

Atmos. Chem. Phys. Discuss., referee comment RC2
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Comments on acp-2020-1324

Anonymous Referee #2

Referee comment on "Secondary aerosol formation from dimethyl sulfide – improved mechanistic understanding based on smog chamber experiments and modelling" by Robin Wollesen de Jonge et al., Atmos. Chem. Phys. Discuss.,
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Review summary:

This study presented the chamber experiment and model simulation for the OH-derived oxidation of DMS to form secondary aerosol. In order to simulate the aerosol formation, a multiphase DMS oxidation mechanism was implemented and compared with chamber data. The results from this study improve the understanding of the DMS oxidation pathway. However, some modifications are necessary to clarify the results and conclusions in this study. Overall, a major revision is needed before publication in ACP.

Comments:

- Page 3 line 57. What is meaning of "model predictions under said conditions"? Do authors imply "acid conditions" or "side conditions"? Word "said conditions" appeared in numerous places. Please change this word to the clear word that can be understandable by readers. Please also check spellings and typos.
- Page 3 Line 80-85. The authors state there is potential particles and organic contaminates from room air due to the inflow of air to the chamber during sampling. Why did not the authors use the similar setup with the humid experiments that directly use clean air added to the chamber to makeup the shrunken volume for the dry exp? The room air which contained a significant concentration of ammonia may influence an inorganic ion balance, aerosol hygroscopicity and sulfuric acid formation. In addition, some hydrocarbons can modify the gas chemistry.
- Figure 1. 1A: please add explanation for "woLWC". 1B: Is the OH concentration set to a constant number during the entire simulation period? If yes, it maybe not necessary to plot Figure 1B. Instead, explain this in the main text. 1C: cannot understand this the drawing. Which one is the Teflon film? What is the meaning of blue colored things? Is it water or moisture? Why RH is only up to 70%? Was there a horizontal gradient in RH and Temperature inside the chamber?

- Table 2. Please add necessary footnotes for the abbreviations used in the Table. It is difficult to understand the meaning of the variables because acronyms appeared later in the manuscript.
- Page 5, line 109. Butanol is hydrophilic. Is there any gaseous butanol loss to the water layer on the wall during the butanol experiments?
- Page 6, line 120. Is the unit for the water concentration on the wall correct? Should it be g per surface area of the wall?
- Page 6, line 134. Please check if the unit for the dissolved ammonium sulfate on wall is correct. The unit of salt on the wall water could be a mass per liquid volume or the mass per air volume?
- Page 6, line 135. Although outdoor ammonia concentration is usually as low as 1 ppb, the indoor ammonia concentration can usually be much higher (Ampollini, Laura, et al 2019). Is the ammonia of 2 ppb from indoor environment used here reasonable? Is there any measurements of gaseous ammonia concentrations to support this value?
- Page 7, line 167. Add “,” after “NO₂”.
- Page 7, line 173. Is the unit of V wrong?
- Page 7, line 175-180. Why is the concentration of ozone in some experiments (i.e., DMS1) low as 1 ppb as seen in Table 1? If the ozone concentration is lower than 1 ppb, how can the authors say that the secondary aerosol formation is most sensitive to ozone for all experiments?
- Page 8, line 194. The meaning of $R(g)$ and $R(aq)$ is unclear. Are they represent reactions? What is their unit ?
- Page 8 line 199. “denote” -> “denotes”. Remove “;” before “K⁻¹”.
- Table S2. The scientific notation in computer code (i.e., Fortran) usually uses “D” to signify double precision numbers but it is uncommon to be used in scientific documentation such as paper. It would be better to change to “E” instead of “D”.
- Page 9, line 213. Why does the chemical mechanisms also include isoprene chemistry mechanisms? Is there any precursors contain isoprene species in the kinetic model?
- Page 10, line 260. “represent” -> “represents”. Line 262, “represent” -> “represents”.
- Page 11, line 283. What is the protocol to setup the cloud conditions? Are they randomly setup?
- Section 3. The place of this section is odd. The authors mainly discuss the simulation of ambient scenarios. However, the figure appeared in Page 22. It would be better to move the explanation to the section for atmospheric implication.
- Page 11, line 300. It is not clear to use the word “Initially”. When is the initial time? The early stage of experiment or the model development stage?
- Page 12, line 303. What is the meaning of “slow down” and “promoting” here? Does it imply the modification of mechanisms or changing experiment setup?
- Page 13, line 342. “previously to slow” -> “previously too slow”.
- Page 12, section 4.1. When authors discussed about measurements (observations), it is unclear which measurements were used and which model run it refers to. For example, Page 13, line 338: where is data for “observed and modelled SA and MSA PM”? Do the authors perform the sensitivity test for the thermal decay rates of CH₃SO₃?
- Section 4.1. What is the simulated mass fraction of MSA from different pathways? Which pathway is more dominant to form MSA and SA?
- Page 14, line 364. “HPMTF may oxidize in cloud droplets” -> “HPMTF may be oxidized in cloud droplets”.
- Page 14, line 366. Does the model include partitioning of OH radicals between the gas phase and the aqueous phase? The partitioning of OH radicals is not discussed in the previous sections.
- Page 14, line 378-379. How can NO_x concentrations be estimated by using ozone formation? Where was this resulted estimation shown in the manuscript? As shown in Table 1, NO_x is lower than 2 ppb. How much uncertainty is included in NO_x?
- Section 4.3. This section is improper to be discussed in the results section. The chamber contaminations should be discussed in the experimental section.
- Page 16, line 407. Does it mean the green color organic showed in Figure 3b is fully by

organic contamination?

- Page 21, line 507. "when the UV light intensity" is high?
- Page 21, line 508. What is the percent of DMS oxidation through OH and O₃ pathways for this simulation?