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Thermodynamic Modeling of Organic-Inorganic Aerosols with the Group-Contribution Model AIOMFAC

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Liquid aerosol particles are - from a physicochemical viewpoint - mixtures of inorganic salts, acids, water and a large variety of organic compounds (Rogge et al., 1993; Zhang et al., 2007). Molecular interactions between these aerosol components lead to deviations from ideal thermodynamic behavior. Strong non-ideality between organics and dissolved ions may influence the aerosol phases at equilibrium by means of liquid-liquid phase separations into a mainly polar (aqueous) and a less polar (organic) phase. A number of activity models exists to successfully describe the thermodynamic equilibrium of aqueous electrolyte solutions. However, the large number of different, often multi-functional, organic compounds in mixed organic-inorganic particles is a challenging problem for the development of thermodynamic models. The group-contribution concept as introduced in the UNIFAC model by Fredenslund et al. (1975), is a practical method to handle this difficulty and to add a certain predictability for unknown organic substances. We present the group-contribution model AIOMFAC (Aerosol Inorganic-Organic Mixtures Functional groups Activity Coefficients), which explicitly accounts for molecular interactions between solution constituents, both organic and inorganic, to calculate activities, chemical potentials and the total Gibbs energy of mixed systems (Zuend et al., 2008). This model enables the computation of vapor-liquid (VLE), liquid-liquid (LLE) and solid-liquid (SLE) equilibria within one framework. Focusing on atmospheric applications we considered eight different cations, five anions and a wide range of alcohols/polyols as organic compounds. With AIOMFAC, the activities of the components within an aqueous electrolyte solution are very well represented up to high ionic strength. We show that the semi-empirical middle-range parametrization of direct organic-inorganic interactions in alcohol-water-salt solutions enables accurate computations of vapor-liquid and liquid-liquid equilibria.

References

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