USER'S GUIDE

of

TOUGH2-EGS: A Coupled Geomechanical and Reactive Geochemical Simulator for Fluid and Heat Flow in Enhanced Geothermal Systems

VERSION 1.0

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ABSTRACT

TOUGH2-EGS is a numerical simulation program coupling geomechanics and chemical reactions for fluid and heat flows in porous media and fractured reservoirs of enhanced geothermal systems. The simulator includes the fully-coupled geomechanical (THM) module, the fully-coupled geochemical (THC) module, and the sequentially coupled reactive geochemistry (THMC) module. The fully-coupled flow-geomechanics model is developed from the linear elastic theory for the thermo-poro-elastic system and is formulated with the mean normal stress as well as pore pressure and temperature. The chemical reaction is sequentially coupled after solution of flow equations, which provides the flow velocity and phase saturation for the solute transport calculation at each time step. In addition, reservoir rock properties, such as porosity and permeability, are subjected to change due to rock deformation and chemical reactions. The relationships between rock properties and geomechanical and chemical effects from poro-elasticity theories and empirical correlations are incorporated into the simulator.

This report provides the user with detailed information on both mathematical models and instructions for using TOUGH2-EGS for THM, THC or THMC simulations. The mathematical models include the fluid and heat flow equations, geomechanical equation, reactive geochemistry equations, and discretization methods. Although TOUGH2-EGS has the capability for simulating fluid and heat flows coupled with both geomechanical and chemical effects, it is up to the users to select the specific coupling process, such as THM, THC, or THMC in a simulation. There are several example problems illustrating the applications of this program. These example problems are described in details and their input data are presented. The results demonstrate that this program can be used for field-scale geothermal reservoir simulation with fluid and heat flow, geomechanical effect, and chemical reaction in porous and fractured media.

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1 INTRODUCTION

The geomechanical effect on performance of fractured and porous media reservoirs has gained the attention for understanding fluid and heat flow and stresses induced phenomena, such as formation subsidence, stress induced change in reservoir properties, and borehole failure. Numerical modeling of efficient coupled fluid flow and geomechanics is complex and has been carried out historically in three separate areas: geomechanical modeling, reservoir simulation, and fracture mechanics (Setari et al., 2000; Setari and Walters, 2001; Longuemare et al., 2002). On the other hand, the strong impacts of geochemical reaction on the EGS reservoirs have been observed in the EGS fields in the past few years. For example, Xu et al. (2004b) presented the reactive transport model of injection well scaling and acidizing at Tiwi field in Philippines. The typical chemical reactions between fluids and rock minerals in EGS reservoirs, the mineral dissolution and precipitation, should be fully evaluated and predicted in order to assist the development of geothermal energy.

TOUGH2 (Pruess et al., 1999) is a general-purpose numerical simulator for multi-dimensional fluid and heat flows of multiphase, multi-component fluid mixtures in porous and fractured media. It provides a flexible and comprehensive framework for EGS reservoir simulation. In addition, TOUGHREACT (Xu et al., 2004a) provides the capability to simulate the reactive geochemical transport in variably saturated geologic media. TOUGH2-EGS is developed based on the framework of TOUGH2 and TOUGHREACT by integrating the EOS3 of TOUGH2 family 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 sequentially. The solute transport and chemical reaction are solved iteratively until the chemical states reach equilibrium.

This report provides a comprehensive description of the mathematical formulation, numerical methods, and specifications for preparing input data for TOUGH2-EGS, along with illustrative sample problems. Section 2 covers the TOUGH2-EGS mathematical model including the derivation and discussion of the governing mass, energy, stress and solute transport equations. Section 3 discusses the numerical discretization, the simulation procedures and organization of thermo-physical and stress arrays, in order to assist the user for understanding the program implementation. Section 4 provides the instructions of compiling and executing TOUGH2-EGS. Section 5 contains the detailed description of TOUGH2-EGS input data and input files. Section 6 presents the example problems, including analytical verification for the mechanical model, geomechanical effect modeling, chemical reaction simulation, and application for coupled geomechanical and geochemical effects.

2 MATHEMATICAL MODEL

2.1 Formulation 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. Fluid flow is described with a multiphase extension of Darcy's law; in addition, there is diffusive mass transport in all phases. Heat flow is governed by conduction and convection, also including sensible as well as latent heat effects. Following Pruess et al. (1999), the governing mass and heat balance equations in each subdomain or REV (Representative Elementary Volume) of an EGS reservoir can be written in the form:

$$\frac{d}{dt}\int_{V_n}\mathbf{M}^{\kappa}dV_n = \int_{\Gamma_n}\mathbf{F}^{\kappa}\bullet\mathbf{n}d\Gamma_n + \int_{V_n}q^{\kappa}dV_n \tag{2.1}$$

where κ = 1, ..., NK (total number of components) and n =1,…, NEL (total number of grid blocks).

The integration in Equation 2.1 is over an arbitrary subdomain V_n of the flow system under study, which is bounded by the closed surface Γ_n. The quantity ***M*** appearing in the accumulation term (left hand side) represents mass or energy per volume, ***F*** denotes mass or heat flux, and q denotes sinks and sources. ***n*** is a normal vector on surface element $d\Gamma_n$, pointing inward into V_n.

In evaluation of the terms in Equation 2.1, mass accumulation, flux, source, and sink must be calculated at each Newton iteration step. The general form of the mass accumulation term is:

$$M^{\kappa} = \sum \phi S_{\beta}\rho_{\beta}X_{\beta}^{\kappa} \tag{2.2}$$

where κ = 1, ..., NK, and β=*1, …NPH* (total number of phases). ϕ is effective porosity, ρ_β is density of phase β, S_β is the saturation of phase β, and X_β^κ is the mass fraction of component κ in phase β. Before the calculation of mass accumulation, the parameters on the right hand side of Equation 2.2 are calculated as functions of primary and secondary variables.

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

$$M^{\kappa} = (1-\phi)\rho_R C_R T + \phi \sum_{\beta} S_{\beta}\rho_{\beta}u_{\beta} \tag{2.3}$$

$\kappa = NK+1$ (NK+1 denotes the heat component) and β=1,…, NPH. Here ρ_R and C_R are grain density and specific heat of the host rock respectively, T is temperature, and u_{β} is specific internal energy in phase β.

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

$$\mathrm{F}_{\beta} = -\mathrm{k}_0\left(1+\frac{\mathrm{b}}{\mathrm{P}_{\beta}}\right)\frac{\mathrm{k}_{\mathrm{r}\beta}\rho_{\beta}}{\mu_{\beta}}(\nabla \mathrm{P}_{\beta} - \rho_{\beta}\boldsymbol{g}) \tag{2.4}$$

β=1,…, NPH

Advective mass flux is a sum over phases,

$$F^{\kappa}\Big|_{adv} = \sum_{\beta} X_{\beta}^{\kappa} F_{\beta} \tag{2.5}$$

where k_0 is absolute permeability, b is the Klinkenberg factor (Klinkenberg, 1941) for gas slippage effect (b=0 when β=aqueous phase), $k_{r\beta}$ is relative permeability to phase β, μ_{β} is viscosity, P_{β} is pressure in the β phase, and $\boldsymbol{g}$ is the vector of gravitational acceleration. The diffusive fluxes are evaluated by the formulation:

$$J_{\beta}^{\kappa} = -\phi\tau_{\beta}\rho_{\beta}d_{\beta}^{\kappa}\nabla X_{\beta}^{\kappa} \tag{2.6}$$

where d_{β}^{κ} is the molecular diffusion coefficient for component κ in phase β, τ_{β} is the tortuosity which is a function of rock property and phase saturation, and X_{β}^{κ} is mass fraction of component κ in phase β.

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

$$F^{\kappa} = -[(1-\phi)K_R + \phi \sum_{\beta=1,2,3} S_\beta K_\beta]\nabla T + f_\sigma \sigma_0 \nabla T^4 + \sum_{\beta=1,2} h_\beta F_\beta \tag{2.7}$$

where K_R is thermal conductivity of the rock, K_β is thermal conductivity of phase β, T is temperature, h_β is specific enthalpy of phase β, f_σ is radiant emittance factor, and σ_0 is the Stefan-Boltzmann constant.

2.2 Formulation of geomechanics in porous medium

This new coupling method assumes that boundaries of each block element can move as an elastic material and obey the generalized Hooke's law. The mean normal stress is selected as an additional primary variable in the model.

Under the assumption of linear elastic with small strain for thermo-poro-elastic system, the equilibrium equation can be expressed in three dimensional as follows (Jaeger et al., 2007)

$$\sigma_{kk} - \left[\alpha P + 3\beta K(T - T_{ref})\right] = 2G\varepsilon_{kk} + \lambda(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}), k = x, y, z \tag{2.8}$$

where σ is the normal stress, α is the Biot's coefficient, β is the linear thermal expansion coefficient, K is the bulk modulus, λ is the Lame's constant, G is the shear modulus, and ε is the strain. The subscript k stands for the directions. Summing over the x, y and z components of Equation 2.8 gives the Hooke's law for poro-thermo-elastic medium:

$$\frac{\sigma_{xx} + \sigma_{yy} + \sigma_{zz}}{3} - \alpha P - 3\beta K\left(T - T_{ref}\right) = \left(\lambda + \frac{2}{3}G\right)\left(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz}\right) \tag{2.9}$$

Rewrite Equation 2.9 with mean normal stress and volumetric strain:

$$\sigma_m - \alpha P - 3\beta K\left(T - T_{ref}\right) = \left(\lambda + \frac{2}{3}G\right)\varepsilon_v \tag{2.10}$$

where σ_m and ε_v are the mean normal stress and volumetric strain, respectively.

One fundamental relation in the linear elasticity theory is that strain can be expressed in terms of a displacement vector, *u*. The displacement vector points from the new position of a volume element to its previous one. The strain tensor is related to the displacement vector by

$$\overline{\overline{\varepsilon}} = \frac{1}{2}\left[\nabla\overline{u} + (\nabla\overline{u})^T\right] \tag{2.11}$$

which can be also written as:

$$\varepsilon_{jk} = \frac{1}{2}\left[\frac{\partial u_k}{\partial x_j} + \frac{\partial u_j}{\partial x_k}\right], (k, j) = x, y, z; x_l = x, y, z \tag{2.12}$$

Under the static equilibrium conditions,

$$\nabla \cdot \overline{\overline{\sigma}} + \overline{F} = 0 \tag{2.13}$$

where $\overline{\overline{\sigma}}$ is the stress tensor and $\overline{F}$ is the body force vector.

Substitute Equation 2.8 into Equation 2.12, leading to the three explicit equations:

$$\alpha\frac{\partial P}{\partial x} + 3\beta K\frac{\partial T}{\partial x} + 2G\frac{\partial \varepsilon_{xx}}{\partial x} + \lambda\frac{\partial(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz})}{\partial x} + 2G\frac{\partial \varepsilon_{yx}}{\partial y} + 2G\frac{\partial \varepsilon_{zx}}{\partial z} + F_x = 0 \tag{2.14}$$

$$\alpha\frac{\partial P}{\partial y} + 3\beta K\frac{\partial T}{\partial y} + 2G\frac{\partial \varepsilon_{yy}}{\partial y} + \lambda\frac{\partial(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz})}{\partial y} + 2G\frac{\partial \varepsilon_{yx}}{\partial x} + 2G\frac{\partial \varepsilon_{yz}}{\partial z} + F_y = 0 \tag{2.15}$$

$$\alpha\frac{\partial P}{\partial z} + 3\beta K\frac{\partial T}{\partial z} + 2G\frac{\partial \varepsilon_{zz}}{\partial z} + \lambda\frac{\partial(\varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz})}{\partial z} + 2G\frac{\partial \varepsilon_{yz}}{\partial y} + 2G\frac{\partial \varepsilon_{xz}}{\partial x} + F_z = 0 \tag{2.16}$$

With relation of Equation 2.11, Equations 2.14-16, the following equations in terms of the displacement vector are obtained:

$$\alpha\frac{\partial P}{\partial x} + 3\beta K\frac{\partial T}{\partial x} + (2G + \lambda)\frac{\partial^2 u_x}{\partial x^2} + \lambda\frac{\partial^2 u_y}{\partial x \partial y} + \lambda\frac{\partial^2 u_z}{\partial x \partial z} + G(\frac{\partial^2 u_x}{\partial y^2} + \frac{\partial^2 u_y}{\partial x \partial y}) + G(\frac{\partial^2 u_x}{\partial z^2} + \frac{\partial^2 u_z}{\partial x \partial z}) + F_x = 0 \tag{2.17}$$

$$\alpha\frac{\partial P}{\partial y} + 3\beta K\frac{\partial T}{\partial y} + (2G + \lambda)\frac{\partial^2 u_y}{\partial y^2} + \lambda\frac{\partial^2 u_x}{\partial x \partial y} + \lambda\frac{\partial^2 u_z}{\partial y \partial z} + G(\frac{\partial^2 u_y}{\partial x^2} + \frac{\partial^2 u_x}{\partial x \partial y}) + G(\frac{\partial^2 u_y}{\partial z^2} + \frac{\partial^2 u_z}{\partial y \partial z}) + F_y = 0 \tag{2.18}$$

$$\alpha\frac{\partial P}{\partial z} + 3\beta K\frac{\partial T}{\partial z} + (2G + \lambda)\frac{\partial^2 u_z}{\partial z^2} + \lambda\frac{\partial^2 u_y}{\partial z \partial y} + \lambda\frac{\partial^2 u_x}{\partial x \partial z} + G(\frac{\partial^2 u_z}{\partial x^2} + \frac{\partial^2 u_x}{\partial x \partial z}) + G(\frac{\partial^2 u_z}{\partial y^2} + \frac{\partial^2 u_y}{\partial y \partial z}) + F_z = 0 \tag{2.19}$$

Equations 2.17-2.18 can be rearranged as

$$\alpha\frac{\partial P}{\partial x}+3\beta K\frac{\partial T}{\partial x}+(G+\lambda)(\frac{\partial^2 u_x}{\partial x^2}+\frac{\partial^2 u_y}{\partial x\partial y}+\frac{\partial^2 u_z}{\partial x\partial z})+G(\frac{\partial^2 u_x}{\partial x^2}+\frac{\partial^2 u_x}{\partial y^2}+\frac{\partial^2 u_x}{\partial z^2})+F_x=0 \qquad (2.20)$$

$$\alpha\frac{\partial P}{\partial y}+3\beta K\frac{\partial T}{\partial y}+(G+\lambda)(\frac{\partial^2 u_x}{\partial x\partial y}+\frac{\partial^2 u_y}{\partial y^2}+\frac{\partial^2 u_z}{\partial y\partial z})+G(\frac{\partial^2 u_y}{\partial x^2}+\frac{\partial^2 u_y}{\partial y^2}+\frac{\partial^2 u_y}{\partial z^2})+F_y=0 \qquad (2.21)$$

$$\alpha\frac{\partial P}{\partial z}+3\beta K\frac{\partial T}{\partial z}+(G+\lambda)(\frac{\partial^2 u_x}{\partial x\partial z}+\frac{\partial^2 u_y}{\partial y\partial z}+\frac{\partial^2 u_z}{\partial z^2})+G(\frac{\partial^2 u_z}{\partial x^2}+\frac{\partial^2 u_z}{\partial y^2}+\frac{\partial^2 u_z}{\partial z^2})+F_z=0 \qquad (2.22)$$

Equations 2.20-2.22 can be expressed in a condensed form as

$$\alpha\nabla P+3\beta K\alpha\nabla T+(\lambda+G)\nabla(\nabla\bullet\bar{u})+G\nabla^2\bar{u}+\bar{F}=0 \qquad (2.23)$$

which is the thermo-poro-elastic Navier equation.

Equation 2.23 has two terms containing the displacement vector and taking the divergence of it results in the following explicit equations

$$\alpha\frac{\partial^2 P}{\partial x^2}+3\beta K\frac{\partial^2 T}{\partial x^2}+(G+\lambda)\frac{\partial}{\partial x}(\frac{\partial^2 u_x}{\partial x^2}+\frac{\partial^2 u_y}{\partial x\partial y}+\frac{\partial^2 u_z}{\partial x\partial z})+G\frac{\partial}{\partial x}(\frac{\partial^2 u_x}{\partial x^2}+\frac{\partial^2 u_x}{\partial y^2}+\frac{\partial^2 u_x}{\partial z^2})+\frac{\partial F_x}{\partial x}=0 \qquad (2.24)$$

$$\alpha\frac{\partial^2 P}{\partial y^2}+3\beta K\frac{\partial^2 T}{\partial y^2}+(G+\lambda)\frac{\partial}{\partial x}(\frac{\partial^2 u_x}{\partial x\partial y}+\frac{\partial^2 u_y}{\partial y^2}+\frac{\partial^2 u_z}{\partial y\partial z})+G\frac{\partial}{\partial x}(\frac{\partial^2 u_y}{\partial x^2}+\frac{\partial^2 u_y}{\partial y^2}+\frac{\partial^2 u_y}{\partial z^2})+\frac{\partial F_y}{\partial x}=0 \qquad (2.25)$$

$$\alpha\frac{\partial^2 P}{\partial z^2}+3\beta K\frac{\partial^2 T}{\partial z^2}+(G+\lambda)\frac{\partial}{\partial z}(\frac{\partial^2 u_x}{\partial x\partial z}+\frac{\partial^2 u_y}{\partial y\partial z}+\frac{\partial^2 u_z}{\partial z^2})+G\frac{\partial}{\partial z}(\frac{\partial^2 u_z}{\partial x^2}+\frac{\partial^2 u_z}{\partial y^2}+\frac{\partial^2 u_z}{\partial z^2})+\frac{\partial F_z}{\partial z}=0 \qquad (2.26)$$

Adding Equations 2.23-2.25 together and changing the order of differentiation:

$$\begin{aligned}
&\alpha(\frac{\partial^2 P}{\partial x^2}+\frac{\partial^2 P}{\partial y^2}+\frac{\partial^2 P}{\partial z^2})+\frac{\partial F_x}{\partial x}+\frac{\partial F_y}{\partial y}+\frac{\partial F_z}{\partial z}+3\beta K(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2})+\\
&(G+\lambda)\frac{\partial^2}{\partial x^2}(\frac{\partial u_x}{\partial x}+\frac{\partial u_y}{\partial y}+\frac{\partial u_z}{\partial z})+G(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2})\frac{\partial u_x}{\partial x}+\\
&(G+\lambda)\frac{\partial^2}{\partial y^2}(\frac{\partial u_x}{\partial x}+\frac{\partial u_y}{\partial y}+\frac{\partial u_z}{\partial z})+G(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2})\frac{\partial u_y}{\partial y}+\\
&(G+\lambda)\frac{\partial^2}{\partial z^2}(\frac{\partial u_x}{\partial x}+\frac{\partial u_y}{\partial y}+\frac{\partial u_z}{\partial z})+G(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2})\frac{\partial u_z}{\partial z}=0
\end{aligned} \qquad (2.27)$$

Equation 2.27 may be written as the following equation with only one term of displacement vector.

$$\alpha\nabla^2 P + 3\beta K\nabla^2 T + (\lambda + 2G)\nabla^2(\nabla\bullet\bar{u}) + \nabla\bullet\bar{F} = 0 \qquad (2.28)$$

The divergence of the displacement vector is the volumetric strain

$$\nabla\bullet\bar{u} = \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z} = \varepsilon_{xx} + \varepsilon_{yy} + \varepsilon_{zz} = \varepsilon_v \qquad (2.29)$$

Combine Equations 2.29 and 2.10:

$$\nabla\bullet\bar{u} = \varepsilon_v = \frac{\sigma_m - \alpha P - 3\beta K\left(T - T_{ref}\right)}{\left(\lambda + \frac{2}{3}G\right)} \qquad (2.30)$$

Substitute Equation 2.30 to 2.28:

$$\alpha\nabla^2 P + 3\beta K\nabla^2 T + \frac{\lambda + 2G}{\lambda + \frac{2}{3}G}\nabla^2(\sigma_m - \alpha P - 3\beta K(T - T_{ref})) + \nabla\bullet\bar{F} = 0 \qquad (2.31)$$

The coefficient of the third term in Equation 2.31 is only a function of Poisson’s ratio υ

$$\frac{\lambda + 2G}{\lambda + \frac{2}{3}G} = \frac{3(1-\upsilon)}{(1+\upsilon)} \qquad (2.32)$$

Equation 2.31 then becomes

$$\frac{3(1-\nu)}{(1+\nu)}\nabla^2\sigma_m + \nabla\bullet\bar{F} - \frac{2(1-2\nu)}{(1+\nu)}(\alpha\nabla^2 P + 3\beta K\nabla^2 T) = 0 \qquad (2.33)$$

Equation 2.33 is the governing geomechanical equation for TOUGH2-EGS and the mean normal stress is the additional primary variables in parallel to pore pressure and temperature variables. The volumetric strain is another geomechanical variable, which can be solved with the relationship of Equation 2.30.

Finally, for the multi-porosity medium represented by multiple interacting continua (MINC) (Pruess and Narasimhan, 1982, 1985; Pruess, 1991), the governing geomechanical equation may be written as

$$\frac{3(1-\nu)}{(1+\nu)}\nabla^2\sigma_m + \nabla\bullet\bar{F} - \sum_j \frac{2(1-2\nu)}{(1+\nu)}(\alpha_j\nabla^2 P_j + 3\beta_j K_j \nabla^2 T_j) = 0 \qquad (2.34)$$

where subscript j refers to a multi-porosity continuum or one MINC block in MINC-method.

2.3 Formulation of reactive geochemistry

The governing equation for chemical transport has the same structure as the mass conservation of Equation 2.1. The aqueous species are subject to transport in the liquid phase as well as to local chemical interactions with solid and gas phases. Transport equations are written in terms of total dissolved concentrations of chemical components, which are concentrations of the basis species plus their associated aqueous secondary species (Yeh and Tripathi, 1991; Steefel and Lasaga, 1994; Walter et al., 1994; Lichtner, 1996; Xu and Pruess, 2001). Advection and diffusion processes are considered for chemical transport, and the diffusion coefficients are assumed to be the same for all species. The local chemical interactions in the transport equations are represented by reaction source/sink terms. Each chemical component in the liquid phase follows the general governing Equation 2.1 with the following accumulation and flux terms.

$$M^k = \phi S_k C_{kl} \qquad (2.35)$$

$$F^k = v_l C_{kl} - \left(\tau\phi S_l D_l\right)\nabla C_{kl} \qquad k = 1 \ldots N_l \qquad (2.36)$$

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

It is convenient to select a subset of aqueous species as basis species (or component or primary species) for representing a geochemical system. All other species are called secondary species that include aqueous complexes, precipitated and gaseous species (Reed, 1982; Yeh and Tripathi, 1991; Steefel and Lasaga, 1994). The number of secondary species must be equal to the number of independent reactions. Any of the secondary species can be represented as a linear combination of the set of basis species such as

$$C_i = \sum_{j=1}^{N_c} v_{ij} C_j \qquad i = 1 \ldots N_R \tag{2.37}$$

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. Likewise, the concentration of aqueous complex can be expressed as function of that of primary species.

Aqueous complexation reactions are assumed to be at local equilibrium. By making use of the mass action equation to the dissociation of the i^{th} aqueous complex, concentrations of aqueous complexes can be expressed as functions of the concentrations of basis species:

$$c_i = K_i^{-1} \gamma_i^{-1} \prod_{j=1}^{N_c} c_j^{v_{ij}} \gamma_j^{v_{ij}} \tag{2.38}$$

where c_i is molar concentration of the i^{th} aqueous complex, and c_j is molar concentration of the j^{th} basis species, γ_i and γ_j are thermodynamic activity coefficients, and K_i is the equilibrium constant.

The mineral saturation ratio can be expressed as

$$\Omega_m = X_m^{-1} \lambda_m^{-1} K_m^{-1} \prod_{j=1}^{N_c} c_j^{v_{mj}} \gamma_j^{v_{mj}} \qquad m = 1 \ldots N_p \tag{2.39}$$

where m is the equilibrium mineral index, X_m is the mole fraction of the m^{th} mineral phase, λ_m is its thermodynamic activity coefficient (for pure mineral phases X_m and λ_m are taken equal to one), and K_m is the corresponding equilibrium constant.

At equilibrium, we have

$$SI_m = \log_{10} \Omega_m = 0 \tag{2.40}$$

where SI_m is called the mineral saturation index.

Kinetic rates could be functions of non-basis species as well. Usually the species appearing in rate laws happen to be basis species. In this model, we use a rate expression given by Lasaga et al. (1994):

$$r_n = f(c_1, c_2, ..., c_{NC}) = \pm k_n A_n \left|1 - \Omega_n^\theta\right|^\eta \quad n = 1...N_q \tag{2.41}$$

where positive values of r_n indicate dissolution, and negative values precipitation, k_n is the rate constant (moles per unit mineral surface area and unit time), which is temperature dependent, A_n is the specific reactive surface area per kg H_2O. Ω_n is the kinetic mineral saturation ratio defined as in Equation 2.39. The parameters θ and η must be determined from experiments; usually, but not always, they are taken equal to one. The temperature dependence of the reaction rate constant can be expressed reasonably well via an Arrhenius equation (Steefel and Lasaga, 1994). Since many rate constants are reported at 25°C, it is convenient to approximate rate constant dependency as a function of temperature, thus

$$k = k_{25} \exp\left[\frac{-E_a}{R}\left(\frac{1}{T} - \frac{1}{298.15}\right)\right] \tag{2.42}$$

where E_a is the activation energy, k_{25} is the rate constant at 25°C, R is universal gas constant, and T is absolute temperature.

Carroll et al. (1998) noted that the rates of amorphous silica precipitation based on Rimstidt and Barnes (1980) are about three orders of magnitude lower than those observed in geothermal systems. Carroll et al. (1998) presented experimental data on amorphous silica precipitation for more complex geothermal fluids at higher degrees of supersaturation, and also for a near-saturation simple fluid chemistry. Under conditions far from equilibrium, the rate law for amorphous silica precipitation has been expressed as:

$$r = kA(\Omega)^\theta \tag{2.43}$$

This rate does not tend to zero as Ω goes to one, and therefore, a modification was made to this law so that it tends to zero as Ω approaches one

$$r = kA\left[\Omega^{\theta} - \frac{1}{\Omega^{2\theta}}\right] \tag{2.44}$$

The kinetic rate constant k in Equations 2.41 and 2.42 only considers the most well-studied mechanism in pure H_2O (neutral pH). Dissolution and precipitation of minerals are often catalyzed by H^+ (acid mechanism) and OH^- (base mechanism). For many minerals, the kinetic rate constant k includes exchange of these three mechanisms (Lasaga et al., 1994) as,

$$\begin{aligned} k &= k_{25}^{nu}\exp\left[\frac{-E_a^{nu}}{R}\left(\frac{1}{T}-\frac{1}{298.15}\right)\right] + k_{25}^{H}\exp\left[\frac{-E_a^{H}}{R}\left(\frac{1}{T}-\frac{1}{298.15}\right)\right]a_H^{n_H} \\ &+ k_{25}^{OH}\exp\left[\frac{-E_a^{OH}}{R}\left(\frac{1}{T}-\frac{1}{298.15}\right)\right]a_{OH}^{n_{OH}} \end{aligned} \tag{2.45}$$

where superscripts or subscripts *nu*, H, and OH indicate neutral, acid and base mechanisms, respectively; a is the activity of the species; and n is power term (constant). Note that parameters θ and η (see Equation 2.41) are assumed the same for each mechanism. The rate constant k can be also dependent on other species such as Al^{3+} and Fe^{3+}. Two or more species may involve in one mechanism. A general form of species dependent rate constants (extension of Equation 2.45) is coded as,

$$k = k_{25}^{nu}\exp\left[\frac{-E_a^{nu}}{R}\left(\frac{1}{T}-\frac{1}{298.15}\right)\right] + \sum_i k_{25}^{i}\exp\left[\frac{-E_a^{i}}{R}\left(\frac{1}{T}-\frac{1}{298.15}\right)\right]\prod_j a_{ij}^{n_{ij}} \tag{2.46}$$

where superscripts or subscripts i is the additional mechanism index, and j is species index involved in one mechanism that can be primary or secondary species. The codes considers up to five additional mechanisms and up to five species involved in each mechanism.

