Modelling the geochemical impact of hydrogen interaction with minerals and aqueous species using GEM-Selektor geochemical modelling package

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Prior to implementing large-scale underground hydrogen storage, its practicality regarding possible interaction among existing phases in the reservoir is critical. Geochemical modelling and study of possible reactions that could occur as a consequence of hydrogen injection, is one of the key steps in assessing feasibility of large scale underground hydrogen storage.

The available dataset from the upper Austria Molasse basin was used to build a geochemical model. The geochemical model involving hydrogen, formation water and minerals was setup using GEM-Selektor (GEMS) package. The SUPCRT92 thermodynamic database of GEMS, was selected as the core database for the modelling. Thermodynamic data of the mineral assemblage has been reviewed and solid solutions for clay minerals were created and integrated into the core thermodynamic database.

Initial equilibrium status of the reservoir considering formation water, minerals and gas phase at *in situ* P = 107 bar and T = 40°C was evaluated and then new equilibrium status of reservoir re-evaluated by considering hydrogen in the system. Despite limitations and uncertainties of geochemical modelling, such as not considering kinetic rates in the modelling, the main results can be summarized as follows: (1) as H_2 introduced, CH_4 is formed, (2) H_2 only appears in the gas phase when enough amount of H_2 gets injected, (3) there is a decreasing trend in the contribution of H_2 to reactions in aqueous, gas, and mineral phases with increasing amount of injected H_2, (4) there is an increasing trend in pH as H_2 is injected, and (5) as the system is titrated by H_2, some mineral alterations (dissolution and precipitation) are observed. These results will be validated by further experimental data.

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