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Development of Comparative Toxicity Potentials of 14 cationic metals in freshwater

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HIGHLIGHTS

- CTPs vary 2.4–6.5 orders for Al, Be, Cr(III), Cu and Fe(III) in different waters.
- Most toxic metals are Al and Cu in acidic water (pH < 6.4), but Cd in other water.
- Emission weighted CTPs based on EU waters were recommended as site generic CTPs.
- Most site generic CTP was higher or similar to default CTP in USEtox and USES-LCA.
- New CTPs were within ~2 orders of magnitudes compared to USEtox and USES-LCA CTPs.

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ABSTRACT

Site-dependent and site-generic Comparative Toxicity Potentials (CTPs) (also known as Characterization Factors (CFs)) were calculated for 14 cationic metals (Al(III), Ba, Be, Cd, Co, Cr(III), Cs, Cu(II), Fe(II), Fe(III), Mn(II), Ni, Pb, Sr and Zn), to be applied in Life Cycle Impact Assessment. CTPs were calculated for 7 EU-archetypes, taking bioavailability and speciation pattern into account. The resulting site-dependent CTPs showed up to 2.4–6.5 orders of magnitude variation across archetypes for those metals that form stable hydroxyl compounds in slightly alkaline waters (Al(III), Be, Cr(III), Cu(II) and Fe(III)), emphasizing the importance of using site-dependent CTPs for these metals where possible. For the other metals, CTPs stayed within around 0.9 orders of magnitude, making spatial differentiation less important. In acidic waters (pH < 6.4), Al(III) and Cu(II) had the highest CTPs, while Cd ranked highest in other waters. Based on the site-dependent CTPs, site-generic CTPs were developed applying different averaging principle. Emission weighted average of 7 EU-archetype CTPs was recommended as site-generic CTP for use in LCA studies, where receiving location is unclear. Compared to previous studies by Gandhi et al. (2010, 2011a), new site-dependent CTPs were similar or slightly higher for Cd, Co, Ni, Pb and Zn, but 1–2 orders of magnitude higher for Cu. Compared to the default site-generic CTPs in the frequently used characterization models USES-LCA and USEtox, new site-generic CTPs were mostly higher or similar, within up to ~2 orders of magnitude difference.

1. Introduction

Life Cycle Assessment (LCA) "quantifies all relevant emissions and resources consumed and the related environmental and health impacts and resource depletion issues that are associated with any goods or services (products)" (EC-JRC, 2010). Life Cycle Impact Assessment (LCIA) translates the emissions inventory from the product life cycle into an environmental profile presenting the potential contributions to a broad selection of environmental impacts. Ecotoxicity potential of an emission is calculated applying Comparative Toxicity Potentials (CTPs), which represent the ecotoxicological impacts caused by a unit emission of substance to certain environmental recipients via different pathways of exposure (Hauschild, 2005). Most models for deriving CTPs are developed based on environmental models simulating behavior of organic substances (Adams et al., 2000). Unlike organic compounds, metals speciate into several forms with different fate characteristics, bioavailability and toxicity that vary with spatially differentiated environmental conditions (Mason, 2013). Though

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several LCIA studies have been carried out addressing spatial differentiation in metal ecotoxicity characterization modeling (Pennington et al., 2005; Sleeswijk and Heijungs, 2010), they have failed to appropriately account for the multiple possible species of metals. The Clearwater Consensus Workshop (Diamond et al., 2010) recommended principles for modeling freshwater CTPs for metals, following which Gandhi et al. (2010, 2011a) developed a framework and applied it to 6 metals: Cobalt(II), Copper(II), Cadmium(II), Nickel(II), Lead(II) and Zinc(II). They found CTPs to vary up to 3 orders of magnitude in different freshwater archetypes, largely due to variations in the metal speciation and bioavailability. Between different freshwater archetypes, not only the absolute value of the metal CTPs, but also the relative ranking of metal CTPs are changed (Gandhi et al., 2011b). These findings demonstrate the importance of taking metal speciation into consideration when calculating cationic metal CTPs also for other metals than those covered by Gandhi and co-workers.

Due to the fact that metal emissions are normally reported in LCA as total emissions, ignoring emission locations, site dependent CTPs are rarely applied in LCA. These points to the importance of looking into how site-generic CTPs can be derived from site-specific CTPs and how sensitive the site-generic factors are to the applied averaging principles.

This study aims at developing CTPs for Aluminum(III), Barium(II), Beryllium(II), Cesium(I), Chromium(III), Iron(II), Iron(III), Manganese(II) and Strontium(II) taking into account speciation patterns in different freshwater archetypes, applying the framework developed by Gandhi et al. (2010) with minor modifications. CTPs for Cd, Co, Cu, Ni, Pb and Zn were recalculated to ensure the methodological consistency and hence compatibility across all metals. Site-generic CTPs were calculated for all metals applying different averaging principles, and the best approach was identified.

