Manuscript #: egusphere-2023-93

Response to Anonymous Referee #2

We would like to extend our appreciation to the reviewer for the time and constructive comments. The comments are reproduced below along with the author response. The changes made to the manuscript were in red color.

Comment 6

"These physicochemical parameters are universalized for five major precursor groups in UNIPAR (Table 1)." What does this mean?

Response: The sentence has been revised to clearly explain what five major precursor groups are as follows,

"These physicochemical parameters are unified for five major precursor groups (aromatics, alkanes, terpene, sesquiterpene, and isoprene) as shown in Table 1."

Reviewer response:

While you have changed "universalized" to "unified", it is still unclear to me what this means. Do you mean that physicochemical parameters are the same for aromatics, alkanes, terpene, sesquiterpene, and isoprene? This appears to be the case looking at Table 1 (although I note the value is 51 for isoprene and 50 for all the others). Could you say the "physicochemical parameters are the same for the five major precursor groups"?

Response: The sentence has been revised as follows,

"Each precursor group uses a single set of physicochemical parameter arrays associated with lumping species: for example, 50 arrays for aromatics; 50 arrays for alkanes; 50 arrays for terpene; 50 arrays for sesquiterpene; and 51 arrays for isoprene."

Comment 8

Have the emissions been validated? A bias in these emissions could mean the SOA model is getting the right/wrong answers for the wrong reasons in some cases. Fig 3 suggests a low bias in SOA which might come in part from an emissions bias.

Response: The emission data used in this study are based on California ARB(Air Resources Board)'s regional inventories and their own estimates and emission monitoring data for local sources. The emission processing went through QA/QC procedures.

Reviewer response:

It is good to see the authors are using a validated emission inventory. The use of the California ARB's regional inventory and a citation to its documentation and evaluation should be included in the main text.

Response: The following sentences were added to the Section 2.2 and the Acknowledgments section.

"Emission inputs are based on California Air Resources Board regional inventories and provided by the Bay Area Air Quality Management District (BAAQMD, 2023)." (Sect. 2.2). The website address for emission inputs has been included in the reference in the revised manuscript.

"Emissions and meteorological inputs for the 2018 California regional modeling were provided by the Bay Area Air Quality Management District." (Acknowledgments section)

Comment 13

"The underestimation of SOA mass can be attributed to missing precursor HCs and unidentified chemistry in the gas and aerosol phases. For example, the SOA model is currently missing phenols, branched and cyclic alkanes, and polyaromatic hydrocarbons (i.e., naphthalene)."

Original comment: I'm not clear this is true without an evaluation of the emissions of the precursor species.

Response: The parameters in UNIAPR are continuously updated with the better gas mechanisms and expanded to include missing hydrocarbons. To support this information, we added citations as follows,

"For example, the precursor HCs such as phenols (Bruns et al., 2016; Majdi et al., 2019; Choi and Jang, 2022),

branched and cyclic alkanes (Chan et al., 2013; Gentner et al., 2017; Madhu et al., 2023), and polyaromatic hydrocarbons (i.e., naphthalene) (Riva et al., 2015; Wang et al., 2021) are currently missing in the UNIPAR model."

Reviewer response:

I don't view this as an acceptable response, and it does not address my concerns. I understand that UNIPAR undergoes constant development (and that is a good thing) but that is not the issue at hand here. The issue at hand is whether the omission of these key species is a major driver of the SOA low bias or whether the low bias is being caused by deficiency in the model elsewhere.

A range of citations have been given but no context provided, and this is insufficient. It is the job of the author to provide convincing evidence to support their claim. These papers may refer to the SOA yield from the various omitted species, but it is not clear. The authors should highlight key features of these papers both in their response to the reviewers, and in the main text for the benefit of other readers. They should make it clear if these omitted species do indeed produce SOA at appreciable yields.

One of UNIPAR's key aims to simulate SOA well so drivers of its biases must be explored in detail. To fully support their claim that the underestimation of SOA is attributable to these missing precursors, rather than another deficiency in the mechanism, the authors should estimate the production of SOA from these missing species (regional emissions times approximate SOA yield) and show how this extra SOA production term might help resolve the model low bias by putting it into context with the SOA production currently included in this version of UNIPAR for the simulations considered.

Response: It is difficult to estimate the SOA mass associated with missing hydrocarbons in the regional scales without model parameters for each precursor. Most laboratory studies report SOA yields from the oxidation of hydrocarbons at high concentrations, and focus on aerosol characterization without parameterization for missing hydrocarbons. The sentence that was commented by the reviewer has been revised and this reads now,

"The precursor HCs such as phenols (Bruns et al., 2016; Majdi et al., 2019; Choi and Jang, 2022), branched and cyclic alkanes (Chan et al., 2013; Gentner et al., 2017; Madhu et al., 2023), and polycyclic aromatic HCs (PAHs) (i.e., naphthalene) (Riva et al., 2015; Wang et al., 2021) are currently missing in the UNIPAR model. For example, all alkanes in this study are treated with linear alkanes, increasing some uncertainties. Branched alkane SOA can be slightly overestimated by substituting it with linear alkanes at the same carbon length, but cyclic alkanes can be underestimated by using linear alkanes (Madhu et al., 2022; Madhu et al., 2023). Zhang and Ying (2012) reported that PAHs including naphthalene, methylnaphthalene and dimethylnaphthalene can contribute to 4% of the anthropogenic SOA mass. Pye et al. (2022) reported in their regional simulation using the Community Regional Atmospheric Chemistry Multiphase Mechanism (CRACMM) that a significant amount of phenolic compounds is missing in the current model. They estimated that most phenol mass (69%) is directly emitted with the balance from benzene oxidation, and cresols are mainly chemically produced (80%). The missing emissions of phenol and cresol can account for 30% of the total aromatic SOA mass (Pye et al., 2022). The SOA formation from low volatility aromatic HCs (aromatics substituted with long-chain alkyl groups) is also missing in the SOA simulation of this study."

Comment 24

Data Accessibility. In the interests of community modelling and FAIR principles, I would like to see the code and model data uploaded to a freely accessible repository such as Github or Zenodo.

Response: The code of the CAMx-UNIPAR model is available upon request in Github.

CAMx-UNIPAR ver. 1.1, which included aromatics and biogenic daytime, is available in GitHub. The updated CAMx-UNIPAR ver. 1.2 has been preparing to include various precursors including alkanes (linear and branched alkanes), updated aromatics, and day/night biogenics. The updated version will include more hydrocarbons than the simulation of this study.

Reviewer response:

This response has only partially answered my original comment. The code of the CAMx-UNIPAR should be freely available on GitHub (not available on request) and the web address clearly provided.

There is also no comment on the availability on model data. This must be made available on a repository such as Zenodo and clearly signposted in the text so as to be inline with Copernicus' data accessibility policy.

Response: The code of CAMx-UNIPAR and model data (meteorological and emission inputs) will be provided upon request. The code of CAMx-UNIPAR has been updating to include more precursors, and the user manual

needs to be prepared. When CAMx-UNIPAR is ready for the manual and updated parameters for essential precursors, CAMx-UNIPAR will be freely available for publics. In current, code to run the CAMx-UNIPAR model in this study is available upon request with appropriate purpose. In addition, the use of input data needs permission from BAAQMD.

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