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Interactive comment on “Modeling the formation and properties of traditional and non-traditional secondary organic aerosol: problem formulation and application to aircraft exhaust” by S. H. Jathar et al.

Anonymous Referee #1

Received and published: 2 June 2012

In this work, the authors present an approach to model secondary organic aerosol that is thought to be formed from low-volatility organic emissions. Here they apply the methodology to model SOA formation from oxidation of aircraft exhaust, incorporating relevant oxidation mechanisms, such as multigenerational oxidation, and employing more realistic parameters. This model represents an improvement over the Robinson 2007 approach, as the authors have noted. I strongly encourage the authors place this work in better context, in order for this methodology to be effectively adopted in atmospheric models. Otherwise the manuscript overall is well written, and the approach is

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novel and important. Publication of this paper is recommended, after considering the following comments.

Major comments:

- The biggest concern I have is that the model parameters are very source dependent, which is a result of the difference in compounds emitted. This will imply that many different sources will need to be included into such a model (e.g. different fuel types, different engine conditions etc.), each requiring a different set of parameters {a1,b1,c1,d1}. This has not been a problem for current models, because the precursor-specific approach used currently for T-SOA allows for straightforward lumping of precursors (simply by chemical similarities). Lack of compound-specific information for the hybrid approach will not allow for that, and would make this approach very computationally expensive. However, requiring that a very complete and detailed knowledge of organic compounds for each emission source be known seems philosophically at odds with the volatility basis set approach. The authors should address this dilemma, and perhaps a balanced approach to solving this problem.

- In section 4.3.2, the authors stated that the parameters were determined for each experiment individually. I am concerned about the robustness of these parameters, since they are semi-empirical. How do the parameters vary in the different JP8-Idle experiments? The authors should investigate if some of the parameters are in fact coupled (i.e. multiple combinations for the parameters can give the same overall aerosol concentration). This is very important in assessing if these parameters can be applied universally.

- Another issue I would like the authors to address is: does this approach only apply for fossil fuel combustion emissions? Using the same set of stoichiometric yields {a1,b1,c1,d1} for all volatility bins is justified if compounds in different volatility bins are chemically similar (branched, cyclic, straight-chain alkanes), which is true for fossil fuels. But it might not apply for other sources, such as biomass burning. A brief discus-

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sion on how to deal with other types of emissions would be very helpful for a modeller who wants to adopt this approach.

Minor comments:

- Introduction: A definition of SVOC and IVOC in terms of their C* would be helpful.
- pg. 9947 In 23: Instead of "defined", the authors should use "classified" or "denoted"
- pg. 9948 In 22: Please provide a reference that suggests the UCM is mostly branched/cyclic alkanes
- pg. 9948 In 22: I don't understand the criticism about using naphthalene as a surrogate for IVOC. Naphthalene is expected to produce more SOA than alkanes of the same vapor pressure or carbon number, which would imply any estimates would be an overestimation. But in Pye and Seinfeld (2010), scaling up from naphthalene still does not make IVOC a significant SOA precursor globally, and this work shows that IVOC as the dominant precursor. I think the problem is that emissions of IVOCs are significantly underestimated.
- pg. 9950 In 24-25: While there can be different oxidation pathways, Heald et al. (2010) shows that on average the O/C and H/C ratios seem to follow the addition of acid group. Do the fitted parameters show a similar trend?
- pg. 9965 In 19-21: Technically that is not true. There is no experimental evidence in this work showing that SOA is in fact from IVOCs, but rather the authors postulated that all the unexplained SOA comes from POCs and proceeded to build a framework to model their production.
- pg. 9974 Table 2: The last 2 rows appear to be the same. Maybe there is a mistake?
- pg. 9981 Fig. 6: Some of the trends in SOA data look strange (e.g. FT-Idle), where there are sudden changes in measured SOA growth. Is that an artifact of the wall loss correction?

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- In multiple occasions, the authors compared the SOA yields of branched alkanes and n-alkanes, but it is unclear whether they are comparing yields of branched alkanes to those of n-alkanes *of the same carbon number*, or *of the same vapor pressure*. This is an important distinction to make, as the volatility bins are based on vapor pressures, whereas comparing branched to straight-chain alkanes imply they are of the same carbon number.

Reference:

Heald, C.L. et al., Geophys. Res. Lett., 37, L08803, doi:10.1029/2010GL042737, 2010

Pye, H. O. T. and J. H. Seinfeld, Atmos. Chem. Phys. 10, 4377-4401, doi:10.5194/acp-10-4377-2010, 2010

Interactive comment on Atmos. Chem. Phys. Discuss., 12, 9945, 2012.

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