Mechanistic and Multi-Element Isotope Modeling of Organic Contaminant Degradation

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We propose a multi-element isotope modeling approach to simultaneously predict the evolution of different isotopes during the transformation of organic contaminants. The isotopic trends of different elements are explicitly simulated by tracking position-specific isotopologues that contain the isotopes located at fractionating positions. Our approach provides a mechanistic description of different degradation pathways that accounts for the influence of both primary and secondary isotope effects during contaminant degradation. The proposed modeling approach is versatile and can be applied to a wide variety of traditional and emerging organic pollutants as well as biotic and abiotic transformation processes. In this study we show applications on microbial degradation of toluene, methyl tert-butyl ether (MTBE) and nitrobenzene observed in previous experimental studies. Our model successfully predicts the multi-element isotope data (both 2D and 3D), and accurately captures the distinct trends observed for different reaction pathways. The approach provides an improved and mechanistic methodology to interpret multi-element isotope data and to predict the extent of multi-element isotope fractionation that goes beyond commonly applied modeling descriptions and simplified methods based on the ratio between bulk enrichment factors or on linear regression in dual-isotope plots.