Abstract

A major concern in development of fractured reservoirs in Enhanced Geothermal Systems (EGS) is to achieve and maintain adequate injectivity, while avoiding short-circuiting flow paths. The injection performance and flow paths are dominated by the permeability distribution of fracture network for EGS reservoirs. The evolution of reservoir permeability can be affected by rock deformation, induced by the change in temperature or pressure around the injector, and chemical reactions between injection fluid and reservoir rock minerals. Thus the change in permeability due to geomechanical deformation and mineral precipitation/dissolution could have a major impact on reservoir long-term performance. A coupled thermal-hydrological-mechanical-chemical (THMC) model is in general necessary to examine the reservoir behavior in EGS.

This paper presents a numerical model, TOUGH2-EGS, for simulating coupled THMC processes in enhanced geothermal reservoirs. This simulator is built by coupling mean stress calculation and reactive geochemistry into the existing framework of TOUGH2 (Pruess et al., 1999) and TOUGHREACT (Xu et al., 2004a), the well-established numerical simulators for geothermal reservoir simulation. The geomechanical model is fully-coupled as mean stress equations are solved simultaneously with fluid and heat flow equations. After solution of the fluid, heat, and stress equations, the flow velocity and phase saturations are used for reactive geochemical transport simulation in order to sequentially couple reactive geochemistry at each time step.

We perform coupled THMC simulations to examine a prototypical EGS reservoir for permeability evolution at the vicinity of the injection well. The simulation results demonstrate the strong influence of rock deformation effects in the short and intermediate term, and long-term influence of chemical effects. It is observed that the permeability enhancement by thermal-mechanical effect can be counteracted by the chemical precipitation of minerals, initially dissolved into the low temperature injected water. We analyze the sensitivity of temperature of injected water on the coupled geomechanical and geochemical effects, and conclude that the temperature of injected water could be modified to maintain or even enhance the reservoir permeability and the injection performance.

Introduction

The successful development of enhanced geothermal systems (EGS) highly depends on the reservoir fracture network of hot dry rock (HDR) and its hydraulic properties, especially the reservoir permeability. The geomechanical processes under subsurface reservoir condition are prevalent in the EGS applications. For example, Tsang (1999) investigated and claimed that hydraulic properties of fracture rocks are subjected to change under reservoir mechanical effects. Rutqvist et al. (2002) presented the correlations between reservoir in-situ stress and the porosity, permeability and capillary pressure. It is also well known that the EGS production processes, such as the cold water injection and steam or hot fluid extraction, have strong thermo-poro-elastic effects on EGS reservoirs.

On the other hand, the strong impacts of geochemical reaction on the EGS reservoirs have been observed in the commercial EGS fields and studied for carbon dioxide (CO₂) based geothermal system in the past few years. Kiryukhin et al. (2004) modeled the reactive chemical process based on the field data from tens of geothermal fields in Kamchatka (Russia) and Japan. In addition, Xu et al. (2004b) presented the reactive transport model of injection well scaling and acidizing at Tiwi field in Philippines. Montalvo et al. (2005) studied the calcite and silica scaling problems with exploratory model for Ahuachapan...
and Berlin geothermal fields in El Salvador. Jung et al. (2013) performed reactive transport modeling to study fluid-rock interactions for CO2-based geothermal system to minimize the uncertainty of EGS development. Thus the typical chemical reactions between fluids and rock minerals, as well as the mineral dissolution and precipitation, should be fully evaluated and predicted in order to assist the development of geothermal energy.

Numerical modeling of efficiently coupled fluid flow and geomechanics (THM) is complex and has been carried out historically in three separated areas: geomechanical modeling, reservoir simulation, and fracture mechanics (Setari et al., 2000; Setari and Walters, 2001; Longuemare et al., 2002). It is also challenging to model the THC processes mathematically and numerically due to the complexity of multiphase fluid flow, water-rock interaction and the strong non-linearities in the conservation equations (Zhang et al. 2012). The research and practice efforts have been put in this direction and a few EGS reservoir simulation tools are developed. For example, Rutqvist et al. (2002) linked TOUGH2 (Pruess et al., 1999) and FLAC3D (Itasca, 1997) for modeling THM process. Wang and Ghassemi (2012) presented a three dimensional thermal-poroelastic model with finite element methods for geothermal reservoir simulation. Fakcharoenphol et al. (2012) developed the fully implicit flow and geomechanics model for EGS reservoirs. The coupled THC simulators, TOUGHREACT (Xu et al., 2004a) and UTCHEM (Fathi et al., 2009), have the capability to model the multi-components multi-phase fluid flow, solute transport and chemical reactions in groundwater and petroleum systems respectively. However, the single programs coupling THC processes are rarely available. Taron et al. (2009) introduced one “modular” approach to generate a coupled THMC simulator by coupling the capabilities of TOUGHREACT with the geomechanical framework of FLAC3D. Compared with single coupled program, although the modular approach may be more rapid and less expensive, it may result in the issues of flexibility and accuracy (Xiong et al., 2013).

