Geochemical reactions at lithological boundaries controlled by downward advection of CO$_2$-enriched brine – A reactive-transport modelling study at pore scale

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Abstract

Reactive transport modelling at the pore scale explores the changes in the geometry of the pore network and the respective chemical gradients due to the fluid-mineral reactions. The advantage of a pore scale model is the true representation of flow and water chemical heterogeneity and respective local reaction rates within the porous rock and therefore avoids the simplification of treating the sedimentary rock as a homogeneous medium. This approach requires a spatial discretisation in the micrometre-range, which typically prohibits model domains with a volume larger than about a cm$^3$. However, modelling of pore scale processes is particularly powerful to investigate transport and reactions at lithological boundaries. Sub-meter scale intraformational baffles with sharp or gradational lithological boundaries are common in reservoirs. These baffles are typically enriched in clay minerals and have a lower porosity and lower permeability relative to the adjacent sandstone units. Therefore, they are known to act as flow barriers and their boundaries may be discrete zones of chemical reactions.

Formation water below the CO$_2$ plume becomes enriched in dissolved CO$_2$ causing an increase in its density to the point when downward advection of the CO$_2$-enriched water commences. In return, deep formation water ascends creating fluid convection in the reservoir, which is the primary cause of solubility trapping. As pointed out above, intraformational baffles form flow barriers causing lateral spreading of the CO$_2$-enriched water with a low pH over the upper surface of intraformational baffles. The flux of CO$_2$-enriched water into the intraformational baffle and rates of fluid-rock reactions at the upper boundary and within the baffle currently remain unknown. However, the contact zone between the low-pH water and clay-mineral rich lithological units is expected to be characterised by extensive geochemical reactions. The objective of this study is to investigate coupled transport and geochemical processes at the upper boundary of intraformational baffles exposed to the downward advection of CO$_2$-enriched, low-pH formation water.

We developed a multicomponent reactive-transport model at pore scale by coupling the transport equation solver COMSOL to the geochemical reaction solver iPHREEQC C++ library using the java-based COMSOL-PHREEQC interface, iCP. A feature of the model is the implementation of the fluid-mineral boundary layer where kinetically controlled mineral dissolution and precipitation can occur. Realistic pore network geometries and 2-dimensional mineral distributions at lithological boundaries are derived from QEMSCAN images and will be used to develop pore scale models. A representative fluid inflow velocity and composition is derived from the literature and model domain boundaries will be kept open in order to allow fluid transport in all directions. We expect mineral dissolution primarily along preferential flow paths whereas mineral saturation and precipitation occurs in pore network areas with no or low flow velocities. The nature of mineral dissolution and precipitation will depend on the primary mineral composition. A reaction front migrating into the intraformational
baffle and controlled by molecular diffusion is expected in case of intraformational baffles with very low permeability. Once the diffusion length is large enough, reactions become kinetically controlled and the system transitions into a steady state.

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