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Title: Development of characterization factors for metals in coastal seawater

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Short Abstract: Metal ecotoxicity Characterization Factors (CFs) in coastal seawater were not developed in USEtox for Life Cycle Impact Assessment (LCIA), due to lack of appropriate ecotoxicity data and inadequate consideration of metal bioavailability in seawater. Taking into account the speciation behavior of metals in seawater and using effect data exclusively for marine organisms, two sets of spatially differentiated CFs were developed for the metals Cd, Co, Cu(II), Ni, Pb and Zn in coastal seawater. One set of CFs (CF_{sw-sw}) addresses the direct metal emission to coastal seawater while the other set (CF_{fw-sw}) represents the ecotoxicity potential of metals in coastal seawater caused by metal emission to freshwater followed by transport to the seawater compartment, taking into account the fate of metal in freshwater and in the estuary.

CF is the product of three factors: Fate Factor (FF), Bioavailability Factor (BF), and Effect Factor (EF). The multimedia fate model of USEtox was used to calculate the FF. WHAM 7.0 was used to model metal speciation underlying the BF. Free Ion Activity Model (FIAM) was used to model EF. The results showed that for a given metal, FF in seawater was higher than in freshwater, due to longer residence time of the water in the coastal seawater than in freshwater. The difference between FF in seawater and freshwater was smaller since the difference in water residence time was partially neutralized by metal removal in estuaries. Metal BFs in seawater were similar or slightly higher than in freshwater due to the lower DOC and SPM concentration in seawater. For most metals, EFs were lower in seawater than freshwater, due to lower sensitivity of seawater biota to metals. As a general observation, CF_{fw-sw} was lower than CF_{sw-sw} due to metal removal in freshwater and estuary, but the difference was modest for most metals. For Pb, seawater CF were up to 1-4 orders of magnitude higher than freshwater CF. But for the other metals, seawater CFs were similar to freshwater CFs, indicating that the higher FF and BF in seawater were largely counterweighed by the lower EF for these metals. The variation of CFs in different coastal seawaters were up to ca. 2-3 orders of magnitude for one metal, indicating the importance of using spatial differentiated CFs. Compared with USES-LCA default CF_{sw-sw} , the new CF_{sw-sw} were at least 3 orders of magnitude lower for all metals except Pb, of which USES-LCA CF_{sw-sw} fall within the range of this study. This implied that for some metals, ecotoxicity CFs in coastal seawater might be overestimated in previous LCIA methods.

Keywords: LCIA, ecotoxicity, marine, metal