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Atmospheric Chemistry and Physics Discussions



# *Interactive comment on* "Predicting Secondary Organic Aerosol Phase State and Viscosity and its Effect on Multiphase Chemistry in a Regional Scale Air Quality Model" *by* Ryan Schmedding et al.

**Anonymous Referee #1**

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In this work the authors implement an SOA phase separation scheme into the chemical transport model CMAQ and explore the implications of this additional mechanism on a variety of aerosol properties such as organic phase partitioning and rates of acid-catalyzed reactions. Several different assumptions and sensitivity simulations are explored, including reduced anthropogenic emissions, increased Henry's law coefficient, and modified separation assumptions. Impacts on isoprene epoxydiol (IEPOX) as measured during the SOAS campaign are highlighted.

This additional mechanism represents an important step in the evolution of SOA mod-



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Discussion paper

eling in CTMs, and the authors have covered a great deal of territory in their analysis. I do have some concerns and questions that I would like to see addressed before publication, in particular the handling of organic water and explanation for worsened OC mass agreement with observations. Furthermore, while the text of this manuscript is generally well-composed, the figure quality is overall fairly low, and I believe substantial work is needed to bring the visuals up to ACP standards.

Specific comments:

- To estimate organic water, it is assumed that "10% of the aerosol water was present in the organic phase, within the range of organic water reported by Pye et al. (2017)." However, Fig 12 of the cited paper shows the fraction of organic water to vary significantly, and even exceed 60% in some areas. With this in mind, "within the range" appears to be a massive simplification of expected conditions. How was this 10% number chosen? What could be the expected consequences of a more explicit organic water mechanism (or even simply a greater amount of organic water in the SE)? Another sensitivity case study may be appropriate here.
- As the authors note in their conclusions, organic hydrophobicity is not considered in this work, including impacts of aging. This seems to me to be a very significant (though understandable) omission, and worthy of more discussion than currently provided.
- Page 19: Which species specifically contribute to the modeled change in O:C with elevation?
- Section 2.7: For the specific locations examined, how well did the modeled O:C values match observations?
- Page 27: The authors argue that the worsened NMB of hourly PM2.5 organic carbon mass vs. observations is likely explained by poorly constrained Henry's law

coefficients (and perhaps other parameters). This may be true, but I do not find Figure S6 to be compelling evidence for the argument. Visual and statistical examination of the differences found when using a modified Henry's law coefficient seems to indicate that its importance is actually very low in terms of impacts on overall OC mass. How can such modest "improvements" be considered evidence supporting this explanation for worsened model performance?

- The authors note that previous work in which phase-separation was included in a box model showed a drastic improvement in NMB (-66.2% to -36.3%). Why would this work not show such improvements? Are there any major differences in the handling of Henry's law coefficients or other parameters that could explain the differences in the performance of the CTM implementation?

- Figures throughout the manuscript and supplementary materials are formatted poorly, overall. Text, colors, positioning, labels, and spacing should all be examined carefully. In particular:

  - Fig 2: Panel and colorbar labels are missing completely.
  - Fig 3: This figure is presented as a timeseries, but the text describes it exclusively in terms of the diurnal cycle. I see no benefit to including individual dates, and it's very hard to tell day from night as shown. I suggest a change to diurnal averages.
  - Fig 7 B and C, and Fig 8: Panel labels for maps needed.
  - Fig 9: Statistical information insets are very hard to read. A transpose of the table may help.
  - Fig 10: Panel labels are missing. In addition, the colorbar chosen for this map is particularly difficult to interpret. A two-tone version in which zero is white or grey would help.
  - Figure S6: y-axis is missing label and units.

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