In this paper we present one coupled THMC simulator for geothermal reservoir modeling, TOUGH2-EGS. It is developed based on the framework of TOUGH2 and TOUGHREACT by integrating the Equation of State (EOS) for water and air components with geomechanics and reactive geochemistry effects. In TOUGH2-EGS, the fluid and heat flow equations are solved simultaneously with mean normal stress equation before modeling chemical reaction effects. After solving flow and geomechanics equations, the fluid velocity, phase saturation, and temperature distribution are used for solute transport calculation at each time step. The solute transport and chemical reaction are solved iteratively until the chemical states reach equilibrium.

This paper provides a comprehensive description of the mathematical formulation, numerical methods, and program architecture for TOUGH2-EGS, along with one illustrative THMC example. We first introduce the TOUGH2-EGS mathematical model including the derivation and discussion of the governing mass, energy, stress and solute transport equations. Then we discuss the numerical discretization, program architecture and the simulation procedures. Finally, one application example for simulating the THMC processes at the vicinity of the injection well is presented.

**Mathematical Model**

**Formulation of Fluid and Heat Flow.**

The TOUGH2-EGS simulator is developed based on a general mathematical and numerical framework, which solves mass and energy balance equations of describing fluid and heat flow in multiphase, multi-component systems, coupled with geomechanics and reactive geochemistry. Following Pruess et al. (1999), the governing mass and heat balance equations in each subdomain or REV (Representative Elementary Volume) of the EGS reservoir can be written in the form:

$$\frac{d}{dt} \int_{V_n} M^k dV_n = \int_{\Gamma_n} F^k \nabla n d\Gamma_n + \int_{V_n} q^k dV_n$$  \hspace{1cm} (1)

where \(k = 1, 2\) (component water or air) and \(n = 1, \ldots, \text{NEL}\) (total number of grid blocks).

In evaluation of the terms in Equation (1), mass accumulation, flux, source and sink must be calculated at each Newton iteration step. The general form of the mass accumulation term is:

$$M^k = \sum_p \phi S_{\beta\phi} \rho_{\beta} X^k$$  \hspace{1cm} (2)

The heat accumulation term includes contributions from the rock matrix, aqueous and gaseous phases and is given by equation:

$$M^3 = (1-\phi) \rho R C_p T + \phi \sum_p S_{\beta\phi} \rho_{\beta} A_{\beta}$$  \hspace{1cm} (3)
where the subscript 3 means that heat is treated as the third component in the general balance Equation (1).

The mass fluxes of aqueous and gaseous phases are determined by a multiphase version of Darcy’s law, written in the form:

\[ F_{\beta} = -k_{0}(1 + b \frac{1}{P_{\beta}}) \frac{k_{r\beta} \rho_{\beta}}{\mu_{\beta}} (\nabla P_{\beta} - \rho_{\beta} g) \]  

(4)

The heat flux term accounts for conduction, advection and radiation heat transfer and is given by:

\[ F^{k} = -(1 - \phi)C_{R} + \phi \sum_{\rho} S_{\rho} C_{\beta} \nabla T + \sum_{\rho} h_{\rho} F_{\rho} + f_{\alpha} \sigma_{0} \nabla T^{4} \]  

(5)

**Formulation of Geomechanics.**

The TOUGH2-EGS geomechanical equations are based on the classical theory of elasticity extended to porous and non-isothermal media. In the theory of elasticity, the stress-strain behavior of an isothermal elastic material is described by Hooke’s law, which can be extended to porous media with pore pressure and non-isothermal influence.

\[ \sigma_{kh} = \left( \alpha P + 3 \beta K \left( T - T_{\text{ref}} \right) \right) = \lambda \left( \epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz} \right) + 2G\epsilon_{kk}, k = x, y, z \]  