The precipitation of a mineral can be suppressed up to a given, positive saturation index value, $\log(\Omega)_w$. Within this "supersaturation window", the mineral is not allowed to precipitate. The mineral precipitates if its saturation index $\log(\Omega) \geq \log(\Omega)_w$, and dissolves if $\log(\Omega) < 0$. The size of the window can be set to decrease exponentially with temperature as follows:

$$\log(\Omega)_{w,T} = \log(\Omega)_{w,T}^{0}\exp(-4.61(T-T^0)/(T_1-T^0)) \tag{2.47}$$

where $log(\Omega)_{w,T}$ is the window at the current temperature T and $log(\Omega)^0_{w,T}$ is the initial (input) window at temperature T_0. T_1 is the temperature at which the window is one hundredth the size of the initial window. Values of $log(\Omega)^0_{w,T}$, T_0, and T_1 are provided in input parameters.

2.4 Hydraulic properties correlations

The hydraulic properties of EGS reservoirs, such as porosity, permeability and capillary pressure are subjected to change due to geomechanical and geochemical effects.

2.4.1 Stress induced correlation

The correlation between hydraulic properties, such as porosity/permeability and stress has been intensively investigated. We describe the dependence of permeability and porosity on effective stress in TOUGH2-EGS in this section. Effective stress was initially defined as the difference between the normal stress and the pore pressure by Terzaghi (1936) and was generalized by Biot and Willis (1957) as:

$$\sigma' = \sigma - \alpha P \tag{2.48}$$

where α is the Biot or effective stress coefficient. A couple of widely accepted correlations between effective stress and hydraulic properties have been incorporated into TOUGH2-EGS.

Rutqvist et al. (2002b) presented the following function for porosity, obtained from laboratory experiments on sedimentary rock by Davies and Davies (1999)

$$\phi = \phi_r + (\phi_0 - \phi_r)e^{-a\sigma'} \tag{2.49}$$

where ϕ_0 is zero effective stress porosity, ϕ_r is high effective stress porosity, and the exponent a is a parameter related specific rock. An associated correlation for permeability in terms of porosity also has been presented

$$k = k_0 e^{c(\frac{\phi}{\phi_0}-1)} \tag{2.50}$$

where *c* is also rock specific parameter. For fracture network, Rutqvist et al. (2002b) defined the aperture width b_i in the direction *i* as function of effective stress

$$b_i = b_{0,i} + \Delta b_i = b_i + b_{\max}(e^{-d\sigma'} - e^{-d\sigma_0'}) \tag{2.51}$$

where subscript *0* refers to initial conditions, Δb_i is the aperture change, which is function of maximum "mechanical" aperture b_{max}, initial and current effective stress σ_0' and σ', and fracture specific parameter *d*. Fracture porosity is correlated to the aperture b_i as:

$$\phi = \phi_0 \frac{b_1 + b_2 + b_3}{b_{1,0} + b_{2,0} + b_{3,0}} \tag{2.52}$$

and permeability in direction *i* is correlated to fracture aperture of other directions *j* and *k* as:

$$k_i = k_{i,0} \frac{b_j^3 + b_k^3}{b_{j,0}^3 + b_{k,0}^3} \tag{2.53}$$

McKee et al. (1988) derived a relationship between porosity and effective stress from poro-elasticity theory for incompressible rock grains:

$$\phi = \phi_0 \frac{e^{-c_p(\sigma' - \sigma_0')}}{1 - \phi_0(1 - e^{-c_p(\sigma' - \sigma_0')})} \tag{2.54}$$

where c_p is average pore compressibility. They also related permeability and porosity with Carman-Kozeny equation:

$$k = k_i \frac{(1-\phi_i)^2}{(1-\phi)^2}\left(\frac{\phi}{\phi_i}\right)^3 \tag{2.55}$$

These relationships fit laboratory and field data for granite, sandstone, clay and coal. Ostensen (1986) studied the relationship between effective stress and permeability for tight gas sands:

$$k^n = D\ln\left[1 + \left(\frac{\sigma'^*}{\sigma'}\right)^2\right] \tag{2.56}$$

where exponential n is 0.5, D is a parameter, and σ'^* is effective stress for zero permeability, obtained by extrapolating measured square root permeability versus effective stress on a semi-log plot.

Verma and Pruess (1988) presented a power law expression relating permeability to porosity:

$$\frac{k-k_c}{k_0-k_c}=(\frac{\phi-\phi_c}{\phi_0-\phi_c})^n \tag{2.57}$$

where k_c and ϕ_c are asymptotic values of permeability and porosity, respectively, and exponent n is a parameter.

Gutierrez and Lewis (2001) presented expressions for solid volume change with pressure and effective stress. These expressions can be integrated to yield an expression for solid volume

$$V_s\left(P,\sigma\right)=V_{s,r}\left[1+\frac{1-\phi_r}{K_s}\left(P-P_r\right)-\frac{1}{K_s}\left(\sigma-\sigma_r\right)\right] \tag{2.58}$$

where subscript r refers to reference conditions. The bulk volume is related to the volumetric strain as following equation

$$V=V_r\left(1-\varepsilon_v\right) \tag{2.59}$$

where V is the bulk volume. The definition of porosity relates to solid volume and bulk volume as

$$\phi=1-\frac{V_s}{V} \tag{2.60}$$

Combining above three equations yield porosity as a function of pressure, temperature and effective stress

$$\phi=1-\frac{\left(1-\phi_r\right)\left[1+\frac{1-\phi_r}{K_s}\left(P-P_r\right)-\frac{1}{K_s}\left(\sigma-\sigma_r\right)\right]}{\frac{1-\varepsilon_v}{1-\varepsilon_{v,r}}} \tag{2.61}$$

2.4.2 Mineral precipitation/dissolution induced correlations

Reservoir porosity in matrix and fractures are directly related to the rock mineral volume, which is subjected to change as a result of precipitation and dissolution. The porosity of the medium (fracture or matrix) is given by

$$\phi = 1 - \sum_{m=1}^{Nm} fr^m - fr^u \tag{2.62}$$

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

The correlation of change in permeability due to chemical reaction may be different for fracture and matrix. In fracture medium, the permeability changes can be approximated using the porosity change and an assumption of plane parallel fractures of uniform aperture (cubic law; Steefel and Lasaga, 1994). The modified permeability, k, is given by

$$k = k_i \left(\frac{\phi}{\phi_i} \right)^3 \tag{2.63}$$

where k_i and ϕ_i are the initial permeability and porosity respectively. This law gives the zero permeability only under zero fracture porosity, which is not true in most experimental and natural systems. Therefore a much strong relationship between permeability and porosity can be developed with fracture aperture. The initial aperture b_0 can be calculated with following cubic law:

$$b_0 = \left(12 k_0 s\right)^{1/3} \tag{2.64}$$

where k_0 is the initial fracture permeability and s is the fracture spacing. The permeability resulting from the change in aperture, is given by

$$k = \frac{\left(b_0 + \Delta b\right)^3}{12 s} \tag{2.65}$$

where Δb is the aperture change resulting from mineral precipitation and dissolution. Xu et al. (2004a) presented the relation between Δb and porosity of the fracture medium.

$$\Delta b = \frac{(\phi - \phi_0)}{\phi_0} b_g \tag{2.66}$$

where b_g is the initial aperture for precipitation, or called geometric aperture, which can be obtained from the ratio of the initial porosity ϕ_0 to the fracture surface area A_f:

$$b_g = \phi_0 / A_f \tag{2.67}$$

For the matrix permeability change, the Carman-Kozeny relation as Equation 2.55 and Verma and Pruess (1988) as Equation 2.57 can be used to correlate the permeability with the porosity change.

2.4.3 Geomechanical and geochemical effects

The change in rock properties under combined geomechanical and geochemical effects may be obtained by coupling them together. The resulting porosity change is calculated as the summation of geomechanical and geochemical induced changes as follows:

$$\phi = \phi_0 + \Delta\phi_m + \Delta\phi_c \tag{2.68}$$

where ϕ_0 is the initial porosity, $\Delta\phi_m$ is the mechanical induced porosity change, and $\Delta\phi_c$ is the chemical induced porosity change. The $\Delta\phi_m$ and $\Delta\phi_c$ are described as section 2.4.1 and 2.4.2.

For matrix medium, the permeability change is given by either Carman-Kozeny or Verma and Pruess correlations as Equation 2.55 or 2.57.

For fracture medium, the permeability change could be obtained by cubic law as equation 2.59, or through aperture changes:

$$b = b_0 + \Delta b_m + \Delta b_c \tag{2.69}$$

Where b is the fracture aperture, the subscript $_0$ is the initial state; m and c stand for mechanical and chemical induced change, respectively, which are also described in section 2.4.1 and 2.4.2.

The updated permeability and porosity are used to scale capillary pressure according to the relation by Leverett (1941):

$$P_c = P_{c0} \frac{\sqrt{(k/\phi)_0}}{\sqrt{k/\phi}} \tag{2.70}$$

3 NUMERICAL MODEL AND CODE ARCHITECTURE

3.1 Space and times discretization

The continuous space and time variables must be discretized for numerical simulation. We are using the integral finite difference method (IFDM) (Edwards, 1972; Narasimhan and Witherspoon, 1976) as shown in Figure 3-1, for space discretization. IFDM avoids any reference to a global system of coordinates, and thus offers the advantage of being applicable to regular or irregular discretization in one, two, and three dimensions. The IFDM also makes it possible, by means of simple preprocessing of geometric data, to implement double- and multiple-porosity methods for modeling flow in fractured media. Time will be discretized fully implicitly as a first-order backward finite difference.

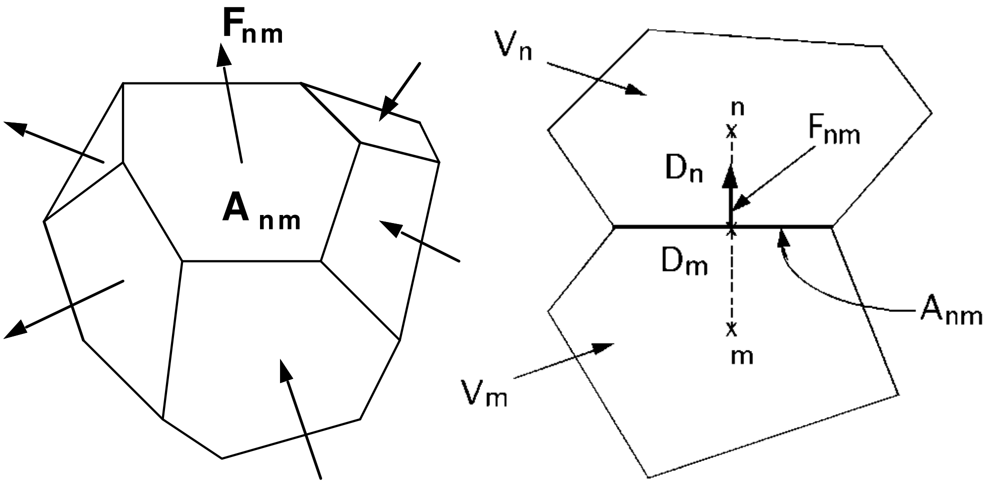


Figure 3-1 Space discretization for the integral finite difference method (Pruess et al., 1999)

Time and space discretization of Equation 2.1 results in a set of coupled non-linear equations, which can be written in residual form as follows (Pruess et al., 1999):

$$R_n^{\kappa}(x^{t+1}) = M_n^{\kappa}(x^{t+1}) - M_n^{\kappa}(x^{t}) - \frac{\Delta t}{V_n}\{\sum_m A_{nm} F_{nm}^{\kappa}(x^{t+1}) + V_n q_n^{\kappa,t+1}\} = 0, \kappa = 1,2,3 \qquad (3.1)$$

where the vector x^t consists of primary variables at time t, R_n^k is the residual of component k (component 1 is water, 2 is air and 3 is the energy) for grid block n, M denotes mass or thermal energy per unit volume for a component, V_n is the volume of the block n, q denotes sinks and sources of mass or energy, Δt denotes the current time step size, $t+1$ denotes the current time, A_{nm} is the interface area between neighboring blocks n and m, and F_{nm} is the "flow" term (fluid flow, heat transfer, and advective and diffusive mass transport) between them.

Equation 2.33 expresses the mean stress in terms of the pore pressure and body forces. It is discretized using the Integral Finite Difference method over volume element, V, with outer surface, Γ. Applying the divergence theorem to the Laplacian operators in Equation 2.33 gives

$$\int\left(\frac{3(1-\nu)}{(1+\nu)}\nabla\sigma_m+\bar{F}-\frac{2(1-2\nu)}{(1+\nu)}(\alpha\nabla P+3\beta K\nabla T)\right)\cdot\hat{n}d\Gamma=0 \tag{3.2}$$

The surface integral can be expressed as a discrete sum of averages over surface segments

$$\sum_j\left(\frac{3(1-\nu)}{(1+\nu)}\nabla\sigma_m+\bar{F}-\frac{2(1-2\nu)}{(1+\nu)}(\alpha\nabla P+3\beta K\nabla T)\right)_j A_j=0 \tag{3.3}$$

where j is the neighboring grid blocks. The boundary conditions for Equation 3.3 are a reference temperature, pressure, and stress at some distance from a given grid block.

The finite difference approximation for Equation 3.3 in residual form is

$$R_n^4(x^{t+1})=\sum_j\left(\frac{3(1-\nu)}{(1+\nu)}\frac{\sigma_j-\sigma_i}{s_{ij}}-\frac{2(1-2\nu)}{(1+\nu)}\alpha\frac{p_j-p_i}{s_{ij}}-\frac{2E}{(1+\nu)}\beta\frac{T_j-T_i}{s_{ij}}+\rho_{tot}g\hat{k}\cdot\hat{n}\right)_{ij}A_{ij}=0 \tag{3.4}$$

The model solves four equations (Equation 3.1 and 3.4) simultaneously for four primary variables (pressure, air mass fraction/gas saturation, temperature, and mean normal stress) for each grid block. The Newton/Raphson method is used for solving the equations, which can be expressed as

$$-\sum_i\left.\frac{\partial R_n^{\kappa,t+1}}{\partial x_i}\right|_p(x_{i,p+1}-x_{i,p})=R_n^{\kappa,t+1}(x_{i,p}),\kappa=1,2,3,4 \tag{3.5}$$

where $x_{i,p}$ represents the value of i^{th} primary variable at the p^{th} iteration step.

Equation 3.5 solves four equations with Newton/Raphson method, corresponding to four components, water, air, energy and stress. There are also four primary variables in the system summarized as Table 3-1.

Table 3-1 Primary variables setup up for solving Equation 3.5

Phase Condition	Primary Variables			
	1	2	3	4
Single Phase Liquid	Liquid pressure P_l	Air mass fraction X	Temperature T	Stress σ
Single Phase Gas	Gas pressure P_g	Air mass fraction X	Temperature T	Stress σ
Two phase	Gas pressure P_g	Gas saturation plus 10 S_g+10	Temperature T	Stress σ

The accumulation term of the component *k* mass balance has the general form

$$\frac{d}{dt}\int_0^{V(t)} M_k dV \tag{3.6}$$

The upper limit in the integral indicates that grid block volume changes with time. The finite difference approximation for Equation 3.6 is

$$\frac{((VM_k)^{n+1}-(VM_k)^n)}{\Delta t} \tag{3.7}$$

Grid block volume and bulk strain are related by

$$V = V_0(1-\varepsilon_v) \tag{3.8}$$

where V_0 is initial grid block volume.

3.2 Multi-porosity flow model

Figure 3-2 illustrates the classical double-porosity concept for modeling flow in fractured porous media as developed by Warren and Root (1963). The flow domain is composed of matrix blocks of low permeability, embedded in a network of interconnected fractures. In these reservoirs, the fractures have larger permeability and smaller porosity relative to those of the porous rock matrix. As a result, a pressure change in the reservoir would travel through fracture much faster than through the rock matrix. The classical double-porosity approach assumes that global fluid flow occurs mostly through the fracture with pseudo-steady exchange between the fracture and matrix, which is also dependent on pressure and temperature difference between them.

However, the assumption of pseudo-steady exchange between fracture and matrix is not valid for many systems, such as complex, multiphase flow or large matrix volumes (Wu and Pruess, 1988), because the time scale associated with flow through the matrix is too large. We model the multi-porosity media with Multiple Interacting Continua (MINC) approach (Pruess and Narasimhan, 1982, 1985; Pruess, 1991). In the MINC conceptual model, flow within the matrix is described more accurately by subdividing the matrix into nested volumes, as shown in Figure 3-3, with flow occurring between adjacent nested matrix volumes, as well as between the fractures and the outer matrix volume. The idea of MINC approach is that the local changes in matrix conditions will be controlled by the distance from the fractures. The volume with same distance to the fracture comprises one MINC block. Flow within the matrix is one-dimensional transient flow, and MINC approach reduces to the classical double porosity model if there is only one matrix subdivision.

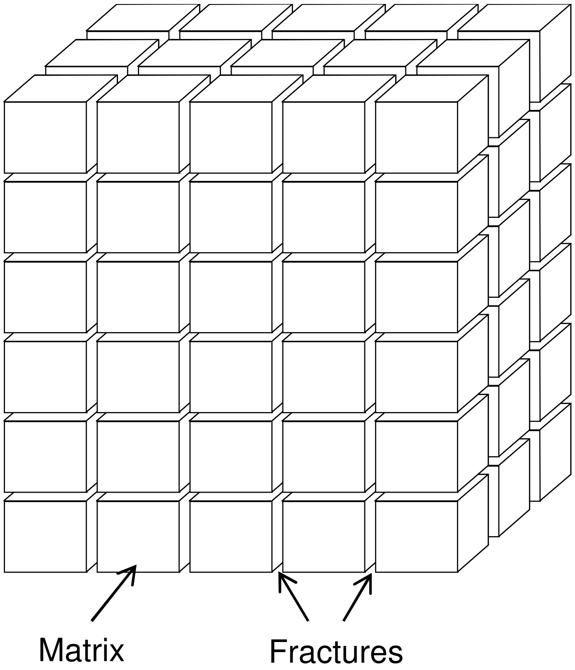


Figure 3-2 Schematic of "double porosity" model for a fractured porous medium (Warren and Root, 1963).

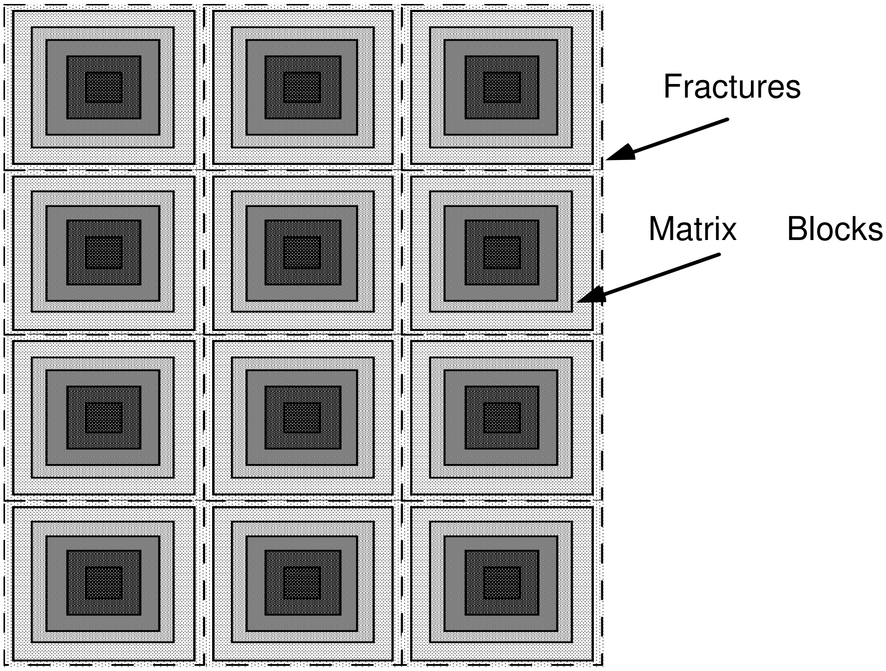


Figure 3-3 Subgridding in the approach of "multiple interacting continua" (MINC) (Pruess, 1991).

The MINC grid blocks can be generated with MESHMAKER function in our codes. For any given fractured reservoir, flow problem, selection of the most appropriate gridding scheme must be based on a careful consideration of the physical and geometric conditions of flow. The MINC approach may not be applicable to systems in which fracturing is so sparse that the fractures cannot be approximated as a continuum.

Considering a simulation domain discretized into N_v grid blocks with N_k components. For the single-porosity approach, there are N_k+2 equations, N_k mass conservation equations, one momentum conservation equation and one energy equation, associated with each grid block, and total $N_v(N_k+2)$ equations for the entire simulation domain. For MINC approach with N_ϕ multi-porous continua in each grid block, there are N_k+1 equations, N_k mass conservation equations, one energy equation for each porous continuum, and one momentum equation for the entire grid block, therefore total $N_v(1+N_\phi(1+N_k))$ equations for the entire simulation domain. The number of equations for single and multi-porosity medium are summarized as Table 3-2.

Table 3-2 Summary of equations for single and multi-porosity medium

Porosity System	Number of Global Grid Blocks (GGB)	Local Grid Block (LGB)	Mass and Energy Conservation Equations/LGB	Momentum Conservation Equations/LGB	Total Equations/LGB	Total Equations
Single	N_v	1	$1+N_k$	1	$2+N_k$	$(2+N_k)N_v$
Multi	N_v	N_ϕ	$(1+N_k)N_\phi$	1	$(1+N_k)N_\phi+1$	$[(1+N_k)N_\phi+1]N_v$

3.3 Simulation logic and procedures

Figure 3-4 describes the program process. It mainly includes two modules, the geomechanical and geochemical modules. Although the figure shows the THMC process, the two modules can be run independently only for THM or THC according to the selection of a user in the input files.

The THMC coupling logic is as follows: The input files, including rock hydrologic and geomechanical properties, computing parameters, solute and chemical parameters, etc., are read into the program. Before stepping into the main cycle, the program initializes the stress state and chemical state variables at initial condition. For each time step, the THM variables are firstly solved and the results, such as fluid velocity, phase saturations, and temperatures, will be used to solve solute transport and chemical reactions. The solute transport and chemical reactions are solved iteratively until chemical state converges. The time control cycle repeats until the target time is reached.

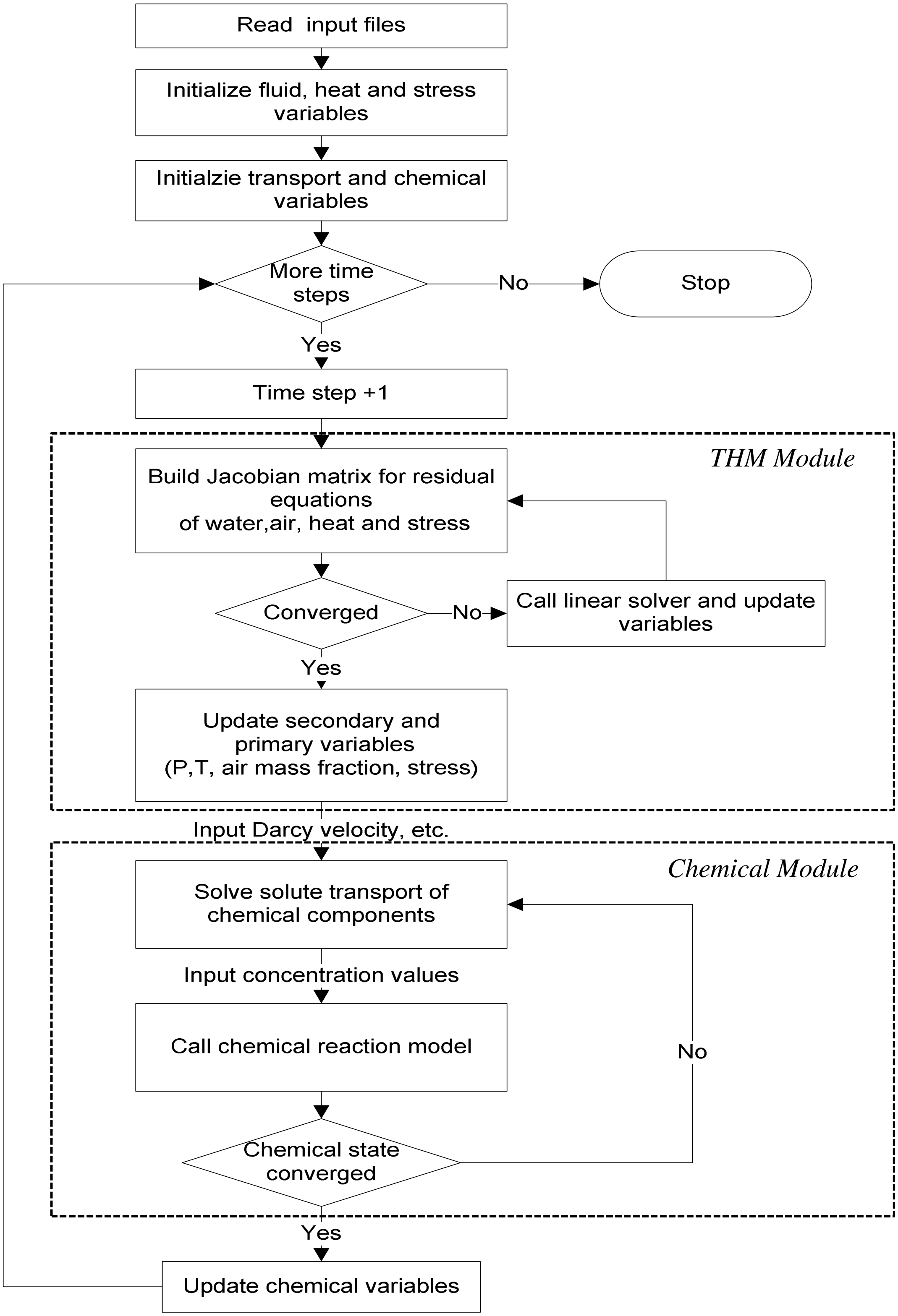


Figure 3-4 The simulation logic and procedures

3.4 *Code architecture and data structure*

The model architecture is summarized in Figure 3-5. In TOUGH2-EGS, *NEL* is the total number of grid blocks; *NK* is two as the number of components. Each element has *NKx* primary variables as Table 3-1, stored sequentially in a one-dimensional array *X*; first the *NKx* variables for grid block *#1*, then the *NKx* variables for grid block *#2*, and so on, as shown in Figure 3-6. The starting location for primary variables for grid block *N* is *NLOC+1*, where *NLOC=(N-1)*NKx*. The thermophysical and stress properties are needed to assemble the mass- and energy-balance equations for all volume elements, which are considered as secondary variables are stored sequentially in a large array *PAR*.

