Kinetic reactive transport modelling of CCS disaster scenarios: CO_2 or brine leakage from a CO_2 reservoir into a freshwater aquifer

Zsuzsanna Szabó[1], Nóra Edit Gál[1], Éva Kun[1], Csilla Király[2], Teodóra Szőcs[1], György Falus[1]

[1]Department of Hydrogeology and Geochemistry, Mining and Geological Survey of Hungary, Columbus u. 17-23., Budapest 1145, Hungary

[2]Geographical Institute, Research Centre for Astronomy and Earth Sciences, Hungarian Academy of Sciences, Budaörsi út 45., Budapest 1112, Hungary

The biggest CCS potential in Hungary, with an estimated storage capacity of one gigaton of CO_2, is connected to the saline aquifers of the Pannonian Basin, SE-Hungary. In total, 13 potential CO_2 geological storage reservoirs, i.e. high porosity structures containing saline water have been identified in the Great Hungarian Plain. An initial assessment period closed in 2014 which included determining the geological and technical viability, estimating storage volume and evaluating the basic environmental aspects of selected structures. A second assessment period started in 2015 including the study of the geochemical reactivity of reservoir and cap rocks. Since the management of any possibility of CO_2 migration out of a storage formation is considered essential in a full scale deployment of CO_2 geological storage, the new phase also focuses on the evaluation of worst-case leakage scenarios. These scenarios are connected to the unlikely, but possible contamination of drinking water supplies at shallower depths above the saline water/CO_2 reservoirs.

Present study, therefore, evaluates disaster scenarios of CO_2 escape and brine displacement to these protected freshwater aquifers in the vicinity of potential CCS sites in Hungary. These scenarios selected represent the two endmembers of the leakage cases, i.e. upward migration of CO_2 or CO_2-enriched brine (in our case simply brine). Their study is primarily possible by the application of geochemical modeling (batch and reactive transport). The applied worst-case CO_2 or brine leakage modelling approach is presented through the example of the well-studied Mezőtúr area which is characterized by regional and intermediate flow systems with a dominant upward flow, comprising a regional discharge area. Besides studying the effects of leakage, reactive transport modelling is a helpful tool also to support a monitoring system design. As a result, if an early detection system is successfully deployed partially relying on the achieved modeling results and leakage is detected, methods are available to efficiently manage these disaster events.

Geochemical modelling connected to CCS is frequently performed by the computer program PHREEQC which is designed to perform a wide variety of aqueous geochemical calculations including thermodynamic and kinetic, as well as batch-reaction and one-dimensional (1D) transport calculations. All these types of calculations have been applied and a 1D reactive transport modelling approach considering kinetic mineral dissolution and precipitation reactions and incorporating cation exchange capacity of Ca-montmorillonite clay has been the most informative. Besides providing ion-concertation and mineral composition change data, the conductivity of the solution and the porosity changes in the rock can also be predicted. The model is possible to extend to 2D simulations by MODFLOW PHT3D module.

The kinetic reactive transport modelling carried out in this work has highlighted the importance of considering the ion-exchange capacity of clays and using the most realistic transport parameters. In the final models presented, for the effect of disastrous CO_2 inflow into the shallow drinking water aquifer, calcite dissolves and dolomite precipitates as opposed to the reference case, the system without CO_2. Furthermore, the dissolution of albite and illite in the rock is predicted making dawsonite formation favoured. Estimated total porosity increases at the entry point of CO_2 by approximately 0.4% per year. However, at further distances a minor porosity decrease might be expected. In the case of brine inflow into the system, the reference reactions intensify. This leads to expected minor increase in porosity along the flow path. Models for both scenarios (CO_2 or brine leakage) predict the increase of ion-concentrations in the freshwater some exceeding drinking water limit values which represent a real risk of CCS. Exploring possibilities of monitoring, CO_2 inflow to freshwater reservoir would be expected to decrease the pH, however, depending on the amount and kinetics of buffering minerals present in the host rock it might not change pH significantly. Electrical conductivity of water is, however, estimated and suggested to be the best parameter to measure for cost-effective monitoring of both worst-case leakage scenarios.