Geophysical Research Abstracts
Vol. 20, EGU2018-1896-1, 2018
EGU General Assembly 2018

Towards a Monte Carlo approach for the nucleation study of neutral and ionic sulfuric acid clusters

Christoph Köhn, Martin Andreas Bødker Enghoff, and Henrik Svensmark
Technical University of Denmark, DTU Space, Lyngby, Denmark (koehn@space.dtu.dk)

The nucleation of molecular clusters is estimated to contribute about half of all cloud condensation nuclei, globally. A central molecule in nucleation is sulfuric acid. Because of their interaction with sulfuric acid dipoles and their relative higher stability clusters with a central hydrogen sulfate ion hereby play an important role in the process of nucleation.

We here present a particle Monte Carlo code to study the growth of sulfuric acid clusters as well as of clusters with central hydrogen sulfate ions as a function of the ambient temperature. For that purpose we have extended our previously developed Monte Carlo model studying the formation of neutral clusters by the motion, clustering and evaporation of ionic clusters.

We initiate a swarm of sulfuric acid molecules of sizes of 0.15 nm with densities between 10^7 and 10^8/cm^3 with and without the addition of hydrogen sulfate ions at temperatures between 200 and 300 K. After every time step, we update the position and velocity of particles as a function of size-dependent diffusion coefficients. For the update of the particle velocity, we take into account the electromagnetic interaction between ions and neutrals which show an effective charge because of their dipole structure. If two particles encounter, we merge them and add their volumes and masses. Inversely, we check after every time step whether a polymer evaporates based on evaporation coefficients from literature. We present very preliminary results on the spatial and size distribution of neutral and ionic clusters for different initial particle densities and temperatures. We investigate how the presence of ions changes the nucleation rate and compare it with values from literature.