Impure CO₂ reacting with Bunter Sandstone

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Geological CO₂ storage may be applied to reduce CO₂ emissions to the atmosphere. Captured CO₂ streams commonly contain impurities like NO_x, SO_x, H₂, O₂ and H₂S. When these impure CO₂ streams are injected into subsurface formations, it is crucial to understand and predict geochemical reactions within storage reservoirs. Reactive transport simulations are routinely used to predict the geochemical reactivity of reservoir rocks, both on spatial and temporal scales. In clusters of various CO2 sources temporally variable CO₂-stream compositions can be expected. By studying a hypothetical cluster of power plants and industrial sources a novel and innovative methodological approach has been established for implementing impurities in reactive transport simulations using TOUGHREACT V3.0-OMP.

Our method combines both of the commonly applied approaches: additional brine injection and trace gas transport. In this hybrid approach a pre-calculated amount of dissolved impurity species is injected into the various grid cells of the reservoir model. The amount of dissolved impurity species to be injected into each individual grid cell is calculated based on a gas saturation profile of a pure ${\rm CO}_2$ injection scenario. Hence, spatially distributed gas phase transport of impurity species is mimicked by "moving the location" of impurity dissolution.

As a generic reservoir formation an averaged Bunter Sandstone mineralogy, typical for the North German Basin, has been used. Simulations including SO_2 and NO_2 in the CO_2 stream effectuate dissolution of Ca^{2+} -bearing carbonates (i.e. calcite and dolomite) as well as precipitation of anhydrite. These coupled reactions result in a geotechnically negligible porosity decrease.