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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Simulation of organic aerosol formation during the CalNex study: updated mobile emissions and simplified secondary organic aerosol parameterization for intermediate volatility organic compounds" *by* Quanyang Lu et al.

Anonymous Referee #2

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Summary: This study summarizes the development of a new SOA model and emissions inventory to explore the contribution of IVOCs to SOA formation in California. New IVOC source profiles are developed for gasoline engines, diesel engines, food cooking, wood smoke, and all other sources. A new VBS model is parameterized to predict SOA formation under typical conditions. Calculations are carried out using CMAQ for the region surrounding Los Angeles and for the entire state of California during the months of May-June 2010. The major conclusions of the study are that

(i) gasoline sources emit 4 times more NMOG than diesel sources, (ii) diesel emits 3x more IVOC than gasoline, (iii) mobile sources contribute $\sim$1 μg m-3 of SOA at Pasadena (incl IVOC contributions), (iv) the additional SOA from mobile source IVOCs does not close the gap with measured SOA concentrations, (v) missing IVOC sources cannot realistically be explained by mobile sources, and (vi) missing IVOC sources could plausibly be related to VCPs.

Comments:

1. Line 129: The constraint to limit the SOA model to fewer than 79 additional species seems artificial. While it is true that regulatory applications of CMAQ may not want to implement calculations with large numbers of species, exploratory scientific applications of CMAQ could easily add this number of species to the SOA model. Several examples have been published in the literature (see for example papers by Ying et al. using CMAQ).

2. Line 157, eq 1: The SOA mode formulation used in the current study does not allow for fragmentation. It may not be possible to fit the coefficients in the model to adequately explain SOA formation under the full range of atmospheric aging at different VOC/NOx ratios with this limitation. Some discussion of this limitation should be included in this section that introduces the simplified SOA model.

3. Line 194: change "and" to "by"?

4. Line 213: using diesel POA as a surrogate for all other combustion sources besides mobile, cooking, and biomass seems like a bit of a simplification. It may not matter much for the overall SOA analysis, but is this really appropriate for sources like aircraft? Or structure fires? Or natural gas combustion? Using diesel POA volatility for these sources could significantly bias the results around some localized sources.

5. Line 228: The authors go to great trouble to estimate the amount of additional POA that was not measured during emissions testing due to low concentrations in sampling

equipment, and then describe this material as semi-volatile using POA volatility distributions (line 208). It isn't clear that this gives a different (better) answer than just leaving the original POA emissions at their nominal values and describing this material as essentially non-volatile. It would be instructive to other readers if the authors could quantify these two treatments of POA (or refer to previous publications where this has been done and summarize the results).

6. Line 250: off-road gasoline does not account for a majority of emissions, but shouldn't off-road gasoline engines (non-catalyst) have their own unique profiles?

7: Line 251: off-road diesel is a major source of emissions. It definitely seems like a stretch to use the on-road diesel profile to describe off-road diesel emissions. The uncertainty introduced by this issue should be analyzed in the paper.

8. Line 262: Fragmentation and functionalization are accounted for, but in a biased manner. All of the SVOC and IVOC emitted in the current study will eventually make SOA due to the absence of fragmentation in the mechanism. The formation rates are tuned to account for the net effects over some pre-defined range of aging, but this simplistic model cannot capture the behavior correctly over the full lifetime. It is beyond the reasonable scope to change the simple model in the current paper, but the authors should properly describe it's limitations.

9. Line 312: EMFAC emissions factors are cited as a source of uncertainty, but line 199 states that mobile on-road and non-road emissions are calculated by MOVES 2014a. Which is it?

10. Line 325: The paper should also acknowledge that unknown chemical reactions leading to the formation and reaction of IVOCs could play a role in model error.

11. Figure 6 lower right panel: each of these sites has a different representative atmospheric aging time. The fact that some over-predict and some under-predict as the emissions are scaled up and down may reflect the fact that the functionalization / frag-

mentation processes have been combined into a single lumped parameter that works at one time scale but not at others. This possibility should be discussed in the results and model formulation sections.

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