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A new inorganic atmospheric aerosol phase equilibrium model (UHAERO)

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Abstract. A variety of thermodynamic models have been developed to predict inorganic gas-aerosol equilibrium. To achieve computational efficiency a number of the models rely on a priori specification of the phases present in certain relative humidity regimes. Presented here is a new computational model, named UHAERO, that is both efficient and rigorously computes phase behavior without any a priori specification. The computational implementation is based on minimization of the Gibbs free energy using a primal-dual method, coupled to a Newton iteration. The mathematical details of the solution are given elsewhere. The model computes deliquescence behavior without any a priori specification of the relative humidities of deliquescence. Also included in the model is a formulation based on classical theory of nucleation kinetics that predicts crystallization behavior. Detailed phase diagrams of the sulfate/nitrate/ammonium/water system are presented as a function of relative humidity at 298.15 K over the complete space of composition.

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