METAL MIXTURES MODELLING

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METAL BIOAVAILABILITY

Fact Sheet Two

Introduction

Metals are released to aquatic ecosystems from a variety of natural and anthropogenic sources (Figure 1).

Figure 1. Natural and anthropogenic sources of metals to aquatic environments.

Considerable progress has been made in the past three decades in our understanding of how metals can affect aquatic ecosystems when present at sufficiently high concentrations. In particular, we now have a much better understanding of how differences in water chemistry can affect metal toxicity. Much of this information has been incorporated into new water quality standards that ensure the protection of aquatic plants and animals, based upon bioavailability (portion of the total quantity of substance which can interact with organisms to cause toxicity; Figure 2). This Factsheet provides additional background information on single metal biotic ligand models (BLMs). Additional information on our understanding of metal mixtures and their regulation, as well as development of mixture BLMs (mBLMs) can be found in subsequent Factsheets.

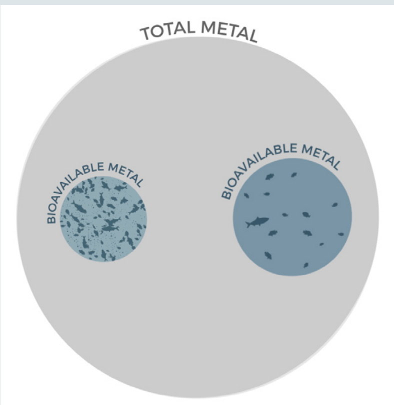

Figure 2. The bioavailable fraction of metal, the proportion that the organism experiences in the water, can be a relatively small fraction of the total amount of metal present and can vary depending on the water chemistry.

How are individual metals regulated?

Historically, water quality standards for metals have often been based on the hardness of the water, and this is one factor which affects metal bioavailability and ultimately, toxicity. However, there are other factors which can have a more important overall effect on metal bioavailability, such as water pH and the concentration of dissolved organic matter. The ways in which these water quality parameters interact with metals and each other to influence metal bioavailability have now been extensively studied leading to the development of new models such as the BLM. BLMs are used to predict metal toxicity as a function of water chemistry, and are now routinely being used in setting metal water quality standards in many parts of the world.

While water quality standards for regulating individual metals in aquatic systems are now well-developed, we know that multiple metals are present both naturally and due to anthropogenic influences in aquatic systems. Consequently, consideration of metal mixtures presents an important scientific and regulatory challenge that is now beginning to be addressed. When multiple metals are present, they can interact to influence the relative bioavailability of each metal and also interact within an aquatic organism to influence toxicity, making regulation of metal mixtures more complicated than for individual metals.

To meet this challenge, there has been a concerted effort to extend existing single metal BLMs to account for the bioavailability and toxicity of metal mixtures. Efforts to date have been quite successful and indicate modelling tools like mBLMs could be used to regulate metal mixtures in the future (metalsintheenvironment.com).

Is water chemistry important for the aquatic toxicity of metals?

The chemical characteristics of the water in which exposure occurs is as important a consideration as organism sensitivity to the metal of interest when assessing potential ecological effects in aquatic systems. Historically, the key water chemistry characteristic that has been accounted for in regard to predicting potential metal toxicity is hardness. Calcium, one of the main components of water hardness has been shown to compete with some metals for uptake by organisms. However, the scientific evidence indicates for many metals other factors like dissolved organic carbon (DOC) and pH can be as, or more, important than water hardness.

These water chemistry characteristics can influence the form or species of the metal in the water column and so govern the potential ecotoxicological effect. Bioavailability of metals to aquatic organisms can be considered to be a combination of the physico-chemical factors governing metal behaviour and the specific physiological characteristics of the organisms (Figure 3). Effectively this means that a measure of bioavailability will reflect the exposures that organisms in the water column actually ‘experience’. The distribution of metal between different components of the solution, like complexes with organic matter or inorganic species, can be calculated reliably for simple systems using an equilibrium speciation model. The “speciation” of the metal describes the different forms that the metal is present in.

What are Biotic Ligand Models?

A BLM is a type of equilibrium chemical speciation model that can predict metal bioavailability to aquatic organisms given information about the water chemistry and the sensitivity of the organisms. They do this by calculating the distribution of the metal between the solution, inorganic ligands and organic matter that bind metals, and the organisms. In order to do this, the behaviour of other ions present in the water, like sodium, magnesium, and calcium, also needs to be considered.

The BLM is a combination of two chemical equilibrium models, one of which describes the inorganic behaviour of the metal in the solution, and the other describes its interactions with organic matter and the organism, which is treated as just another ligand in the system. Other ions present in the water can affect the interactions of the metal with both the organisms and organic matter in the solution (Figure 3). Historic hardness based thresholds took account of the effect of some these other ions (e.g., calcium) on metal interactions with the organism, but did not take account of any of the other factors which affect bioavailability. Metals bind to the gills (or other respiratory surface) of the organism, and it is the concentration of metal at the gill that determines the toxicity.

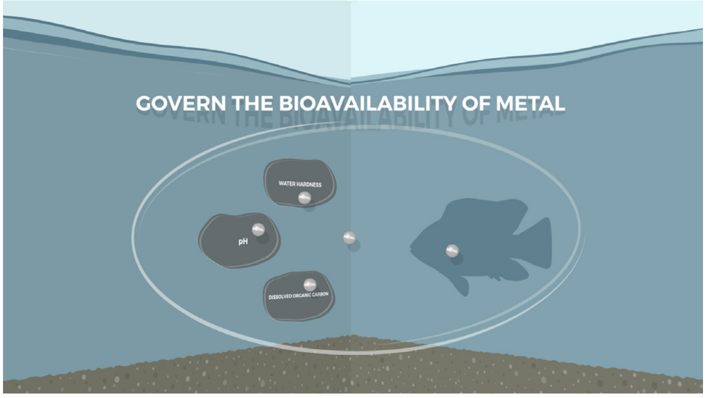

Figure 3. Bioavailability of a metal to an aquatic organism can be predicted from the Biotic Ligand Models, from measurements of water chemistry.

Overall the most important single factor in defining metal toxicity is usually the DOC concentration, which forms complexes with metals making them less bioavailable. pH also has a similar effect on metal toxicity to that of calcium, but as the effect is due to competition from protons lower toxicity is typically observed at low pH. Hardness concentrations and pH often co-vary in natural waters, so soft waters usually have a low pH, and hard waters typically have a high pH. The competing effects of hardness and pH on metal toxicity balance each other out to some extent, meaning that overall the DOC concentration is usually the single most important parameter.

Summary

Water chemistry can influence the behaviour, fate and ecotoxicity of trace metals. Biotic ligand models provide a method to predict both chronic and acute effects for single metals from measurements of water quality. However, metals are often present as mixtures in the environment, leading to interest in the development of models and regulations for metal mixtures. Additional information on metal mixtures and development of mBLMs can be found at metalsintheenvironment.com.