

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 #2

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The manuscript describes a detailed modeling study of the effect of liquid–liquid phase separation on vapor–liquid equilibrium of semi-volatile organics and water. Also, the effects of relative humidity and solution non-idealities are investigated. The results show that solution non-idealities and RH-dependent liquid–liquid phase separation are affecting on the gas/particle partitioning. Because liquid–liquid phase separation can happen in aerosols, the topic of the manuscript is relevant. Therefore, I recommend this paper for publication after minor corrections.

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General comments

The manuscript is very well written. Due to the thorough description of the model and results, the manuscript is a bit lengthy. However, the detailed description can be justified by the fact that liquid–liquid equilibrium calculations are not that common in aerosol modeling.

It looks like the model is suitable mainly for simulating laboratory experiments, but is the model applicable for atmospheric aerosols or even simplified representations of ambient aerosols? For example, are these currently modeled alcohols and polyols common in the atmosphere, e.g., compared with abundances of organic acids? Due to their electrolytic nature organic acids are likely to partition to the water-rich phase, but are there any other common type of atmospheric organics capable of forming an organic-rich phase?

Specific comments

Due to the differences between compositions of ambient aerosol and currently modeled mixtures, do the authors think that their results can be generalized (e.g. the modified C_j^* definition)?

When comparing O:C ratios of current organics with those of the ambient aerosol (Sect. 4.3), it should be kept in mind that in the atmosphere increased O:C ratios usually mean high concentrations of organic polyacids, and their properties are different than those of the polyols.

Technical corrections

Page 12498, line 12: “thermodynamic properties of the *phase diagram*” maybe e.g. multicomponent mixtures?