EGUsphere, referee comment RC1
https://doi.org/10.5194/egusphere-2022-681-RC1, 2022

Comment on egusphere-2022-681

Anonymous Referee #1

Referee comment on "Modeling the influence of chain length on secondary organic aerosol (SOA) formation via multiphase reactions of alkanes" by Azad Madhu et al., EGUsphere, https://doi.org/10.5194/egusphere-2022-681-RC1, 2022

This paper presents a comparison between a modeling study and chamber measurements. It reaches conclusions that should be of interest to the atmospheric chemistry modeling community with regard to the relative importance of SOA mass creation processes. The paper is well written, with clear figures and discussion. I have two requests for improvement:

1) This work is a development of a previous work by some of the same workers (Zhou et al 2019), and it is not always immediately apparent what is new work and what is a restatement of that previous work. The text should clarify the distinction. The restated sections should be condensed and appropriate reference should be made to the prior work.

2) This study should add at least one sensitivity test that attempts to model the morning spike seen in the chamber observations, to support the authors' assertion about its origin.

The standard review questions follow:

1. Does the paper address relevant scientific questions within the scope of ACP?

Yes, this work is well within the shpere of interest of ACP. The paper presents a process-model simulation of the formation of SOA from a selection of precursors representative of diesel fuel emissions. The authors use parameterized product distributions, and extrapolate these distributions to larger precursors than those available in the model's chemical mechanism.

2. Does the paper present novel concepts, ideas, tools, or data?

The simulations using the extrapolated parameterizations are compared to new chamber data. The comparisons are improved by the addition of the auto-oxidation process to the model training set, and by the consideration of wall losses in the chamber.

3. Are substantial conclusions reached?

The authors conclude that reactions in the wet inorganic phase make no significant contribution to SOA mass from the species considered: gas-particle partitioning is far more important. This result should be useful to future modeling studies.

4. Are the scientific methods and assumptions valid and clearly outlined?

The scientific method combines several previously-published concepts and equations, which are clearly outlined.

5. Are the results sufficient to support the interpretations and conclusions?

The interpretations and conclusions follow logically from the model/chamber comparisons. The Figures illustrate the analysis nicely.

- Line 300: discussion of Figure 3. I agree that C9D, C10D and C11C show good model-data comparisons. Comparisons C9C and C10B are not so good, and look more like comparisons C11A and C11B, which are said to be poor. The text should be clearer about this distinction. This comment des not detract from the paper's overall conclusions.
- IMPORTANT. This study should add at least one sensitivity test that attempts to model the morning spike seen in the chamber observations, to support the authors' assertion about its origin. (Line 325)

6. Is the description of experiments and calculations sufficiently complete and precise to allow their reproduction by fellow scientists (traceability of results)?

The experiments appear to be well documented.

7. Do the authors give proper credit to related work and clearly indicate their own new/original contribution?

In general, yes, credit is given. However this work is a development of a previous work by the same group (Zhou et al 2019), and it is not always immediately apparent what is new work and what is a restatement of that previous work. The model description, especially Sections 3.2 & 3.4, appears to be taken almost verbatim from Zhou et al 2019. That work should be acknowledged early in each relevant section and the authors should clearly say in the model description what parts of the model system are reused from that prior work, and what parts are new. Consideration should be given as to whether any of these sections can be simplified and shortened by referring the reader to the previous work. The same applies to Figure 1, which appears to be almost identical to Figure 1 of Zhou (2019)

8.Does the title clearly reflect the contents of the paper? 9.Does the abstract provide a concise and complete summary?

The title and abstract are clear and complete. I suggest that the model name should be added to the paper title.

10. Is the overall presentation well structured and clear?

The presentation and structure are generally clear. For specific minor points, see my list below.

11. Is the language fluent and precise?

The language is mostly fluent, precise and clear. I have a couple of minor requests for clarity, detailed below.

12. Are mathematical formulae, symbols, abbreviations, and units correctly defined and used?

- The symbols and abbreviations are much easier to follow after studying Figure 1.
- Section S4, Table S2: It is unfortunate that the accommodation coefficient alpha_w,i, and the polarizability alpha_i have such similar symbols, and that these could be

confused with the mass-based stoichiometric coefficient alpha_i introduced in section 3.2. It might be appropriate to change one of these symbols, or at least to explicitly acknowledge the possibility for confusion.

13. Should any parts of the paper (text, formulae, figures, tables) be clarified, reduced, combined, or eliminated?

- The model description could be condensed by properly acknowledging and referring to the previous work, as already mentioned.
- Line 131-132, 197, 215 etc: This reviewer finds the abbreviations "or" and "in" confusing in the text because they can be mistaken for ordinary words. Please spell out the words "organic" & "inorganic" unless the abbreviations are used in combination with other symbols? Or, at a minimum, give them bold italic font to differentiate them from normal text.

14. Are the number and quality of references appropriate?

This is generally a good (but not exhaustive) guide to the recent literature on the relevant topics.

- The following works are cited in the text but are missing from the reference lists: Line 198: Pankow (1994); Line 272: Yap (2011); SI: Roldin (2019).
- Line 142: Pye 2019 and Xavier 2019 are not appropriate references for the identification of auto-oxidation reactions: they are modeling papers. It would be better to cite an early lab study (e.g. Sahetchian et al, Combust. Flame 1991; Crounse & Nielsen. J. Phys. Chem. Lett., 2013)

15. Is the amount and quality of supplementary material appropriate?

The supplementary material is helpful and appropriate.

- Tables S4, S5: please provide a key to or explanation of the chemical compound code names?

Other specific comments (major):

- Line 158: Please briefly discuss the conceptual movement of the reaction products between reactivity levels in your 51-box matrix. What does this represent, in a chemical-physical sense? Are there any constraints on the sum of all the dynamic alpha_sub_i values?

Specific comments (minor):

- Line 45: please correct the reference (Robinson et al., 2007)
- Lines 46-73: Please mention the names of the models used in Hodzic (2010), Cappa (2013), Zhang & Seinfeld (2013)
- Line 50: Note that, since Lee-Taylor et al used the larger linear alkanes as surrogates for all larger species, the fact that the majority of SOA precursors in their model were linear alkanes is a logical outcome of those SOA species having larger carbon numbers.
- Lines 61-65: Perhaps "neglect" would be kinder than "fail to consider"? The previous authors are likely well aware of the limitations of their approaches, and (at least in one case) mention those limitations explicitly.
- Line 86: "… the typical ozone mechanisms.." This seems vague. Did this study use several ozone mechanisms or just one?
- Line 133: "OMAR" needs subscripts.
- Lines 272-274: This sentence is confusing. Please rearrange it?
- Line 305: Do you mean "from" instead of "form"?
- Line 321, 323: Do you mean figure 5 instead of fig 6?
- Line 322: Do you mean figure 4 instead of fig 5?
- Line 341: why is it notable that previous experiments used H2O2 as a low-NOx OH source? What are the implications? Please discuss.
- Line 357: please specify whether you mean the relative or absolute contribution of OM_{AR}?
- Line 370: do you mean Figure S6 instead of Fig 5?
- Line 625, 655: "OCEC is missing its "/"