Geochemically coupled 2D models reproduce the formation of transition zones within potash seams

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In Germany, salt deposits play an important role as industrial raw material as well as sites for energy storage. However, in geological fault zones, the contact with migrating groundwater can lead to the formation of geogenic caverns that are filled with gas and brine. These brine occurrences belong to the most significant risks in salt mining as they can cause mine flooding and land subsidence. Especially within highly soluble potash seams, the interactions between brine and salt rock result in cavernous structures surrounded by moisture penetration zones (hereinafter referred to as transition zones). In order to facilitate an early detection and a safe long-term retention of geogenic caverns, the temporal and spatial development of these transition zones was simulated.

In a first step, the software PHREEQC (Parkhurst & Appelo, 2013) and a polytherm dataset for the hexary system Na-K-Mg-Cl-SO₄-Ca-H₂O from THEREDA were used to investigate the dissolution behavior of different potash salts. A titration model based on thermodynamic equilibrium showed that the components within a potash seam are only partly converted into secondary minerals. Brine composition and precipitations mainly depend on the ratio between kieserite and sylvite and the dissolution process only stops if water, kieserite or sylvite is fully depleted. As a consequence, 1 kg of brine can influence several tens of kilograms of potash salt. A 1D model in PHREEQC implied that the transition zone between a cavernous structure and the unaffected rock can be divided into different mineralogical regions, containing secondary minerals like glaserite, leonite or kainite besides halite. A comparison with measured data from a natural brine occurrence validates the model results. However, these models do not include temporal or spacial scaling.

The titration model in PHREEQC was then used as a basis for the coupling of chemistry and hydraulics which is done in Python. Transport processes free and forced convection as well as diffusion are taken into account. A 2D model of the potash seam was built considering the stratification of the rock as well as changing permeabilities due to geological fault zones and dissolution and precipitation. Cavern and transition zone are assumed to be porous media which coincides with field measurements from K+S. In the area of the dissolution front, the amount of dry potash salt that is made available for chemical reactions is controlled by a dissolution rate. Apart from that, thermodynamic equilibrium is assumed within the transition zone but a temporal
scaling is still given based on the exchange rate. Besides sensitivity analyses, several scenario analyses for varying initial and boundary conditions have been done. The results are compared to a natural transition zone in a german mine and provide important insights into the long-term development of natural cavern systems within potash seams.

References: