

Review of the manuscript “Isoprene derived secondary organic aerosol in a global aerosol chemistry climate model”

In the manuscript the authors describes a semi-explicit isoprene oxidation scheme and the explicit treatment of SOA formation from 6 isoprene oxidation products in the global chemistry climate model ECHAM-HAMMOZ.

I find the method used to simulate isoprene SOA (iSOA) very novel and encouraging and I definitely think that this kind of explicit treatment of SOA formation from known oxidation products are necessary in order to improve the knowledge about SOA formation and anthropogenic impact (e.g. NO_x) on SOA formation in the atmosphere. The manuscript is generally well written and clearly structured and I recommend that the manuscript should be accepted for publication after a minor revision where the authors carefully addressed my comments.

General comments:

I miss references in the main text to the supplement and the reactions R1-R22. This is needed for clarity.

On Page 5, L9 and on several other places in the manuscript you refer to the isoprene oxidation products in Table 1 as low volatility compounds (LVOC) since their saturation vapor pressures (p_0^*) at 298.15 K is below 0.01 Pa. I presume that you mean their pure-liquid saturation vapor pressures. Further, this is not the common p_0^* limit for LVOC which e.g. according to Donaue et al., Faraday Discuss. 2013, 165, 91–104 is compounds with C^* in the range of $10^{-0.5}$ to $10^{-3.5}$ $\mu\text{g m}^{-3}$ which approximately correspond to a p_0^* range of 4×10^{-6} to 4×10^{-9} Pa. Instead 0.01 Pa is somewhere on the limit between SVOC and IVOC. Thus, only LISOPOOHOOH in Table 1 can be referred to as LVOC at 298.15 K.

On Page 6-7 and in Figure 1 you refer to the yields of the iSOA precursors as if they were fixed yields. E.g. On Page 6, L9-10 you write that: “LISOPOOHOOH has the highest yield of the LVOC considered here, 9% of isoprene end up as LISOPOOHOOH”.

First of all, what do you mean with this yield? Is it the molar or mass yield that is 9 %?

Secondly, how can these yields have a fixed value? If the gas-phase mechanism explicitly simulates the formation of the different iSOA precursors their yields should vary depending on the concentrations of NO, O₃, OH, NO₃ etc. Maybe it is the global average yields derived with the model? If this is the case please state that.

The section 2.1.2 is somewhat confusing when you discuss the SALSA-VBS system that apparently is not used in the present study but then in Figure 5 you still present results where you use the VBS method.

On Page 10, L12-13 you write: “Loss processes for SOA in HAM-SALSA include sedimentation, deposition and wash out in the aerosol phase.” But should it not

be “Loss processes for SOA in HAM-SALSA include, apart from evaporation, sedimentation, deposition and wash out in the aerosol phase.”

I don't understand why/how the pH of the aerosol particles can differ by several order of magnitudes if the only inorganic species is ammonium bisulfate. I guess the pH is only calculated for the inorganic aqueous phase. Is the 4 order of magnitude difference in pH only related to the average RH at different locations? Please clarify this in the text on page 10 and also refer to the figure in the supplement.

I miss labeling (e.g. a, b, c) of the panels in all figure and the figure text to figure 2 need to describe what the two panels actually display.

In the results section on Page 14 and maybe on some other places you use the terms “quite big” and “quite high”. Try to avoid using these vague statements and instead write concrete numbers (e.g. contributes to 30 % of the SOA mass instead of contributes to quite big amounts of the SOA mass).

On Page 14, L10 you state that LSOPOOHOOH-SOA is extremely low volatile but it is not. At least not at 298.15 K (see the comment concerning LVOC above).

Concerning the uncertainty of the estimated saturation vapor pressures (Section 3.3). I think it is good that you discuss the uncertainties related to the functional group contribution methods used to estimate the pure liquid saturation vapor pressures.

In publication by Kurtén et al., J. Phys. Chem. A 2016, 120, 2569–2582 it is stated that: “Unfortunately, the basis data sets of existing group contribution based empirical parametrizations for determining saturation vapor pressures of organic molecules (e.g., SIMPOL, or the widely used and generally successful Nannoolal et al. approach) do not contain complex polyhydroperoxides (or multiply substituted peroxy acids), and the parametrizations may therefore not be reliable for HOMs.” LSOPOOHOOH can be considered as a HOM with two hydroperoxide functional groups.

Thus, according to the results from Kurtén et al., 2016 it may have been more appropriate to use the EVAPORATION method which also is provided via UManSysProp (Topping et al., 2016). With EVAPORATION/Nannoolal I get a p_0^* (298.15 K) of 10^{-5} Pa, e.g. 38 times higher than the value you used at 298.15 K. In fact according to EVAPORATION LSOPOOHOOH is not a LVOC but a SVOC ($C^* \approx 1 \mu\text{g m}^{-3}$) at 298.15 K.

Technical corrections:

Write out that ISOP(OOH)₂ refers to dihydroxy dihydroperoxide in the abstract

Page 4, L16: Change from “... and its evaluation it is referred ...” to e.g. “... and its evaluation the reader is referred ...”

Page 4, L33: Change from “The semi-explicit isoprene oxidation with 147 reactions constitutes a major of these reactions in JAM3.”

e.g. to:

“Thus, the 147 reactions in the semi-explicit isoprene oxidation scheme

constitute a substantial fraction of these reactions in JAM3.”

Page 5, L20: Change from “ For simplicity there are ...” to “ For simplicity they are ...”

On Page 15, L24: I think it should be “lifetime” and not “life time”. Try to reformulate the wording “huge wet deposition loss”.

On Page 17, L3: Remove “is” after iSOA and remove one “motivated” on L5.

On Page 17, L14: What do you mean with VBS classes 0, 1 and 10? If it is C* in $\mu\text{g m}^{-3}$ non of these species are LVOC at 298.15 K according to e.g. Donahue et al., 2013.