Modeling whole body trace metal concentrations in aquatic invertebrate communities: A trait-based approach ☆

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ABSTRACT

Trace metal risk assessment and environmental quality standard definition require realistic models that quantify metal exposure and accumulation by biota. In the present study we propose a novel trait-based approach to predict whole body concentrations of metals in aquatic invertebrates from concentrations measured in different environmental compartments. Field data from a large riverine floodplain was used to calibrate and test the model. The prediction performance of the trait-based model was unbiased and uncertainty was below the twofold of measured concentrations for the four studied metals (Ni, Cu, Cd, Pb). The relative contribution of feeding, respiration and locomotion patterns as well as metal concentrations in three environmental compartments provided insights into the importance of different uptake pathways. The relation with the sediment (i.e., to what degree taxa live in or directly on the sediment) was shown to be the most important trait to predict metal accumulation. Overall, this study demonstrated the potential use of bioecological traits for the modeling of whole body metal concentrations of entire aquatic invertebrate communities.

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1. Introduction

Metal risk assessment and environmental quality guidelines are currently mostly based on data from a few model species. However, aquatic invertebrates in the natural environment are diverse concerning their biological and ecological traits (e.g, feeding, life history, locomotion (Schmidt-Kloiber and Hering, 2015; Tachet et al., 2000). These diverse traits lead to different interactions and exposure pathways towards trace metals in the field. The environment (physico-chemical characteristics of the field site), invertebrate species characteristics (accumulation strategy, traits) and metal concentrations in ambient water and food influence whole body concentrations. Whole body metal concentrations can serve as estimates for potential internal exposure and indicate

bioavailable metal concentrations in the environment. Several models to estimate whole body concentrations with statistical approaches have been described: chemical speciation modeling (De Jonge et al., 2014; Iwasaki et al., 2013; Stockdale et al., 2010), body weight (Hendriks and Heikens, 2001), or general regression methods (Esbaugh et al., 2012; Solà and Prat, 2006; van Griethuysen et al., 2004; van Hattum et al., 1991). The integration and quantification of biotic factors is the main challenge of statistical approaches. A good method which includes biotic factors should provide a model that is transferable among species and even among systems. Biological traits seem a promising approach to make the same statistical model adaptable to different macro-invertebrate species. Feeding guilds, which can be seen as a simplified ecological trait, were tested to explain bioaccumulation (Goodyear and McNeill, 1999). They found no apparent link between accumulation and feeding guilds. However, feeding patterns are more complicated than the simple feeding guild classification and are better represented by a fuzzy coded system (Chevenet et al., 1994; Moog, 1995). Fuzzy coded traits have been used as response metrics in various biomonitoring contexts (Arce et al., 2014;

Archaimbault et al., 2009; Culp et al., 2011; Mondy and Usseglio-Polatera, 2014; Van den Brink et al., 2013) but also in the estimation of the exposure to organic pollutants (Ippolito et al., 2012; Liess et al., 2008). This estimation of the exposure was only applied to single species and has not yet been generalized for an entire community. Some authors argued that phylogenetic relationships are more important than traits to determine uptake. However, while the phylogenetic signal holds at the family level, it becomes mostly insignificant at lower taxonomic levels (Buchwalter et al., 2008; Poteat and Buchwalter, 2014a). To our knowledge, detailed trait information has not been tested in metal uptake models to date.

The objective of this study was to test the integration of bio-ecological traits into a statistical model for whole body concentrations of aquatic invertebrates that can be applied to a whole community. We characterised the distribution of traits in macro-invertebrate communities of a large river floodplain. Traits that are likely to influence metal exposure (e.g., feeding patterns, locomotion type) were used as parametric terms within a statistical model. At the same time, we tested the influence of phylogeny by including family as predictor for whole body metal concentrations. To account for different accumulation kinetics, a regression tree model which is able to model non-linear predictor-response relationships and a linear model were tested. Prediction performance is important for possible applications in risk assessment and variable selection is important to elucidate mechanisms. As there is always a trade-off between the two, several techniques to select predictors were explored.

Whole body concentrations of a wide range of aquatic invertebrates were determined at different sites of the Rhône floodplain. In parallel, trace metals were measured in water, sediment and suspended particulate matter (SPM). Major ions and dissolved organic carbon (DOC) were also measured.

With this data, we constructed a model that searches to establish a quantitative link between metal concentrations in environmental compartments and concentrations in invertebrates. The following questions were addressed:

1. How large is the variation of the trait distribution between sites?
2. Do traits improve the quality of predictions?
3. Which model terms (e.g., traits, sediment metal concentrations, water metal concentrations) are important and are there differences between metals?
4. Does the information on taxonomy influence the model outcome?
5. What are the implications of these results for the application of such models in environmental risk assessment and for the refinement of environmental quality guidelines?

