Molecular Dynamics Simulation of Heterogeneous Nucleation of Aerosols from Water Vapor

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Heterogeneous nucleation of water vapor was simulated by molecular dynamics. This is an essential study to understand how solid particle size and configuration can directly influence aerosol growth in the atmosphere. Solid precursor particles that act as seeds with different shapes (sphere or cube) and sizes were inserted into multiple supersaturated water vapor systems. The focus is to find how the shape of particles will affect heterogeneous growth and condensation. A constant particle number, temperature, volume ensemble was used. Two different shape types and three different sizes of aluminum particles were tested. A single particle was inserted inside a supersaturated vapor system. The Yasuoka-Matsumoto method was used to calculate how quickly condensation occurs on the particle surface and how the seed interacts with sponatneously forming nuclei. Previous studies on monatomic vapor systems have shown that though the different particle shapes have similar surface areas, condensation is faster for the cube by one order of magnitude. Aerosol growth from water vapor, however was not affected by the intial seed configuration. The difference in the growth mechanism was clarified through this work.