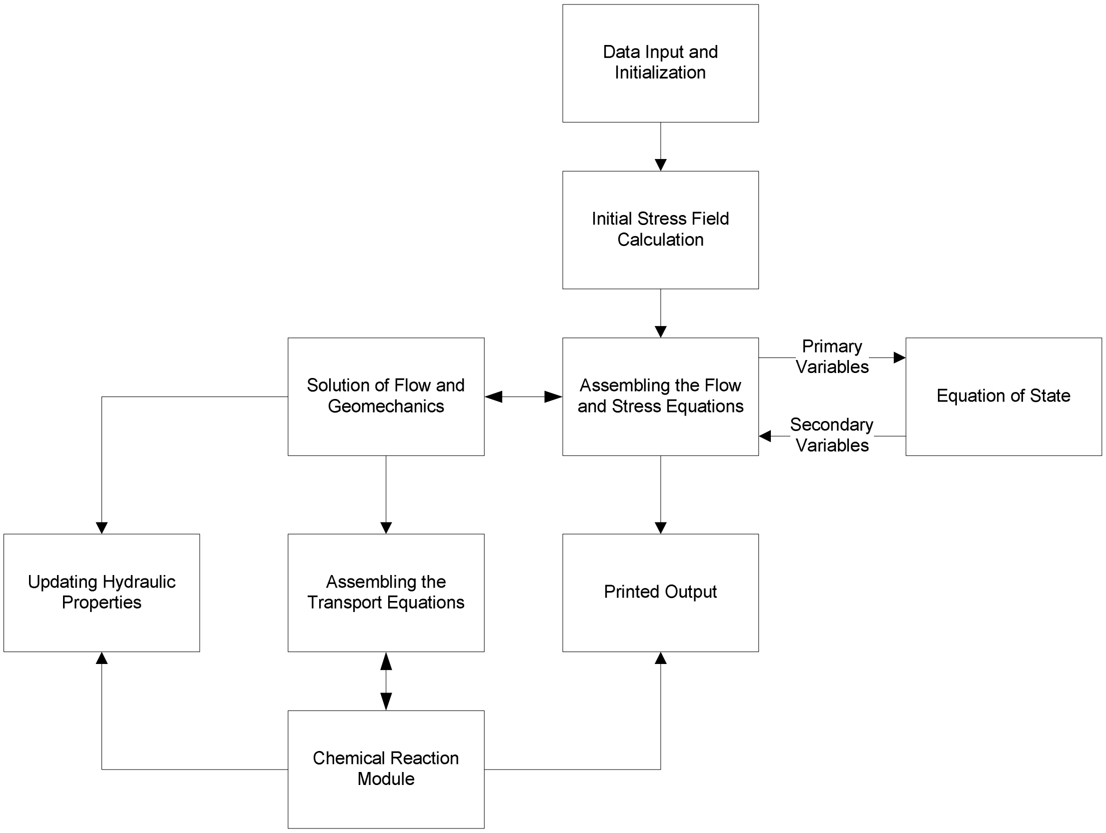
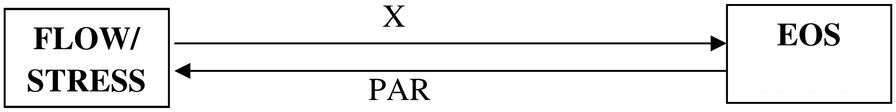


Figure 3-5 Model Architecture of TOUGH2-EGS

As shown in Figure 3-6, the first group of *NB (=8)* secondary parameters includes the parameters needed for the accumulation and flow terms. Starting in the location *NB+1*, there are *NK* component mass fractions, so that the total number of secondary parameters per fluid phase is *NBK* = *NB*+*NK*. By TOUGH2 convention, the *NBK* gas phase parameters come first, followed by *NBK* parameters for the aqueous phase. The *NPH*NB*K phase-specific parameters are followed by 9 other parameters, including geomechanical variables and temperature, etc. Therefore there total *NPH*NBK+9* secondary variables. There are another *NEQ* (number of equations) set of secondary variables, which are used for evaluating numerical derivatives. The TOUGH2 user guide (Pruess, 1991) gives the detailed description on it.



Volume Element	**Primary Variables**
#1	X(1)
	...
	X(NKx)
#2	**X(NKx+1)**
	...
	*X(2*NKx)*
	…
#N	X(NLOC+1)
	...
	X(NLOC+NKx)
	…
#NEL	...
	X(NEL*NKx)

Volume Element **SECONDARY PARAMETERS**

			gas phase	aqueous phase
#1	phase saturation	S	PAR(1)	PAR(NBK+1)
	relative permeability	Kr	PAR(2)	…
	viscosity	μ	PAR(3)	…
	density	ρ	PAR(4)	…
	specific enthalpy	h	PAR(5)	…
	capillary pressure	P_c	PAR(6)	…
	diffusion factor 1	a	PAR(7)	…
	diffusion factor 2	b	PAR(8)	…
	<u>mass fractions</u>			
	component 1	X^1	PAR(NB+1)	…
	…			
	component NK	X^{NK}	PAR(NB+NK)	PAR(2*NBK)
	mean stress		PAR(NSEC-8)	
	mean stress		PAR(NSEC-7)	
	stain $(1-\varepsilon_v)$		PAR(NSEC-6)	
	Permeability (kz)		PAR(NSEC-5)	
	Permeability (ky)		PAR(NSEC-4)	
	Permeability (kx)		PAR(NSEC-3)	
	Porosity (ϕ)		PAR(NSEC-2)	
	temperature	T	PAR(NSEC-1)	
	(miscellaneous)		PAR(NSEC)	
	(second set of secondary parameters: X(1) incremented)			
			PAR(NSEC+1)	
			…	
			PAR(2*NSEC)	
			…	
			PAR((NEQ+1)*NSEC)	
#2	…			
…	…			
#NEL	…			

Figure 3-6 Structure of thermophysical and stress property arrays in TOUGH2-EGS

4 USING TOUGH2-EGS

4.1 Compilation

The code was written in standard Fortran 77, which can be compiled in any platform with compiler supporting Fortran 77. The Table 4-1 shows all the source files and its descriptions for TOUGH2-EGS.

Table 4-1. Lists of source files of TOUGH2-EGS

File name	Description
eos3.f	Equation of state module for water and air components for EGS reservoirs
meshm.f	Mesh maker for generating grid blocks
react_coupled.f	Main coupling program for chemical reactions
t2cg2.f	TOUGH2 main program
t2f.f	TOUGH2 subroutines
t2react.f	Subroutines of chemical reactions program
t2solv.f	Conjugate gradient linear equation solvers
chempar.fi	INCLUDE file for PARAMETER statements of reactive geochemical transport
common.fi	INCLUDE file for common blocks for reactive geochemical transport
perm_cap.fi	INCLUDE file for PARAMETER statements related to porosity, permeability and capillary changes due to mineral dissolution and precipitation;
t2_old.fi	INCLUDE file for PARAMETER statements of dimensioning major arrays

Since Fortran 77 has no constraints on the features of routine checkup and array boundaries, the following compiling options are required to successfully compile the source codes. We take the Intel Fortran compiler as the example to show how to set the options:

- Set Project Properties->Fortran->Diagnostic->Check Routine Interface to No
- Set Project Properties->Fortran ->Data->Default Real to 8 bytes
- Set Project Properties->Fortran->Run-time->Check Array and String Bound to No

The other compilers should have the similar options, which are required to set to proper values for the compiling.

4.2 Execution

The executable “TOUGH2_EGS.exe” can be run in Windows system by simply double click. The prompt of the running execution:

> ***PLEASE TYPE A FLOW INPUT FILE NAME (INCLUDING EXTENSION)***

Here type the main input file name, which includes the description for the flow parameters and computation parameters for geomechanics and chemical reactions.

> ***PLEASE TYPE A MAIN OUTPUT FILE NAME (INCLUDING EXTENSION)***

Here type the main output file name, which includes the computation results of flow and geomechanics simulation.

There are three input files for mechanical and chemical simulations, and only one input file for mechanical simulation.

Main input file: This file includes rock properties, time-stepping information, geometric grid information, initial and boundary conditions, and data related to multi-phase fluid and heat flow simulation. The flow input is the same as the original TOUGH2 V2 (see the manual; Pruess et al., 1999), with some additional data blocks for geomechanical and geochemical setting. This file name is defined and input by the users.

Transport input file - “solute.inp”: This file contains various flags and input parameters for calculations of reactive transport, such as diffusion coefficients, tolerance limits for convergence of transport and chemical iterations, printout flags for mineral and aqueous species, and the configuration of model zones with different chemical composition. The filename is fixed as “solute.inp” and the users do not need to type this file as input, but do need to prepare it in the folder.

Chemical reaction input file – “chemical.inp”: This file is used to define the geochemical system (i.e. the type and number of aqueous component species and minerals considered in the simulation). It also includes the initial compositions of water, mineral, and gas zones configured in file solute.inp, and kinetic data for minerals (rate constants, surface areas, etc.).

In addition to the three input files above, the program needs a thermodynamic database file. The file name is specified in solute.inp file. This file contains reaction stoichiometry, dissociation constants (log(K)), and regression coefficients of log(K) as a function of temperature.

If performing coupled geomechanical simulation only, the transport input file, chemical reaction input file and thermodynamic database file are not needed. They are required to perform coupled geochemical simulations.

Table 4-2. Keywords of data blocks of main input file

KEYWORD	FUNCTION
TITLE (first record)	One data record (single line) with a title for the simulation problem
MESHM	Optional; parameters for internal grid generation through MESHMaker
ROCKS	Hydrogeologic parameters for various reservoir domains or rock types
MULTI	Optional; specifies number of fluid components and balance equations per grid block; applicable only for certain fluid property (EOS) modules
SELEC	Used with EOS-modules to supply thermophysical property data
START	Optional; one data record for more flexible initialization
PARAM	Computational parameters; time stepping and convergence parameters;
RPCAP	Optional; parameters for relative permeability and capillary pressure functions
TIMES	Optional; specification of times for generating printout
*ELEME	List of grid blocks (volume elements)
*CONNE	List of flow connections between grid blocks
*GENER	Optional; list of mass or heat sinks and sources
INDOM	Optional; list of initial conditions for specific reservoir domains
*INCON	Optional; list of initial conditions for specific grid blocks
NOVER (optional)	Optional; if present, suppresses printout of version numbers and dates of the program units executed in a TOUGH2-EGS run
SOLVR	Introducing solver parameters;
REACT	Parameters for chemical reactions
GRMOD	Optional; setting individual properties for specific grid blocks
FOFT	Optional; list of grid blocks for time-dependent output
COFT	Optional; list of connections for time-dependent output
GOFT	Optional; list of sink/source grid blocks for time-dependent output
ENDCY (last record)	One record to close the TOUGH2-EGS main input file and initiate the simulation
ENDFI	Alternative to “ENDCY” for closing a TOUGH2-EGS main input file; will cause flow simulation to be skipped; useful if only mesh generation is desired

§Blocks labeled with a star * can be provided as separate disk files, in which case they would be omitted from the main input file.

5 DESCRIPTION OF INPUT FILES

In this chapter, we are going to describe the detailed format for the input files mentioned above. The start for each record for the input data block are in bold and underlined like **<u>BOLD</u>**, and the keywords and variables in each data block are in **BOLD**.

5.1 Main Input files format

The main input file uses the TOUGH2 convention for the keywords of input data blocks. The Table 5-1 list the key words of the input data blocks for the main input file. This section presents the data input format of the main input file for TOUGH2-EGS.

TITLE	is the first record of the input file, containing a header of up to 80 characters, to be printed on output. This can be used to identify a problem. If no title is desired, leave this record blank.
MESHM	introduces parameters for internal mesh generation and processing. The MESHMaker input has a modular structure which is organized by keywords. Detailed instructions for preparing MESHMaker input are given in Section 5.2.

<u>Record MESHM.1</u>

Variable: WORD

Format: A5

WORD	enter one of several keywords, such as RZ2D, RZ2DL, XYZ, and MINC, to generate different kinds of computational meshes.

<u>Record MESHM.2</u>

A blank record closes the MESHM data block.

ENDFI	is a keyword that can be used to close a TOUGH2 input file when no flow simulation is desired. This will often be used for a mesh generation run when some hand-editing of the mesh will be needed before the actual flow simulation.
ROCKS	introduces material parameters for up to 27 different reservoir domains.

Record ROCKS.1

Variable: MAT, NAD, DROK, POR, (PER (I), I = 1, 3), CWET, SPHT

Format: A5, I5, 7E10.4

MAT	material name (rock type).
NAD	if zero or negative, defaults will take effect for a number of parameters (see below); ≥1: will read another data record to override defaults. ≥2: will read two more records with domain-specific parameters for relative permeability and capillary pressure functions. ≥3: will read three more records with domain-specific parameters for rock mechanics and stress-porosity, stress-permeability relations.
DROK	rock grain density (kg/m^3)
POR	default porosity (void fraction) for all elements belonging to domain "MAT" for which no other porosity has been specified in block INCON. Option "START" is necessary for using default porosity.
PER (I)	absolute permeability along the three principal axes, as specified by ISOT in block CONNE.
CWET	formation heat conductivity under fully liquid-saturated conditions (W/m ˚C).

SPHT	rock grain specific heat (J/kg ˚C). Domains with SPHT > 104 J/kg ˚ C will not be included in global material balances. This provision is useful for boundary nodes, which are given very large volumes so that their thermo-dynamic state remains constant. Because of the large volume, inclusion of such nodes in global material balances would make the balances useless.

Note: if SPHT < 0, then a table for temperature-dependent rock grain specific heat needs to be input following Record ROCKS.1.1.

<u>Record ROCKS.1.1</u> (optional, NAD ≥ 1 only)

Variable: COM, EXPAN, CDRY, TORTX, GK

Format: 5E10.4

COM	pore compressibility (Pa^{-1})
EXPAN	linear temperature expansivity (1/ ˚C)
CDRY	formation heat conductivity under desaturated conditions (W/m ˚C), default is CWET
TORTX	tortuosity factor for binary diffusion.
GK	Klinkenberg parameter *b* (Pa^{-1}) for enhancing gas phase

<u>Record ROCKS.1.2</u> (optional, NAD ≥ 2 only)

Variable: IRP, (RP(I), I= 1,7)

Format: I5, 5X,7E10.4

IRP	integer parameter to choose type of relative permeability function (see Appendix B).

RP(I)	I = 1, ..., 7, parameters for relative permeability function (Appendix C).

Record ROCKS.1.3 (optional, NAD ≥ 2 only)

Variable: ICP, (CP(I), I = 1,7)

Format: I5, 5X,7E10.4)

ICP	integer parameter to choose type of capillary pressure function (see Appendix C).
CP(I)	I = 1, ..., 7, parameters for capillary pressure function (Appendix C).

Repeat records 1, 1.1, 1.2, and 1.3 for any number of reservoir domains.

Record ROCKS.1.4 (optional, NAD≥3 only)

Variable: IRPOPT, IRKOPT, IPORPERM, POIRAT, YOUNGM, CBIOT, TREF

Format: 2I5, I10, 7E10.4

IRPOPT	Stress-porosity correlation options
IRKOPT	Stress-permeability correlation options
IPORPERM	Porosity-permeability correlation options. This option will be used in the following two scenarios: (1) In the coupled geomechanical and geochemical simulations, the total permeability change is calculated from porosity change due to mechanical and chemical effects for given IPORPERM options. (2) If IRKOPT is not given for geomechanical simulations, the stress induced permeability change will be also calculated from stress induced porosity change for given IPORPERM options.

POIRAT	Poisson ratio
YOUNGM	Young’s module
CBIOT	Biot’s coefficient.
TREF	Reference temperature.

<u>Record ROCKS.1.5</u> (optional, NAD≥3 only)

Variable: RCKPAR(I),I=1,8

Format: 8E10.4

RCKPAR	The parameters for porosity and permeability correlations with stress

Repeat records 1, 1.1, 1.2, and 1.5 for up to 27 reservoir domains.

<u>Record ROCKS.2</u> A blank record closes the ROCKS data block.

ICOUP the keyword to specify the coupling process for the simulation

<u>Record ICOUP. 1</u>

Variable: ISTCAL, ICHCAL

Format: 2I10

ISTCAL	the flag to specify the geomechanical coupling process. = 1 coupling geomechanical process = 0 no geomechanical coupling
ICHCAL	the flag to specify the reactive chemical process = 1 coupling chemical reaction process =0 no chemical reaction coupling

The coupling process is controlled with ISTCAL and ICHCAL, which enables TH, THM, THC and THMC coupled simulation. See Table 5-1 for the coupling options summary.

Table 5-1 Coupling Options Summary

Coupling Options	**Value of ISTCAL**	**Value of ICHCAL**
T-H	0	0
THM	1	0
THC	0	1
THMC	1	1

START (optional) a record with START typed in columns 1-5 allows a more flexible initialization. More specifically, when START is present, INCON data can be in arbitrary order, and need not be present for all grid blocks (in which case defaults will be used). Without START, there must be a one-to-one correspondence between the data in blocks ELEME and INCON.

PARAM introduces computation parameters, time stepping information, and default initial conditions.

Record PARAM.1

Variables: NOITE, KDATA, MCYC, MSEC, MCYPR, (MOP(I), I = 1, 24), TEXP, BE

Format: 2I2,3I4,24I1,E9.4,4E10.4

NOITE specifies the maximum number of Newtonian iterations per time step (default is 8)

KDATA specifies amount of printout (default is 1)

= 0 or 1: print a selection of the most important variables.

= 2: in addition, print mass and heat fluxes and flow velocities.

= 3: in addition, print primary variables and their changes.

If the above values for KDATA are increased by 10, printout will occur after each Newton-Raphson iteration (not just after convergence).

MCYC	maximum number of time steps to be calculated
MSEC	maximum duration, in CPU seconds, of the simulation (default is infinite).
MCYPR	printout will occur for every multiple of MCYPR steps (default is 1).
MOP(I)	I = 1,24 allows choice of various options, which are documented in printed output from a TOUGH2-EGS run.
MOP(1)	if unequal 0, a short printout for non-convergent iterations will be generated. MOP(2) through MOP(6) generate additional printout in various subroutines, if set unequal 0. This feature should not be needed in normal applications, but it will be convenient when a user suspects a bug and wishes to examine the inner workings of the code. The amount of printout increases with MOP(I) (consult source code listings for details).
MOP(2)	CYCIT (main subroutine).
MOP(3)	MULTI (flow- and accumulation-terms).
MOP(4)	QU (sinks/sources).
MOP(5)	EOS (equation of state).
MOP(6)	LINEQ (linear equations).
MOP(7)	if unequal 0, a printout of input data will be provided. Calculation choices are as follows:

MOP(9) determines the composition of produced fluid with the MASS option (see GENER, below). The relative amounts of phases are determined as follows:

= 0: according to relative mobility in the source element.

= 1: produced source fluid has the same phase composition as the producing element.

MOP(10) chooses the interpolation formula for heat conductivity of rock as a function of liquid saturation (S_l)

= 0: $C(S_l) = CDRY + SQRT(S_l * [CWET - CDRY])$

= 1: $C(S_l) = CDRY + S_l * (CWET - CDRY)$

MOP(11) determines evaluation of mobility and permeability at interfaces.

= 0: mobilities are upstream weighted with WUP (see PARAM.3), permeability is upstream weighted.

= 1: mobilities are averaged between adjacent elements, permeability is upstream weighted.

= 2: mobilities are upstream weighted, permeability is harmonic weighted.

= 3: mobilities are averaged between adjacent elements, permeability is harmonic weighted.

= 4: mobility and permeability are both harmonic weighted.

MOP(12) determines interpolation procedure for time dependent sink/source data (flow rates and enthalpies).

= 0: triple linear interpolation; tabular data are used to obtain interpolated rates and enthalpies for the beginning and end of the time step; the average of these values is then used.

= 1: step function option; rates and enthalpies are taken as averages of the table values corresponding to the beginning and end of the time step.

= 2: rigorous step rate capability for time dependent generation data.

A set of time ti and generation rates qi provided in data block GENER is

interpreted to mean that sink/source rates are piecewise constant and

change in discontinuous fashion at table points. Specifically, generation is assumed to occur at constant rate qi during the time interval [ti,ti+1), and changes to qi+1 at ti+1. Actual rate used during a time step that ends at time t, with ti≤t≤ti+1, is automatically adjusted in such a way that total cumulative exchanged mass at time t

$$Q(t) = \int_0^t q dt' = \sum_{j=1}^{i-1} q_j (t_{j+1} - t_j) + q_i (t - t_i)$$

is rigorously conserved. If also tabular data for enthalpies are given, an

analogous adjustment is made for fluid enthalpy, so preserve $\int qhdt$.

MOP(14) not used in this version

MOP(15) determines conductive heat exchange with impermeable confining layers

= 0: heat exchange is off.

= 1: heat exchange is on (for grid blocks that have a non-zero heat transfer area; see data block ELEME).

MOP(16) provides automatic time step control. Time step size will be doubled if convergence occurs within ITER ≤ MOP(16) Newton-Raphson iterations.

It is recommended to set MOP(16) in the range of 2 - 4.

MOP(17) not used in this version

MOP(18) selects handling of interface density.

= 0: perform upstream weighting for interface density.

> 0: average interface density between the two grid blocks. However, when one of the two phase saturations is zero, upstream weighting will be performed.

MOP(19) not used in this version

MOP(20) not used in this version

MOP(21) select the linear equation solver.

= 0 or 1: defaults to MOP(21) = 3, DSLUCS, Lanczos-type preconditioned bi-conjugate gradient solver.

= 2: DSLUBC, bi-conjugate gradient solver.

= 3: DSLUCS, (default).

= 4: DSLUGM, generalized minimum residual preconditioned conjugate gradient solver.

= 5: DLUSTB, stabilized bi-conjugate gradient solver.

= 6: LUBAND, banded direct solver.

All conjugate gradient solvers use incomplete LU-factorization as a default preconditioner. Other preconditioners may be chosen by means of a data block SOLVR.

MOP(22)	not used in this version
MOP(23)	not used in this version
MOP(24)	determines handling of multiphase diffusive fluxes at interfaces. = 0: harmonic weighting of fully-coupled effective multiphase diffusivity. = 1: separate harmonic weighting of gas and liquid phase diffusivities.

TEXP	parameter for temperature dependence of gas phase diffusion coefficient.
BE	(optional) parameter for effective strength of enhanced vapor diffusion; if set to a non-zero value, will replace the parameter group 0 for vapor diffusion.

Record PARAM.2

Variables: TSTART, TIMAX, DELTEN, DELTMX, ELST, GF, REDLT, SCALE

Format: 4E10.4, A5, 5X,3E10.4

TSTART	starting time of simulation in seconds (default is 0).
TIMAX	time in seconds at which simulation should stop (default is infinite).
DELTEN	length of time steps in seconds. If DELTEN is a negative integer, DELTEN = - NDLT, the program will proceed to read NDLT records with time step information. Note that - NDLT must be provided as a floating point number, with decimal point.

DELTMX	upper limit for time step size in seconds (default is infinite).
ELST	writes a file for time versus primary variables for selected elements at all the times, when ELST = RICKA.
GF	magnitude (m/sec^2) of the gravitational acceleration vector. Blank or zero gives "no gravity" calculation.
REDLT	factor by which time step is reduced in case of convergence failure or other problems (default is 4).
SCALE	scale factor to change the size of the mesh (default = 1.0).

Record PARAM.2.1, 2.2, etc.

Variables: DLT(I), I = 1, 100

Format: 8E10.4

DLT(I)	Length (in seconds) of time step I. This set of records is optional for DELTEN = - NDLT, a negative integer. Up to 13 records can be read, each containing 8 time step data. If the number of simulated time steps exceeds the number of DLT(I), the simulation will continue with time steps equal to the last non-zero DLT(I) encountered. When automatic time step control is chosen (MOP (16) > 0), time steps following the last DLT (I) input by the user will increase according to the convergence rate of the Newton-Raphson iteration. Automatic time step reduction will occur if the maximum number of Newton-Raphson iterations is exceeded (parameter NOITE, record PARAM.1)

Record PARAM.3

Variables: RE1, RE2, U, WUP, WNR, DFAC

Format: 6E10.4

RE1	convergence criterion for relative error (default= 10^{-5}).
RE2	convergence criterion for absolute error (default= 1).

U	not used in this version
WUP	upstream weighting factor for motilities and enthalpies at interfaces (default = 1.0 is recommended). $0 \leq \text{WUP} \leq 1$.
WNR	weighting factor for increments in Newton/Raphson - iteration (default = 1.0 is recommended). $0 < \text{WNR} \leq 1$.
DFAC	increment factor for numerically computing derivatives (default value DFAC $=10^{-k/2}$, where k, evaluated internally, is the number of significant digits of the floating point processor used; for 64-bit arithmetic, DFAC $\approx 10^{-8}$).

Record PARAM.4

Introduces fluid and heat flow primary variables (first three primary variables in Table 3-1), which are used as default initial conditions for all grid blocks that are not assigned by means of data blocks INDOM or INCON. Option START is necessary to use default INCON.

Note: The fourth primary variable, stress, will be initialized in the keyword GENER and variable GX.

Variables: DEP (I), I = 1, 3

Format: 3E20.14

DEP	The number of primary variables, 3, is normally assigned internally in the EOS module, and is usually equal to the number NEQ of equations solved per grid block. See data block MULTI for special assignments of 3. Different sets of primary variables are in use for different EOS modules.
INDOM	introduces domain-specific initial conditions. These will supersede default initial conditions specified in PARAM.4, and can be overwritten by element-specific initial conditions in data block INCON. Option START is needed to use INDOM conditions.

Record INDOM. 1

Variables: MAT

Format: A5

MAT	name of a reservoir domain, as specified in data block ROCKS.

Record INDOM.2

A set of primary flow variables assigned to all grid blocks in the domain specified in record INDOM. l. Different sets of primary variables are used for different EOS modules.

Variables: Xl, X2, X3

Format: 3E20.13

Record INDOM.3

A blank record closes the INDOM data block. Repeat records INDOM. l and INDOM.2 for as many domains as desired. The ordering is arbitrary and need not be the same as in block ROCKS.

INCON	introduces element-specific initial conditions.

Record INCON.1

Variables: ELNE, NSEQ, NADD

Format: A5, 2I5

ELNE	code name of element.
NSEQ	number of additional elements with the same initial conditions (used only for 5-character element name).
NADD	increment between the code numbers of two successive elements with identical initial conditions (used only for 5-character element name).