(6)

The above Hooke’s law equation for poroelastic medium has three components in x, y and z directions. Sum them over gives the following equation in terms of mean normal stress and volumetric strain (Xiong et al., 2013).

\[ \sigma_{m} = \alpha P - 3 \beta K \left( T - T_{\text{ref}} \right) = \left( \lambda + \frac{2}{3} G \right) \epsilon_{v} \]  

(7)

Two other fundamental relations in the theory of linear elasticity are the relation between strain tensor and the displacement vector:

\[ \mathbf{\varepsilon} = \frac{1}{2} \left( \nabla \mathbf{u} + \nabla \mathbf{u}^{T} \right) \]  

(8)

and the static equilibrium equation:

\[ \nabla \sigma + \mathbf{F}_{b} = 0 \]  

(9)

We combine Equation (6), (8) and (9) to obtain the thermo-poro-elastic non-isothermal Navier equation:

\[ \alpha \nabla P + 3 \beta K \nabla T + \left( \lambda + G \right) \nabla \left( \nabla \mathbf{g} \mathbf{\varepsilon} \right) + G \nabla^{2} \mathbf{u} + \mathbf{F}_{b} = 0 \]  

(10)

Equation (10) has two terms containing the displacement vector and taking the divergence of it results in an equation that has one term containing the divergence of the displacement vector:

\[ \alpha \nabla^{2} P + 3 \beta K \nabla^{2} T + \left( \lambda + 2G \right) \nabla^{2} \left( \nabla \mathbf{g} \mathbf{\varepsilon} \right) + \nabla \nabla \mathbf{F}_{b} = 0 \]  

(11)

The divergence of the displacement vector is the sum of the normal strain components, the volumetric strain:

\[ \nabla \mathbf{g} \mathbf{\varepsilon} = \frac{\partial u_{x}}{\partial x} + \frac{\partial u_{y}}{\partial y} + \frac{\partial u_{z}}{\partial z} = \epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz} = \epsilon_{v} \]  

(12)

Finally combining Equations (11), (12) and (7) yields an equation relating mean normal stress, pore pressure, temperature and body force:
\[
\frac{3(1-v)}{(1+v)} \nabla^2 \sigma_m + \nabla g_F = \frac{2(1-2v)}{(1+v)} \left( \alpha \nabla^2 P + 3 \beta K \nabla^2 T \right) \tag{13}
\]

where \(v\) is the Poisson’s ratio, substituting the \(\lambda\) and \(G\) of the original equations with the appropriate relationships.

Equation (13) is the governing geomechanical equation for TOUGH2-EGS, and mean normal stress is another primary variable solved simultaneously with primary thermodynamic variables for mass and energy conservation equations.

**Formulation of Chemical Reactions.**

The TOUGH2-EGS chemical reactions module sequentially solves solute transport and chemical reactions. The solute transport gives the solution of chemical concentration for each species, and the effects of chemical reactions on the change of concentrations are fed back to solute transport through sink/source term.

**Solute Transport.**

The solute transport occurring in the liquid phase also follows the general mass balance equation (1), where accumulation and flux terms may be expressed

\[
M^k = \phi S_k C_{kl} \tag{14}
\]

\[
F^k = v_i C_{kl} - \left( \tau \phi S_i D_l \right) \nabla C_{kl} \quad k = 1 \ldots N_l
\tag{15}
\]

where \(N_l\) is the total number of chemical components (species) in the liquid phase; \(C_{kl}\) is the concentration of the \(k\)th species in liquid phase; \(v_i\) is the Darcy velocity, \(D_l\) is the diffusion coefficient.

In order to reduce the computation workload and conveniently define the chemical system, a subset of aqueous species could be selected as basis species (primary species). All other species (secondary species), including aqueous complexes and precipitated species, can be represented as a linear combination of basis species as

\[
C_i = \sum_{j=1}^{N_c} v_{ij} C_j \quad i = 1 \ldots N_R
\tag{16}
\]

where \(N_c\) is the number of the primary species and \(N_R\) is the number of the secondary species, \(j\) is the primary species index and \(i\) is the secondary species index, \(v_{ij}\) is the stoichiometric coefficient of \(j\)th primary species in the \(i\)th reaction.

