Responses to Referee #1

Farrell et al. present an interesting investigation into the impact of various organic aerosol phase state parametrizations on the prediction of IEPOX-SOA phase states using CMAQ. This represents a significant development for the CMAQ modelling community. However, before I can recommend publication in an EGU journal, major modifications with respect to context and presentation need to be made. Overall, the manuscript reads more like a combination of model description and evaluation. In this context, it might be better suited to publication in Geoscientific Model Development (GMD) instead of ACP.

We thank the Referee for their thorough review of our manuscript and have made modifications to address issues with figures.

We were intentional about submitting this article to ACP (as opposed to GMD), given ACP's aims and scope. In this article we describe and implement new physiochemical processes (by way of differing phase state parameterizations) in the formation of IEPOX derived aerosols. While the developments made here are significant to the formation of IEPOX derived aerosols, and potentially other heterogeneous reactive uptake in the formation of other aerosols, we do not develop a new model, nor a new module within CMAQ. In this work, we implement code within an existing module but still use all of the existing CMAQ infrastructure.

General comments:
Version 5.3.2 of CMAQ was published in 2020. Since then, there have been two major updates to CMAQ, which is now available as version 5.5. Please explain why you are relying on an outdated version of CMAQ. As far as I can tell, your code adjustments are not included in the official CMAQ repository. Can your code modifications be transferred to the current and future versions of CMAQ?

We thank the reviewer for raising this point and the opportunity to explain our design choices. CMAQv5.3 was the version of the model that we chose when first embarking on this study in 2020. At the time, the updates encoded in this version were novel for this specific application - namely the inclusion of hygroscopicity parameters so that water uptake attributed to oxygenated organic aerosols could be tracked and modeled. This allowed us to model organic coating phase state dynamically with the plasticizing effect of water. Major updates to CMAQ between v5.3 and v5.5 include but are not limited to updates to deposition, updates to emissions treatments, output of diagnostic variables, and the addition of a new chemical mechanism. While becoming a more state-of-the science from v5.3 to v5.5, the updates (water associated with organic aerosol) most critical for our work were in v5.3.

The representation style is generally good. However, the figures require significant quality improvements and harmonisation. Figure 3 is completely unreadable. No information can be obtained from panels (e) and (f). Figures 1 and 4 also have quality issues, with some text being illegible. Please harmonise the layout of Figures 2, 3 and 6. Figure 3 has latitudes and longitudes, but the other two do not.

We thank the reviewer for noting this. Illegible figures are indeed attributed to Word manuscript to a pdf conversion issues. We have corrected this issue, including increasing figure resolution and harmonizing figures 2, 3, and 6.

Line 39: Does the 99.99% indicate that the reactive uptake is completely suppressed?

After taking the average of percent changes in the IEPOX reactive uptake parameter (gamma_IEPOX) for each modeled grid cell, the maximum of those reductions was 99.99%. So – the implementation of phase separation and phase state does not always completely suppress IEPOX reactive uptake, but can in certain grid cells for the episode modeled. The way we phrase this, nonetheless, is confusing and we have therefore made the following change:

> observationally-derived field measurements. The implementation of phase separation and phase state parameterizations resulted in times and grid cells where IEPOX reactive uptake is completely supressed.~~, on average, decreased IEPOX reactive~~

Line 39: Please specify what you are referring to with 'mixed model performance'. Do you mean numerical performance or when evaluating predictions with observations?

We have made the following changes to avoid confusion:

> 40 ~~uptake by up to 99.99% compared to Base CMAQ, resulting in mixed model performance.~~ While modelled positive bias in 2-methyltetrol concentrations were decreased ~~performance improved~~ with phase separation and phase state updates, modelled methyltetrol sulfates and total IEPOX-SOA concentrations further underpredicted field observations in comparison to Base CMAQ.

Line 41: I assume that 'Base CMAQ' refers to the same CMAQ version without your modifications with otherwise the same model setup?

