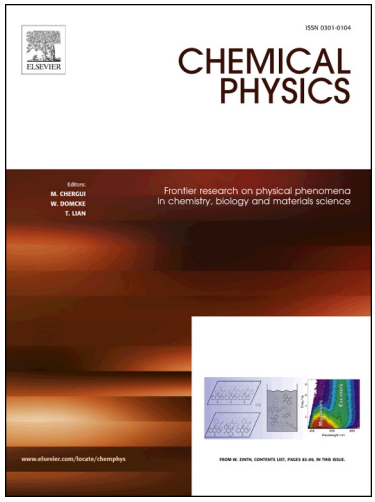

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Influence of Temperature on the Swelling Pressure of Bentonite Clay

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ABSTRACT

The swelling pressures of bentonites have been studied extensively due to their potential use as a barrier in radioactive waste disposal repository. Due to the radioactive decay of the waste, the temperature will increase in the repositories. Several experimental studies of the temperature dependence of the swelling pressure of smectites have been published while theoretical studies have received less attention. Atomic level simulations have been proven to be useful in broadening the understanding of clay materials in various conditions. Therefore, molecular dynamics simulations were carried out to predict thermal effects on the swelling pressure of a sodium smectite clay. The study focused on two temperature regimes. In the first regime, the clay was placed in a frozen environment and heated while the second regime involves heating the clay-water system from room temperature. At low temperatures gradual melting is observed and the onset of the swelling takes place around 250 K. At temperatures in the range of 300 K-600 K a slight increase in the swelling pressure is observed. The results can be used to rationalize experimental findings in the swelling pressure studies of smectite clays.

Keywords: Sodium smectite, Radioactive waste, Thermal effect, Molecular dynamics.

Graphical Abstract