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Aerosol activation behaviour predicted using a primitive form of the Köhler equation

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The Aerosol Diameter Dependent Equilibrium Model (ADDEM) (Topping et al 2005a,b) has been used to make predictions of the sub-saturated water uptake of aerosol particles based on composition measured by an Aerodyne Aerosol Mass Spectrometer and by HPLC / 1H-NMR analysis. The model, which has been presented in the literature, relies on two separate activity coefficient models for calculating the non-ideality of the solution and surface tension models or parameterisations for treating the influence of curvature. To do this ADDEM is based around an iterative solution of the primitive Köhler equation. The Köhler equation is often found in various guises in the literature when describing warm cloud activation, the merits of these techniques discussed recently in the literature (McFiggans et al 2005). By relying on a primitive form one requires either an explicit thermodynamic model for calculating the water activity or a parameterised fit derived experimentally. ADDEM currently requires information solely on the organic functionality and not molecular weight of individual species. The mathematical modelling framework can depend on what information is required, i.e. critical super-saturations for a particle of a given dry size and composition, equilibrium size for a given RH or the equilibrium RH for a given wet diameter. These will be discussed in turn. Here we present results based on marine boundary layer measurements. The sensitivity to various model parameters has been made in the sub-saturated humid regime leading to the conclusion that the relative importance of the Raoult and Kelvin effects switches as one moves into the super-saturated humid regime. However, an interesting result from this study shows that differences between parameterized and calculated surface tensions, using the functionality assigned to the organic fraction when calculating the contribution from the Raoult effect, can lead to significant differences in calculated critical super-saturations. This effect may be due

to model inaccuracy or inappropriate choice of model compound. In any case, this sensitivity to surface tension in real atmospheric aerosol particles containing organic material shows the importance in realistically capturing the composition effects.

Topping, D. O., G. B. McFiggans and H. Coe, A curved multi-component aerosol hygroscopicity model framework: Part 1 – Inorganic compounds, *Atmos. Chem. Phys.*, **5**, 1205-1222, SRef-ID: 1680-7324/acp/2005-5-1205, 2005

Topping, D. O., G. B. McFiggans and H. Coe, A curved multi-component aerosol hygroscopicity model framework: Part 2 – Including organic compounds, *Atmos. Chem. Phys.*, **5**, 1223-1242, SRef-ID: 1680-7324/acp/2005-5-1223, 2005

McFiggans, G., P. Artaxo, U. Baltensperger, H. Coe, M. C. Facchini, G. Feingold, S. Fuzzi, M. Gysel, A. Laaksonen, U. Lohmann, Th. F. Mentel, D. M. Murphy, C. D. O'Dowd, J. R. Snider, E. Weingartner, The Effect of Physical and Chemical Aerosol Properties on Warm Cloud Droplet Activation, *to appear imminently in Atmospheric Chemistry & Physics Discussions*, 2005b