Correct. The only change we made to out of the box Base CMAQ (that downloaded from github), was that we use a different pseudo first-order rate constant for the formation of methyltetrol sulfates (AIEOS) than the default. This pseudo first-order rate constant is from Riedel et al. 2016 and was chosen to be consistent with the IEPOX heterogeneous reactive uptake modeled in Schmedding et al., 2020 (Riedel et al., 2016; Schmedding et al., 2020). We have clarified this in the methods section:

185 Where $k_{particle}$ is the pseudo-first-order rate constant (s^{-1}) that takes into account the opening of the epoxydiol group on IEPOX by a proton (acid) followed by a nucleophilic attack (by sulfate, water, or monomer IEPOX-SOA species) on the free carbo-cation formed from this opening, and is represented by the following equation (Eddingsaas et al., 2010; Pye et al., 2013):

$$k_{particle} = \sum_{i=1}^{N} \sum_{j=1}^{M} k_{i,j}[nuc_i][acid_j] \quad (5)$$

190 Where $k_{i,j}$ are individual acid-nucleophile rate constants defined by Supplemental Table 3. A slight alteration was made to Base CMAQ and all of the phase state sensitivity model runs with regard to Eq. 5 in that in this study we use the individual third-order rate constant for AIEOS from Riedel et al., 2016, instead of the default from Piletic et al., 2013, to be consistent with Schmedding et al., 2020 (Piletic et al., 2013; Riedel et al., 2016; Schmedding et al., 2020)

Line 93: Please elaborate why 10% was chosen for previous studies.

Absolutely. The assumed 10% of water associated with the organic coating was chosen in Schmedding et al., 2020 based on the lower bound of day-time ALW associated with the organic aerosols predicted in Pye et al., 2017 (Pye et al., 2017; Schmedding et al., 2020). The lower bound of ALW during the day was chosen as opposed to that of night-time since most IEPOX reactive uptake is expected to occur during the day (when isoprene is released from vegetation). While explanation of this is pertinent to justifying design choices in Schmedding et al., 2020, we decide to leave this out of our introduction for brevity and readers can always refer to this article for more details.

Line 142: I assume that AIETET and other name given in parenthesis are the names of the corresponding species in the CMAQ mechanism. Indicating this could be beneficial for readers that are not familiar with CAMQ.

These are species that are a part of the SAPRC07tic_ae7i chemical mechanism and aren't necessarily specific to CMAQ. I have made the following changes for better clarity:

from the EPA's National Emissions Inventory (NEI) 2011 version 2. Biogenic emissions were predicted using the Biogenic
140 Emissions Inventory System (BEIS) version 3.6.1, with biogenic isoprene emissions scaled up by a factor of 1.5 to better match isoprene measured at the Centreville, AL SOAS site (CTR) as detailed in (Pye et al., 2017). The State Air Pollution Research Center version 07tic with extended isoprene chemistry and aero7i treatment of SOA (SAPRC07tic_ae7i) was used as the chemical mechanism (Xie et al., 2013) as it explicitly tracks 2-methyltetrols (corresponding to AIETET in the SAPRC07tic_ae7i mechanism) and methyltetrol sulfates (corresponding to AIEOS in the SAPRC07tic_ae7i mechanism, also
145 known as IEPOX organosulfate) (Pye et al., 2013). These are the predominant IEPOX-derived SOA species permitting the tracking of the influence of sulfate aerosols on the acid-driven multiphase chemistry (reactive uptake) of IEPOX (Budisulistiorini et al., 2015a, 2015b; Budisulistiorini et al., 2017; Pye et al., 2013).

Line 157: How was the Vogel-Tamman-Fulcher equation modified?

The Vogel-Tamman-Fulcher equation was modified to 1) conform to $\eta_\infty = 10^{-5}$ Pa s (Angell, 1991) and 2) the fragility parameter (D) was modified to depend on O:C ratios (using the O:C ratios and fragility parameters for 95 organic aerosol species) for ease of implementation into air quality models as O:C ratios of organic species are widely encoded. These modifications are documented in DeRieux et al., 2018 (DeRieux et al., 2018). I have added in the Angell, 1991 citation to account for this modification #1.

> here-on-out as $T_g(w_{org})$. The $T_g(w_{org})$: T ratios were then used determine the viscosity of the organic coating (η_{org}) (Eq. 3-6 shown in Fig. 1) using a modified Vogel-Tamman-Fulcher equation (Angell, 1991; DeRieux et al., 2018; Fulcher, 1925; Schmedding et al., 2020; Tammann et al., 1926; Vogel, 1921). Equations for the viscosity of the aerosol (i.e., Eq. 3-6) and

Line 169: Is the 'numerical precision' given as a general comment on CMAQ's performance or are you referring to calculated precision (single vs double precision in Fortran)?

