

Response to Anonymous Referee #1

We would like to thank the reviewer for the time and the constructive comments on our work. The comments are reproduced below along with the author response. The changes made to the manuscript or supporting information were in red color.

Comment 1

The authors should better state how innovative their work is. Except the Yu et al., 2022 paper for the Korus campaign in South Korea, are there other examples where a detailed multiphase aerosol model like UNIPAR was integrated into a 3D model system? This should be pointed out.

Response: Very rarely have detailed multiphase aerosol models, such as UNIPAR, been applied to the 3D model. We added the novelty of UNIPAR in Section 2.1 and reads now,

“The CAMx-UNIPAR of this study simulates SOA formation via multiphase reactions of ten aromatics, three biogenics (isoprene, terpene, and sesquiterpene), and three alkane groups as summarized in Table 1. The lumping species, which are generated by using semi-explicitly predicted products of the oxidation of HCs, are involved in multiphase partitioning and aerosol-phase reactions to form SOA mass. The prediction of stoichiometric coefficients associated with the lumping species from the oxidation of ten aromatics (MCM v3.3.1(Jenkin, 2004)) potentially increases the accuracy of the prediction of aromatic SOA formation under varying emissions. For biogenic HCs, recently identified biogenic oxidation mechanisms that yielded low-volatility products have been applied to the prediction of lumping species. For example, the peroxy radical autoxidation mechanism (Roldin et al., 2019) is known to form highly oxygenated organic molecules (HOMs) (Molteni et al., 2019). Additionally, HOMs form via the accretion reaction to form ROOR from RO₂ species (Bates et al., 2022; Zhao et al., 2021). These HOMs are included in biogenic lumping species in the current CAMx-UNIPAR. In order to represent day and night chemistry, CAMx-UNIPAR is equipped with the oxidation-path-dependent stoichiometric coefficients from individually processed reactions of biogenic HCs with three major oxidants (OH radicals, ozone, and nitrate radicals) (Han and Jang, 2023). Thus, nighttime SOA formation, which is dominated by oxidation via ozone and nitrate radicals, can be simulated in CAMx-UNIPAR. By using the recent chamber study by Madhu et al. (2022), the lumping species generated from the oxidation of long-chain alkanes ranging from C₉ to C₂₄ have been newly integrated with CAMx-UNIPAR, which increases the predictability of SOA formation from intermediate volatility organic compounds (IVOCs). Alkane gas mechanisms include autoxidation of alkoxy radicals to form HOMs (Madhu et al., 2022; Crouse et al., 2013; Bianchi et al., 2019; Roldin et al., 2019). Importantly, the estimation of activity coefficients of lumping species in both the organic phase and the inorganic aqueous-phase enables the simulation of multiphase partitioning of lumping species and their aerosol phase reactions. Aqueous reactions in CAM-UNIPAR facilitate the evaluation of the impact of humidity, aerosol acidity, and aerosol-phase state on SOA formation in regional scales.”

Comment 2

While the Central valley might be an interesting place with significant organic aerosol pollution, the available data from four sites of the standard air quality network are in my sense rather poor for detailed model evaluation. They only provide daily averages each three days, so we have 12 OC data points for each of the four sites. I would propose two options: either apply the model to an intensive field campaign giving information on precursor gases, oxidants, and organic aerosol composition, ideally including tracers for different formation pathways and precursors. This would be in my mind highly interesting, and I recommend thinking in this way.

Response: The simulation of the air quality in the Central valley, CA was the first case to demonstrate CAMx-UNIPAR to regional simulation in the USA domain. We utilized the emissions of hydrocarbons based on SAPRAC07 gas mechanisms in this simulation. SAPRAC07 was chosen because it can explicitly cover hydrocarbon species. However, preexisting emissions of hydrocarbons was mostly established on CB6 in regional models. The emission based on SAPRAC07 species was available in the database from BAAQMD in CA. BAAQMD provided emission and meteorological input data for the CAMx-UNIPAR simulation. In the future, CAMx-UNIPAR will be tested using different gas mechanism platform such as CB6 to demonstrate the model on various field observations. In order to response to the reviewer, we added the sentence into the end of manuscript and reads now,

“In the future, emission species will be integrated with Carbon Bond 6 (CB6) gas mechanism (Yarwood et al., 2010), which is frequently used for hydrocarbon gas oxidation, and applied to CAMx-UNIPAR to demonstrate the model on various field observations.”

