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Linking observable stable isotope fractionation to transformation pathways of organic pollutants

M. Elsner (1), L. Zwank (2), D. Hunkeler (3), R.P. Schwarzenbach (4)

(1) Institute of Groundwater Ecology, GSF Neuherberg/München, Germany, (2) CRTE, Luxembourg, (3) University of Neuchatel, Switzerland, (4) ETH Zürich, Switzerland

Measuring stable isotope fractionation of carbon, hydrogen and other elements by compound specific isotope analysis (CSIA) is a new, innovative approach to assess organic pollutant degradation in the environment. Central to this concept is the Rayleigh equation which relates degradation-induced decreases in concentrations directly to concomitant changes in bulk (= average over the whole compound) isotope ratios. The extent of *in situ* transformation may therefore be inferred from measured isotope ratios in field samples, provided that an appropriate enrichment factor (ε_{bulk}) is known. This ε_{bulk} value, however, is usually only valid for a specific compound and for specific degradation conditions.

We therefore developed an evaluation procedure that takes into account (a) non-reacting positions within a compound as well as (b) effects of intramolecular isotopic competition so that enrichment factors ε_{bulk} can now be converted into estimates of apparent kinetic isotope effects. Reevaluation of existing ε_{bulk} literature values result in consistent ranges of AKIE values that generally are in good agreement with previously published data in the (bio)chemical literature and are typical of certain degradation reactions. Hence, the evaluation scheme bridges a gap between basic and environmental (bio)chemistry. It provides insight into factors that control the magnitude of bulk isotope fractionation factors and serves as a basis to even *identify degradation pathways* using only the observable bulk isotope fractionation in an organic substrate.