

***Interactive comment on* “Effects of uncertainties in the thermodynamic properties of aerosol components in an air quality model – Part I: Treatment of inorganic electrolytes and organic compounds in the condensed phase” by S. L. Clegg et al.**

Anonymous Referee #1

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This is a valuable addition to the body of literature on the subject of modeling the thermodynamics of aerosol formation. I do not have any substantive criticisms of the work or conclusions and think it could be published in its present form, although I might question whether the paper needs to be this long given the relatively modest conclusions. It might make more of an impact if it could be shortened, perhaps by omitting the analysis of the time-dependence and focusing on one simulation time that encapsu-

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lates all of the differences between the AIM approach and the simpler thermodynamic model in UCD-CACM? Similarly, there is little effect of size-segregation in the UCD-CACM model on the distribution of compounds between the various phases, especially when compared to the bulk-averaged AIM model. Perhaps that discussion could also be shortened? There is not a problem with the manuscript in its current length, it just seems unwieldy, with a lot of work to reach the pay-offs in Section 4.

A discussion of the possible effects of the missing UNIFAC interaction parameters, -ONO₂, for instance, would be useful. UNIFAC is commonly used for aerosol modeling, but with the recognized importance of organic nitrates and carbonyl nitrates in aerosol formation, the lack of that group might limit the utility of UNIFAC if the effect of the interaction parameters is large. Similarly, other groups might exist in the formal definition of UNIFAC (e.g., an aromatic NO₂ group) but not have interaction parameters for critical main groups (e.g., interaction of -NO₂ with -COOH). It would be useful to list the places where UNIFAC is incomplete and the possible consequences. If the interaction terms are unimportant, one might question whether any UNIFAC interaction terms are required for the organics. This might greatly simplify activity calculations.

Specific corrections.

1. Clegg (2004) P-4, reference appears to be missing from list. Probably should be Clegg and Seinfeld (2004).

Interactive comment on Atmos. Chem. Phys. Discuss., 7, 10971, 2007.

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