Response to the Editor

We are very grateful to the editor for the careful evaluation and constructive suggestions, which have helped us further clarify and improve the manuscript. Before addressing the editor's comments point by point, we briefly summarize the main revisions made in response to these final suggestions. The editor's comments are shown in **bold blue text**, while our responses and the corresponding revised manuscript text are shown in black text. All line numbers refer to the revised manuscript.

In response to the editor's comments, we made several targeted revisions to improve the manuscript. Specifically, we expanded the discussion of key model assumptions and limitations, clarified that the lumped product classes shown in Fig. 1 may be dominated by organosulfates rather than organonitrates, improved the discussion of potential causes of model evaluation biases, and clarified the scope and limitations of the molecular-species evaluation. Relevant recent references were added accordingly.

1.) Lines 253-255: I think the authors need to state one limitation of their assumption that no further oxidation of 2-methyltetrol sulfates (i.e., IEPOX's main organosulfate derivative) has been shown to occur in both lab-generated aerosol particles (Chen et al., 2020, ES&T Letters; Xu et al., 2024, ES&T Letters) and more recently in cloud/fog/aerosol water mimics (Royer et al., 2026, ACS ES&T Air). The oxidation compounds from 2-methyltetrol sulfates identified from these lab studies were also found in ambient PM2.5 samples. I think the authors need to acknowledge that one limitation of their model is that they didn't consider heterogeneous or aqueous-phase oxidation of these products.

Response: We thank the editor for highlighting this important limitation. We agree that, although the omission of further oxidation is consistent with previous modeling studies, it represents a limitation in the treatment of 2-methyltetrol sulfates (2-MTS), which are represented within the lumped AIEOSN species. We have therefore revised the corresponding paragraph to acknowledge recent evidence for heterogeneous and aqueous-phase OH oxidation of 2-MTS and have added Chen et al. (2020), Xu et al. (2024), and Royer et al. (2026) to the reference list.

Lines 258–265:

Once ISOA from IEPOX, HMML, and MAE is formed, no further oxidation is represented in the model, consistent with previous modeling studies (Budisulistiorini et al., 2017; Marais et al., 2016; Schmedding et al., 2019). However, this assumption represents a limitation in the treatment of 2-methyltetrol sulfates (2-MTS), major IEPOX-derived organosulfates represented within the lumped AIEOSN species, because 2-MTS have been shown to undergo heterogeneous OH oxidation

in laboratory-generated aerosol particles (Chen et al., 2020; Xu et al., 2024) and aqueous-phase OH oxidation in cloud, fog, and aerosol water mimics (Royer et al., 2026). Several oxidation products have also been detected in ambient fine aerosols (Chen et al., 2020).

2.) Figure 1: The authors need to clarify that the species binned in AIEOSN and AHMSON may be dominated by the organosulfates and not the organonitrates through this scheme. Furthermore, as shown recently by Cooke et al. (2025, ES&T), HSO4- is a much weaker nucleophile for IEPOX than sulfate. This is consistent with important kinetic work from Prof. Matthew Elrod's group from Oberlin College, which also find nitrate is a weaker nucelophile than sulfate and tertiary organonitrates can be rapidly hydrolyzed by water or sulfate to form 2-methyltetrols and 2-methyltetrol sulfates (e.g., Darer et al., 2011, ES&T).

Response: We thank the editor for this helpful suggestion. We agree that the lumped AIEOSN and AHMOSN product classes should not be interpreted as containing equal contributions from organosulfates and organonitrates. We have revised Sect. 2.1.2 to clarify that both classes include organosulfates and organonitrates but may be dominated by organosulfates. We have also added relevant kinetic evidence concerning the lower nucleophilicity of HSO_4^- and nitrate relative to sulfate and the rapid conversion of tertiary organonitrates by water or sulfate. The revised text further clarifies that the internal organosulfate/organonitrate composition is not explicitly resolved within these lumped model classes (lines 249–254).

Figure 1 has also been updated to distinguish the H_2O-mediated product branches, labeled with H^+ and AeroWater, from the lumped inorganic-nucleophile addition product branches, labeled with SO_4^{2-}, NO_3^-, and HSO_4^-, consistent with the product-class definitions used in the model. The caption of Fig. 1 has been revised accordingly to clarify the interpretation and potential organosulfate dominance of AIEOSN and AHMOSN (lines 268–275). Because the model does not explicitly resolve their internal organosulfate/organonitrate fractions, no quantitative weighting is assigned to these products in the schematic.

The references for Cooke et al. (2024), Mael et al. (2015), and Darer et al. (2011) have also been added to the reference list. The cited Cooke et al. paper was formally published in 2024, and we have cited it using its final publication year.

Lines 249–254:

AIEOSN and AHMOSN are lumped product classes that include both organosulfates and organonitrates but may be dominated by organosulfates. Recent kinetic evidence indicates that HSO_4^- is substantially less nucleophilic toward IEPOX than SO_4^{2-} (Cooke et al., 2024), while nitrate is weaker than sulfate in related epoxide systems (Mael et al., 2015). Tertiary organonitrates can also be rapidly hydrolyzed by water to form polyols or undergo nucleophilic substitution by sulfate to form organosulfates (Darer et al., 2011). The internal organosulfate/organonitrate composition of these lumped classes is not explicitly resolved in the model.