**Mineral Dissolution and Precipitation.**

The mineral dissolution/precipitation due to the reactions between the injected water and the reservoir rock or fluid is the main interest with respect to reactive geochemistry for EGS reservoir modeling. The mineral saturation ratio can be expressed as

\[
\Omega_m = X_m^{-1} \lambda_m^{-1} K_m^{-1} \prod_{j=1}^{N_c} c_j^{v_{mj}} \tag{17}
\]

where \(N_p\) is the number of minerals at equilibrium conditions, \(m\) is he equilibrium mineral index, \(\Omega_m\) is mineral saturation ratio, \(X_m\) is the mole fraction of the \(m\)th mineral phase, \(\lambda_m\) is its thermodynamic activity coefficient (\(X_m\) and \(\lambda_m\) are taken to one for pure mineral phases), and \(K_m\) is the corresponding equilibrium constant. At equilibrium condition

\[
SI_m = \log \Omega_m = 0 \tag{18}
\]

where \(SI_m\) is the mineral saturation index.

Under kinetic mineral dissolution/precipitation condition, the kinetic rate could be functions of non-primary species. We usually consider the species appearing in rate laws as the primary species. In our model, we use the rate expression given by Lasaga et al. (1994)
where \( N_q \) is the number of minerals at kinetic conditions, the positive values of \( r_n \) indicate dissolution and negative values for precipitation, \( k_n \) is the rate constant (moles per unit mineral surface area and unit time) which depends on the temperature, \( A_n \) is the specific reactive surface area per kg H2O. \( \Omega_n \) is the kinetic mineral saturation ratio defined as Equation (17). The parameters \( \theta \) and \( \eta \), can be determined from experiment, usually assumed to be unity. The reaction rate constant \( k_n \) is dependent on temperature and usually rate constants are reported at 25°C.

**Time and Space Discretization.**

The general mass and energy balance Equation (1) is discretized in space using integral finite difference method (IFD; Narasimhan and Witherspoon, 1976). The fully implicit approach is taken in the time discretization. By introducing proper average volume and approximating surface integrals to a discrete sum of averages over surface segments, the Equation (1) has the residual form as the following with time and space discretization.

\[
R_n^{k}\frac{t_{n+1}}{t_n} = M_n^{k} - M_n^{k} - \frac{\Delta t}{V_n} \left[ \sum_{m} A_{nm} F_{nm}^{k} + V_n q_n^{k} \right] = 0
\]

where \( R \) is the residual of component \( k \) (\( k = 1 \) and 2 stands for components of water and air, and 3 stands for energy; \( k \) could be also primary species in the solute transport) for grid block \( n \), \( t+1 \) donates the current time level, \( m \) donates the neighboring grid blocks of \( n \), \( A_{nm} \) and \( F_{nm} \) are the interface area and flux between them.

The mean normal stress is another primary variable and solved simultaneously with heat and fluid flow equations. Accordingly Equation (13) should be discretized to the same as form as Equation (20). Applying the divergence theorem and approximating surface integrals to a discrete sum over surface segments, the mean stress governing equation has the following discretized residual form

\[
R_n^{\mu}\frac{t_{n+1}}{t_n} = \sum_{m} \left[ 3(1-\nu) \nabla \sigma + F \right] / (1+\nu) - 2(1-2\nu) \left( \alpha NP + 3\beta KT \right) A_{mn} = 0
\]

where \( m \) is the neighboring grid blocks of \( n \) and \( A_{mn} \) is the interface area between them. After solving the THM process, the Darcy velocity and phase saturation are used to compute solute transport and chemical reaction, which also follows the similar numerical method.

**THMC Effects on Reservoir Properties**

Rock deformation and chemical reactions affect fluid flow in several ways, such as hydraulic properties, mass accumulation and capillary pressure. The following section explains how TOUGH2-EGS incorporate the effects to the model.

**Porosity and Permeability.**

The relationship between effective stress \( \sigma' \) and porosity \( \phi \) has been investigated through many research efforts (Ostensen et al., 1986; McKee et al., 1988; Davies et al., 2001; Rutqvist et al., 2002). Our mechanical model implements those correlations and the user can choose the proper one according to the specific reservoir conditions.

\[
\phi_m = \phi(\sigma')
\]

where the subscript \( m \) stands for mechanical effects on porosity. The chemical reaction model considers the porosity change due to mineral dissolution/precipitation as follows.

\[
\phi_c = 1 - \sum_{m=1}^{N_m} f_r m - f_r^a
\]

where \( N_m \) is the number of reactive minerals and \( f_r m \) is the mineral fraction in the containing rock \( (V_{mineral}/V_{medium}) \), \( f_r^a \) is the non-reactive fraction.

