

Interactive comment on “Computation of liquid-liquid equilibria and phase stabilities: implications for RH-dependent gas/particle partitioning of organic-inorganic aerosols” by A. Zuend et al.

Anonymous Referee #1

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This paper highlights a process which captures a level of detail largely neglected in models of SOA partitioning. Results suggest that commonly held assumptions regarding assumed phase state may be invalid and as such, studies such as the one presented here are crucial for adequately parameterising process representations in large scale models

I think this paper is highly significant and should be published in ACP. The description of processes studied and required theoretical frameworks is quite refreshing.

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I have only a few minor, rather philosophical, queries:

General points

The authors restrict the calculations to two separate liquid phases. This is understandable given the complexity of the calculations. However, would this assumption hold for more complex organic systems which a broader range of functionality, polarity etc? In essence, can the conclusions derived in this study really be generalised to interpret much more complex systems, such as smog chamber ensemble studies?

Do the authors think that the interfacial energy between separate phases in actualy aerosol particles might influence overall gibbs energy of the system to alter the generalised conclusions reported here? There have been few studies analysing the potential sensitivity of size dependent deliquescence, for example, to interfacial energies.

Specific point.

In section 2.4.2 the authors mention how a specific system may not be perfectly represented within a group contribution method which has been constrained to a specific subset of organic functionality. This has been found in simpler studies using updated parameters within the UNIFAC framework. Given the many combinations of functional groups which would require fitting, do the authors think that there is ultimately a level of accuracy beyond which model predictions will never be attainable given restrictions in bulk analytical techniques (i.e. solubility, evaporation etc). Whilst this is a rather philosophical question, it is an interesting discussion nonetheless.

Interactive comment on Atmos. Chem. Phys. Discuss., 10, 12497, 2010.

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