Experimental and Theoretical Characterization of Metal Complexation with Humic Acid

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ABSTRACT

This study investigated the bonding of calcium and magnesium to specific sites in humic acid as a function of pH, temperature, and trace metal concentrations. Other metals were investigated but not in detail. Using a surface complexation model with well-defined phenolic and carboxylic sites in humic acid, the fractions of calcium/magnesium and trace metals that bond with the various sites were quantified. These sites were also classified as monodentate or bidentate. The goal of the study was to understand the conditions that favor calcium/magnesium bonding to bidentate humic acid. Therefore, adsorption measurements were performed followed by surface complexation simulations. The total metal and labile metal ion formed in the ultrafiltrate were determined by inductively coupled plasma mass spectrometry and square-wave anodic stripping voltammetry, respectively. The results showed that the adsorption capacity of each metal to humic acid was influenced by pH and metal loading. For example, zinc(II) and copper(II) were statistically different in their adsorption capacities. The Morel and Dzombak surface complexation models showed stronger lead and copper interactions with monodentate sites compared to bidentate sites. The phenolic sites were weakly involved in bonding, and the bonding capacities of calcium and magnesium ions to phenolic or carboxylic were pH dependent. For example, lead(II) used only 5% of bidentate carboxylic–phenolic sites at 45°C showing 95% favorable calcium/magnesium bonding to these sites in humic acid. These results may allow substantial scale reduction.