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IRON AND ALUMINIUM SPECIATION IN SWEDISH FRESHWATERS

Implications for geochemical modelling

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ABSTRACT

Speciation governs transport and toxicity of trace metals and is important to monitor in natural waters. Geochemical models that predict speciation are valuable tools for monitoring. They can be used for risk assessments and future scenarios such as termination of liming. However, there are often large uncertainties concerning the speciation of iron and aluminium in the models, due to the complicated chemistry of these metals. Both are important in governing the speciation of other metals, due to (i) their capacity to form minerals onto which metals can adsorb and (ii) their ability to compete for binding sites to natural organic matter (NOM). Aluminium is also potentially toxic and is therefore closely monitored in acidified freshwaters. In this study different phases of iron in Swedish lakes were characterised. This required a good method for preconcentrating the iron colloids. A new method was developed in this thesis that uses an anion-exchange column to isolate the iron colloids prior to characterisation with extended X-ray absorption fine structure (EXAFS) spectroscopy. Iron was present as ferrihydrite in particles but was also strongly monomerically complexed to NOM in two Swedish lakes. Based on the results an internally consistent process-based geochemical equilibrium model was presented for Swedish freshwaters. The model was validated for pH ($n = 9\ 400$) and inorganic monomeric aluminium (Al_i) ($n = 3\ 400$). The model could simulate pH and Al_i simultaneously, and be used for scenario modelling. In this thesis, modelling scenarios for decreases and complete termination of liming are presented for the 3 000 limed Swedish lakes. The results suggest that liming can be terminated in 30 % of the Swedish lakes and decreased in many other lakes.

Keywords: Geochemical equilibrium modelling; pH; adsorption to ferrihydrite; metal-NOM complexation; liming; EXAFS spectroscopy

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