

Interactive comment on “A curved multi-component aerosol hygroscopicity model framework: 1 – Inorganics” by D. O. Topping et al.

D. O. Topping et al.

Received and published: 3 February 2005

Response to anonymous referee #3

The authors would like to thank you for your general comments and support of the work which has been presented in the paper. The remarks made are addressed below.

Specific comments

‘..it could be considered to be implemented in a chemistry model. The authors should comment on what computational resources are needed for running the model. Would it be feasible to implement it in, say, a box model, 1D model or 3D model?’ Response - we are currently implementing ADDEM within a box model to assess its suitability; our intention is to compare it with thermodynamic routines used in 3-D models within

Full Screen / Esc

Print Version

Interactive Discussion

Discussion Paper

the box modelling framework to establish regimes of particular importance concerning differences in thermodynamic descriptions. A robust profile of computational burden and comparisons with other existing models will form the focus of future work. Any resource requirements would at present be resource specific and this is not helpful in a general paper

‘..the authors should also state clearly in the abstract and summary for which range of temperature and RH the model will give reliable results. Will it for instance be applicable for the upper troposphere as well as for the lower troposphere?’ Response - This will be clarified in the revised version of the paper. The variation of the Gibbs free energy of formation with temperature for each species is accounted for as shown in the text. However, the range of ambient conditions for which the equilibrium model will give reliable results is largely dictated by the accuracy of the activity coefficient model. For the H^+ - NH_4^+ - SO_4^{2-} - NO_3^- - H_2O model excluding Na^+ and Cl^- , Clegg et al (1998a) derived interaction parameters designed to make predictions over the temperature range $<200K-330K$. The ability of such parameters to reproduce behaviour in such regions has been analysed by Clegg et al (1998a). Though Clegg et al (1996) showed that the activity coefficient varies over $0-50^{\circ}C$ by as much as 5%, if one wishes to include the ions Na^+ and Cl^- then interaction parameters are only available for $298.15K$. For this system, the activity model is valid for concentrations from infinite dilution to saturation (with respect to the solid phases), and to about 40 mol per kg for acid sulphate systems which can remain liquid to concentrations approaching the pure acid (Clegg et al 1998b). It should be noted however that the model was designed primarily for lower tropospheric conditions, thus although the activity coefficient model can deal with system (1) across a broad temperature range, there is no treatment of ice formation or acid hydrates which may become important at lower temperatures. Thus for a purely aqueous aerosol alone, then the model is expected to give reliable results in both the lower and upper troposphere for systems excluding Na^+ and Cl^- . It is difficult to ascertain an absolute lower RH boundary for which the model will be accurate as this will depend upon the relative composition and temperature. However, an example given

in the text shows the vast improvement this activity model attains over Pitzer's molality based model for higher concentrations, and it is expected that the equilibrium model will give reliable results for various supersaturated solutions at an RH as low as 20%. .

P. 8639/8640: 'In Eqns. (13) and (14) the Kelvin term is the same in both but different symbols are used for the variables. They should be the same.' Response - this has been corrected.

P. 8645, l. 13: 'It should be 'Eq. (13)' instead of 'Eq. (8)' Response - this has been corrected.

P.8647, l. 21: 'suggest to abbreviate GF_thermodynamic to GF_th' Response - text changed to GF_thermo

P8651, l. 10: 'some text is lost in this line.' Response - this has been corrected. It should read 'The adjustment in for each solid component results in no need to adjust the values of for the ions or gaseous components.'

P. 8652: 'Figure 8 shows standard deviations. From the text it is not clear to me how these standard deviations are calculated. Please clarify. Also the labels (a), (b), (c), (d) are missing in the figure.' Response - This is clarified in the revised text. For figure 8a and 8b, three different surface tension models, described in the text, were used to calculate three different growth factors. The standard deviation between these different outputs was then calculated. The same process is repeated in figures 8c and 8d but using two different solution density mixing rules. The figures now also have the appropriate labels.

Table 1: ' I suggest to reduce the number of digits in column "Adj. DeltaG_f".' Response - As discussed in section 7.1.1 the predicted deliquescence point of the different solids was found to be particularly sensitive to the choice of Gibbs free energy used. The accuracy with which the values are presented in table 1 is used to reflect this and represent those values which minimise the difference between predicted and observed

[Full Screen / Esc](#)[Print Version](#)[Interactive Discussion](#)[Discussion Paper](#)

deliquescence points.

Figure 3 - 'the unites of the x-axis label are missing' Response - this has been corrected

Figure 6 - 'the x-axis label is missing.' Response - This has been corrected

Figure 9 - 'the label (a) and (b) are missing. In the bottom figure the y-axis label is missing' Response - these features have been corrected.

Missing references: Hameri (2002), Tang (1981), Tang (1986), Wagman et al. (1982).
Response - These references have been added to the bibliography.

Interactive comment on Atmos. Chem. Phys. Discuss., 4, 8627, 2004.

Full Screen / Esc

Print Version

Interactive Discussion

Discussion Paper