Comment 3

As an alternative, authors could conduct a more operational evaluation. To my knowledge, the CSN and IMPOROVE networks contain more the 100 sites with OM data. Performing a simulation over a wider area and period would allow a truly statistical analysis of model ability to simulate SOA. From a computer point of view, is a longer situation possible?

Response: We agree with the reviewer. In the future, CAMx-UNIPAR will be evaluated in different regions and different time. As discussed in the response to comment 2, The CAMx-UNIPAR simulation of this study was restricted by the emission data, which was coupled with hydrocarbon species in SAPRAC07 mechanism. The emission data which have a fixed domain were provided by BAAQMD, so the modeling domain cannot be extended. Furthermore, wildfire occurred frequently in California. We selected the season where wildfire is inactive in 2018, which was winter months.

Comment 4

I think that figures 4 and 5 are not coherent with figure 6. From what I see, figure 6 shows a bit less than half of aromatic SOA with respect to alkane SOA averaged over the period (roughly both contributions have similar spatial contributions) while in figures 4 and 5 the aromatic contribution is very low. The same incoherence seems to appear for sesquiterpene SOA, in figure 6 it is with terpene the major SOA contributor in San José, but in figures 4 and 5 it is nearly absent. In section 2.5 it is said, that sesquiterpene emissions are negligible. Please check these figures.

Response: In Fig. 6, please notice that each SOA species has different scale. To clearly show the color-bar scales, the font size increased in the revised manuscript.

Comment 5

Beyond this incoherence, it is astonishing that the aromatic contribution is so low, and the alkane one so high. In the conclusion it is said that these are partly long alkane chains, probably in the IVOC range. This should be made clearer already before the conclusion, when talking about emissions in section 2.5

Response: The very low contribution of aromatic SOA is strongly associated with the low level of aromatic emissions in CA as shown in Fig. 2. Long chain alkanes significantly contribute to IVOCs, which emitted from automobile exhaust and plants. In this paper, the SOA mass from alkanes were simulated based on emission recently reported by the EPA (Pye et al., 2022) and the study by McDonald et al. (2018). Stoichiometric coefficients associated with lumping species were estimated with the recent study by Madhu et al., (2022). Based on this protocol, alkane SOA has been first time simulated using CAMx-UNIPAR. As shown in Fig. 2, alkane is dominant among anthropogenic precursors. In our model, alkane precursors are split into three groups based on their volatility. In particular, the fractions of alkanes which have more than C13 (IVOC) is significant (approximately 60% of all alkanes). The information about alkane has been updated in Section 2.2, and the uncertainty of alkane SOA overprediction has been added in Section 4 as follows,

“Long chain alkanes are important IVOCs, which are emitted from automobile exhaust (Pye and Pouliot, 2012; Ensberg et al., 2014) and plants (Simoneit, 2002; Yao et al., 2009; Li et al., 2022). Laboratory studies showed that SOA yields from long chain alkanes are high suggesting their significance in ambient SOA mass (Lim and Ziemann, 2009; Tkacik et al., 2012; Presto et al., 2010; Srivastava et al., 2022). In the model, alkanes in different carbon chain lengths are split into three groups due to their different SOA formation potential: C9-C14, C15-C19, and C20-C24 (Table 1).” in Section 2.2

“Additionally, the uncertainty of emissions in long-chain alkanes might be high. The deposition flux of IVOCs onto PM and various ground-level surfaces can increase with increasing IVOC molecular weight due to their low volatility. Hitherto, the impact of multiphase partitioning on IVOCs emissions or the dry deposition is poorly treated in the regional models. Omitting dry deposition of IVOCs could overpredict SOA production (Bessagnet et al., 2010).” in Section 4

Comment 6

The detailed model results about species contribution cannot be evaluated from the measurements available from this paper. They should be discussed in depth based on intensive campaigns elsewhere, beyond the discussion with the KORUS campaign. In the same order of ideas, is the 10 -35% simulated contribution of in-particle

formation expected from literature, has such a contribution already been simulated, observed in the field or in a chamber?

