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Simplified models of transport and reactions in conditions of CO_2 storage in saline aquifers

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Simple hydrogeochemical models may serve as tools of preliminary assessment of CO_2 injection and sequestraton impact on the aquifer and cap-rocks. In order to create models of reaction and transport in conditions of CO_2 injection and storage, the TOUGHREACT simulator, and the Geochemist's Workbench software were applied. The chemical composition of waters for kinetic transport models based on the water - rock equilibrium calculations.

Analyses of reaction and transport of substances during CO_2 injection and storage period were carried out in three scenarios: one-dimensional radial model, and two-dimensional model of CO_2 injection and sequestration, and one-dimensional model of aquifer – cap-rock interface. Modeling was performed in two stages. The first one simulated the immediate changes in the aquifer and insulating rocks impacted by CO_2 injection (100 days in case of reaction model and 30 years in transport and reaction model), the second – enabled assessment of long-term effects of sequestration (20000 years). Reactions' quality and progress were monitored and their effects on formation porosity and sequestration capacity in form of mineral, residual and free phase of CO_2 were calculated. Calibration of numerical models (including precipitation of secondary minerals, and correction of kinetics parameters) describing the initial stage of injection, was based on the experimental results.

Modeling allowed to evaluate the pore space saturation with gas, changes in the composition and pH of pore waters, relationships between porosity and permeability changes and crystallization or dissolution minerals. We assessed the temporal and spatial extent of crystallization processes, and the amount of carbonates trapping. CO_2 in mineral form. The calculated sequestration capacity of analyzed formations reached $n \cdot 100$ kg/m3 for the: dissolved phase – CO(aq), gas phase – $CO_2(g)$ and mineral phase, but as much as 101 kg/m3 for the supercritical phase – $SCCO_2$. Processes of gas and pore fluid migration within the analyzed aquifers were characterized based on the two-dimensional model. Their mechanism is controlled by, changing with time, density contrasts between supercritical CO_2, the initial brine, and the brine with CO_2 dissolved.

When modeling the impact of CO_2 storage on the aquifer and cap-rock interface we noted, that decrease in porosity, resulting from a positive balance of secondary minerals volume, was visible mainly in aquifer rocks. Porosity remained almost constant in cap-rocks, to the advantage of sealing of the repository. We also observed, that mineralogical changes at the interface zone, differ from those which occur in central parts of aquifer and cap-rock. This can be explained by high gas saturation in the aquifer roof, and by formation of a front of pore fluids migrating outwards from the interface zone. Due to these mechanisms, at the base of cap-rock, the phenomenon of CO_2 desequestration may temporarily occur, associated with the dissolution of carbonate minerals.

The simplified models described, may be applicable in assessment of carbon dioxide trapped by dissolution and in mineral phases, and also evaluation of petrostructural consequences of CO_2 injection into saline aquifers. This allows estimation of suitability of given formations for CO_2 sequestration.

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