

Review of Advanced modelling of gas chemistry and aerosol dynamics with SSH-aerosol v 2.0

This manuscript describes the development and updates of the model SSH-aerosol, which can be utilized to simulate the formation of secondary aerosols, and evolution of both the primary and secondary aerosols. This involves simulating the gas-and particle phase heterogenous chemistry and aerosol dynamics. Various test cases ranging from aerosol dynamic processes and gas-particle phase chemistry were simulated and presented in the manuscript to show model capabilities. The manuscript is well written, with the supplement/guide serving as a detailed blueprint for potential users to test and implement the model. The SSH-aerosol model serves as an interesting tool to simulate aerosol dynamics under different environmental scenarios and would surely benefit the modelling and experimental community. I recommend the publication of this manuscript, after the authors have addressed the following comments/suggestions.

General comments:

I would recommend adding a figure outlining the different inputs and modules and their workflow. This could also serve the purpose of being a visual reference for any user trying the model.

Add figure letters (e.g. Figure4, a, b or c) to avoid confusion.

While discussing results (e.g. L 303-306, Figure 8 etc.), the authors states what the results shows, but don't discuss why that's happening. The readers will appreciate if they get to know for e.g., why SOA yields are increasing/decreasing in the presence of NO_x.

Nucleation: This section has not been discussed in depth but rather just glossed over.

Model computational time: How much impact does different configurations (gas+SOA schemes) have on the computational time. Since this model can be couple to a 3-d model, how realistic is it to use particle phase and viscosity calculation with the coupled 3-d model since its includes discretised particle layer calculations.

Minor comments:

L 35: "atmospheric chambers"- I believe the correct terminology would be atmospheric smog chambers.

L 43: "Several aerosol box models exist". I think this line is unnecessary. Either remove it or club it with the next line.

L56-57: One must be careful in formulating such descriptions. MCM is an explicit gas phase oxidation mechanism, not a SOA formation scheme. It is coupled to a SOA formation scheme and therefore should be categorized as a chemical scheme and not a SOA scheme.

L65-66: Some examples of different reduction strategies could be included.

L89: "repertories" to repositories

L 99: what kind of solver is used to deal with the ODE systems? How will it affect the computational time?

L 110: How are the saturation vapor pressures generated? Nannolal/Evaporation/SIMPOL or another mechanism?

L211 – 213: does this mean that one can use 2 or more chemistry schemes at the same time? For example, one can use CB05 for estimating a reaction products conc., say X and another explicit scheme to use the [X] in their respective chemical schemes? If so, does it only work for first generation oxidation products or more complex oxidation products as well? Are these conc. profiles interpolated to the timestep of the SOA chemical scheme?

L214-216: This part is unclear. Does it mean one can have a specific combination for each precursor + SOA scheme? E.g. alpha-pinene using MCM + beta caryophyllene using RACM2? if so how would one account for example RO₂ from ap +RO₂ (bcarp) reaction products from different chemical schemes, in case the resulting RO₂ is not present in either scheme?

L223-224: There are different vapor pressure estimation methods on the UManSysProp. Which method was used?

L234: is this analogous to “lumped RO₂” species? Is this RO₂ pool rereferring to RO₂ from one precursor alone or can it refer to lumped RO₂ from all of MCM or a subset of precursors?

L 236: what does “ARR” stand for?

L 243: “TBRO₂” is not referenced in the equation above or explained anywhere else.

Figure 2: This makes sense since MCM doesn't yet include a fully developed peroxy radical autooxidation scheme for beta caryophyllene. It would be interesting to perform such tests with alpha-pinene.

Section 3.2 My one suggestion here to improve readability would be to have a table detailing the explicit and reduced mechanism, with a shorthand representing each. For e.g near explicit mech for monoterpenes could be denoted by $\text{Exp}_{\text{mcm+pram}}$ or something like that. It could make it easier for readability without one having to go back and forth to see what the respective mechanisms were.

L281: This should be right panel.

L 294: upper right panel?

L296-294: Referring to Fig 4: these differences are barely visible in the plot. Perhaps the authors will think about providing percentage increase or decrease w.r.t the reference to indicate the difference.

L 299-303: why is that?

Figure 3: what is the reference scheme? it should be mentioned in the caption.
Is the related to NO₂ conc.?

L 364-365: Since H₂O is based on smog chamber experiments, was wall losses considered when simulating SOA for species which was compared to H₂O? I suspect the SOA yields for species where H₂O was used for comparison would differ if wall losses of organics would be considered.

L 378-380: why does the H₂O mechanism overestimate the SOA mass?

L398: "interface the index of the layer at the interface". what does this represent or mean?
Also $K_{bin, interface}$, p_i and the corresponding $M_o^{bin, interface layer}$ is not defined.

L 413: "f". This needs more explanation here. For e.g., what does a value $f=0.2$ indicate?
how is f determined?

L 430: "Compounds not affected to a specific molecular structure". what does this mean?

Figure 9: I assume that since this is an organic phase there would be no charged compounds would be present in the particle phase. But when the RH increases compounds in the particle phase are bound to break and form cations and anions. How will this affect the viscosity especially in the presence of acids?

Figure 9: Add panel letters to make it easy to follow. how does the c panel which is bottom left change if you have varying RH for alcohol+acid + varying RH?

L480: parameter k . Is this a function of water conc. and pH?

L 505: K_{oligo}^{max} , hoe is this determined?

L505: $a_{monomer}$, I would suggest representing this as η or $\sum(a_{A, monomer})$, both in the equation 24 and here.

Eq. 28: is this nomenclature based on H₂O or MCM or other chemical schemes?

L 587: SOAP. Does the model account for the formation of salts in the particle-phase?

Figure 13: please improve the legend. It's hard to read it in its current form.

Nucleation: Have the authors considered to couple ACDC for more complex termolecular acids and bases?