

Response to the comments of the Editor and the Reviewers

Ms. Ref. No.: egusphere-2025-229

Title: Influencing Factors of Gas-Particle Distribution of Oxygenated Organics in Urban Atmosphere and Deviation from Equilibrium Partitioning: A Random Forest Model Study

Editor Comments

1. *Thank you for revising your manuscript. Please provide a further revised manuscript addressing the minor technical points outlined by the final review, prior to publication.*

Also, ACP prefers titles that highlight the scientific results/findings or implications of the study. Please adjust the title of your manuscript to address this.

Reponses:

Thank you very much for your suggestion. We have revised the title as follows:

Influencing Factors of Gas-Particle Distribution of Oxygenated Organics in Urban Atmosphere and Deviation from Equilibrium Partitioning: A Random Forest Model Study.

Referee Comments

1. *In response to reviewer 3 comment 4 the authors write:*

'In line 121, we clarified "These fragments were excluded from the gas/particle partitioning analysis". So the fragment did not bias the G/P ratio of OOMs.

By comparing with the OC measured with the thermal-optical method, the OOMs measured with the FIGAERO-CIMS accounted for only $26 \pm 8\%$ of the total OA ($OC \times 1.4$). So this study focused only on detectable OOMs by iodide ionization scheme, not all aerosol organic compounds.'

It seems the authors did not quite understand the bias referred to in the comment. To clarify, the detection of thermal fragments implies the thermal decomposition of some compounds in the FIGAERO, presumably including the OOMs the authors investigated. By excluding the fragments, although they should be excluded, some of the signal originating from the OOMs of interest is excluded from the particle phase data. This will lead to an underestimation of the particle phase data, and therefore an overestimation of the detected G/P partitioning ratio. I

would like the authors to either explain how they were able to counteract this bias with their analysis, or clearly state that there is a slight bias towards lower particle phase concentrations in the data they present in the paper.

Reponses:

Thank you for pointing out the misunderstanding. Our analysis is valid for the OOMs that did not decompose at all. On the other hand, those OOMs that fully thermal-decomposed were naturally excluded from our analysis. For those OOMs undergoing partial thermal decomposition, to unknown extent, in the particle phase, our analysis might underestimate their particle-phase concentrations, thus biasing towards higher G/P ratios. We tend to believe that once an OOM is thermally unstable in the FIGAERO, it decomposes completely. However, we were unable to validate this hypothesis using the method in our analysis.

In lines 116-130, we have revised the text:

“Thermal desorption may cause OOM decomposition in the particle phase. According to our earlier study on the same dataset using a K-means clustering method (Wang et al., 2024), on average, 25.1% of particle-bound OOM species number and 26.8% of OOM mass detected by the FIGAERO-CIMS could be attributed to thermal decomposition fragments ([Supplementary Materials Text S2](#)). These fragments were excluded from the gas/particle partitioning analysis. The overlap of non-fragment particle-bound OOM species with those gas-phase OOM species resulted in 123 species, which were chosen as the target species for subsequent partitioning analysis. Based on our previous work ([Figure S1](#)) (Wang et al., 2024), these 123 OOM species were classified to 41 aromatic species (33.7%), 35 monoterpene-derived species (28.3%), 14 isoprene-derived species (11.4%), 11 aliphatic species (8.7%), 10 biomass burning tracers (8.1%), 3 sulfur-containing species (2.4%) and 9 other unknown species (7.3%). [Notably, we cannot rule out the possibility that some of these 123 OOMs underwent partial thermal decomposition in the particle phase to an unknown extent. This could lead to an underestimate of their particle-phase concentrations and, in turn, bias the results toward higher G/P ratios.](#)”

2. On line 153 the authors write:

‘Based on the saturation concentrations of HOM detected by Tröstl et al. (2016)...

I would like to note that those are modelled saturation concentrations, not measured, so the word detected is misleading. The study also assumes certain structures that have not been directly observed.

Reponses:

In lines 154-158, we have revised the text as follows:

Based on the saturation concentrations of HOMs modeled by Tröstl et al. (2016), Mohr et al. (2019) applied an updated version of SIMPOL-type parameterization described by Donahue et al. (2011) to estimate C^* from the numbers of carbon, oxygen, and nitrogen atoms of an organic species (n_C , n_O , and n_N), but emphasizing the increased importance of OOH groups.

3. On lines 469-472 the authors write:

‘Since O_3 is not expected to change $(\frac{G}{P})_{eq}$, the negative impact of O_3 on $(\frac{G}{P})_{obs}/(\frac{G}{P})_{eq}$ ratio could be explained by the fact that high O_3 concentrations are likely to deplete gas-phase OOMs at a faster rate than particle-phase OOMs, thereby reducing $(\frac{G}{P})_{obs}$.’

By stating “by the fact that high O_3 ...” the authors imply this is established knowledge. If this is an established fact the authors should provide a source for this claim, otherwise it should be reworded to show that it is a hypothesis, or speculation, by the authors.

Reponses:

In lines 468-471, we add a citation Kaur Kohli et al., 2023 and revised the text as follows:

Since O_3 is not expected to change $(\frac{G}{P})_{eq}$, the negative impact of O_3 on $(\frac{G}{P})_{obs}/(\frac{G}{P})_{eq}$ ratio could be explained by the speculation (Kaur Kohli et al., 2023) that high O_3 concentrations are likely to deplete gas-phase OOMs at a faster rate than particle-phase OOMs, thereby reducing $(\frac{G}{P})_{obs}$.

References

Kaur Kohli, R., S., R. R., R., W. K., and Davies, J. F.: Exploring the influence of particle phase in the ozonolysis of oleic and elaidic acid, Aerosol Sci. Technol., 58, 356-373, <https://doi.org/10.1080/02786826.2023.2226183>, 2023.