# Reconstruction of Water Quality from Adsorbed Heavy Elements in Sediment: Surface Complexation Modeling of Trace Uranyl Adsorption on Iron Oxide

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Since the birth of the earth, the earth's surface environment has undergone various changes. How the nature of water on the earth (water quality) has been responded to the environmental changes is essential to understand the origin and evolution of life. Also, the understanding of the changes of water quality that had been occurred in planets which possess water is essential to evaluate the possibility of existence of life. The most important and fundamental parameter that indicates the chemical nature of water is pH. It controls the chemical behavior of elements in water via dissolution, precipitation and complexation, and dominates the transfers of energy and substance through water. In geology, the past water quality is reconstructed from proxies left in sediments and fossils (geological records) at the time, but there is no versatile proxy of pH at the moment.

Natural water contains various trace elements. These trace elements adsorb to mineral surface depending on water condition such as pH. Therefore it is possible to consider that trace elements adsorbed on mineral record the information about the water quality during the adsorption. Thermodynamic adsorption model called “surface complexation modeling (SCM)” can theoretically predict the adsorption behavior of trace elements as a function of water quality. Application of SCM inversely is capable to predict the water quality from adsorption behavior of trace elements. The goal of the present study is to develop the methodology for the reconstruction of water quality using SCM from the trace elements information of sediments.

One of heavy elements contained in relatively high concentration in natural water is uranium (U). U thermodynamically exists as a hexavalent valence U(VI) under the condition that the oxygen partial pressure is approximately $10^{-50}$ atm or higher. U(VI) possesses relatively high solubility and therefore high mobility, but U(VI) has the nature for strongly adsorbing on iron oxide. U(VI) adsorption on iron oxide is frequently observed in nature. For example, previous study reported that U(VI) concentration of the sediments core from the continental ancient lake (Lake Hovsgol) varies with age. It is pointed out that the fluctuating U concentration may be explained by adsorption and desorption processes on iron oxide.

In this study, we conducted the adsorption experiments of trace amounts of uranium with iron oxide at laboratory and tried to parameterize the adsorption behavior using SCM from the obtained experimental results. Then we attempted to reconstruct the paleo water quality of Lake Hovsgol using the constructed surface complex modeling.

Keywords: adsorption, trace heavy element, iron oxide

 