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Isotope pattern deconvolution as rising tool for isotope tracer studies in environmental research

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During the last decade stable isotope tracers have emerged as versatile tool in ecological research. Besides 'intrinsic' isotope tracers caused by the natural variation of isotopes, the intentional introduction of 'extrinsic' enriched stable isotope tracers into biological systems has gained significant interest. Hereby the induced change in the natural isotopic composition of an element allows amongst others for studying the fate and fluxes of metals, trace elements and species in organisms or provides an intrinsic marker or tag of particular biological samples. Due to the shoreless potential of this methodology, the number of publications dealing with applications of isotope (double) spikes as tracers to address research questions in 'real world systems' is constantly increasing.

However, some isotope systems like the natural Sr isotopic system, although potentially very powerful for this type of application, are still rarely used, mainly because their adequate measurement/determination poses major analytical challenges; as e.g. Sr is available in significant amounts in natural samples. In addition, biological systems underlie complex processes such as metabolism, adsorption/desorption or oxidation/reduction. As a consequence, classic evaluation approaches such as the isotope dilution mass spectrometry equation are often not applicable because of the unknown amount of tracer finally present in the sample.

Isotope pattern deconvolution (IPD), based on multiple linear regression, serves as simplified alternative data processing strategy to double spike isotope dilution calculations. The outstanding advantage of this mathematical tool lies in the possibility of deconvolving the isotope pattern in a spiked sample without knowing the quantities of enriched isotope tracer being incorporated into the natural sample matrix as well as the degree of impurities and species-interconversion (e.g. from sample preparation).

Here, the potential of IPD for environmental tracer studies is critically discussed, where special emphasis is set on evaluating different data processing strategies on the example of enriched stable Sr isotopes.[1] The analytical key parameters such as blank (Kr, Sr and Rb), variation of the natural Sr isotopic composition in the sample, mass bias, interferences (Rb) and total combined uncertainty are considered.

A full metrological protocol for data processing using IPD is presented based on data gained during two transgenerational marking studies of fish, where the transfer of a Sr isotope double spike (^{84}Sr and ^{86}Sr) from female spawners of common carp (*Cyprinus carpio* L.) and brown trout (*Salmo trutta f.f.*)[2] to the centre of the otoliths of their offspring was studied by (LA)-MC-ICP-MS.

[1] J. Irrgeher, A. Zitek, M. Cervicek and T. Prohaska, J. Anal. At. Spectrom., 2014, 29, 193-200.

[2] A. Zitek, J. Irrgeher, M. Kletzl, T. Weismann and T. Prohaska, Fish. Manage. Ecol., 2013, 20, 654-361.