Using WHAM-FTOX to understand proton and metal mixture toxicity in the laboratory and field

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It is a well-attested fact that the uptake and toxicity of cationic metals to organisms are dependent on the chemistry of the exposure medium. Considerable research effort has been devoted to development of modelling tools to understand, explain and predict these medium effects. Predominant among the developed models is the Biotic Ligand Model (BLM), which considers exposure to be directly related to metal bound to specific uptake sites (biotic ligands) on the target organism, with chemical speciation in the medium and competition for binding to the biotic ligand(s) accounted for. Similarly to the BLM, WHAM-FTOX is based around the concept of computing amounts of metal bound to the organism. However, rather than computing amounts of metals bound to assumed specific biotic ligands, WHAM-FTOX assumes that exposure to metals is proportional to the amount of metal bound by all weak-acid coordination sites on or in the organism, in equilibrium with the surrounding medium. An overall toxic response for mixtures of cations (metals and protons) is quantified as a toxicity function F_{TOX}, given by

$$F_{TOX} = \sum \alpha_i \Theta_i$$

where the exposure to each cation is given by Θ_i (the fractional occupancy of binding sites) and α_i is a toxicity coefficient specific to each cation. Amounts of bound cations are computed using the WHAM chemical speciation model, taking the amounts bound to humic acid (HA) as proxies for amounts bound to organisms. This approach has the advantage that constants for cation binding are already available, rather than needing to be derived as with the BLM, and that mixture effects are readily computed. Furthermore, the toxic effects of proton binding can be included in the mixture exposure modelling.

Initial applications of WHAM-FTOX focused on describing field community effects in freshwaters impacted by acidification and metal contamination in a number of locations including the UK and North America. Subsequent work has focused on modelling accumulation and mixture effects in laboratory toxicity tests. Most recently, the model has been used in a meta-analysis of single metal–single species laboratory toxicity data with the aim of providing a unifying picture of toxic effects through time and across metals and organisms. Collectively, this body of work demonstrates the utility of WHAM-FTOX as a unifying tool for understanding and predicting the toxicity of cation mixtures from the laboratory to the field, from single species to whole communities. Prospects for the future include the use of the model to predict mixture field effects based on calibration to laboratory data.