Reviewer 2

Interactive comment on "Modeling of Gas-Wall Partitioning of Organic Compounds Using a Quantitative Structure-Activity Relationship" by Sanghee Han, Myoseon Jang*, and Huanhuan Jiang

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We thank reviewer 2 for the valuable comments on the manuscript.

Overall comment:

Han et al. use a quantitative structure-activity relationship to predict gas-wall partitioning of semi-volatile organic compounds in chamber experiments. They explore the effects of relative humidity of gas-wall partitioning and the influences on SOA mass predictions. The approach is new and interesting. However, I have several questions and comments that needs to be addressed before I am convinced that this approach is promising to be used by other chamber users.

Summary of response to the reviewer 2:

1) Through additional experiments, we characterize the chemical composition of the organic layer (OM_{wall}) on the surface of both the Teflon film chamber wall and the unused Teflon film by using FTIR spectra (Fig. R3, please find the responds to comment 4 from reviewer 1)
2) The limitation of the extraction method to characterize of OM_{wall} was discussed (response b to comment 1).
3) The suitability of the QSAR-base GWP model to other products from oxidation of reactive hydrocarbons was discussed.
4) The GWP model was derived using the actual sampling time by including the duration to introduce organic vapor into the West chamber and the sampling duration (total 17.5 minutes). To demonstrate the feasibility of the GWP model, we conducted the additional chamber experiment with the short time lag (12.5 minutes) from time =0.
5) The detail information about the determination of the descriptor for the GWP predictive polynomial equation was discussed and this was added to the revised SI.

The detail responses to the comments from Reviewer 2 are following:

Major comments:

Comment 1) The elemental composition of $M_{wall\text{-}OM}$ is determined as $C_{15}H_{24}O_4$. It is interesting that the authors use one composition to represent the presumably tens or hundreds of different SVOC deposited on the wall. In addition, there will be SVOC wall loss even in a completely new chamber wall without pre-deposited SOA particles and vapors. Therefore, it is not clear to

me how does the $M_{wall\text{-}OM}$ alone affect vapor wall loss. Further, does the wiping collect all the organic matter mass on the wall (Line 117)?

Response:

Please also find the response to comment 4 from reviewer 1 and the response to comment 1 from reviewer 3.

a. *Composition of OM on wall:* In order to response the reviewer, we measured FTIR spectra of the organic matter collected from the Teflon film wall inside the UF-APHOR chamber at different time. We also included the FTIR spectrum of organic mass originating from the unused Teflon film as seen in Fig. R3 for response to reviewer 1. Regardless of aging time associated with chamber history, a strong aliphatic carbon peak (wax-like material) appeared in all spectra. Teflon would be the most hydrophobic polymer. Wax-like aliphatic compounds are ubiquitous in the ambient atmosphere due to the emissions from vehicle combustions, vegetation, and industries. This wax-like compounds can deposit onto the Teflon film. Teflon film can be exposed to ambient air by numerous ways (manufacturing sites, transportation from the manufacturing site to laboratories or Teflon film bag manufacturers, and ventilation of the chamber with the ambient air after each chamber experiment). Thus, most Teflon film surfaces are contaminated by wax-like materials in the ambient air. Prior to each experiment, the outdoor chamber air is cleaned with a clean air generator under the ambient sunlight for 2-3 days. However, the wax-like matter is not completely removed.

b. *Extraction method of OM:* It is a good point. We agree with the review's concern about the extraction method. We tested with several solvent (methylene chloride, acetonitrile, and acetone). The resulting spectra are similar even with different solvent. A small quantity of inorganic salts can be appeared with polar solvent, but the main composition is wax-like matter. The evaporation procedure may impact compositions of OM_{wall} but it would be small because the chamber is vented with the clean air and the volatile compounds are evaporated. The large uncertainty in the characterization of OM_{wall} would be the OM extraction efficiency associated with a wiping method. This wax-like material may penetrate into the certain layers of Teflon film near the surface and influence the property of Teflon film. As we mention in Section S2 (Mass concentration of $M_{wall\text{-}OM}$ and its molecular weight), the mass of OM_{wall} measured using the wiping method was lower (30%-50%) than that with the solvent extraction by socking into a large amount of several solvents (methylene chloride, acetonitrile, and acetone). In this study, the mass of OM_{wall} was determined with the solvent extraction method and the MW_{OM} of OM_{wall} was determined by using FTIR data associated with the wiping method.

