Simulation of Reactive Transport in Porous Media: A Benchmark for a COMSOL-PHREEQC-Interface

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Abstract

In geothermal energy systems where heat bearing fluids are circulating through different wells, the rock-fluid interaction and dissolution or precipitation of chemical components will change the porosity and therefore the permeability of the aquifer. In this context, such reactive transport processes can significantly influence the hydraulic properties of porous media, and further determine the long-term performance and reliability of the geothermal system. In addition, high temperature or pressure gradients and dynamic feedback cycles often pose challenges on predicting the influence of the relevant processes.

The novel reactive transport simulation interface COMSOL_PHREEQC, developed by Wissmeier & Barry (2011), combines the capabilities of COMSOL Multiphysics® and PHREEQC by providing a MATLAB®-based coupling interface between both programs. COMSOL Multiphysics® is applied to model thermal and hydraulic transport processes. The aqueous geochemical reactions and rock-fluid-interactions occurring in the aquifer are simulated with the geochemical modeling framework PHREEQC. Compared to using COMSOL's built-in reactive transport simulator, the new interface employs the capability of PHREEQC to simulate equilibrium, adsorption and kinetic reactions based on the mass action laws. At the same time, it takes different activity correction models into account, which are required by the thermal and pressure conditions in geothermal energy systems.

The functionality of the coupling tool is demonstrated on an example ("calcite"), described by Shao et al. (2012). In this example, a 50 cm long column initially contains calcite and is filled with water. During the experiment, the column is flushed with a solution containing MgCl2. At the front of the plume, calcite will dissolve and dolomite will precipitate temporarily.
Shao et al. used OpenGeoSys code combined with ChemApp, PHREEQC and GEMIPM2K to simulate this experiment. The results from COMSOL_PHREEQC will be compared and discussed in this presentation.

Reference

1. Haibing Shao et al., Reactive Transport, In: Olaf Kolditz et al. (Eds.), Thermo-Hydro-Mechanical-Chemical Processes in Fractured Porous Media, Springer, Berlin/Heidelberg, 313-344 (2012).
2. Laurin Wissmeier & David Andrew Barry, Simulation tool for variably saturated flow with comprehensive geochemical reactions in two- and three-dimensional domains, Environmental Modelling & Software, 26, 210-218 (2011)