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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Model evaluation of NO₃ secondary organic aerosol (SOA) source and heterogeneous organic aerosol (OA) sink in the Western United States" *by* J. L. Fry and K. Sackinger

Anonymous Referee #1

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Overall comments: The paper addresses an issue of atmospheric relevance, but some of the implementation is not entirely clear. Many of the comments below stem from the need to better understand the heterogeneous sink, and if the conclusions hold after the comments are addressed, the paper may be suitable for publication.

1. Some simplifications do not seem necessary.

a. For example, equation (2) and Table 1 indicate a fixed yield of aerosol is used for each lumped parent hydrocarbon. What conditions (organic aerosol concentration,

temperature) is this yield valid for? Could you use a yield curve and calculate the yield for the organic aerosol concentration predicted by WRF? The mass yield of 5% might be more realistic given nighttime aerosol loadings.

b. For equation (7), could the fraction of the semivolatile in the gas and aerosol phases be calculated instead of using a cutoff?

2. Can you clarify how OLI and OLT were used? It is my understanding that the olefinic bonds are mapped to OLI and OLT and the rest of the carbon is mapped to another species. How do you assemble back the parent hydrocarbon that serves as the SOA precursor? What is the molecular weight? Are there significant amounts of compounds other than monoterpenes that make up OLI and OLT?

3. Figure 3. Do colors also have meaning?

4. Page 5196-5198: Additional clarification is needed on the conversion between functional groups of bulk aerosol vs whole molecules of individual species (for use in vapor pressure calculations, mechanism species, etc.)

a. Page 5197, Line 1: Each starting molecule is assumed to have only one functional group. Given that organic aerosol tends to have OM/OC of 1.4-2.1, is this a realistic assumption?

b. The average carbon number of 27 seems high. That seems valid for primary organic aerosol, but given the ubiquity of multifunctional organic aerosol and SOA/OOA, it seems high. Alves et al. carbon numbers are based on PM10 measurements and they attributed the >C20 compounds to vascular plants. Does that match up with the aerosol WRF predicts? Following the previous comment, given how oxidized ambient aerosol is, would you not expect a much shorter carbon backbone?

c. Given the functional group composition on the bottom of page 5196, the assumption that each starting molecule has only one functional group, and the specification of the carbon number distribution, is the composition of aerosol over specified?

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12, C1373–C1375, 2012

5. Table 3: The assumption of 100% unsaturated aerosol and 97% aliphatic aerosol both increase the aerosol loss rate relative to the base sink. Why is that?

6. Is there any reasonable combination of parameters (ie low aerosol yield, shorter carbon backbone, more functional groups, higher uptake coefficient for aliphatic sites, etc) that would make the source and sink within an order of magnitude of each other?

7. Page 5192, line 2: '(51)' seems out of place.

8. Page 5196: insert definition of variables for equation 4 in text.

9. Page 5196, line 17, is there a reference for the 2 g/cm3 density?

10. Title should be revised. "Model evaluation.." implies that a model has been evaluated. What about "Model investigation. . .."

Interactive comment on Atmos. Chem. Phys. Discuss., 12, 5189, 2012.