We thank the reviewer for their question and have made the following changes to clarify the paragraph:

> When $w_s = 0$, the aggregated OA phase state equation (Eq. 82) collapses into ~~is equal to~~ the mass fraction weighted aggregated ~~T_gs, previously referred to as the~~ dry phase state equation, represented by $T_{g,org}$ (Dette et al., 2014; Li et al., 2021; Li et al., 2020):
>
> $$T_{g,org} = w_a T_{g,a} + w_b T_{g,b} \quad (14)$$
>
> ~~.~~ Given there ~~numerical precision of CMAQ and the likelihood of very small w_s values characteristic of dry OAs yet still greater than zero~~ was never an occurrence during our modeling where ~~the occurrence of~~ $w_s = 0$ ~~was minimal~~, we ~~. A recent~~

> ~~publication~~ use ~~defined the~~ equation 14 when ~~dry phase state as~~ $w_s \leq 0.1$ (Rasool et al., 2021), signifying a dry aggregate glass transition temperature that does not consider water uptake to the organic shell. While our implementation of phase separation and phase state in CMAQ did~~does~~ not implement in-model conditionals to switch between using $T_g(w_{org})$ and $T_{g,org}$ ~~phase state equations~~ based off of these w_s thresholds~~values~~, we identify dry aerosol phase state instances offline ~~using this threshold and refer to it as $T_{g,org}$~~.

Line 214: What influence do you expect from assuming an activity coefficient of 1?

In assuming an activity coefficient of 1, we are assuming that like partitions onto like, when in reality, a partitioning species is often chemically different to the existing aerosol it partitions onto. In being able to capture this nuance, an effective saturation concentration, as opposed to a pure saturation, is calculated (where this activity coefficient is not equal to 1). In CMAQ's semi-volatile partitioning scheme, effective saturation concentrations are used, as these are derived

from chamber experiments that track the partitioning of an individual (or category) of semi-volatile species on to existing (and chemically different) aerosols. The importance of this would be more significant with relation to the treatment of semi-volatile organic aerosol partitioning as opposed to our application here. In this study we only calculate these C^0 values for the purpose of calculating Tgs and do not change anything with semi-volatile partitioning. For example, in all of our model runs, the semi-volatile organic partitioning scheme uses the original C^0 for AIETET (10^{-9} μg/m^3 – which is the value at which created aerosol species do not re-volatilize and remain locked in the particle phase), and not our updated C^0 value.

The impact of mixtures on an individual specie's glass transition temperature is currently not well known, and has not been formulated for all CMAQ species and existing aerosol mixtures, and therefore we make this assumption that the activity coefficient is 1. We, however, now realize the confusion this poses and make the following changes:

and their structures were coded into the Simplified Molecular Input Line Entry System (SMILES) coding notation (Anderson, 1987). Once SMILES were coded, they were input into the OPEn structure–activity/property Relationship App (OPERA)
330 (Mansouri et al., 2018), where p_0 were estimated and then used to calculate C^0 using the following relationship ~~assuming that the activity coefficient is 1~~ (Donahue et al., 2006; Pankow, 1994; Zhang et al., 2019b):

$$C^0 = \frac{M10^6 p_0}{RT} \quad (184)$$

Line 242 and 244: Please provide approximate pressure altitudes for layer 18, 28, and 35.

Thank you for the suggestion. We have made the following changes:

