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Atmospheric Chemistry and Physics
Discussions

Interactive comment on "Uncertain Henry's Law Constants Compromise Equilibrium Partitioning Calculations of Atmospheric Oxidation Products" *by* Chen Wang et al.

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This manuscript describes in detail a modeling experiment to determine the best approach to describe partitioning of organic gases (thousands of compounds tested) into the particle-phase's aqueous and organic medium. The authors employ 3 modeling approaches to describe partitioning with a focus on highly oxidized material. The authors also offer comparison and a critique of an approach currently implemented in an atmospheric model based on volatility. The authors make a compelling argument for their main thesis: "The large uncertainty in Kw/g predictions for highly functionalized organic compounds needs to be resolved to improve the quantitative treatment of SOA formation." Predicted organic aerosol amounts in atmospheric models will be highly

dependent on and sensitive to the chosen partitioning parameterizations, which are highly uncertain. The authors identify a key knowledge gap. I recommend the paper for publication provided adequate response and revision to the comments provided below.

Response: Thanks for the comments.

My biggest challenge understanding this paper was Figure 3, which I believe is the most important. Perhaps there is a way to draw in 3 dimensions to make more clear? It is confusing to have the vertical purple line "without aqueous phase" drawn in the aqueous phase. It is also confusing to just have this scenario for only the ppLFER experiments. Casual readers will not understand what the circled dots in the Figure 3c are.

Response: We have simplified Figure 3 and added two more figures (S13 and S14) in the supporting information to make the figures more understandable (see figures below). The text in the manuscript has been modified accordingly.

Lines 383-387 have been changed to: "The blue dotted lines represent a cloud scenario where LWC is 0.3 g/m3 and OM is 10 μg/m3. Figures S13 and S14 in the supporting information show an aerosol scenario without an aqueous phase and a cloud scenario without a separated organic phase because all of the OM is dissolved in the aqueous phase (see also Figure S12 (c) and (d))."

The following sentence was added at the end of line 433 "Those compounds are not sufficiently soluble in water to partition to the cloud and are not sufficiently volatile to be in the gas phase."

"Figure S12" on line 408 and 411 was replaced with "Figure S15".

Line 448 has been changed to: "The number of compounds on the right side of the blue dotted boundary in Figure S13 does not vary substantially with different predictions."

Why do there appear to be 'straight' lines in the dots for all models, most pronounced for 0 and 1 functional groups?

Response: There are no straight lines in the dots in Figure 3 so nothing has been changed.

Page 4, Line 71/72: May an additional reason for the study and importance of VOC oxidation products be that in addition to their higher affinity, they have a great atmospheric abundance?

Response: On line 72, we add “and a great atmospheric abundance.”

Figure 2: can the method for ‘possible outlier’ and ‘extreme value’ be explicitly stated here

Response: The “possible outliers”, i.e., the circles, are values that are either 1.5×IQR or more above the third quartile or 1.5×IQR or more below the first quartile, where IQR is the range between the first and third quartile of the boxplot, called interquartile range (IQR). The asterisks or stars are “extreme outliers”, which are either 3×IQR or more above the third quartile or 3×IQR or more below the first quartile.

Editorial: p. 7, Line 159: “value” should be “values”

Response: Changed.

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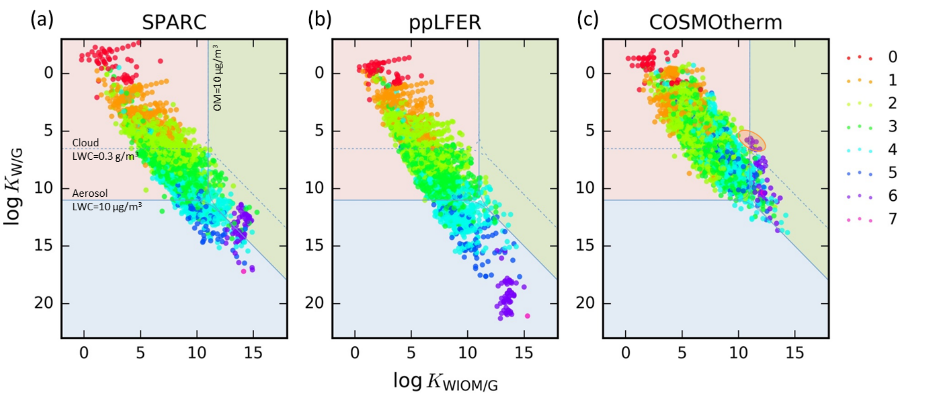

Fig. 1. Figure 3

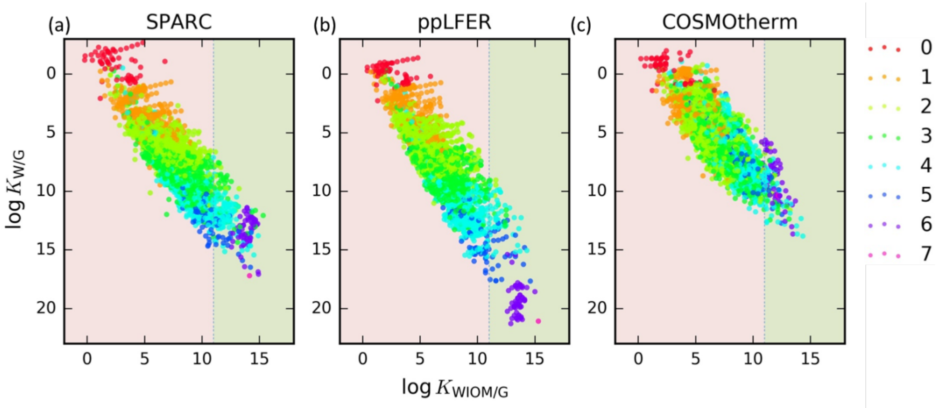

Fig. 2. Figure S13

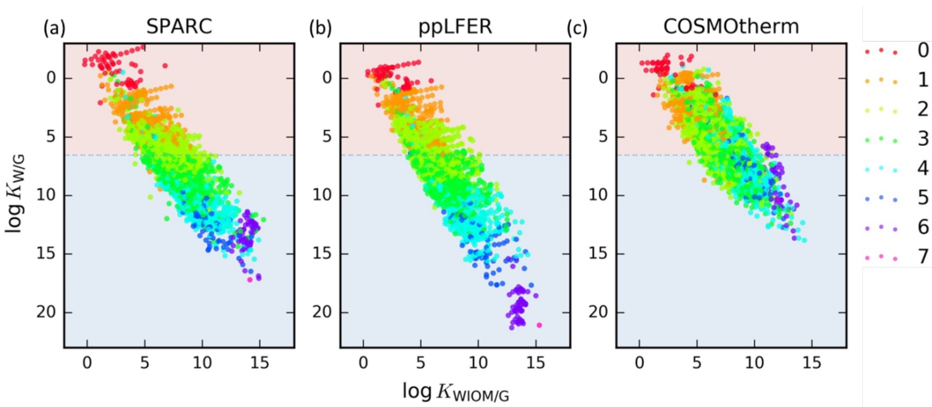

Fig. 3. Figure S14