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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Model-measurement comparison of functional group abundance in α-pinene and 1,3,5-trimethylbenzene secondary organic aerosol formation" *by* G. Ruggeri et al.

Anonymous Referee #1

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General Comments

In this manuscript the authors compare results of Master Chemical Mechanism (MCM) simulations of the functional group composition of secondary organic aerosol (SOA) formed from reactions of a-pinene (APIN) and 1,3,5-trimethylbenzene (TMB) with measured values determined by FTIR analysis in order to demonstrate the utility of this approach for evaluating chemical reaction models. The systems chosen for study are popular ones since APIN is an important biogenic VOC and TMB is representative of anthropogenic aromatic emissions. The manuscript is concise and well written, and the authors do a good job of comparing model and measurement results, providing plausible explanations for discrepancies when possible. Because there are in many

cases significant differences, and both the simulations and measurements have considerable uncertainties, it is difficult to determine the source of the discrepancies. One conclusion is therefore that more measurements of chamber systems are needed using a variety of tools in order to develop databases of reliable chemical data for model comparisons. In general, however, I think the approach presented here has promise, and that the manuscript presents a useful demonstration of how models can be tested using more detailed chemical data rather than just SOA yields and O/C ratios. I think the paper is suitable for publication in ACP, but have a couple questions the authors should address.

Specific Comments

1. The comparison of measurements with simulations of the low-NOx TMB reaction seems problematic, since FTIR does not measure peroxides, which dominate the simulated SOA composition. I don't see any explicit mention of this.

2. When certain FG, like peroxides, are not measured by FTIR, how are the reported concentrations of the other FG affected? I do not see an "unidentified" component of SOA in the pie diagrams.

3. Is there molecular information available from other experiments conducted under roughly similar conditions that can be used to determine if the major molecular components predicted by the MCM are reasonable, which may help in determining whether the model or measurements are the source of discrepancies in some comparisons?

4. Are there simpler systems that might be modeled and analyzed?

Technical Comments

None.

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