

Interactive comment on “Interpretation of organic components from positive matrix factorization of aerosol mass spectrometric data” by I. M. Ulbrich et al.

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We thank V. Lanz for his comments, which concern three minor points about references to his previous work in our paper. We've repeated selections from his comments here in italics. Our replies follow each excerpt.

1) We did not use the rotmat matrix to derive the optimum solution. If we stucked to this criterion, we would have selected the 2-factorial solution (local minimum max(rotmat) vs. number of factors) as can be derived from Fig. 2c, p. 1509 (Lanz et al., 2007). We characterized the different solutions by different mathematical diagnostics (such as the maximum rotmat element).

[Response]: The Lee et al. (1999) and the Lanz et al. (2007) papers do discuss

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max(rotmat) as A metric (*one of several* criteria) to determine the number of factors. We did not say, nor mean to imply, that it was used as THE metric (the *only* criterion) to determine the optimal number of factors. We will modify the sentence to read, “Some have used the criterion of a solution with the least rotation (lowest maximum value of Rotmat) as one of several qualitative metrics for making the determination of the number of factors (Lee et al., 1999; Lanz et al., 2007).”

The point that we are trying to make in the paper is that in the synthetic datasets, where the correct factorization is known, the max(RotMat) criterion would give a *wrong and misleading* indication of number of factors (5 factors for the 2-factor case, 6 factors for the 3-factor case). Therefore we have some amount of evidence that the max(Rotmat) criterion may lead one away from the right solution and would not recommend it as even A metric (one of several) for choosing the number of factors for a real dataset. Of course we cannot rule out that max(RotMat) may have some benefit in other datasets. However, a typical ambient dataset has no control case with which to indicate whether its use as A metric indicates a correct or incorrect number of factors, so we do not recommend using this metric until further studies are carried out that prove its usefulness.

2) *Lanz et al. (2006) should not be cited (p. 6740): in view of Lanz et al. (2007), the ACPD-version is obsolete.*

[Response]: Readers have access to both the ACPD and ACP versions, and over the last year we have pointed out the existence of the ACP version of the Lanz et al. paper to 2 separate researchers who were interested in PMF and were still using the ACPD version. Since both versions are available, we believed that we served science best by making clear that the difference between our results regarding max(rotmat) and those of Lanz et al. apply to both the 2006 and 2007 versions. However, to minimize confusion, we will remove the citation to the ACPD version.

3) *For several data sets we found that defining a too large number of factors, single m/z's may partly be represented by one single factor. This behaviour can be observed*

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for matrices estimated by different versions of the AMS data analysis software (also for v1.36 or later). Therefore, the reference Lanz et al. (2007) is not appropriate at this instance. Therefore we suggest to delete “Lanz et al., 2007” on p. 6743, line 3.

[Response]: We thank V. Lanz for the clarification of this point. In our experience with several datasets, this behavior only appeared when we were using outdated error estimates from older versions of the Q-AMS data analysis code. One exception is a dataset in Houston where very large fluorinated pump oil particles were present and caused single m/z factors to appear, but that situation is unusual for ambient datasets. Since Lanz et al. did not report which version of the Q-AMS code was used for their error calculations, nor an unusual situation such as the presence of fluorinated pump oil particles, we assumed that this behavior arose for similar reasons in their case. Given the new information provided by V. Lanz in his comment, we agree that the citation is inaccurate and will be removed. The revised sentence will read: “Nonsensical behavior of the factors (MS with one dominant fragment, or TS that oscillate between zero several $\mu\text{g}/\text{m}^3$ over 5-min periods) were observed when using error estimates from older versions of the Q-AMS data analysis software, but not when v1.36 was used.”

It would still be of interest to determine why the above behavior is different in our experience vs. that of Lanz et al. This should be a topic of future discussion, and we are happy to collaborate with V. Lanz to clarify this point.

Interactive comment on Atmos. Chem. Phys. Discuss., 8, 6729, 2008.

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