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Numerical Modeling and Simulation of Fully Coupled Processes of Reactive Multiphase Flow in Porous Media

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Abstract. In this paper, we consider a finite volume approach for modelling multiphase flow coupled to geochemistry in porous media. Reactive multiphase flows are modelled by a highly nonlinear system of degenerate partial differential equations coupled with algebraic and ordinary differential equations. We propose a fully implicit scheme using a direct substitution approach (DSA) implemented in the framework of the parallel open-source platform DuMu^X. We focus on the particular case where porosity changes due to mineral dissolution/precipitation are taken into account. This alteration of the porosity can have significant effects on the permeability and the tortuosity. The accuracy and effectiveness of the implementation of permeability/porosity and tortuosity/porosity relationships related to mineral dissolution/precipitation for single-phase and two-phase flows are demonstrated through numerical simulations.

AMS subject classifications: 76S05, 65M08, 76T10, 74F25

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1 Introduction

Reactive transport modelling is involved in many applications related to subsurface energy and environmental issues. We can mention, no exhaustively, the geological sequestration of CO_2 in saline aquifers, the management of nuclear waste, enhancement of oil

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recovery, groundwater remediation or deep geothermal energy. A detailed description of these applications and the numerical codes dedicated to reactive transport modelling can be found for instance in [1], [2] or [3].

Equations governing such phenomena consists of a set of nonlinear degenerate system of advection-diffusion partial differential equations (related to the flow) coupled to algebraic relations and ordinary differential equations (related to the chemistry). In the literature, several strategies can be considered to deal with this set of coupled equations. In the pioneering contribution [4], the authors present several implicit and sequential approaches for solving reactive transport problems. Global implicit approaches (GIA) tackle the full system of equations while sequential approaches decouple the flow and the chemistry. Due to the strong coupling of the flow and reactive transport equations, a standard approach is to use a GIA to ensure stability in the solution. Although this guarantees numerical stability of the solution, it does not guarantee a nonlinear convergence. This complexity makes difficult the analysis of the entire nonlinear problem. A separation of the different physics can improve the understanding and result in a better design of nonlinear solvers for the reactive transport problem. It is why sequential approaches are more widespread than GIA. Moreover, sequential approaches are easier for implementation since existing codes and specific methods can be used for each sub-problem (flow, transport, chemistry). In [5–7], we developed and integrated in the DuMu^X framework a sequential approach. DuMu^X [8, 9] is a free and open-source parallel simulator for flow and transport processes in porous media, based on the Distributed and Unified Numerics Environment DUNE [10]. Our strategy splits the global problem into two sub-problems. The first sub-problem computes a two-phase compositional flow where only species present in both phases are treated implicitly. Exchanges between phases are totally solved in this step and the contribution of the other species is treated explicitly. The second sub-problem calculates a reactive transport problem where flow properties (Darcy's velocity for each phase, saturation of each phase, temperature, density,...) are given by the first step. Nonetheless, sequential approaches introduce operator splitting errors [11, 12] and restrictions on the time-step are mandatory to ensure mass conservation. In [4], the authors described the GIA as research tools for one-dimensional investigations due to their complexity and their high computational requirements. Thanks to the advance of high-performance computing in the last decades, these restrictions are no longer relevant. So, to improve the robustness of the scheme and the possible accuracy loss due to the time-splitting involved by sequential approaches, we switched to a GIA for a single-phase multicomponent flow with reactive transport in [13]. Our strategy has been validated by numerous numerical examples including 2D and 3D simulations and parallel calculations.

In this work, we propose to extend GIA developed in [13] to deal with reactive two-phase flows and consequently to drop out the sequential approach considered in [5–7]. Moreover, we are interested in expanding the range of possible applications by considering some examples where porosity and permeability changes must be taken into account. Indeed, the simulation of permeability and tortuosity evolution due to porosi-