2. Methods

2.1. General framework

CTP (PAF. day. m^3/kg) is the product of three factors: Fate Factor (FF; day), Bioavailability Factor (BF; dimensionless) and Effect Factor (EF; PAF. m^3/kg) (Gandhi et al., 2010):

$$CTP = FF \cdot BF \cdot EF \quad (1)$$

FF can be understood as residence time of total metal in freshwater environment. EF represents the ecotoxicity of truly dissolved metal, expressed as potentially affected fraction (PAF) of freshwater species. FF and EF are made compatible through BF, which is the fraction of truly dissolved metal within total metal. These parameters are further documented in Appendix A in Supplementary Information (SI).

2.2. Variation of freshwater chemistry and averaging across archetypes

7 typical Europe freshwater archetypes (EUFwArcs) were selected (Gandhi et al., 2011a) representing the variation of freshwater chemistries in Europe mainland, exclude Romania, Bulgaria and Serbia (Table S1 in SI). Each EUFwArc contains data for a set of water parameters (Suspended Particulate Matter (SPM), pH, temperature, Dissolved Organic Carbon (DOC), Particulate Organic Carbon (POC), Fe oxides, Mn oxides, Al oxides, Fe^{3+}, Al^{3+}, Ca^{2+}, Mg^{2+}, K^+, Na^+, Cl^- and SO_4^{2-}). These parameters were chosen by Gandhi and co-workers due to their major influence on the speciation of Cu, Ni and Zn. We further confirmed that it is the same set of parameters which controls speciation of the other metals covered by this study (Lofts and Tipping, 2011). For each combination of metal and EUFwArc, a CTP was calculated using Eq. (1).

To derive generic CTPs, the following approaches were tested on each metal. Assuming that there is an equal probability of receiving metal emission in each water archetype, we tested the geometric mean (CTP_{EUGeo}) and arithmetic mean (CTP_{EUAve}) of seven EU CTPs, where less weight is put on extreme archetypes when using geometric mean. We also calculated a central tendency CTP (CTP_{EUCent}) for each metal in a hypothetical "central tendency freshwater" with medium values of the concentration of major ions, DOC and pH across EUFwArcs, neglecting spatial variability. Considering that the probability of a given metal emission occurring to a specific archetype is directly correlated with the total annual metal emission to that archetype, we developed an EU emission weighted CTP (CTP_{EUWt}) according to Eq. (2), basing the weighting factors (WF) for the individual archetypes on the total annual metal emission that they receive (Table S2 in SI). Emission-based WF were calculated for each of the seven water archetypes for six of the metals (Cd, Cr, Cu, Ni, Pb and Zn), as the share of the reported annual waterborne metal emissions from industrial facilities that can be expected to go to that water archetype. For the other metals, the arithmetic mean across the WFs for the six metals was used as proxy. This is a reasonable assumption since the waterborne metal emissions were mainly from the same sources, namely urban waste water treatment plants, thermal power stations, mining and metal production (Nriagu and Pacyna, 1988; E-PRTR, 2011).

$$CTP_{Wt} = \sum_{i=1}^{n} CTP_i \cdot WF_i \quad (2)$$

where CTP_i is the metal CTP in water archetype *i*. WF_i is the weighting factor of water archetype *i*. *n* is the number of water archetypes.

In lack of better data, CTPs developed for Europe are often used for global LCIA applications (Hauschild et al., 2013). To check whether European CTPs are reasonable proxies of global CTPs, water chemistry parameters were assembled for 6 continents (Asia, Africa, Australia, Europe, North America and South America) and world average rivers and lakes (Table S3 in SI). Each of these water chemistries represents the average composition of freshwater in the given geographic context, where the variability of water chemistry within one geographic context is neglected. Using these data, CTPs were calculated for each continent and the world average rivers and lakes (CTP_{Wd}) respectively. Volume weighted CTP across continents ($CTP_{WdVolWt}$) were then calculated according to Eq. (2), by using the share of freshwater total volumes in each continent as weighting factors (Table S4 in SI). Here we assume that the damage caused by metal emission to an archetype can be judged by the relative volume share of these archetypes in the environment, since metals will eventually cause ecotoxicity in the entire water body. We also developed a surface runoff area weighed CTP across continents (CTP_{WdArWt}) by using the share of surface runoff area in each continent as WF (Table S4 in SI). This weighting method implies the assumption that each unit of surface runoff area has the same probability of receiving metal emission.

2.3. Selection of models and parameter calculations

2.3.1. Fate model and FF calculation

We assumed that metals were emitted in the form of total metal, regardless of speciation. This is in consistence with the fact that life cycle inventories usually only report total metal emission concentration. Multimedia fate model of USEtox (Rosenbaum et al., 2008) was adapted to calculate FF. Being developed from model comparison of all relevant existing LCIA models, it represents a