Response: The contributions of SOA mass in-particle phase (OMH) in this study are generally consistent with the literature. We have added additional discussion about OMH in the revised manuscript (Section 3.2) as below,

“The predicted contributions of OMH to the total SOA using UNIPAR ranged from 23% to 41%. The fractions of oligomeric matter (OMH) from anthropogenic HCs (aromatics and alkanes) ranged from 41% to 47% and those of biogenic HCs ranged from 13% to 18%. The anthropogenic OMH fractions are consistent with reported values predicted by Pye and Pouliot (2012) in regional scales in the US domain. For example, they reported that the oligomeric SOA simulated mainly from alkanes and partly from polycyclic aromatic hydrocarbons (PAHs) accounted for about half of the anthropogenic SOA in the US domain. In the regional simulation by Yu et al. (2022), the SOA mass were simulated with both the two-product SOA (SOAP) model and the UNIPAR SOA model during the KORUS-AQ campaign. The contributions of OMH to the total SOA are on average 31% and 40% with SOAP SOA model and the UNIPAR SOA model, respectively.”

Comment 7

The paper's quality in English wording is not sufficient. This can easily be improved. I put some examples below.

Response: The manuscript has been thoroughly reviewed by the native English speaker.

Comment 8

Line 55: "To compensate the underestimation of SOA, the SOA model employed high partitioning-base model parameters, emerging gas mechanisms to form low-volatile products via autoxidation (Mayorga et al., 2022; Jokinen et al., 2015; Pye et al., 2019), or nighttime oxidations of HC with nitrate radical and ozone (Zaveri et al., 2020; Gao et al., 2019)." This suggests that the mentioned processes do not occur in the atmosphere, or at least are overestimated. Both statements are not proven.

Response: The sentence has been revised as below,

“To improve the prediction of SOA, SOA models have employed large partitioning-based parameters, gas mechanisms to form low-volatile products via autoxidation...”

Comment 9

Line 82: "In this study, the CAMx–UNIPAR model was extended to alkane SOA and nighttime chemistry of biogenic HCs." and Line 87: "In addition, the UNIPAR model has recently been expanded to simulate biogenic SOA based on three major paths (i.e., OH radicals, ozone and nitrate radicals) being capable of nighttime SOA formation (Han and Jang, 2023) that was dominated by oxidation with ozone and nitrate radicals." From this it is not clear where these changes are first presented, in the present work or already in Han and Jang (2023). Or the first comparison to field data is done here? (it becomes clear from table 1 and looking into the papers but should be made clear in the text).

Response: To clearly show the new additions in the CAMx-UNIPAR of this study, the last paragraph of Section 1 has been revised as follows,

“In this study, the CAMx–UNIPAR model has been updated to include the SOA formation from long-chain alkanes and nighttime chemistry of biogenic HCs. Long-chain alkanes are regarded as essential precursors for SOA formation (Aumont et al., 2012; Madhu et al., 2022). Madhu et al. (2022) have recently added an autoxidation mechanism into alkane semi-explicit oxidation mechanisms, improving the predictability of alkane SOA using the UNIPAR model against their chamber study. The resulting alkane model parameters have been newly implemented into CAMx-UNIPAR. In addition, the UNIPAR model of this study has been expanded to simulate biogenic SOA based on three major oxidation paths (i.e., OH radicals, ozone and nitrate radicals) being capable of nighttime SOA formation that is dominated by oxidation with ozone and nitrate radicals (Han and Jang, 2023).”

