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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 #1

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The Couvidat et al. manuscript reports on a series of parameterizations implemented in a model for secondary organic aerosol (SOA). Model simulation results are compared with experimental data obtained from the Euphore chamber, using both anthropogenic and biogenic precursors. The model used is the SOAP model, which uses surrogate compounds for each precursor that best reproduce the bulk properties of the SOA formed (e.g., O/C and H/C ratios). SOAP model parameterizations are developed for anthropogenic and biogenic precursors, and to represent oligomerization and acid-

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catalyzed uptake of aldehydes. Sensitivity of model simulations to increased particle viscosity and vapor wall loss are considered. While there are some complex processes that are well represented in the model, and these complex processes are treated in a single model framework, the manuscript lacks clear direction. The objectives of the modeling are not clear, nor are the scientific contributions. Development of SOA models has been rapidly advancing over the last 20 years; parameterizations for all of the processes described in this manuscript have been developed and applied. The application of different parameterizations is not particularly novel, nor does it clearly advance the state of the science. It is suggested that this manuscript undergo major revisions prior to publication. The manuscript may be improved by focusing on one of the parameterizations (e.g., oligomerization) and comparing more rigorously to other model parameterizations and a broader suite of published studies. The manuscript should also be read carefully for clarity and grammatical errors. This will also improve the manuscript and increase its potential impact.

Comments: The mechanism parameters for aromatics were developed largely from chamber studies that are now 10+ years old. For at least some of the compounds of interest, more recent data are available. For example: Hildebrandt et al., ACP 2015 (toluene) and Li et al., ACP 2016 (aromatics, low NOx). The same is true of the parameters used to represent oligomerization. See for example, Kundu et al., ACP 2016 (oligomers from limonene). There may be good reasons for using the particular studies/data chosen, but those reasons should be articulated.

Abstract, lines 6-7: replace "were" with "where"

p.3, line 20: It is recommended that the authors be more specific about the ranges of conditions covered by the experiments, particularly for atmospherically-relevant conditions that are outside the available datasets.

p.5, line 3-4: Chamber data studies are referenced twice.

p. 7, lines 27-30: How are "short", "big", and "bigger" oligomers defined?

p. 11, lines 11-15: Can more be said about the underlying reasons for differences between the model simulations in this work with those of Santiago et al. 2012? Particularly from the perspective of describing the likely processes in the experimental studies.

p. 11, lines 31-33: It is suggested that this section be rewritten to clarify that the model simulations are over/under predicting in different chemical regimes. It is not clear as written. p. 15: The discussion of the consideration of vapor wall loss is incomplete and perhaps misleading. The measurement/model agreement will reflect both the model parameterizations (as indicated), but also the experimental conditions. In this case, underestimation by inclusion of vapor wall loss may largely be due to the fact that vapor wall loss was negligible in the Euphore chamber under the experimental conditions. There is not good scientific support for broadly applying a 3-fold decrease in SVOC volatility and a single vapor wall loss parameterization for all SOA models developed using the Odum approach as applied to all Teflon chamber studies. The extent of wall loss involves competing kinetic processes, and will be highly dependent on the chamber and the experimental conditions.

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