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EQSAM4 – Aerosol water parameterization for atmospheric modeling

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We introduce version 4 of the EQuilibrium Simplified Aerosol Model (EQSAM4). The model is designed for atmospheric modeling and based on CPU efficient parameterizations that allow a sufficiently fast and accurate estimation of the overall aerosol liquid water content (AWC) and the required Relative Humidity of Deliquescence (RHD) – central in atmospheric chemistry and climate modeling. The main advantage of the revised model is its simplicity and predictive capability. The concept is based on a set of analytical functions (all of the form $a^x x$) that approximate the computationally comprehensive minimization of the Gibbs free energy and therefore allows to non-iteratively calculate the RHD based AWC of a droplet distribution that is in equilibrium with the ambient air, containing either single or mixed solutes. Our equations are a function of relative humidity (RH) and only require a single parameter $\nu_{i(aq)}$ for the entire range (0-1) of water activity ($a_{w(aq)}$). $\nu_{i(aq)}$ acts as an effective solute-solute and solute-solvent ion−ion and surface interaction parameter. $\nu_{i(aq)}$ is pre-scribed in EQSAM4 by look-up tables and determined by fitting our analytical equations to measurements assuming approximately flat surfaces. To account for surface tensions, or other size effects, $\nu_{i(aq)}$ can be altenratively derived from other empirical coefficients, or reference models, through the various relations presented. AWC distributions calculated with a global chemistry-climate model (EMAC) indicate that the EQSAM4 parameterizations are in general agreement with the more explicit thermodynamic model ISORROPIA2. AWC box model results of major single salt solutions (i.e. containing NaCl, NH_4NO_3, $(NH_4)_2SO_4$, NH_4HSO_4, $NaHSO_4$), and the corresponding mixed solutions, further nicely compare with those of the thermodynamic reference model E-AIM. The AWC of mixed solutions can be optionally obtained with EQSAM4 by calculating mean values of $\nu_{i(aq)}$ from all single solutes in the mixed solution. This new mixing rule of EQSAM4 complements the widely used additive approach of partial water masses of single solutes (ZSR-relation).