

Atmos. Chem. Phys. Discuss., referee comment RC2
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Comment on acp-2021-118

Anonymous Referee #2

Referee comment on "Evolution of OH reactivity in NO-free volatile organic compound photooxidation investigated by the fully explicit GECKO-A model" by Zhe Peng et al., Atmos. Chem. Phys. Discuss., <https://doi.org/10.5194/acp-2021-118-RC2>, 2021

In this manuscript, the authors analyzed OH reactivity during oxidation of three types of volatile organic compounds by using a fully explicit chemical mechanism, GECKO-A. The authors focused on the simulations under the low NO condition.

One of my concern is that simulation results are reported in this manuscript without any validation. Of course, I understand that experimental studies of OHR under low NO condition have not been conducted, but this point should be further examined in future studies.

Another concern is that aerosol formation is not considered in this simulation. In Line 164: the authors showed that major intermediates/products under low NO condition have high C*. However, multi-functional compounds have important contributions to OHR as in Figures 3, S4, and S5, and vapors deposit onto chamber walls. Thus, I don't think gas-particle partitioning is negligible. The authors noted that aerosol concentration is very low under low-NO condition in the ambient air (remote atmosphere). However, not in the context of atmospheric analysis, but in the context of the interpretation of chamber experiments, contributions of gas-particle partitioning could be significant. Thus, in my opinion, the authors' demonstration with gas-wall partitioning but without gas-particle partitioning is misleading; contributions of gas-wall partitioning could be overestimated. I recommend the authors to consistently simulate gas-particle-wall partitioning, particularly for the chamber cases.

Even with these concerns, this manuscript includes useful information about the OHR of VOCs, as well as the oxidation pathways of VOCs. Thus, I recommend this manuscript for publication after my concerns adequately addressed.

Specific comments

Line 72: Why is it difficult to achieve low-NO conditions in chambers?

Line 130: Another than what? Explanation of a kinetic solver is not given so far.

Line 118: Parameters for the chamber should be explicitly given (chamber volume, area, and coefficient of eddy diffusion).

Line 305: This is not the case at higher OH exposure ($> 10^{12}$ molecules cm^{-3} s) or for some of the sensitivity cases.

Figure 1: The authors conducted several sensitivity simulations for RH, UV, initial OHR, but they did not discuss the variability of these simulation results. In the course of my comment for Line 305, the argue of the authors is not necessarily true for all the sensitivity cases. If the authors leave results of these sensitivity simulations, rationale and some discussion of these sensitivity simulations are necessary.

In addition, it is difficult to discriminate the lines of multiple sensitivity simulations. Line styles or symbols should be adequately selected for clearer visibility.

Figure S4: Legend for "organic peroxy" is not shown.