

Comments on 'Precursors and formation of secondary organic aerosols from wildfires in the Euro-Mediterranean region', Majdi, et al., (2018)

Summary/recommendation:

This paper was an interesting modelling study on capturing both precursor vapors and SOA from wildfires. The authors updated a pre-existing SOA formation scheme in order to run several sensitivity simulations that detail the sensitivity of their model to precursor sources and concentrations as well as aging mechanisms on smoke OA. However, many portions of the paper were made difficult to follow due to missing (mainly minor) details. I recommend that this study be published but with minor revisions. I request that the authors consider the following points as they revise this manuscript:

General comments:

Pg 2, line 15: the definition of OA_{tot} is confusing, given that 'aerosol' usually refers to the particle phase concentrations only. If this is the sum of the particle and gas phase, do the authors mean that the gas phase species are only those who are low enough in volatility to participate in partitioning? Or all the gas phase species, including VOCs and IVOCs? Please clarify this.

pg 3, line 27 Please qualify what is meant by "misclassified" here

Section 2.1: the authors should consider adding more explanation as to what the original H^2O scheme was (and what its purpose is), and what additions/changes the authors are specifically making to H^2O . It's a little unclear if the details being described on pg 4 through line 6 on pg 5 are of the original H^2O model? The first 2 sentences of this section (starting on pg 4, line 18) would benefit from having the appropriate H^2O citations added.

Pg 5, lines 23-24. The authors state that the one-product model correctly reproduces the experimental data; there is a small amount of spread between the model and experimental data. Can the authors briefly quantify that error? Same for the analysis given for fig 2 (lines 16-17 of pg 6)

Pg 6, lines 1-2: can the authors briefly discuss what error might be anticipated to be introduced by using ACIDMAL as a high-NO_x surrogate given the lack of data for this mechanism? Same for the cresol chemical mechanism, lines 13-15 of page 6?

Pg 11 lines 13-16: can the authors briefly explain their rationale for choosing USC>6 compounds to undergo the same OH oxidation mechanisms as phenol or naphthalene?

Section 2.2: The acronyms should be well defined: what are BBPOAIP, BBPOAmP and BBPOAhP? I strongly suggest making sure all acronyms in this work are well-defined the first time they are used. Also, consider re-defining major (uncommon) acronyms at the beginning of new sections for any readers who may be skipping sections. These aren't defined to my knowledge until section 5.2. 'P' is never defined that I saw--pressure? There is a missing citation or statement on line 6 (currently shows up as a questions mark). Also, it should be made clear in the text to which volatility bin BBPOA0, BBPOA1, etc belongs to.

Pg 12 lines 15-18: It's not clear from the text or appendix D what the fragmentation and functionalization scheme is. It would be helpful to have the fragmentation and functionalization rates or fractions explicitly expressed. Or is the given reaction rate with OH of $4e10^{-11}$ supposed to account a combined probability of fragmentation and functionalization? The units on this reaction rate seem incorrect, they are listed as molecules⁻¹ cm³ s⁻¹, where often reaction rates are expressed as molecules cm⁻³ s⁻¹. Please comment on the units. Also, a brief look through Donahue et al. (2013) does not show where the specific value of $4e10^{-11}$ came from--perhaps another citation is also necessary here? Can the authors comment on this as well. Finally, it should be stated what happens to fragmentation products--are they placed into higher volatility bins or are they "lost" and no longer tracked in the model? The authors should consider adding more details on all of the issues raised here in the text.

Section 3 lines 30-31: I suggest writing out what ISORROPIA and SOAP stand for.

Page 13, line 6 and Table E1: I suggest adding 1 sentence explanation of what the reactivity factor is. In Table E1 this is listed as Reactivity fo, consider changing to something like Reactivity factor (fo).

Section 4 page 13 line 12: It would be helpful to let the reader know that the emissions estimate of toluene and xylene will be discussed in the next section. Same for when NMOG is discussed in this section.

Pg 14: What is Un in the Multstep-UnNMOG-withVOCs?

pg 14 lines 8-12: can the authors comment on by ~ how much (I assume a range) lower Donahue et al (2005)'s calculation of the enthalpy of vaporization was than the SIMPOL.1 calculations? I recommend including the range of $\Delta(H_{\text{vap}})$ s from SIMPOL.1 either in the text or in table 1.

Section 5.1: can the authors comment on how representative they believe woodfire stove smoke emissions are of wildfires?

Section 5.3, lines 32-33 (first sentence of the section): would the left panel of Fig 7 technically be showing POA_{tot}? Since these are the OA_{tot} precursors?

Section 6.1. Pg 21 lines 3-5: Can the authors briefly justify the choice of using Multistep-withVOCs for this figure?

Page 21 lines 9-10: from which model run(s) does this data come from?

Pg 23, lines 10-13: how were the differences within “the fire plume” determined? What’s meant by the fire plume here? How well can the model resolve an individual plume? Please explain this further.

Two more general comments: Are the model results being compared to actual observations? If instead they are being compared to work done in the first author’s other ACPD paper, this should be made more clear and the comparisons could be spelled out more explicitly.

This work would benefit from a discussion of the pros/cons of each model simulation type, and whether or not any model simulations appear to better represent the real atmosphere. Much work was clearly done here, but the paper currently does not seem to have the “why this matters/how it improves upon previous work” factor yet that will allow it to become an easily useful guide and reference for other members of the community.

Figures/tables:

Figures 1-4 would benefit from being made in a higher-quality format rather than the excel default graphs.

Figure 11: It should state in the figure caption and/or on the figure which model simulation is being used to make this figure.

Figure 12: from what data/model simulation(s) was this pie chart constructed? This should be stated in the figure caption and in the text.

Figure 13: the colorbars should have units with them (% and mass concentrations?). This colorbar is a little hard to interpret, are we to take that the tan regions are anywhere between 0-5 or 8% different? Can the authors make the colorbars for each % difference plot the same, they’re currently changing by between 5 and 11 units. I suggest considering a non-linear colorbar to see more structure within the -5 to 5% difference range.

Technical comments:

Page 2 line 7: suggest rewriting to PM is composed of organic and inorganic compounds, dust, and black carbon (Jimenez et al., 2009).

Page 2 line 13: do the authors mean that both POA and SOA are composed of compounds of different volatilities? Suggest clarifying this sentence.

Page 20 line 11: un should be Un in the simulation name.

Page 20 line 21: this would make more sense if it was written something like “Across our cases, 28 to 42%...”