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Comment

Interactive comment on “Particle partitioning potential of organic compounds is highest in the Eastern US and driven by anthropogenic water” by A. G. Carlton and B. J. Turpin

Anonymous Referee #2

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Overall Comment and Recommendation:

This is a well written and timely study that examines the importance of liquid water and water soluble organic gases on organic aerosol formation in the eastern U.S. The authors use version 4.7 of the Community Multiscale Air Quality (CMAQ) model in order to conduct their study for July 2003. My major concern with this current version of the manuscript is with the model simulations. Specifically, the model simulations lack inclusion of explicit chemistry related to isoprene epoxydiols (IEPOX) (Paulot et al., 2009, Science; Surratt et al., 2010, PNAS; Lin et al., 2012, ES&T) and methacrylic acid epoxide (MAE) (Lin et al., 2013, PNAS). Considering that most of the measurable isoprene

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SOA tracers in ambient PM_{2.5} come from these two gas-phase water soluble epoxides (Lin et al., 2013, ACPD), it seems the model is missing an important class of water soluble species. Without including these species, the authors may be underestimating the controllable fraction even more than they currently think in this manuscript. I think the authors need to acknowledge this as an issue (or limitation) of the model in this area of the country. Please note that I'm aware of a study that is trying to incorporate these new chemistries into the CMAQ model, but it is currently under review. As a result of the latter, it may not be expected that the authors include this at the present time. I should stress here that isoprene epoxides have been linked with sulfate aerosols as a major source of organic aerosol in this region (Lin et al., 2013, ACPD; Budisulistiorini et al., 2013, ES&T). Specifically, their reactive uptake onto acidified sulfate aerosols (and thus wet sulfate aerosols) and subsequent aerosol-phase chemistry has been demonstrated (Lin et al., 2012, ES&T; Lin et al., 2013, PNAS). In an ideal world, it would be appropriate for the authors to include the isoprene-derived epoxides (MAE and IEPOX) in their simulations, especially since their oxirane ring-opening reactions are critical to SOA formation. For example, by H₂O acting as a nucleophile, you get the famous (and quite abundant) 2-methyltetrols and 2-methylglyceric acid from IEPOX and MAE hydrolysis, respectively.

In addition to the lack of inclusion of explicit isoprene epoxides, why are the authors not using the Xie et al. (2012, ACPD) modified mechanism (SAPRC07) for their gas-phase simulations? It seems the modified SAPRC07 model might be more appropriate than the 99 mechanism. Do the authors agree?

With these major questions, I must recommend that this paper be accepted with major revisions noted above. I do think this is an incredibly relevant topic to ACP's mission and the study is clearly well thought out by these leaders in aqueous phase chemistry.

Minor Comments:

It seems strange there is only a results section and no discussion section in this

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manuscript. In addition, I thought for ACP publications there should also be a conclusions section, right?

Interactive comment on Atmos. Chem. Phys. Discuss., 13, 12743, 2013.

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13, C4573–C4575, 2013

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