Record INCON.2 specifies fluid and heat equation primary variables.

Variables: Xl, X2, X3

Format: 3E20.14

A set of fluid and heat primary variables for the element specified in record INCON.l. INCON specifications will supersede default conditions specified in PARAM.4, and domain-specific conditions that may have been specified in data block INDOM.

Record INCON.3

A blank record closes the INCON data block. Alternatively, initial condition information may terminate on a record with '+++' typed in the first three columns, followed by time stepping information. This feature is used for a continuation run from a previous TOUGH2 simulation.

SOLVR: (optional) introduces a data block with parameters for linear equation solvers.

Record SOLVR.1

Variables: MATSLV, ZPROCS, OPROCS, RITMAX, CLOSUR

Format: I1, 2X, A2, 3X, A2, 2E10.4

MATSLV: selects the linear equation solver.

= 1: Default (DSLUCS)

= 2: DSLUBC.

= 3: DSLUCS.

= 4: DSLUGM.

= 5: DLUSTB.

= 6: LUBAND.

ZPROCS selects the Z-preconditioning (Moridis and Pruess, 1998). Regardless of user specifications, Z-preprocessing will only be performed when iterative solvers are used ($2 \leq MATSLV \leq 5$), and if there are zeros on the main diagonal of the Jacobian matrix.

= Z0: no Z-preprocessing (default for NEQ=1)

= Z1: replace zeros on the main diagonal by a small constant (1.e-25; default for NEQ≠1)

= Z2: make linear combinations of equations for each grid block to achieve non-zeros on the main diagonal

= Z3: normalize equations, followed by Z2

= Z4: affine transformation to unit main-diagonal submatrices, without center pivoting

OPROCS: selects the O-preconditioning (Moridis and Pruess, 1998).

= O0: no O-preprocessing (default, also invoked for NEQ=1)

= O1: eliminate lower half of the main-diagonal submatrix with center pivoting

= O2: O1, plus eliminate upper half of the main-diagonal submatrix with center pivoting

= O3: O2, plus normalize, resulting in unit main-diagonal submatrices.

= O4: affine transformation to unit main-diagonal submatrices, without center pivoting

RITMAX selects the maximum number of CG iterations as a fraction of the total number of equations (0.0<RITMAX≤1.0; default is RITMAX=0.1)

CLOSUR convergence criterion for the CG iterations (1.e-12≤CLOSUR≤1.e-6; default is CLOSUR=1.e-6)

FOFT: (optional) introduces a list of elements (grid blocks) for which time-dependent data are to be written out for plotting to a file called FOFT during the simulation.

Record FOFT.1

FOFT is an element name. Repeat for up to 100 elements, one per record.

Variables: EOFT (I)

Format: A5

Record FOFT.2 A blank record closes the FOFT data block.

COFT: (optional) introduces a list of connections for which time-dependent data are to be written out for plotting to a file called COFT during the simulation.

Record COFT.1

ECOFT is a connection name, i.e., an ordered pair of two element names.

Variable: ECOFT (I)

Format: A10

Repeat for up to 100 connections, one per record.

Record COFT.2

A blank record closes the COFT data block.

GOFT: (optional) introduces a list of sinks/sources for which time-dependent data are to be written out for plotting to a file called GOFT during the simulation.

Record GOFT.1

Variables: EGOFT (I)

Format: A5

EGOFT is the name of an element in which a sink/source is defined. Repeat for up to 100 sinks/sources, one per record. When no sinks or sources are specified here, by default tabulation will be made for all.

Record GOFT.2 A blank record closes the GOFT data block.

NOVER: (optional) one record with NOVER typed in columns 1-5 will suppress printing of a summary of versions and dates of the program units used in a TOUGH2 run.

DIFFUSION (optional; needed only for NB≥8) introduces diffusion coefficients.

Record DIFFU.1

Diffusion coefficients for mass component #1 in all phases (I=1: gas; I=2: aqueous; etc.)

Variables: FDDIAG(I,1),I=1,NPH

Format: 8E10.4

Record DIFFU.2

Variables: FDDIAG(I,2),I=1,NPH

Format:8E10.4

FDDIAG diffusion coefficients for mass component #2 in all phases (I=1: gas; I=2: aqueous; etc.) provide a total of NK records with diffusion coefficients for all NK mass components.

SELEC: (optional) introduces a number of integer and floating point parameters that are used for different purposes in different TOUGH2 modules.

Record SELEC.1

Variables: IE (I), I=1, 16

Format: 16I5

IE (I) number of records with floating point numbers that will be read (default is IE(1) = 1; maximum values is 64).

Record SELEC.2, SELEC.3, ..., SELEC.IE(1)*8

provide as many records with floating point numbers as specified in IE(1), up to a maximum of 64 records

Variables: FE(I), I=1,IE(1)*8

Format: 8E10.4

RPCAP introduces information on relative permeability and capillary pressure functions, which will be applied for all flow domains for which no data were specified in records ROCKS.1.2 and ROCKS.1.3. A catalog of relative permeability and capillary pressure functions is presented in Appendix B and Appendix C, respectively.

Record RPCAP.1

Variables: IRP, (RP (I), I = 1, 7)

Format: I5, 5X, 7E10.4

IRP: integer parameter to choose type of relative permeability function (see Appendix B).

RP (I) I = 1, ..., 7 parameters for relative permeability function (Appendix B).

Record RPCAP.2

Variable: ICP, (CP (I), I = 1, 7)

Format: I5, 5X, 7E10.4

ICP integer parameter to choose type of capillary pressure function (see Appendix C).

CP(I) I = 1, ..., 7 parameters for capillary pressure function (Appendix C).

TIMES permits the user to obtain printout at specified times (optional). This printout will occur in addition to printout specified in record PARAM.1.

<u>Record TIMES.1</u>

Variables: ITI, ITE, DELAF, TINTER

Format: 2I5, 2E10.4

ITI	number of times provided on records TIMES.2, TIMES.3, etc., (see below; restriction: ITI ≤ 100).
ITE	total number of times desired (ITI ≤ ITE ≤ 100; default is ITE = ITI).
DELAF	maximum time step size after any of the prescribed times have been reached (default is infinite).
TINTER	time increment for times with index ITI, ITI+1, ..., ITE.

<u>Record TIMES.2, TIMES.3</u>, etc.

Variables: TIS (I), I = l, ITI

Format: 8E10.4

TIS (I)	list of times (in ascending order) at which printout is desired.

ELEME introduces element (grid block) information.

<u>Record ELEME.1</u>

Variables: ELEM, NSEQ, NADD, MA1, MA2, VOLX, AHTX, PMX, X, Y, Z

Format: A5,2I5,A3,A2,6E10.4

ELEM	five-character code name of an element.
NSEQ	number of additional elements having the same volume and belonging to the same reservoir domain (used only for 5-character element name).

NADD	increment between the code numbers of two successive elements. (Note: the maximum permissible code number NE + NSEQ *NADD is $\leq$ 99 and used only for 5-character element name)
MA1, MA2	a five-character material identifier corresponding to one of the reservoir domains as specified in block ROCKS. If the first three characters are blanks and the last two characters are numbers then they indicate the sequence number of the domain as entered in ROCKS. If both MA1 and MA2 are left blank the element is by default assigned to the first domain in block ROCKS.
VOLX	element volume (m^3).
AHTX	interface area (m^2) for heat exchange with semi-infinite confining beds.
PMX	permeability modifier (optional, active only when a domain 'SEED' has been specified in the ROCKS block), will be used as multiplicative factor for the permeability parameters from block ROCKS. Simultaneously, strength of capillary pressure will be scaled as 1/SQRT (PMX). PMX=0 will results in an impermeable block. Radom permeability modifiers can be generated internally. The PMX may be used to specify spatially correlated heterogeneous fields, but users need their own preprocessing programs for this, as TOUGH2 provides no internal capabilities for generating such fields.
X, Y, Z	Cartesian coordinates of grid block centers. These may be included in the ELEME data to make subsequent plotting of results more convenient. Repeat record ELEME.1 for the number of elements desired.

Record ELEME.2

A blank record closes the ELEME data block.

CONNE introduces information for the connections (interfaces) between elements.

Record CONNE.1

Variables:	ELEM1, ELEM2, NSEQ, NAD1, NAD2, ISOT, D1, D2, AREAX, BETAX, SIGX
Format:	A5,A5,4I5,5E10.4)
ELEM1	code name of the first element.
ELEM2	code name of the second element.
NSEQ	number of additional connections in the sequence (used only for 5-character element).
NAD1	increment of the code number of the first element between two successive connections (used only for 5-character element).
NAD2	increment of the code number of the second element between two successive connections (used only for 5-character element).
ISOT	set equal to 1, 2, or 3; specifies absolute permeability to be PER (ISOT) for the materials in elements (EL1, NE1) and (EL2, NE2), where PER is read in block ROCKS. This allows assignment of different permeability, e.g., in the horizontal and vertical direction.
D1, D2	distance (m) from first and second element, respectively, to their common interface.
AREAX	interface area (m^2).
BETAX	cosine of the angle between the gravitational acceleration vector and the line between the two elements. GF * BETAX > 0 (<0) corresponds to first element being above (below) the second element.
SIGX	"radiant emittance" factor for radiative heat transfer, which for a perfectly "black" body is equal to 1. The rate of radiative heat transfer between the two grid blocks is

$$G_{rad} = SIGX * \sigma_0 * AREAX * \left(T_2^4 - T_1^4\right) \tag{5.1}$$

where σ_0 = 5.6687e-8 J/m^2 K^4 s is the Stefan-Boltzmann constant, and T_1 and T_2 are the absolute temperatures of the two grid blocks. SIGX may be entered as a negative number, in which case the absolute value will be used, and heat conduction at the connection will be suppressed. SIGX = 0 will result in no radiative heat transfer.

Repeat record CONNE.1 for the number of connections desired.

Record CONNE.2

A blank record closes the CONNE data block. Alternatively, connection information may terminate on a record with '+++' typed in the first three columns, followed by element cross-referencing information. This is the termination used when generating a MESH file with TOUGH2-EGS.

REACT Parameter choices for reactive transport simulation

Record REACT.1

Variables: MOPR (20)

Format: 20I1

MOPR Flags show options for chemical reaction calculation.

MOPR(1) > 0	writes the transport coefficient matrix, Darcy velocities, porosities, and other transport data in the runlog.out file during calculations of aqueous species and gas transport. For debugging uses only.
MOPR(2) > 0	writes source terms, old and new aqueous concentrations, and various other parameters in the runlog.out file during transport calculations. Also outputs the permeability, porosity, and capillary pressure correction factor at each grid block in the runlog.out file. For debugging uses only.

MOPR(3)	This option to allow the # of digits past the decimal to be printed out for chemistry output files. Zero or blank gives the earlier default, which was originally 4 digits. The # of digits is up to 8.
MOPR(4) = 1	Printout two files for (1) mass balance information and (2) mineral saturation index vs. grid block at specified times. The two file names are fixed as mbalance.out and min_SI.dat.
=2	Pringout another file rctn_rate.out for mineral reaction rate information
=3	Print out another file rct_sfarea.out for mineral reaction surface area
= 0	No printout the two output files.
MOPR(5)-MOPR(20):	Not used now. Leave them blank.

GRMOD set properties for a grid block range. Properties are set for a grid block index range KJI given by

$$KJI = (I-1)*NUMI + (J-1)*NUMJ + (K-1)*NUMK + KJI0 \qquad (5.2)$$

where index *I* varies from *I1* to *I2*, index *J* varies from *J1* to *J2*, and index *K* varies from *K1* to *K2*. For MINC (Multiple Interacting Continua) simulations, *KJI* refers to the primary grid (before subdivision into multiple interacting continua) and the parameter *JMINC* refers to one of the continua. Continua in a MINC grid block are assumed to be numbered consecutively from 1 to *NMINC* (number of multiple interacting continua), for example, in a double-porosity fracture-matrix system, fracture is 1 and matrix is 2.

Record GRMOD.1

Variables: TYPE, NUMI, NUMJ, NUMK, KJI0, JMINC

Format: A5, 5X, 5I10

TYPE	must be “COEFS.”
NUMI	gridblock index multiple for I.
NUMJ	gridblock index multiple for J.
NUMK	gridblock index multiple for K.
KJI0:	gridblock index offset.
JMINC	MINC index, 1≤JMINC≤NMINC.

Record GRMOD.2.1

Variables: PROP, ISOT, I1, I2, J1, J2, K1, K2, VALUE

Format: A5, I5,6(I10),E10.4

PROP	Property identifier must be PERM, permeability, m^2.
IDIR	Permeability direction, ISOT = 1, 2, or 3.
I1	Start index for gridblock index multiple I.
I2	End index for gridblock index multiple I.
J1	Start index for gridblock index multiple J.
J2	End index for gridblock index multiple J.
K1	Start index for gridblock index multiple K.
K2	End index for gridblock index multiple K.
VALUE	Property value.

Record GRMOD.2.2

Variables: PROP, I1, I2, J1, J2, K1, K2, VALUE

Format: A5, 5X,6(I10),E10.4

PROP Property identifier, options are:

POROS - porosity;

PRESS - pressure, Pa;

PVAR2 - primary variable position 2;

PVAR3 - primary variable position 3;

TEMPR - temperature, °C;

STRES - mean stress, Pa.

The variables *I1*, *I2*, *J1*, *J2*, *K1*, *K2* and *VALUE* have the same meaning as previous record.

Record GRMOD.2.3

Variables: PROP, I1, I2, J1, J2, K1, K2, IVALUE

Format: A5, 5X,6(I10),I10

PROP Property identifier, options are:

BNDST - boundary status for mean stress equation, values are

0: gridblock does not border surroundings;

1: gridblock borders surroundings;

MATRG - material region.

The variables *I1*, *I2*, *J1*, *J2*, *K1*, *K2* have the same meaning as previous record

IVALUE	Property value (integer).

Record GRMOD.3

A blank record closes the GRMOD data block.

Data specified from a GRMOD.1 record are in effect until they are overwritten by that from a subsequent record. Any number of GRMOD records may appear. Entered grid block properties overwrite previous ones.

GENER introduces sinks or sources, or specify initial stress for specified grid blocks.

Record GENER.1

Variables: EL1, SL1, NSEQ, NADD, NADS, LTAB, TYPE, ITAB, GX, EX,HX

Format: A5, A5, 4I5, 5X, A4, A1, 3E10.4)

EL1	code name of the element containing the sink/source, or reference initial stress.
SL1	code name of the sink/source or reference initial stress. The first three characters are arbitrary; the last two characters must be numbers.
NSEQ	number of additional sinks/sources with the same injection/production rate, or same reference initial stress (not applicable for TYPE = DELV).
NADD	increment between the code numbers of two successive elements with identical sink/source, or reference initial stress.
NADS	increment between the code numbers of two successive sinks/sources only for 5-character element).
LTAB	number of points in table of generation rate versus time. Set 0 or 1 for constant generation rate. For wells on deliverability, LTAB denotes the number of open layers, to be specified only for the bottommost layer.

TYPE specifies different options for fluid or heat production and injection. For example, different fluid components may be injected, the nature of which depends on the EOS module being used. Different options for considering wellbore flow effects may also be specified.

HEAT	introduces a heat sink/source
WATE	component 1(water), injection only
COM1	component 1 (water), injection only
COM2	component 2, injection only
MASS	mass production rate specified.
DELV	well on deliverability, i.e., production occurs against specified bottomhole pressure. If well is completed in more than one layer, bottommost layer must be specified first, with number of layers given in LTAB. Subsequent layers must be given sequentially for a total number of LTAB layers.
RSTR	reference inital stress at a specified elevation and temperature used only for stress initialization
DELT	heat loss occurs against a specified temperature

ITAB unless left blank, table of specific enthalpies will be read (LTAB > 1 only)

GX constant generation rate; positive for injection, negative for production; GX is mass rate (kg/sec) for generation types COMl, COM2, and MASS; it is energy rate (J/s) for a HEAT sink/source.

For wells on deliverability, GX is productivity index PI (m^3);

For reference stress calculation, GX is reference initial stress (Pa). The stress of other grid blocks will be calculated from this reference stress under stress equilibrium condition.

For heat loss against a specified temperature, GX is heat transfer coefficient (J/s-m^2)

EX fixed specific enthalpy (J/kg) of the fluid for mass injection (GX>0). For wells on deliverability against fixed bottomhole pressure, EX is bottomhole pressure P_{wb} (Pa), at the center of the topmost producing layer in which the well is open.

HG thickness of layer (m; wells on deliverability with specified bottomhole pressure only).

<u>Record GENER.l.l</u> (optional, LTAB > l only)

Variables: Fl(L), L=l, LTAB

Format: 4E14.7

F1 generation times

<u>Record GENER.1.2</u> (optional, LTAB > 1 only)

Variable: F2 (L), L=1, LTAB

Format (4E14.7)

F2: generation rates.

<u>Record GENER.1.3</u> (optional, LTAB > 1 and ITAB non-blank only)

Variables: F3 (L), L=1, LTAB

Format: 4E14.7

F3 specific enthalpy of produced or injected fluid.

Repeat records GENER.1, 1.1, 1.2, and 1.3 for the number of sinks/sources desired.

Record GENER.2

A blank record closes the GENER data block.

Alternatively, generation information may terminate on a record with ‘+++’ typed in the first three columns, followed by element cross-referencing information.

ENDCY closes the TOUGH2 input file and initiates the simulation.

Note on closure of blocks CONNE, GENER, and INCON

The ordinary way to indicate the end of any of the above data blocks is by means of a blank record. There is an alternative available if the user makes up an input file from files MESH, GENER, or SAVE, which have been generated by a previous TOUGH2 run. These files are written exactly according to the specifications of data blocks ELEME and CONNE (file MESH), GENER (file GENER), and INCON (file SAVE), except that the CONNE, GENER, and INCON data terminate on a record with "+++" in columns 1-3, followed by some cross-referencing and restart information. TOUGH2 will accept this type of input, and in this case there is no blank record at the end of indicated data block.

5.2 Input Formats for MESHMAKER

The MESHMaker module performs internal mesh generation and processing. The input for MESHMaker has a modular structure and a variable number of records; it begins with keyword MESHM and ends with a blank record.

At the present time there are three sub-modules available in MESHMaker: keywords RZ2D or RZ2DL invoke generation of a one or two-dimensional radially symmetric R-Z mesh; XYZ initiates generation of a one, two, or three dimensional Cartesian X-Y-Z mesh; and MINC calls a modified version of the GMINC program (Pruess, 1983) to sub-partition a primary porous medium mesh into a secondary mesh for fractured media, using the method of “multiple interacting continua” (Pruess and Narasimhan, 1985). The meshes generated under keyword RZ2D or XYZ are internally written to file MESH. The MINC processing operates on the data in file MESH, so that invoking the RZ2D or XYZ options, or assignment of ELEME and CONNE blocks in the INPUT file must precede the MESHMaker/MINC data. We shall now separately describe the preparation of input data for the three MESHMaker sub-modules.

5.2.1 Generation of radially symmetric grids

Keyword RZ2D (or RZ2DL) invokes generation of a radially symmetric mesh. Values for the radii to which the grid blocks extend can be provided by the user or can be generated internally (see below). Nodal points will be placed half-way between neighboring radial interfaces. When RZ2D is specified, the mesh will be generated by columns; i.e., in the ELEME block we will first have the grid blocks at smallest radius for all layers, then the next largest radius for all layers, and so on. With keyword RZ2DL the mesh will be generated by layers; i.e., in the ELEME block we will first have all grid blocks for the first (top) layer from smallest to largest radius, then all grid blocks for the second layer, and so on. Apart from the different ordering of elements, the two meshes for RZ2D and RZ2DL are identical. Assignment of inactive elements would be made by using a text editor on the RZ2D-generated MESH file, and moving groups of elements towards the end of the ELEME block, past a dummy element with zero volume. RZ2D makes it easy to declare a vertical column inactive, facilitating assignment of boundary conditions in the vertical, such as a gravitationally equilibrated pressure gradient. RZ2DL on the other hand facilitates implementation of areal (top and bottom layer) boundary conditions.

RADII is the first keyword following RZ2D; it introduces data for defining a set of interfaces (grid block boundaries) in the radial direction.

<u>Record RADII.1</u>

Variables: NRAD

Format: I5

NRAD number of radius data that will be read. At least one radius must be provided, indicating the inner boundary of the mesh.

Record RADII.2, RADII.3, etc.

Variables: RC(I), I = 1, NRAD

Format: 8E10.4

RC(I)	a set of radii in ascending order.

Record EQUID. L

Equidistant introduces data on a set of equal radial increments.

Variables: NEQU, DR

Format: I5, 5X, E10.4

NEQU	number of desired radial increments.
DR	magnitude of radial increment.

Note: At least one radius must have been defined via block RADII before EQUID can be invoked.

Record LOGAR. 1

Logarithmic introduces data on radial increments that increase from one to the next by the same factor ($R_{n+1} = f \bullet R_n$).

Variables: NLOG, RLOG, DR

Format: A5, 5X, 2E10.4

NLOG	number of additional interface radii desired.
RLOG	desired radius of the last (largest) of these radii.
DR	reference radial increment: the first R generated will be equal to f • DR, with f internal determined such that the last increment will bring total radius to RLOG.f < 1 for decreasing radial increments is permissible. If DR is set equal

to zero, or left blank, the last increment DR generated before keyword LOGAR will be used as default.

Additional blocks RADII, EQUID, and LOGAR can be specified in arbitrary order.

Note: At least one radius must have been defined before LOGAR can be invoked. If DR = 0, at least two radii must have been defined.

LAYER introduces information on horizontal layers, and signals closure of RZ2D input data.

Record LAYER. L

Variables: NLAY

Format: I5

NLAY number of horizontal grid layers.

Record LAYER.2

Variables: H(I), I = 1, NLAY

Format: 8E10.4

H(I) a set of layer thicknesses, from top layer downward. By default, zero or blank entries for layer thickness will result in assignment of the last preceding non-zero entry. Assignment of a zero layer thickness, as needed for inactive layers, can be accomplished by specifying a negative value.

The LAYER data close the RZ2D data block. Note that one blank record must follow to indicate termination of the MESHM data block. Alternatively, keyword MINC can appear to invoke MINC-processing for fractured media (see below).

5.2.2 Generation of rectilinear grids

XYZ invokes generation of a Cartesian (rectilinear) mesh.

Record XYZ.l

Variables: DEG

Format: E10.4

DEG	angle (in degrees) between the Y-axis and the horizontal. If gravitational acceleration (parameter GF in record PARAM.2) is specified positive, -90° < DEG < 90° corresponds to grid layers going from top down. Grids can be specified from bottom layer up by setting GF or BETA negative. Default (DEG = 0) corresponds to horizontal Y- and vertical Z-axis. X-axis is always horizontal.

Record XYZ.2

Variables: NTYPE, NO, DEL

Format: A2, 3X, I5, E10.4

NTYPE	set equal to NX, NY or NZ for specifying grid increments in X, Y, or Z direction.
NO	number of grid increments desired.
DEL	constant grid increment for NO grid blocks, if set to a non-zero value.

Record XYZ.3 (optional, DEL = 0. or blank only)

Variables: DEL (I), I = 1, NO

Format: 8E10.4

DEL(I)	a set of grid increments in the direction specified by NTYPE in record XYZ.2. Additional records with formats as XYZ.2 and XYZ.3 can be provided, with X, Y, and Z-data in arbitrary order.

Record XYZ.4 a blank record closes the XYZ data block.

Note that the end of block MESHMaker is also marked by a blank record. Thus, when MESHMaker/XYZ is used, there will be two blank records at the end of the corresponding input data block.

5.2.3 MINC processing for fractured media

MINC invokes post processing of a primary porous medium mesh from file MESH. The input formats in data block MINC are identical to those of the GMINC program (Pruess, 1983), with two enhancements: there is an additional facility for specifying global matrix-matrix connections ("dual permeability"); further, only active elements will be subjected to MINC-processing, the remainder of the MESH remaining unaltered as porous medium grid blocks.

PART is the first keyword following MINC; it will be followed on the same line by parameters TYPE and DUAL with information on the nature of fracture distributions and matrix-matrix connections.

Variables: PART, TYPE, DUAL

Format: 2A5, 5X, A5

PART identifier of data block with partitioning parameters for secondary mesh.

TYPE a five-character word for selecting one of the six different proximity functions provided in MINC (Pruess, 1983).

ONE-D: a set of plane parallel infinite fractures with matrix block thickness between neighboring fractures equal to PAR(l).

TWO-D: two sets of plane parallel infinite fractures, with arbitrary angle between them. Matrix block thickness is PAR(l) for the first set, and PAR(2) for the second set. If PAR(2) is not specified explicitly, it will be set equal to PAR(l).

THRED: three sets of plane parallel infinite fractures at right angles, with matrix block dimensions of PAR(l), PAR(2), and PAR(3), respectively. If PAR(2) and/or PAR(3) are not explicitly specified, they will be set equal to PAR(l) and/or PAR(2), respectively.

STANA:	average proximity function for rock loading of Stanford large reservoir model (Lam et al., 1988).
STANB:	proximity function for the five bottom layers of Stanford large reservoir model.
STANC:	proximity function for top layer of Stanford large reservoir model.

Note: a user wishing to employ a different proximity function than provided in MINC needs to replace the function subprogram PROX(x) in file meshm.f with a routine of the form:

```
FUNCTION PROX(x)

PROX = (arithmetic expression in x)

RETURN

END
```

It is necessary that PROX(x) is defined even when x exceeds the maximum possible distance from the fractures, and that PROX = 1 in this case. Also, when the user supplies his/her own proximity function subprogram, the parameter TYPE has to be chosen equal to ONE-D, TWO-D, or THRED, depending on the dimensionality of the proximity function. This will assure proper definition of innermost nodal distance (Pruess, 1983).

DUAL is a five-character word for selecting the treatment of global matrix flow.

blank:	(default) global flow occurs only through the fracture continuum, while rock matrix and fractures interact locally by means of interporosity flow (“double-porosity” model).
MMVER:	global matrix-matrix flow is permitted only in the vertical; otherwise like the double-porosity model; for internal

consistency this choice should only be made for flow systems with one or two predominantly vertical fracture sets.

MMALL: global matrix-matrix flow in all directions; for internal consistency only two continua, representing matrix and fractures, should be specified (“dual-permeability”).

Record PART.l

Variables: J, NVOL, WHERE, (PAR(I), I = 1, 7)

Format: 2I3, A4, 7E10.4

J total number of multiple interacting continua (J < 36).

NVOL total number of explicitly provided volume fractions (NVOL < J). If NVOL < J, the volume fractions with indices NVOL+l, ..., J will be internally generated; all being equal and chosen such as to yield proper normalization to 1.

WHERE specifies whether the sequentially specified volume fractions begin with the fractures (WHERE = ‘OUT ‘) or in the interior of the matrix blocks (WHERE = 'IN ').

PAR(I) I = 1, 7holds parameters for fracture spacing (see above).

Record PART.2.1, 2.2, etc.

