Atmos. Chem. Phys. Discuss., 11, C4833–C4834, 2011
www.atmos-chem-phys-discuss.net/11/C4833/2011/

Atmospheric Chemistry and Physics Discussions

Interactive comment on "Simulating the oxygen content of ambient organic aerosol with the 2D volatility basis set" *by* B. N. Murphy et al.

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Received and published: 12 June 2011

1. *As noted above, the base-case model results for the mean OA concentration and O/C ratio compare remarkably well with the ambient measurements, especially considering the large uncertainties in many model inputs and the fact that the community regularly reports 1-2 order-of-magnitude discrepancies in OA predictions. The study is presented as if the modeling was carried out with complete ignorance of the measurements. Is this the case, or did the modelers peak at the field results before completing the modeling, and if so, were any base-case parameters or other components of the model selected or adjusted in order to improve agreement? I don't view this as a problem, but it should be discussed lest readers be misled as to some of the reasons for the remarkable agreement, which I would view as bordering on the miraculous.*

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Interactive Discussion

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No, the modeling was not carried out in complete ignorance of the experiments. However, it was not clear before we completed this work, that one could successfully predict the large extent of oxygenation that was observed by using realistic reaction rates and believable transformations for each oxidation generation (i.e. the number of oxygens added). To answer this question, one needs atmospherically relevant emission rates, photolysis rates, oxidant chemistry, and removal processes. This work merely serves to address that concern of feasibility. The base rate constants for chemical aging used here are the same as those of our recent previous work with the 1-D VBS (Murphy and Pandis, 2009). We do not intend to suggest that the particular model configuration we have used is the ultimate answer to the problem of atmospheric organic compound aging, but merely a useful tool. We will continue to look at the uncertainties closely from a variety of angles in future work. We have added some discussion to make this point clear in the text.

2. *Although outside the scope of this paper, it would be very interesting if the authors carried out a similar study in their smog chamber with a mixture of aromatics, alkanes, and terpenes, in which they would have even better knowledge of the precursors and the oxidation conditions. To my knowledge, this has not been done. I think the authors have typically used chamber data to obtain parameterizations for use in ambient models, but not to test their models for a simulated complex atmospheric system. Presumably the model could perform as well or better than it did in the field.*

This idea is quite promising and we are currently pursuing these types of experiments in order to constrain the model even further. This mixture system of precursors could well be an interesting intermediate step between the simplicity of one-precursor systems and a realistic atmosphere. We hope to develop for the next application a model that successfully addresses both these complex laboratory systems as well as the atmospheric context we have presented in the current work.

Interactive comment on Atmos. Chem. Phys. Discuss., 11, 8553, 2011.