Coupling chemical and hydrodynamic simulations for long-term prediction of mineralization in heterogeneous CO_2 storage systems

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Long-term reactive transport simulations involving multiphase hydrodynamics and chemical reactions in heterogeneous settings are computationally extremely challenging and therefore prone to oversimplifications. A one-way coupling approach between hydrodynamics and reactive chemistry was therefore developed [1], [2] adapted to the typical conditions of underground CO_2 storage: the time scale of chemical processes is much larger than that of the hydrodynamics, and no significant alteration of petrophysical reservoir properties attained before substantial hydraulic equilibrium is reached. Main advantage of this coupling strategy is the ability to efficiently use well resolved hydrodynamic simulations performed on grids in the order of millions of elements and only a few batch geochemical simulations, thus preserving the complexity of both processes. We demonstrate that the discrepancies between fully coupled and one-way coupled simulations fall in the range of 20-30% in the most unfavourable cases. The procedure used to validate the one-way coupling involved batch simulations of the reference geochemical model, then performing both, unreactive and fully coupled 3D reactive transport simulations, and finally applying the one-way coupling scheme based on the unreactive and geochemical batch model. Thereto, the TOUGHREACT [3] simulator was used. The most influential parameters for the converging of the two couplings are the degree of refinement of the spatial grid, the complexity and rate of mineral reactions, and a cut-off value for the minimum concentration of dissolved CO_2 allowed to originate precipitates.

The one-way coupling enabled the estimation of the mineral trapping potential at the Ketzin CO_2 storage pilot site in Germany [4] over a time span of over 15.000 years otherwise inaccessible by fully coupled reactive transport simulations.

[1]Klein *et al* (2013) *Int J Greenh Gas Con* **19**, 720-730 [2]Kempka *et al* (2013) *Energy Procedia* **37**, 5419-5426 [3] Xu *et al* (2010) *Comput Geosci* **37(6)**, 763–774 [4] Martens *et al* (2012) *Environ Earth Sci* **67(2)**, 323-334