Monte Carlo based Determination of Arbitrary Shaped Particle Steady State Charge Distributions and Unipolar Charging Rates

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ABSTRACT

Electrical mobility analysis is the predominant method by which aerosol nanoparticle size distribution functions are determined in both field and laboratory settings. To correctly determine the size distribution from electrical mobility analysis, it is necessary to know precisely the charged fraction of particles as a function of particle “size”. Considerable effort has thus been made to determine the diffusion charging rate for spherical particles, i.e. the rate at which ions collide with and transfer charge to particles, such that in an environment of equal positive and negative ion concentrations, particles arrive at a known diameter-dependent steady state charge distribution. For non-spherical particles, however, the diffusion charging rate and steady-state charge distributions remain unknown, leaving ambiguities in all electrostatic based analyses of non-spherical particles. Motivated 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.

Specifically, the dimensionless diffusion charging rate for particles of any shape can be expressed as a function of the diffusive Knudsen number, i.e. the ratio of the colliding ion persistence distance to a clearly defined descriptor of the particle size, and a ratio of the surface potential energy of the particle to the thermal energy of the background gas. Similarly, the steady state charge distribution on an arbitrary shaped particle, under any background gas conditions, and for any ion properties, can be extracted from simulations. Finally, the results of simulations are compared to the commonly used results of Fuchs’s flux matching theory, and it is shown that Fuchs’s approach becomes invalid under conditions of unipolar charging of particles outside the continuum regime.

BIOSKETCH

Chris Hogan is a McKnight Land-Grant Assistant Professor in the department of Mechanical Engineering at the University of Minnesota. He received a BS degree in Biological & Environmental Engineering from Cornell University in 2004, and a PhD degree in Energy, Environmental, & Chemical Engineering from Washington University in 2008, where he was a student of Pratim Biswas. After studying as a Postdoctoral Associate at Yale University in 2008-2009, he joined the faculty at the University of Minnesota in July 2009. He is the recipient of the 2011 Sheldon K. Friedlander Award for “Outstanding PhD dissertation in a field of aerosol science and technology”, and a Japan Society for the Promotion of Science Fellowship in 2010. Currently, his laboratory group, the Nanoparticle Physics Laboratory, focuses on the analysis of mass, momentum, and energy transport processes in nanoparticle-laden aerosols and colloids.