New simulation model for predicting bentonite clay swelling in nuclear waste disposal

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Bentonite clay is planned to be used as a key barrier in the deep geological disposal of high-level nuclear waste. To ensure the safety of disposal, it is crucial to understand and predict the swelling behaviour of bentonite clay. The swelling property is, however, regulated by multiple structural and environmental factors. A new spring model developed at the University of Eastern Finland simulates the atomic-level interactions among the components of clay-water system, reproducing the swelling trends and swelling pressures measured by experiments with good accuracy.

The central function of bentonite clay is to protect the waste canisters, so that these canisters do not get in contact with underground water and other possible corrosive agents, such as bacteria. The plasticity of bentonite clay also helps the canister to stay intact against mechanical forces, such as rock movements or earthquakes. Therefore, the swelling behaviour of the bentonite buffer is crucial for disposal safety. Swelling pressure, as an important quantitative indication of the swelling potential of bentonite clays, is hence considered as a key criterion in the selection of candidate smectite clay minerals.

The structure and physio-chemical nature of bentonite is very complex, and moreover, the swelling behaviour depends on multiple interrelated structural and environmental factors. The joint effects are, however, difficult to be investigate experimentally. The study employed a

molecular dynamics technique to investigate the effects of multiple factors on the swelling behaviour of clay, and developed a spring model to simulate the atomic-level interactions among the components of clay-water system.

The swelling pressure of Na- and Ca-clays with varying layer charge and charge distribution was systematically analysed. In Na-clays with layer charges of -0.5 to -1.0e per unit cell, the swelling pressure correlates inversely with the layer charge. Montmorillonite-like clays bearing dominant octahedral charges have a higher swelling pressure than beidellite-like clays that bear dominant tetrahedral charges. In contrast to Na-clays where substantial swelling pressure readily develops after initial hydration, Ca-clays are seen to lose their swelling pressure as soon as the swelling initiates. The model also found that an increase in water salinity decreased the swelling pressure, and a decrease was more evident in calcium chloride solutions than in sodium chloride solutions. In addition to the qualitative prediction of swelling pressure, the new spring model also shows quantitative agreement with experimental measurements.

The new computational approach can be extended to other clay systems and is expected to be useful in the prediction and comparison of the swelling pressure of bentonite clay over a range of potential candidate materials and variations in the clays, either in the context of deep geological disposal of nuclear waste or other industrial applications relating to swelling clays.

The findings were originally published in *Journal of Physical Chemistry C*.

More information: Linlin Sun et al. Estimation of Montmorillonite Swelling Pressure: A Molecular Dynamics Approach, *The Journal of Physical Chemistry C* (2015). DOI: 10.1021/acs.jpcc.5b04972