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Coupled THMC modeling of CO_2 injection by finite element methods

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ABSTRACT

Geological CO_2 sequestration has been proposed to mitigate greenhouse gas emissions. Massive CO_2 injection into subsurface formation involves interactions among pressure and temperature change, chemical reactions, solute transport, and the mechanical response of the rock; this is a coupled thermal–hydraulic–mechanical–chemical (THMC) process. Numerical modeling of CO_2 injection around the wellbore area can provide information such as changes in rock properties as well as stress and pressure changes, and this helps better predict injectivity evolution and leakage risk. In this paper, a fully coupled THMC model based on finite element methods is presented to analyze the transient stress, pressure, temperature and chemical solute concentration changes simultaneously around an injection well. To overcome these numerical oscillations in solving the transient advection–diffusion equations involved in the heat transfer and solute transport processes, we employ a stabilized finite element approach, the subgrid scale/gradient subgrid scale method (SGS/GSGS). A hypothetical numerical experiment on CO_2 saturated water injection into a carbonate aquifer is conducted and preliminary results show that the fully coupled model can successfully analyze stress and pressure changes in the rock around a wellbore subjected to thermal and chemical effects.

1. Introduction

Massive CO_2 sequestration is proposed to mitigate greenhouse gas emissions; salt caverns, depleted oil and gas reservoirs, and deep saline aquifers have been considered as medium- to long-term (100–10,000 yr) geological sequestration media (Bachu and Stewart, 2002). It has been suggested that 7 Gt of CO_2 might be sequestered every year, approximately 30% of annual anthropogenic CO_2 emissions (Gessinger, 1997). Injection of such large amounts of CO_2 requires suitable strata injectivity to keep costs to a reasonable level and also requires well and cap-rock integrity to reduce leakage risk (Streit and Hillis, 2004). This demands a better understanding of permeability alterations and a clear description of stress and pressure changes in the storage formation and cap-rock during injection.

Massive CO_2 injection into salt caverns, aquifers or depleted hydrocarbon reservoirs induces a range of strongly coupled thermal, hydraulic, mechanical and chemical processes (THMC) including heat transfer, multiphase fluid flow, geomechanical response (strains and stresses), solute transport, and geochemical reactions between the fluids and formation minerals. Researchers are making efforts toward fully coupled THMC modeling of CO_2 injection from different degrees and combinations of coupling among thermal, hydraulic, mechanical and chemical effects (Andre et al., 2007; Bachu and Dusseault, 2005; Bachu and Rothenburg, 2003; Celia and Nordbotten, 2009; Chalaturnyk and Gunter, 2004; Class et al., 2009; Comerlati et al., 2003; Dusseault et al., 2004; Hawkes et al., 2004; Izgec et al., 2008; Johnson et al., 2005; Kumar et al., 2005; Le Gallo et al., 2006; Lichtner and Lu, 2006; Nghiem et al., 2004; Prévost et al., 2005; Pruess et al., 2003; Rutqvist and Tsang, 2005; Rutqvist et al., 2002, Rutqvist et al., 2006; Xu et al., 2003). The very few fully-coupled THMC models have addressed the large-scale problem, while the wellbore scale has not been paid much attention (Cailly et al., 2005; Gaus et al., 2008). To predict effectively the potential for hydraulic fracturing and shear failure, useful information for injection design and leakage prevention, it is necessary to identify the stresses and pressure change around the injection well. Since both CO_2 injection in greenhouse gas storage and water/gas injection in petroleum industry involve petroleum boreholes, within a general petroleum geomechanics perspective (Dusseault, 1999, 2003a,b), we use a fully-coupled THMC model to analyze stress and pressure changes in the rock around a borehole during CO_2 injection. Heat transfer, fluid flow, geomechanics behavior and reactive chemical transport are solved simultaneously in the mathematical model presented. Due to the complexity of the problem, we restrict our

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model to single phase flow and elastic porous media in this preliminary study.

In Section 2 we introduce the basic ideas behind fully-coupled THMC modeling during CO_2 injection and corresponding formulations by finite element methods (FEM). A simple FEM verification example is given in Section 3, a hypothetical numerical experiment on CO_2 saturated water injection into a carbonate aquifer is conducted in Section 4, and conclusions are given in Section 5.

2. Fully coupled THMC modeling framework for CO_2 injection by FEM

Fully coupled THMC modeling of CO_2 injection integrates theories of poroelasticity, thermoelasticity, elastoplasticity, and reactive solute transport (Bear, 1988; Biot, 1941; Charlez, 1997; Coussy, 1995; Detournay and Cheng, 1993; Steefel and Lasaga, 1994; Zimmerman, 1991). This combination allows us to address situations of strong coupling among thermal flux, reactive solute transport, fluid flow, and porous medium deformations.

Based on thermoporoelastic theory for single phase fluid flow through deformable porous media, a general equilibrium equation in terms of effective stress can be written as (Lewis and Schrefler, 1998; Yin et al., 2010):

$$G\nabla^2\mathbf{u} + (G+\lambda)\nabla \operatorname{div}\mathbf{u} - \left(1-\frac{K}{K_m}\right)\nabla p - K\beta_s\nabla T = 0 \tag{1}$$

G and λ are the Lamé elastic constants, **u**, p and T denote displacement, pore pressure and temperature respectively. β_s is the volumetric thermal expansion coefficient of the skeleton, and K and K_m are bulk moduli for the bulk skeleton and the matrix mineral respectively.

