General Comments

In this manuscript the authors describe a study in which they compared results of a computational model with experiments conducted on the oxidation of benzene and phenol by OH radicals. The model is an updated version of the Master Chemical Mechanism (MCM) and the experimental results are mass concentrations of secondary organic aerosol (SOA) formed in a laboratory study reported in the literature. The model includes a mechanism that has been expanded to include new gas-phase reactions developed using computational chemistry and literature methods and data, gas-particle and gas-wall partitioning, photolysis, and multiphase chemistry. The authors present a very thorough evaluation of the model by comparing results of the unmodified MCM and multiple versions of the modified mechanisms with each other and with SOA measurements conducted under a range of conditions (NOx, seed particles, etc.). Sensitivity analyses are also performed and a reduced version of the model is compared to the more complete version.
This study is very well done. The modifications to the MCM are extensive and carefully and thoroughly justified. The results are clearly explained and interpreted, and the paper is well-written and well-organized. The study represents a significant improvement to our understanding of the complex chemistry involved in the oxidation of aromatic compounds, a topic which has challenged scientists for decades. I recommend publication in ACP after the following very minor comments are addressed.

The authors thank the reviewer for their feedback and comments on the article. The following paragraphs detail the responses to each comment and the changes made to the manuscript.

Specific Comments

1. How would this model be used in the atmosphere under conditions where RO2 + RO2 radicals are important, since RO2 radicals from other VOC reactions will be present?

Our reply: The benzene reaction scheme presented in this study details the reactions involving the peroxy radicals produced through benzene oxidation, i.e. only the "generated" peroxy radicals are considered. In atmospheric conditions, peroxy radicals have multiple origin sources. In SSH-aerosol v2.0, the contribution of RO2 radicals originating from other VOC oxidation mechanisms is accounted for through the*RO2pool* species. Multiple *RO2pool* can be defined as the sum concentration of several specified peroxy radicals, considered as "background" peroxy radicals. Additional reactions may be included in the oxidation scheme to take into account new product formation, representing the interactions between background RO2 with benzene oxidation products and assess their role in benzene SOA formation. We have clarified this aspect in the revised manuscript.

Sentences added to the manuscript: **It should be noted that, in the present simulations, the peroxy radicals considered are only formed through benzene oxidation. The inclusion of "background" RO2 radicals from other precursors would increase the contribution of bimolecular RO2 reactions and could enhance SOA formation.**

2. Figure 7. It appears that the proper treatment of glyoxal partitioning and oligomer formation can have a large effect on predicted SOA formation. What about the role of other oxidation products in oligomer formation? Are multiphase reactions likely to be the major model uncertainty for SOA predictions?

Our reply: We thank the reviewer for this comment. Simulations show that the assumption of irreversible partitioning does not accurately represent SOA mass and that accounting for glyoxal hydration decreases SOA formation under the simulated conditions. The formation and uptake of hydrated glyoxal reduces HO2 concentration thus decreasing the oxidation capacity of the system, while its direct contribution through gas–particle partitioning has a limited effect on total SOA mass. In a similar fashion, oligomerization of other high volatility VOCs could transfer mass from the gas to the particle phase while simultaneously removing reactive compounds from the gas phase, modifying oxidant concentrations and the subsequent formation of low volatility products. Our results indicate that multiphase processes can substantially affect SOA formation, but the impact of their contribution is difficult to constrain and is expected to vary with atmospheric conditions. Recent work on photoinduced intraparticle chemistry of biomass burning organic aerosol oxidation suggests that photoinduced radical chemistry can drive very rapid oxidation within organic particles (Zhang et al., 2026). Hence the following sentences were added to the conclusion:
The representation of intraparticle chemistry remains a source of uncertainty. Recent experiments on biomass-burning organic aerosol indicate that photoinduced radical chemistry within particles can lead to fast atmospheric aging (Zhang et al., 2026). Triplet excited states and other photochemically generated reactive species may be particularly relevant for phenolic compounds, which are abundant in biomass burning emissions.

3. I understand that the model results for SOA mass are compared to experiments because that is the best data available. In the future the authors might consider presenting model predictions of the functional group composition of the SOA. I suppose one could calculate this from data in Figure 11 but presenting it for a range of laboratory conditions would be better. This could inspire experimentalists to measure those quantities and would provide a more rigorous evaluation of the model than the SOA mass comparison, which can be good or bad for many different reasons.

Our reply: The authors agree with the reviewer. Accurately determining the composition of the particulate phase experimentally would allow for better differentiation of the mechanisms developed for modeling. This line of research is all the more important given that toxicity of aerosols might be directly related to their composition. Supplementary Material S10 has been added, presenting the composition of the particulate phase in terms of functional groups for the 16 experiments and using all three Mech1, Mech2, and Mech3 mechanisms. In addition, a repository containing raw simulation results has been added as an appendix, which would allow for comparison with experimental results regarding composition.

Sentences added to the manuscript: **In addition to total SOA mass, the simulated particle-phase composition provide some additional information on the mechanisms. The proportion of each functional group is detailed in Supplement S10 and indicate an important increase in the mass fraction of highly oxygenated SOA, particularly hydroperoxides, at the expense of alkyl and hydroxyl groups. This enhanced contribution of hydroperoxides is qualitavely consistent with Borrás and Tortajada-Genaro (2012), who identified hydroperoxides as the dominant functional group in SOA (see Supplement S11). As hydroperoxides are not similarly dominant in our simulation, their formation might still be under-estimated in our mechanism. Because organic peroxides can contribute to aerosol oxidative potential (Wang et al., 2023), the differences in SOA composition predicted by Mech2 may have implications for aerosol toxicity.**

Technical Comments

1. Line 133: Should be 11.8%.

Our reply: The comma has been replaced with a period.

References

Borrás, E. and Tortajada-Genaro, L. A.: Secondary Organic Aerosol Formation from the Photo-Oxidation of Benzene, Atmos. Environ., 47, 154–163, https://doi.org/10.1016/j.atmosenv.2011.11.020, 2012.

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