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Position-specific isotope modeling of organic micropollutants transformation through different reaction pathways - DTU Orbit (08/11/2017)

Position-specific isotope modeling of organic micropollutants transformation through different reaction pathways

The degradation of organic micropollutants occurs via different reaction pathways. Compound specific isotope analysis is a valuable tool to identify such degradation pathways in different environmental systems. We propose a mechanism-based modeling approach that provides a quantitative framework to simultaneously evaluate concentration as well as bulk and position-specific multi-element isotope evolution during the transformation of organic micropollutants. The model explicitly simulates position-specific isotopologues for those atoms that experience isotope effects and, thereby, provides a mechanistic description of isotope fractionation occurring at different molecular positions. To demonstrate specific features of the modeling approach, we simulated the degradation of three selected organic micropollutants: dichlorobenzamide (BAM), isoproturon (IPU) and diclofenac (DCF). The model accurately reproduces the multi-element isotope data observed in previous experimental studies. Furthermore, it precisely captures the dual element isotope trends characteristic of different reaction pathways as well as their range of variation consistent with observed bulk isotope fractionation. It was also possible to directly validate the model capability to predict the evolution of position-specific isotope ratios with available experimental data. Therefore, the approach is useful both for a mechanism-based evaluation of experimental results and as a tool to explore transformation pathways in scenarios for which position-specific isotope data are not yet available.

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