Comment 10

Around line 190 : deriving POA from a fixed POA/EC ratio is uncertain, even more since the used ratio has been derived some 20 years ago. No control is possible using daily measurements. This is in line with my above remark that the used observational data-set is not suitable for in depth model evaluation.

Response: We agree with the reviewer. As discussed in the responses to comment 2 and 3, CAMx-UNIPAR will be evaluated in various domains and periods using different gas mechanism such as CB6.

Comment 11

Line 270: it is not specifically figure “Fig. 4(e-h)” here.

Response: Fig. 4(e-h) is correct for the time series of the simulated SOA species and pie charts.

Comment 12

Line 274: “For example, the fraction of alkane SOA was higher than that of terpene SOA in all sites except Sacramento.” Is this SOA from the ALK5 lumped species? Does this include long chain alkanes, of intermediate volatility. Please state this before the conclusion section.

Response: Alkane SOA includes long chain alkane (up to C24). As discussed in the response to comment 5, the description of alkane has been modified in the revised manuscript (Section 2.2).

Comment 13

Lines 410 – 427: there is a long discussion on the potential NO_x and SO₂ reduction impact on BSOA formation. I encourage the authors to add a test simulation where they test such scenarios over their model domain.

Response. We agree to the reviewer. In the future, we will simulate the impact of acidity on SOA formation with better emission data in the different locations. The sensitivity of SOA formation to SO₂ emissions is complex because the increased acidity due to increased SO₂ can reduce ammonium nitrate, which is hygroscopic and influences aqueous reactions. In this paper, the impact of NO_x on SOA formation has been discussed to response to the reviewer. Section 3.5 “Impact of NO₂ on SOA formation” in “Results and Discussion” has been added into the revised manuscript. The newly added Table 3 shows the correlation coefficients between NO₂, nitrate and the SOA mass associated with each HC excluding low PBL height periods. Based on the formaldehyde-to-NO₂ ratio (FNR) at Figure S14, the four urban sites of this study are VOC-limited condition (high NO_x levels). Under the VOC-limited condition, SOA production is typically correlated to NO₂ with a negative relation. However, SOA simulations of this study are positively correlated to NO₂. Biogenic SOA is more strongly correlated with NO₂ than anthropogenic SOA. This information has been discussed in the revised paper (Section 3.5 and Fig. S14) and reads now,

“3.5 Impact of NO₂ on SOA formation

To understand the impact of NO₂ on SOA formation, the correlation coefficients (R) between NO₂, nitrate, and SOA mass associated with each HC were estimated as shown in Table 3. The simulations of NO₂, nitrate and SOA during low PBL height periods were excluded. The formaldehyde-to-NO₂ ratio (FNR) is typically used to denote NO_x levels. When FNR is less than 1, it represents VOC-limited condition (Duncan et al., 2010; Hoque et al., 2022). Based on the spatial distribution of FNR in Fig. S14, the four urban sites of this study were VOC-limited (high NO_x levels) condition. Under this environment, a typical SOA production in daytime is negatively correlated with NO₂ concentrations (Presto et al., 2005; Yang et al., 2020; Madhu et al., 2022). However, all correlation coefficients between NO₂ and SOA mass shown in Table 3 were positive. Biogenic SOA was more strongly correlated with NO₂ (larger positive R) than anthropogenic SOA.

As discussed in Section 3.2 and 3.3, biogenic HCs, particularly terpene, react with a nitrate radical to form low-volatile products and effectively increase SOA mass. NO₂ is linked to the formation of nitrate radicals at night and thus, it can be positively related to biogenic SOA mass. Increased nighttime biogenic SOA (Fig. 5) can influence OMP of anthropogenic SOA and it can weaken the negative correlation between NO₂ and anthropogenic SOA formation. For example, the last column in Fig. 5, which displays the diurnal variation of the total SOA concentrations, evinces the influence of terpene SOA on anthropogenic SOA mass. Anthropogenic SOA mass gradually increased with increasing terpene SOA mass after sunset (5 PM) when the production of OH radical was nearly inactive. As shown in Fig. S15, a rapid change in the PBL height appeared between 3PM and 5PM, and no change appeared in the PBL height after 7PM. Thus, the influence of the lowered PBL height on changes in anthropogenic SOA mass after 7PM can be excluded. Under the Central Valley’s environments in this study, ammonia was rich, temperature was relatively low, and humidity was high. The high concentration of NO₂ in this region is favorable to form inorganic nitrate aerosol, which can promote aqueous phase reactions of organic species. Evidently, a strong positive correlation appeared between inorganic nitrate concentrations and SOA mass (R: 0.41–0.86 in Table 3) declining a conventional negative correlation between NO_x concentration and anthropogenic SOA formation at high NO_x levels.”