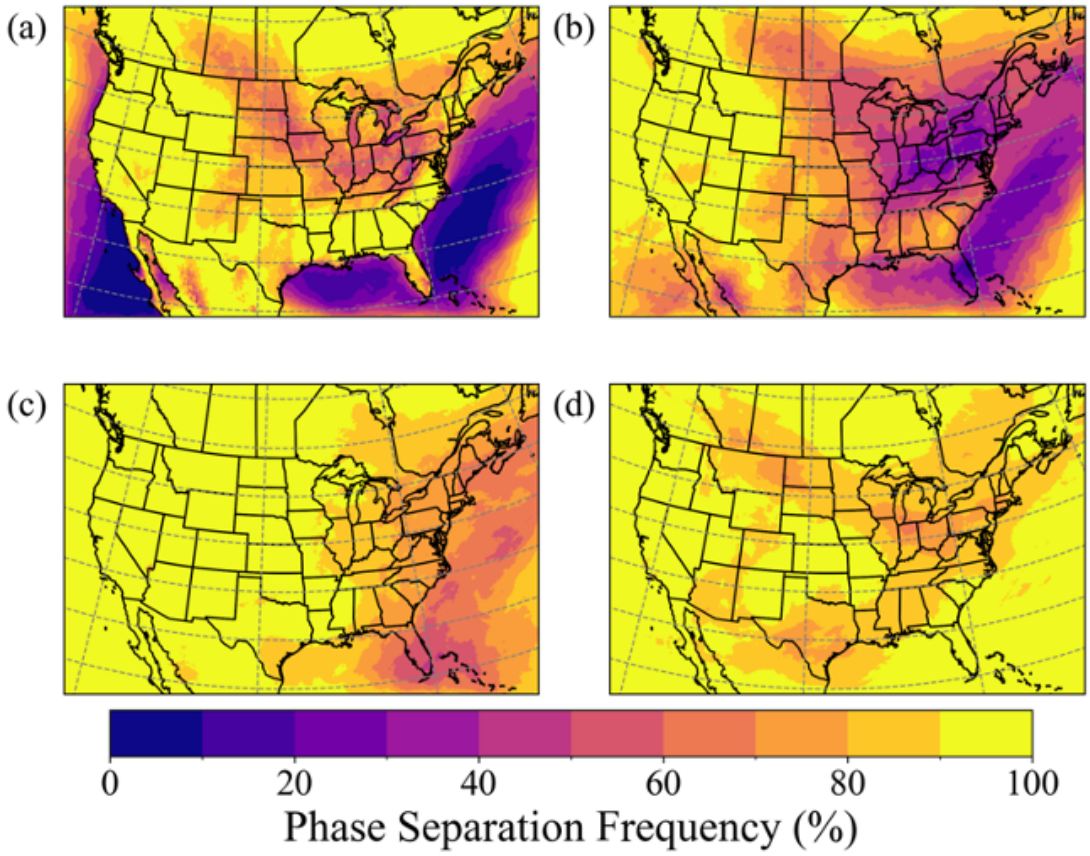


Figure 2. Frequency of modelled aerosol phase separation for the SOAS 2013 Field Campaign episode (June 1st – July 15, 2013) at layer 1 (surface layer; 1-0.9975 atm (a)), layer 18 (corresponding to ~1.8km; 0.82-0.8 atm (b)), layer 28 (corresponding to ~8km; 0.4-0.35 atm (c)), and layer 35 (corresponding to ~17km; 0.05-0 atm (d)) across hourly model estimations.

Line 259-261: How about representing these conditions in a table?

We thank the reviewer for this recommendation and note that these conditions are illustrated in Figure 4.

Line 266: Do you expect this transition to be valid for other seasons as well?

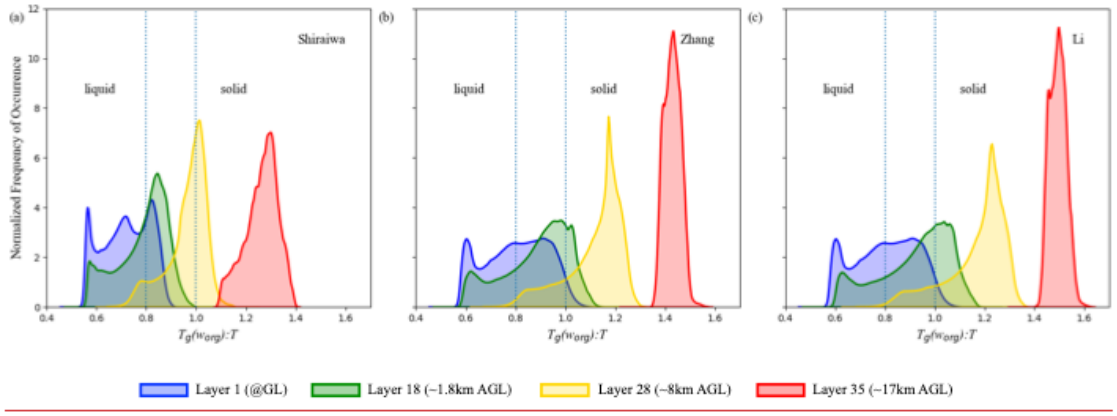
We exclusively modeled a summer-time episode, as this is the time of year for peak isoprene emissions. There may be a decrease in this gradient during other seasons when both temperatures are cooler and relative humidity is lower in the southeast and make the following additions in text to comment on this:

