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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 #1

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This manuscript describes application of the statistical oxidation model (SOM) to predict OA concentrations in a regional chemical transport model. The modeling focuses primarily on the time period for the 2005 SOAR campaign, though there are also some comparisons to the 2010 CalNex campaign. This is the third in a series of papers regarding application of SOM to regional models, and focuses primarily on impacts of I/SVOCs and NOx on predicted OA concentrations.

Overall the manuscript is appropriate for ACP. However, before publication the authors should work to improve the clarity of presentation. As described in my comments below, the manuscript is at times hard to follow.

One note on the manuscript format: I can't use the line numbers. The pdf I can see has line numbers from 0-9 that repeat. Thus in my comments I try to cite the page number and quote the relevant text where possible.

(1) The manuscript is long and at times hard to follow. While the various topics (e.g., POA partitioning, NOx effects, model-measurement comparison) are placed into organized subsections, there is still a lot of information that the reader needs to keep track of throughout the manuscript. There are nine different case studies (Table 3), each at high and low NOx, and a number of SOA pseudo-species (aI-SOA, aV-SOA_aromatic, etc.). Maybe his level of complexity is unavoidable because of the scope of the study. Nonetheless, I found myself having to go back and forth between the Methods and Results sections.

(2) It's not clear to me what the take-home message of this manuscript is. The most striking result, in my opinion, is shown in Figure 3. This figure shows that vapor wall losses are the largest available "knob" for changing SOA predictions. Including vapor wall losses has a bigger impact on SOA predictions than NOx effects or the inclusion of I/SVOC SOA. Maybe this issue is addressed in more detail in Cappa (2016), but it seems like it deserves more attention in this manuscript. The fact that the SOA predictions are strongly dependent on what amounts to an uncertainty in smog chamber data (because the vapor wall loss is calculated rather than directly sampled) is potentially troubling.

(3) Emissions: I would suggest toning down the rhetoric on whether certain gasoline and diesel vehicle emission profiles are representative for use in chemical transport models. On both page 3 and pages 20-21 the authors are critical of using either the Schauer et al emissions profiles or of scaling POA emissions to estimate IVOCs. It is

a fair criticism that the Schauer emissions profiles are dated (though maybe not too out of date for the 2005 modeling period for SOAR), and that there seem to be better IVOC estimates than scaling POA emissions. However, the authors use the May et al emissions profiles, which include gasoline vehicles up through model year 2010 and DPF-equipped diesel vehicles, and offer no comment on how those profiles might also be inappropriate for a 2005 modeling period. At the very least, it seems like the diesel emissions profile in the model should not include the DPF vehicles tested by May et al, unless there is evidence of significant DPF diesel traffic in California prior to the 2007 change in federal emissions limits for diesels.

(4) NOx effects are included in the final model prediction using equations 1-4. These equations are introduced in the Methods section, but the implications of the various corrections are not discussed. Then on page 16 it is noted that a logarithmic function is used. Since NOx effects are a major focus of this paper, the choice of the logarithmic function needs to be discussed in more detail. For instance, why is a logarithmic function used? Is there a physical basis for using this functional form?

(5) Abstract: "IVOCs did not contribute significantly to SOA mass concentrations in the urban areas" A 15% contribution of IVOCs to SOA does not seem insignificant.

(6) Page 6 "Seven SOM grids were used" I think this means that the SOA from the 9 classes were tracked separately. Please clarify.

(7) What are units of delta_LVP in Table 1?

(8) Bottom of page 7 - alkane seems to be mistyped as "alke"

(9) Page 9 - IVOCs are modeled as either a C13 or C15 alkane, but above and in Table 1 it is stated that IVOCs are modeled as a C12 hydrocarbon. Please clarify.

(10) VOC speciation from May et al - is this only for vehicles relevant to the 2005 fleet?

(11) Figure 2 - It would help to label locations of LA and Riverside.

(12) Page 16 - "In central Los Angeles" - how many grid cells are covered by "central" LA and the whole of LA?

(13) Page 17 compares SOA concentrations in LA and Riverside, and states that a difference of 0.2 ug/m3 of SOA between Riverside and LA is evidence of higher SOA in downwind areas. What is the resolving power of the model (if this were a measurement I would think of the minimum detection limit or precision)? What is the minimum concentration difference that can be claimed as meaningfully different between two locations?

(14) Figure 3 - panels are not labeled as (a) and (b) as noted in the caption.

(15) Last line of page 18, the POA reductions between the Traditional and SVOC model case are "more realistic." More realistic than what? The expected POA reduction from May et al (which was not a modeling study)? It seems like the appropriate comparison for how realistic the model predicted POA concentration is comes from comparing to something like AMS data, not by the fractional evaporation in nonvolatile versus semivolatile POA cases.

(16) The top of page 30 suggests that missing VOCs from consumer products might be a reason for low predictions at CSN sites. I don't find this explanation very convincing for several reasons. First, the IMPROVE sites are also under predicted (negative bias for both CSN and IMPROVE), so it's not clear there is a missing source of urban VOCs. Figure 3 shows that SOA predictions are most sensitive to vapor wall losses, which could easily account for SOA under predictions. Since adding 80 tons/day of IVOC emissions (Figure 1) barely impacts SOA formation (in the case without vapor wall loss), the corresponding source associated with personal care products would need to be huge to make up for the missing SOA.

(17) Page 33 "under and over predicted the H:C and O:C" I think this is reversed. O:C is under predicted.

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