Variables: VOL(I), I = 1, NVOL

Format: 8E10.4

VOL (I) volume fraction (between 0 and 1) of continuum with index I (for WHERE = ‘OUT’) or index J+ l - I (for WHERE = ‘IN’). NVOL volume fractions will be read. For WHERE = ‘OUT’, I = 1 is the fracture continuum, I = 2 is the matrix continuum closest to the fractures, I = 3 is the matrix continuum adjacent to I = 2, etc. The sum of all volume fractions must not exceed 1.

5.3 Input format for chemical reactions

There are three input files needed for chemical reaction simulation besides the main input file, transport data file “solute.inp”, geochemical data file “chemical.inp” and thermodynamic database file.

Different from the main input file, there are no keywords for data block for the chemical input but the record order determines the input meaning. This part will describe the input format of those files.

5.3.1 Transport input file – solute.inp

The first record of this input file is for writing title, comments and remarks; followed by 12 data records. Some records can be omitted in certain conditions. Prior to each record there is always a heading (comment) line. Some variables in data records are not required under certain conditions. In such cases one should leave them blank or input an arbitrary value. Next, we describe the content of each record, indicating the description of each variable and its corresponding FORTRAN format for appropriate reading.

Record 1 Title

Variable: TITLE

Format: A76

TITLE title, comments and remarks.

Record 2 Option variables for reactive geochemical transport

Variable: ISPIA INIBOUND ISOLVC RCOUR NGAS1 ICHDUMP KCPL ICO2H2O NUMDR

Format: I5 I5 I5 F5.2 I5 I5 I5 I5 I5

ISPIA indicator of iteration scheme between transport and reaction. ISPIA = 2 is normally used.

0 - sequential iteration between transport and chemistry

2 - sequential no iteration (fully explicit reaction source terms)

INIBOUND	indicator of identifying boundary water solution (including pumping/injection at the internal grid blocks). 0 - not identifying 1 - identifying (normally used)
ISOLVC	a flag of the linear equation solver for transport. It is the same as the original TOUGH2 V2, ISOLVC = 5 is normally used. 2 - DSLUBC, a bi-conjugate gradient solver 3 - DSLUCS, a Lanczos-type bi-conjugate gradient solver 4 - DSLUGM, a general minimum residual solver 5 - DLUSTB, a stabilized bi-conjugate gradient solver
RCOUR	is both a variable and a flag to limit the time step size. RCOUR > 0.0 limits the maximum time step size to RCOUR
NGAS1	indicator of including gaseous chemical species transport 0 - Not included 1 - Included

If gas partial pressure remains constant with time, put NGAS1=0

ICHDUMP	is a flag to enable printing of chemical speciation results at each grid block and each time step (0 = disabled, 1=enabled). It should be enabled for debugging purposes only, or to track small problems. If this option is enabled, the program will abort after outputting speciation results for the first 1000 grid blocks and/or time steps, to avoid accidentally filling up disk space.

KCPL	is a flag to consider feedback effects of changes of porosity, permeability, and capillary pressure due to mineral dissolution and precipitation on fluid flow. 0 - not considering 1 - considering 2 - only monitor the changes (printout), but does not affect fluid flow.
ICO2H2O	is a flag to consider effects of CO2 and H2O reaction source/sink terms on fluid flow calculations. ICO2H2O is only used for EOS2 and ECO2 flow modules. For other flow modules, put ICO2H2O = 0. 0 - not considering 1 - considering only CO2 reaction source/sink terms 2 - considering both CO2 and H2O reaction source/sink terms
NUMDR	is flag of method for calculating derivatives of mineral kinetic rates with respective to concentrations of primary species. 0 - Analytical method (normally used) 1- Numerical method

Record 3. Option variables for reactive geochemical transport

Variable: SL1MIN, D1MIN, STIMAX, CNFACT

Format: 4E10.4

The first three parameters are used for skipping geochemical speciation calculations at grid blocks where conditions of saturation, inter grid block distance, or ionic strength are outside of the valid ranges of the model. The geochemical calculations are skipped at grid blocks where: the liquid saturation is less than SL1MIN; the minimum distance to the center of any adjacent block is less than D1MIN; or the stoichiometric ionic strength is more than STIMAX.

For typical boiling simulations, use SL1MIN less or equal to 10^{-3}. Set D1MIN = 0.0 (disabled) unless absolutely necessary. With this program version, STIMAX can be up to 6 mol/kg H2O for NaCl dominant solution. STIMAX should not be 20 greater than 2.0 because of limitations regarding the calculation of activity coefficients at elevated ionic strength.

CNFACT	is a weighting factor for mineral and gas reaction source terms in the transport equations (1.0 = fully implicit source terms, 0.0 = fully explicit source terms). This parameter has an effect only if sequential iterations are enabled (ISPIA = 0). In this program version, CNFACT always defaults to 1.0 if a non-zero value is input (implicit only). Simulations with CNFACT = 0.0 using sequential iterations will produce the same results as simulations without sequential iterations (explicit source terms) but requires increased computing time and therefore should be avoided.

<u>Record_4.1 through 4.6. Output files names</u>

Variable: THERMO_in , OUTiter, OUTplot, OUTsolid, OUTgas, OUTtime

Format: A20, each file name occupies one line.

THERMO_in	name of thermodynamic data file
OUTiter	iteration information
OUTplot	aqueous concentrations for grid blocks at specified times defined in main input file
OUTsolid	solid concentrations (mineral abundances and exchanged species concentrations) for all grid blocks at specified times defined in main input file
OUTgas	gas pressures for all grid blocks at specified times defined in main input file
OUTtime	aqueous and solid concentrations vs. time at specified grid blocks defined in SOLUTE.INP

Record 5. Weighting parameters and diffusion coefficients

Variable: WTIME, WUPC, DIFUN, DIFUNG

Format: 2F10.0, 2E10.3

WTIME	time weighting factor, ranging from 0 to 1. WTIME = 1 (implicit) is suggested.
WUPC	upstream weighting factor, ranging from 0 to 1. WUPC = 1 (fully upstream) is suggested.
DIFUN	diffusion coefficients (m^2/s) of the medium for aqueous species. The tortuosity is defined in rock property block of the flow input
DIFUNG	diffusion coefficients (m^2/s) of the medium for gaseous species.
DIFUNG < 0	the program computes gaseous diffusion coefficient as function of temperature and pressure.

Record 6. Data related to convergence criteria

Variable: MAXITPTR, TOLTR, MAXITPCH, TOLCH, MAXITPAD, TOLAD, TOLDC, TOLDR

Format: I5, E10.3, I5, E10.3, I5, E10.3, E10.3, E10.3,

MAXITPTR	maximum number of iterations allowed between solving transport and geochemistry; if MAXITPTR=1, it executes sequential non-iterative approach where transport and chemistry are sequentially solved without iteration procedure (normally is suggested).
TOLTR	relative tolerance of concentration for transport iteration; a value between 1.0E-03 to 1.0E-06 is suggested.
MAXITPCH	maximum number of iterations allowed for solving whole geochemical system.

TOLCH	relative tolerance of concentration for whole chemical system; a value between 1.0E-03 to 1.0 E-06 is suggested.
MAXITPAD	maximum number of iterations allowed for solving sorption via surface complexation.
TOLAD	relative tolerance of concentration for solving sorption; a value between 1.0E-03 to 1.0E-06 is suggested.
TOLDC	relative concentration change (between two consecutive time steps) tolerance for quasi-stationary state (QSS); a value between 1.0E-03 to 1.0E-06 is suggested; if not using QSS approximation set equal to zero. When KCPL>0 and ICO2H2O>0 in Record_2, set equal to zero.
TOLDR	relative dissolution and/or precipitation rate change tolerance for quasi-stationary state (QSS); a value between 1.0E-03 to 1.0E-06 is suggested; if not using QSS approximation set equal to zero. When KCPL>0 and ICO2H2O>0 in Record_2, set equal to zero.

Record 7. Writing control variables

Variable: NWTI, NWNOD, NWCOM, NWMIN, IWCOMT, ICONFLAG, MINFLAG

Format: 7I5

NWTI	writing frequency in time for some selected grid blocks (NWNOD)
NWNOD	number of grid blocks for writing time evolution
NWCOM	number of chemical components (specious) for writing
NWMIN	number of minerals for writing
IWCOMT	0 - writing the aqueous species concentrations

1 - writing the total aqueous component concentrations;

ICONFLAG A flag for aqueous concentration unit in output files

0- mol/kg H2O

1 - mol/l liquid

MINFLAG A flag for unit of mineral abundances in output files

0 - Change (from t=0) of mineral abundance in mol/m^3 medium

1 - Change of mineral abundance in volume fraction (dimensionless)

2 - Mineral abundance in volume fraction (dimensionless)

Record 8. List of grid blocks for printing time evolution results

Variable: EL

Format: 15A5

EL Five-character code name of a grid block. The name must be specified in main input file or mesh file. If NWNOD=0 in Record_7, leave a blank line.

Record 9. Pointer of the number of components to be printed out

Variables: (IWCOM (I), I=1, NWCOM)

Format: 15I5

IWCOM (I): vector component numbers

Record 10. Pointer of the number of minerals to be printed out

Variable: IWMIN (I), I=1, NWMIN

Format: 20I5

IWMIN (I)	vector of the number of minerals for writing. If NWMIN=0 in Record_7, leave a blank line.

Record 11. Default values for chemical property zone related to grid blocks

Variable: IZIWDF, IZBWDF, IZMIDF, IZGSDF, IZADDF, IZEXDF, IZPPDF, IZKDDF

Format: 8I5

IZIWDF, IZBWDF, IZMIDF, IZGSDF, IZADDF, IZEXDF, IZPPDF, and IZKDDF are default values of IZIW, IZBW, IZMI, IZGS, IZAD, IZEX, IZPP, and IZKD in the following record, respectively.

Record 12. Chemical property zone related to grid blocks

Variable: EL, NSEQ, NADD, IZIW, IZBW, IZMI, IZGS, IZAD, IZEX, IZPP, IZKD

Format: A5, 10I5

Remark: Repeat as many times as required, and ends with a blank record.

EL	grid block name
NSEQ	number of additional grid blocks having the same chemical properties
NADD	increment between the code numbers of two successive grid blocks
IZIW	initial water zone number
IZBW	boundary inflow (including injecting at internal blocks) water zone number

IZMI	mineral zone number
IZGS	gas zone number
IZAD	adsorption zone number
IZEX	ion exchange zone number
IZPP	zone number for porosity-permeability relation
IZKD	linear adsorption Kd zone number

The chemical properties for each zone are specified in chemical.inp file.

<u>Record 13. List of grid blocks connected to external gas reservoir (such as atmosphere)</u>

Remark: Repeat as many times as required, and ends with a blank record.

Variable: EL, DISG, (PFUGB (IG), IG=1, NGAS)

Format: A5, 5E10.3

EL	grid block name
DISG	=A/D, where A is interface area and D is distance to the interface (m)
PFUGB	gaseous species partial pressure (bar) at the reservoir, repeat as the number of gaseous species

5.3.2 Geochemical input file - chemical.inp

<u>Record 1. Title</u>

Variable: TITLE

Format: A76

TITLE	title, comments and remarks in one line

<u>Record 2. Label</u>

Variable: LABEL

Format: A76

LABEL	comments which will appear in the output file

5.3.2.1 Definition of the geochemical system

It contains the information on the aqueous species, minerals, gases, surface complexes, species with linear adsorption Kd and decay, and exchangeable cations involved in the system. The names must be written according to those labeled in the thermodynamic database file.

<u>Record 3. Label</u>

Variable: LABEL

Format: A76

LABEL	comments which will appear in the output file

Primary species

<u>Record 4. Label</u>

Variable: LABEL

Format: A76

LABEL	comments which will appear in the output file

<u>Record 5. Primary aqueous species</u>

Variable: NAPRI

Format: A20 (write NAPRI within single quote, such as ‘h+’)

Remark: Repeat Record-5 as many times as number of primary species

NAPRI	name of the primary species. It must be consistent with that in the thermodynamic database file.

Aqueous complexes

The aqueous complex block (Records 6 and 7) can be omitted. In this case, all possible aqueous complexes found in the database file are automatically used.

Record 6. Label

Variable: LABEL

Format: A76

LABEL comments which will appear in the output file

Record 7. Aqueous complexes

Variable: NAAQX

Format: A20

Remark: Repeat Record-7 as many times as number of aqueous complexes

NAAQX name of the aqueous complex. It must be consistent with that appeared in the database file. Omit NAAQX if no aqueous complexes are required. However, the species '*' is always needed to indicate the end of the list.

Minerals

Record-8. Label

Variable: LABEL

Format: A76

LABEL comments which will appear in the output file.

The following three records are repeated as many times as number of minerals.

Record 9.1. Mineral record 1

Variable: NAMIN, IKIN, IDISPRE, ISS, M1

Format: A20 (write NAMIN within single quotes such as 'calcite'), 4I (free)

Remark: Minerals can be entered in any order as long as the minerals at equilibrium precede those under kinetic constraints. The specified minerals consist of reactants and any possible products. Their names must match exactly the names of minerals in the database. Minerals with identical stoichiometries (i.e. quartz and cristobalite) cannot both be specified at equilibrium, but can be specified under kinetic constraints. Minerals at equilibrium are defined with one record (per mineral). Minerals under kinetic constraints require more records (per mineral).

NAMIN	name of the mineral phase. It must be consistent with that in the database. Omit NAMIN if no minerals are required. However, the species '*' is always needed to indicate the end of the list.
IKIN	a flag for the type of mineral: 0 for minerals at equilibrium, and 1 for those under kinetic constraints.
IDSPRE	a flag for the type of kinetic constraints: 1 for dissolution only, 2 for precipitation only, and 3 for both (mineral can either precipitate or dissolve). Always set IDSPRE = 0 if IKIN = 0 and IDISPRE > 0 if IKIN = 1.
ISS	an index for a solid solution mineral end member. All end members for a specified phase are given the same ISS value: ISS = 1 for each end member of the first solid solution, ISS = 2 for each end member of the second solid solution, and so on (numbers cannot be skipped). Records for each member can appear in any order in the mineral records.
M1	an index for a mineral that may be precipitated in a dry grid block (liquid saturation < sl1min that is specified in solute.inp file) if there is water flux into the grid block, and/or if the grid block dries out. The mineral with M1 = 1 precipitates first, with M1 =2 second, and so on. If this flag is set to zero, then the mineral will not be formed in the dry grid block.

If IKIN = 1 and IDSPRE = 1 or 3, Record9.2 is required to define dissolution rate law parameters

Record 9.2. Mineral record 2

Variable: RKF, IDEP, CK1, CK2, EA, ACFDISS, BCFDISS, CCFDISS

Format: F, I, 6F (all are free format)

RFK	the coefficient k25 in the Equation 2.42
IDEP	a flag for rate constant dependence on pH or multiple mechanisms. If IDEP = 0, pH dependent rate constants and multiple mechanisms are not considered. If IDEP = 1, Record 9.3 needs to include information on the rate dependence on pH. If IDEP = 2, Record 9.4 and Record 9.5 need to include information on the rate constants contributed from additional mechanisms.
CK1, CK2	the exponents η and θ for Equation 2.41
EA	the activation energy (KJ/mol).
ACFDISS, BCFDISS, and CCFDISS	should be set to zero, unless a different form of rate constant dependence with temperature is desired. This alternate form is: log (k) = a + b*T + c/T, where T is absolute temperature in K and log is in base 10. To enable this option, RFK must be set to 1.0, EA must be set to zero, CK1 and CK2 can be set to any values, and ACFDISS, BCFDISS, and CCFDISS must be specified as the coefficients a, b, and c, respectively, in the above expression. If IKIN = 1 and IDSPRE = 2 or 3 Record 9.6 is required to define precipitation rate law parameters.

Record 9.3. Mineral record 3

Variable: PH1, SLOPE1, PH2, SLOPE2

Format: 4F (all are free format)

Record 9.4. Mineral record 4

Variable: NDIS

Format: F (free format)

NDIS	is the number of additional mechanisms contributed to the rate constant (see Equation 2. 46)

Record 9.5. Mineral record 5

Variable: NAPRE, RKDSP, EXPDSP

Format: 3F (free format)

Remark: This record must be repeated as many as NDIS times (a maximum of five additional mechanisms can be considered).

RKDS	is k_j in Equation 2.46 where *i* is the additional mechanism index.
EADS	is the activation energy (KJ/mol) for each additional mechanism.
NSPDS	is the number of species involved in each mechanism (a maximum of five species can be considered).
NADIS	is the name of species involving in the mechanism that must be in the list of primary or secondary species. NADIS and the following variable
EXPDSP	must be repeated as many as NSPDS times.
EXPDSP	is the power term in Equation 2.46.

Record 9.6. Mineral record 6

Variable: RKPREC, IDEPREC, CK1PREC, CK2PREC, EAPREC, ACFPREC, BCFPREC, CCFPREC, RNUCL, NPLAW

Format: F, I, 7F, I (all are free formats)

The first 8 input parameters are listed in the same order and have the same functions as those described above for mineral dissolution, except that the parameters apply to mineral precipitation instead of dissolution.

RNUCL	the initial volume fraction ($V_{mineral}/V_{solid}$) to be assumed for calculating initial effective surface area if the mineral is not present at the start of a simulation but precipitates as a new reaction product.
NPLAW	precipitation law index. NPLAW = 0 for Equation 2.41 and 2.46. NPLAW = 1 for Equation 2.44

Record 9.7. Mineral record 7

This record is only required for a mineral with precipitation.

Variable: SSQK0, SSTK1, SSTK2

Format: 3F (free)

SSQK0	log (Q/K) gap (super-saturation window, see Equation 2.47). A zero value represents no gap.
SSTK1	temperature (in °C) at which to begin reducing gap.
SSTK2	temperature (in °C) endpoint at which the gap has diminished to nearly zero (1% of original value). The gap decreases exponentially from the first (SSTK1) to the second (SSTK2) temperature value, and SSTK2 must always be greater than SSTK1.

Gaseous species

Record-10. Label

Variable: LABEL

Format: A76

LABEL	comments which will appear in the output file

Record-11. Gases

Variable: NAGAS

Format: A20 (write NAGAS within single quotes such as ‘co2(g)’)

Remark: Repeat Record-11 as many times as number of gaseous species

NAGAS	name of a gaseous species. It must be consistent with that in the chemical thermodynamic database file. Omit NAGAS if no gaseous species are required. However, the species ‘*’ is always needed to indicate the end of the list.

Surface complexes

Record-12. LABEL

Variable: LABEL

Format: A76

LABEL	comments which will appear in the output file

Record-13. Surface complexes

Variable: NAADS

Format: A20

Remark: Repeat Record-13 as many times as number of surface species

NAADS	name of surface complex. Omit NAADS if no surface complexes are required. However, the species ‘*’ is always needed to indicate the end of the list.

Aqueous species (primary) with Kd and decay

Record-14. LABEL

Variable: LABEL

Format: A76

LABEL	comments which will appear in the output file

Record-15. Species with Kd and decay

Variable: NAKDD, DECAYC

Format: A20

Repeat Record-15 as many times as species with Kd and decay

NAKDD	name of the aqueous primary species with Kd and/or decay. These names must appear in the above mentioned .primary species record. of the input file.
DECAYC	decay constant (in 1/s). For the species with only Kd adsorption and without decay, set DECAYC equal to zero.

Exchangeable cations

Record-16. Label

Variable: LABEL

Format: A76

LABEL	comments which will appear in the output file

Record-17. Label

Variable: LABEL

Format: A76

LABEL	comments which will appear in the output file

Record-18. Data related with exchangeable cations

Variable: NAEXC IMS IEX EKX

Format: A20 I I F (the last three variables are free format)

Remark: Repeat Record-18 as many times as number of exchangeable cations

NAEXC	name of exchangeable cation. Omit NAEXC if no exchangeable cations are required. However, the species '*' is always needed to indicate the end of the list.
IMS	If IMS = 1, the cation is used as reference for the exchange reactions (normally Na+). For the rest of cations IMS must be 0.
IEX	exchange convention type used in the calculations: 1= Gaines-Thomas; 2= Vanselow; 3= Gapon. The value of IEX must be the same for all the exchanged cations.
EKX	exchange coefficient of the cation with respect to the reference cation. If IMS = 1, then EKX = 1.0.

Initial and boundary water solutions

Record-19. Label

Variable: LABEL

Format: A76

LABEL	comments which will appear in the output file

Record-20. Label

Variable: LABEL

Format: A76

LABEL	comments which will appear in the output file

Record-21. Data related with the number of aqueous solutions

Variable: NIWTYPE NBWTYPE

Format: I I (all are free format)

NIWTYPE	number of types of aqueous solution initially present in the system.
NBWTYPE	number of types of boundary (including pumping/injection at the internal grid blocks) solution.

Data related to aqueous solutions

This part describes the different types of aqueous solutions (initial and boundary). Repeat the following Records 22, 23 and 24 a number of times equal to (NIWTYPE + NBWTYPE), starting with initial solutions, and then boundary solutions.

Record-22. Identification of the solution

Variable: IWTYPE TC2 ITC2

Format: I, F, I (all are free format)

IWTYPE	number of the initial or boundary solution. The value of IWTYPE varies from 1 to NIWTYPE, then starts again with 1 up to NBWTYPE.
TC2	temperature of the solution (^{o}C).
ITC2	set zero for this version

Record-23. Label

Variable: LABEL

Format: A76

LABEL	comments which will appear in the output file

Record-24. Data related to the chemical definition of the solution

Variable: NAPRI ICON CGUESS CTOT NADUM ICTOT

Format: A20, I, F, F, A20, I

Remark: Repeat Record-24 as many times as number of primary species

NAPRI	name of the aqueous primary species. The name of the species must coincide with those previously listed as primary species in the definition of the system, although the order may change. Names must be included between single quotes, such as ‘h+’. The species ‘*’ indicates the end of the list.
ICON	flag indicating the type of constraint controlling the solute content which is given under CTOT. 1 = the concentration of the species is constrained by the total concentration CTOT, except for water which is assumed unity. 2 = the concentration of the species calculated through charge balance. 3 = the activity of the species is fixed during the inialization. In this case, the following two variables: CGUESS = CTOT = the fixed activity. For example, if the pH of an initial water is fixed at 7, we set CGUESS = CTOT = 10^{-7} for H+ activity.
CGUESS	initial guess for the concentration (mol/kg) of the primary species.
CTOT	total dissolved component concentration (mol/kg).
NADUM	is not used in this version
ICTOT	is not used in this version, place zero.

5.3.2.2 Initial mineral zones

This part describes the different mineral zones initially forming the system.

Record-25. Label

Variable: LABEL

Format: A76

LABEL	comments which will appear in the output file

Record-26. Label

Variable: LABEL

Format: A76

LABEL	comments which will appear in the output file

Record-27.

Variable: NMTYPE

Format: I4

NMTYPE	Number of mineral zones forming the system. If mineral is not considered in the system, place NMTYPE = 1.

The following Records 28, 29 and 30 must be repeated NMTYPE times.

Record-28.

Variable: IMTYPE

Format: I4

IMTYPE	number of the mineral zone

Record-29. Label

Variable: LABEL

Format: A76

LABEL	comments which will appear in the output file

Record-30. Data related to the composition of the mineral zone

Variable: NAMIN VOL IKIN

Format: A20 F I (the last two variables are free format)

NAMIN	name of the mineral present in the system. The name of the mineral must be included among those previously listed in the definition of the system, although the order may change, and it is not needed to repeat the complete list. Names must be included between single quotes, such as ‘calcite’. The mineral ‘*’ indicates the end of the list of minerals.
VOL	is the initial volume fraction of the mineral, excluding liquid (mineral volume divided by total volume of solids). The sum of VOL’s need not add up to 1. The remaining solid volume fraction is considered un-reactive.
IKIN	A flag for the type of mineral: 0 for minerals at equilibrium, and 1 for those under kinetic constraints. When IKIN=1, the following record (Record-30-1) is required.

<u>Record-30-1.</u>

Variable: RAD, AMIN , IMFLG

Format: F, F, I (all are free format)

RAD	radius of mineral grain (in m) used to calculate surface area for initial formation of secondary phase. If RAD = 0, the initial surface area is calculated from RNUCL in Record-9-6.
AMIN	specific reactive surface area. Its unit depends on the following flag IMFLG
IMFLG	A flag for surface area conversion IMFLG = 0 for cm2/g mineral IMFLG = 1 for m2 rock area/m3 medium IMFLG = 2 for m2/m3 mineral

5.3.2.3 Initial gas zones:

This part describes the different initial gas zones in the system.

<u>Record-31. Label</u>

Variable: LABEL

Format: A76

LABEL comments which will appear in the output file

Record-32. Label

Variable: LABEL

Format: A76

LABEL comments which will appear in the output file

Record-33.

Variable: NGTYPE

Format: I4

NGTYPE number of gas zones forming the system. If gaseous species is not considered in the system, place NGTYPE = 1

The following records 34, 35 and 36 must be repeated NGTYPE times.

Record-34.

Variable: IGTYPE

Format: I4

IGTYPE number of the gas zone

Record-35. Label

Variable: LABEL

Format: A76

LABEL comments which will appear in the output file

Record-36. Data related to the composition of the gas zone

Variable: NAGAS VOLG

Format: A20 F (the last one is free format)

NAGAS name of the gaseous species present in the system. The name of the gas must be included among those previously listed in the definition of the system, although the order may change, and it is not needed to repeat the complete list.

Names must be included between single quotes. The gas ‘*’ indicates the end of the list.

VOLG partial pressure of the gaseous species (in bar).

Zones for permeability-porosity relationship

Record-37. Label

Variable: LABEL

Format: A76

LABEL comments which will appear in the output file

Record-38. Label

Variable: LABEL

Format: A76 (write LABEL within .single quotes.)

LABEL comments which will appear in the output file

Record-39.

Variable: NPPZON

Format: I4

NPPZON Number of permeability zones. If permeability change is not considered in the simulation, place NPPZON = 1.

The following records, 40, 41 and 42 must be repeated NPPZON times.

Record-40.

Variable: IPPZON

Format: I4

IPPZON number of order of the permeability zone

Record-41. Label

Variable: LABEL

Format: A76

LABEL comments which will appear in the output file

Record-42. Data related to zone for permeability-porosity relationship

Variable: ipptyp, apppar, bpppar

Format: I, 2F (All are free format)

Ipptyp, apppar, bpppar the index for the permeability law, which is used to correlate permeability from the reaction induced porosity change. When coupling geomechanical and geochemical together, the keyword IPORPERM in the ROCKS section will override it. And apppar and bpppar is the parameters for the correlation calculation.

Surface adsorption zones

This part describes the characteristics of the zones with different surface adsorption properties present in the system. The capability of TOUGHREACT for surface complexes has not been tested in the present version. The purpose is to reserve a space for future use.

Record-43. Label

Variable: LABEL

Format: A76 (write LABEL within .single quotes.)

LABEL comments which will appear in the output file

Record-44. Label

Variable: LABEL

Format: A76

LABEL comments which will appear in the output file

Record-45.

Variable: NDTYPE

Format: I4

NDTYPE number of surface adsorption zones.

Record-46. Label

Variable: LABEL

Format: A76 (write LABEL within .single quotes.)

LABEL comments which will appear in the output file

Record-47. Data related to the adsorption zone

Variable: IDTYPE SUPADS TSS

Format: I4 Free Free

IDTYPE number of the surface adsorption zone.

