

Improved estimation of sediment source contributions by concentration-dependent Bayesian isotopic mixing model

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The implementation of compound-specific stable isotope (CSSI) analyses of biotracers (e.g. fatty acids, FAs) as constraints on sediment-source contributions has become increasingly relevant to understand the origin of sediments in catchments. The CSSI fingerprinting of sediment utilizes CSSI signature of biotracer as input in an isotopic mixing model (IMM) to apportion source soil contributions. So far source studies relied on the linear mixing assumptions of CSSI signature of sources to the sediment without accounting for potential effects of source biotracer concentration. Here we evaluated the effect of FAs concentration in sources on the accuracy of source contribution estimations in artificial soil mixture of three well-separated land use sources. Soil samples from land use sources were mixed to create three groups of artificial mixture with known source contributions. Sources and artificial mixture were analysed for $\delta^{13}\text{C}$ of FAs using gas chromatography-combustion-isotope ratio mass spectrometry. The source contributions to the mixture were estimated using with and without concentration-dependent MixSIAR, a Bayesian isotopic mixing model. The concentration-dependent MixSIAR provided the closest estimates to the known artificial mixture source contributions (mean absolute error, MAE = 10.9%, and standard error, SE = 1.4%). In contrast, the concentration-independent MixSIAR with post mixing correction of tracer proportions based on aggregated concentration of FAs of sources biased the source contributions (MAE = 22.0%, SE = 3.4%). This study highlights the importance of accounting the potential effect of a source FA concentration for isotopic mixing in sediments that adds realism to mixing model and allows more accurate estimates of contributions of sources to the mixture. The potential influence of FA concentration on CSSI signature of sediments is an important underlying factor that determines whether the isotopic signature of a given source is observable even after equilibrium. Therefore inclusion of FA concentrations of the sources in the IMM formulation is standard procedure for accurate estimation of source contributions. The post model correction approach that dominates the CSSI fingerprinting causes bias, especially if the FAs concentration of sources differs substantially.