The general form of the continuity equation for fluid flow, incorporating Darcy's Law, can be expressed as follows (Lewis and Schrefler, 1998; Yin et al., 2010):

$$\nabla^T\left(-\frac{k}{\mu}\nabla p\right) + \left(\frac{\alpha-\phi}{K_m}+\frac{\phi}{K_w}\right)\frac{\partial p}{\partial t} + \alpha\frac{\partial \varepsilon}{\partial t} - [(\alpha-\phi)\beta_s + \phi\beta_w]\frac{\partial T}{\partial t} = 0. \tag{2}$$

where α is Biot's coefficient, equal to 1.0-K/K_m, k is the permeability of the porous medium, ϕ is the porosity and μ is the viscosity of the fluid. β_w is the volumetric thermal expansion coefficient of the fluid. The permeability is updated based on the porosity change at each time step after the temporal discretization introduced later for the whole system equation.

Then the general form of the energy balance equation, including the thermal convection and thermal conduction terms, can be expressed as follows (Lewis and Schrefler, 1998; Yin et al., 2010):

$$\nabla^T[-\lambda_T\nabla\mathbf{T}] + \rho_w c_w v\nabla\mathbf{T} + T\left[(1-\phi)c_s\frac{\rho_s}{K_m}+\phi c_w\frac{\rho_w}{K_w}\right]\frac{\partial \mathbf{p}}{\partial t} + [-\phi c_w\rho_w\beta_w T - (1-\phi)\rho_s c_s\beta_s T + (1-\phi)\rho_s c_s + \phi\rho_w c_w]\frac{\partial \mathbf{T}}{\partial t} + Q_h = 0. \tag{3}$$

Here, λ_T is the porous medium thermal conductivity, c_l is the specific heat capacity (the subscript l represents the solid, s, and water, w), ρ_l is the density, Q_h is an external sink or source, and, as before, v is the Darcy velocity. In this work, the change of density and viscosity of fluids with temperature is ignored. For a particular problem, the specific boundary condition can be incorporated when solving Eq. (3).

Finally, considering that there are N aqueous species and M mineral species involved in the chemical reactions between the fluid and rock during CO_2 injection, the general form of the equation for solute transport of ith aqueous species, including both the solute diffusion and convection terms, is written as follows:

$$\nabla^T(D_i\nabla C_i) + \phi\frac{\partial C_i}{\partial t} + v_w\nabla C_i = R_i, \quad i = 1,\cdots,N \tag{4}$$

where C_i is aqueous phase concentration of the ith species defined as moles of species per unit volume of solution, D_i is the dispersion coefficient, R_i is the reaction rate, and v_w is the Darcy velocity of the fluid. The general form of the continuity equation for the jth species in the solid phase is written as follows:

$$\frac{\partial C_j}{\partial t} = R_j, \quad j = 1,\cdots,M \tag{5}$$

where C_j is the solid phase concentration of the jth mineral species defined as moles of species per bulk volume of rock, and R_j is the reaction rate. The rate law for the mineral dissolution and precipitation reaction is:

$$R_j = A_j k_j\left(1-\frac{Q_j}{K_{eq.j}}\right) \tag{6}$$

where A_j is the reactive surface area for mineral j, k_j is the rate constant of mineral j, $K_{eq,j}$ is the chemical equilibrium constant for mineral reaction j and Q_j is the chemical affinity of mineral reaction j. R_j is taken as positive for precipitation and negative for dissolution. The rate of formation/consumption of the different aqueous species in Eq. (5) is obtained from $R_i = v_{ij}\,R_j$, where v_{ij} is the stoichiometric coefficient.

Approaches to solve the reactive transport equations above can be divided in two groups: one-step methods and two-step methods. In one-step methods, the solute transport and chemical reactions are solved simultaneously (Celia et al., 1989; Lichtner and Lu, 2006; Miller and Benson, 1983; Steefel and Lasaga, 1994; Valocchi et al., 1981; White, 1995). In two-step methods, the solute transport and chemical reactions are solved separately (Barry et al., 1996; Bryant et al., 1986; Cederberg et al., 1985; Clement, 1997; Engesgaard and Kipp, 1992; Herzer and Kinzelbach, 1989; Kirkner et al., 1984; Miller and Rabideau, 1993; Walsh et al., 1984; Walter et al., 1994; Wheeler and Dawson, 1988; Xu et al., 1999; Yeh and Tripathi, 1991; Zysset et al., 1994). Since the latter approach is recognized to be more mathematically robust than the first one, a two-step method is employed here to handle the reactive solute transport equations. With this two-step method, to couple the reactive solute transport to the other stress, pressure, and temperature fields mentioned previously, the pure solute transport equation excluding the reaction rate terms will be solved with other equilibrium equations, mass balance equations and energy balance equations simultaneously while the chemical reactions are solved immediately based on the solute concentrations obtained. Then we have the new concentrations and the induced porosity and permeability changes can be updated. The chemical reactions can be solved by Newton–Raphson iteration and predictor–corrector methods (Xu et al., 1999; Zysset et al., 1994) whereas the fully coupled multi-field equations can be solved by the finite element methods that are introduced in the following section.

Because of its power and flexibility, the finite element method (FEM) is widely applied in numerical modeling of petroleum geomechanics related multi-field problems that couple stress and deformation, multiphase flow, heat transfer, solute transport, etc. (Dusseault et al., 1998; Gambolati et al., 2001; Gutierrez and Lewis, 1998; Jing and Hudson, 2002; Settari and Mourits, 1998; Yin et al., 2009, 2010). Based on the traditional Galerkin finite element method, the final matrix form of