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

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Organic compounds are produced in vast quantities for industrial and agricultural use, as well as for human and animal healthcare [1]. These chemicals and their metabolites are frequently detected at trace levels in fresh water environments where they undergo degradation via different reaction pathways. Compound specific stable isotope analysis (CSIA) is a valuable tool to identify such degradation pathways in different environmental systems. Recent advances in analytical techniques have promoted the fast development and implementation of multi-element CSIA. However, quantitative frameworks to evaluate multi-element stable isotope data and incorporating mechanistic information on the degradation processes [2,3] are still lacking.
In this study we propose a mechanism-based modeling approach 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. We validate the proposed approach with the concentration and multi-element isotope data of three selected organic micropollutants: dichlorobenzamide (BAM), isoproturon (IPU) and diclofenac (DCF). The model precisely captures the dual element isotope trends characteristic of different reaction pathways and their range of variation consistent with observed multi-element (C, N) bulk isotope fractionation. The proposed approach can also be used as a tool to explore transformation pathways in scenarios for which position-specific isotope data are not yet available.

[1] Schwarzenbach, R.P., Egli, T., Hofstetter, T.B., von Gunten, U., Wehrli, B., 2010. Global Water Pollution and Human Health. Annu. Rev. Environ. Resour. doi:10.1146/annurev-environ-100809-125342.
[2] Jin, B., Haderlein, S.B., Rolle, M., 2013. Integrated carbon and chlorine isotope modeling: Applications to chlorinated aliphatic hydrocarbons dechlorination. Environ. Sci. Technol. 47, 1443–1451. doi:10.1021/es304053h.
[3] Jin, B., Rolle, M., 2014. Mechanistic approach to multi-element isotope modeling of organic contaminant degradation. Chemosphere 95, 131–139. doi:10.1016/j.chemosphere.2013.08.050.