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A curved multi-component aerosol hygroscopicity model framework: Part 1 – Inorganic compounds

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Abstract. A thermodynamic modelling framework to predict the equilibrium behaviour of mixed inorganic salt aerosols is developed, and then coupled with a technique for finding a solution to the Kohler equation in order to create a diameter dependent hygroscopic aerosol model (Aerosol Diameter Dependent Equilibrium Model – ADDEM). The model described here provides a robust and accurate inorganic basis using a mole fraction based activity coefficient model and adjusted energies of formation for treating solid precipitation. The model framework can accommodate organic components, though this added complexity is considered in a companion paper, this paper describes the development of the modelling architecture to be used and predictions of an inorganic model alone. The modelling framework has been developed to flexibly use a combination of mixing rules and other potentially more accurate techniques where available to calculate the water content. Comparisons with other state-of-the-art general equilibrium models and experimental data are presented and show excellent agreement. The Kelvin effect can be considered in this scheme using a variety of surface tension models. Comparison of predicted diameter dependent phenomena, such as the increased relative humidity for onset of deliquescence with decreasing diameter, with another diameter dependent model is very good despite the different approach used. The model is subject to various sensitivities. For the inorganic systems studied here, the model is sensitive to choice of surface tension scheme used, which decreases for larger aerosol. Large sensitivities are found for the value of dry density used. It is thus likely that the history of the aerosol studied in a hygroscopic tandem differential mobility analyser (HTDMA), specifically the nature of the drying process that will influence the final crystalline form, will create systematic uncertainties upon comparisons with theoretical predictions. However, the magnitudes of all of the above sensitivities are potentially less than those introduced when using a semi ideal growth factor analogue for certain conditions.

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