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A new atmospheric aerosol phase equilibrium model (UHAERO): organic systems

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Abstract. In atmospheric aerosols, water and volatile inorganic and organic species are distributed between the gas and aerosol phases in accordance with thermodynamic equilibrium. Within an atmospheric particle, liquid and solid phases can exist at equilibrium. Models exist for computation of phase equilibria for inorganic/water mixtures typical of atmospheric aerosols; when organic species are present, the phase equilibrium problem is complicated by organic/water interactions as well as the potentially large number of organic species. We present here an extension of the UHAERO inorganic thermodynamic model (Amundson et al., 2006c) to organic/water systems. Phase diagrams for a number of model organic/water systems characteristic of both primary and secondary organic aerosols are computed. Also calculated are inorganic/organic/water phase diagrams that show the effect of organics on inorganic deliquescence behavior. The effect of the choice of activity coefficient model for organics on the computed phase equilibria is explored.

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