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Evaluating uncertainties in geochemical modelling for CO_2 storage: multivariate sensitivity analysis of database entries

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Geochemical and reactive transport modelling are powerful tools used for the assessment of the stability and long-term safety of CO_2 storage sites. Due to the complexity of the natural systems and the consequent experimental difficulties, and despite the large effort of the scientific community in filling the gaps, the data which forms the available thermodynamical and geochemical databases needed for the simulations are incomplete and patchy, and include measurement errors, inconsistencies, fitting and extrapolation errors (i.e. unknown or partial dependency on temperature and pressure). Such sources of uncertainty are usually disregarded by the modellers (end-users) and not easy to quantify.

The goal of the study is to assess the reliability of chemical simulations for simple and more complex settings, in a range of conditions relevant for CO_2 storage in depleted gas reservoir, taking as reference the Altmark gas field (Germany). The considered temperatures range from 25 to 130 °C and pressures up to 200 bar, accompanied by a high salinity of the involved brines. More in detail, the data we are focusing on are on one hand Pitzer coefficients, required to model with sufficient accuracy the activities of the dissolved species due to the high ionic strength of the formation fluids; on the other hand, the equilibrium constants of aqueous and mineral reactions. We performed a systematic multivariate sensitivity analysis based on randomly generated small perturbations of the parameters tabulated in available databases, in order to investigate the propagation of the errors through the chemical speciation system. The geochemical simulator PHREEQC was used in the test cases. We show that with perturbations of less than 5% in the initial equilibrium constants and Pitzer parameters, which is already optimistic for the considered range of ionic strengths and temperatures, the response on the simulations in unfavorable cases can reach relative differences in the order of 15%. This compares in magnitude to uncertainties arising from other unknown features of the underground like spatial heterogeneity or uncertainties in reaction kinetics. More complex settings with an increased number of reacting mineral phases may, however, not necessarily show increased discrepancies.