SUPADS: specific adsorbent surface of the solid phase per unit volume of solution

TSS Total adsorption sites per volume of solution

Linear Kd zones

This part describes the different linear adsorption Kd zones initially in the system.

Record-48. Label

Variable: LABEL

Format: A76

LABEL comments which will appear in the output file

Record-49. Label

Variable: LABEL

Format: A76 (write LABEL within .single quotes.)

LABEL comments which will appear in the output file

Record-50.

Variable: KDTYPE

Format: I4

KDTYPE: number of Kd zones in the system. If Kd adsorption is not considered in the simulation, place KDTYPE = 1

The following Records 51, 52 and 53 must be repeated KDTYPE times.

Record-51.

Variable: IDTYPE

Format: I4

IDTYPE number of the Kd zone

Record-52. Label

Variable: LABEL

Format: A76 (write LABEL within .single quotes.)

LABEL	comments which will appear in the output file

Record-53. Data related to the Kd zone

Variable: NAME , SDEN2, VKD2

Format: A20, F, F (the last two variables are free real number)

NAME	the name of aqueous primary species with Kd, which can be listed in any order. The species spelling must be the same as defined previously.
SDEN2	the solid density (in kg/dm3).
VKD2	is value of Kd (in (l/kg which is mass/kg solid divided by mass/l solution). If SDEN2=0.0, VKD2 automatically represents retardation factor.

Cation exchange zones

This part describes the characteristics of the zones with different cation exchange capacity present in the system.

Record-54. Label

Variable: LABEL

Format: A76

LABEL	comments which will appear in the output file

Record-55. Label

Variable: LABEL

Format: A76

LABEL: comments which will appear in the output file

Record-56.

Variable: NXTYPE

Format: I4

NXTYPE	number of cation exchange zones.

Record-57. Label

Variable: LABEL

Format: A76 (write LABEL within .single quotes.)

LABEL	comments which will appear in the output file

Record-58. Data related to the cation exchange zone

Record-58 must be repeated NXTYPE times. If NXTYPE is zero omit this card. No *' is required to indicate the end of the list of cation exchange zones.

Variable: IXTYPE CEC

Format: I F (all are free format)

IXTYPE	number of the cation exchange zone.
CEC	cation exchange capacity

End of reading chemical input

This part allows the user to be sure that the chemical data have been entirely read.

Record-59. Label

Variable: LABEL

Format: A76 (write LABEL within .single quotes.)

LABEL	comments which will appear in the output file

Record-60. Label to check the end of chemical data input

Variable: LABEL

Format: A76 (write LABEL within .single quotes.)

LABEL	This label must be ‘end’.

Thermodynamic Data File

Aqueous species, minerals, and gases contained in CHEMICAL.INP must be found in this thermodynamic database file. The name of the database file is specified in SOLUTE.INP. The format of the database file is free. For most problems, the database files supplied with sample problem of chemical reactions in the source codes package may be used without addition and modification. If any aqueous species, mineral, and gas are not contained in the supplied database file or one desires to use different thermodynamic data, users must add them to the database file.

5.4 Output from TOUGH2-EGS

5.4.1 Main output file:

TOUGH2-EGS produces a variety of printed output, most of which can be controlled by the user. Information written in the initialization phase to the standard output file includes PARAMETER settings in the main program for dimensioning of problem-size dependent arrays, and disk files in use. This is followed by documentation on settings of the MOP-parameters for choosing program options, and on the EOS-module. During execution TOUGH2 can optionally generate a brief printout for Newtonian iterations and time steps. Standard output at user-specified simulation times or time steps is generated by a subroutine OUT (each EOS module comes with its own routine OUT). This output provides some time-stepping information, and a complete element-by-element report of thermodynamic state variables and other important parameters. Additional optional output is available on mass and heat flow rates and velocities, and on diffusive fluxes of components in phases. Changes in thermodynamic state variables during a time step may also be printed. There are some minor differences in naming conventions used by different EOS-modules. Here we summarize the main output parameters in alphabetical order.

Table 5-2 List of output variables

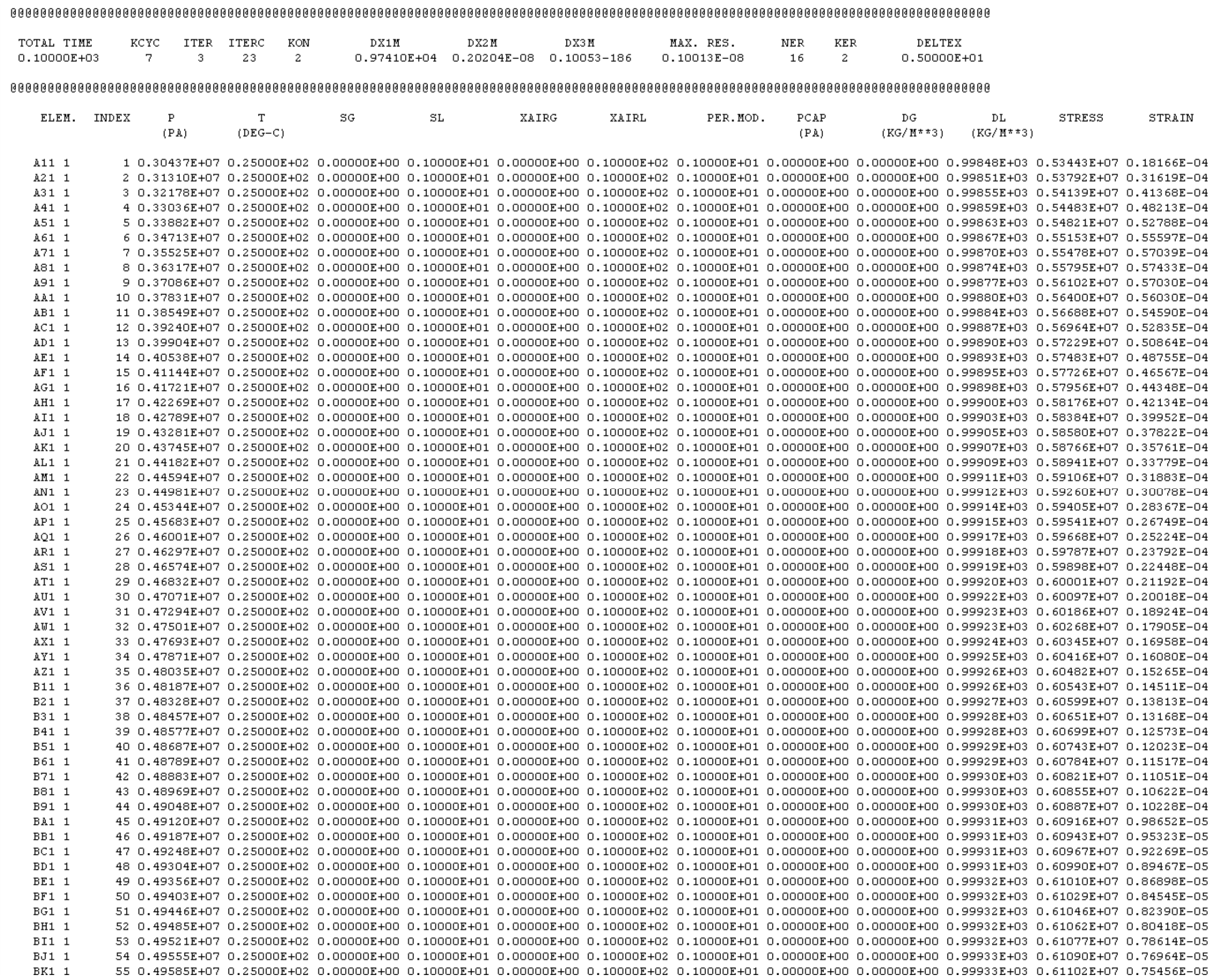
DELTEX	time step size, seconds
DG	gas phase density, kg/m^3
DL	liquid (aqueous phase) density, kg/m^3
DT	time step size, seconds
DW	water (aqueous phase) density, kg/m^3
DX1, DX2, etc.	changes in first, second, etc. thermodynamic variable
DX1M, DX2M, DX3M	maximum change in first, second, and third primary variable in current time step
ELEM	code name of element
ELEM1, ELEM2	code name of first and second element, respectively, in a flow connection
ENTHALPY	flowing specific enthalpy for mass sinks/sources, J/kg
FF(GAS), FF(LIQ)	mass fraction of flow in gas and liquid phases, respectively (mass production wells only)

FLO(BRINE)	total rate of brine flow, kg/s (positive if from ELEM2 into ELEM1)
FLOF	total rate of fluid flow, kg/s (positive if from ELEM2 into ELEM1)
FLO(GAS)	total rate of gas flow, kg/s (positive if from ELEM2 into ELEM1)
FLOH	total rate of heat flow, W (positive if from ELEM2 into ELEM1)
FLO(LIQ)	total rate of liquid (aqueous phase) flow, kg/s (positive if from ELEM2 into ELEM1)
GENERATION RATE	sink (> 0) or source (< 0) rate, kg/s (mass), W (heat)
INDEX	internal indexing number of elements, connections, sinks/sources
ITER	number of Newtonian iterations in current time step
ITERC	total cumulative number of Newtonian iterations in simulation run
KCYC	time step counter
KER	index number of equation with largest residual
K(GAS)	gas phase relative permeability

K(LIQ)	liquid (aqueous) phase relative permeability
KON	convergence flag; KON = 2: converged; KON = 1: not converged
MAX. RES.	maximum (relative) residual in any of the mass and energy balance equations
NER	index number of element (grid block) with largest residual
P	pressure, Pa
PER.MOD.	permeability modification coefficient
PCAP	capillary pressure, Pa
PSAT	saturated vapor pressure, Pa
P(WB)	flowing bottomhole pressure (production wells on deliverability only), Pa
RH	Relative humidity
SG	gas saturation
SL	liquid saturation
SOURCE	code name of sink/source
ST	simulation time, in seconds
STRAIN	volumetric strain.
STRESS	mean normal stress.
SW	water (aqueous phase) saturation
T	temperature, ˚C

TOTAL TIME	simulation time, in seconds
VEL(GAS)	gas phase pore velocity, m/s (positive if from ELEM2 into ELEM1)
VEL(LIQ)	liquid (aqueous) phase pore velocity, m/s (positive if from ELEM2 into ELEM1)
VIS(LIQ)	liquid (aqueous) phase viscosity, Pa-s
X1, X2, etc.	first, second, etc. thermodynamic variable
XAIRG	mass fraction of air in gas phase
XAIRL	mass fraction of air in liquid phase

For a certain time-step plot, the outputted profile is as the Figure 5-1.



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 TOTAL TIME     KCYC   ITER  ITERC   KON        DX1M         DX2M         DX3M          MAX. RES.      NER    KER         DELTEX
 0.10000E+03      7      3     23     2       0.97410E+04  0.20204E-08  0.10053-186    0.10013E-08     16      2        0.50000E+01

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    ELEM.  INDEX      P           T            SG           SL            XAIRG        XAIRL        PER.MOD.     PCAP          DG           DL          STRESS       STRAIN
                     (PA)       (DEG-C)                                                                        (PA)       (KG/M**3)    (KG/M**3)

   A11 1        1 0.30437E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99848E+03 0.53443E+07 0.18166E-04
   A21 1        2 0.31310E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99851E+03 0.53792E+07 0.31619E-04
   A31 1        3 0.32178E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99855E+03 0.54139E+07 0.41368E-04
   A41 1        4 0.33036E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99859E+03 0.54483E+07 0.48213E-04
   A51 1        5 0.33882E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99863E+03 0.54821E+07 0.52788E-04
   A61 1        6 0.34713E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99867E+03 0.55153E+07 0.55597E-04
   A71 1        7 0.35525E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99870E+03 0.55478E+07 0.57039E-04
   A81 1        8 0.36317E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99874E+03 0.55795E+07 0.57433E-04
   A91 1        9 0.37086E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99877E+03 0.56102E+07 0.57030E-04
   AA1 1       10 0.37831E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99880E+03 0.56400E+07 0.56030E-04
   AB1 1       11 0.38549E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99884E+03 0.56688E+07 0.54590E-04
   AC1 1       12 0.39240E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99887E+03 0.56964E+07 0.52835E-04
   AD1 1       13 0.39904E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99890E+03 0.57229E+07 0.50864E-04
   AE1 1       14 0.40538E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99893E+03 0.57483E+07 0.48755E-04
   AF1 1       15 0.41144E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99895E+03 0.57726E+07 0.46567E-04
   AG1 1       16 0.41721E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99898E+03 0.57956E+07 0.44348E-04
   AH1 1       17 0.42269E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99900E+03 0.58176E+07 0.42134E-04
   AI1 1       18 0.42789E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99903E+03 0.58384E+07 0.39952E-04
   AJ1 1       19 0.43281E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99905E+03 0.58580E+07 0.37822E-04
   AK1 1       20 0.43745E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99907E+03 0.58766E+07 0.35761E-04
   AL1 1       21 0.44182E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99909E+03 0.58941E+07 0.33779E-04
   AM1 1       22 0.44594E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99911E+03 0.59106E+07 0.31883E-04
   AN1 1       23 0.44981E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99912E+03 0.59260E+07 0.30078E-04
   AO1 1       24 0.45344E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99914E+03 0.59405E+07 0.28367E-04
   AP1 1       25 0.45683E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99915E+03 0.59541E+07 0.26749E-04
   AQ1 1       26 0.46001E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99917E+03 0.59668E+07 0.25224E-04
   AR1 1       27 0.46297E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99918E+03 0.59787E+07 0.23792E-04
   AS1 1       28 0.46574E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99919E+03 0.59898E+07 0.22448E-04
   AT1 1       29 0.46832E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99920E+03 0.60001E+07 0.21192E-04
   AU1 1       30 0.47071E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99922E+03 0.60097E+07 0.20018E-04
   AV1 1       31 0.47294E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99923E+03 0.60186E+07 0.18924E-04
   AW1 1       32 0.47501E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99923E+03 0.60268E+07 0.17905E-04
   AX1 1       33 0.47693E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99924E+03 0.60345E+07 0.16958E-04
   AY1 1       34 0.47871E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99925E+03 0.60416E+07 0.16080E-04
   AZ1 1       35 0.48035E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99926E+03 0.60482E+07 0.15265E-04
   B11 1       36 0.48187E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99926E+03 0.60543E+07 0.14511E-04
   B21 1       37 0.48328E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99927E+03 0.60599E+07 0.13813E-04
   B31 1       38 0.48457E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99928E+03 0.60651E+07 0.13168E-04
   B41 1       39 0.48577E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99928E+03 0.60699E+07 0.12573E-04
   B51 1       40 0.48687E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99929E+03 0.60743E+07 0.12023E-04
   B61 1       41 0.48789E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99929E+03 0.60784E+07 0.11517E-04
   B71 1       42 0.48883E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99930E+03 0.60821E+07 0.11051E-04
   B81 1       43 0.48969E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99930E+03 0.60855E+07 0.10622E-04
   B91 1       44 0.49048E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99930E+03 0.60887E+07 0.10228E-04
   BA1 1       45 0.49120E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99931E+03 0.60916E+07 0.98652E-05
   BB1 1       46 0.49187E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99931E+03 0.60943E+07 0.95323E-05
   BC1 1       47 0.49248E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99931E+03 0.60967E+07 0.92269E-05
   BD1 1       48 0.49304E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99931E+03 0.60990E+07 0.89467E-05
   BE1 1       49 0.49356E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99932E+03 0.61010E+07 0.86898E-05
   BF1 1       50 0.49403E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99932E+03 0.61029E+07 0.84545E-05
   BG1 1       51 0.49446E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99932E+03 0.61046E+07 0.82390E-05
   BH1 1       52 0.49485E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99932E+03 0.61062E+07 0.80418E-05
   BI1 1       53 0.49521E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99932E+03 0.61077E+07 0.78614E-05
   BJ1 1       54 0.49555E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99933E+03 0.61090E+07 0.76964E-05
   BK1 1       55 0.49585E+07 0.25000E+02 0.00000E+00 0.10000E+01 0.00000E+00 0.10000E+02 0.10000E+01 0.00000E+00 0.00000E+00 0.99933E+03 0.61102E+07 0.75456E-05
```

Figure 5-1 snapshot of the main out file

5.4.2 Output files for chemical reactions

5.4.2.1 Fixed-name output files

solute.out	Echo of input file solute.inp. This file lists the data read from input file SOLUTE.INP, including all transport parameters, chemical zone configuration, and other run specific parameters.
chemical.out	Echo of input file chemical.inp. This file lists the data read from input files chemical.inp and chemical database, including initial water, rock, and gas compositions, equilibrium constants and stoichiometries of chemical reactions, kinetic data, and linear adsorption Kd values and decay constants for certain species.

runlog.out	Log of the simulation progress. This file is constantly updated during a simulation. It lists some run input parameters and all run-related messages, including error messages.
chdump.out	chemical speciation data. This file contains results of geochemical speciation calculations for each initial water composition input into the model. It also lists these data for grid blocks where chemical convergence fails (not reaching specified convergence criteria). They include a printout of chemical mass balances (total mass balance and aqueous species mass balance). For debugging purposes or for small grids, if the flag ICHDUMP in the solute.inp input file is set equal to 1, geochemical speciation results will be output in the chdump.out file for every grid block at every time step. As a precaution to avoid filling up disk space, results of speciation calculations are output only for the first thousand grid blocks and/or time steps, after which the program will abort.
savechem	save of geochemical data for restart. This can be used to perform a series of chemical reactions runs, in which geochemical conditions obtained in one run, and written to disk file savechem, are used as initial conditions in a subsequent run. The restart run for reactive geochemical transport simulation must be used together with a restart of the flow simulation (see p. 61 of the TOUGH2 V2 manual; Pruess et al., 1999). For a restart run, file name savechem must be changed to, inchem, and save to incon (same as in the original TOUGH2).

In addition, the chemical reaction module has two optional output files, one for mass balance information and the other for mineral saturation index vs. grid block at specified times. The two file names are fixed as mbalance.out and min_SI.dat. The reaction rate and surface area can also be printed out into files rct_rate.out and rct_sfarea.out respectively. Printing those files or not is controlled by parameter MOPR(4) in flow.inp file.

5.4.2.2 User-specified output files:

The names of these files must be specified in the input file SOLUTE.INP, and cannot be left blank. The output files are described below:

Iteration Data	This file lists numbers of flow, transport and chemical iterations used to reach convergence at each time step.
Aqueous species plot data	This file contains times, grid block coordinates (m), liquid saturation, temperature (°C), pH, and aqueous species concentrations at all grid blocks for times specified in the FLOW.INP file. The number and type of species to this output is specified by flags in the input file SOLUTE.INP. This file is in a TECPLOT-compatible format.
Solid phase plot data	This file contains time, grid point coordinates (m), temperature (°C), mineral abundance, exchanged species concentrations at all grid blocks for time steps specified in the main input file. This file is also in a TECPLOT-compatible format.
Gas phase plot data	This file contains time, grid point coordinates (m), temperature (°C), and gaseous partial pressures at all grid blocks for times specified in the FLOW.INP file. This file is also in a TECPLOT-compatible format.
Time evolution file	This file contains grid block identifier, time, liquid saturation, temperature, pH, aqueous species concentrations, mineral abundances, and gas pressures, exchanged species concentrations for specific grid blocks and time intervals, as specified in the input file SOLUTE.INP.

6 EXAMPLE PROBLEMS

Couples of sample problems are included in this section. They may be used as benchmarks for testing the codes' capabilities and for verifying any changes to the recent codes. The input data files for each problem also can be used as templates to facilitate preparation of new simulations. There are total eight examples problems. The first three examples illustrate the accuracy of the geomechanical model against the analytical solutions. The fourth and fifth examples show the coupled THC and THM simulations, and compared to other simulators for validation. The sixth example demonstrates the field application for THM simulations. The seventh example demonstrates the coupled THMC simulation for one prototypical EGS reservoir. The last example shows the simulation in dual porosity systems with THM model.

6.1 1-D consolidation

6.1.1 Problem description

The 1-D consolidation problem is a porous permeable column that undergoes uniaxial strain in the vertical direction only. The column is subjected to a constant load on the top, the fluid boundary pressure is set to zero gauge right after the load is imposed, and only vertical displacement takes place as shown in Figure 6-1.

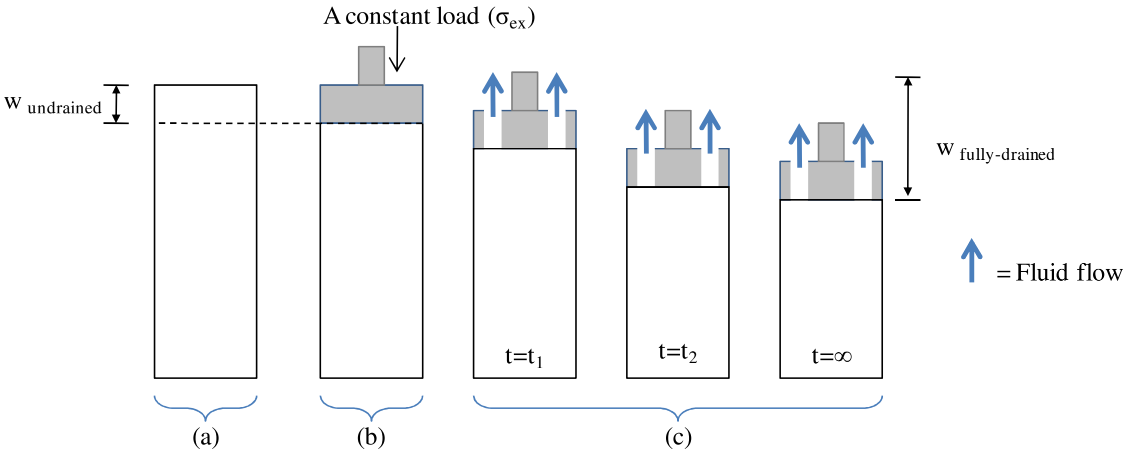


Figure 6-1 Evolution of the column displacement for an 1-D consolidation problem; (a) The initial condition (no compaction); (b) the column is subjected to a constant load, pressure is being increased and no fluid is drained (undrained condition); (c) Fluid is drained from the column and pressure is being decreased (drained condition): Charoenwongsa et al. (2010).

6.1.2 Numerical simulation setup

We simulated this problem in two steps. The first step was the load application to produce the pore pressure increase, shown in Figures 6-1a to 6-2b. We started from a relaxed state where pore pressures and mean stress were initialized at 3.0 MPa and 5.0 MPa, respectively. Then, the additional vertical stress of 3.0 MPa was imposed at the column top that induced a pore pressure increase in the column after the system equilibrated; see the input data in Figure 6-2. ‘OPTIO’ 5 in ‘GRMOD’ entry was used to allow the in-equilibrium stress initialization. The model was run without sink or source term until reaching the equilibrium where the pore pressure was increased due to the additional load. Then, the ‘SAVE’ file which is the results from the initialization was renamed to ‘INCON’ which would be used as the initial condition for the next runs.

For uniaxial deformation in an isothermal medium, the additional mean stress can be calculated from the additional vertical stress, and pore pressures as follows:

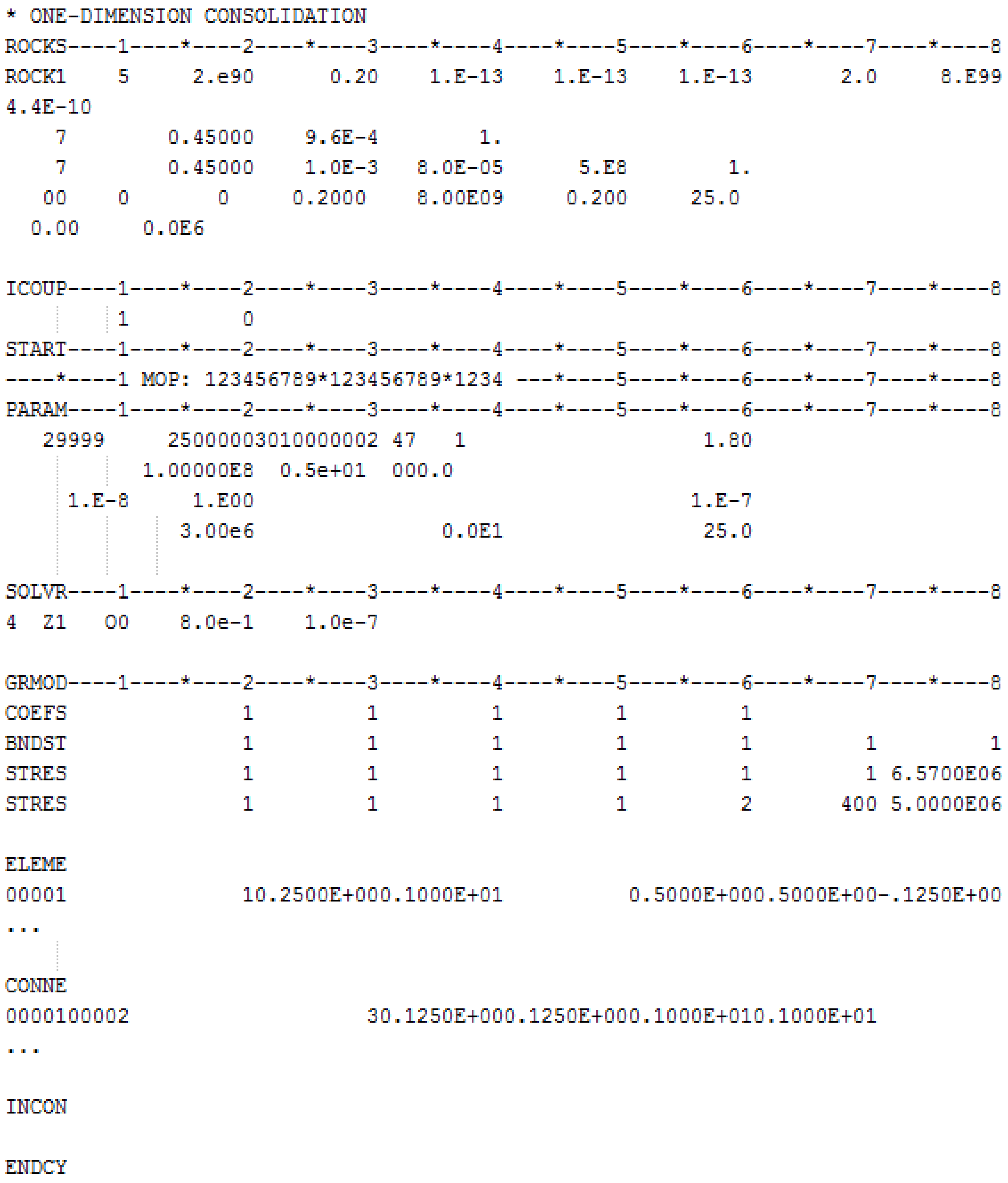
$$\Delta\sigma_m = \frac{1}{3}\frac{(1+\nu)}{(1-\nu)}\left(\Delta\sigma_{zz} - \alpha\Delta p\right) + \alpha\Delta p \tag{6.1}$$

where ν is the Poisson’s ratio, α is Biot constant, σ_{zz} is the z direction stress and σ_m is the mean effective stress.

The second step was simulation of fluid drainage, shown in Figure 6-1c. The column was initially at the above equilibrated state. We set the pore pressures at the column top to the initial pore pressures (3.0MPa). We also set the mean stress at the column top to that calculated from Equation 6.1 using the constant additional vertical-direction stress (3.0MPa). Fluid then drained out of the column top as the pore pressures in the column returned to the initial values see the input data in Figure 6-3. The detailed input data is shown in Table 6-1.

Table 6-1 Input parameters used in simulation of the 1-D consolidation problem

Parameters	**Value**	**Unit**
Rock properties (Berea sandstone)		
Elastic modulus (E)	8.0	GPa
Poisson ratio (ν)	0.20	
Porosity (ϕ)	0.20	
Permeability (k)	1.00×10^{-13}	m^2
Biot coefficient (α)	0.20	
Fluid properties		
Water viscosity (μ)	0.89	Pa.s
Water compressibility (c_w)	4.55×10^{-10}	Pa^{-1}
Initial and Boundary Conditions		
Pressure at relaxed condition	3.0	MPa
Mean stress at the relaxed	5.0	MPa
Imposed additional vertical stress	3.0	MPa



