



EGUsphere, referee comment RC2
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Comment on egusphere-2022-667

Anonymous Referee #1

Referee comment on "Source apportionment of VOCs, IVOCs and SVOCs by positive matrix factorization in suburban Livermore, California" by Rebecca A. Wernis et al., EGU sphere, <https://doi.org/10.5194/egusphere-2022-667-RC2>, 2022

Wernis et al. present a comprehensive source apportionment of atmospheric VOCs, IVOCs and SVOCs for an Eastern US suburban area, which can be considered representative enough to provide insights into the various sources of complex atmospheric organic carbon in such settings. They deploy a novel instrument in order to access a broad volatility range in their source apportionment which is considered a real step forward. The combined gas chromatographic and mass spectrometric approach provides unique capabilities of compound identification, and the authors take great care in analyzing their PMF-obtained variability in the data. This manuscript shows that in suburban areas, organic compounds associated with personal care products are present in many ways. In addition, it also shows that classical source profiles such as gasoline emissions can have distinct features in such purely suburban areas. In that sense this manuscript clearly improves our understanding of the diverse sources of organic compounds in the atmosphere.

The manuscript is well-written and the scientific approach seems solid to me. I especially like how the authors took great care in differentiating between source apportionment and possible lifetime differences in their discussion of the different factors. However, I find it currently very cumbersome to go through the manuscript and relate the identification of the different PMF factors with the shown Figures and Tables. In addition, I would also appreciate a more thorough discussion on the uncertainty of the individual factor profiles, potentially explaining some of the "cross-talk" between different factors. Therefore, I hope that the following comments can help to improve the clarity of the manuscript and help to better streamline the main messages.

Major comments:

- I find it very cumbersome to swap between the different plots (Fig.1-3, Fig. 5) during

the discussion of each factor and it currently is a lot of work to thoroughly go through the manuscript. The following points should be improved:

- In my opinion, each factor should be associated with a single figure showing the time-series, the diurnal variation and the factor profile. In return, Fig.5, Fig. 3 and Fig.1 (anyways roughly shown in Fig. 4 c) could be removed or put into the SI.
- For the factor profile (Fig 2.) it would be nice to add the names of the most prominent peaks, or at the very least mention the number of the compound as given in Table 1 in the text. This would help the reader to much faster connect the compound to the profile.
- In that sense, I would appreciate if during the discussion of the factors also the relative contributions of different compounds to that factor compared to other compounds (maybe call it relative contribution) could be mentioned and not only the relative contribution of a compound to that factor compared to their contribution to other factors (maybe call it relative split) would be mentioned. This should provide insights into which compounds are the most dominant one. Subsequently the authors should be careful with their wording when using phrases such as “minor contribution” to make clear which type of contribution they mean.
- For Figure 2 (i.e. the subplots in the future factor specific Figures), I would suggest that the x-axis gets some coloring where IVOC/VOC compounds are and where SVOC compounds are. This would help to better assign the contributions of the different modes of the cTAG to the factors and reduce the need of the overly lengthy Table 1, which I would suggest moving to the SI to keep the main text better accessible.
- Please check careful that all axes have units. Fig. 5 is really difficult to put into context without a map of Livermore and its surroundings and the location of the measurement station indicated on it. I really suggest the authors to add such a map.
- When discussing the factor profiles, the authors find several compounds showing up in factors where they wouldn't be primarily attributed to. I appreciate the authors discussion on these points, but I miss an overall error estimate of the individual source profiles, which might explain some of the interesting assignments (e.g., siloxanes and palmitoleic acid in Factor 3 and diesel markers in the primary biogenic factor). If the authors can use bootstrapping on their dataset (removing or doubling randomly datapoints and rerunning PMF), this should allow them to assign errorbars to the individual contributions given in Figure 2, which could indicate that some assignments are more uncertain than others (as the authors already explain for example in their discussion about palmitoleic acid in Factor 3).

Minor comments:

- Page 3, lines 94-95: It would help the reader to directly give the corresponding saturation mass concentrations to the given alkene equivalents.
- Page 4, line 111-112: Quickly recall for the reader what you mean by total ion chromatograms (total signal in mass spectrometer) and especially single ion chromatograms (specific mass identified by the mass spectrometer).
- Page 8, line 235: Q_{exp} is not defined in the main text yet, so it would be good to refer to the SI here once again.
- Page 14, line 276: Do I understand correctly, that the percentages in brackets give the contribution of the individual compound to that factor compared to its contribution to other factors? Please specify what these numbers mean (see major comment)
- Page 15, line 283 and line 304: Either I have difficulties in understanding the rose plot, or that southwest enhancement does not look very mild to my eyes. Please consider

revising these statements. Also for other factors I am not convinced if a few occurrences from other directions outweigh a dominant occurrence from one direction to conclude that the factor has no or mild directional dependence.

- Page 22, line 477: The very early morning peak of Factor 5 puzzles me, as I do not believe that typical wake-up time (commuter preparing for work which should induce the personal care product emissions) in Livermore is 4 am. However, as noted later, it is consistently a bit earlier than the gasoline factor, which is very plausible. Maybe there is some daylight-saving-time related shift, which could explain both peaks to be so early in the day.
- Page 22, line 496: "Methyl salicylate and α -isomethyl ionone are low-volatility IVOCs, measured on the SVOC channel" seems to be a direct contradiction. A compound which is an IVOC cannot be of low-volatility, as it would be an LVOC then (not even SVOC). Moreover, why is it an IVOC if measured in the SVOC channel? Please revise this statements and clarify.