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Derivation of freshwater quality criteria for zinc using interspecies correlation estimation models to protect aquatic life in China

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HIGHLIGHTS

- Interspecies correlation estimation (ICE) models were used to predict toxicity data for zinc in China.
- There were no significant differences between the ICE- and the measured-based SSDs and HC5s.
- The most sensitive species to zinc were invertebrates, especially crustaceans.
- A combination of measured and ICE-derived data will prove useful to derive water quality criteria.

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ABSTRACT

Species sensitivity distributions (SSDs) are usually used in the development of water quality criteria and require a large number of toxicity values to define a hazard level to protect the majority of species. However, some toxicity data for certain chemicals are limited, especially for endangered and threatened species. Thus, it is important to predict the unknown species toxicity data using available toxicity data. To address this need, interspecies correlation estimation (ICE) models were developed by US EPA to predict acute toxicity of chemicals to diverse species based on a more limited data set of surrogate species toxicity data. Use of SSDs generated from ICE models allows for the prediction of protective water quality criteria, such as the HC5 (hazard concentration, 5th percentile). In the present study, we tested this concept using toxicity data collected for zinc. ICE-based-SSDs were generated using three surrogate species (common carp (*Cyprinus carpio*), rainbow trout (*Oncorhynchus mykiss*), and *Daphnia magna*) and compared with the measured-based SSD and corresponding HC5. The results showed that no significant differences were observed between the ICE- and the measured-based SSDs and HC5s. Furthermore, the examination of species placements within the SSDs indicated that the most sensitive species to zinc were invertebrates, especially crustaceans. Given the similarity of SSD and HC5s for zinc, the use of ICE to derive potential water quality criteria for diverse chemicals in China is proposed. Further, a combination of measured and ICE-derived data will prove useful for assessing water quality and chemical risks in the near future.

1. Introduction

Species sensitivity distributions (SSDs) are widely used in ecological risk assessment and the development of water quality criteria (Solomon et al., 1996; ANZECC and ARMCANZ, 2000; Wheeler et al., 2002a). A significant purpose of SSD analysis is to determine a chemical concentration protective of most species in the environment, usually the 95% protection level, known as the HC5 (Van Straalen and Van Rijn, 1998). The HC5 has been used for setting quality objectives for the environment in Europe and North America. Ecological risk assessments require characterizing the effects of multiple chemicals on a diversity of ecological receptors using toxicity data for only a limited number of species. Regulatory activities such as Registration, Evaluation and Authorization of Chemicals (REACH), International Council of Chemical Associations (ICCA) and Canada's Domestic Substance List will also create new demands for toxicity data (Bodar et al., 2002; European Commission, 2007). SSDs are dependent upon available data sets and can differ in distribution, taxonomic diversity, and sample size (Wheeler et al., 2002b; Maltby et al., 2005). Recommendations of minimal sample sizes necessary for meaningful estimations have varied with the data set and estimation methodology (Stephen et al., 1985; ECB, 2003). With adequate representation of diverse taxa,

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eight species have been considered a sufficient number of observations in the water quality criteria in USA (Stephen et al., 1985). Similar taxa requirements have also been illustrated in the water quality guidelines in other countries (ANZECC and ARMCANZ, 2000; CCME, 2007; RIVM, 2007). In general, aquatic toxicity data for species were derived from actual laboratory tests. However, the number of species tested was limited by test procedure, species availability, time and expense, especially for threatened and endangered species. Therefore, it is important to investigate how to use the limited toxicity data to predict non-tested species.

Recently, the US EPA has developed interspecies correlation estimation (ICE) models to fill in data gaps in species sensitivity distributions. ICE models predict acute toxicity effects of aquatic and wildlife species based on toxicity results from surrogate species (Asfaw et al., 2003; Ellersieck et al., 2003; Raimondo et al., 2007, 2010; Awkerman et al., 2008). The entire data base of acute toxicity used in the development of aquatic Web-ICE models consisted of 5487 test results of 180 species and 1258 chemicals (Raimondo et al., 2010). ICE models are log-linear least-square regressions of acute toxicity data corresponding to chemical-species pairs. The resultant regression can be used to predict the acute toxicity of a chemical to another species. There are at least three advantages for using ICE models: (1) prediction of diverse species toxicity data based on a limited measured dataset; (2) reduced animal use; and (3) generation of sufficient toxicity data to derive protective criteria. Unfortunately, the development of ICE models for predicting chronic toxicity is problematic due to substantially fewer toxicity values compared to acute databases. ICE models have been employed in toxicity extrapolation of aquatic invertebrates and fish. For example, Dyer et al. (2006) introduced the use of ICE models to generate SSDs and recommended additional assessment and validation of ICE-based HC5s. Moreover, the SSDs derived from ICE and measured toxicity data used to derive US EPA's ambient water quality criteria (AWQC) dataset were compared (Dyer et al., 2008). The applications of ICE for wildlife, such as birds and mammals have also been conducted (Raimondo et al., 2007; Awkerman et al., 2008), suggesting that ICE models can also be used to generate SSDs comparable to those derived from measured wildlife toxicity data.

