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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 #3

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Reviewer comments on "Simulating secondary organic aerosol in a regional 1 air quality model using the statistical oxidation model – Part 3: Assessing the influence of semi-volatile and intermediate volatility organic compounds and NOX," acp-2018-616

This work describes an update to the UCD/CIT chemical transport model, specifically by the inclusion of the SOM organic aerosol model. The impacts of various improvements are described and investigated, such as the inclusion of SVOC and IVOC oxida-

tion. In general, the methods are well described, and the results are reasonable. The manuscript is well within the scope of the journal, and warrants publication with minor revisions as described below.

Major comments: 1) The manuscript is fairly lengthy and detailed. While this is reasonable for a detailed description of model improvements, it can make it difficult to keep track of the main points at times. I wonder if some of the results could be boiled down to really the key points, and some of the subtleties moved to the supplement.

2) As a chemistry-minded member of our community, a frequent point of confusion for me is in discussion of IVOC with lack of precision around the chemical composition being represented. In this case, IVOC is being used to mean non-speciated intermediate volatility combustion emissions, which are primarily branched and cyclic aliphatics and some aromatics. Yet they are represented by n-alkanes (which likely differ in their SOA yields), and are somehow grouped separately than "long alkanes and aromatics", despite this being a reasonable description of these IVOCs (I presume the latter refers to speciated emissions?). It would be helpful to be more precise in the language and consider in the discussion what these emissions likely are.

Technical comments: This line numbering approach is maddening bordering on useless. Please in the future use unique line numbers for all lines on a given page, or better yet use continuous line numbers throughout the document. When I copy and paste into notepad, I see digits before the final appear and are continuous, so perhaps this is just a conversion issue?

Page 1, paragraph 1: extra space before "gas/particle"

Page 3, line 3: remove comma after "formed"

Page 3, paragraph 1: IVOCs are not necessarily unique from "aromatics and long alkanes", in fact as the authors point out that is in large part what they contain (plus cylic and polycyclic aliphatics), so the wording seems a bit off. I would also direct the

authors to Gentner et al., PNAS, 2012 (doi: 10.1073/pnas.1212272109), for a detailed analysis of the composition of combustion emissions in the IVOC range (e.g. diesel fuels), and that work in general that suggested substantial OA formation from diesel fuel components (i.e. IVOCs). Similarly Worton et al. (ES&T, 2014, doi: 10.1021/es405375) found POA from all sources to "look like" motor oil, which was heavily cyclized and branched.

Page 4, paragraph 2: 500 ppbv is very high NOx indeed - are these general trends applicable to more ambient-relevant conditions?

Page 4, paragraph 3: Should be "i.e., Henze", because the authors mean "in other words", not "for example"

Method descriptions of UCD/CIT and SOM are clear and well-written

Page 6, paragraph 2: Though dodecane probably has an approximately appropriate volatility and chain-length, the true chemical composition of combustion related I/SVOCs contains much for branching and cyclization. For future work I would recommend generating an SOM grid for a branched alkylcyclohexane or some similar such compound, if possible.

Page 7, last line: misspelled alkane

Page 8, paragraph 2: Gentner et al. (2012) estimated that branching and cyclization, which likely dominate I/SVOCs decrease SOA yields by a factor of around 3 (based on compiled chamber data available at that time). The assumption of a linear alkane SOM grid could consequently have a significant impact on SOA produced in this work. The authors point to Gentner and Caravaggio to justify that "alkanes" are the substantial fraction, but this somewhat obscures the fact that these alkanes are not linear, which may be important

Page 14, paragraph 1: I'm a bit confused, if measured OA:OC is 1.8-2.1, but are the authors using 1.6?

Figure 1 and discussion therefore: The terminology of splitting "IVOC" and "long alkane and aromatics" is a bit confusing, since the IVOCs are being modeled as long alkanes, and is comprised of alkanes and aromatics. I would recommended something more like "speciated" and "unspeciated", or "lumped". It's not totally clear to me what is a long alkane, and what is an IVOC, but perhaps I missed it in the methods?

Page 17, end of paragraph 1: What might explain this underestimation in SOA? Particularly given that the use of linear alkanes as proxies likely overestimates the SOA yield of some of these groups? Do the later changes to the model fix this regional underestimation?

Page 17, end of paragraph 1: missing a period

Page 20, paragraph 3: "Our simulations imply that IVOCs as a bulk class of SOA precursors may not contribute substantially to ambient SOA levels." Again, I'm not quite sure what to make of this statement, as long alkanes may include species that would be considered IVOCs, so I'm a bit confused by imprecision in language around these compound classes.

Page 22: The authors discuss the impact of faster reaction times, but what about the impact of high volatility preventing wall loss. Does a C6 compound really suffer substantial wall loss, given its ability to re-partition to the gas phase? I would expect most losses to be centered in the IVOC range (less reversibly absorbing to the walls)

Page 26, paragraph 2: The discussion of equations 1-4 is a bit unclear. It would be helpful to remind the reader of the implications of each equation.

Figure 8, Table 4 and discussion thereof: What does it mean from a practical sense that the correlations here are so poor. While I acknowledge the biases and averages are not unreasonable, the model appears unable to capture the temporal variability of these measurements - is that simply due to poor resolution in emissions databases, or is there additional important complexity being ignored? The concern of course is that it

might be telling us something more fundamental about the assumptions or applications of the model.

Figure 9: It's not clear why an O:C of 0.078 was chosen. I imagine it comes from the measurements, but it's not obvious where this is stated. Update: I see it is stated later, this should be brought forward to discussion of the figure or the caption.

Page 34 paragraph 3: Given how big a role vapor wall loss correction plays in the model, it would be helpful to have some discussion of how exactly it is being corrected for. This manuscript just references previous studies, but it warrants some overview here.

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