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Exemplifying the Effects of Parameterization Shortcomings in the Numerical Simulation of Geological Energy and Mass Storage

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Numerical simulations of hydraulic, thermal, geomechanical, or geochemical (THMC-) processes in the subsurface have been conducted for decades. Often, such simulations are commenced by applying a parameter set that is as realistic as possible. Then, a base scenario is calibrated on field observations. Finally, scenario simulations can be performed, for instance to forecast the system behavior after varying input data. In the context of subsurface energy and mass storage, however, these model calibrations based on field data are often not available, as these storage actions have not been carried out so far. Consequently, the numerical models merely rely on the parameter set initially selected, and uncertainties as a consequence of a lack of parameter values or process understanding may not be perceivable, not mentioning quantifiable. Therefore, conducting THMC simulations in the context of energy and mass storage deserves a particular review of the model parameterization with its input data, and such a review so far hardly exists to the required extent.

Variability or aleatory uncertainty exists for geoscientific parameter values in general, and parameters for that numerous data points are available, such as aquifer permeabilities, may be described statistically thereby exhibiting statistical uncertainty. In this case, sensitivity analyses for quantifying the uncertainty in the simulation resulting from varying this parameter can be conducted. There are other parameters, where the lack of data quantity and quality implies a fundamental changing of ongoing processes when such a parameter value is varied in numerical scenario simulations. As an example for such a scenario uncertainty, varying the capillary entry pressure as one of the multiphase flow parameters can either allow or completely inhibit the penetration of an aquitard by gas. As the last example, the uncertainty of cap-rock fault permeabilities and consequently potential leakage rates of stored gases into shallow compartments are regarded as recognized ignorance by the authors of this study, as no realistic approach exists to determine this parameter and values are best guesses only. In addition to these aleatory uncertainties, an equivalent classification is possible for rating epistemic uncertainties describing the degree of understanding processes such as the geochemical and hydraulic effects following potential gas intrusions from deeper reservoirs into shallow aquifers.

As an outcome of this grouping of uncertainties, prediction errors of scenario simulations can be calculated by sensitivity analyses, if the uncertainties are identified as statistical. However, if scenario uncertainties exist or even recognized ignorance has to be attested to a parameter or a process in question, the outcomes of simulations mainly depend on the decision of the modeler by choosing parameter values or by interpreting the occurring of processes. In that case, the informative value of numerical simulations is limited by ambiguous simulation results, which cannot be refined without improving the geoscientific database through laboratory or field studies on a longer term basis, so that the effects of the subsurface use may be predicted realistically. This discussion, amended by a compilation of available geoscientific data to parameterize such simulations, will be presented in this study.