**Atmospheric
Chemistry
and Physics
Discussions**

Interactive
Comment

Interactive comment on "The sensitivity of
secondary organic aerosol component
partitioning to the predictions of component
properties – Part 1: A systematic evaluation of
some available estimation techniques" *by*
G. McFiggans et al.

Anonymous Referee #2

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Referee comments

A review of "The sensitivity of secondary organic aerosol component partitioning to
the predictions of component properties – Part 1: A systematic evaluation of some
available estimation techniques" by McFiggans et al.

Overview

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Interactive Discussion

Discussion Paper

The study is based on the previous work of the authors where different methods for estimating saturation vapor pressure of atmospherically relevant semi-volatile organic compounds were evaluated. Here the work is extended to consider mixtures of organic compounds, and also different metrics are used in the evaluation. The approach and the results of the manuscript are novel and the work is, potentially, within the scope of Atmospheric Chemistry and Physics. However, at its current form, I'm quite hesitant to recommend the manuscript for publication in ACP, i.e. major changes are needed. My main criticisms are the following:

1. Description of the methodology. At its current form, it is extremely difficult to understand exactly how the compounds making up the considered mixtures are generated (Sections 2.3 and 2.4). Furthermore, the applied methods for calculating saturation vapour pressures remain somewhat vague (Section 2.2). Finally, several assumptions made in choosing the properties of the considered are not adequately justified (Section 2.3).

2. Atmospheric relevance of the results. The authors based their main conclusions on the investigation of "synthetic" mixtures of organic compounds which, so it seems at least, do not necessarily bear relevance to the atmosphere. The authors should justify the use of such mixtures or consider a different set of mixtures which would be, in the light of the current knowledge on the composition of the atmosphere, atmospherically relevant.

Detailed comments associated with these points are given below.

Major comments

1. Section 2.2. Please split the description of the vapour pressure models into further paragraphs so that the boiling point estimation methods are described in the first, and the saturation vapour pressure models in the second. Also, please summarize the applied combinations in a separate table or in the end of the section.

2. Section 2.3, second paragraph. Please justify the two applied restrictions. In particular, why the total concentration of the compounds decreases linearly with the carbon number? Secondly, the requirement that the total condensed mass is fixed under the base case assumptions is somewhat counterintuitive – to me, keeping the total mass in the system (gas & particle phases) fixed would be more intuitive. Also in many applications, the people would be interested in knowing how large errors to the SOA mass (rather than to the total concentration) are caused by the choice of the saturation vapour pressure estimation methods.

3. Section 2.3, third paragraph. Please describe explicitly the probability distributions which give the probability that a functional group is attached to a carbon skeleton. Judging from Figure 1, the distributions are Gaussian. This choice should be justified because given the absence of a comprehensive picture on the composition of atmospheric SOA, an intuitive choice would be to use uniform distributions. Also, is it guaranteed that does the method lead to generation of compounds that 1) exist, and 2) if so, are they present in the atmosphere at all? Please discuss.

3. Section 2.3., third paragraph. Please describe more in detail the applied method. Also, the last sentence ("To summarise...") should be clarified. Finally, the authors could give some examples of the individual compounds that result from the generation procedure to illustrate possible outcomes.

4. Section 2.4, page 15390, lines 23-30. The authors conclude that "...the selected conditions adequately serve to illustrate the sensitivities". Again, the authors fail to justify that the generated mixtures reflect the composition of the atmosphere. I agree with the authors that it is not possible to address the issue comprehensively, but I'd suggest that the authors generate mixtures (with a smaller degree of randomization) that are based on the available information on the atmospheric, semi-volatile organics and investigate whether the main conclusions of the study still hold.

Minor comments

1. Introduction. Please describe and justify briefly the metrics used in the study.

2. Introduction, sixth paragraph, page 15384. The usage of the terms such as "uptake" and "condensation" do not reflect the fact that the atmospheric gas/particle partitioning is a reversible process. Please change the terminology accordingly.

3. Section 2.3, third paragraph. Please list the considered functional groups in a separate table. Are they all found in atmospheric organic compounds?

4. Section 2.5. Please provide references and a brief discussion that motivates the use of the last three metrics.

5. Section 3.2. Please explain the contents of Figure 6 in more detail. For example, what do the blue and green boxes and symbols signify?

6. Page 15394, line 25. I do not see how the discussed feature is "...somewhat predictable...", please elucidate.

7. Page 15398, line 9. The meaning of the expression "...atmospherically relevant functionality Tong et al. (2008)." is unclear.

8. Figures. Please describe the figures in detail in the captions rather than in the text because with the current form, it is hard to extract key findings from the text.

9. Figure 1. Why the probability distributions are (at least shown as) continuous? Shouldn't they be discreet with respect to the carbon number?

10. Figure 4. What calculations does the line "Act" represent?

Technical comments

1. Introduction, last paragraph. Please state the publishing status and (preliminary) titles of the companion manuscripts.

2. Figures 3 and 4. Title of the y-axis is missing, please provide.

3. Figure 5. The scale of the y-axis is missing, please p

Interactive comment on Atmos. Chem. Phys. Discuss., 10, 15379, 2010.

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