Tracing the degree of structural H- and O-isotope exchange in smectite during bentonite-water interactions over a thermal gradient

Bentonites are rocks formed when ash from volcanic eruptions settles and is compacted over thousands of years. During this time, most of the ash is chemically changed into a type of clay mineral called smectite. Smectite is the primary component of bentonite rocks. The structure of smectite is like a sandwich, whereby, one octahedral sheet is between two tetrahedral sheets and these three sheets combine to form a layer. The sheets are arranged in an ideal chemical structure, like building blocks set in a pattern. However, in nature, other elements may substitute into the structure, creating deviations from the ideal pattern. These substitutions take place quite predictably because they are controlled by the amount specific elements are attracted to each other and their sizes; this creates different types of smectites with different chemical and structural characteristics. The 3-sheet layers of a smectite can be stacked together, where the contact between the layers is called the interlayer space. This interlayer space can open or expand to allow positively charged particles (cations) and water molecules inside. Water molecules contain the elements hydrogen (H) and oxygen (O). H has two stable isotopes, ^{1}H and ^{2}H, while O has three, ^{16}O, ^{17}O, and ^{18}O. Stable isotopes do not undergo radioactive decay like radiogenic isotopes, which makes them useful to track interactions between rocks, minerals, and fluids.

The stable H- and O-isotope composition in smectite can be used to track the interaction between bentonite rocks and water. Tracking can be done because the layers of the smectite have the elements O and H in it and since the structure and water contain the same elements, they can trade or share H- and O-isotopes, meaning the ratio of ^{2}H to ^{1}H may be higher in the rock or water depending on the conditions they were exposed to (amount of heat). It is generally known that greater exchange of isotopes will happen at higher temperatures and that exchange will be more for H and less for O. What is not known, is the degree of exchange that will happen between the smectite OH and water, as a function of temperature. It is also unclear how the substitutions in the different types of smectites will change the degree of isotope exchange between smectite and water. A change in the way a specific smectite interacts with water when heated, can indicate that it (and hence the bentonite rock) has lost or had some of its useful expansion characteristics changed, which may make it not as effective for the application it was intended.

The expansion and liquid adsorption abilities make smectite-rich bentonite rocks beneficial in everyday life. Applications for bentonites range from cat litter and pharmaceuticals to use in landfills or nuclear waste storage as geotechnical barriers. Currently, radioactive waste from nuclear power generation is stored at or near the Earth’s surface, leaving it vulnerable to natural and human hazards. A safer alternative in the form of underground Deep Geologic Repositories (DGR) is being studied and constructed in several countries. The concept involves emplacing metal canisters with nuclear waste in a storage facility ~500m underground for the ~1 million years needed for radioactive waste to decay to a safe level. Bentonites are a very important component of the DGR environment and are being studied for use as a geotechnical barrier to protect the metal canisters from corrosion and prevent leakage into groundwater systems. Radioactive decay generates heat, so the bentonite barrier must also provide effective containment at temperatures of ~100°C. A fundamental and comprehensive understanding of how different bentonites interact with heat and water in the DGR environment is of vital importance for determining their ability to provide long-term effective containment and functionality for local and global safety.

The primary objective of this project is to track how much H- and O-isotope exchange will happen between the smectite structure of a specific bentonite and water, as temperature increases, to understand if the usefulness of the bentonite will be compromised. This will be done using different bentonites, from the Alternative Buffer Material 2 & 5 experiments at the underground Äspö Hard Rock Laboratory in Sweden, that were saturated with water and heated at different temperatures for up to 7 years.

Data comparison between the samples, saturation water, and unheated reference materials will be used to track the amount of H- and O-isotope exchange at different temperatures and how the chemical and structural differences in each bentonite contribute to these changes. This will help identify any changes to the useful properties of a bentonite, including its adsorption and containment abilities.
A combination of reliable and new state-of-the-art equipment and scientific methods of H and O isotopes composition determination, including one recently developed by the applicant, will help in producing both quality data and results.

This project has potential impacts to answer fundamental questions about bentonite rock-water interactions that have persisted in the scientific literature for decades and can also provide useful information regarding the stability of different types of bentonite for the safe, long-term containment of nuclear waste.