

Modelling long-time CO₂ migration and loss behaviour in CO₂ underground storage sites using process-based basin modelling software

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Geological sequestration of CO₂ provides a promising solution to reduce net emissions of greenhouse gases into the atmosphere. Saline aquifers offer the advantage of combining large storage volumes with abundant occurrence in the subsurface. CO₂ storage sites have to be environmentally safe with respect to CO₂ leakage. Due to the fact that the long-time (10^3 - 10^4 a) sealing of the cap rock and faults cannot be tested directly by experiments, modelling studies are of utter importance for storage site assessment. Many processes considered are accounted for in hydrocarbon migration modelling tools (e.g. pVT, hydrocarbon composition, capillary pressure, clay smear along faults). Two further challenges have to be addressed in modelling CO₂ behaviour in deep storage sites: (1) its supercritical state and (2) geochemical reactivity.

The transport mechanism from the storage site into the caprock is thought to be diffusion-controlled and therefore a relative slow process. Due to the fact that for thoughtfully selected storage sites the overlying shale's thickness may be 100s of meters and with low permeabilities, leakage through the caprock is rather unlikely, but this has to be also proven. Probably more important, cracks and faults are potential CO₂ migration pathways. A fault is neither a seal nor a conduit per se (Allan, 1989). The degree of fracturing and composition of authigenic and non-authigenic mineral phases in the fault zones will have a delicate influence on the sealing probability of the fractured zone. With a reactive supercritical CO₂ phase the chemical interaction with the mineral phases in the fault system has to be evaluated. In addition, migration distances for the CO₂ to leave the storage site are potentially shorter than in unfaulted and unfractured structures.

We are currently developing a module to be integrated into the in-house software SEMI MC (Secundary Migration Multi Component; Sylta, 2004), combining equation of state partitioning of CO₂, formation waters and potentially other chemical compounds in the system (i.e. N₂, CH₄, H₂S, higher hydrocarbons) with physicochemical behaviour of CO₂ at the storage site. Main physicochemical processes to be integrated into this model are (1) viscous fingering, (2) vertical/lateral diffusion of CO₂ from the supercritical CO₂ phase into the caprock and into microfaults and faults, and (3) dissolution/precipitation of mineral species utilising thermodynamic and kinetic data sets. We will evaluate the significance of these CO₂-related processes with respect to fault-scale distances. It is evident from the number and character of processes that interferences between physicochemical and migration transport processes are possible and have to be addressed. SEMI MC has demonstrated its capability to predict hydrocarbon accumulation in structural and stratigraphic traps including migration via faults. In

order to extend the modelling tool we will implement appropriate flash calculations for the described physicochemical processes which will eventually give rise to loss functions for CO₂.

Overall, geochemical and solute transport processes may have profound implications on the storage safety of geological CO₂ storage sites on a basin-wide scale. We are planning to apply the updated modelling software to a selected case site, and to carry out sensitivity studies.

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