

Interactive comment on “Positive Matrix Factorization of Organic Aerosol: Insights from a Chemical Transport Model” by Anthoula D. Drosatou et al.

Anonymous Referee #1

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Drosatou et al. present a study in which chemical transport model predictions of organic aerosol over Europe are used in a PMF (and ME-2) analysis to determine what types of organic aerosol factors exist in model predictions. The use of a chemical transport model means that the PMF factors can be directly examined in terms of their sources and identity. The major findings include the composition of POA factors in terms of potential SOA contributions and expected error as well as identification of 2 types of SOA or OOA-like factors in a variety of locations. They show that the two types of SOA do not separate anthropogenic and biogenic SOA and the separation is mainly based on age. This is a useful analysis and comments below focus on two main areas.

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Main comments:

1. Methodology

a. How would results be different if source information (for example the chemical identity of POA and bbPOA) was not used in the PMF analysis of model output? If the volatility of the model-predicted OA was the only chemical information in the PMF analysis, would you get similar results? This may provide insight into how results from this work translate to AMS analysis in which sources may not be very chemically distinct due to fragmentation.

b. PMF appears to have been performed on a site by site basis. Can this be clarified? The analysis generally always leads to two SOA (or OOA) factors, but the composition of the SOA factors varies by site. How many SOA factors would be obtained if all locations from the model were used in one PMF analysis? An analysis along these lines could help inform questions in the second main comment regarding how different the two OOA factors are in different locations or studies.

c. What information is introduced by the PMF analysis of model output that is not otherwise available? Could the same “factors” be obtained by determining how much POA, SOA-sv, bSOA, aSOA, etc correlate or covary and making two groups?

d. How was the boundary condition OA at the edge of the domain specified and evaluated? If the boundary OA was not assigned a C^* of 0.01 ug/m^3 , would it have ended up in a different factor?

2. Meaning of two SOA or OOA factors

a. Is the proliferation of terms in literature (LO/MO-OOA, OOA-1/2, LV/SV-OOA) indicating true site to site variability in the OOA components or is it just a nomenclature choice?

b. The authors argue that the designation of the two AMS factors based on volatility is somewhat misleading due to overlap in their volatility. I was not convinced that this

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designation was misleading (based on Figure 10) but do agree that it is a simplification. What is the best description of the two factors given that they likely overlap on many metrics (volatility, O:C, age, etc) and age, O:C, and volatility covary?

c. How should CTMs evaluate their predictions compared to AMS data beyond SOA vs OOA? Can the analysis here be used to provide a range of agreement where models can be assumed “in agreement?”

Minor comments:

1. Lines 22-28 of the abstract are useful, but could be condensed. Mentioning the fraction of the POA factor that is secondary (e.g. lines 477-478) would be even more useful.

2. Lines 81-104 are missing the MO- and LO-OOA designations (Xu et al. 2015 PNAS <https://doi.org/10.1073/pnas.1417609112>) in the discussion and how those fit with the other AMS PMF factors from literature.

3. Line 134: what version of SAPRC was used?

4. Paragraph starting at line 250: Clarify that there was no observed POA or bbPOA factor in observations or model for Melpitz.

5. Figure 3: Could boundary OA and POA+S/IVOC-SOA be added to panel (b)? Could SOA (excluding boundary and S/IVOC-SOA) be added to panel (a)? How much value does the PMF factor bring compared to classifying boundary and S/IVOC-SOA as one type and all other SOA as one type?

6. Figure 7: How were the locations chosen?

7. Figure 7: What would you expect the NME to be for typical urban, suburban, or rural conditions (add to plot)?

8. Did the model include any aqueous SOA? Where would that appear in the PMF analysis?

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Editorial comments:

1. Line 126: “a regional three-dimensional CTM” is duplicated within the sentence.
2. Figure 1: Needs (a) and (b) labels or titles.
3. Figure 2: Could be on same panel in different colors
4. Figure 4: Could go in SI
5. Figure 11: switch columns 3 and 4 so that both Melpitz and Finokalia data reads as increasing age going left to right.

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