Response to Referee #1

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.

We thank the reviewer for the support and helpful comments. We address specific comments below.

1. **Comment** : 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.

   Response: We note that peroxides concentrations were not reported in the study by Sax et al., but is not beyond the capability of analysis by FTIR as there are absorption bands in the infrared window for hydroperoxides and organic peroxides. However, the reviewer's point with respect to model-measurement comparison in this work is worth clarifying in the manuscript. In our pie charts in Figure 3, only the measured mole fraction of OA is shown.

   In Methods Section 2.4, we have added the sentence:

   "For model-measurement comparison, we select the subset of FGs that are reported by measurement and use relative metrics normalized only by the measured fraction of OA."

2. **Comment**: 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.

   Response In response to the previous comment, we report relative concentrations of the measured fraction. While it is possible to include an unidentified or remaining fraction in the model simulation pie charts, we do not know how large this fraction should be for the FTIR measurements. We have therefore added in the caption of Figure 3 the phrase:

   "The mole fractions reported in simulations are summed with respect to the subset of FGs that are reported by measurement to facilitate direct comparison."

3. **Comment**: 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?

   Response: There are some analyses of gas phase composition which we now include in our analysis.

   In Results Section 3.1.1:

"Pinonic acid is the second largest contributor to COOH FG, which is consistent with previous reports of pinonic acid being a major contributor to SOA in APIN photooxidation over a range of NO_x conditions Eddingsaas et al. (2012)."

And in Results Section 3.2.1: "As for APIN-lNO_x , pinonic acid is the second largest contributor to COOH FG; consistent with observations in similar experiments (Eddingsaas et al., 2012)."

We hope that this manuscript will encourage the adoption of FTIR as a complementary tool for OA analysis and that such joint measurements will become available in the future.

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

   Response α-pinene dark ozonolysis is a classic, well-studied system (e.g., Yu et al., 1999) which may provide constraints and simplification in interpretation. At present time, we selected simulations for which experimental values were available, but hope that there will be opportunities for further exploration in future studies.

   The reasoning for selecting these particular systems have now been explicitly added to the beginning of Methods Section 2:

   "We target our model simulations to mimic SOA formation in environmentally controlled chambers for which FG measurements are available."

References

Eddingsaas, N. C., Loza, C. L., Yee, L. D., Seinfeld, J. H., and Wennberg, P. O.: alpha-pinene photooxidation under controlled chemical conditions - Part 1: Gas-phase composition in low- and high-NOx environments, Atmospheric Chemistry and Physics, 12, 6489–6504, doi:10.5194/acp-12-6489-2012, 2012.

Yu, J. Z., Cocker, D. R., Griffin, R. J., Flagan, R. C., and Seinfeld, J. H.: Gas-phase ozone oxidation of monoterpenes: Gaseous and particulate products, Journal of Atmospheric Chemistry, 34, 207–258, doi:10.1023/A:1006254930583, 1999.