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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Aqueous-phase mechanism for secondary organic aerosol formation from isoprene: application to the Southeast United States and co-benefit of SO_2 emission controls" *by* E. A. Marais et al.

Anonymous Referee #2

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In this study the isoprene aqueous SOA chemistry is considered and incorporated into the chemical transport model GEOS-Chem. The detailed formation pathways are successfully reproduced and their relative contributions to isoprene SOA are evaluated. The results of the sensitivity of isoprene SOA to the changes of SO2 emissions will help make countermeasures against air pollution. I found that the study was conducted very well and the manuscript is written clearly. I have below specific comments that the authors should consider and implement in the revised manuscript.

Specific comments:

1. Following IUPAC recommendations, I would suggest terming Gamma as "reactive uptake coefficients", rather than using "reactive uptake probabilities".

2. SOA particles are assumed as aqueous droplets in this study. Under low humidity of below ∼50% RH, isoprene SOA were shown to be semi-solid or solid (Saukko et al., ACP, 12, 7517, 2012; Song et al., ACP, 2015), and in that case there will be strong kinetic limitations of gas-particle partitioning (e.g., Perraud et al., PNAS, 109, 2836, 2012; Shiraiwa & Seinfeld, GRL, 39, L24801, 2012). This study compared the simulated results with aircraft observations within the boundary layer. While as the altitude increases to the top of the boundary layer, particles might become semi-solid or solid upon decrease of temperature (e.g., Koop et al., PCCP, 13, 19238, 2011). Although investigation of particle phase is not a priority of this research, it would be very helpful to add some discussion, justification and potential bias of assumed liquid phase state for simulation uncertainties.

3. Regarding eq (1): Gas-phase diffusion seems to be neglected, as gas diffusivity is not explicitly treated in eq (1). If this is true, this should be explicitly mentioned. Several studies have clearly shown that gas diffusion can play an important role in SOA growth (e.g., Tang et al., ACP, 14, 9233, 2014; Riipinen et al., ACP, 11, 3865, 2011). Please clarify and discuss.

4. It would also be helpful to show the comparison of observed and simulated meteorological parameters (e.g., T and RH). They are related to particle phase determination; RH impacts the sulfate aerosol size distribution as shown in Section 3 and IEPOX sulfate formation (Liao et al., 2015); T impacts the isoprene emission as shown on Line 8, Page 32020, and meteorological parameters impact the prediction of chemical fields.

5. In the Sect. 2, I suggest including discussion on uncertainties of kaq and the potential impacts on the following simulated results.

6. How much uncertainties are expected in column HCHO measured by OMI? (first paragraph of Section 4).

7. Line 19, Page 32020 says that the H+ -catalyzed channel is a larger contributor compared to the sulfate channels. Is this result applicable to all of the simulated areas? How about the results for higher altitudes? As shown in Fig. 2, this study seems not to consider the reactions involving SO42- leading to organosulfate formation. Will this impact the result that a direct role of sulfate in IEPOX SOA is not important? It is not clear for me whether the term of knuc[nuc][H+] in eq(2) already include organosulfate formation. Please clarify.

8. Aerosol pH seems to be very critical in simulating SOA mass due to an importance of acid-catalyzed reactions. pH is modeled based on ISOROPPIA. Do you have field measurements of aerosol pH and could it be compared with modeled pH? How much uncertainty would you expect in the modeled pH?

9. Page 32021, Line 5: will nitrate take similar effects as sulfate to increase aqueous volume and acidity?

Technical corrections: - P32019, Line 4, Abad et al., 2015 is missing in the section of References.

Interactive comment on Atmos. Chem. Phys. Discuss., 15, 32005, 2015.