Using triple-isotope analysis for quantifying the contribution of three competing pathways to total degradation

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Compound-specific stable isotope analysis (CSIA) has been used for the determination of specific degradation pathways by analyzing the stable isotopes of two elements. This 'dual-isotope' or two-dimensional isotope' analysis also allows for an estimation of the contribution of two different pathways contributing both to the overall degradation and stable isotope fractionation. Recent CSIA approaches also allow for investigating the simultaneous stable isotope fractionation effects for three different elements. Such information on the stable isotope fractionation of three different elements of a degradable compound could be used for a quantitative analysis of the contribution of different degradation pathways in systems with three different pathways, but up to know there is no theoretical concepts providing such quantitative estimate.

The aim of the present study is to overcome this shortage and to present such theoretical concept for the quantification of single pathway contribution to the overall biodegradation in systems with three parallel degradation pathways. For this purpose the approach of Centler et al. (2013) for the analysis of dual-isotope analysis has been expanded to consider the fractionation of three different elements affected by three different pathways. The obtained analytical expression allows for the quantification of each pathway to total degradation based stable isotope enrichment factors and measured stable isotope signatures. The applicability of the concept is demonstrated using data from Wijker et al. (2013).

Centler, F., Hesse, F., and Thullner, M. (2013) *Journal of Contaminant Hydrology*, 152, 97-116.

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