2. Methods

2.1. Study area and trace metal determination in environmental compartments

We measured trace metals in water, sediment, SPM and aquatic invertebrates in twelve sites of the French Rhône River floodplain. Sampling sites were distributed in the floodplain as follows: six sites upstream of Lyon and six sites downstream of Lyon, with three connected and three disconnected secondary channels in each sector. Water quality variables such as dissolved organic carbon (DOC), pH and major cations and anions (Na^+, Mg^{2+}, Ca^{2+}, K^+, Cl^-, SO_4^{2-} and NO_3^-) allowed modeling of the metal speciation to obtain free ion concentrations and provided site specific water characteristics for the model. A detailed presentation of the sampling sites

and procedures is available in (Hug Peter et al., 2017, Peter et al., 2014). Briefly, we sampled the dissolved ($0.45 \mu m$ filterable) fraction, the suspended particulate matter (material retained on a $0.45 \mu m$ membrane filter) and the surficial sediment (5 cm) fractions for metal analysis. We measured conductivity and pH on site. Water was sampled for DOC ($0.72 \mu m$ Whatmann, glass fibre filter) analysis and for major ions (Milex HA 0.45 μm, Millipore, nitrate cellulose filter). Invertebrates were collected with hand nets and by direct collection to obtain a sufficient number of individuals for the subsequent analysis. For the analysis of whole body concentrations, they were rinsed with 1 mM ethylenediaminetetraacetic acid (analytical grade, Merck, Darmstadt, Germany) for 20 min and then with Milli-Q water. Freeze dried arthropods were reduced to powder while molluscs were digested directly. Concentrated HNO_3 and H_2O_2 (4:1 v/v) (Suprapur reagents, Merck, Darmstadt, Germany) were added to the biological material and left overnight and the digestion was terminated at $80°C$ during 1 h. The digestion protocol for SPM on filters and a sediment subsample followed the first step of the method proposed by the European Community Bureau of Reference (Rauret et al., 2000, 1999). This extraction method was chosen to extract the exchangeable and carbonate bound trace metals. Analysis of Na^+, Mg^{2+}, Ca^{2+}, K^+, Cl^-, SO_4^{2-} and NO_3^- was performed in filtered water samples within two days after sampling with Ion chromatography (Dionnex ICS-3000, Thermo Fisher Scientific, Dreieich, Germany). The concentration of DOC was measured with a Shimadzu TOC analyzer. Cd, Cu, Ni and Pb analysis in water and digestats was conducted by inductively coupled mass plasma spectrometry (ICP-MS) (Agilent 7700, Morges, Switzerland). Details of analytical procedures can be found in Hug Peter et al., 2017. We modeled metal speciation in the dissolved phase using Visual MINTEQ (v 3.0, KTH, Dept of Land and Water Resources Engineering, Stockholm, Sweden). Metal complexation by humic substances was modeled with the Non-ideal competitive adsorption coupled with a Donnan phase (NICA-Donnan) model (Benedetti et al., 1996). The ratio of dissolved organic matter (DOM) to DOC was set at 1.65 and 50% of DOM was assumed to be humic acid.

2.2. Invertebrate traits and community data

For the characterisation of the invertebrate communities in the twelve study sites, we used abundance data from the monitoring program of the "Plan Rhône" (Lamouroux et al., 2015). Two sampling years were selected for each site. Invertebrate traits were obtained from two sources: the freshwaterecology. info web database (Schmidt-Kloiber and Hering, 2015) and the Tachet database (Usseglio-Polatera et al., 2000). Feeding strategy was extracted from the freshwaterecology database, coded at the species level. More information on respiration and locomotion was available from the Tachet database, so these two traits were taken from this source, coded at the genus level. In both databases, bio-ecological traits of aquatic invertebrates are quantified with a fuzzy coded ten point assignment system. Within a trait (e.g., feeding strategy), ten points are distributed among the different categories (e.g., active filtering, predator), representing the ecology/biology of the species based on expert knowledge and published sources. A detailed description of the freshwaterecology. info database is provided in Schmidt-Kloiber and Hering (2015). The fuzzy coded information was transformed to percentage by trait. The same traits were also used in the whole body concentration modeling. A rarefied theoretical community was generated after pooling of all the samples of a sampling date. This procedure allows to reduce bias due to sampling inequalities. We multiplied the site x taxon matrix by the traits x taxon matrix to obtain a site x trait matrix.