Effects of pH on Ice Nucleation by Kaolinite

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Heterogeneous ice nucleation refers to ice nucleation initiated by an ice nucleating particle (INP). Important INPs include mineral dust particles and biological particles. Nucleation processes are affected by cloud conditions, for example, the cloud pH. Clouds are generally acidic and have a range of pH values. Alkaline particulates significantly increase the cloud water pH leading to near-neutral or even basic clouds. The effect of cloud pH on ice nucleation has not been extensively studied. We investigate the effect of pH on immersion freezing by kaolinite employing both droplet freezing experiments and molecular dynamics simulations. In droplet freezing experiments, kaolinite suspensions are mixed with various concentrations of HNO_3/NaOH solutions in order to cover a wide pH range. Our laboratory experiments show that freezing temperatures are similar under acidic and neutral conditions, but decrease under basic conditions. This suggests that kaolinite remains active under acidic conditions but partly loses its nucleating ability under basic conditions. To model kaolinite particles immersed under different pH conditions, modified kaolinite Al-surfaces are investigated using molecular dynamics simulations. The basal Al-surface undergoes protonation under acidic conditions and deprotonation under basic conditions. We simulate multiple surface proton coverages on the basal Al-surface, and relate the surface proton coverage to pH through pKa values reported in the literature. The pH range for which we observe ice nucleation in simulations agrees well with our droplet freezing experiments. The possibility of ice nucleation by various kaolinite edges is also considered, but for these surfaces nucleation is not observed in simulations at 230 K.