Finite-Elements Simulation of the Fate of Carbon Dioxide Trapped in Deep Saline Aquifers

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Introduction

In this study, we consider the injection of CO_2 into a multi-layered deep aquifer covered by an impermeable layer of rock for the purpose of permanent geological sequestration. CO_2 sequestration is viewed as a promising approach to reduce the emission of greenhouse gases into the atmosphere. The storage concept is based on different trapping mechanisms that prevent the injected CO_2 from being released into the atmosphere or into drinkable water reservoirs; those mechanisms, which depend on the properties of injected CO_2 and on the composition of the liquid and solid phases, are characterized by different time scales, ranging from weeks to thousands of years.

Computational Fluid Dynamics (CFD) can greatly help in the modeling of such a complex and rich fluid phenomenon. The multiphase-multicomponent nature of this flow has to be coupled to the chemical reactions characterizing the interactions of the different species inside the same phase or between different phases, like the dissolution of CO_2 into the aqueous phase as well as its precipitation into carbonate minerals. This requires an effective handling of a high number of equations and variables.

In this study order we adopt the Finite Element Method (FEM) coupled with the reduction scheme of Kräutle, Knabner and Hoffmann [8, 9, 10]. The general idea is to take specific linear combinations of equations (which is done in each phase separately) in order to isolate the equilibrium reaction rates each in a single transformed equation. Afterwards, provided that one is not interested in the equilibrium reaction rates, these equations can be dropped. Finally, the equilibrium equations are used to eliminate certain variables by defining a resolution function, which further reduces the size of the system. The advantage of this method compared to other transformation techniques is that in the transformed equations, all transport operators depend linearly on transformed concentration variables after solving and substituting the algebraic equations into the remaining equations. This avoids the generation of additional nonzero entries in the Jacobian.

Methodology

Typically, CO_2 is injected in its supercritical state where it adopts properties midway between a gas and a liquid. More precisely, it has the low viscosity of a gas and the high density of a liquid. Therefore, we employ the equation of state (EOS hereafter) of Duan [6] to compute the density of CO_2. We use the approach of Garcia [4] to define the function f_l that represents the molar liquid phase density. Regarding the solubility of CO_2 in water, Henrys law, is invalid at the high pressure conditions prevailing at a deep underground CO_2 storage site. We use the EOS of Spycher and Pruess [7] to define the interphase mass exchange of CO_2. For the viscosity of the gas phase, an approach of Fenghour et al. [5] is used. Since the coefficient functions described above are given only implicitly, their evaluation may be computationally expensive. Therefore, lookup tables are initially generated and cubic splines are used to evaluate the coefficient functions and their derivatives during the simulation.

Cases

We start from the reaction network described in the work of [2]. Firstly a uniform layer is considered in terms of rock composition, porosity and permeability. This initial case is then extended to a more realistic multilayered structure. In this way the leackage of CO_2 into superior layers of drinkable water can also be studied. The effects of permeability, porosity and of the different models to represent capillary pressure and relative permeability (Brooks-Corey vs. van Genuchten) are considered. The cases presented will demonstrate the ability of our approach to capture the different CO_2 sequestration mechanisms like *hydrodynamic, capillary, solution* and *mineral* trapping.

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