

Numerical simulation of fluid–rock interaction upon CO₂ injection into a carbonate-hosted saline aquifer

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We run reactive transport simulations to understand the transient chemical processes that occur in a carbonate-dominated aquifer during and after the injection of CO₂. The model, its design and its initial and bounding physico-chemical conditions, are patterned after the Upper Muschelkalk-Gipskeuper aquifer-seal pair in the Molasse Basin in Northern Switzerland. Porosity and permeability measurements on samples from the Muschelkalk indicate a strong correlation. Both the porosity and permeability distribution reflect natural heterogeneity related to the sedimentary, diagenetic and tectonic history of the aquifer. The heterogeneous permeability structure of the aquifer controls the dynamics and the shape of the CO₂ plume and thus affects the efficiency of residual and solubility trapping. The dissolution of CO₂ into the brine entails a lowering of the *pH* and hence the dissolution of the primary carbonate mineralogy. Because the brine remains at local equilibrium with the carbonates, the dynamics of the CO₂ plume and the CO₂-enriched brine is reflected by the mineral alteration pattern. Although the drop in *pH* is associated with carbonate dissolution, the *pH* recovers in certain regions of the aquifer faster than in others, thus leading to a complex pattern of carbonate dissolution and reprecipitation. This evolving pattern of carbonate dissolution/reprecipitation implies that chemical constituents that are initially incorporated in or that coexist with primary carbonate minerals may be released into the fluid, then later removed from the fluid by reprecipitation when conditions have changed.

Mass balance calculations suggest that CO₂ injection into a carbonate rock releases additional CO₂ due to mineral dissolution. Thus trapping of CO₂ in a carbonate aquifer requires that the seal remains tight over long periods of time. The increase in reservoir pressure during injection, the dynamics of the CO₂ plume and the perturbation of chemical conditions in the reservoir will initiate mass transfer across the aquifer-seal interface and initiate chemical reactions on either side of the interface. We explore the extent of species mobilization and transfer across the reservoir/seal interface, identify the type of reactions that occur as well as their implications for the tightness of the caprock.

Organic facies variation from well data on the bituminous Miocene units, Northwestern Anatolia (Sevinç/Ağapınar-Eskişehir), Turkey

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In the region, the Miocene units consist of conglomerate, sandstone, claystone, coal, marl, siltstone, bituminous shale and limestone. Some 60 samples of bituminous units from the Miocene succession were collected from ES-07 well, in the north-western part of Turkey (Sevinç/Ağapınar-Eskişehir). 24 core samples were screened for total organic carbon (TOC) content. Selected samples were then analyzed by Rock-Eval pyrolysis. Visual kerogen analysis and vitrinite reflectance measurements were also undertaken. Detailed data from bituminous Miocene sediments made it possible to construct an organic facies framework using different zonations. Organic facies type B, C, CD and D were identified in the investigated units. Alteration colors of organic materials are yellow and dark yellow. Spore colors of these samples are yellow and dark yellow (SCI:2-3.5). Organic facies B is related to bituminous shale lithofacies. This facies is characterized by average values of HI around 509 (equivalent to type II Kerogene), TOC around 7.77%, and an average of S2 of 40.81 mg HC/g of rock. This facies is laminated and well bedded, and usually contains a higher percentage of terrestrial residual organic matter. Organic facies C is related to marl, coaly marl and coal lithofacies. This facies is composed of organic matter with average values HI around 153 (equivalent to Type II/III Kerogene), TOC around 28.05 and S2 between 3.97 and 83.77 mg HC/g sample. Organic facies C is the “gas-prone” facies. The organic matter is dominated by terrestrial debris in various stages of oxidization. Most coals are organic facies C. The organic facies CD is related to the coaly marl, marl and shale lithofacies. This facies is characterized by average values of HI around 73 (equivalent to Type III Kerogene), TOC around 13.10%, and an average of S2 of 13.97 mg HC/g of rock. An organic facies D, associated with marl, sandy marl, coaly marl and limestone lithofacies, displays values of HI around 163 (equivalent to Type III Kerogene) and TOC around 2.94%. S2 varies between 0.01 and 5.53 mg HC/g of rock.