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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.

Anonymous Referee #2

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This article describes a new PMF tool to support the interpretation of Aerosol Chemical Speciation Monitor (ACSM) and Aerosol Mass Spectrometer (ASM) data. Creation of this tool is very timely and useful. The article is well written, clearly structured, and represents a useful contribution to the literature. In the manuscript, the rotational ambiguity of PMF/ME-2 models was thoroughly examined by comparing unconstrained and constrained G and F matrices. These are very useful approaches to finding more reasonable sources and identifying the stability of a PMF solution. The primary references used for comparison are a fully constrained chemical mass balance (CMB) and

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a fully unconstrained PMF analysis ($f_{\text{peak}}=0$). Since PMF users would examine the rotational ambiguity using the f_{peak} , 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 f_{peak} yielded an unsatisfactory outcome. More details could be provided as this seems like a key argument for using the ME-2 approach. 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 profiles. 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 identified, or both. 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 profile 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. 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 benefits of this approach were explored and described in the paper, were alternate approaches, beyond the full CMB, explored and rejected?

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