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Atmos. Chem. Phys. Discuss., referee comment RC1
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Comment on acp-2021-649

Anonymous Referee #1

Referee comment on "Prediction of secondary organic aerosol from the multiphase reaction of gasoline vapor by using volatility–reactivity base lumping" by Sanghee Han and Myoseon Jang, Atmos. Chem. Phys. Discuss., https://doi.org/10.5194/acp-2021-649-RC1, 2021

General comments:

Han and Jang provide some modeling insights on the photooxidative fates of gasoline emissions, using an SOA growth model with corrective terms that account for gas-wall partitioning phenomena that may bias kinetic inferences from experimental chamber data. Simulations across a range of NOx and seed aerosol conditions were developed and compared to observations of ambiently irradiated aerosols in the University of Florida atmospheric chamber, showing reasonable consistency between estimated and measured SOA mass. Further, the authors report broad-strokes sensitivity analyses for a variety of initial conditions and model parameters.

While the core content of the authors' work is interesting and relevant to the field at large, some minor revisions focusing on the reworking of introduction and discussion would be necessary prior to its wider release. In particular, further explanation and disambiguation of certain experimental or modeling decisions would be helpful to better reinforce the authors' assertions in their analysis. Therefore, I recommend this manuscript for publication upon the resolution of the following questions and comments.

Specific Comments:

- A major takeaway of this manuscript is that it is necessary and important to implement corrections for gas-wall partitioning into SOA models. While perhaps an obvious statement to make, I believe it would be useful to underscore that GWP is a largely unavoidable artifact of the experimental data that informs SOA models and is not based

in ambient atmospheric phenomena. The authors note that GWP can vary through several different operational and experimental factors; providing illustrative ranges for wall-loss rate coefficients, similar to the Introduction section of Cappa et al. 2016 (Cappa et al., 2016) will help contextualize the magnitude of these contributions to overall mass balances to the reader.

- Overall: Given that there are many acronyms and abbreviations used throughout this manuscript, it may be helpful (though perhaps not necessary) to include a glossary or list of abbreviations in the SI to improve general readability.
- Section 2 and Table 1: The information provided is likely enough to approximate or infer the duration and magnitude of sunlight that the University of Florida chamber is exposed to in each run. However, it may be helpful for the authors to provide rough estimations for the maximum actinic flux for each day so that the reader can more easily get a feel for the ranges of irradiance across experiments, much like how the ranges of temperatures and relative humidity values are presented. For instance, it is not immediately apparent that the approximate duration between dawn until dusk is 10 hours in January/December, which better justifies the experiment length mentioned on Line 84. The authors provide a reference sunlight intensity that is used in their models, though taken in the end of a Spring season instead of a Winter season. Do the authors expect differences in seasonal incident sunlight to contribute to any potential inconsistencies in results?
- Line 55: As written, it is not clear what parameter(s) the negative biases from wall losses are affecting in SOA models.
- Line 58, "FS is 1 in SA and 0.33 in AS, indicating the aerosol acidity." It is not immediately clear what the authors mean by "indicating" in this context. Is it meant that fractional sulfate can be used as a proxy for initial aerosol acidity? What ranges of FS would be expected for ambient aerosol?
- Line 83, "before sunrise:" given that vapor wall losses are a major feature of this paper, do the authors expect that the amount of time that the initial gasoline vapor spends in the chamber prior to photoreaction will contribute to variance in yields?
- Line 84: Similar to a broader comment above, does the experimental run in March have any notably different behavior compared to the runs that took place in January/December?
- Section 4.1: This section refers explicitly to multiple figures and tables in the supplemental information, and is difficult to interpret without having these figures open; as such, it would likely make sense that some of this information is moved into the body of the manuscript itself. Further, the first paragraph has a majority of its text describing these figures, making it difficult to parse the main assertions and conclusions that the authors are trying to articulate. This section should be reworked to improve its readability.
- Section 4.2: While it is true that the majority of the observed chamber data shows agreement with the authors' OM_T model, it may be helpful to include percentage errors or residuals between model and data. Potential trends in model inaccuracy across different chamber experiments and/or times-of-day would be easier to infer.
- Line 306: When the authors refer to "uncertainty," is it correct to state that they are performing a sensitivity analysis of sorts similar to what they perform in the preceding section, though by adjusting (phenomenological) model parameters rather than environmental conditions? Do the authors expect similar sensitivity trends if GWP factors are taken into account?

Technical Corrections:

- Line 38: Missing space on “bias.”
- Line 82: “flam ionization” should be “flame ionization.”
- Line 350: “…but oligomer is less favorable…” should be checked for grammar.
- Line 351: “This is because…” should have be checked for grammar.
- Figure 2: There is no indication in text or in the caption of which set of markers corresponds to which dataset.
- Figure 3: What does the 9% error refer to? Instrumental resolution? Standard deviation/error across multiple samples? It would make more sense to present this error in absolute terms (i.e., in units of $\mu g/m^{-3}$).

References:

Cappa, C. D., Jathar, S. H., Kleeman, M. J., Docherty, K. S., Jimenez, J. L., Seinfeld, J. H., and Wexler, A. S.: Simulating secondary organic aerosol in a regional air quality model using the statistical oxidation model-Part 2: Assessing the influence of vapor wall losses, 16, 3041–3059, https://doi.org/10.5194/acp-16-3041-2016, 2016.