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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Simulating secondary organic aerosol in a regional air quality model using the statistical oxidation model – Part 3: Assessing the influence of semi-volatile and intermediate volatility organic compounds and NO_X" *by* Ali Akherati et al.

Anonymous Referee #2

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The manuscript describes the update of a chemical transport model, specifically the UCD/CIT model in which the SOM model has been embedded, to predict OA and SOA in California. The modeling period studied is 14 days during late July and early August 2005. The major advance in this work, compared to previous work publish by same group, is the addition of primary IVOCs and SVOCs to the model including treating POA as semi-volatile, while accounting for vapor wall losses during chamber experiments and molecular fragmentation. The authors also examine how NOx levels

impact SOA predictions in the updated model.

The paper is well written, of interest to ACP readers, and appropriate for publication once the following comments have been addressed. I have listed one general comment immediately below followed by more specific and minor comments. Lastly, there is a problem with the manuscript formatting and the line numbers are not displayed correctly in the pdf document. I have thus used the page number and paragraph to indicate the relevant sections of the text.

Length of manuscript: I found the manuscript very long to read, but well-written and clear. I think the scope of the research mostly justifies the length of the manuscript. The sole exception is the section regarding future OA concentrations in 2035. This section felt very much like it was "tacked-on" and it is not well developed. Given the uncertainties in the model, how accurate is the model when projected to 30 years into the future? Sensitivity studies should be run to identify how the predictions vary with different model assumptions as was done for the 2005 simulations. Furthermore, what is the value of running a simulation for only a two week period in 2035? If one wants to inform future policy decisions, it would be better to run the simulation for a much longer period (e.g. a few months). Ultimately, it seems like this work is best left for another manuscript, and deleting this part would also shorten the length of the current manuscript.

Specific Comments:

Introduction, page 3, paragraph 2: The text here stating that SOA formation schemes have been rarely validated against experimental data is too strong or needs to be nuanced. One can, for example, cite the following modeling studies where P-S/IVOCs are treated and models are compared against measurements.

Fountoukis et al. Atmos. Chem. Phys. 2016, 16, 3727-3741.

Murphy et al. Atmos. Chem. Phys. 2017, 17, 11107-11133.

Zhang et al. Atmos. Chem. Phys. 2015, 15, 13973-13992.

Page 8, second paragraph: what is meant by "carbon-equivalent linear alkane"? Is it reasonable to assume that linear alkanes can be used to estimate OH reaction rate constants of SVOCs, given that branched alkanes represent a large portion of POA mass?

Section 2.2.2, last paragraph: Is it correct to state that the model is consistent with Gordon et al.? From the text, it seems that the yields in the model are different versus the Gordon et al. smog chamber studies, but it is expected that the difference in SOA yields will be compensated for by the fact that emissions are different relative to work of Zhao et al.

Section 2.2.3: It would improve the manuscript if the choice of the equation where there is a logarithmic dependence on the VOC/NOx ratio, among the four equations presented, were better justified based on chemical reasons. Currently, the justification is essentially based on the observation that this equation results in the highest SOA prediction.

Table 3: A clarifying question: were the vapor wall losses corrected for VOCs in all the simulations? Even in the traditional case? This is what is indicated by the table, but in the text below it is simply stated "no correction for chamber vapor wall losses", which would seem to exclude also the application of the correction to the VOCs.

Page 19, last sentence: using a 20% yield as an approximate SOA mass yield seems too low, given that earlier in the same paragraph estimated yields for SVOC oxidation ranged from 33% to 86%. I also think the oxidation rate constant is a little low, given that octadecane and nonadecane (for example) have rate constants that are greater than 2e-11 cm-3 molecules-1 s-1, and these compounds likely represent a lower limit as oxidation rates increase with alkane branching. Also, how was the wind speed of 5 miles per hour chosen?

Page 20: The statement saying IVOCs as a bulk class of SOA precursors may not contribute substantially to ambient SOA levels is too strong. There is an important contribution, especially if one only considers anthropogenic SOA, even though that contribution may be less than that from traditional VOCs.

Page 21, first paragraph, last sentence: I don't disagree with the value of the work presented in the manuscript, but, in my opinion, what is really unique is the incorporation of these 4 elements into a chemical transport model. It seems that should be mentioned somewhere in this sentence.

Page 32, Line 3: I think there is a typo here and the measured value given is incorrect and should be 1.9 rather than 2.2.

Page 32, first paragraph, last sentence: The comparison of HOA to POA from mobile sources is rather good. It would be worthwhile to point that out.

Figure S5: Why do the b-alkanes have an enhancement of less than 1 under high NOx conditions? Doesn't correcting for the wall losses always increase the SOA yield?

Minor comments:

Table 1: Simply for the sake of clarity, the order of the molar yields should be indicated. Do they progress (left to right) from the addition of 1 to 4 oxygen atoms per reaction, or is it the opposite order?

Table 2: There is an "&" symbol in the footnotes of the table, but I cannot find the matching symbol in the table or table caption.

Page 7: There appears to be a typo on the last line of this page.

Section 2.2.3: Were the IVOCs and gas phase SVOCs used to calculate the modeled VOC:NOX ratios? These compounds would contribute to the HO2 budget, although likely less than the VOCs.

Page 16, last paragraph: a reference should be provided for the measured mass concentrations of POA over the open ocean west of California.

Page 28: What was the measured aromatic concentration ratio between 2005 and 2010 at the Los Angeles-North Main Street site?

Page 29, last sentence: it should be clarified that the 27 measurements available for comparison are measurements taken at IMPROVE sites. (At least I think that is the case, it is not entirely clear from the manuscript.)

Page 34, lines 1 – 2: There may be a typo here. I thought the argument was the timescales for SOA formation are LONGER than the timescales for transport out of the urban airshed.

Page 36, references: The reference from the American Lung Association doesn't seem to be correct as it contains a link to a website about air quality in Fort Collins, Colorado. In addition, the organization name is shortened as if it is an author's name.

Supporting information: Some of the tables and figures and their matching captions are split across different pages. For readability, each figure and table should appear entirely on one page with it's caption.

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