```
* ONE-DIMENSION CONSOLIDATION
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
ROCK1    5     2.e90      0.20    1.E-13    1.E-13    1.E-13       2.0     8.E99
4.4E-10
    7        0.45000    9.6E-4        1.
    7        0.45000    1.0E-3   8.0E-05      5.E8        1.
   00    0       0     0.2000    8.00E09     0.200     25.0
  0.00     0.0E6

ICOUP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
         1         0
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   29999     25000003010000002 47   1                   1.80
           1.00000E8  0.5e+01  000.0
     1.E-8     1.E00                                   1.E-7
              3.00e6               0.0E1                25.0

SOLVR----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
4  Z1   O0    8.0e-1    1.0e-7

GRMOD----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
COEFS              1         1         1         1         1
BNDST              1         1         1         1         1         1         1
STRES              1         1         1         1         1         1 6.5700E06
STRES              1         1         1         1         2       400 5.0000E06

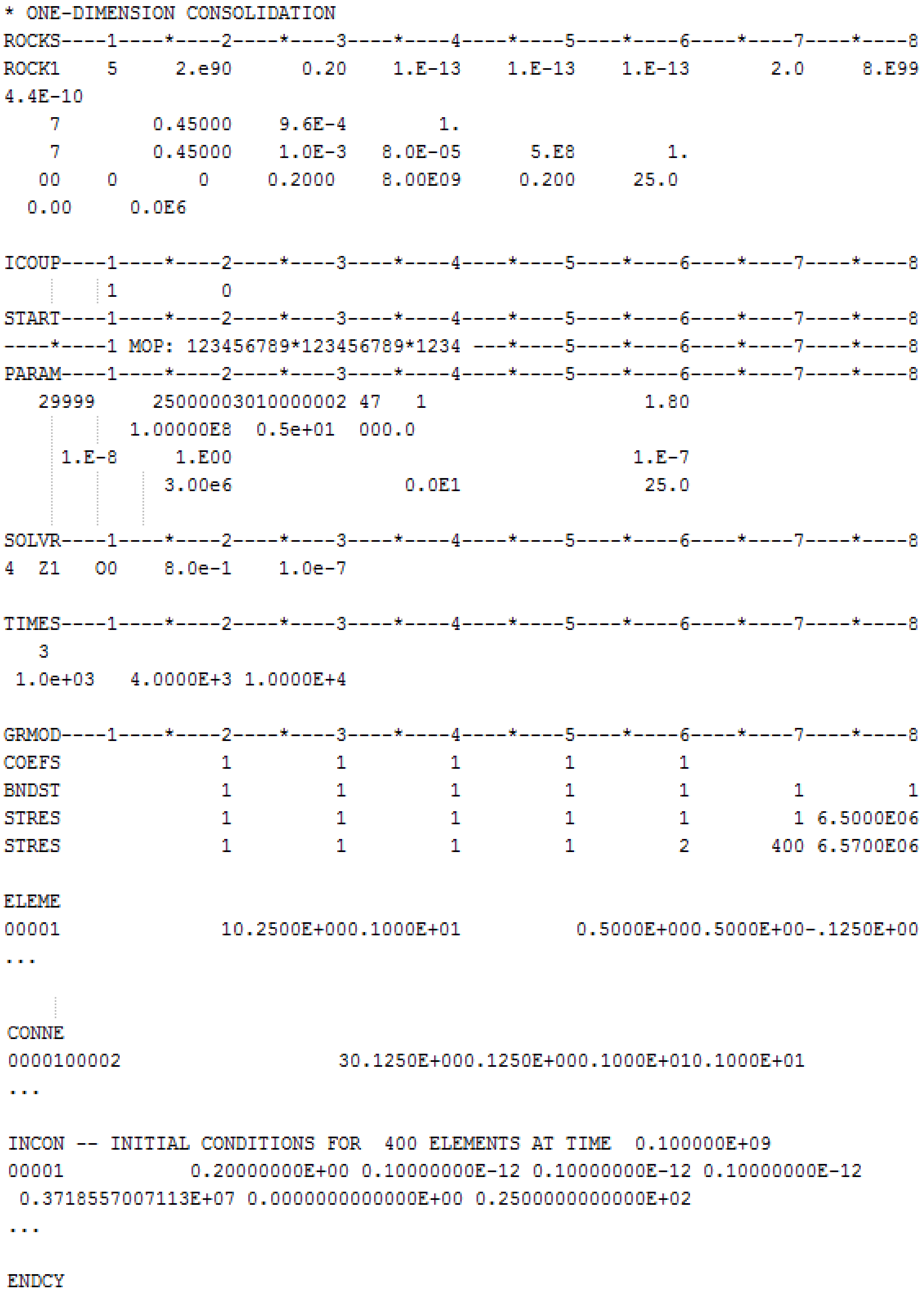
ELEME
00001              10.2500E+000.1000E+01          0.5000E+000.5000E+00-.1250E+00
...

CONNE
0000100002                   30.1250E+000.1250E+000.1000E+010.1000E+01
...

INCON

ENDCY
```

Figure 6-2 Input data for the initialization of 1-D consolidation



```
* ONE-DIMENSION CONSOLIDATION
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
ROCK1    5     2.e90      0.20    1.E-13    1.E-13    1.E-13       2.0     8.E99
4.4E-10
    7        0.45000    9.6E-4        1.
    7        0.45000    1.0E-3   8.0E-05      5.E8        1.
   00    0       0     0.2000    8.00E09     0.200     25.0
  0.00     0.0E6

ICOUP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
         1         0
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   29999     25000003010000002 47   1                   1.80
           1.00000E8  0.5e+01  000.0
     1.E-8     1.E00                                   1.E-7
              3.00e6               0.0E1                25.0

SOLVR----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
4  Z1   O0    8.0e-1    1.0e-7

TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   3
 1.0e+03   4.0000E+3 1.0000E+4

GRMOD----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
COEFS              1         1         1         1         1
BNDST              1         1         1         1         1         1         1
STRES              1         1         1         1         1         1 6.5000E06
STRES              1         1         1         1         2       400 6.5700E06

ELEME
00001              10.2500E+000.1000E+01          0.5000E+000.5000E+00-.1250E+00
...

CONNE
0000100002                   30.1250E+000.1250E+000.1000E+010.1000E+01
...

INCON -- INITIAL CONDITIONS FOR  400 ELEMENTS AT TIME  0.100000E+09
00001           0.20000000E+00 0.10000000E-12 0.10000000E-12 0.10000000E-12
 0.3718557007113E+07 0.0000000000000E+00 0.2500000000000E+02
...

ENDCY
```

Figure 6-3 Input data during the drained condition of 1-D consolidation

6.1.3 Comparison of analytical solution and numerical results

The comparison result in Figure 6-4 indicates that our numerical results produce essentially the same answers to analytical models, which lends creditability to our computational approach.

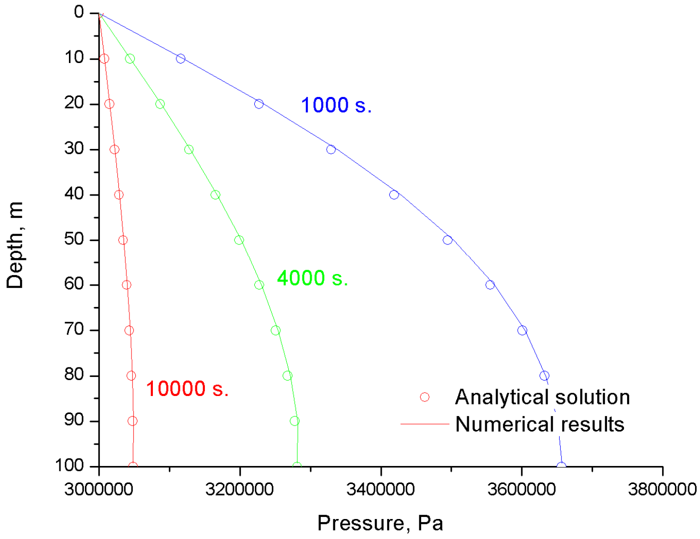


Figure 6-4 The comparison between numerical results and analytical solutions for pressure profiles

6.2 1-D heat conduction

6.2.1 Problem description

The 1-D heat conduction problem is a non-permeable column that undergoes uniaxial strain in the vertical direction only. The column is subjected to a constant temperature on the top. Only heat conduction takes place. Here, ‘OPTIO’ 4 in ‘GRMOD’ entry was used to generate vertical displacement from the top column.

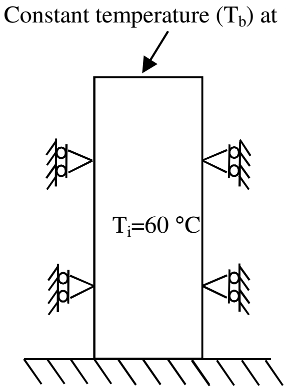


Figure 6-5 Problem description for 1-D heat conduction

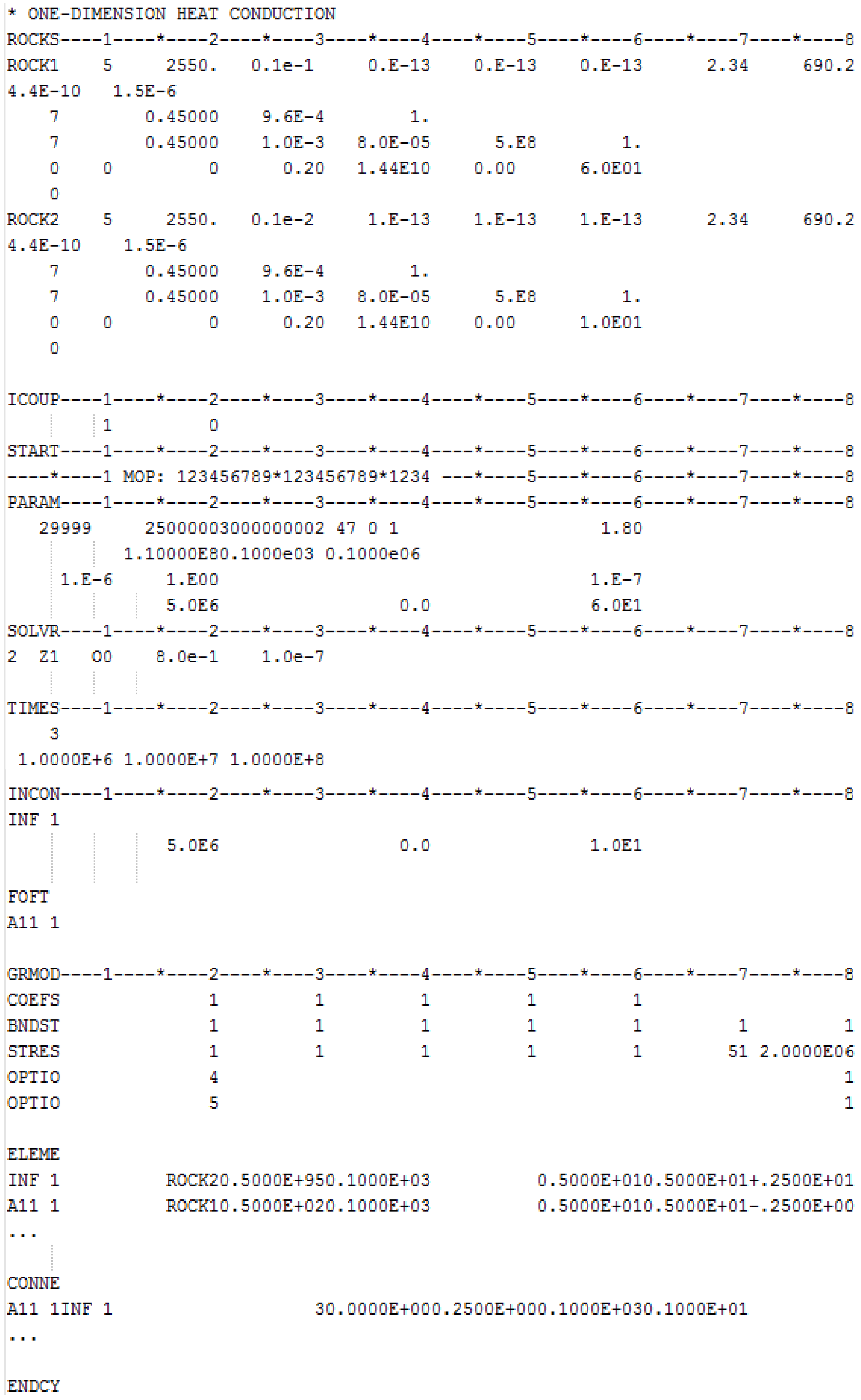
6.2.2 Numerical simulation setup

A non-permeable solid column with very small porosity was initialized with the temperature of 60 °C. A low temperature of 10 °C was imposed at the top column. Detailed input data are shown in Table 6-2, and the input data is shown in Figure 6-6.

The Table 6-2 shows the input parameters, and Figure 6-5 shows the input file used in the simulation of the 1-D heat conduction in a deformable rock column problem.

Table 6-2 Input parameters for the 1D heat conduction problem

Parameters	**Value**	**Unit**
Rock properties (Berea sandstone)		
Elastic modulus (E)	14.40	GPa
Poisson ratio (ν)	0.20	
Porosity (ϕ)	0.01	
Heat conduction (k_T)	2.34	W/m°K
Heat capacity (c_v)	690	J/kg°K
Linear thermal expansion(β)	$1.5\text{x}10^{-6}$	$°K^{-1}$
Initial and Boundary Conditions		
Initial temperature condition	60	°C
Initial mean stress	2.0	MPa
A temperature at the top boundary	10	°C



```
* ONE-DIMENSION HEAT CONDUCTION
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
ROCK1    5     2550.   0.1e-1     0.E-13    0.E-13    0.E-13      2.34     690.2
4.4E-10   1.5E-6
    7        0.45000    9.6E-4        1.
    7        0.45000    1.0E-3   8.0E-05      5.E8        1.
    0    0         0      0.20   1.44E10    0.00      6.0E01
    0
ROCK2    5     2550.   0.1e-2     1.E-13    1.E-13    1.E-13      2.34     690.2
4.4E-10    1.5E-6
    7        0.45000    9.6E-4        1.
    7        0.45000    1.0E-3   8.0E-05      5.E8        1.
    0    0         0      0.20   1.44E10    0.00      1.0E01
    0

ICOUP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
         1         0
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
----*----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   29999     25000003000000002 47 0 1                   1.80
           1.10000E80.1000e03 0.1000e06
     1.E-6     1.E00                                   1.E-7
               5.0E6                 0.0               6.0E1
SOLVR----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
2  Z1   O0    8.0e-1    1.0e-7

TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    3
 1.0000E+6 1.0000E+7 1.0000E+8
INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
INF 1
               5.0E6                 0.0               1.0E1

FOFT
A11 1

GRMOD----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
COEFS              1         1         1         1         1
BNDST              1         1         1         1         1         1         1
STRES              1         1         1         1         1        51 2.0000E06
OPTIO              4                                                           1
OPTIO              5                                                           1

ELEME
INF 1          ROCK20.5000E+950.1000E+03          0.5000E+010.5000E+01+.2500E+01
A11 1          ROCK10.5000E+020.1000E+03          0.5000E+010.5000E+01-.2500E+00
...

CONNE
A11 1INF 1                   30.0000E+000.2500E+000.1000E+030.1000E+01
...

ENDCY
```

Figure 6-6 TOUGH2-EGS input file for 1-D heat conduction problem

6.2.3 *Comparison of analytical solution and numerical results*

The comparison result in Figure 6-6 indicates that our numerical results produce essentially the same answers to analytical models.

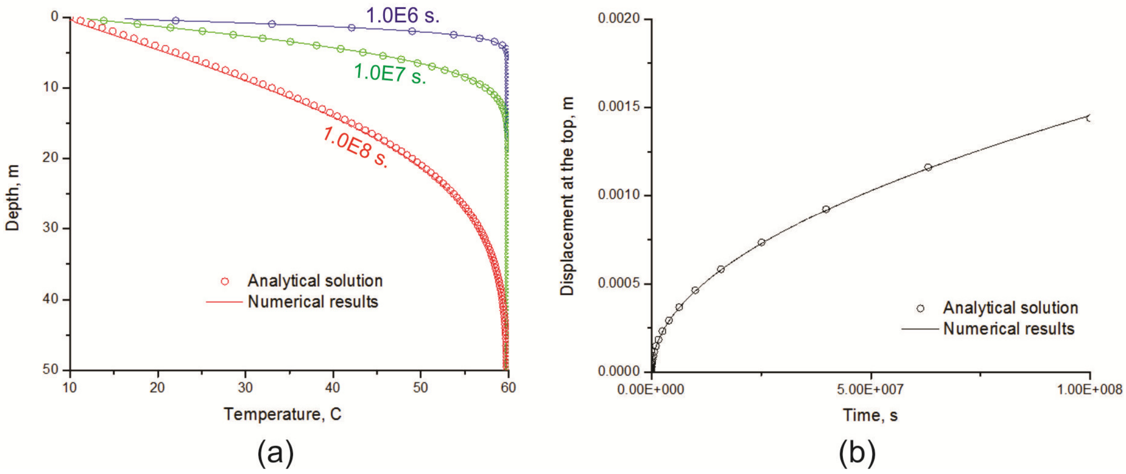


Figure 6-7: The comparison between numerical results and analytical solutions: (a) pressure profiles and (b) the displacement of the top column.

6.3 2-D compaction

6.3.1 *Problem description*

A constant compressive force is applied to the top of a fluid-filled poroelastic material, inducing an instantaneous uniform pore pressure increase and compression (Figure 6-8). Afterwards, the material is allowed to drain laterally. Because the pore pressure near the edges must decrease due to drainage, the material there becomes less stiff and there is a load transfer to the center, resulting in a further increase in center pore pressure that reaches a maximum and then declines. This pore pressure behavior is called the Mandel-Cryer effect (Mandel, 1953) and Abousleiman and et al., (1996) present an analytical solution to the above problem that we compare our simulated results to.

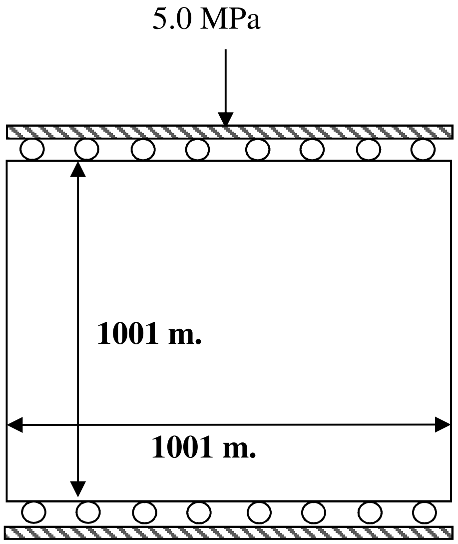


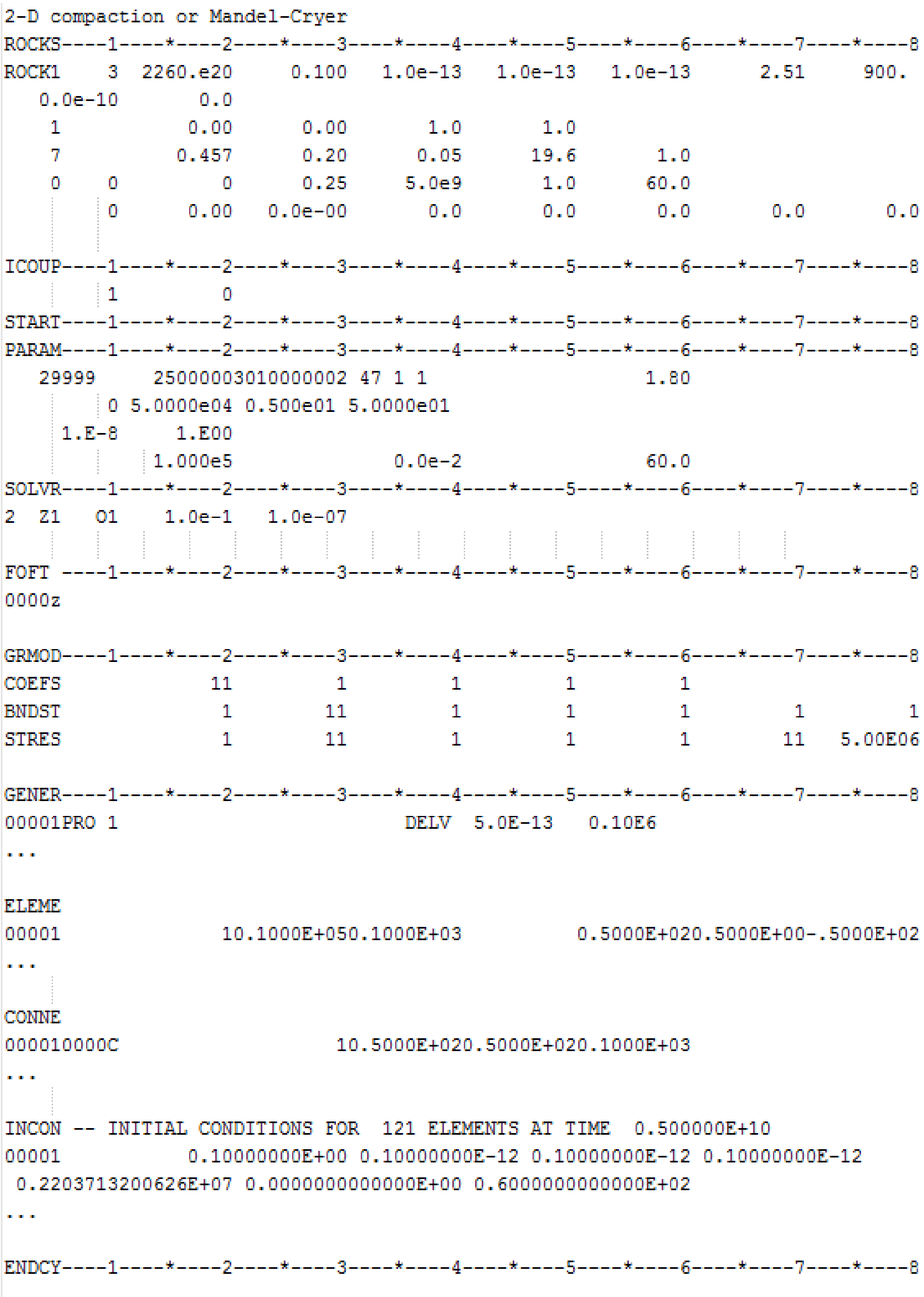
Figure 6-8 Problem description for 2-D compaction

6.3.2 Numerical simulation setup

Similar to 1-D consolidation problem, we simulated this problem in two steps. The first step was to simulate the application of force that induced the pore pressure increase. We started from the initial state where pore pressure and mean stress were initialized at 0.1 MPa and 0.1 MPa, respectively. Then, the addition stress was imposed of 5.0 MPa was imposed and produced the pore pressure increase. We allowed the system to reach equilibrium. We next simulated fluid drainage. The system was allowed to drain from both sides with the pressure of 0.1 MPa. See the table 6-3 for simulation parameters and Figure 6-8 for the sample input files.

Table 6-3 input parameters used in simulation of the 2-D compaction problem

Parameters	**Value**	**Unit**
Rock properties		
Elastic modulus (E)	5.0	GPa
Poisson ratio (ν)	0.25	
Porosity (ϕ)	0.10	
Permeability (k)	$1.00\text{x}10^{-14}$	m^2
Biot coefficient (α)	1.0	
Fluid properties		
Water viscosity (μ_w)	0.89	Pa.s
Water compressibility (c_w)	$4.5\text{x}10^{-10}$	Pa^{-1}
Initial and Boundary Conditions		
Pressure at relaxed condition	0.1	MPa
Mean stress at related condition	0.1	MPa
Additional stress on the top	5.1	MPa
Pressure at the lateral sides	0.1	MPa



```
2-D compaction or Mandel-Cryer
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
ROCK1    3  2260.e20     0.100   1.0e-13   1.0e-13   1.0e-13      2.51      900.
   0.0e-10       0.0
    1           0.00      0.00       1.0       1.0
    7          0.457      0.20      0.05      19.6       1.0
    0    0         0      0.25     5.0e9       1.0      60.0
         0      0.00   0.0e-00       0.0       0.0       0.0       0.0       0.0

ICOUP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
         1         0
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   29999     25000003010000002 47 1 1                   1.80
         0 5.0000e04 0.500e01 5.0000e01
     1.E-8     1.E00
             1.000e5              0.0e-2                60.0
SOLVR----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
2  Z1   O1    1.0e-1   1.0e-07

FOFT ----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
0000z

GRMOD----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
COEFS             11         1         1         1         1
BNDST              1        11         1         1         1         1         1
STRES              1        11         1         1         1        11   5.00E06

GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
00001PRO 1                         DELV  5.0E-13   0.10E6
...

ELEME
00001              10.1000E+050.1000E+03          0.5000E+020.5000E+00-.5000E+02
...

CONNE
000010000C                   10.5000E+020.5000E+020.1000E+03
...

INCON -- INITIAL CONDITIONS FOR  121 ELEMENTS AT TIME  0.500000E+10
00001           0.10000000E+00 0.10000000E-12 0.10000000E-12 0.10000000E-12
 0.2203713200626E+07 0.0000000000000E+00 0.6000000000000E+02
...

