

Interactive comment on “Applications and limitations of constrained high-resolution peak fitting on low resolving power mass spectra from the ToF-ACSM” by H. Timonen et al.

Anonymous Referee #1

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This paper discusses the application of high resolution peak fitting commonplace in HR-AMS analysis to the TOF-ACSM. While this instrument is not designed to produce data over UMR (like the Q-ACSM), it may be possible to obtain some information and will be of much interest to those operating such instrument. The paper employs the current state-of-the-art regarding peak resolution within the AMS community and critically assesses its ability to deliver usable data. Recommendations for data analysis and future instrument modifications (e.g. addition of a m/z calibration source) are given.

The paper is methodical and well written. I have a few comments, but these are mostly minor. This paper is well suited to AMT and will provide a useful reference for future data inversion. It may also have applications to other mass spectrometric techniques.

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Comments:

In general, there are a lot of figures, possibly more than is needed to support the main article, so some could probably be moved into the supplement. I would also observe that only about half of the figures are referred to in the text, which might imply that some of them are not vital. However, some of the methodological figures (e.g. 1 and 2) should be retained, as these help to illustrate the specific steps described.

Page 5 line 3: I am not sure what is meant by 'background ions' because ions are unlikely to persist in the electric fields of a time-of-flight mass spectrometer. If the authors are referring to scattered ions or electrons, they should specify this.

Page 5 line 10: More detail should be given here, specifically the low-pass filter algorithm and parameters and the actual width of the box used. I would note that step ii could leave a slightly positive offset in peak-free data depending on the amount of noise, so the authors should comment on whether this is an issue.

Page 6, line 11: An example should be given for step iii

Page 9, line 8: 'Mass defect' is probably more appropriate than 'mass excess', as these can be negative.

Page 16: The ability of the AMS to detect sea salt is not universally well established. The results here should be compared against Ovadnevaite et al. (2012, Doi 10.1029/2011jd01737).

Page 20, line 5: There is no need to refer to 'poor woman's PMF' by name; the technique has had other nicknames over the years (e.g. 'poor person's PMF', 'marker method'), so it is probably best just referring to the paper.

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