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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Modeling of Gas-Wall Partitioning of Organic Compounds Using a Quantitative Structure–Activity Relationship" *by* Sanghee Han et al.

Anonymous Referee #2

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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.

Major comments:

1. The elemental composition of Mwall-OM is determined as C15O4H24. It is interesting that the authors use one composition to represent the presumably tens or hundreds

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Discussion paper

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 Mwall-OM alone affect vapor wall loss. Further, does the wiping collect all the organic matter mass on the wall (Line 117)?

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.

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.

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.

Minor comments:

1. Line 8, PaDEL-Descriptor, a software that calculates. . .

2. Table S2 and S3: There are several coefficients that have a p-value greater than 0.05, are those all included as descriptors?

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): 3472-3509.

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