Atmos. Chem. Phys. Discuss.,
https://doi.org/10.5194/acp-2017-1178-RC2, 2018

Atmospheric Chemistry and Physics Discussions

Interactive comment on "Simulating secondary organic aerosol from anthropogenic and biogenic precursors: comparison to outdoor chamber experiments, effect of oligomerization on SOA formation and reactive uptake of aldehydes" *by* Florian Couvidat et al.

Anonymous Referee #2

Received and published: 29 March 2018

Couvidat et al. develop updates to a secondary organic aerosol (SOA) model and report their findings on how those updates perform against chamber SOA measurements made with mixtures of biogenic and anthropogenic precursors. They find that, in general, the updates help improve the model-measurement comparison but offer nuanced insights on the role of NO, oligomerization, vapor wall losses, reactive uptake of pinonaldehyde, and particle phase on SOA formation.

The area of study undertaken by the authors is very important, that of understanding the processes that determine the formation, composition, evolution, and properties of SOA from oxidation of organic precursors. Findings here will help develop simplified mechanisms for atmospheric models. However, the manuscript in its current form does not do well in communicating the methods and, in some cases, the results and implications of the modeling efforts (see some comments below for details). What makes the manuscript even harder to understand is that there are numerous grammatical mistakes and phrasing/style issues. These need to be fixed before the manuscript can be reviewed again, in addition to achieving the quality desired in a journal like Atmospheric Chemistry and Physics. Although I believe this is important and novel work, I cannot make a judgement at this point based on the manuscript submitted for review. Hence, I do not recommend publication in ACP until the issues I discuss below are resolved, the presentation quality is significantly improved, and the manuscript is sent out for review again.

Major Comments:

1. Details on experimental methods and data: There is very little description of the experimental methods used to provide context to the modeling in this work. For example, how big is the Euphore facility? Given the size, was it correct to use the same wall loss rate as that used by the Caltech chamber to model vapor wall losses? Was it a Teflon chamber? What was the motivation to use a mix of precursors instead of using a single precursor? Were these photooxidation experiments or ozonolysis experiments (especially for the biogenic mixture)? Was an OH precursor used and if yes, which one? What photochemical ages were achieved? Was ozone produced? If yes, how much? Were these experiments seeded? What instrumentation was used to measure aerosol mass concentrations? How were the data corrected for wall losses? What are the uncertainties in the measurement data? Answers to these questions and more that bear relevance to the modeling need to be provided as part of section 2.1.

2. Details on modeling methods: Various details of the modeling approach are missing

that make it hard to understand the simulated processes. For example, (page 4, lines 30-32), why was the wall loss rate for vapors used in this work based on the Caltech chamber. A vapor wall loss rate could be estimated for the Euphore facility based on the calculations laid out in the supporting information of Zhang et al. (PNAS, 2014). Why was this not done? Also, the vapor wall loss rate only defines the loss rate of vapors. The affinity of these compounds to stick to the walls was modeled by Zhang et al. (PNAS, 2014) and later shown by Krechmer et al. (ES&T, 2016) to be a function of the vapor pressure of the species. Was this modeled similarly? In the mechanism section (page 5, lines 1-31), the abbreviations for the different species are obvious but it would be worthwhile to explicitly specify them, e.g., API is never defined. Perhaps, include this information in the tables as a legend. Why is only the number mean used to model particle size and not use the entire aerosol size distribution?

3. Structure, grammar, phrasing, and style: In terms of structure, I did not understand the order of the figures. I would recommend that the figure numbers be ordered in the order they show up in the manuscript. Further, the grammar, phrasing and style could be significantly improved. Here is a sample of mistakes I found just in Section 3.3 on page 13: (a) line 8: 'they dynamic of the uptake', (b) line 18: 'specific of the compound', and (c) line 18-19: 'probably provides a good estimate and order of magnitude.'. The manuscript is littered with such mistakes.

Minor comments: 1. Page 2, line 13: Consider citing the chemical transport model study of Cappa et al. (ACP, 2016) that simulated the influence of vapor wall losses on organic aerosol (OA) mass concentrations in urban areas.

2. Page 2, line 14: Jathar et al. (ACP, 2016) have showed – similar to the findings in this work – that oligomerization may not play an important role in affecting SOA mass concentrations but may change the SOA composition. Consider citing.

3. Page 3, line 17: How big is the Euphore facility?

4. Page 4, line 29: What does chamber is closed mean?

5. Page 5, line 23-29: Are the different O:Cs possibly from differences in OA mass concentrations in the different experiments?

6. Page 11, line 7-8: Is particle number or mass used to determine particle wall loss rates? Why are the particle wall loss rates different for with and without oligomerization?

7. Page 11, line 28: Could the differences in SOA formation be explained as a function of the VOC/NOx ratio expressed in ppbC/ppb, similar to previous work?

8. Page 12, line 17: Use 'fragmentation' instead of 'fractionalization'.

9. Page 14, line 7-8: Sentence is unclear and needs more explanation.

10. Page 14, line 14-15: What figure shows a factor of 3 difference for the simulation that includes the loss of vapors to the walls.

11. Page 14, line 23: What do stoichiometric coefficients mean here?

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