395 ~~present~~ in the organic coating ~~foraeross~~ all model simulations, with a distinct transition going from east to west (Fig. 3 a-c). The southeast U.S. is known to experience hot and humid summers with both increased temperatures and increased ALW, which results in the expected plasticizing of~~to plasticize~~ the organic coating. In this study we only simulated Summer 2013, however expect that this spatial trend in organic coating phase state calculated may be different during other seasons with changes in emissions, RH, and T.

400

Figure 4: I recommend listing the simulation name in each sub-figures heading in addition to (a), (b), and (c).

We have made the following changes to Figure 4:



430 **Figure 4.** The normalized frequency of occurrence of organic coating phase states (when $w_s > 0.1$; ($T_g(w_{org}):T$)) across the surface spatial domain and for the entire simulation period (hourly model estimations) for modeled layers 1 (blue, GL = ground level), 18 (green, 1.8 km AGL = above ground level), 28 (yellow, 8 km AGL), and 35 (red, 17 km AGL). Shown are the estimates using the Shiraiwa (a), Zhang (b), and Li (c) simulations. Distributions were normalized so that the area under each curve was equal to 1. Dotted blue lines representing the bounds for the three different phase states: liquid, semi-solid, and solid.

Table 2: The text in column 'Species Description' is hardly readable.

We thank the reviewer for raising this issue. This column, given its illegibility was removed and readers can refer to Supplemental Table 1 for species descriptions.

Line 330-332: Did you perform sensitivity simulations for this assumption? How would this affect your predictions?

We thank the reviewer for raising this point. We did not perform sensitivity simulations for this assumption, however we anticipate that both the $Tg(worg)$ or the Tg,org for predicted by the Shiraiwa simulations would increase, leading to predictions of a more viscous phase state, as stated. Although we choose ammonium oxalate as the proxy for AGLY's volatility, this is still a lumped species in CMAQ, whose properties require further investigation. One aim of this paper is to raise awareness to species that require further investigation prior to further aerosol phase state treatment in air quality models, which is what we intended to do in pointing out this discrepancy.

Line 376: Please specify which reduction corresponds to which phase state simulation.

We thank the reviewer for raising this point. These reductions are illustrated in Figure 6. We have made the following changes:

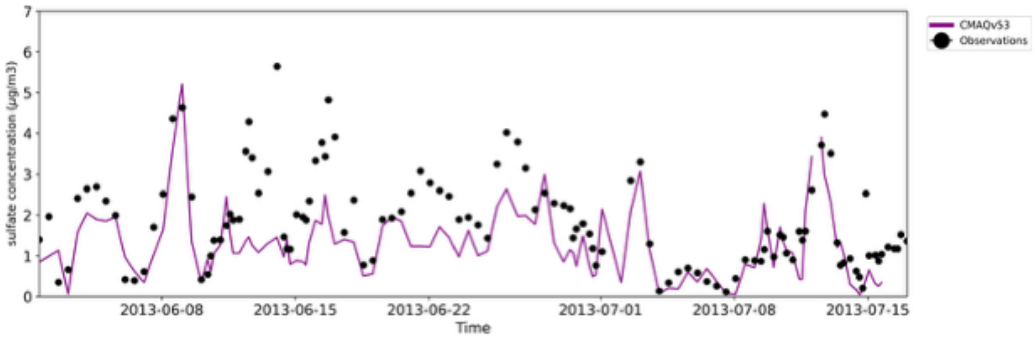
520 reduction). In the Southeast U.S. (where IEPOX concentrations peak (Fig. S1)) predicted reductions in γ_{IEPOX} range from 20-80% depending on the phase state simulation used (Fig. 6). At the LRK SOAS site, γ_{IEPOX} were reduced to values ranging from 3.5×10^{-4} to 4.84×10^{-4} and are in closer agreement to values in Budisulistiorini et al. (Budisulistiorini et al., 2017).

