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Integrated Prediction Model for Cadmium Toxicity in Oxidized Freshwater Sediment: Emphasis on the Role of Fe Oxides and Validation with Hyalella azteca

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The evaluation of metal toxicity in sediment has traditionally involved measuring sulfide concentrations and considering organic carbon content through the sediment biotic ligand model. This model operates on the assumption that the predominant formation of insoluble metal sulfides (MeS) renders the metals unavailable for uptake by benthic organisms. Specifically, in cases where the quantity of metals exceeds that of sulfides, the model postulates that the surplus metals will partition to organic carbon. It holds relevance in anoxic environments where sulfides and organic carbon play pivotal roles in metal binding. However, heavy metals susceptible to redox changes may be released from both MeS and organic carbon, particularly in oxidized sediments. Literature indicates elevated concentrations of dissolved Cadmium under oxidizing conditions compared to reduced sediments. Such liberated metals subsequently re-adsorb onto Fe oxides, another significant phase for metal binding.

To enhance cadmium toxicity prediction, we propose an advanced model that considers contributions from both Fe oxides and organic carbon, in addition to sulfide, in oxidized sediment. Partition coefficients (K_d) for both phases were determined using the Windermere Humic Aqueous Model, version 7 (UK Centre for Ecology and Hydrology, 2012), and the relationship with pH was derived through curve fitting to optimize data fitting. Previous studies' data align well with the predicted K_d values. A comprehensive model equation for determining a total K_d, incorporating these K_d values of Fe oxides and organic carbon contents, was formulated. Upon comparison with experimental data from sediment samples collected from 21 different regions in South Korea, the model exhibited accurate predictions within one order of magnitude.

To validate the proposed model, a toxicity test was conducted using a benthic invertebrate, *Hyalella azteca*, with the same sediment samples. While the previous model predicted toxicity, the observed mortality was less than 24%, indicating non-toxicity to the organism. The new model accurately assessed toxicity and serves as a valuable tool for predicting cadmium toxicity in oxidized sediment.