Coupling Multiphysics with Geochemistry: The COMSOL-PhreeqC Interface

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Abstract

Phreeqc is a freely available computer program for simulating chemical reactions and 1D transport processes in aqueous systems (Parkhurst and Appelo, 1999). It is perhaps the most widely used geochemical code in the scientific community and is openly distributed. The program is based on equilibrium chemistry of aqueous solutions interacting with minerals, gases, solid solutions, exchangers, and sorption surfaces, but also includes the capability to model kinetic reactions with rate equations that are user-specified in a very flexible way by means of BASIC statements directly written in the input file. Several couplings between conservative transport codes and PHREEQC have been done in the past (Parkhurst et al, 2004, Šimunek et al, 2006), even with COMSOL (Wissmeier and Barry, 2011). The common methodology is based on the Sequential Non Iterative Approach (SNIA) which is based on the operator splitting concept: the transport of the aqueous components and the chemical reactions are solved in two different steps. Here we present a coupling based on the same SNIA concept. The approach followed has mainly focused on keeping the key capabilities of both codes: the flexibility of COMSOL for solving all kind of PDE systems and the wide range of chemical calculations of Phreeqc. This has been achieved with enough performance to face highly coupled non-linear Thermal Hydraulic Mechanical and Chemistry problems (THMC) for problems around 100k elements. Furthermore, some optional coupling between both codes like temperature effects on chemistry and density or porosity changes due to chemical reactions has been enabled. The development is based on a Java interface which uses the COMSOL Java API and the IPhreeqc dynamic library (Charlton and Parkhurst, 2010) accessed through the JNA wrapping library. The chemical step has been parallelized using shared memory to optimize the simulations on multi-core processors. The numerical tool has been extensively verified by comparison of simulation results of 1D, 2D and 3D benchmark examples solved with other reactive transport simulators. An example of 3D reactive transport simulations in clay material is shown to illustrate the capabilities and the potential of the framework. This example is based on the thermo-hydro-chemical (THC) evolution of a deposition hole of a spent nuclear fuel repository. Variable saturated flow and reactive transport simulations have been performed to study the expected geochemical behavior of the clay barriers. Figure 1 shows the different meshes and domains used depending on the phenomenon simulated. COMSOL-Phreeqc is a powerful and flexible tool which allows solving highly coupled THMC problems. Furthermore it leaves the Phreeqc input unchanged, which makes it easy to use for experienced geochemical users. The SNIA approach has its limitations but the approximation is sufficient for most cases (Barry et al, 1996; Saaltink et al, 2001).

Reference

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Figures used in the abstract

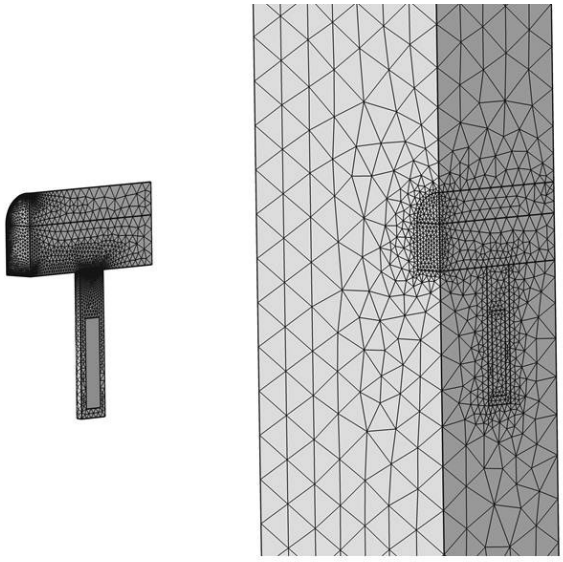

Figure 1: Left – mesh used for flow and reactive transport phenomena. Right – mesh used for thermal phenomenon.