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Experimental validation of Swy-2 clay standard's PHREEQC model

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One of the challenges of the present century is to limit the greenhouse gas emissions for the mitigation of climate change which is possible for example by a transitional technology, CCS (Carbon Capture and Storage) and, among others, by the increase of nuclear proportion in the energy mix. Clay minerals are considered to be responsible for the low permeability and sealing capacity of caprocks sealing off stored CO_2 and they are also the main constituents of bentonite in high level radioactive waste disposal facilities. The understanding of clay behaviour in these deep geological environments is possible through laboratory batch experiments of well-known standards and coupled geochemical models. Such experimentally validated models are scarce even though they allow deriving more precise long-term predictions of mineral reactions and rock and bentonite degradation underground and, therefore, ensuring the safety of the above technologies and increase their public acceptance. This ongoing work aims to create a kinetic geochemical model of Na-montmorillonite standard Swy-2 in the widely used PHREEQC code, supported by solution and mineral composition results from batch experiments.
Several four days experiments have been carried out in 1:35 rock:water ratio at atmospheric conditions, and with inert and CO_2 supercritical phase at 100 bar and 80 ^{0}C relevant for the potential Hungarian CO_2 reservoir complex. Solution samples have been taken during and after experiments and their compositions were measured by ICP-OES. The treated solid phase has been analysed by XRD and ATR-FTIR and compared to in-parallel measured references (dried Swy-2). Kinetic geochemical modelling of the experimental conditions has been performed by PHREEQC version 3 using equations and kinetic rate parameters from the USGS report of Palandri and Kharaka (2004). The visualization of experimental and numerous modelling results has been automatized by R.
Experiments and models show very fast reactions under the studied conditions and increased reactivity in presence of $scCO_2$. A model sensitivity analysis has pointed out that the continuously changing solution composition results cannot be described by the change of the uncertain reactive surface area of mineral phases in the model and still several orders of magnitude different ion-concentrations are predicted. However, by considering the clay standard's cation exchange capacity divided proportionally among interlayer cations of Na-montmorillonite, the measured variation can be described on an order of magnitude level. It is furthermore indicated that not only the interlayer cations take part in this process but a minor proportion of other, structural ions as well, differently in the reference and $scCO_2$ environments. Experimental methodological aspects of the work, such as solution sampling, solid sample post-experimental treatment, solution and solid sample analysis sensitivity, expected experimental by-products etc. are also to be addressed.