

Interactive comment on “Predicting the glass transition temperature and viscosity of secondary organic material using molecular composition” by Wing-Sy Wong DeRieux et al.

Anonymous Referee #2

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Summary:

This ACPD article describes a modeling method to estimate the glass transition temperature and viscosity of organic mixtures and secondary organic aerosols (SOA) with molecular weight up to 1100 g mol⁻¹. This work continues the work that the authors published before, but the difference is that previous work can only predict organics with molar masses up to 450 g mol⁻¹ while this work extends the molar mass region twice as much as the previous work. The scientific significance of this study is that the current model is able to predict the glass transition temperatures and viscosities of oligomers instead of just small organic molecules, which can be applied those oligomer-rich SOA

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systems. I like that even though the paper focus on molecular mass >450 g/mol, the fitting equation still fit for molecular <450 g/mol, and the results are even better. This study describes the modeling process, and then utilizes experimental data to verify the model. The experimental data add credibility to the modeling results. Overall, the manuscript is sound and after addressing the following issues, it is suitable to be published on ACP.

Major Comments:

In Figure 1, it looks like there are only 8 compounds whose molar masses are larger than 450 g/mol, which is quite few compared with the number of compounds whose molar masses are below 450 g/mol. Would the limited number of compounds with higher molar masses causing a skew when modeling their viscosity and glass transition temperatures?

In Figure 4 (a), the author uses measured viscosity data of alpha-pinene SOA to model the viscosity trend with RH. The author seems to heavily rely on the data from Renbaum-Wolff because that set of data covers a wider RH. However, in Renbaum-Wolff et al. specified that their data was only the water-soluble part of SOA, while all the other measured data listed in the plot were based on the whole SOA. The model does not seem to distinguish these two differences and mix all the data together. Wouldn't this approach lead to inaccuracy to predict the viscosity of total SOA? Maybe it is better for the author to use the measured viscosity of total SOA to predict SOA's viscosity, and leave the water-soluble part of the SOA to another plot and estimate its viscosity individually.

Figure 4(b) was based on Song et al. 2015 data and Bateman et al. 2015 data. I checked Song et al. 2015 and found out that their data was based on SOA condensation from the potential aerosol mass (PAM) reactor (Song, Liu et al. 2015). In the ambient environment, it has shown that the majority of the isoprene SOA is formed by heterogeneous reactions with the acidic sulfate particles, rather than condensation of

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semi-volatile species (Lin, Zhang et al. 2013, Surratt, Chan et al. 2010). Heterogeneous reactions of isoprene products will be able to form more oligomers and lead to a lower viscosity (Gaston, Riedel et al. 2014). Therefore the experimental data from Figure 4(b) may not represent the ambient isoprene SOA viscosity. At the very least the author should make it clear in the manuscript (both Figure 4(b) and Figure 10) about the limitation of this study so more motivation is put for others to perform experimental viscosity measurement on ambient-like isoprene SOA particles generated from heterogeneous reactions.

In Figure 9 and 10, the author used ESI and APPI data to model the viscosity value of biomass burning aerosols. Biomass burning aerosols typically also contain inorganic components as well but the author neglects that part and only take the organic component into consideration. How would the inorganic components affect the viscosity of the total aerosols? Maybe the author should be a bit more specific when they mention biomass burning particles?

Minor Comments:

Lines 120-122: When the author says :” Specifically, data for 76 aliphatic alcohols, 39 carbohydrates and their derivatives...”, do all these compounds have molar masses larger than 450 g/mol? It sounds like it because the way the author phrase the sentence. If not, the author may want to revise this sentence to make it more clear and indicate which compounds have molar masses > 450. Table 1, nc(0) symbol is not centered in the table; Line 786, the parenthesis after 2014 is missing; Line 792, the letters are partially overlapping with the table

References:

Gaston, C. J., et al. (2014). "Reactive Uptake of an Isoprene-Derived Epoxydiol to Submicron Aerosol Particles." *Environ. Sci. Technol.* 48(19): 11178-11186. Lin, Y. H., et al. (2013). "Epoxide as a Precursor to Secondary Organic Aerosol Formation from Isoprene Photooxidation in the Presence of Nitrogen Oxides." *Proc. Natl. Acad. Sci.*

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