Application of Spectroscopic Methods to Sorption Model Parameter Estimation

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Macroscopic data for the sorption of Co(II), Cd(II) and Sr(II) to α-Al₂O₃ were used in conjunction with x-ray absorption spectroscopy (XAS) data to estimate triple layer (TLM) surface complexation model parameters. The XAS results showed that Co(II) and Cd(II) sorbed as inner-sphere surface complexes and that Sr(II) sorbed as an outer-sphere complex. In addition, surface precipitation was observed only in the case of Co(II) sorption. Surface complexation model reactions were selected based on the XAS results for each divalent metal ion, and surface acidity constants were determined using potentiometric titration data. A solid solution version of the TLM that appears to be consistent with the spectroscopic data was used to describe the sorption of Co(II). The modeling results predicted that Co(II) sorption is dominated by mononuclear surface complexes at low surface coverage and by Co(II)/Al(III) surface precipitates at high surface coverage. In order to model the Cd(II) sorption data throughout the range of data presented by Honeyman (1984), it was necessary to incorporate a second high energy surface hydroxyl site. In contrast to the Co(II) data, it was not necessary to incorporate a solid solution model to predict sorption data collected at high coverage. The effects of ionic strength on Sr(II) adsorption to α-Al₂O₃ could be described using two outer sphere reactions. The results shown in this chapter demonstrate the effectiveness of surface complexation models when the selection of surface reactions and parameter estimation are constrained by independent measurements.

INTRODUCTION

The prevalence of toxic metal ions in contaminated aqueous and terrestrial environments represents a significant environmental risk. Effective pollution con-