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Molecular dynamics simulations of semi-volatile organic aerosol particles containing water, black carbon, and α-pinene secondary organic compounds

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Atmospheric black carbon (BC) is known to contribute significantly to the Earth's climate. However, detailed quantification of this effect remains elusive due to uncertainty regarding the contribution of BC to the cloud condensation nuclei (CCN) budget. A significant portion of this uncertainty is associated with the poorly understood impact of aging on BC hygroscopicity and CCN activity. In this work, we carried out molecular dynamics (MD) simulations aimed at examining one aging mechanism: the influence of secondary organic aerosol (SOA) on systems containing BC, liquid water, and air. In particular, we simulated systems in which water-air interfaces were exposed to BC and SOA (either jointly or separately) and examined the resulting structural, energetic, and physical properties. Coronene molecules were used as model compounds for BC, while 3-Methyl-1,2,3-butanetricarboxylic acid (MBTCA), a humic-like substance (HULIS) that is an oxidation product of α-pinene, was used as a SOA. Results suggest that MBTCA reduces the surface tension of water, enhancing the CCN ability of BC. The molecular descriptions in this study provide insights into the effects of α-pinene SOA aging on aerosol properties and its contribution to cloud formation.