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Reactive transport modeling to quantify swelling of clay-sulfate rocks

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The processes underlying the swelling of clay-sulfate rocks are complex and have been the subject of numerous previous investigations. In general, the transformation of anhydrite into gypsum, which is accompanied by a volume increase of 61 %, is considered the main mechanism of swelling. The process is typically initiated by a change in hydraulic conditions, followed by influx of water and a change in geochemistry. However, hydraulic and geochemical changes in the swelling zone, which may be induced by construction measures and borehole drillings, remain difficult to assess.

In this study, a numerical reactive transport model was developed for a study site in SW-Germany, where geothermal drillings led to significant swelling in clay-sulfate rocks, heaves at the ground surface and large damage of houses. A dual-domain reactive transport modeling approach was employed to investigate and quantify the importance of groundwater influx and geochemical reactions within the swelling zone. The observed swelling process was conceptualized through (i) a mobile domain that accounts for water flux and solute transport along preferential flow paths (PFP); and (ii) an immobile 'reactive' domain considering the rate-limited transformation of anhydrite into gypsum. The model was calibrated by optimizing adjustable model parameters until the calculated volume changes that result from the simulated transformation of anhydrite into gypsum agreed with geodesic heave measurements at the ground surface. The calibrated model is capable of closely replicating the heave measurements that were taken prior to the mitigation measures that were implemented at the site. The reaction rate constants for anhydrite dissolution and gypsum precipitation that were determined during the model calibration were, not unexpectedly, lower than the corresponding constants reported from laboratory experiments. It was found that transport by PFP as well as the mass transfer between the mobile and immobile domains and therefore water availability - impose a strong control on the magnitude and spatial extent of the simulated swelling process. With the calibrated model, we investigated various transient water influx scenarios representing hydrological changes after mitigation measures took effect. The scenario model predictions were validated against geodesic heave measurements.