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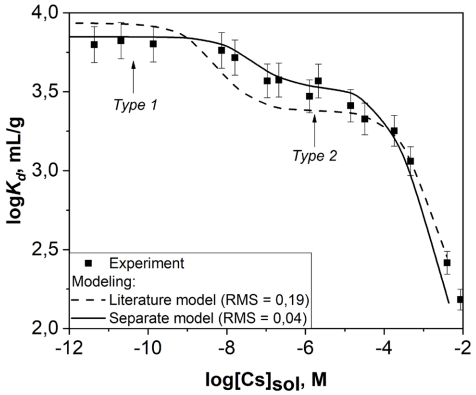
Cesium interaction with bentonite clays: role of unique properties in sorption modeling

IRINA MENSHIKOVA-TONYAN[1], ANNA SEMENKOVA[1], VALENTINA SVITELMAN[2], VICTORIA KRUPSKAYA[3], ANNA ROMANCHUK[1] AND STEPAN KALMYKOV[1]

[1]Lomonosov Moscow State University
[2]Nuclear Safety Institute of Russian Academy of Sciences
[3]Institute of Geology of Ore Deposits, Petrography, Mineralogy and Geochemistry (IGEM) RAS



To guarantee the safety of high-level radioactive waste (HLW) over hundreds of thousands of years, it is essential to establish protective engineering barrier systems. Bentonite clays, known for their low water permeability and high sorption capacity, are considered a key material for such barriers. Among the radionuclides requiring attention are Cs isotopes, which are byproducts of uranium fuel fission and are notable for their high environmental mobility and biotoxicity. To ensure the long-term safety of HLW disposal sites, it is crucial to develop mathematical models that describe sorption processes.

In this work, we compare the behavior of Cs in its interaction with 11 different bentonite clays to determine the dependence of sorption on their individual characteristics such as CEC, SSA, and mineral composition. Samples of bentonite clays from all over the world were used: lesser-studied deposits were represented by samples from Dash-Salakhly (Republic of Azerbaijan), Taganskoye (Kazakhstan), Kutch (India), widely studied clays included samples MX-80 (USA), FEBEX (Spain), Kunipia-F (Japan) and other.

Sorption isotherms in wide range of Cs^+ concentrations were investigated. Almost for all samples 2 plateaus on Cs sorption isotherms were observed, that indicates the existence of different types of sorption sites. The presence of multiple sorption sites is independent of the composition of clay minerals.

Existing approaches to the description of cesium sorption include models with different types of sites. The results of simulation with 6 literature approaches showed the best correlation with experimental data for approaches using two types of sites. However, these approaches did not accurately describe all dependencies, and obtained concentrations of sorbed sites did not correspond to their individual characteristics.

To improve the accuracy of modeling, approaches based on optimization of reaction constants and concentrations of sorption sites were proposed. The parameters were optimized for each specific isotherm, as well as for all dependencies together. Based on the optimization results, the values of the constants $\log K_1$ = 6.48 for highly and $\log K_2$ =1.35 for low-selective centers with separate optimization and $\log K_1$ = 6.00 and $\log K_2$ =1.61 for joint optimization, respectively, were proposed.

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