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How does the packing density of a metal screen affect the mechanism for catching highly charged nanoparticles?

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ABSTRACT

Highly charged aerosol nanoparticles of a molecular size (< 5 nm) exhibit complex behaviors caused by random (Brownian) motion and electrostatic interactions (image force) with solid surfaces. The classical single fiber theory, however, can only partially describe the complex filtration mechanism of highly charged nanoparticles. We began this study by employing the Langevin Dynamics (LD) Method to simulate the random motion and deposition of highly charged nanoparticles on a single fiber. The single fiber efficiencies predicted by the LD simulation did not agree with data from experiments using electrosprayed highly charged molecular ions. To explain this mismatch and search for other factors that could potentially affect the capturing mechanism, we investigated the influence of the mesh structure. While the image force exerted a significant influence as the packing density decreased, the influence tended to oppose the theoretical predictions. These results suggested that the fiber-fiber interaction in a wire screen with high packing density significantly influences the collection of multiply charged molecular ions. A new theoretical model describing the influence of inter-fiber interaction will be required to clarify how highly charged molecular ions are captured by image force.

1. Introduction

The special, size-dependent properties of nanoparticles have been attracting increased attention. As nanotechnologies burgeon, industry requires efficient but cost-effective separation technologies that can prevent worker exposure to, and the environmental release of, nanoparticles. Air filtration, one of the most conventional and cost-effective ways to separate nanoparticles from gases, is seriously constrained by the high pressure drop through high-performance filters. Electrical effects have been studied in search of a possible mechanism to increase the collection efficiency without increasing the pressure drop (Brown, 1993).

When a charged particle approaches a conductive surface, it induces a so-called image force with an equal but opposite charge located at the same distance on the other side of the surface. In the case of a metallic filter or mesh, the image force attracts the particle toward the surface, causing the particle to migrate in that direction. The migration velocity depends upon the charge on the particle and the drag forces that oppose the motion. Because the particle is smaller than the mean free path, λ, of the gas molecule, the drag force acting upon the particle scales as the particle diameter, d_p, is squared. Hence, image force strongly influences the collection of very small or highly charged particles.

When these electrical effects are exploited for practical application, an understanding of the behavior of nanoparticles in filtration

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is important to prevent nanoparticle leakage. The behavior of a charged nanoparticle in a filter is difficult to understand, however, as the combination with Brownian motion complicates the electrical motion. Several investigations of this complex motion have been performed using wire screens (meshes) as model filters, as the geometries of real filters are too complex to permit accurate analysis (Alonso, Alguacil, Santos, Jidenko, & Borra, 2007; Heim, Attoui, & Kasper, 2010; Omori et al., 2016; Thomas, Mouret, Cadavid-Rodriguez, Chazelet, & Bémer, 2013). Alonso et al. (2007) measured the filtration efficiency of a metal mesh for particles of 25–65 nm in diameter carrying + 1 - + 3 elementary charges. They explained the collection efficiency by image force and Brownian diffusion using a fitting parameter. Heim et al. (2010) confirmed that collection efficiencies could be expressed according to Alonso's prediction using a metal mesh for singly charged nanoparticles ($d_p = 1.2 - 8$ nm). Several years later, Omori et al. (2016) confirmed fair agreement between the predicted values and experimentally obtained data on the collection efficiency of highly charged molecular ions ($d_p = 2.6$ 4.8 nm, $p = +2$ - $+7$) by a metal mesh. The efficiency with which metal meshes can collect charged nanoparticles has been predictable since their study, but the predictions have not agreed with the theory. This discrepancy may be traceable to the high packing densities of the metal meshes used. When a filter or mesh has a high packing density, the classical single fiber theory fails to account for the interactions between the tightly packed fibers when describing the collection efficiency.

In the present study we sought to better understand the behavior of charged nanoparticles in a neutral metal mesh by clarifying the influence of the packing density. We began by calculating the particle trajectories around an isolated cylinder by numerical simulation with the Langevin Dynamics Method (LD simulation), a useful mathematical tool for modeling the dynamics of molecular systems (Wu & Brooks, 2003). Based on the trajectories, we then calculated the single fiber efficiencies to compare them with previous theoretical correlations and our previous experimental data (Omori et al., 2016). We also investigated the limitations of the single fiber theory by measuring the collection efficiencies of highly charged macromolecular ions by metal meshes composed of fibers of the same diameter packed at different densities.

2. Classical single fiber theory (CFT) for charged nanoparticles

In the diffusion regime, the total single fiber efficiency, η_T, is expressed as the sum of the single fiber efficiencies of Brownian diffusion, η_D, image force, η_{IM}, and the combined effect of diffusion and image force, η_{DIM}, in the following equation (Alonso et al., 2007):

$$\eta_T = \eta_D + \eta_{IM} + \eta_{DIM} \tag{1}$$

The single fiber collection efficiency by Brownian diffusion, η_D, is expressed by Eq. (2) (Cheng & Yeh, 1980):

$$\eta_D = 2.7Pe^{-2/3}, \tag{2}$$

where *Pe,* the Peclet number, is given by,

$$Pe = \frac{ud_f}{D}. \tag{3}$$

A number of investigations on collection efficiency by image force have been performed. Theoretically, the image force effect acting on filtration efficiency scales as,

$$\eta_{IM} = \beta\sqrt{K_{IM}}, \tag{4}$$

where,

$$K_{IM} = \left(\frac{\varepsilon_f - 1}{\varepsilon_f + 1}\right)\frac{Cp^2e^2}{12\pi^2 u\varepsilon_0 d_p {d_f}^2} \tag{5}$$

is the dimensionless image force parameter (Brown, 1993; Yoshioka, Emi, Hattori, & Tamori, 1968), C is the Cunningham slip correction factor, p is the number of charges on the particle, e is the elementary charge, μ is the air viscosity, u is the air flow velocity, and d_f is the fiber diameter. The prefactor, β, in Eq. (4) is a constant of proportionality that has taken different values in previous works. Conventional filtration theory suggests that the prefactor of single fiber efficiency by image force is given by Eq. (6) (Brown, 1993; Yoshioka et al., 1968):

$$\beta = \frac{2}{\zeta^{1/2}}, \tag{6}$$

where ζ is the hydrodynamic factor.

The prefactor has also been investigated experimentally. Lundgren and Whitby (1965) reported a β value of 1.5 in experiments on highly charged solid spherical particles of 0.1 and 1 µm in diameter filtered through three types of filter medias with low packing densities (felt, urethane, glass). Yoshioka et al. (1968) proposed a β value of 2.3 from experiments on the collection of charged oil droplets by a neutral glass filter (a = 0.01). Alonso et al. (2007) measured the collection efficiencies of metal meshes for nanoparticles in a 25 − 65 nm diameter range carrying 1 − 3 elementary charges. They asserted that the pure image force was negligible in the strong diffusional regime ($10^{-7} < K_{IM} < 10^{-5}$) and proposed the empirical equation $\eta_{DIM} = 9.7\sqrt{K_{IM}}$ ($\eta_{DIM} = 29.7{K_{IM}}^{.59}$), where η_{DIM} was proportional to the square root of the K_{IM} assumed from combination of diffusion and image force from their experiments.