In addition, we have added the description about the NO_x and SO₂ impacts on SOA mass into Section 4 in the revised manuscript, and reads now,

“As discussed in Section 3.5, the anthropogenic SOA formation can be influenced by the amount of biogenic SOA, and vice versa. Hence the impact of NO₂ on SOA formation can be varied with the composition of precursor HCs. The SOA mass in California urban area possibly would decrease as NO_x decreases because of the dominance of

terpene SOA, which has a strongly positive correlation with NO₂ as shown in Table 3. For the polluted urban area where anthropogenic SOA is dominant and NO_x is rich, SOA formation can be negatively correlated with NO_x. Under this situation, SOA mass increases with lowering NO_x. The impact of SO₂ change on SOA formation is complicated due to the aerosol acidity and the amount of wet-inorganic aerosol. The reduction of SO₂ drops aerosol acidity and thus, it can reduce SOA mass. However, the reduced aerosol acidity with decreasing SO₂ under ammonia-rich environments can increase the deposition of nitric acid forming ammonium nitrate that is very hygroscopic. The ERH of ammonium nitrate is lower than that of ammonium sulfate and increases wettability of aerosol. Increased ammonium nitrate mass increases partitioning of polar organics onto the wet aerosol and enhances the reactions of reactive organic species in aqueous phase.”

Comment 14

*In table 1, I guess that SOA data means chamber data for validation of parts of the UNIPAR model. Please correct. I do not understand why 50 *4 stoichiometric coefficients are needed.*

Response: Yes, SOA data is chamber data. The word “SOA data” has been replaced by “Chamber data”. We added information into the footnote “c” in Table 1. The description of four different stoichiometric coefficient sets is also described in footnote “b” in Table 1.

Comment 15

For regional simulations, I think Yu et al. 2022 should appear more often except for alkanes.

Response: We have cited the paper by Yu et al. (2022) in numerous places of this manuscript and Table 1.

Comment 16

Line 45: “The SOA model has been simulated in regional and global scales” This is a strange formulation. You could say : “themodel has been to simulate at regional and global scales”

Response: “in regional and global scales” has been replaced by “at regional and global scales”

Comment 17

Line 69: “established on UNIPAR » in, within?”

Response: “The model parameters and equations established on UNIPAR” has been replaced by “The model parameters and equations in UNIPAR”

Comment 18

Line 99 : “as follow » with an « s ».

Response: “as follow” has been replaced by “as follows”

Comment 19

Line 101 : “For the SOA formation in multiphase ...” -> “For the multiphase SOA formation ...”

Response: “For the SOA formation in multiphase” has been replaced by “For the multiphase SOA formation”

Comment 20

Line 107 : “volatility-reactivity base » -> « volatility-reactivity based”

Response: “volatility-reactivity base” has been replaced by “volatility-reactivity based”

Comment 21

Line 115 : “are used to manage their multiphase partitioning” -> may be : “are used to determine their multiphase partitioning”

Response: “are used to manage their multiphase partitioning” has been replaced by “are used to determine their multiphase partitioning”

Comment 22

Line 422: “where aromatic SOA is MORE dominant than that in California”

Response: This sentence has been removed in the revised manuscript.

Comment 23

Line 436: “can yield lower SOA yields” please reformulate

Response: “can yield” has been replaced by “have”

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