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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Modeling secondary organic aerosol in an urban area: application to Paris, France" *by* F. Couvidat et al.

Anonymous Referee #1

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General Comments

In this manuscript the authors used two related models to simulate SOA formation in Paris, for comparison with results of field measurements of OC and EC. SOA is simulated using the H2O (Hydrophilic/Hydrophobic Organic) model, which employs surrogate compounds to represent different classes of SOA species and accounts for the differences in partitioning of organic compounds to aqueous and organic phases. Simulations were conducted with the standard H2O model (H2O-Ref) and also with a modified version (H2O-Mech) that used a more molecular based approach to simulate aging of primary and aged SVOC. In general the model results agree well with the measurements. The paper is clearly written and the results are discussed in sufficient detail, with the authors providing reasonable possible explanations for situations when

the results and measurements do not agree. The paper presents a useful evaluation of an approach to SOA modeling that is worthy of publication. The paper will be suitable for ACP once the following comments have been addressed.

Specific Comments

1. Table 1. Please explain why PAHs make up 30% of the primary SVOC emissions. This sounds incredibly high. It seems that this value is based on data from Schauer et al. (1999). Is this 30% value relative to the total mass of SVOC that was identified in their study or the total SVOC mass? Usually 80-90% of the total mass is present in an unresolved complex mixture that is dominated by branched and cyclic alkanes.

2. Page 23477, lines12-13: The yields of products from reactions of aromatics with OH are generally dominated by ring-opened products containing aldehyde groups that should oligomerize, with intact aromatic products being a relatively small fraction. In addition, these ring-opened products are unsaturated and so react with OH radicals much faster than aromatic compounds and thus lead to rapid aging. Both of these factors are likely to lead to much more SOA than would be simulated with the H2O-Mech model.

3. Page 23481lines 15-18: A little discussion of the criteria of performance quoted here would be helpful. What is the basis for these? Are they widely accepted?

4. The results regarding the sources of SOA in Figure 13 seem surprising. Recent results from the CalNex study in the Los Angeles area indicate that SOA is dominated by aromatic sources (Bahreini et al., Geophys. Res. Lett., 2010). Furthermore, I am not aware of other studies that have suggested that sesquiterpenes could be such a large source of SOA, especially in an urban area. Is there some reason why things should be so different in Paris?

5. As a non-modeler I am always amazed at how good the agreement tends to be between models and ambient measurements, such as shown in Figures 4, 5, and 8. The

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modeling I have seen of chamber reactions involving a single compound and oxidant and very well controlled conditions rarely does as well. So this leads me to a question: To what extent were the many parameters and assumptions used in this modeling study adjusted to improve agreement with the ambient data, or was the modeling done completely "blind" and then compared with no further adjustments? This is not clear to me from the manuscript.

6. Some discussion regarding the likely sensitivities of the modeling results to the assumptions and parameters chosen for the study would be helpful.

Technical Comments

Page 23478, line 12: I think NO3 is meant to be NO2.

Interactive comment on Atmos. Chem. Phys. Discuss., 12, 23471, 2012.