Experimental determination of isotope enrichment factors – bias from mass removal by repetitive sampling - DTU Orbit (24/12/2018)

Application of compound-specific stable isotope approaches often involves comparisons of isotope enrichment factors (ε). Experimental determination of ε-values is based on the Rayleigh equation, which relates the change in measured isotope ratios to the decreasing substrate fractions and is valid for closed systems. Even in well-controlled batch experiments, however, this requirement is not necessarily fulfilled, since repetitive sampling can remove a significant fraction of the analyte. For volatile compounds the need for appropriate corrections is most evident and various methods have been proposed to account for mass removal and for volatilization into the headspace. In this study we use both synthetic and experimental data to demonstrate that the determination of ε-values according to current correction methods is prone to considerable systematic errors even in well-designed experimental setups. Application of inappropriate methods may lead to incorrect and inconsistent ε-values entailing misinterpretations regarding the processes underlying isotope fractionation. In fact, our results suggest that artifacts arising from inappropriate data evaluation might contribute to the variability of published ε-values. In response, we present novel, adequate methods to eliminate systematic errors in data evaluation. A model-based sensitivity analysis serves to reveal the most crucial experimental parameters and can be used for future experimental design to obtain correct ε-values allowing mechanistic interpretations.

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