\Delta q_0}{q_\infty}(q_\infty - q_0) \tag{1}$$

Depending on the equilibrium charge q_∞, the impact charge varies linearly between 0 and the "initiating impact charge" Δq_0 [10]; the initial charge varies from q_∞ to 0. This equation was first derived in the condenser model framework but its validity was shown in the relaxation model too. The essential difference between these theories is how the equilibrium charge and the charge acquired by an uncharged particle, Δq_0, are handled.

2.1. Equilibrium charge

According to the condenser model theory [11], Eq. (1) can be rearranged to yield:

$$\Delta q = \frac{\varepsilon_r \varepsilon_0 S}{z_0}(V_c - V_e) = \frac{\varepsilon_r \varepsilon_0 S}{z_0}\left(V_c - \frac{2z_0}{\pi \varepsilon_r \varepsilon_0 D_p^2} q_0\right) \tag{2}$$

It's quite evident that the equilibrium charge can be considered to be the initial charge that a particle must possess to cancel the potential caused by the difference in work functions of the touching materials. It was shown [8], however, that the equilibrium charge does not depend on the work function of the metal target but rather it depends only on the particle diameter and relative dielectric constant of the particle. They proposed that as a particle separates from a surface, the potential difference is kept equal to the contact potential difference by a tunnelling effect. In the ~ 1.0 nm tunnelling region the potential difference increases as the contact gap increases because of a reduction of capacitance between the separating surfaces. The potential difference is limited by the gas breakdown process, so that the charge acquired by a particle lowers or relaxes until a potential, equal to the breakdown potential, is induced by the remaining charge on the particle, called "equilibrium charge". Apart from gaseous pressure that controls breakdown potential, as described within Paschen's law, the particle diameter and the relative dielectric constant also play a fundamental role in determining the electrostatic field around a particle near a metal plate: when a particle is larger than the spatial scale of field variation, the image charge generated by the charged particle induces in turn polarization on the particle with an infinite series of higher order polarization, which is enhanced by the permittivity of the particles.

First, the equilibrium charge of a dielectric particle with a uniform charge distribution is addressed and then the equilibrium charge of a dielectric particle with initial charge distributed only on a small surface sector is addressed. The equilibrium charge for a uniform initial distribution, $q_{\infty,\mathrm{u}}$, and the critical contact gap, $d_{\mathrm{c,u}}$, is evaluated by solving the following system of coupled equations, where equality between the breakdown potential V_s and the potential of particles $V_{\mathrm{p,u}}$ and their first derivatives must be set:

$$V_\mathrm{s}(d_{\mathrm{c,u}}) = V_{\mathrm{p,u}}(d_{\mathrm{c,u}}, q_{\infty,\mathrm{u}}) \tag{3a}$$

$$\frac{\partial V_\mathrm{s}}{\partial d}(d_{\mathrm{c,u}}) = \frac{\partial V_{\mathrm{p,u}}}{\partial d}(d_{\mathrm{c,u}}, q_{\infty,\mathrm{u}}) \tag{3b}$$

In order to calculate the potential field around the particle, the re-expansion technique developed by Matsuyama et al. [12] was used.

Another system of equations, in the same form of the previous one, has to be solved to obtain q_∞ and the critical contact gap d_c for a non-uniform initial charge distribution. The system has to be iteratively solved to find the charge distributed on a surface sector described by a solid angle θ_c. The following boundaries of charge distribution:

$$\begin{aligned} \sigma(\theta) &= \sigma \ \text{for} \ 0<\theta<\theta_\mathrm{c} \\ \sigma(\theta) &= 0 \ \text{for} \ \theta_\mathrm{c}<\theta<\pi \end{aligned} \tag{4}$$

induce a potential curve touching the Paschen's curve. In this second case the equilibrium charge becomes smaller as the charging angle θ_c decreases.

For both charge distributions, the numerical solution has been carried out for 25 different particle diameters, ranging from 10 to 1000 μm, and for relative dielectric constants of 1, 2 and 5. Since it has been reported that the relative permittivity of ash is close to four [13] and the permittivity of glass, used in previous experiments of tribo-electrification, is around five [4], these two values were used to approximate those for the particle studied by Li [6]. For the non-uniform charge distribution, calculations were performed using dimensionless variables for charging angles from 5° up to 15°, following the procedure of Matsuyama and Yamamoto [10].