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Research article

Limitations of experiments performed in artificially made OECD standard soils for predicting cadmium, lead and zinc toxicity towards organisms living in natural soils

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Development of comparative toxicity potentials of cationic metals in soils for applications in hazard ranking and toxic impact assessment is currently jeopardized by the availability of experimental effect data. To compensate for this deficiency, data retrieved from experiments carried out in standardized artificial soils, like OECD soils, could potentially be tapped as a source of effect data. It is, however, unknown whether such data are applicable to natural soils where the variability in pore water concentrations of dissolved base cations is large, and where mass transfer limitations of metal uptake can occur. Here, free ion activity models (FIAM) and empirical regression models (ERM, with pH as a predictor) were derived from total metal EC50 values (concentration with effects in 50% of individuals) using speciation for experiments performed in artificial OECD soils measuring ecotoxicological endpoints for terrestrial earthworms, potworms, and springtails. The models were validated by predicting total metal based EC50 values using backward speciation employing an independent set of natural soils with missing information about ionic composition of pore water, as retrieved from a literature review. ERMs performed better than FIAMs. Pearson's *r* for $\log_{10}$-transformed total metal based EC50s values (ERM) ranged from 0.25 to 0.74, suggesting a general correlation between predicted and measured values. Yet, root-mean-square-error (RMSE) ranged from 0.16 to 0.87 and was either smaller or comparable with the variability of measured EC50 values, suggesting modest performance. This modest performance was mainly due to the omission of pore water concentrations of base cations during model development and their validation, as verified by comparisons with predictions of published terrestrial biotic ligand models. Thus, the usefulness of data from artificial OECD soils for global-scale assessment of terrestrial ecotoxic impacts of Cd, Pb and Zn in soils is limited due to relatively small variability of pore water concentrations of dissolved base cations in OECD soils, preventing their inclusion in development of predictive models. Our findings stress the importance of considering differences in ionic composition of soil pore water when characterizing terrestrial ecotoxicity of cationic metals in natural soils.

1. Introduction

Addressing liquid-phase speciation in calculation of comparative toxicity potentials (CTP) for application in hazard ranking and toxic impact assessment requires that both the bioavailability factor and the effect factor used in the CTP calculation must be based on immediately bioavailable toxic metal forms (Gandhi et al., 2010; Owsianiak et al., 2013; Dong et al., 2014). The bioavailability factor used in CTP calculations is expressed as the fraction of metal present in the directly bioavailable, toxic forms, relative to the reactive metal concentration (Owsianiak et al., 2013). The effect factor indicates the average toxic potency of the directly bioavailable, toxic forms of a metal. This effect factor is derived from free ion based HC50 values, the hazardous concentration of toxic metal forms affecting 50% of the species, calculated as a geometric mean of EC50 values for individual species (i.e. the concentration with

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(lethal) effects in 50% of the individuals of a species). As EC50s are based on either free ion or truly dissolved metal concentrations (i.e. including free ions and inorganic complexes) they can be derived using either terrestrial biotic ligand models (TBLM), empirical regression models (ERM), or free ion activity models (FIAM) (Owsianiak et al., 2013; Qiu et al., 2013). ERMs can be considered as an intermediate approach between relatively simple FIAMs, which assume that the ecotoxic response is proportional to metal free ion activity in the pore water, and more complex TBLMs, which assume that the ecotoxic response is proportional to the amount of metal ions bound to biotic ligand as influenced by protons and base cations. Protons and base cations compete with toxic metal ions for binding to the biotic ligand of the exposed organism.

Currently, the development of free ion based EC50 values for cationic metals in soils is constrained by the availability of terrestrial effect data of sufficient quality needed to derive them. The major limitation of reported effect data is incomplete information about ionic composition of soil pore water in the tested natural soils, which influences both speciation pattern of a metal and the ecotoxic response through competitive binding of protons and sometimes base cations to biotic ligand(s) (Steenbergen et al., 2005; Thakali et al., 2006a,b; Voigt et al., 2006). Incomplete information about soil properties has led to disregarding speciation in the effect factor of Zn, resulting in an underestimation of the CTP (Plouffe et al., 2015a, 2016). It is thus important to find alternative sources of data, which can be used to derive models predicting EC50 values of metals in soils based on directly available, toxic metals forms.

Ecotoxicological effect data measured in artificial soils, like OECD soils, could potentially be tapped as a source of data for calculation of free ion based HC50 values as the composition of the OECD soils is known and pore water compositions can be estimated. Indeed, in the ECOTOX database (U.S. Environmental Protection Agency, 2012) the majority of ecotoxicity tests for common cationic metals with the terrestrial earthworm *Eisenia fetida* were conducted in artificial soils (59, 95 and 86% of all experiments with *E. fetida* for Cd, Pb and Zn, respectively). Some metals have data from artificial soils only (e.g. Au, Ti). It is therefore of interest to evaluate the applicability of models built on effect data measured in artificial OECD soils for predicting metal ecotoxicity in natural soils while considering variability in properties of natural soils.

