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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Improved AIOMFAC model parameterisation of the temperature dependence of activity coefficients for aqueous organic mixtures" *by* G. Ganbavale et al.

Anonymous Referee #2

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The authors introduce a new and improved parameterization of the temperature dependence of activity coefficients in the AIOMFAC model for organic species in aqueous organic and water-free organic mixtures. This is a daunting task, and the presented work is comprehensive and of high quality. The manuscript can be published in ACP after the following comments are properly addressed.

Comments:

1. A more detailed discussion on the limitations and applicability of the new parameterization is needed than what is presented in section 5.3. Can the authors give

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more specific guidelines on what types of complex multifunctional, high molecular weight species (including oligomers) the current model can and cannot handle?

2. The authors mention in the introduction "Thermodynamic phase equilibrium calculations allow to determine whether the aerosol phase is a liquid (or viscous amorphous phase), a crystalline solid, or a mixture of solid and liquid phases and to what degree semivolatile species partition to the condensed phases." The question is can AIOMFAC actually predict or distinguish between liquid and viscous (semisolid) amorphous phases? If so, how is viscosity and temperature dependence of viscosity predicted (or taken into account)? A discussion on these points should also be included in section 5.3.

3. Finally, these limitations of the model should be briefly mentioned in the abstract and the conclusions section.

Interactive comment on Atmos. Chem. Phys. Discuss., 14, 16907, 2014.