

Modeling interactions at the tributyltin–kaolinite interface

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Received 12 November 2002; received in revised form 22 October 2004; accepted 25 October 2004

Abstract

Tributyltin (TBT) is a common pollutant in natural environments and the interaction with mineral surfaces largely determine its solubility, speciation, bioavailability, and transport in aqueous systems. The present work aimed at quantifying the TBT adsorption using kaolinite and a kaolinite-rich sediment as sorbent materials. Experiments were conducted under conditions that are important from an environmental perspective. Proton adsorption data were determined for kaolinite as a function of pH and electrolyte concentrations to ascertain intrinsic acidity constants and site density values. The pH_{zpc} of kaolinite sample KGa was determined at 4.9 by surface titration.

The generalized diffused double layer model (DLM) was used to quantify both, proton and TBT adsorption. Following intrinsic acidity and TBT binding constants resulting from the TBT/kaolinite system were used: $>\text{SOH} \Rightarrow >\text{SO}^- + \text{H}^+$, $\log K = -5.4$; $>\text{SOH} + \text{H}^+ \Rightarrow \text{SOH}_2^+$, $\log K = 4.6$; $>\text{XNa} + \text{H} \Rightarrow \text{XH} + \text{Na}^+$, $\log K_{\text{X/H}^+} = -1.1$; $>\text{SO}^- + \text{TBT}^+ \Rightarrow >\text{SOTBT}$, $\log K = 3.5$; $>\text{XNa} + \text{TBT}^+ \Rightarrow \text{Na}^+$, $\log K_{\text{X/TBT}} = 1.0$. All surface-active variable charge sites on kaolinite, namely $>\text{AlOH}$ and $>\text{SiOH}$ are grouped and collectively refer to as $>\text{SOH}$ in this paper. $>\text{XNa}$ refers to ion exchange sites. Modeling of TBT adsorption onto kaolinite was conducted distinguishing selective (high affinity) sites ($>\text{S}_5\text{OH}$) in addition to non-selective sites ($>\text{SOH}$). The inclusion of $>\text{S}_5\text{OH}$ was essential in order to quantify TBT adsorption successfully, while the inclusion of $>\text{XNa}$ was optional. The reduction of surface coverage values by a 10-fold TBT adsorption modeling is in agreement with the results of molecular model calculations of the system. Parameters calculated for the monophase kaolinite were subsequently used to quantify the TBT adsorption onto kaolinite-rich sediment.

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Keywords: TBT; DLM; Kaolinite; Adsorption; Surface complexation; Sediments
