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Evaluating the uncertainty in geochemical modelling for CO_2 storage. The example of Ketzin.

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Several sources of uncertainty are associated with geochemical modelling of reservoirs considered for CO_2 storage : on one hand only few available data are generally available for a particular reservoir, which are affected by measure errors, and whose representativity is in most cases questionable; on the other hand, the phenomenological description itself of the chemical fluid-rock interactions relies heavily on experimental determination of physical observables, which are summarized in a thermodynamical and chemical databases used by the numerical simulators. The latter is for example the case of the CO_2 disposal in saline aquifer, where the high ionic strength of the formation fluid requires a Pitzer ion interaction model to evaluate with sufficient accuracy the activities of the considered species. Typically, parameters for Pitzer model are discordant following different authors and data related to a conspicous number of relevant ions are often unavailable or unreliable -i.e. derived for different P/T conditions or ionic strength of the solution -, which makes very difficult to estimate the accuracy of the predictions.

This contribution presents our effort in evaluating the reliability of chemical simulations in the case of Ketzin on-shore CO_2 storage project. Based on available fluid and mineralogic analysis, an initial equilibrium model was determined, i.e. matching both the observed fluid composition and the saturation with the mineral phases present in the sandstone layer of the Stuttgart formation which constitutes the reservoir. A sensitivity analisys based on small perturbations of such initial model was then performed, in order to assess the influence of measurement errors and possibly define a compositional range which can be assumed in spatially variable simulations. This step is then followed by the sensitivity to the Pitzer parameters that are collected in the chemical database used throughout this study; both the parameters themselves and their dependence on temperature are investigated. To reduce the number of degrees of freedom of all possible simulations while dealing with systems with several components, some strategies from the theory of Experimental Design have been applied; all modelling was performed using the chemical equilibrium and speciation program `PHREEQC` and a newly developed interface to the statistical environment `R`.

Finally, simple 1D reactive transport simulations modelling the injection of pure CO_2 were made to highlight the influence of spatially variable initial concentrations, of the solubility model for CO_2 in saline water and the dissolution and precipitation kinetics of selected minerals.