The Unipolar Charging Rate and Bipolar Charge Distribution for Nonspherical Particles

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The charging of particles via collisions with ions (diffusion charging) is an integral step in many nanoparticle characterization systems and control technologies. Considerable prior effort has hence been devoted to the determination the diffusion charging rate, i.e. the rate at which ions collide with and transfer charge to particles. With knowledge of this rate, both the increase in net charge on particles in unipolar ion environments, and the steady-state charge distribution on particles in bipolar ion environments can be determined. However, prior analyses are limited to spherical particles; for non-spherical particles, the diffusion charging rate and steady-state charge distributions remain unknown, leaving ambiguities in all electrostatic based analyses of non-spherical particles. Motived by this issue, we have utilized a combination of Brownian dynamics and molecular dynamics simulations to examine (1) the collision rate between particles of arbitrary shape and ions, and (2) the steady state charge distribution on arbitrary shaped particles in the presence of realistic ion populations (with mass and diffusion coefficient distributions determined by tandem differential mobility analysis-mass spectrometry). Results for both of these simulations are provided in this presentation.

In unipolar charging, the collision kernel, which defines the collision rate between particles and ions of known number concentrations, is parameterized by the dimensionless collision kernel H for all shapes, and depends upon the diffusive Knudsen number, Kn_D, the ratio of the ion mean persistence path to a well-defined particle length scale. This particle length scale is a combination of the orientation averaged projected area PA and the Smoluchowski radius R_s of the particle. In the continuum ($Kn_D \rightarrow 0$) and free molecular ($Kn_D \rightarrow \infty$) regimes, the dimensional collision kernel collapses to a particle geometry independent function, expressed in terms of Ψ_E and Ψ_I, the potential energy to thermal energy ratios for the Coulomb and image potentials, respectively. Dimensionlessly, these functions lead to $H = 4\pi Kn_D^2$ as $Kn_D \rightarrow 0$ and $H = (8\pi)^{1/2} Kn_D$ as $Kn_D \rightarrow \infty$. In the transition regime (finite Kn_D), as shown in Figure 1 the dimensionless collision kernel is shown to be geometry independent for conducting particles, depending only on a suitably defined Kn_D.

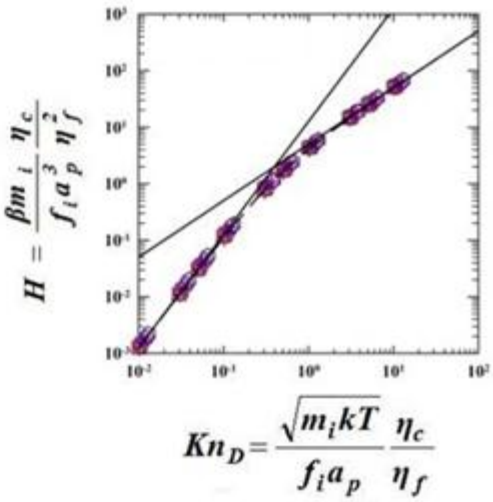

Figure 1. The dimensionless collision kernel, H, as a function of the diffusive Knudsen number, Kn_D, determined from Brownian dynamics calculations of particle charging by unipolar ions. Plotted points represent results for particles of varying geometry and varying number of charges, yet all collapse to a single dimensionless curve. The solid lines shown represent the $Kn_D \rightarrow 0$ and $Kn_D \rightarrow \infty$ limiting expressions.

To study bipolar charging, a Brownian dynamics method is also employed, but which circumvents ion-particle collision rate calculation while still enabling determination of the steady state charge distribution on non-spherical aerosol particles. BD calculations are performed using both monodisperse and measured polydisperse ion properties under atmospheric pressure, room temperature conditions. In the examination of non-spherical particles (aggregates, linear chains and cylinders), two models are employed: (1). accumulated charge distributes itself along particle surfaces, and (2). accumulated charge is immobile. Independent of model, it is found that particles having a Projected Area (PA) to diffusion based surface area (πR_s^2) ratio close to unity have similar bipolar charge distributions to spheres sphere of the same mobility diameter. However, model specific behavior is observed for highly non-spherical particles ($PA/\pi R_s^2 < 0.5$). With distributed charge, highly non-spherical particles acquire more charges than an equivalent mobility sphere in the sub 100 nm range, yet acquire less charge than spheres in the submicrometer range. Conversely with immobile charges, non-spherical particles are found to be more charged than equivalent mobility diameter spheres in both the nano- and submicrometer size ranges.