



## **An alternative to fully coupled reactive transport simulations for long-term prediction of chemical reactions in complex geological systems**

Marco De Lucia, Thomas Kempka, and Michael Kühn

GFZ German Research Centre for Geosciences, Hydrogeology, Potsdam, Germany

Fully-coupled reactive transport simulations involving multiphase hydrodynamics and chemical reactions in heterogeneous settings are extremely challenging from a computational point of view. This often leads to oversimplification of the investigated system: coarse spatial discretization, to keep the number of elements in the order of few thousands; simplified chemistry, disregarding many potentially important reactions. A novel approach for coupling non-reactive hydrodynamic simulations with the outcome of single batch geochemical simulations was therefore introduced to assess the potential long-term mineral trapping at the Ketzin pilot site for underground CO<sub>2</sub> storage in Germany [1],[2]. The advantage of the coupling is the ability to use multi-million grid non-reactive hydrodynamics simulations on one side and few batch 0D geochemical simulations on the other, so that the complexity of both systems does not need to be reduced.

This contribution shows the approach which was taken to validate this simplified coupling scheme. The procedure involved batch simulations of the reference geochemical model, then performing both non-reactive and fully coupled 1D and 3D reactive transport simulations and finally applying the simplified coupling scheme based on the non-reactive and geochemical batch model. The TOUGHREACT/ECO<sub>2</sub>N [3] simulator was adopted for the validation. The degree of refinement of the spatial grid and the complexity and velocity of the mineral reactions, along with a cut-off value for the minimum concentration of dissolved CO<sub>2</sub> allowed to originate precipitates in the simplified approach were found out to be the governing parameters for the convergence of the two schemes. Systematic discrepancies between the approaches are not reducible, simply because there is no feedback between chemistry and hydrodynamics, and can reach 20 % - 30 % in unfavourable cases. However, even such discrepancy is completely acceptable, in our opinion, given the amount of uncertainty underlying the geochemical models.

### References

- [1] Klein, E., De Lucia, M., Kempka, T. Kühn, M. 2013. Evaluation of longterm mineral trapping at the Ketzin pilot site for CO<sub>2</sub> storage: an integrative approach using geochemical modelling and reservoir simulation. *International Journal of Greenhouse Gas Control* 19: 720-730, doi:10.1016/j.ijggc.2013.05.014
- [2] Kempka, T., Klein, E., De Lucia, M., Tillner, E. Kühn, M. 2013. Assessment of Long-term CO<sub>2</sub> Trapping Mechanisms at the Ketzin Pilot Site (Germany) by Coupled Numerical Modelling. *Energy Procedia* 37: 5419-5426, doi:10.1016/j.egypro.2013.06.460
- [3] Xu, T., Spycher, N., Sonnenthal, E., Zhang, G., Zheng, L., Pruess, K. 2010. TOUGHREACT Version 2.0: A simulator for subsurface reactive transport under non-isothermal multiphase flow conditions, *Computers & Geosciences* 37(6), doi:10.1016/j.cageo.2010.10.007