Numerical simulation of reactive single phase multicomponent flows in porous media: a sequential coupling between DuMuX and PHREEQC

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Résumé

Reactive transport modeling is widely used in several environmental applications such as CO2 sequestration and nuclear waste disposal. Significant efforts are made to improve the capacity of the models in comprehensively representing the reactive transport processes. Among these efforts, DuMuX with a modular-based structure allows for efficient modeling of the multi-physical processes in porous media and implementing constitutive relations. Despite the capacity of DuMuX in integrating the full complexity of hydraulic and chemical coupled processes on a reservoir scale, its use is still relatively limited due to the constraints in integrating with realistic chemical descriptions of fluids and rocks. Therefore, the aim of this study is to decouple the hydraulic and chemical sub-problems and solve the latter with a geochemical code for handling complex chemical systems. Among the variety of geochemical codes, the software package PHREEQC, a code for simulating aqueous speciation and reaction path, has obtained popularity due to the convenience of defining and solving the desired geochemical system via basic scripts. Coupling DuMuX with PHREEQC brings the convenience of efficient modeling of the multi-physical processes together with access to the rich chemical database of PHREEQC and flexibility in defining the chemical system.

A reactive single phase multicomponent flow process in porous media is considered. Chemical reactions can involve solutes, sorbed species, and minerals. The problem is modeled by Darcy's law for the conservation of momentum and a mass conservation law is written in an element-based approach.The system is closed by a mass action law for each equilibrium reaction and an ordinary differential equation for each kinetic reaction. The coupling between the hydraulic transport part in DuMuX and the chemical reaction part in PHREEQC has been done through a sequential non-iterative approach (SNIA) using PhreeqcRM. PhreeqcRM is called in each time step as the reaction engine for updating the values of element concentrations which are given by DuMuX after a transport step. For the spatial discretization, we used a cell-centered finite volume method combining an upwind scheme for the convective terms and a two-point flux approximation for the diffusive terms. An implicit Euler scheme is used for time discretization.

Firstly, we validated our coupling approach on a 1D single phase reactive flow and a well-known calcite dissolution benchmark. The results of the concentration of mobile elements as well as minerals obtained with coupled DuMuX-PHREEQC are compared with the reference solution given by PHREEQC. Calcium and carbonate are initially at equilibrium in the solution. With the progressive introduction of magnesium, calcite mineral starts to dissolve and dolomite precipitates. A very good accordance between results is observed. The extension of this sequential coupling to deal with multiphase reactive flows is in progress. The first

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results obtained by coupling the two platforms are encouraging and promising, and open up new prospects for efficient modeling of multiphase reactive transport for a variety of realistic applications in the subsurface.