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Kinetic and Thermodynamic Modeling Approaches of Selenium by Man-Made and Natural Geological Barriers for Nuclear Waste Management

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Some components of nuclear wastes like ^{79}Se should be taken into consideration due to extremely long half-lives and potential migration ability through the environment. Clay minerals are suggested as a barrier material in radioactive waste management; however they have some deficiencies to retard anionic radioisotopes like selenium due to structural properties. Modification of these minerals may help to improve their retardation ability toward these anionic radioisotopes. There are two predominant reasons for limiting selenium in water: a major limiting factor is the possible damage to plants and crops and selenium can represent reproductive dangers for human.

The study of sorption kinetics is significant as it provides valuable insights into the reaction pathways and into the mechanism of sorption reactions. The reaction can be defined by a sequence of processes that control the rate, diffusion of ions through particle film, diffusion through the particle and chemical reaction with the functional groups. This paper is dedicated to kinetic performance for selenium removal by selenium selective adsorbent. Batch kinetic experiments were performed using a solution containing 250 mg Se/L (pH 4.0) and 40 mg of inorganic pillared bentonite (OPBent) at three different temperatures and at a certain shaking rate. The selenium concentrations of the samples were monitored by taking the samples from the solution at defined times. The samples were analyzed by high resolution gamma spectroscopy system. The kinetic data obtained were evaluated using classical kinetic models and diffusion/reaction models. The transport mechanism of selenium which comprises a diffusion process from aqueous phase to organo-inorgano-bentonite was described by two kinetic models consisting of derived equations: the homogenous particle diffusion model (HPDM) and the shell progressive model (SPM). The effective particle diffusion coefficient D_{eff} values derived from both the HPDM and SPM equations were compared. The mechanism of selenate sorption by OPBent has been postulated from the experimental results.

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