Zinc is widespread in Chinese freshwaters. According to statistics, the concentration levels of zinc in Chinese freshwaters range from 2 to 330 $\mu g\,L^{-1}$, and much higher in sediments (Wu, 2012). Zinc is an essential trace element. When the internal dose exceeds certain content, it might cause adverse effects through combination with biological macromolecules to the organisms, such as reduction of enzyme activity, gene expression changes, reproduction, and development (Poynton et al., 2007, 2008; Wu, 2012). China has recently begun water quality criteria research. Until now, only limited chemicals have been derived for their water quality criteria. Therefore, in this paper, as an application case study for China, ICE was used to predict toxicities to diverse species in order to develop a SSD and hazard criterion (HC5) for zinc and compared to recently developed water quality criteria in China. The accuracy of the comparison is discussed below.

2. Material and methods

2.1. Data sources and data processing

In the present study, two separate datasets were used: (1) measured zinc toxicity data and (2) data derived from interspecies correlation estimations (ICEs). Acute toxicity data from the open literature was combined with acute toxicity data from the US EPA's ECOTOX database (http://cfpub.epa.gov/ecotox/) constituted the total measured zinc toxicity dataset. Further, the ICE zinc dataset came from the on-line ICE database (http://epa.gov/ceampubl/fchain/webice/). Inclusion of Chinese species in the two datasets was based on the following principles: (1) if the species is native to China and (2) species is introduced species from abroad and now exist in China. Acute toxicity data were ranked and assigned percentiles. The data were then fitted with log–logistic distribution to construct SSDs. The acute HC5 for SSDs was determined by the Origin 8.0 statistical software (USA, Origin Lab Company). Species ranks from the two distributions were examined to determine the similarities of species placement in the SSD curves. The smaller the cumulative probability is, the more sensitive the species. Hence species in the first quartile of the SSD curve were thought as the most sensitive species.

2.2. Measured zinc toxicity data collection

Measured toxicity data for zinc were collected from the open literature and the ECOTOX database, managed by US EPA. The zinc forms used in the analysis contained zinc chloride, zinc sulfate, zinc acetate, zinc nitrate, zinc oxide and zinc sulfide, yet all data were expressed as $\mu g\,L^{-1}$. Data were subjected to rigorous quality assurance guidelines (Buckler et al., 2003). Briefly, aquatic acute toxicity tests found within the database or literature included the following characteristics: 96-h LC50 or EC50 for fish; 48-h LC50 or EC50 for invertebrates; the toxicological endpoints of zinc to fish and invertebrates mainly concerned about death effects, such as immobility, respiratory inhibition, and lethal effect; water hardness was between 30 and 60 mg of $CaCO_3$/L; pH ranged from 6 to 8; temperatures were appropriate per species (e.g., 12–15 °C for rainbow trout; ~20 °C for *Daphnia magna*); the majority of exposures included flow-through as well as static/renewal; finally, species occurring in China were considered. In addition, when more than one acute (e.g., LC50 or EC50) value was available for per species, geometric species mean acute toxicity values were calculated. Based on the criteria mentioned above, the total number for aquatic acute animal toxicity records for zinc contained 22 families, 33 genus and 40 species, including fish, invertebrates and amphibians (Wu et al., 2011). The detailed information about the acute toxicity data are listed in Table 1.

2.3. ICE data set

US EPA has developed both the ICE software (Asfaw et al., 2003) and the additional robust ICE models for aquatic and wildlife species that were available from the Internet (http://www.epa.gov/ceampubl/fchain/webice/index.htm). The on-line ICE platform was used in this study. Web-based ICE provides interspecies extrapolation models for acute toxicity via a user-friendly interface. Test results in the database met the following conditions: 96 h LC50/EC50 for fish; 48 h LC50/EC50 for most invertebrates; fish weighing 0.2–0.5 g; fish were less than 3 months old or less than 50 mm in length. Besides, the toxicological endpoints of zinc to fish and invertebrates restricts to those linked to death such as immobility, respiratory inhibition, and lethal effect. Because of the availability of few correlations between algae and animal taxa, we focused our work on only the invertebrate and fish species.

Based on geometric means from the measured database, Web-ICE was seeded with acute toxicity values for *Daphnia magna*, *Cyprinus carpio* and *Oncorhynchus mykiss* (691 $\mu g\,L^{-1}$, 7050 $\mu g\,L^{-1}$ and 1014 $\mu g\,L^{-1}$, respectively) to predict acute toxicity values for several invertebrate and vertebrate species. It is relevant to note that these three species are widespread in China.