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Geoscientific Model Development Discussions

Interactive comment on "A simplified parameterization of isoprene-epoxydiol-derived secondary organic aerosol (IEPOX-SOA) for global chemistry and climate models" *by* Duseong S. Jo et al.

Anonymous Referee #2

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General Comments

The manuscript presents a simplified parameterization of isoprene-epoxydiols (IEPOX) derived secondary organic aerosol (SOA) that exhibits both computational economy and reproducibility of the explicit or full chemistry (Marais et al., 2016) in simulating IEPOX SOA in global chemistry and climate models. The new parameterization was developed based on an approximate analytical fitting in a box model to reproduce the formation yield and time scale of gas-phase intermediates and SOA from isoprene represented by the full chemistry. Three variations of the simplified parameterization

were discussed and evaluated along with fixed yield and VBS against full chemistry in GEOS-Chem v11-02-rc for IEPOX SOA simulations. Simulations by two out of the three new parameterizations generally captured the tropospheric burden of IEPOX-SOA and spatio-temporal profiles of those simulated by the full chemistry while fixed yields and VBS failed to do so. At the same time, the simplified parameterizations were at least 5 times faster than the full chemistry. The study also highlighted the importance of diurnal variation of chemical/meteorological fields to different parameterizations under comparison in the study. As a result, PAR3, the closest to the full chemistry in structure, resembled the full chemistry the best in terms of the response to the diurnal variation of chemical/meteorological fields.

The manuscript is written well and easy to follow. The new parameterization was concluded to be a good alternative to the full chemical mechanism for accurate and fast simulations of IEPOX-SOA in climate model applications. The method used to develop the parameterizations is very repeatable in simplifying other SOA mechanisms and updatable with continuing advance in isoprene SOA mechanisms. Below are several major and minor comments, which need to be addressed and clarified:

Specific Comments Major 1) Organic coating effects were considered as mentioned in Section 2.2 and results were plotted as Figure S1. First of all, the equations and parameters used in the implementation of organic coating effects were not described. Was the resistor representation of uptake coefficient γ by Gaston et al., (2014) used here? What were the values of the parameters used then? Was the dependency on the types of organic matters generated in simulations considered? These need to be clarified. Second, the goal of the paper is to improve computational efficiency while retaining the ability to predict ground level IEPOX-SOA relative to the full chemistry. However, the inclusion of organic coating is intended to be realistic, which seems to be beyond the scope. From my understanding, the coating effect was only implemented in the full chemistry where γ was modeled explicitly. In other words, the coating effect is now getting "fitted" into the new parametrization intrinsically as well as the uncer-

tainties going along with it. Please clarify whether this is the case or not. If it is, the uncertainties must be discussed. In addition, my worry is that this would make the future efforts to differentiate the inhibiting effects induced by different SOA types under varying environmental conditions hard to implement without fitting a new set of parameters for each type of organic coating. One should expect that variables like organic types, thickness of the coating, and relative humidity would change the effect of organic coating on reactive uptake.

2) Line134-136: overestimation compared to the measurements? The organic coating effect is strongly influenced by the composition of the coating and ambient relative humidity, changing the diffusion coefficient of IEPOX in the coating layer. Therefore, not just the Henry's law constant and the mass accommodation coefficient but the parameterization for organic coating (e.g., diffusion coefficient of IEPOX in the coating layer) could also affect the apparent uptake rate (or heterogenous reaction rate in some literature). It seems that the coating parameterization implemented in this work was not strong enough to counteract the increase in surface as shown by Figure S1, which contradicts with Zhang et al., 2018. Authors should address this or explain why the result is contradictory to the literature. Again, authors should provide the detailed description of the parameterization of the coating effect, and discuss its limitations and uncertainties. 3) Line 140: I found the statement here problematic. Literature effective Henry's law constant for IEPOX spans three orders of magnitude (Gaston et al., 2014; Nguyen et al., 2014; Pye et al., 2013; Sareen et al., 2017), the effect of which on uptake coefficient might not be trivial as stated here. Pye et al., 2013 tested the sensitivity of predicted IEPOX SOA to the Henry's law constant. With an increase in the Henry's law constant by a factor of 7, the predicted IEPOX SOA increased by a factor of 5. This scalability indicates that future update on the Henry's law constant may require a full re-evaluation of the parameterization. Besides, author should also note that the Henry' law constant for IEPOX dissolution into the organic layer would be different from that into aqueous aerosol. Zhang et al., estimated the Henry's law constant for IEPOX into the alpha-pinene SOA coating to be 1-5x10^6 M/atm by fitting a resistor model using

experimental data (Zhang et al., 2018). Authors should justify why Henry's law constant was not altered to accommodate the implementation of organic coating.

4) Figure 3: PAR2 and PAR3 overpredicted IEPOX SOA in source regions. Is this also a result of differing influence of the diurnal variation profiles of chemical fields compared to the full chemistry? Are there any other reasons? Although this paper focuses on evaluating the new parameterization against the full chemistry, the natural question to ask is does it improve the model performance against measurements? No indication was given in that sense. If the full chemistry model with the coating effect tends to overestimate IEPOX SOA vs. measurements in the source regions, the new parametrizations would worsen the model performance. If the full chemistry underestimates IEPOX SOA, the overestimation of PAR2 and PAR3 offsets the underestimation to some extent and may improve the model performance. The phrase "more accurate" appears a few times in the manuscript including in the conclusion. It should be more carefully used otherwise misleading.

Minor 1) Figure 1: Which mechanism/parameterization was used to calculate the yields for each step in this figure? Please clarify.

2) Line 400 Figure 4C: Is there a seasonal pattern if the northern and southern hemisphere can be plotted separately?

Technical Corrections: Figure 2(a): Was IEPOX-SOA molar yield or IEPOX yield plotted here? The caption didn't match with axis labels.

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