Comment 2) There is increasing evidence that secondary organic aerosols from oxidation of VOCs such as alpha-pinene consist of LVOCs and ELVOCs that contain -OOH functional groups (Bianchi et al., 2019). The authors need to broaden the discussions on the implications/limitations of using the descriptor to estimate gas-wall process and its effects on SOA mass predictions regarding -OOH and (E)LVOCs.

Response:

In order to respond to the reviewer, the feasibility of QSAR on the prediction of GWP of the compound containing -OOH was discussed in the revised manuscript.

"There is increasing evidence that SOA from oxidation of the reactive hydrocarbon such as α-pinene contains both low volatility organic products and extremely low volatile organic products with -OOH functional groups (Bianchi et al., 2019). The QSAR-base model of this study is also capable of supporting the prediction of the GWP of the products with –OOH functionality."

Comment 3) As a figure in the main text, Figure 3 deserves more description and discussions. The observed time sequences of 1-heptanoic acid and 2,5-dimethylphenol do not show a downward trend as the predicted time sequences at 40% RH. The authors need to provide more explanation.

Response:

The observed gas-phase concentration of 1-heptanoic acid and 2,5-dimethylphenol do not show a decreasing trend as the predicted values because they can rapidly reach to equilibrium at 0.4 RH. As discussed in the section 4.3, the longer $\tau_{GWP,i}$ was found for SVOCs with the higher $K_{w,i}$. By reducing volatility, the SVOC has a greater $K_{w,i}$ with a large carbon number or strong hydrogen bonding. Both 1-heptanoic acid and 2,5-dimethylphenol are the compounds with small carbon numbers and strong hydrogen bonding. However, strong hydrogen bonding cannot increase $K_{w,i}$ a lot under the lower RH than 0.5. As seen in Fig. S4, the surface of Teflon film (OM_{wall}) is relatively hydrophobic and the water contend in OM_{wall} (or surface Teflon film) is very little before 0.5 RH (Fig. S5). It suggesting that $K_{w,i}$ of the SVOCs with polar functional group is similarly small under lower RH than 0.5. In addition, a longer $\tau_{GWP,i}$ was found for SVOCs with large $\alpha_{w,i}$, which is smaller with increasing molecular size.

Comment 4) Line 104: It is confusing here. Are there particles in these experiments or not? Figure 2 indicates there are no particles but line 104 indicates there are particles.

Response:

The sentient has been revised and reads now,

"No particle appeared after vaporizing organic chemicals into the chamber air based on particle data, which was monitored using a scanning mobility particle sizer (SMPS, TSI 3080, Shoreview, MN, USA) and a condensation particle counter (CPC, TSI 3022A, Shoreview, MN, USA)."

Minor comments:

Comment 5) Line 8, PaDEL-Descriptor, a software that calculates. . .

Response:

The sentence pointed by the reviewer has been corrected.

Comment 6) Table S2 and S3: There are several coefficients that have a p-value greater than

0.05, are those all included as descriptors?

Response:

Several descriptors show larger p-value than 0.05. In particular, the high p-value of E_i and $H_{a,i}$ indicates that those are insignificant (p-value > 0.05) to the $\ln(\gamma_{w,i})$. The definition of insignificant parameters was considered to determine the reasonable GWP predictive polynomial equation. E_i can partially involve by other terms of the $K_{w,i}$ (Eq. 11) because E_i is calculated based on the molecular weight and density. Thus, E_i was eliminated from the polynomial equation. $H_{a,i}$ was included as a descriptor of the polynomial equation to consider energetic contribution of hydrogen bonding interactions between hydrogen accepting SVOCs and hydrogen donating wall composition. Then, based on the adjusted R^2 values in linear regressions, parameters $H_{d,i}$, $H_{a,i}$, α_i, and S_i were applied to the derivation of the QSAR-based polynomial equation.

Reference:

Bianchi, Federico, et al. "Highly oxygenated organic molecules (HOM) from gas-phase autoxidation involving peroxy radicals: A key contributor to atmospheric aerosol." Chemical reviews119.6 (2019): 3472-350