Calibration of XRF core scanners for quantitative geochemical logging of soft sediment cores

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Rapid on-line analysis of soft sediment cores by XRF core scanners has become increasing popular during the past decade, because it allows near-continuous geochemical profiles to be acquired with a minimum of analytical effort. Conversion of core-scanner output to element concentrations has been perceived as problematic, because specimens are inhomogeneous and the measurement geometry is poorly constrained. We propose a log-ratio model to solve the long-standing problem of XRF-core-scanner calibration based on a combination of theoretical concepts from XRF-spectrometry, empirical evidence, and principles of compositional data analysis. This new model provides accurate and precise predictions of sediment composition from XRF core-scanner output with $2(D-1)$ parameters only, where D equals the number of chemical elements. The model accommodates the inherent non-linearity of the relation between relative intensities and concentrations and provides unbiased (i.e. accurate) estimates. Tests on a sediment core collected offshore NW Africa (GeoB7920) show that the average relative standard deviation of predicted element concentrations is less than 2%. This level of precision is attainable with 50 randomly selected calibration specimens. Our results show that XRF core scanning can be developed into a rigorous quantitative measurement technology if improved control over input errors can be achieved. This will enable large amounts of high-resolution quantitative geochemical data to be routinely acquired from sediment cores.

Isotopic composition from six Mo reference solutions measured by MC-ICP-MS

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There is no internationally-certified Mo isotopic reference standard to date. As proposed by Anbar (2004), certification of an international reference standard for inter-lab comparison should be a high priority for the Mo stable isotope community.

Here we report the isotopic composition of six Mo reference solutions, NIST SRM 3134 (lot#891307), JMC-Mo Sie (lot #602332B), JMC-Mo Wen (lot#13989C), Merck (lot#170334), Aldrich (lot#207306) and Prolabo, using the isoprobe and Nu instrument MC-ICP-MS at CRPG and ENS-Loyn of France with the “Sample-standard bracketing” method.

The results of standard measurements from several measuring sessions showed, within individual sessions (1-2 days), the standard solutions yields 2 times the standard deviation reproducibility between 0.02 and 0.11 per mil on ratio 96Mo/95Mo, 0.05 and 0.13 per mil on 97Mo/95Mo, 0.06-0.17 per mil on ratio 98Mo/95Mo. The averaging precision for different sessions over time is better than session uncertainties with 0.03 per mil for 96Mo/95Mo, 0.04 per mil for 97Mo/95Mo, and 0.06 per mil for 98Mo/95Mo.

The JMC Sie and JMC Wen Mo solutions were analyzed several times against NIST Mo solution. The grand mean of all analytical sessions yields a 2 times the standard deviation of less than 0.1 per mil for the ratios 96Mo/95Mo and 97Mo/95Mo, which is consistent with the reported literature value and our internal precision. Our measurements show that there is no significant fractionation occurred between JMC Mo solutions with different lot.

Similarly, the Merck, Aldrich and Prolabo Mo solutions also is close to zero for their isotopic compositions relative to NIST 3134 Mo solution, suggesting their Mo isotopic compositions is homogeneous.

Therefore, the results show that there is no significant fractionation among the six Mo reference solutions and the good internal reproducibility is obtained with 0.06‰ of two times standard deviations for 97Mo/95Mo by the correction of the “Sample-standard bracketing” method compared with the “isotopic double spike” method.