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Discussions

Interactive comment on "Peak fitting and integration uncertainties for the Aerodyne Aerosol Mass Spectrometer" *by* J. C. Corbin et al.

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Corbin et al. report a novel approach for the estimation of the uncertainties associated with the PIKA peak height values which is to be welcomed and sure to provoke interesting discussion. They refer in places to the recently-published work of Cubison et al. (AMTD 2014, in press AMT 2015) which studied the same problem from a somewhat different angle. However, particularly in sections 4.2 and 4.3, the methodology taken by the authors to study the fitting errors associated with overlapping peaks is very similar to the work of Cubison et al. and the authors are thus asked to reference this accordingly.

Presently, the methodology is introduced and it is noted on P3496 L22 that "Ion-

counting imprecisions, as addressed by Cubison et al. (2014), are not included for simplicity". We ask the authors to recognise that they performed similar simulations to those reported in Cubison et al., only that 1) counting noise was disregarded in order to focus on the influence of the m/z calibration and 2) the m/z calibration bias was held constant for a given set of iterations. This is important as their Figures 9 and 10 are simply a different representation of the results presented in Figure 5 of the Cubison et al. AMTD article; in this case however without the inclusion of counting noise which is why these still represent novel graphics and should still justifiably be published.

The observations that the peak heights of isolated ions (for the constrained peak fitting scenario studied here) are accurately retrieved (P3494 L10) and that well-separated peaks in a multiple-peak system behave analogously to isolated peaks (P3493 L9) were also reported by Cubison et al. and should be cited in the appropriate places in the text.

The conclusion on P3489 L21 is also that same as concluded in Cubison et al. in their section 3.6: "The optimal experimental setup for a given ion pair is where χ = χ_d, for then intensity imprecision due to m/Q calibration is negligible but the number of points measured across the peak, is maximised."

The authors may also have misunderstood the treatment of data-point spacing and m/z calibration biases reported in Cubison et al.. Both of these effects were in fact taken into account in the numerical studies presented in that paper, which argued that the limiting precision is described in most cases by either counting error or m/z calibration errors. Changing data-point spacing directly influences the imprecision imposed by counting error and is thus incorporated in the results. When assessing the m/z calibration errors, the scalar of interest was the standard deviation on the distribution of fitted peak position for ALL calibrant peaks. This distribution is, critically, a COMBINATION of both imprecision and biases and is, in fact, the bottom left graph in Figure 5 of Corbin et al.. This Figure does a good job of showing the different contributions to the overall m/z calibration error, which was not described in detail in Cubison et al. Therefore, the statement on page 3496 that these two effects may influence the conclusions reported in Cubison et al. is misleading, and should be removed or altered.

Where Corbin et al. may improve on the error estimates reported in the previous study is in their treatment of the linear uncertainty term. We look forward to further discussions on this topic.

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