

Interactive comment on “A predictive group-contribution model for the viscosity of aqueous organic aerosol” by Natalie R. Gervasi et al.

Anonymous Referee #1

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In “A predictive group-contribution model for the viscosity of aqueous organic aerosol” by Gervasi et al., a model is presented for calculating viscosity of aqueous solutions as a function of temperature and chemical composition. The predictive model treats aqueous mixtures of organics using functional group contribution framework based on GC-UNIMOD (Cao et al. 1993) with activity coefficient predictions from AIOMFAC (Zuend et al. 2008, 2011). Importantly, the predictions for the mixtures rely on predictions of pure composition viscosities, found using the predicted glass transition temperature of DeRieux et al. (2018) for the organic components. Overall, the paper is well written, with nice discussion throughout of the organic chemical composition variation and evolution as a function of temperature and relative humidity in the atmosphere.

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However, while well-written, a compelling case for the use of group contribution method for the aqueous organic mixture was not made in the current form of the manuscript. Arguably, the simple mixing rule of mole fraction-based weighting (eqn 14a) is as good as the proposed AIOMFAC-VISC, and significantly simpler. The authors should also present the results of the mole-fraction based weighed prediction for sucrose, trehalose, as well as the more complex mixtures of Figure 5+, which may demonstrate differences between the simple mixing and AIOMFAC-VISC. Additionally, the authors should consider presenting the results of an activity-based weighing (that is, use the mole-fraction based weighing, but include the mole-fraction activity coefficient for each species based on AIOMFAC calculations, similar to that done by the authors for the combinatoric contributions in eqn. 2). It also seems possible/likely that any variations in the predictions between these approaches for treating the mixture may be small compared to the uncertainty caused by the predictions of the pure component viscosities, and this simpler approach would be much more accessible method to users.

The majority of the model uncertainty comes from the pure component viscosity predictions; if these are done correctly, the mixing model is likely correct. The authors should consider ways to improve the predictions of the pure component viscosities, possibility also using their function group contribution methods. This would significantly strengthen the paper.

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