Under THMC processes, the total porosity change at each time step is given

\[
\phi' = \phi' + \Delta \phi_m^{t+1} + \Delta \phi_c^{t+1}
\]
The total permeability change can be correlated with the porosity
\[ k^{t+1} = k\left(\phi^{t+1}\right) \]  
(25)

**Mass Accumulation.**
The total mass for one REV is subjected to change due to rock deformation. The volumetric strain is included in the mass accumulation formulation to account for it.

\[ M^\ast = \sum_{\mu} \left(1 - \epsilon_\mu\right) \phi_S \rho_\mu X^\ast_\mu \]  
(26)

**Capillary Pressure.**
The change in permeability and porosity lead to the change of capillary pressure. The following J-function is included in our model to correct capillary pressure change.

\[ p_c = p_c^0 \sqrt{\frac{k^0\phi}{k\phi^0}} \]  
(27)

**Program Architecture and Simulation Process**
TOUGH2-EGS reservoir simulator is a single program built on the framework of TOUGH2, fully coupling geomechanics and sequentially coupling reactive geochemistry. The Figure 1 presents the high level architecture of the program, and Table 1 explains each module in details.

As shown in Figure 1, the EOS module in the architecture is relatively independent, which provides the flexibility that the program can be easily adapted to various subsurface systems as long as the proper EOS is provided. For example, the EOS for water and air used in the EGS reservoir could be replaced by EOS of petroleum systems under the same program framework in order to simulate the coupled geomechanical and geochemical process for petroleum reservoirs.

The Figure 2 describes the program process. It mainly includes two parts, the geomechanical and geochemical parts. The program initializes the thermodynamic variables first, and then initializes the mechanical and chemical systems according to the initial equilibrium conditions. The fluid and heat flow equations are solved with geomechanical equations simultaneously in the THM module. The Figure 2 also shows that the connections between THM module and chemical module are the solutions of THM equations, such as fluid velocity, temperature distribution and other thermodynamic variables, which are used as the input for the solute transport and chemical reaction computation. The solute transport and chemical reactions are solved iteratively until chemical state converges. The time control cycle repeats until the target time is reached.

**Application and Discussion**
In the application example, we present one prototypical EGS reservoir to simulate THMC process of the vicinity of the injection well for continuous two years injection. As shown in the Figure 3, the EGS reservoir is overlain by the perfect caprock and the injection well is in the middle of the simulated area. The mesh is generated with radial and vertical (R-Z) dimensions and logarithmic distribution in radial direction to capture the subtle effects around the wellbore. In order to show the geomechanical and geochemical effects under different injection temperature, two simulation runs are performed for 150°C and 100°C injected water respectively.

The reservoir hydraulic properties, including porosity and permeability, are considered dynamically changed due to mechanical and chemical effects. TOUGH2-EGS incorporates various correlations between stress and porosity/permeability, and allows the users to choose the most appropriate one for the specific reservoir. Davies and Davies (1999) presented the correlation between stress and porosity as Equation 28, which is chosen in the simulation. The total porosity change combines the stress and mineral reaction induced effects, and the Carman-Kozeny correlation as Equation (29) is used for the permeability correlation from porosity.

\[ \phi = \phi_r + (\phi_0 - \phi_r)e^{-ao'} \]  
(28)
The exponent parameter $a$ of Equation (28) is related to the real reservoir rock, which can be obtained by experimental test on the relationship between reservoir porosity and confining stress.

\[
k = k_i \left( \frac{1 - \phi}{1 - \phi_i} \right)^a \left( \frac{\phi}{\phi_i} \right)^2
\]

(29)

