

Atmos. Chem. Phys. Discuss., referee comment RC1
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Comment on acp-2021-1002

Anonymous Referee #1

Referee comment on "Secondary organic aerosol formation via multiphase reaction of hydrocarbons in urban atmospheres using CAMx integrated with the UNIPAR model" by Zechen Yu et al., Atmos. Chem. Phys. Discuss.,
<https://doi.org/10.5194/acp-2021-1002-RC1>, 2022

In this manuscript, the authors incorporated their sophisticated SOA model (UNIPAR) with an air quality model (CAMx) and simulated SOA concentrations from different formation pathways and different precursors. Observed concentration of organic matter (OM) is better reproduced by the UNIPAR mode than by a conventional two product model (SOAP). By applying the UNIPAR model, the SOA formation from gas-particle partitioning, in-particle oligomerization, and aqueous-phase reactions are separately calculated, and their contributions have been quantified.

This manuscript is well written and includes useful information about the numerical modeling of SOA formation processes in the ambient air. However, I have several concerns as below. I recommend this manuscript for publication after the following concerns are adequately addressed.

1: Methodology

I am afraid that methodology (model and emissions) is not comprehensively described or adequate references are cited.

- You wrote in L109 that "The mathematical equations used to construct the stoichiometric coefficient array are reported in Section S1" and four parameters (A, B, C, and D) for different precursors and conditions (NO_x level and aging status) are given

in Table 3, . However, I could not find the information how did you consider dependence on NO_x (high/low) and aging degree (fresh/aged) for the calculation of stoichiometric coefficients in the ambient conditions.

- You set six categories for oxidation products: non-reactive (P), slow (S), medium (M), fast (F), very fast (VF), and multifunctional alcohols (MA). Products with these categories are always produced or did you consider any condition dependence?
- Thermodynamic parameters of oxidation products (vapor pressure and vaporization enthalpy) are not explicitly shown.
- Information of emission amounts is not shown. As you estimated the contributions of SOA precursors, total emissions or their distributions are important information. I have two more concerns about emissions:

- You wrote in L255 that "During the wet period, HC emissions increased". It appears from Figures S5 and S6 that daytime temperature is higher during the dry periods than wet, and thus, I speculate that BVOC emissions are higher during the dry period. Quantitative information and reasons for the increase of HC emissions should be given.

- L308: "isoprene SOA is negligible at all sites due to low isoprene emissions". Information of isoprene emissions (preferably with terpene and aromatics) is required.

2: Precursors' contributions:

You wrote in L308 as "Isoprene SOA is negligible at all sites", and concentrations of isoprene SOA was small over the domain as shown in Figure 8 (g) and (h). However, previous observational and simulation studies have indicated that isoprene SOA has important contributions in East Asia in May-June (e.g., Hu et al., Zhu et al., and Ding et al.). I recommend the authors to discuss the differences of your estimate with previous studies.

Hu et al. (2017) doi:10.5194/acp-17-77-2017

Zhu et al. (2018) doi: 10.1016/j.apr.2017.09.001

Ding et al. (2016) doi: 10.1038/srep20411

3: OMH and OMP

You wrote in L324-326 that "Under the dry period (Fig. 3), the predicted SOA mass by the UNIPAR model is dominated by gas-particle partitioning onto organic phase and oligomerization in organic aerosol. During the wet period, SOA production forms mainly through gas-aqueous partitioning and aqueous reactions."

I could not get how did you separate contributions of oligomer SOA and SOA from aqueous-phase reactions (I guess both are categorized OMH). Quantitative information of the contributions of the three pathways is helpful to readers.

4: OM and OC

It is not clear whether you showed organic mass (OM) or organic carbon (OC) in Figures 3-5. I guess OM concentration is calculated by your simulation model, whereas OC concentration is measured by carbon analyzers. Conversion factor from OC to OM (or vice versa) should be explicitly noted.

Specific comments:

L51: References for the following sentence is necessary: "In particular, the current model applied to regional scales suffers from a substantial negative bias under high humidity conditions."

L104: eight aromatics?

L214: VCPs sourced from "residential, commercial, and industrial sectors"?

L300: "OMH attributes to 50% of aromatic SOA": it appears OMH contribution is smaller than 50% in Fig. 7 (during the wet period).

L342: 53% of total anthropogenic VOC emissions in LA?