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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 #1

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This manuscript proposed three parameterization methods to reduce the computational cost of simulating Isoprene-derived SOA in GEOS-Chem using the full chemistry model. The parameterization methods were also compared with the volatility-basis-set and fixed yield methods. The results show that the parameterization methods, especially the third one (PAR3), could generally predict the isoprene-derived SOA spatially while reducing the computational cost of using a full chemistry model. The manuscript also suggests that the VBS approach is not accurate in predicting isoprene-derived SOA because the reactive uptake process is the main process for isoprene-derived

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Discussion paper

SOA formation.

The manuscript has clear logic and it provides a useful and efficient parameterization method to calculate isoprene-derived SOA in global models such as GEOS-Chem. The quality of the manuscript is good and the main argument is valid, thus the manuscript is worth being published in Geoscientific Model Development. My main comments are that it occurred in a few places of the manuscript that the assumptions of the model or the detailed processes are not fully clear. I suggest the authors make appropriate changes to the manuscript in the following sections.

1. Line 80: the author states that Pye et al. 2010 used VBS method to predict isoprene-derived SOA from first-generation products through partitioning. However, in Pye et al. 2013, the reactive uptake aqueous pathway was already incorporated to the VBS method in predicting the isoprene-derived SOA. The new VBS results have been improved and are consistent with field measurements. The author should at least incorporate the latest model improvement approach by Pye et al. in the manuscript when discussing the VBS method. With the latest method incorporating 2-methyltetrol and 2-methylglyceric acid, it is inaccurate to state that "the default VBS mechanism underestimated the observed isoprene SOA formation by a factor of 3 over the southeast US in summer".

2. Line 130-135. The author states that the net effect of the coating effect is to increase the reaction rate of IEPOX with organic coated aerosols. However, both Gaston et al. 2015 and Zhang et al. 2018 show that the uptake coefficient is highly dependent on the diffusion coefficient of IEPOX in the organic layer, the Herny's law of the IEPOX into the organic layer, etc. With different parameters, the resistor model can give drastically different results. The author should explicitly specify what the equations and values were used to calculate the uptake coefficient in Figure S1. Also, why would the uptake coefficient increase at higher organic loading in Figure S1? As shown in Anttila et al., 2006, Gaston et al. 2015, and Zhang et al. 2018, the resistor model will generate monotonically decreasing reactive uptake values as the coating thickness increases.

3. Line 140. I understand that the author is intended to cross compare parameterizations against the full chemistry model for isoprene formation, however it is inaccurate and a bit misleading to state that "Updating the parameterizations developed here with more accurate values of H or α determined in future literature studies would be trivial." The H or α values affect the absolute values of the isoprene-derived SOA significantly, and currently the estimation of the Herny's law constant can vary by two orders of magnitudes. Knowing an accurate value of the Herny's law constant will help bridge the gap between the model and the field measurement, thus these values are not trivial. I suggest the author revise this sentence.

4. Please remove the Nault et al. in prep. citation as unpublished work should not appear in the formal citation.

5. Line 227-230: The author states a numerical fitting method was used to calculate f(ISOPO2-ISOPOOH). Which numerical fitting method was selected and why? How good is the fitting result? Please include some details of this fitting in the manuscript.

7. What is the physical meaning or the rationale of constructing Equation 5c in the current format? Please note that this is a rather complicated fitting equation and I wonder how did the author obtain such format? Why cannot the equation be expressed in other ways? Could the author include the rationale behind constructing this equation in the text, please?

8. Similar question as the previous one: what are the physical meanings of F? Why is it constructed in such a way? Maybe the author can explain more in the manuscript.

9. In Figure 2, the e-fold formation timescale from the analytical model was plotted against the full box model. However, unlike the analytical model that has a definition and equation for the formation timescale, there is no definition of the formation timescale in the full box model. How did the author calculate the formation timescale in the full box model? Please specify.

10. It seems that PAR3 can capture most of the isoprene-derived SOA values when compared with the full chemistry model. However, at isoprene rich areas such as Amazon forest, central Africa and Southeast Asia, the isoprene-derived SOA was overpredicted by PAR3. Are there any reactions causing such overprediction in isoprene-rich areas? It seems to be some sort of systematical error. The author should discuss the drawbacks of PAR3 (such as overprediction in isoprene-rich areas) so as to objectively evaluate the model and educate potential users.

11. Why would the IEPOX uptake rate peak at around 6 pm? It seems that the only variable in the IEPOX uptake rate (Equation 7) is [OH]*k17, which is affected by temperature and the OH contraction. However, the product of these two values should not cause the IEPOX uptake rate to peak at 6 pm. Could the author explain why he IEPOX uptake rate peak at around 6 pm?

Minor Comments:

Please refrain using the word "it" in Line 269 as it makes the sentence confusing. I suggest the author change this part of the sentence to “because of Equation 9 assumes rapid formation of the SOA.”

The author listed the scatter and correlation plots of PAR1 and PAR3 versus the full mechanism box model in Figure S3 and Figure 2. For consistency I suggest include a similar plot for PAR2 in the SI as well.

The phrase "IEPOX condensation rates" in line 391-line 395 should be changed to "IEPOX reactive uptake rates".

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