

**Title: The application of surface complexation modeling to the adsorption of uranium(VI) on natural composite materials**

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**Abstract:** Surface complexation modeling using the component additivity (CA) and the generalized composite (GC) approaches is illustrated for describing uranium(VI) sorption on the carbonate-free Naturita material. The carbonate-free Naturita material was prepared from a natural composite material from the Naturita site, Naturita, Colorado where carbonate minerals were removed using sodium acetate at pH 5. The sorption experiments were conducted over the pH range of 7.0–9.0, total U(VI) concentrations of  $10^{-7}$  to  $10^{-5}$  M, solid concentrations of 50 and 100g/L, and CO<sub>2</sub> partial pressures of atmospheric and 0.02 atm. Uranium(VI) sorption data is successfully simulated using the generalized composite approach with only five adjustable parameters including four bidentate surface species [ $\text{SO}_2\text{HUO}_2^+$ ,  $\text{SO}_2\text{H}_2\text{UO}_2(\text{CO}_3)_2^{2-}$ ,  $\text{YO}_2\text{UO}_2$ , and  $\text{YO}_2\text{UO}_2(\text{CO}_3)_2^{4-}$ ] and a strong U(VI) binding site with a density of  $0.031 \mu\text{mol}/\text{m}^2$ . The CA approach is conducted using diffuse double layer model (DDL) for well characterized carbonate-free Naturita material. The CA approach is successfully applied to predict the U(VI) sorption on the carbonate-free Naturita material through an analysis of the component sorbents. For the CA model, sorption sites in the carbonate-free Naturita material were associated with ferrihydrite-like sites. Site concentrations were based on chemical extraction. Micro-synchrotron X-ray Fluorescence Spectroscopy (micro-SXRF) and micro-X-ray Absorption Near Edge Structure Spectroscopy (micro-XANES) also confirmed the strong association between U(VI) and iron oxide phases.

The CA model presents a better prediction for the same U(VI) sorption data than the GC model based on the goodness-of-fit values. The comparison of the CA and GC approaches shows that the GC approach requires less information and laboratory data. Moreover, the GC approach is useful for immediate and practical application. In order to apply the CA approach, detailed information on mineral surface compositions including characterization and quantification of surface coatings is required.