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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.

F. Canonaco et al.

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Answers to the first referee

General: The only thing that is perhaps a little disappointing is that the authors chose to test it on an entirely new dataset and not perform any benchmarking against any datasets in the literature that have already been heavily studied with other receptor modelling techniques (the Pittsburgh dataset featured in the Ulbrich et al. and Zhang et al. papers or the Zurich datasets investigated in the Lanz et al. papers spring

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to mind). I don't feel this omission would be grounds for rejecting the paper, as the authors already present some pretty convincing results, but its inclusion would add a lot of value.

We added a section (3.2.4) where the profiles and the absolute contributions of the winter data have been compared to the previous study conducted by Lanz et al., 2008.

Title: I ïňĄnd this title misleading because the paper focuses on ACSM data, rather than AMS data. Running title: This is a bit nonspeciïňĄc. Suggest changing to something mentioning ME-2

We explicitly did not mention AMS, since this abbreviation sometimes refers to a measuring instrument. However, referring to aerosol mass spectrometer data is general and covers all instruments that produce such data, including the ACSM. Thus, we would like to keep the title as it is.

Page 6411, line 15: PMF isn't so much a model in itself as an algorithm that employs a 2-dimensional data model.

We agree and replaced model by algorithm

Page 6411, line 19: Meteorological events that cause covariance don't necessarily hinder PMF as such other than by removing available signal. They are merely a source of variance that doesn't help PMF, as opposed to sources of variance that only affect individual factors such as source activity.

We agree with this comment. However, if the variance of single sources is less pronounced compared to the meteorologically induced variances, this might lead to PMF results which do not any longer represent well-defined sources but rather capture the meteorological variability.

Page 6411, line 24 (and elsewhere): Part of me is not entirely comfortable with the term 'CMB', as this could easily be confused with EPA-CMB, which is a speciïňĄc software package (http://www.epa.gov/scram001/receptor_cmb.htm). Unless, that is, the

authors are saying the mathematical approach is identical, in which case they should be speciïñẠc in this detail.

We agree with the referee and replaced on page 6411, line 24 the statement: "If all factor proïñĄles are predetermined, the approach is called chemical mass balance (CMB) with "If all factor profiles are predetermined, the approach is within the spirit of the chemical mass balance (CMB)." This reformulation should avoid confusion with a specific software package and underlines only the similarity with the CMB algorithm.

Page 6411: It should probably be added that ME-2 is particularly beneïñĄcial to the analysis of ACSM data, as compared to the AMS, it has a lower signal-to-noise ratio and cannot resolve peaks with different elemental compositions.

We do not agree and discussed this in the newly created paragraph 4.3 comparison between the PMF2 and the ME-2 solvers. The ME-2 solver offers the possibility to potentially explore the full PMF solution space, which is by far not supported by the PMF2 solver. Hence, the ME-2 solver is beneficial for all types of PMF runs.

Page 6414, line 1: The authors should specify the model of the NOx analyser and the method used for NOx conversion, as instruments employing molybdenum catalysts, while common, are known to suffer artefacts from partial NOz conversion.

We added following sentence: The technique involves a molybdenum converter suffering from artifacts from partial conversion of NOx oxidation products (Steinbacher et al., 2007). These artifacts are however only expected to be important at low concentrations and more during summer

Page 6416, line 8: 'typical' is a very subjective generalisation. I am aware of much more variations than this in publications, so I recommend the authors tone this statement down.

The following sentence has been added to underline the issues with the absolute value of Q/Qexp:

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"Ideally, if the model entirely captured the variability of the measured data and all uncertainties were properly defined a value of Q/Qexp of 1 would be expected. However, several reasons, e.g. transient sources that are not fully modeled, errors in the estimate of the measurement uncertainties and the unknown model uncertainties prevent the use of the absolute Q/Qexp"

Page 6421, line 13: Was a minimum error imposed?

Yes, and we added the following statement at the end of chapter 2: "In addition the measurement uncertainty for points with a signal to noise (S/N) smaller than 2 (weak variables) and a S/N smaller than 0.2 (bad variables) was increased by a factor of 3 and 10, respectively, as in Ulbrich et al. (2009)."

Page 6424, line 22: It should be pointed out that the fact that the CMB approach has the largest UEV is expected, as this is given the least freedom during ïňĄtting.

This is already part of the discussion (4.1). However, we agree with the reviewer that this should be underlined and that's why we extended the paragraph in 4.1 and stressed the large increase of UEV due to the very tight constraint in the CMB approach.

Page 6429, line 3: Change 'extend' to 'extent'

Has been changed

References

Lanz, V. A., Alfarra, M. R., Baltensperger, U., Buchmann, B., Hueglin, C., Szidat, S., Wehrli, M. N., Wacker, L., Weimer, S., Caseiro, A., Puxbaum, H., and Prevot, A. S. H.: Source attribution of submicron organic aerosols during wintertime inversions by advanced factor analysis of aerosol mass spectra, Environ. Sci. Technol., 42, 214-220, doi:10.1021/es0707207s, 2008. Steinbacher, M., Zellweger, C., Schwarzenbach, B., Bugmann, S., Buchmann, B., Ordonez, C., Prevot, A. S. H., and Hueglin, C.: Nitrogen oxide measurements at rural sites in Switzerland: Bias of conventional measurement techniques, Geophys. Res. Atmos., 112, doi:10.1029/2006jd007971s, 2007. Ulbrich, I.

M., Canagaratna, M. R., Zhang, Q., Worsnop, D. R., and Jimenez, J. L.: Interpretation of organic components from positive matrix factorization of aerosol mass spectrometric data, Atmos. Chem. Phys., 9, 2891-2918, 2009.

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