

Interactive comment on “Simulating the SOA formation of isoprene from partitioning and aerosol phase reactions in the presence of inorganics” by R. L. Beardsley and M. Jang

Anonymous Referee #1

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This paper attempts to use the UNIPAR model to predict isoprene derived SOA, including aqueous reactions and organosulfate formation. The model results are validated against a set of chamber experiments. While the topic is certainly an important and interesting one, I find that the paper is generally not clear, concise and not well organized. I suggest that it could possibly be considered for publication after it is modified accordingly.

General concerns:

It is not clear in the introduction section what the authors are trying to accomplish in this paper. There are in fact many models that already exist which model the formation

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of isoprene SOA including aqueous reactions and OS formation etc. . . (McNeill et al., 2012; Pye et al., Gaston et al., 2014, and likely others.). In this case, what is the issue which the authors are trying to address? Is there a clear deficiency in these other models that their model can improve upon? Is there missing chemistry for isoprene in other models? Although there are some places in the paper that hint at what the point of this paper is, it is far from clear and would benefit from stating these facts up front rather than buried somewhere in the paper.

The paper is also generally overly complex and disorganized. A number of equations can be in the supplemental information rather than in the main paper, and the same can be said for the explanation of these equations.

It is not quite clear why the authors would use so many different parameters to describe acidity of the aerosol, and then try to investigate the effect of these parameters on SOA yield. At the end of the day it may be the particle pH that is important for aqueous reactions, but all the other parameters used will also affect the particle pH. For example, LWC affects the acidity, as does the “free sulfate”. Because of this, it is not possible to understand what is actually controlling what process. I would suggest that the authors use one term that describes acidity and in particular the particle pH. The paper would be made much clearer if it was organized in such a way as to separately describe the effects of pH, LWC and sulfate (because SO₄ is responsible for OS and also effects the pH) on the SOA yield, rather than the manner which it is done currently.

Some experiments were conducted with acidic particles. It is unclear how relevant these particles are to the ambient atmosphere. The authors need to compare their aerosol acidities with what might be expected in the atmosphere. The same can be said for the range of VOC/NO_x used in these experiments.

Specific issues:

Pg 33135, line 23-24: If it is acidity of some sort which is required for aqueous reactions to occur how does one explain the OM_AR being the dominant contributor (65%)

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to experiments without any SA seed particles? For that matter, how is an experiment without any seed particles relevant to the ambient atmosphere? The authors are relying upon nucleation of isoprene products to make particles, which only occurs here because they are using ppm levels of isoprene in their chamber. This will not occur in the real atmosphere, and so the authors must explain the utility of such experiments without any pre-existing seed particles.

Pg 33134, lines 1-4: It has already been shown (minerath et al., 2008, barsanti et al. . .) that functional groups such as alcohols and aldehydes are likely to react too slow under realistic atmospheric conditions to make much OS. Including them here may be inducing more OS than is realistic. The authors need to justify including them here.

Pg 33124, lines 5-8: a mechanistic reason(s) for these facts should be included here if possible.

Pg 33124, lines 4: "lowly" is poor grammar. This is also written throughout the paper and should be changed accordingly.

Pg 33125, lines 3-4: poor grammar in this last line. Make it two sentences.

Pg 33126, first paragraph: there is no mention of the issue of semi-volatile gas-phase wall losses. This is a recent area of concern for chamber studies and should at least be mentioned.

Pg 33127, line 2: insert "the" after "on"

Pg 33127, lines 23-27: Some justification or reasoning for selecting these reactivity bins, and how compounds were assigned to these bins would be very useful here.

Pg 33128, lines 8-10: choosing the concentrations of each group based on the maximum HO₂/NO ratio seems arbitrary. The composition will be dependent upon a number of factors such as this ratio, and time etc. . . its not clear why this particular value was selected and what effect this would ultimately have on the final model results.

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Pg 33129, lines 4-10: how similar are the compounds chosen in Bertram et al, to the products of isoprene? Is it valid to use these parameterizations? Also, how well does the UNIPAR model predict the O:C ratio?

Pg 33131, equation: This equation and many of the following ones are miss numbered.

Pg 33133, eq 11: it is not clear how this equation was derived. There are too many equations in this section and the text is rather complex and confusing. I suggest simplifying this page and putting it in the supporting info.

Figure 1: It would be useful to have a gas-phase flow chart associated with this one for the aerosol phase. . .or at least an additional schematic box attached above it.

Figure 2: the compound acronyms in the legend need to be described in the caption.

Figure 3: this figure is nearly impossible to read. It must be made bigger and clarified.

Interactive comment on Atmos. Chem. Phys. Discuss., 15, 33121, 2015.

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