Table 1: Program high level modules

<table>
<thead>
<tr>
<th>Modules</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Data input and initialization</td>
<td>Read and parse the initial parameters from the input files; also initialize the thermodynamic variables, geomechanical and geochemical systems.</td>
</tr>
<tr>
<td>Solution of flow and geomechanics</td>
<td>Solve the fluid and heat flow equations, as well as geomechanical equations simultaneously with linear solver.</td>
</tr>
<tr>
<td>Assembling flow and stress equations</td>
<td>Build the Jacobian matrix according to the mass, energy balance equations and governing geomechanical equation.</td>
</tr>
<tr>
<td>Equation of state</td>
<td>Provide the thermodynamic computation based on equation of state for water and air; use the primary variables to calculate the other variables according to the thermodynamic laws.</td>
</tr>
<tr>
<td>Updating reservoir properties</td>
<td>Update and modify the reservoir properties due geomechanical and geochemical effects.</td>
</tr>
<tr>
<td>Assembling transport equations</td>
<td>Build the Jacobian matrix according to mass balance for each primary species; provide solutions of chemical concentrations for all the species.</td>
</tr>
<tr>
<td>Chemical reaction modules</td>
<td>Compute the chemical reactions with chemical species concentrations as input; the chemical reaction results are fed back to transport equations through sink and source term</td>
</tr>
<tr>
<td>Printed output</td>
<td>Output the simulation results</td>
</tr>
</tbody>
</table>

Figure 1: TOUGH2-EGS high level architecture
Figure 2: TOUGH2-EGS program process

Figure 3: Geometry and mesh configuration of the simulated area

Caprock

Reservoir rock:
T = 240 °C
P = 6.35 MPa
σ = 15.6 MPa

Injection rate = 38 kg/s
In order to represent the real EGS reservoir, the initial reservoir mechanical and chemical properties are mainly taken from the published data of Rutqvist et al. (2002) and Xu et al. (2004b), shown as Table 2 and 3. Table 2 shows the reservoir hydraulic and mechanical properties, and Table 3 shows the primary chemical species in the initial reservoir aqueous system and the injection water. Figure 4 presents the initial mineral volume fraction of reservoir rock, where the unreactive portion does not participate in any chemical reactions.

<table>
<thead>
<tr>
<th>Properties</th>
<th>Values</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s Modulus (GPa)</td>
<td>14.4</td>
</tr>
<tr>
<td>Poisson’s ratio (dimensionless)</td>
<td>0.20</td>
</tr>
<tr>
<td>Permeability (m²)</td>
<td>5.37×10⁻¹⁴</td>
</tr>
<tr>
<td>Porosity (dimensionless)</td>
<td>0.1</td>
</tr>
<tr>
<td>Pore compressibility (Pa⁻¹)</td>
<td>5×10⁻⁷</td>
</tr>
<tr>
<td>Thermal expansion coefficient (ºC⁻¹)</td>
<td>4.14×10⁻⁵</td>
</tr>
<tr>
<td>Rock grain specific heat (J/kg ºC)</td>
<td>1000</td>
</tr>
<tr>
<td>Rock grain density (kg/m³)</td>
<td>2750</td>
</tr>
<tr>
<td>Formation thermal conductivity (W/m ºC)</td>
<td>2.4</td>
</tr>
<tr>
<td>Biot’s coefficient (dimensionless)</td>
<td>1.0</td>
</tr>
<tr>
<td>Initial mean normal stress (MPa)</td>
<td>15.6</td>
</tr>
<tr>
<td>High stress residual porosity (dimensionless)</td>
<td>0.8</td>
</tr>
<tr>
<td>Exponent parameter a of Equation 28 (Pa⁻¹)</td>
<td>2×10⁻⁷</td>
</tr>
</tbody>
</table>

Table 3: The chemical components for reservoir initial water and injection water

<table>
<thead>
<tr>
<th>Chemical Species</th>
<th>Initial Water Concentration (mol/l)</th>
<th>Injection Water Concentration (mol/l)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ca²⁺</td>
<td>3.32×10⁻²</td>
<td>1.0327×10⁻²</td>
</tr>
<tr>
<td>Mg²⁺</td>
<td>8.62×10⁻⁶</td>
<td>1.6609×10⁻⁶</td>
</tr>
<tr>
<td>Na⁺</td>
<td>1.285×10⁻¹</td>
<td>1.2734×10⁻¹</td>
</tr>
<tr>
<td>Cl⁻</td>
<td>1.418×10⁻¹</td>
<td>1.418×10⁻¹</td>
</tr>
<tr>
<td>SiO₂(aq)</td>
<td>1.218×10⁻¹</td>
<td>1.1734×10⁻²</td>
</tr>
<tr>
<td>HCO₃⁻</td>
<td>1.0423×10⁻⁻</td>
<td>1.0423×10⁻⁻</td>
</tr>
<tr>
<td>SO₄²⁻</td>
<td>2.6272×10⁻⁷</td>
<td>2.6272×10⁻⁷</td>
</tr>
<tr>
<td>K⁺</td>
<td>1.5852×10⁻¹</td>
<td>1.5852×10⁻²</td>
</tr>
<tr>
<td>AlO₂⁻</td>
<td>0.059×10⁻⁴</td>
<td>0.0205×10⁻⁴</td>
</tr>
</tbody>
</table>

