3D Computational Fluid Dynamics Modelling of Direct Ultraviolet Photoionization and Charge Recombination of Ultrafine Particles

R.T. Nishida*, A.M. Boies and S. Hochgreb

Department of Engineering, University of Cambridge, Cambridge, CB2 1PZ, UK

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*Presenting author email: rn359@cam.ac.uk

Ultrafine aerosol particles are electrically charged in a range of devices to enable their detection, capture and control. Charging by direct ultraviolet (UV) photoionization is more efficient than other charging mechanisms such as corona discharge, particularly in size ranges below 50 nm diameter. However, the photoionization behaviour of aerosol ultrafine particles is not well understood. Existing models for photoionization are supplemented with empirically-determined constants which vary for particle size and type. Models often neglect or inadequately capture particle and ion wall losses and flow geometry effects. In this work we model the behaviour of UV particle charging and subsequent charge transport and collection in a continuous flow as a means to evaluate photoionization theory and provide tools for quantitative control of ultrafine particle charge states. The models developed in this work demonstrate state-of-the-art capture of particle transport and charging effects leading to predictive design tools and better design of charging-based devices.

Particles are charged directly by absorbing incoming UV photons and emitting electrons, which differs from diffusive charging that relies on the process of ion-to particle collision or recombination. Photons are absorbed, causing the particles to emit electrons, which in turn collide with the surrounding air forming gaseous ions. During continued irradiation, the particles increase in charge state to the Coulomb limit which can reach upwards of 10 charges per particle (Matter *et al.* 1995). Both the charged particles and ions can be moved by an electric field and captured or be allowed to recombine with the particles into neutral molecules. Diffusional losses of both particles and ions to walls can be significant and affect the resulting charge distribution.

The aim of this work is to provide modelling and simulation of these processes. Non-dimensional analysis is used to indicate regimes under which the photocharging process is dominated by diffusion, electric field transport, convection, photoionization, or recombination. A non-dimensional irradiation time is defined to indicate when the steady-state Coulomb limit is reached as a function of particle size, concentration, material, and light wavelength and intensity. Using these techniques, the geometry, flow rate and electric field may be designed to output a controlled charge distribution.

Relations capturing both photoionization and recombination of ions/particles are modelled in 3D computational fluid dynamics (CFD) for the first time. The model incorporates ion/particle advection/diffusion, wall losses, and electric field transport. Upwards of 50 simultaneous species transport equations are solved to allow the resolution of local charge distribution and average charges per particle for multiple charge states.

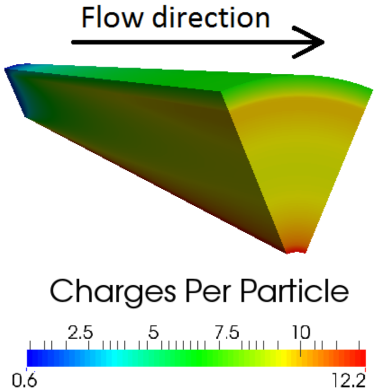

Figure 1. Sample distribution of charges per particle during convective flow under irradiation. The charge level increases in the flow direction due to photoionization.

Previous studies of photo-charging assumed 1D behavior that neglected important 3D phenomena. Results from this 3D study are first verified with existing 1D models for particle charging (Maisels et al., 2002; Maisels et al., 2003). The existing 1D models are then enhanced by incorporating the effect of an external electric field and the validity of assumptions made for diffusional wall losses and external electric field action are evaluated by comparison with results from the CFD model.

The results are presented as a function of parametric variations in the ratios of different terms in the governing equations for particle motion, including charging, transport, and wall loss effects, identifying conditions where simplified models may be valid (or not). Final recommendations are made regarding the level of detail required for the prediction and design of aerosol charging and transport methods.

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