**Atmospheric
Chemistry
and Physics
Discussions**

Interactive comment on "Modeling of secondary organic aerosol yields from laboratory chamber data" by M. N. Chan et al.

Anonymous Referee #1

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Summary

In this manuscript Chan et al. present an updated product-specific model for SOA formation and compare their model to experimental a-pinene ozonolysis data. Five semi-volatile products, identified as important components of a-pinene SOA in previous publications, are chosen as representative compounds. The equilibrium partitioning constants of these species are then estimated from an updated group contribution method and equilibrium partitioning theory is used to predict SOA yield, chemical composition, and temperature dependence. The paper is well-written and some interesting conclusions are drawn. The paper is appropriate for ACP and could be published with relatively minor modifications.

General comments

My major comments have to do with the estimated Kp values and their implications. It seems clear from the paper that most if not all measurable experimental quantities are better fit using Kp = 100, relative to Kp=1. Can the authors comment on the errors in the vapor pressure estimation? Is vapor pressure the most uncertain quantity in the Kp calculation? It seems unlikely that the errors in the group contribution method are two orders of magnitude for all the products.

Can the authors comment further on the relatively poor performance of the Kp=1 case? For example, do any simple oligomerization reactions of the model products produce the 100x reduction in Kp? If not, what functional groups are necessary to produce a ~100 x reduction in Kp?

If the Kp values have to be empirically increased by a factor of 100 for the model to reproduce the data, is there any advantage to the Odum-type fitting over the basis-set method, which appears to fit the low-loading data more accurately?

The authors should further comment on the large alpha values necessary for fitting the data (beyond just stating they are aware of the large values). The sum of the yields is close to or greater than one, which isn't physically realistic under the experimental loadings studied. What does this mean for the model? Does it imply that the Kp values of the products in the experimental studies are even lower than in the Kp 100 case?

How unique are the solutions to the fitting equations? Can the data be fit equally well if the solver is seeded with other values of alpha?

Specific Comments:

P 9471, lines 10-12. The authors state that their O/C ratios are somewhat lower than those of Shilling et al. (Shilling et al., 2009). Did the authors assume atmospheric concentrations of CO_2? Pure air generators generally deplete CO_2 well below atmospheric values (Shilling et al., 2009). The default Aiken et al. code corrects the total CO_2 signal (gas + particle) for atmospheric CO_2 concentrations (Aiken et al., 2008). In

the case of pure air, the code may overestimate gas-phase signal, thereby underestimating particle-phase CO_2 and consequently O/C. Because so many other ion signals are estimated based on the particle-phase CO_2 signal, it is extremely important to accurately quantify particle-phase CO_2.

P9466, lines 26 – 28. Qualitative descriptions such as "weak" and "slight" are not very useful, especially when a quantitative measure is available. A quantitative comparison between the measured T dependence with the modeled T dependence would be much more informative.

P9462, lines 3 – 11. The authors interrupt the flow of the discussion by switching between basis-set and Odum-type fitting routines. I suggest separating the basis set discussion into its own paragraph.

P9470 lines 20-25. Please change the wording of this sentence. If a HR-AMS is available, a-priori knowledge of the composition is not needed. The composition is measured during the course of the experiment. In fact, the authors rely on a-priori knowledge of the chemical composition for their own particle resolved model, so the authors' statement is misleading.

References

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Jenkin, M.: Modeling the formation and composition of secondary organic aerosol from a- and b- pinene with o3, Atmos. Chem. Phys., 2004, 1741-1754, 2004.

Shilling, J. E., Chen, Q., King, S. M., Rosenoern, T., Kroll, J. H., Worsnop, D. R.,

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Interactive Discussion

Discussion Paper

DeCarlo, P. F., Aiken, A. C., Sueper, D., Jimenez, J. L. and Martin, S. T.: Loading-dependent elemental composition of a-pinene soa particles, Atmos. Chem. Phys. , 9, 771-782, 2009.

Interactive comment on Atmos. Chem. Phys. Discuss., 9, 9457, 2009.