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

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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.
We here present a particle Monte Carlo code to study the growth of sulfuric acid clusters as well as its dependence on the ambient temperature and the number of ions. In contrast to common density models, we here trace individual sulfuric acid molecules and hydrogen sulfate ions.
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 amongst all ions as well as 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 [Yu, 2005. J. Chem. Phys., vol. 122, 074501; Yu, 2006. Atmos. Chem. Phys., vol. 6, 5193–5211].
We present the time evolution of the particle number as well as of the size distribution. We also calculate the nucleation rate of clusters with a diameter of 1.7 nm as a function of time and determine how the nucleation rate depends on the initial molecule density, the temperature and the presence of ions.