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Interactive comment on "Constraining condensed-phase formation kinetics of secondary organic aerosol components from isoprene epoxydiols" *by* T. P. Riedel et al.

Anonymous Referee #1

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Combining a box model and chamber experiments, the authors of this work provide constraints to the condensed-phase IEPOX reaction kinetics which lack experimental determination. The rate constants of a series of reactions are estimated by finding the best match to the measured tracer concentrations from filters collected in chamber experiments. Based on the rate constants, SOAformation under atmospherically relevant conditions is simulated, and the authors demonstrate that the results show consistency with a recent field measurement.

Given that isoprene is by far the most emitted volatile organic compound species in the global scale, and that the reactions and uptake of IEPOX represent the most important

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steps of isoprene SOA formation, the current work is valuable and relevant to the scope of ACP. Before the paper is published, the following points should be addressed.

Comment 1

A major weakness of the current work lies in the fact that the rate constants are determined based on a countable number of chamber experiments whose conditions are not fully representative of the ambient atmosphere. A clearer link between the chamber and the ambient conditions should be presented. In particular:

1.1) Are the chamber conditions represent certain ambient conditions? If yes, the authors should mention what types of environment the chamber conditions are intended to simulate. If no, the authors should discuss potential problem of extrapolating the chamber experiments to the ambient.

1.2) The authors can probably consider putting the ambient condition used in the simulation in Sect. 3.3 into Table 1 to make a clearer comparison with the conditions employed in the chamber experiments.

1.3) Specifically, the chamber experiments are performed under dry conditions (i.e. RH < 5%), but this seems to be too low to represent the ambient condition. Can rate constants determined from dry chamber experiment be extrapolate to make implication for the ambient conditions? The authors should justify this in the paper.

1.4) In the simulation for ambient condition (Sect. 3.3.), RH is set at 50 %. Is this why 2-methyltetrol is the major SOA constituents in the ambient simulation, but “Other SOA” is the major constituent measured from the chamber? No explanations are provided to discuss the differences.

1.5) The authors mention that the ambient simulation is in “close correspondence to recent [field] measurements” (page 28302, line 3), but they do not seem very close to the reviewer. Why the major SOA constituents in the chamber and the simulation are different (also see the previous comment). Why sulfate titration is significant in the chamber but not under the ambient conditions? The authors should enrich the discussion to explain these differences.

Comment 2

Although the approach employed in the current work is robust in constraining rate constants that have not been measured experimentally, discussions about the limitations of this approach seems to be lacking from the current manuscript.

2.1) What are the potential danger of fitting multi-variables to match a countable number of chamber experiments? The authors briefly discuss the experimental limitations of the current work in Sect. 4 (Concluding Remark). Instead of mentioning these in the conclusion, the authors are encouraged to make a new section to summarize the potential shortcomings of the method.

2.2) The uncertainties associated with the determined rate constants are currently listed as the standard deviation from the five chamber experiments (Table 3), but the uncertainties should be assessed more statistically. When each rate constant is fitted for the best match to the chamber experiment, can a statistical uncertainty be determined for each constant, instead of the standard deviation of the five experiments?

2.3) Related to the previous comment, some of the uncertainties (Table 3) are so large that the rate constant can potentially be negative. Explanation should be added to address this issue. In particular, the large uncertainty associated with “Other SOA” formation should be discussed, given that “Other SOA” is the major fraction observed in the chamber experiment (Fig. 3).

Comment 3

The assumption of “other SOA” being IEPOX-OS should be better justified, or a sensitivity test should be performed. When “Other SOA” is assumed to be a compound with a larger or a smaller molecular weight, would the prediction of the rate constants be altered significantly?

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Comment 4

I found that the information provided in Table 2 repetitive, making this table less informative. The authors are encouraged to find a better way to present the agreement between the actual measurement and modeled results.

Technical comment:

Page 28296 Line 3: “mostly likely” should be “most likely”.

Interactive comment on Atmos. Chem. Phys. Discuss., 15, 28289, 2015.

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