A mathematical formulation for reactive transport in porous media adapted to CO2 sequestration

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ABSTRACT

Carbon capture and storage (CCS) is currently one of the major options to reduce greenhouse gas emissions from power plants. However, the implementation of CCS has been slowed down by uncertainties about the long term evolution of injected carbon into deep saline aquifers. Reactive transport numerical models [1] are used to predict temperature and pressure variations, brine and gas phases displacement, and chemical effects of gas-water-rock interactions. One of the main challenges of these models is to accurately represent the coupling between transport phenomena and mass transfer occurring in sub-surface porous media.

In this work, we present a new mathematical formulation for reactive transport in porous media. This fully implicit multi-component, multi-phase flow formulation is able to deal with phase appearance and disappearance combined with stoichiometric mass transfer. Our formulation is currently restricted to advective transport and chemical equilibrium equations, however an extension to diffusion processes and kinetic equations is considered. The novelty of our work consists in the extension of concepts used so far to deal only with phase equilibrium [2][3] to both homogeneous and heterogeneous equilibrium reactions.

We implement our mathematical formulation in a three-dimensional multi-phase flow code using the HPC numerical framework Arcane [4]. We first show results obtained with this code applied to numerically challenging test cases in reactive transport modelling such as precipitation and dissolution of minerals or gas-water equilibrium. We then test the code for validation against more realistic benchmark studies and discuss the results.

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