



Effects of different peak fitting strategies for XRF-spectra and their implications for paleoenvironmental studies: an example from powdered loess-paleosol samples

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X-ray fluorescence (XRF) core scanning is influenced by numerous sample-specific effects such as water content, sediment matrix and grain size. All these parameters affect the characteristics of fluorescent X-rays recorded by the detector. Subsequently, the recorded spectra are translated into element-specific counts by mathematical peak fitting strategies allowing for qualitative element tracking along a sediment profile. Down-core changes of these element counts or ratios often serve as a basis for paleoenvironmental interpretation. However, for such studies detailed information about peak fitting procedures is rarely provided. Therefore, we investigate the influence of different peak fitting strategies on elemental count rates derived from XRF (Mo-tube) scanning of powdered samples from the Süttő loess-paleosol sequence, Hungary – a sequence chosen due to its pronounced lithological changes between loess and paleosol sections. In contrast to sediment cores, for dried and powdered samples the effects related to grain size and water content are minimized whereas those related to sediment matrix and lithology are emphasized.

Using the ITRAX XRF core-scanner (Cox analytical systems) peak fitting is accomplished by the processing software Q-Spec (version 8.60). In this software, the mean square error (MSE) indicates the goodness-of-fit of the mathematical model to the actually measured energies. To consider all different lithologies occurring within a sediment profile, a sum-spectrum of all individual sample spectra is calculated. Despite optimizing the fit for the sum-spectrum, first results indicate that drastic changes between loess and paleosols can cause the MSE to increase (reduce the goodness-of-fit) and thus alter the modelled element counts within paleosols. Therefore, succeeding samples with a poor fit are collected in a subset based on a user-defined MSE threshold. Subsequently, a new sum-spectrum is calculated and fitted for this subset separately. First results show that the different fits obtained with this procedure have the potential to change element counts by several percent up to more than 50%, e.g. for Ba and S. Consequently, these results suggest that changes in the goodness-of-fit along a sediment profile may superimpose the variations in the elemental composition related to paleoenvironmental changes.

With this study we attempt to stress the necessity for a more detailed description of peak fitting strategies executed with XRF data for paleoenvironmental studies. We highlight the importance of applying adequate peak fitting strategies to reduce elemental count errors introduced by poorly fitted subsets of samples. This is crucial if peak-fitting-affected elements are interpreted as paleoenvironmental proxies.