Modeling position-specific isotope fractionation of organic micropollutants degradation via different reaction pathways

Jin, Biao; Rolle, Massimo

Publication date: 2016

Document Version
Peer reviewed version

Link back to DTU Orbit

Citation (APA):

General rights
Copyright and moral rights for the publications made accessible in the public portal are retained by the authors and/or other copyright owners and it is a condition of accessing publications that users recognise and abide by the legal requirements associated with these rights.

- Users may download and print one copy of any publication from the public portal for the purpose of private study or research.
- You may not further distribute the material or use it for any profit-making activity or commercial gain
- You may freely distribute the URL identifying the publication in the public portal

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.
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, such as groundwater systems, and are referred to as organic micropollutants. Degradation of various organic micropollutants occurs via different reaction pathways. Compound specific stable isotope analysis (CSIA) is a valuable tool to characterize different degradation pathways of these contaminants in different aquatic systems and under different environmental conditions. 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 transformation of different organic contaminants [2,3] are still lacking.

In this study we propose an integrated modeling approach to simultaneously predict concentration as well as bulk and position-specific multi-element isotope evolution during the transformation of organic micropollutants [4]. The model simulates position-specific isotopologues explicitly incorporating the atoms that experience isotope effects. Thus, it provides a mechanistic description of isotope fractionation occurring at specific molecular positions. We apply the proposed approach to interpret the data available for three selected organic micropollutants: dichlorobenzamide (BAM), isoproturon (IPU) and diclofenac (DCF). The model successfully reproduces the multi-element isotope data, and precisely captures the dual element isotope trends, characterizing the different degradation pathways. Besides illustrating the model capability of mechanistic evaluation of experimental observations, we also show its potential as a predictive and design tool to explore transformation pathways in micropollutants degradation scenarios for which position-specific isotope data are not (yet) available.