It is hypothesized that the difference in ionic composition of the water phase between artificial OECD soils and natural soils will limit the applicability of effect data from experiments carried out in artificial OECD soils. Although average pore water concentrations of base cations in artificial OECD soils (Lock et al., 2006) and natural soils (Owsianiak et al., 2013) are usually within the same order of magnitude (with the exception of Ca^{2+} concentration which on average is by one order of magnitude higher in natural soils), the variability in pore water concentration of base cations is much higher in natural soils, where differences by up to three, (Na^{+}, K^{+}), five (Ca^{2+}) and six (Ca^{2+}) orders of magnitude are observed (Owsianiak et al., 2013). An increase in concentrations of dissolved Mg^{2+} by one order of magnitude decreases toxicity to various terrestrial organisms towards Ni^{2+} by a factor of five (Owsianiak et al., 2013). Thus, the applicability of models based on effect data measured in artificial OECD soils is expected to depend on: (i) ionic composition of the artificial OECD soils used to derive the predictive models, and (ii) the ionic composition of the natural soil(s) where the model is employed for prediction of metal's ecotoxicity. Ionic composition of pore water is rarely measured in ecotoxicity experiments and is not reported in soil databases like ISRIC-WISE3 or the Harmonized World Soil Database (HWSD) (FAO/IIASA/ISRIC/ISS-CAS/JRC, 2009), and is not always possible to calculate (e.g. HWSD does not provide information about exchangeable base cations, which also span a wide range in natural soils). Thus, it is of interest to estimate the implications of the limited information about ionic composition of soil pore water on the performance of models developed based on effect data from experiments carried out in artificial OECD soils. Although there is some variability in properties of artificial OECD soils, which can influence sorption and resulting ecotoxicity, the extent of this variability is smaller compared to the variability in properties of natural soils (Crommentuijn et al., 1997; Bielská et al., 2012, 2017; Hofman et al., 2014; Vašíčková et al., 2015). Geographic variability in properties of natural soils must be considered when computing CTP of metals at a global scale (Plouffe et al., 2016; Owsianiak et al., 2013).

The aim of this study was to evaluate the applicability of free ion based models (FIAM and ERM) derived from effect data measured in artificial OECD soils for predicting ecotoxicity of cationic metals in natural soils at the level of total metal based EC50s. For this purpose, the empirical data from a literature review based solely on data from experiments performed in artificial OECD soils were collected and subjected to speciation modelling to develop FIAMs and ERMs separately for various species of earthworms, potworms, and springtails for acute and chronic endpoints, like mortality, growth, and reproduction. Next, using backward speciation, the models' performance for prediction of total metal based EC50 values in natural soils was tested. To quantify the influence of missing data about pore water concentration of dissolved based cations both in models' development and validation, comparison was made with prediction of published terrestrial biotic ligand models using pore water concentrations of base cations being in average, lower, and higher range of values expected for global soils.

2. Methods

The study involved collection and selection of data from OECD soils based on defined set of criteria, as presented in Fig. 1. Then speciation calculations for the OECD soils to derive FIAMs and ERMs were conducted. Finally, backward speciation calculations to total metal content were done on a data set representing natural soils selected, applying the same criteria as for selection of the data in OECD soils, and the model predictions of ecotoxicity in these soils were evaluated.

2.1. Data collection and selection criteria

Data on metal ecotoxicity were collected from peer-reviewed scientific reports available until March 2015 identified through searching the ISI Web of Science, v. 5.17 (Thomson Reuters, New York, NY), using a combination of keywords: (i) “toxicity”; and (either) (ii) “soil”, or “terrestrial”; and (either) (iii) “Al”, “Ba”, “Be”, “Cd”, “Co”, “Cr”, “Cs”, “Fe”, “Mn”, “Pb”, “Sr”, “Zn”, “aluminum”, “barium”, “beryllium”, “cadmium”, “cobalt”, “chromium”, “cesium”, “iron”, “manganese”, “lead”, “strontium”, or “zinc”; and (either) (iv) “EC50”, “LC50”. For example, one of the used keywords combination was: “toxicity” and “soil” and “Zn” and “EC50”. A complementary search was conducted in ISI in order to collect publications citing references retrieved in the previous step, and those which were cited in the collected publications, but were not found through the initial search. The two latter steps were iterated until no new data were found. Although the ecotoxicity effect data for Cu and Ni is relatively abundant, effect factors of these two metals were already calculated using terrestrial biotic ligand models (Owsianiak et al., 2013). Cu and Ni are thus not considered as priority metals for calculation of effect factors underlying CTP.