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Atmospheric Measurement Techniques Discussions

Interactive comment on "SoFi, an Igor based interface for the efficient use of the generalized multilinear engine (ME-2) for source apportionment: application to aerosol mass spectrometer data" *by* F. Canonaco et al.

F. Canonaco et al.

francesco.canonaco@psi.ch

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Since PMF users would examine the rotational ambiguity using the fpeak, comparison with the unconstrained PMF analysis is interesting, but perhaps not relevant. Isn't the real question here whether using the ME-2 approach offers advantages over the more commonly derived PMF solutions that include exploration of the rotational ambiguity? The paper mentions on line 381 that using fpeak yielded an unsatisfactory outcome. More details could be provided as this seems like a key argument for using the ME-2

approach.

The exploration of the global fpeak that we performed at the beginning involved an increase of Q/Qexp of roughly 5%. We stopped there, due to the fact that either the factor profiles degraded, i.e. they were no longer interpretable, or no net improvement in the correlation between HOA/NOx, LV-OOA/sulfate and SV-OOA/nitrate respectively, was notable. This obviously shows that the fpeak tool is not the proper tool for the examination of the rotational ambiguity of the model solutions (as also confirmed by Paatero in a personal communication) This we also addressed in the newly created section 4.3 comparison between the PMF2 and the ME-2 solvers

A detailed comparison would help readers appreciate the relative merits of the approaches. In terms of the development of the Igor based PMF tool, it would be great if a sensitivity test for the change of uncertainties were included in the tool. The determination of the measurement uncertainties is a crucial point that affects the robustness of the model solution as well. Increased uncertainties can be used in the model in a manner analogous to how the "a-value" approach is applied to constrain source proïňĄles.

The aspect of the uncertainties touched by the referee is very crucial, since the uncertainties play a major role during the model calculation. Normally the uncertainties employed for PMF runs comprise the measurement and the model uncertainties. Although the measurement uncertainties are well known, the model uncertainties are mostly unknown or at least not sufficiently estimated. Employing the variability of retrieved and validated source profiles might be a valid strategy to estimate the model uncertainty and performing the tests the referee is referring too. However, testing systematically possible model uncertainties within the PMF algorithm would go beyond the scope of this study. We share the opinion of the referee that these studies should definitely be conducted. However, we think that only a separate thoroughly scientific study will elucidate the importance of the model uncertainty for the PMF results.

Further, since the article is about the tool, some comments on the ease of use would

help. I was left wondering if the advantage offered by the ME-2 based tool is primarily that it yields “better” solutions, allows optimal solutions to be more easily identiïňĄed, or both.

There is already a small section in the manuscript that highlights the ease of the tool (page 6412, lines 1-7), and the fact that ME-2 offers more options for the exploration of the solution space is also addressed in the newly created paragraph 4.3.

A minor point is that the only evidence provided to support the presence of COA (cooking OA) was the diurnal pattern. NO2, BC, and UV absorbing BC data were used to show strong correlations with HOA and BBOA, but no COA related measurement. Care must be taken to ensure the presence of the factor since the source proïňĄle and contribution of COA were similar to that of HOA. It surprises me how distinct the diurnal trend of COA is (peaking at 12pm and 8 pm). The authors could perhaps also present weekend and weekday differences in the contributions of the HOA and COA factors.

Due to the lack of strong markers for the COA source the only information available to validate a COA factor is the distinct diurnal cycle. This was also true for similar other AMS source apportionment studies, e.g. Mohr et al., 2012, Crippa et al., 2013. We liked the suggestion of the referee very much and added a small section in the supplementary part (6.4.3), where we compared the diurnal cycles (week-days and week-end) for an ME-2 run using the a-value 0.1.

Finally the authors recommend constraining (line 567) “the primary factors (HOA, COA, BBOA), whenever the PMF run reveals indications for such sources in the PMF model result and or in the corresponding residuals”. While the beneïňĄts of this approach were explored and described in the paper, were alternate approaches, beyond the full CMB, explored and rejected?

Different other approaches mentioned in the manuscript, e.g. the individual fpeak or the use of specific pulling equations for the exploration of the solution space and as such to estimate the rotational ambiguity can be interesting as well and we are exploring

such approaches more systematically at the moment. For most users, the approach described here or in Crippa et al. in prep will likely be the most common approach as it is more straight forward to be used.

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