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A thermodynamic model of mixed organic-inorganic aerosols to predict activity coefficients

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Abstract. Tropospheric aerosols contain mixtures of inorganic salts, acids, water, and a large variety of organic compounds. Interactions between these substances in liquid mixtures lead to discrepancies from ideal thermodynamic behaviour. By means of activity coefficients, non-ideal behaviour can be taken into account. We present here a thermodynamic model named AIOMFAC (Aerosol Inorganic-Organic Mixtures Functional groups Activity Coefficients) that is able to calculate activity coefficients covering inorganic, organic, and organic-inorganic interactions in aqueous solutions over a wide concentration range. This model is based on the activity coefficient model LIFAC by Yan et al. (1999) that we modified and reparametrised to better describe atmospherically relevant conditions and mixture compositions. Focusing on atmospheric applications we considered H^+, Li^+, Na^+, K^+, NH^+_4, Mg^{2+}, Ca^{2+}, Cl^-, Br^-, NO^-_3, HSO^-_4, and SO^{2-}_4 as cations and anions and a wide range of alcohols/polyols composed of the functional groups CH_n and OH as organic compounds. With AIOMFAC, the activities of the components within an aqueous electrolyte solution are well represented up to high ionic strength. Most notably, a semi-empirical middle-range parametrisation of direct organic-inorganic interactions in alcohol+water+salt solutions strongly improves the agreement between experimental and modelled activity coefficients. At room temperature, this novel thermodynamic model offers the possibility to compute equilibrium relative humidities, gas/particle partitioning and liquid-liquid phase separations with high accuracy. In further studies, other organic functional groups will be introduced. The model framework is not restricted to specific ions or organic compounds and is therefore also applicable for other research topics.

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