EGUsphere, author comment AC2
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Reply on RC2

Marta Via et al.

Author comment on "*Rolling* vs. *seasonal* PMF: real-world multi-site and synthetic dataset comparison" by Marta Via et al., EGUsphere,
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Reply to Anonymous Referee #2 (Egusphere-2022-269)

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The authors would like to thank this reviewer for the comments and suggestions, which helped improving the quality of this work. A new version of the manuscript has been prepared following the suggestions from the reviewers. We provide below detailed replies to each of the comments in a point□by□point manner. Figures and tables cited in this document can be found in the supplementary annex.

Comments from the reviewer

This paper illustrates the comparison results between rolling and seasonal PMF methods using a synthetic dataset and real-world ambient datasets. They deployed multiple tools in many dimensions to evaluate the comparison results. In general, they found the rolling window PMF method performs slightly better than seasonal PMF method when the source apportionment for long-term dataset is required. The whole paper is well written and organized. I only have a few questions, as shown below.

MAJOR COMMENTS

- **For rolling window method, why were 14 days or 28 days chosen for a timing window. Can other arbitrary days e.g., 7 days or 20 days be applied? I also do not understand why 1 day shift was used. How about the half day or other days.**

The 14-days window-length was proposed in Parworth et al. (2015) as it results in a good compromise between catching the lifetimes of the studied pollutants (~ 5-6 days) and capturing short enough periods to observe inter-window variability. Nevertheless, the window length was further tested in Canonaco et al. (2021) considering the Q/Q_{exp} and the number of non-modelled points as

shown in Figure 1(a) in that study and Figure R2.1. (a) in this document.

The 14-days window is justified as it presents a low Q/Q_{exp} value and minimises the number of non-modelled points. The immediately inferior window length presents a quadrupled number of modelled points therefore it is discarded, even if the Q/Q_{exp} is a bit lower. The 28-days period presents a higher Q/Q_{exp} and non-modelled points percentage, but the difference is not high, therefore this window length could be used if any environmentally-feasible criteria pointed to a better performance with this window length. The reason why the window length was set to the multiples of 7 is that certain sources (e.g., HOA, COA, and BBOA) have stable weekly cycles (Chen et al., 2022) that could help in resolving better results. Therefore, time windows smaller than 7 days might not be a representative subset to conduct PMF. In the case of the present study, the window length modification criterium consisted on checking if the correlation of time series to their external markers overperformed the mathematically-optimised 14-days window length as well as following the guidelines in Canonaco et al., (2021).

The use of an advancing 1-day shift is stablished due to the assumption that the factor profiles remain consistent within a day. Of course, different steps could be tested with alternative assumptions, but changing less than 1/7 data in the time window will have limited effects on the final PMF solutions. Besides, shortening the step will imply increasing computational expense with extra repetitions that one can argue it is not worthwhile.

- **For the seasonal PMF, can the MO-OOA and LO-OOA be compared among different seasons since free PMF was used. The MO-OOA and/or LO-OOA among different seasons might have different spectra and oxidation level. Are the spectra of MO-OOA and LO-OOA the same compared to the rolling method.**

The Figure R2.2 depicts the oxidation ratio f44/f44 for the LO-OOA and MO-OOA factors on the left and for SOA on the right.

The left plot shows close rolling and seasonal dots in all seasons and in the mean of all of them except for the MO-OOA in FMAM. Compared to truth, it can be seen how this issue is related to an f44/f43 overestimation of the seasonal method. In the right graph, it can be seen how in all cases except for JJA, the rolling captures a more oxidised aerosol than the seasonal, which is closer to the *truth*.

- **Is there any difference among the spectra of SOA_{bio}, SOA_{bb} and SOA_{tr}? How were these spectra obtained and which oxidation level was chosen? The similarity of BBOA and SOA_{bb} might obscure the source results.**

There are significant differences between these three SOA factors in terms of oxidation level as can be seen in Figure R1.1 in the RC1 document. These three SOAs were selected blindly from the PMF runner from the spectral database described in Ulbrich et al. (2009) to configure a '*truth*' synthetic dataset.

Figure R2.3(a) aims to depict the significant differences between truth BBOA and SOA_{bb} profiles. In the profiles can already be seen the lower proportion of m/z 43, m/z 44 in BBOA in comparison with the SOA and a much higher concentrations of combustion markers (m/z 60, 73) for the BBOA. Figure R4(b) also depicts much higher proportions of 44, 28 in the SOA_{bb} profile. To summarize, these two factors presented are distinct enough to be separated by

PMF, as shown in the study.

- **Figure 3 b-c, This figure needs to be revised, which shows very small legend and label.**

The figure has been revised and included in the new version of the manuscript as can be seen in Figure R.2.4.

MINOR COMMENTS:

- **Line 307 delete extra “m/z”**

This modification was applied to the manuscript.

- **Line 384, line 394 and line 426 What is “58-OA”? There shall be explanation for the abbreviation name of each PMF factor since some of the readers might not be familiar with these names.**

The following sentence has been added to the manuscript to clarify this factor source:

The 58-related OA, as explained in Chen et al. (2021), is a factor dominated by nitrogen fragments (m/z 58, m/z 84, m/z 94) which appeared as an artefact after the filament replacement in that instrument.

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Please also note the supplement to this comment:
https://egusphere.copernicus.org/preprints/2022/egusphere-2022-269/egusphere-2022-269-AC2-supplement.pdf