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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Role of ozone in SOA formation from alkane photooxidation" *by* X. Zhang et al.

Anonymous Referee #3

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Review of "Role of ozone in SOA formation from alkane photooxidation" by X. Zhang, R. Schwantes, M. Coggon, C. Loza, K. Schilling, R. Flagan, and J. Seinfeld [acp-2013-660].

This paper presents an investigation of the SOA formation from large n-alkanes, focusing on the competition between OH and O3 on the oxidation of dehydrofurans. The paper uses dodecane as the model system. The paper presents experimental data measured in a smog chamber under high and low NOx conditions at different relative humidity (RH). The paper extends existing SOA mechanisms to account for ozonolysis of dihydrofurans. Their analysis suggests that ozonylsis will be the dominant fate of dihydrofurans in most environments. This reduces SOA yields but creates more oxygenated organic aerosol. This is an important effect that should be accounted for in

models (and experiments).

The paper is interesting and well written. The experiments were well done and the model development appears to be well grounded in the existing literature. Large alkanes are likely an important source SOA in urban environments, but there are gaps in our understanding of the underlying chemistry (especially with respect to SOA formation). This paper attacks an interesting gap – the potential role of ozonolysis on SOA formation from alkanes. I recommend that the paper be published after addressing the following comments.

Model evaluation – A strength of the paper is the combination of the measurements and model development. However, these pieces are not well integrated. It is almost as if there are two separate papers. There is only one figure (Figure 10) in which the model is compared with the data. Two parameters are compared – the decay of dodecane and the production of SOA. The fact that the model reproduces the measured decay of dodecane is no surprise – the data were fit to determine the OH concentration. The good agreement with the SOA formation is potentially more interesting. The agreement is excellent; presumably this is because the model has been fit to reproduce the measured SOA. What free parameters that were fit to match the data? How unique is the solution?

The good agreement in SOA data shown Figure 10 could be interpreted by the reader as "validation" of the proposed mechanism. Is this the correct interpretation? Presumably other models / mechanisms could also reproduce the data. The paper presents lots of Figures with just data (Figure 4, 5, 6, 7, 8, 9) or just model results (Figure 3) but few Figures that compare both (only Figure 10). The paper should compare the model predictions against other measured parameters to test whether or not the proposed mechanism is correct.

Role of water / RH – The experiments varied the RH inside the chamber from ∼3% to ∼55%. There was relatively little discussion of these results. For example, it appear

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to slow the decay of C12H23O+ in the AMS. Why was that? I would encourage the authors to add a bit more discussion on the effects of RH to the manuscript. Smog chamber experiments are often done at very low RH. How much affect does RH appear to have on the SOA formation? The effect is directly on the chemistry? Or is it indirect on the partitioning? The experiment did not consider RH greater than 50%, which are very common in the atmosphere. What are the implications of the results if one extrapolates to higher RH?

Experimental matrix – Table 1 provides the experimental matrix. It appears that experiments were done only at each experimental condition once. Is this correct? Given the complexity of smog chamber experiments, the paper should discuss the repeatability of the results.

Typos

Page 24723 line 21 – mˆ3 missing negative sign

Page 24729 line 12 – this should be 44 (f44 is presumably mass fraction of 44 not 43)

Interactive comment on Atmos. Chem. Phys. Discuss., 13, 24713, 2013.