Numerical modeling of coupled two-phase multicomponent flow with reactive geochemical transport in porous media

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1. Introduction

In this talk, we will discuss a new numerical modelling of two-phase multicomponent flow with reactive transport in porous media such as immiscible gas injection in oil reservoirs, gas migration in a nuclear waste repository or long-term fate of injected CO_2 for geological sequestration [1].

We will focus on the numerical modelling of immiscible compressible two-phase flow in porous media with geochemistry. The problem is modelled by the mass balance law for each phase, Darcy-Muskat's law, the capillary pressure law and the coupling with chemistry occurs through reactions rates. In the case of kinetic reactions, these rates are nonlinear functions of the concentrations involved in ordinary differential equations, while for equilibrium reactions, these rates are unknown and replaced by the mass action laws that relate the activities of concerned species.

2. Methodology

A sequential approach solving firstly a two-phase flow model and then the reactive transport problem, has been implemented in the open-source simulator DuMu^X [2].This strategy is schematised in Figure 1:

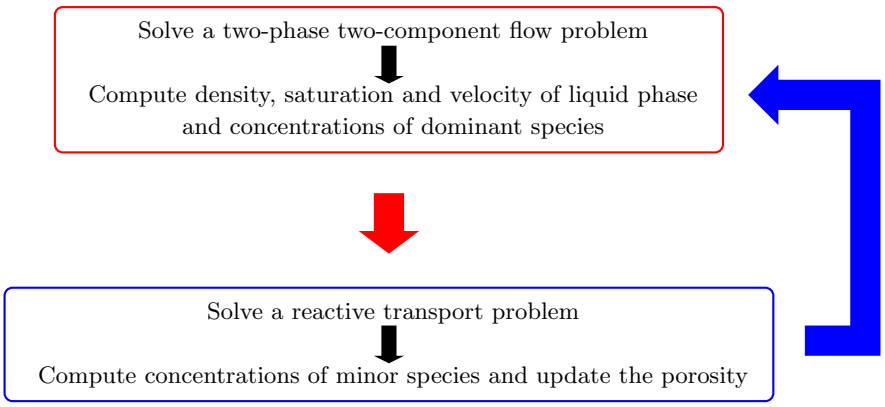


Figure 1: Coupling procedure between flow and reactive transport modules.

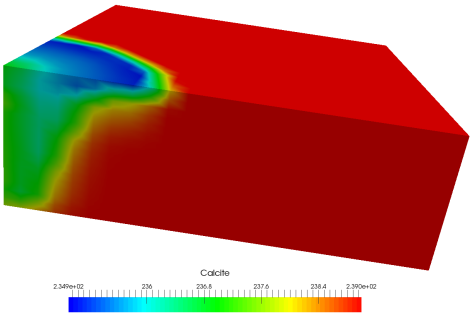
- Firstly, the module 2p2c, based on an implicit finite volume method, is used to solve a two-phase two-component flow model considering that a dominant component exists in each phase. The concentration of other species, assumed as minor, are treated explicitly.
- Secondly, a direct substitution approach is employed to obtain the reactive transport system described by advection dispersion reaction equations coupled to differential algebraic equations to deal with the minor species. Again an implicit finite volume method is used to discretize this system. A new reactive transport module called 1pNc-react was implemented in DuMu^X.

Finally, an efficient coupling between the modules 2p2c and 1pNc-react has been developed. The accuracy and effectiveness of this new simulator is demonstrated through numerical investigation.

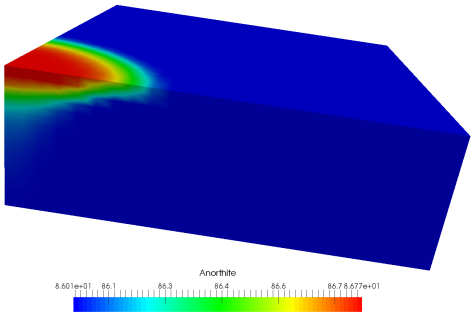
3. Numerical results

To validate our methodology, we have performed a test case proposed in [3]. The domain is three-dimensional and a pure CO_2 steam is injected in a well located $25m$ from the top of the aquifer. The chemical system consists of 12 components involved in 3 equilibrium reactions and 3 kinetic reactions. Injection is performed during 20 years while time of simulation equals 2000 years. The model contains 10000 grid blocks.

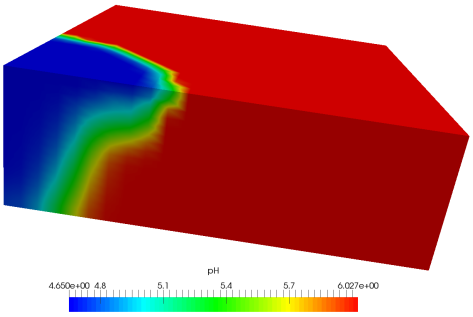
Figure 2 displays concentration of calcite and anorthite at $t = 2000$ years. Initially, their concentration were respectively 238 and 87 mol.m^{-3}. We can see that calcite is dissolved near the injection of CO_2 and precipitated far from the injection while anorthite is dissolved everywhere. The molality of aqueous CO_2 and the pH are also depicted. They are strongly correlated since high concentration of aqueous CO_2 acidifies the liquid phase.



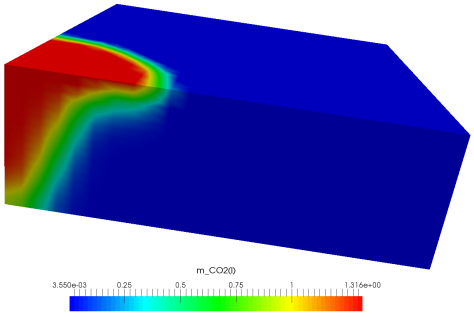
Calcite concentration [mol.m^{-3}]



Anorthite concentration [mol.m^{-3}]



pH



Aqueous CO_2 molality [mol.kg^{-1}]

Figure 2: Profiles at $t = 2000$ years.

References

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