

Geochemical Modelling of CO₂-Water-Rock Interactions for Carbon Storage: Data Requirements and Outputs

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Summary

Geochemical modelling provides the ability to predict the short term and longer term behaviour of CO₂, formation water composition and reservoir minerals in a geological storage site. However, like any predictive capability, there are requirements of input information and limitations on what the models can do. This presentation consists of two parts: the first identifies what the data requirements are and how to integrate them into simulations; the second part involves applying geochemical modelling and the types of outputs that can be expected for potential storage sites and natural analogues. The fundamental data requirements for geochemical modeling are: detailed mineral petrography and composition and formation water chemistry; thermodynamic and kinetic data for the mineral phases present and potential product phases; and rock and reservoir physical characteristics (porosity, permeability, temperature, pressure, etc.). Geochemical modelling includes reaction path modelling to determine the total reactivity or CO₂ storage capability of the rock by applying static equilibrium and kinetics based numerical simulations. This method enables the identification/confirmation of potential product phases and an understanding of the chemical evolution of the system with extent of reaction and time. Applying reactive transport modelling enables an understanding of the spatial and temporal variations in plume migration and the compositional evolution of the water chemistry and mineralogy. The applicability of outcomes is directly related to the complexity of input data and the degree of sophistication of the physical model. Changes in porosity and the resultant implications to permeability over time is a feature of particular relevance to site selection. Natural analogues provide a means of testing the model capabilities and several examples will be discussed.