In order to analyze the temperature sensitivity on mechanical and chemical effects, two simulation runs are performed with above input data for two years, one run with injected water temperature of 150 °C and another with injection temperature of 100 °C. The Figure 5 gives the distributions of temperature and pressure after two years injection for both simulations. The Figure 6 shows the effective stress evolution due to geomechanical effect, and Figure 7 shows the change of mineral volume fraction due to mineral dissolution (negative change) and precipitation (positive change). The horizontal axis represents the distance from the injection well.

Figure 5 shows the temperature and pressure profile after two years water injection, which indicates the low temperature from injected water has propagated to the 150 meter from the injection well. Since the injection rate is same for both cases, the reservoir pressures are very close as shown of Figure 5 for different injection temperature. The small gap between them may be due to the different impact on reservoir properties.
Figure 4: Initial mineral fraction of reservoir rock

Figure 5: Temperature and pressure distribution after 2 years injection

Figure 6: Evolution of effective stress for 150 °C (left) and 100 °C (right) injected water
Figure 6 shows the geomechanical effects around the injection well. The results demonstrate that the low temperature water injection results in the significant decrease of effective stress. The lower temperature has much higher effects of stress decrease. For example, the 100°C injection temperature leads to less than 2 MPa reservoir effective stress compared to more than 4 MPa under 150°C injection. The two plots in Figure 6 also show that the stress profile has the same trend as the temperature profile of Figure 5 for two years injection curves, which implies the stress evolution is mainly due to the low temperature injection. It is also observed that the change of stress propagates faster at early time, reaching to about 70 meters from the injection well in half year and finally 150 meters in two years.

Figure 7 presents the change of mineral fraction of reservoir rock due to chemical reaction. The positive change means the mineral precipitation, over the dissolution, dominates the chemical effects. The two plots have the same trend that the change of mineral fraction increases steadily from half year to two years, and mainly concentrates within the 10 meters areas from the injection well. In addition, the lower injection temperature results in much stronger precipitation effects from Figure 7. For example, the change of mineral fraction under 100°C injected temperature is five times more than that under 150°C.

The geomechanical and geochemical effects are fed back to flow through the change of reservoir properties, such as porosity and permeability. The Equation (28) and (29) are used in the simulation to correlate the reservoir porosity and the stress, as well as the permeability and porosity. Figure 8 gives the permeability contour plots around the injector after two years low temperature water injection.

The low temperature injection has the geomechanical effect of reduced stress, which enhances the porosity and permeability. On the other hand, the low temperature strengthens the chemical precipitation, which undermines the reservoir porosity and permeability. The combined geomechanical and chemical effects could be observed from Figure 8. The area close to the injector has lower permeability due to mineral precipitation effects over the geomechanical influence; beyond that area the effects are more pronounced.
permeability is enhanced due to geomechanical effects over the chemical influence. If the temperature of injected water is reduced as shown on the right plot of Figure 8, the permeability is even undermined in the smaller area close the injector due to stronger precipitation, but higher enhanced permeability in the further area because of the enhancement of geomechanical effects by the lower temperature.

Summary and Conclusions
We present a fully-coupled fluid flow and geomechanics, and sequentially coupled reactive geochemistry program, TOUGH2-EGS, for simulating multiphase flow, heat transfer, rock deformation, and chemical reactions for EGS reservoirs. The fluid and heat flow formulation is based on the framework of TOUGH2 and Equation of State (EOS) for components water and air. The geomechanical formulation is derived from the theory of thermo-poro-elasticity. The flow, heat and stress equations are solved simultaneously in this fully coupled simulator, followed by geochemical simulation. Primary variables in TOUGH2-EGS are pressure, air mass fraction, temperature, and mean total stress. Secondary variables, such as phase saturation, capillary pressure, volumetric strain, etc. are evaluated from their relations with primary variables.