Lines 268–275:

Figure 1: Schematic of the explicit isoprene-derived secondary organic aerosol (ISOA) formation mechanism implemented in CAM6-Chem in this study. Dashed arrows indicate gas-phase reactions, whereas solid arrows indicate particle-phase heterogeneous uptake and product-formation reactions. Species explicitly represented as updated ISOA precursors or product classes in this mechanism are shown in green, and the explicitly represented ISOA formation pathways are shown in orange. AeroWater denotes aerosol liquid water. AIETET denotes IEPOX-derived 2-methyltetrols, and AHMGA denotes HMML/MAE-derived 2-methylglyceric acid. AIEOSN and AHMOSN denote lumped inorganic-nucleophile addition product classes from the IEPOX and HMML/MAE pathways, respectively. These classes include both organosulfates and organonitrates but may be dominated by organosulfates.

3.) Lines 300-303: While I agree, I just want to make sure the authors are aware of work by Molly Frauenheim showing that C5-alkene triols are not the original compounds previously proposed by proving with organic synthesis (Frauenheim et al., 2022, ES&T Letters) and that these actual compounds can react in the atmosphere since they can partition off aerosols where IEPOX reacted to react with gas-phase oxidants producing other isoprene SOA (Frauenheim et al., 2024, ES&T). These exact compounds are not included in models and their potential to undergo gas-phase oxidation chemistry to form new SOA.

Response: We appreciate the editor's clarification and the references to recent work by Frauenheim et al. The relevant $C_5H_{10}O_3$ products as 3-methylenebutane-1,2,4-triol and isomeric 3-methyltetrahydrofuran-2,4-diols using authentic synthetic standards. Accordingly, we replaced the previous "C5-alkene triols" terminology with the structurally neutral term $C_5H_{10}O_3$ reactive uptake products. We also acknowledge that these semivolatile products can repartition from the particle phase to the gas phase and undergo gas-phase OH oxidation to form additional isoprene-derived SOA (Frauenheim et al., 2024). We further clarify that this competing product branch and its subsequent gas-phase oxidation are not explicitly represented in the model and that omission of the branch may lead to excessive allocation of IEPOX-derived carbon to AIETET, contributing to its positive bias. The manuscript has been revised accordingly (Lines 311–317), and both references have been added to the reference list.

Lines 311–317:

First, missing or simplified competing pathways may cause an over-allocation of epoxide precursors to the explicitly represented ISOA products. For example, a fraction of IEPOX-derived carbon may form structurally characterized $C_5H_{10}O_3$ reactive uptake products (Frauenheim et al., 2022). These semivolatile products can repartition from the particle phase to the gas phase and undergo gas-phase OH oxidation to form additional isoprene-derived SOA (Frauenheim et al., 2024). This competing product branch and its subsequent gas-phase oxidation are not explicitly represented in the model. Omission of this branch may therefore lead to excessive allocation of IEPOX-derived carbon to AIETET, contributing to its positive bias.

4.) Finally, the authors need to make clearer that one major limitation of their study is that they don't provide a comparison of model predicted 2-methyltetrol sulfate and 2-MG sulfate versus observations. The reason I raise this issue as a final point is that most studies in the U.S. and around the world show that 2-methyltetrol sulfate (the main organosulfate from IEPOX) can contribute large mass fractions (upwards of 15%) to the organic in PM2.5 (see Hettiyadura et al. 2019, ACP). I'm guessing the authors weren't able to do this comparison due to the lack of available measurements of these two important organosulfates in China? Can you please clarify this final point?

Response: We agree that the absence of a direct species-specific evaluation of 2-methyltetrol sulfate (2-MTS) and 2-methylglyceric acid sulfate (2-MGS) should be stated more clearly as a limitation. This limitation is important because 2-MTS can contribute substantially to fine-particle organic carbon (Hettiyadura et al., 2019). First, sufficiently extensive measurements of these two organosulfates are not available in China to support a robust evaluation of their absolute concentrations. Given this limitation, we instead used the available observations reported by Zhang et al. (2022) from Beijing, Hefei, and Kunming to evaluate the relative contributions of the corresponding product classes in Fig. 2(c). Second, 2-MTS and 2-MGS are not represented as separate model species but are included within the lumped AIEOSN and AHMOSN classes, respectively, which also contain other organosulfate and organonitrate products. Consequently, a one-to-one comparison of their absolute concentrations is not possible. We have clarified the scope of this evaluation in Section 3.1 (lines 356–360) and added Hettiyadura et al. (2019) to the reference list.

Lines 356–360:

Although 2-MTS can contribute substantially to fine-particle organic carbon in some regions (Hettiyadura et al., 2019), available observations of 2-MTS and 2-methylglyceric acid sulfate in China have limited spatial coverage, and the two compounds are not separately resolved within the lumped AIEOSN and AHMOSN classes, respectively. Accordingly, Fig. 2(c) provides a product-class-level comparison of relative contributions rather than a species-specific evaluation of absolute concentrations.