

Interactive comment on “Field and laboratory evaluation of a high time resolution x-ray fluorescence instrument for determining the elemental composition of ambient aerosols” by Anja H. Tremper et al.

Anonymous Referee #1

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General

The manuscript presents a comprehensive lab and field evaluation of the CES Xact 625 XRF spectrometer. Various alternative methods with different time resolutions and particle sizes are compared with the XRF measurements, with generally good agreement to XRF and between methods. Explanations for deviations are given. The manuscript adds to the literature on quality assessment of the Xact online spectrometer, an instrument with great potential for monitoring environmental metals and other elements in airborne particles. The study is more comprehensive than previous studies that

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compare those methods, although some questions with Xact data quality remain.

The structure of the manuscript, the results and the presentation of the material are good. The data has been analyzed and presented with care. The language is impeccable. The topic is relevant and well worth publication in AMT.

Major comments

The study describes intercomparisons of time series of metal concentrations measured with the Xact and with other techniques. The statistical work horse is Deming regression which assigns individual measurement uncertainties to each technique. This approach is straightforward and has been applied in other studies. Comparisons are made between Xact and ICP-MS (with different digestions), ACSM, URG, and XRF (measuring filters with the Xact itself). Data were collected in field studies and in laboratory experiments.

The field studies show good regressions with a slightly positive bias of the Xact vs. ICP-MS, in agreement with previous studies. It is nicely demonstrated that the slope depends on the digestion method used for ICP-MS, and an overestimation of the XRF values compared to the ICP-MS values may turn into an underestimation when using the other digestion method. This makes a generalization of regression results (which technique is best or better?) rather difficult. Comparisons with ACSM and URG suffer from the different size classes sampled (PM_{2.5}, PM₁) and the different particle characteristics (non-sea salt, non-refractory). A comparison then requires additional assumptions to bring the values into closer agreement. This is discussed by the authors, but it also makes the comparisons more qualitative than quantitative. Interesting is the comparison between Xact measurements and filters analyzed with the Xact (Table S1). Slopes ranging from 0.8 to 1.85 with R^2 values > 0.9 (excluding the extreme cases of As and Se) might indicate more serious issues with the calibration of the Xact or with the spectral deconvolution algorithm, even though the number of samples is only 12, and slopes of 1.31 (Ba) and 1.62 (V) are not significantly different from unity,

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according to the authors. Here I would like some comment from the authors.

The laboratory experiment regressions in Fig. S2 show very good agreement between Xact and TEOM, except for some outliers for S. The concentration maxima are extremely high compared to typical ambient concentrations. Except Zn, all elements should be prone to self-absorption effects in XRF analysis when the deposited layer becomes too thick, but no such effect can be seen in the regressions. Are self-absorption effects so well compensated by the Xact software? It would be helpful to add information on particle sizes (as measured with the SMPS) and/or deposit thickness to understand why XRF self-absorption effects do not show up in the graphs.

Minor comments

P7L1: Middlebrook instead of Middlebook P7L34-36: Strange sentence. P8L11: remove one '.' after Table 3. P12L7: remove one '.' after filter measurements. P21 Table 7: Check the arrangement of rows carefully. P17 Fig. 7 and Figs. S3-S5: It might make the graphs more consistent when the coloring of all figures were in agreement. I suggest to color the dots in the Figures S3-S5 in red (HF/HClO₄), and blue (HNO₃/H₂O₂), to correspond to the colors in Fig. 7.

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