The geomechanical and geochemical models have been verified against analytical solutions and other numerical simulators (Fakcharoenphol et al., 2013). For example, we verified the geomechanical model against the analytical solutions of one-dimensional consolidation and heat conduction problems, and two-dimensional Mandel’s problem (Mandel, 1953). We also verified the chemical reaction model against the TOUGHREACT (Xu et al., 2004a). Furthermore, we verified the simulation results of fluid and heat flow against the commercial simulator CMG_STAR (CMG, 2010). The intensive verifications show that TOUGH2-EGS is able to accurately capture the geomechanical and geochemical effects coupled with fluid and heat flow for EGS reservoirs.

The architecture of TOUGH2-EGS provides the flexible numerical framework for coupling geomechanical and reactive geochemical effects, enabling easy integration of Equation of State (EOS) module for the specific reservoir system. An appropriate EOS module provides the thermo-physical parameters, such as fluid density, viscosity, capillarity, etc., to the governing equations. Thus TOUGH2-EGS can be easily adapted to other subsurface systems, such as petroleum reservoirs and CO2 geological sequestration etc.

Compared with other numerical modeling codes for geotechnical analysis of soil, rock, and structural support, such as FLAC3D, our numerical geomechanical model only calculates mean normal stress instead of the total stress tensor. This simplification saves computation workload but cannot analyze the phenomena dependent on shear stress. Overall, TOUGH2-EGS is rigorous in handling the simulations coupled flow, rock deformation, and reactive geochemistry. It can be applied to stress-sensible or geochemistry-sensible reservoirs for analyzing multiphase fluid, heat flow, rock deformation and chemical reactions.

Acknowledgement
This work is supported by the U.S. Department of Energy under Contract No. DE-EE0002762, “Development of Advanced Thermal-Hydrological-Mechanical-Chemical (THMC) Modeling Capabilities for Enhanced Geothermal Systems.” Special thanks are due to the Energy Modeling Group (EMG) of Department of Petroleum Engineering at Colorado School of Mines, supported by Foundation Computer Modeling Group (CMG).

Nomenclature

\( a \) = exponent parameter of Equation (28), Pa\(^{-1}\)  
\( A_{mn} \) = cross area between grid blocks m and n, m\(^2\)  
\( C_i \) = the total concentration of the \( i^{th} \) primary species, mol.L\(^{-1}\)  
\( C_{kl} \) = the concentration of the \( k^{th} \) species in liquid phase, mol.L\(^{-1}\)  
\( C_R \) = specific heat of reservoir rock, J.kg\(^{-1}\) K\(^{-1}\)  
\( D_l \) = the diffusion coefficient of liquid phase, m\(^2\)s\(^{-1}\)  
\( F_b \) = body force per area, Pa  
\( F^k \) = mass or energy flux terms due to advection  
\( g \) = gravitational acceleration, m.s\(^{-2}\)  
\( G \) = shear modulus, Pa  
\( h_\beta \) = specific enthalpy in phase \( \beta \), J kg\(^{-1}\)  
\( k \) = absolute permeability, m\(^2\)  
\( K \) = bulk modulus, Pa  
\( K_R \) = heat conductivity of rock, W.m\(^{-1}\)K\(^{-1}\)  
\( K_\beta \) = heat conductivity of phase \( \beta \), W.m\(^{-1}\)K\(^{-1}\)  
\( k_{\beta} \) = Relative permeability to phase \( \beta \)  
\( M^\phi \) = accumulation terms of the components and energy  
\( P_c \) = capillary pressure, Pa
\(q_k\) = sink or source term of mass or energy component  
\(R_n\) = residual of mass component or energy component  
\(S_\beta\) = saturation of phase \(\beta\)  
\(t\) = time, s  
\(T\) = temperature, °C or K  
\(u\) = displacement, m  
\(u_\beta\) = specific internal energy of phase \(\beta\), J.kg\(^{-1}\)  
\(V_n\) = volume of grid block \(n\), m\(^3\)  
\(\alpha\) = Biot’s coefficient  
\(\beta\) = linear thermal expansion coefficient, °C\(^{-1}\)  
\(\mu_\beta\) = viscosity of phase \(\beta\), Pa.s  
\(\phi\) = porosity  
\(\lambda\) = Lamé’s constant, Pa  
\(\varepsilon\) = strain  
\(\nu\) = Poisson’s ratio  
\(\sigma\) = normal stress, Pa  
\(\rho\) = density, kg.m\(^{-3}\)  
\(\Gamma_n\) = area of closed surface, m\(^2\)

References