Line 381: How was this run-time improvement measured? Is it a simple comparison of run-time provided by the model (ignoring variability introduced by the cluster used)? Or did you use a specific tool to analyze run-time behavior?

We used model run-times output at the end of each model run log file and compared run-times this way.

Figure 7: Between 2013-06-08 and 2013-06-22 it looks as if all models fail to reproduce specific features in the observation. Can you comment on this?

We thank the reviewer for raising this point and the opportunity to discuss this. At the CTR site, all models in this time range seem to underpredict total IEPOX-SOA. There are some instances where the base model best represents total IEPOX-SOA concentrations, indicating that perhaps the phase state of the outer organic shell may be parameterized as too viscous in some of the sensitivity model runs. There are other times where all models, including the base underpredict total IEPOX-SOA. This may indicate missing precursors to IEPOX-SOA formation, like sulfate. While we do not explore sulfate performance at the CTR site, we do explore it at the LRK site (Fig. S7):



95 **Supplementary Figure 74.** Modeled and observed sulfate concentrations at the LRK SOAS site from June 1st to July 15th 2013.

And find generally that during the same periods that AIEOS is underpredicted at LRK, sulfate is also underpredicted. During this time period AIETET is mostly overpredicted which may be due to AIETET remaining in the particle phase after formation in CMAQ, although recent studies anticipate it can re-volatilize (Riedel et al., 2015; Su et al., 2025) and note this in section 3.6:

565 run having a NMB of 1.54. For the model runs accounting for phase separation and phase state, the bias improves with NMBs of 1.26, 1.19, and 1.14 for the Shiraiwa, Zhang, and Li parameterizations, respectively. It is important to note the recent studies have suggested that AIETET can re-volatilize ~~off-gas~~ (Riedel et al., 2015; Su et al., 2025); however, heterogeneous oxidation experiments of IEPOX-SOA have also suggested aged IEPOX-SOA (which produces more functionalized oligomer species) may limit this re-volatilization ~~off-gassing~~ (Armstrong et al., 2022; Hu et al., 2016; Yan et al., 2023). The base CMAQ run
570 underpredicts AIEOS concentrations with a NMB of -0.66. All parameterizations accounting for phase separation and phase

Line 411: Where the WRF simulations used for the meteorology in this study nudged? How do the temperature and RH simulated by CAMQ compare to SOAS observations?

WRF simulations were nudged above the planetary boundary layer height (PBLH), with the exception of soil moisture (which is nudged below the PBLH) – which is common practice for meteorological inputs for CMAQ simulations (Gilliam et al., 2006; Pleim et al., 2009; Pleim et al., 2003). We did not look at temperature and RH performance, however, can note that both variables were nudged indirectly (via soil moisture nudging):

predicted w_s values ranging from 0.1-0.6. Differences in IEPOX-SOA predictions across model runs at the LRK site coincide
565 with both low temperatures and low w_s. While we do not evaluate temperature and RH for our models in this paper, both variables were indirectly nudged in WRF simulations to observations of soil moisture (Gilliam et al., 2006; Pleim et al., 2009; Pleim et al., 2003). AIETET is overpredicted most of the time for all parameterizations (including the base run), with the base run having a NMB of 1.54. For the model runs accounting for phase separation and phase state, the bias improves with NMBs of 1.26, 1.19, and 1.14 for the Shiraiwa, Zhang, and Li parameterizations, respectively. It is important to note the recent studies

Code/Data Availability: I recommend to archive the code adjustments currently only available in GitHub to a permanent storage (e.g., Zenodo) to insure future reproducibility.

I have created a Zenodo page which includes source code (with our code adjustments), along with python scripts used to generate figures and the data used in those figures located here: https://doi.org/10.5281/zenodo.18624097

Units: Throughout the manuscript, various styles for units are used. I strongly recommend harmonizing this in a revised version according to ACP guidelines.

We thank the reviewer for their comment and have reviewed our manuscript for consistency in presenting units both in-text and in figures and in tables.

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