ENDCY----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
```

Figure 6-9 input file for 2-D compaction

6.3.3 Comparison of analytical solution and numerical results

The comparison result in Figure 6-10 indicates that our numerical results produce essentially the same answers to analytical models.

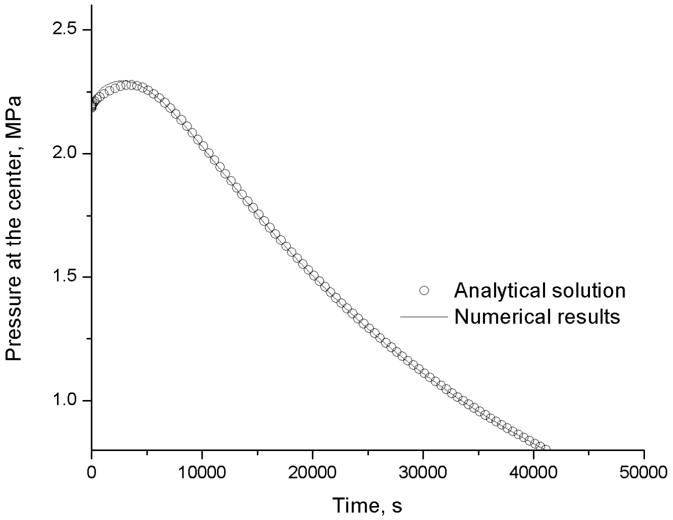


Figure 6-10 The comparison between numerical results and analytical solutions for the pressure profile at the center of the model

6.4 The mineral scaling of Tiwi geothermal field

This example is taken from TOUGHREACT manual (Xu et al., 2004a) and only THC simulation is performed. We are going to compare against the simulation results from TOUGHREACT in this part.

6.4.1 Problem description

Nag-67 is one of the hot brine injectors located to the south-east of the Tiwi production field, Philippines. The well was completed in March 1987 as a deviated hole with a 9 5/8 in. casing shoe set at 917m measured depth (MD), and the top of a 7 in. production liner at 878mMD with the shoe at 2114mMD (1873mtotal vertical depth—TVD). The injectivity of the well decreased significantly with time. The drop in injection capacity was attributed to scaling inside the wellbore as early as October 1992; the liner was found to be reduced in diameter to 5 in. at the depth of 1651 m.

The silica concentration and pH of the brine being supplied to the Nag-67 injector were monitored between 1989 and 2000. Complete brine analyses were also available for every year except 1999 and were used to characterize the saturation state of the brine with respect to other minerals. From this historical chemical record, the degree of amorphous silica saturation in the water sample was determined.

6.4.2 Grid and fluid flow parameters

A120m thick reservoir formation at the bottommost permeable zone of the injection well (Nag-67) was modelled. A simple one-dimensional radial flow model was used, consisting of 50 radial blocks with logarithmically increasing radii (Figure 6-11). The 50 blocks represent a distance of 1000m from the wall of the drilled open hole. Only the fracture network is considered in the model, with the assumption that the fluid exchange with the surrounding low permeability matrix is insignificant. Initial reservoir temperature and pressure were assumed as 260°C and 11.6MPa, respectively. A constant injection temperature of 160°C was used because measured temperature fluctuations were generally small and with a relatively flat average trend.

The injection history of the well was used to define the amount of injected mass versus time (Figure 6-12), and 50% of the total injection rate in Nag-67 was used because spinner surveys showed that the bottommost permeable zone accepted about 50% of the injection.

6.4.3 Geochemical data

The types and initial abundances of primary minerals were determined from the reported Nag-67 alteration mineralogy at the 1798–1920m MD permeable zone, as shown on Table 6-4.

Table 6-4 List of minerals and aqueous species in the simulation

Chemical Species	Initial Water Concentration (mol/l)	Injection Water Concentration (mol/l)
Ca^{2+}	3.32×10^{-3}	1.0327×10^{-3}
Mg^{2+}	8.62×10^{-6}	1.6609×10^{-6}
Na^{+}	1.285×10^{-1}	1.2734×10^{-1}
Cl^{-}	1.418×10^{-1}	1.418×10^{-1}
$SiO_2(aq)$	1.218×10^{-2}	1.1734×10^{-2}
HCO_3^{-}	1.0423×10^{-3}	1.0423×10^{-3}
SO_4^{2-}	2.6272×10^{-4}	2.6272×10^{-4}
K^{+}	1.5852×10^{-2}	1.5852×10^{-2}
AlO_2^{-}	0.059×10^{-4}	0.0205×10^{-4}

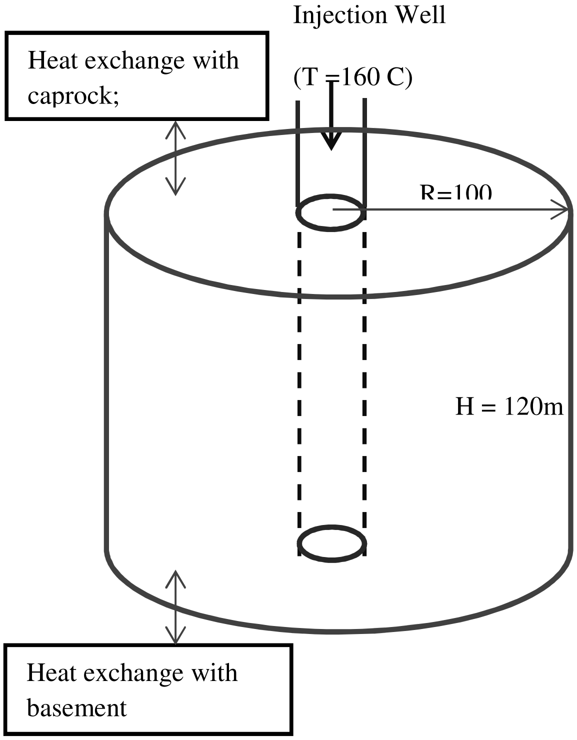


Figure 6-11Simplified model of grid blocks and injection well

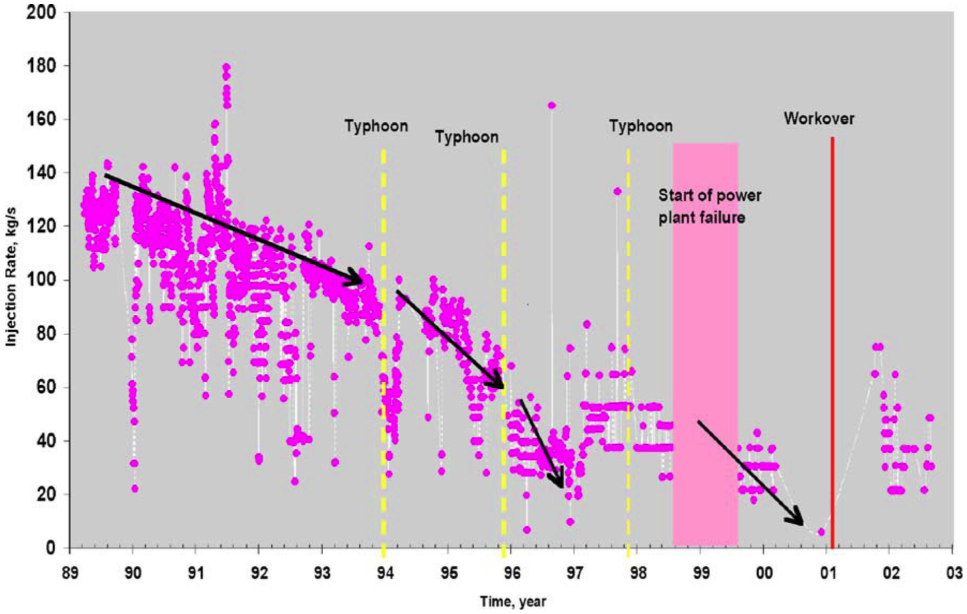


Figure 6-12 Injection history of Nag-67

The composition of the injected brine was provided from historical analytical data. The formation water was reconstituted from the known brine composition as follows. First, the brine was diluted to yield saturation with quartz at the observed reservoir temperature of 260 ◦C (thus reversing the concentrative effect of flashing). The resulting water was then equilibrated with minerals identified in the well mineralogy log (calculating the aluminium concentration using equilibrium with microcline, sodium using albite, pH using calcite, calcium using clinozoisite, and magnesium using clinochlore). Calcite and anhydrite were assumed to react at equilibrium because their reaction rate is typically quite rapid. Other minerals were set to react under kinetic constraints. For other minerals, thermodynamic and kinetic data were taken from various other literature sources.

Besides the main input file as Figure 6-14, there are other two input files required for the chemical reaction simulation, the “solute.inp” and “chemical.inp” as shown in the Figure 6-15 and 6-16. The initial mineral fraction of the reservoir rock for the simulation is shown as the Figure 6-13.

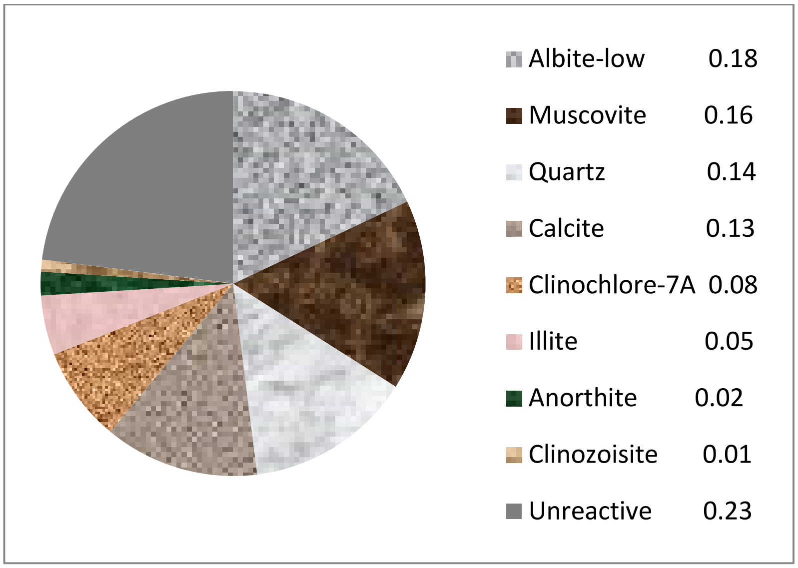
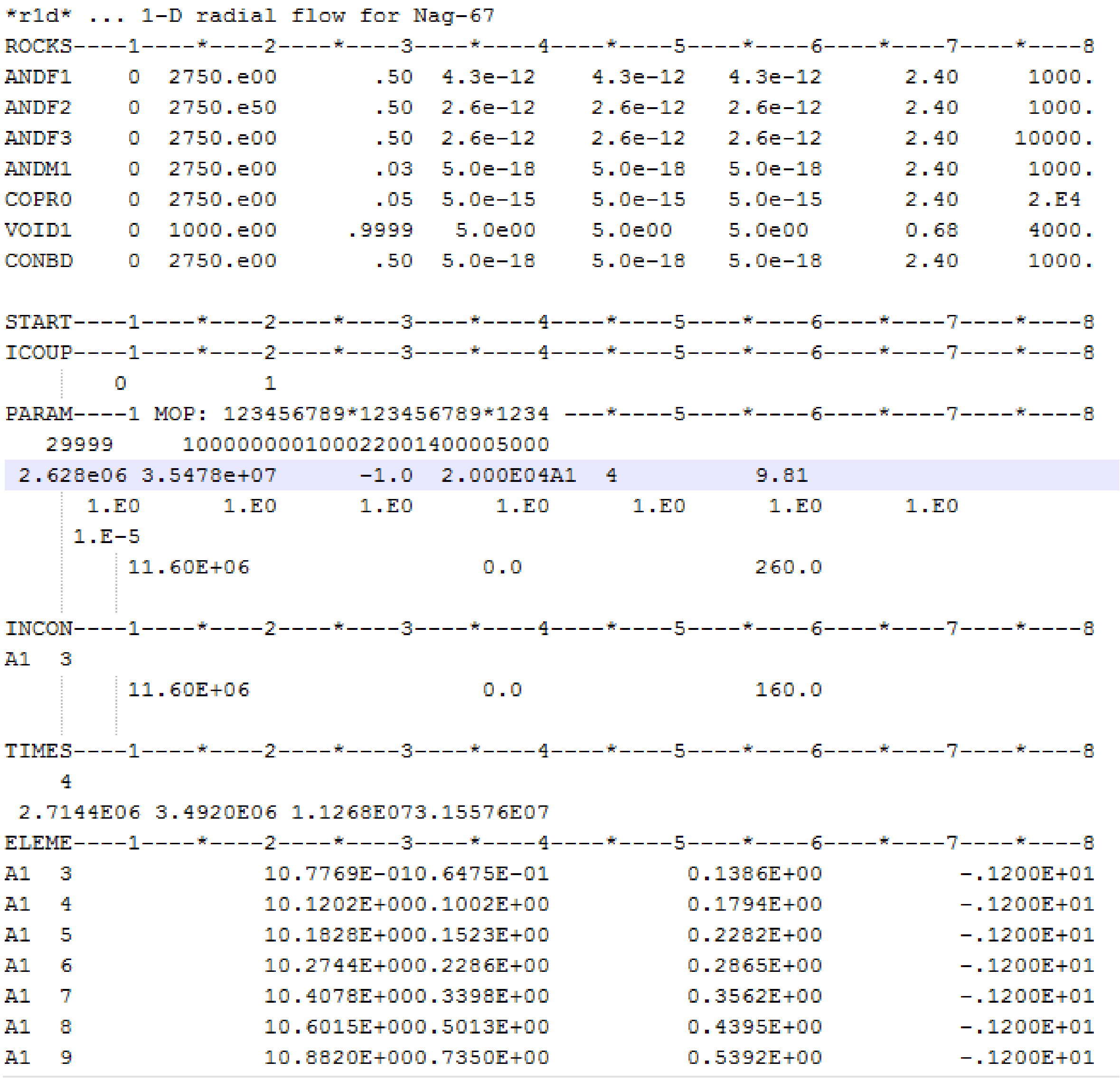


Figure 6-13 The initial mineral volume fraction



```
*r1d* ... 1-D radial flow for Nag-67
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
ANDF1    0  2750.e00       .50  4.3e-12    4.3e-12   4.3e-12      2.40     1000.
ANDF2    0  2750.e50       .50  2.6e-12    2.6e-12   2.6e-12      2.40     1000.
ANDF3    0  2750.e00       .50  2.6e-12    2.6e-12   2.6e-12      2.40    10000.
ANDM1    0  2750.e00       .03  5.0e-18    5.0e-18   5.0e-18      2.40     1000.
COPR0    0  2750.e00       .05  5.0e-15    5.0e-15   5.0e-15      2.40     2.E4
VOID1    0  1000.e00     .9999   5.0e00    5.0e00    5.0e00       0.68     4000.
CONBD    0  2750.e00       .50  5.0e-18    5.0e-18   5.0e-18      2.40     1000.

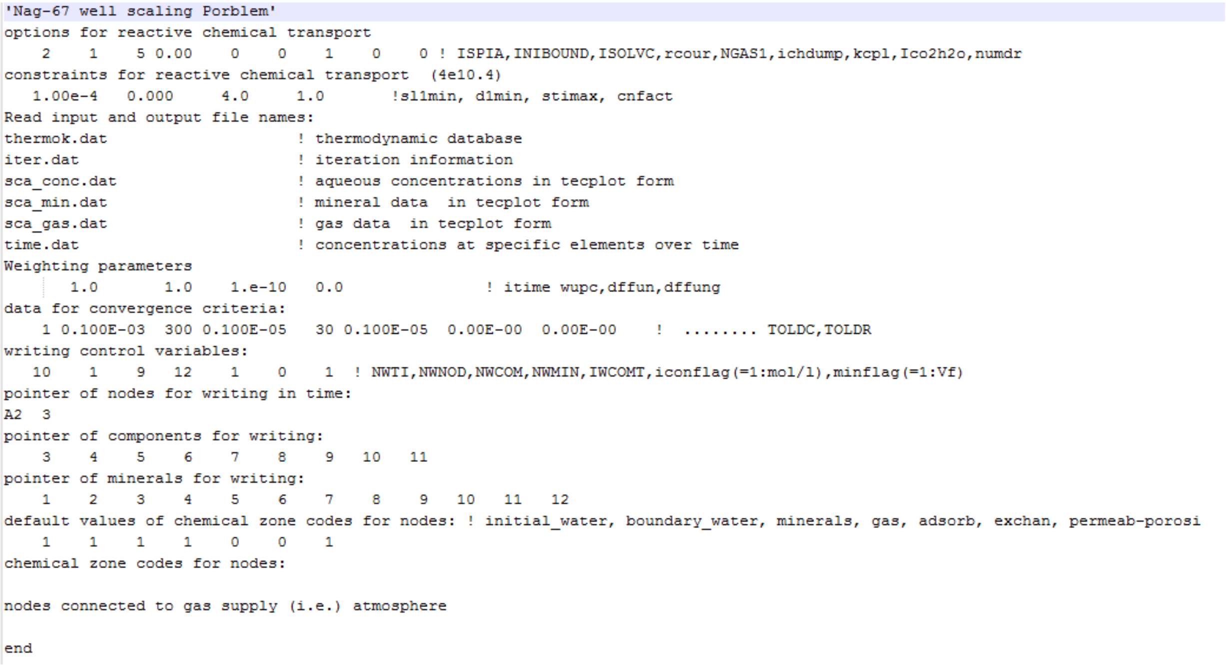
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
ICOUP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
        0          1
PARAM----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
   29999     100000000100022001400005000
 2.628e06 3.5478e+07      -1.0  2.000E04A1  4          9.81
      1.E0      1.E0      1.E0      1.E0      1.E0      1.E0      1.E0
     1.E-5
         11.60E+06                 0.0                 260.0

INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A1  3
         11.60E+06                 0.0                 160.0

TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    4
 2.7144E06 3.4920E06 1.1268E073.15576E07
ELEME----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
A1  3              10.7769E-010.6475E-01          0.1386E+00          -.1200E+01
A1  4              10.1202E+000.1002E+00          0.1794E+00          -.1200E+01
A1  5              10.1828E+000.1523E+00          0.2282E+00          -.1200E+01
A1  6              10.2744E+000.2286E+00          0.2865E+00          -.1200E+01
A1  7              10.4078E+000.3398E+00          0.3562E+00          -.1200E+01
A1  8              10.6015E+000.5013E+00          0.4395E+00          -.1200E+01
A1  9              10.8820E+000.7350E+00          0.5392E+00          -.1200E+01
```

......

Figure 6-14 The main input file of THC simulation

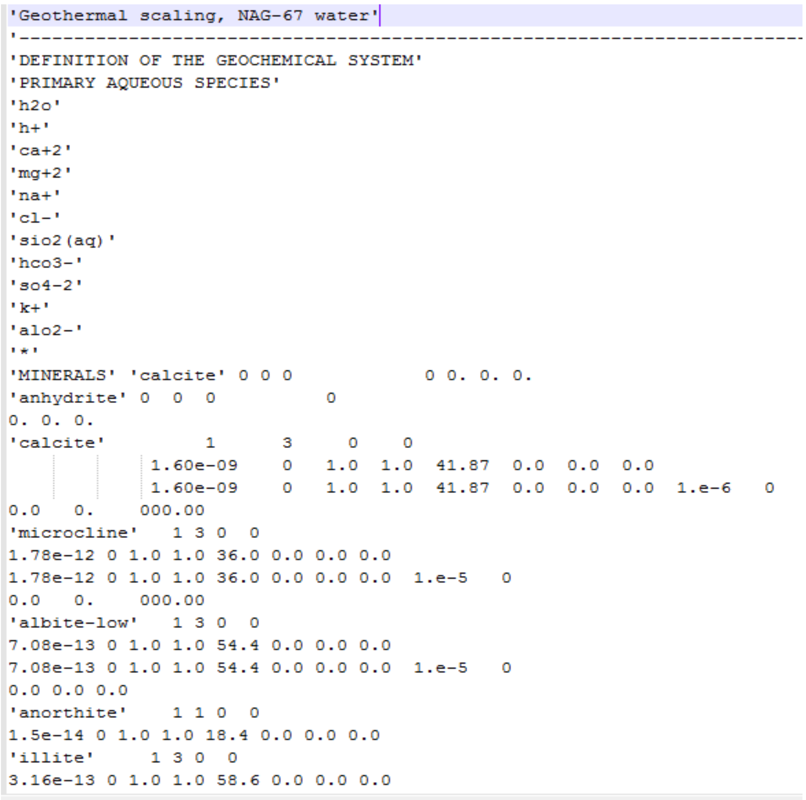


```
'Nag-67 well scaling Porblem'
options for reactive chemical transport
    2    1    5 0.00    0    0    1    0    0 ! ISPIA,INIBOUND,ISOLVC,rcour,NGAS1,ichdump,kcpl,Ico2h2o,numdr
constraints for reactive chemical transport  (4e10.4)
   1.00e-4   0.000     4.0     1.0       !sl1min, d1min, stimax, cnfact
Read input and output file names:
thermok.dat                    ! thermodynamic database
iter.dat                       ! iteration information
sca_conc.dat                   ! aqueous concentrations in tecplot form
sca_min.dat                    ! mineral data  in tecplot form
sca_gas.dat                    ! gas data  in tecplot form
time.dat                       ! concentrations at specific elements over time
Weighting parameters
       1.0       1.0    1.e-10   0.0               ! itime wupc,dffun,dffung
data for convergence criteria:
    1 0.100E-03  300 0.100E-05   30 0.100E-05  0.00E-00  0.00E-00    !  ........ TOLDC,TOLDR
writing control variables:
   10    1    9   12    1    0    1  ! NWTI,NWNOD,NWCOM,NWMIN,IWCOMT,iconflag(=1:mol/l),minflag(=1:Vf)
pointer of nodes for writing in time:
A2  3
pointer of components for writing:
    3    4    5    6    7    8    9   10   11
pointer of minerals for writing:
    1    2    3    4    5    6    7    8    9   10   11   12
default values of chemical zone codes for nodes: ! initial_water, boundary_water, minerals, gas, adsorb, exchan, permeab-porosi
    1    1    1    1    0    0    1
chemical zone codes for nodes:

nodes connected to gas supply (i.e.) atmosphere

end
```

Figure 6-15 The solute.inp file for the simulation



```
'Geothermal scaling, NAG-67 water'
'------------------------------------------------------------------------
'DEFINITION OF THE GEOCHEMICAL SYSTEM'
'PRIMARY AQUEOUS SPECIES'
'h2o'
'h+'
'ca+2'
'mg+2'
'na+'
'cl-'
'sio2(aq)'
'hco3-'
'so4-2'
'k+'
'alo2-'
'*'
'MINERALS' 'calcite' 0 0 0            0 0. 0. 0.
'anhydrite' 0  0  0          0
0. 0. 0.
'calcite'         1      3     0    0
             1.60e-09    0    1.0  1.0  41.87  0.0   0.0   0.0
             1.60e-09    0    1.0  1.0  41.87  0.0   0.0   0.0   1.e-6   0
0.0   0.    000.00
'microcline'   1 3 0  0
1.78e-12 0 1.0 1.0 36.0 0.0 0.0 0.0
1.78e-12 0 1.0 1.0 36.0 0.0 0.0 0.0  1.e-5   0
0.0   0.    000.00
'albite-low'   1 3 0  0
7.08e-13 0 1.0 1.0 54.4 0.0 0.0 0.0
7.08e-13 0 1.0 1.0 54.4 0.0 0.0 0.0  1.e-5   0
0.0 0.0 0.0
'anorthite'    1 1 0  0
1.5e-14 0 1.0 1.0 18.4 0.0 0.0 0.0
'illite'     1 3 0  0
3.16e-13 0 1.0 1.0 58.6 0.0 0.0 0.0
```

Figure 6-16 The chemical.inp file for the simulation

6.4.4 Simulation Results

The well injectivity is dominated by the permeability evolution. The mineral precipitation takes the porous media space and decrease the porosity therefore the permeability is affected by the mineral precipitation and dissolution. See Figure 6-17 as the porosity and permeability evolution of injection well due to mineral precipitation.

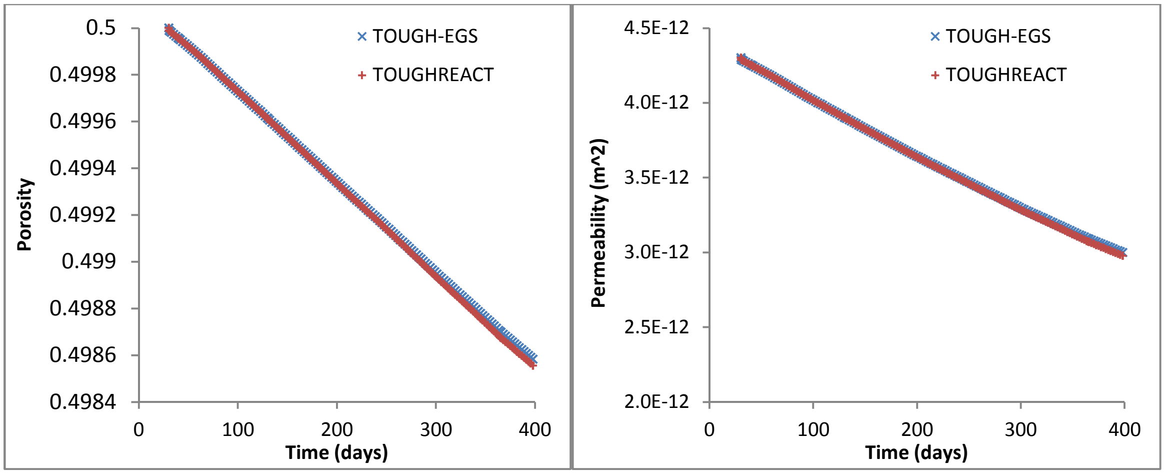


Figure 6-17 Porosity and permeability evolution of injection well due to chemical reaction

The output of fluid and heat flow simulation by TOUGH2-EGS, typically the temperature and pressure, is plotted as Figure 6-18. The horizontal axis is the radial distance from the injection well. Figure 6-19 shows the comparison results of P and T after 1 year simulation.

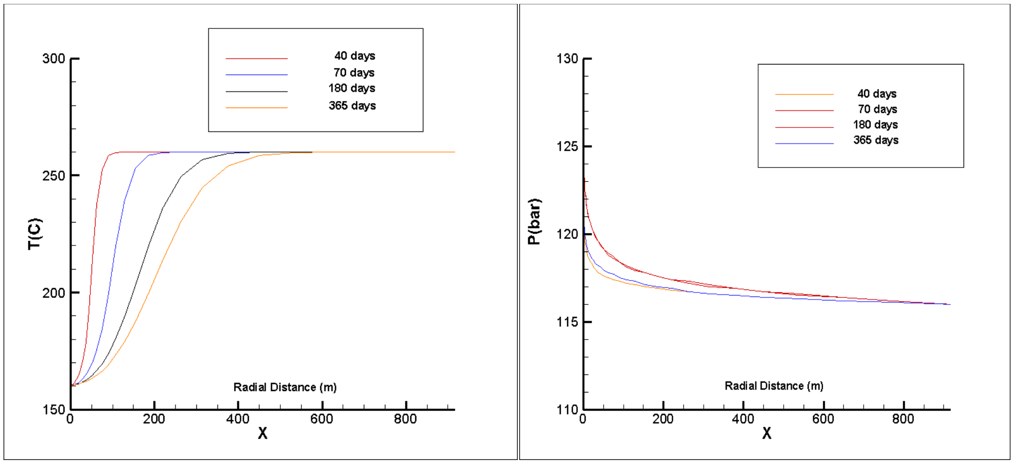


Figure 6-18 Temperature and Pressure evolution by TOUGH-EGS simulation

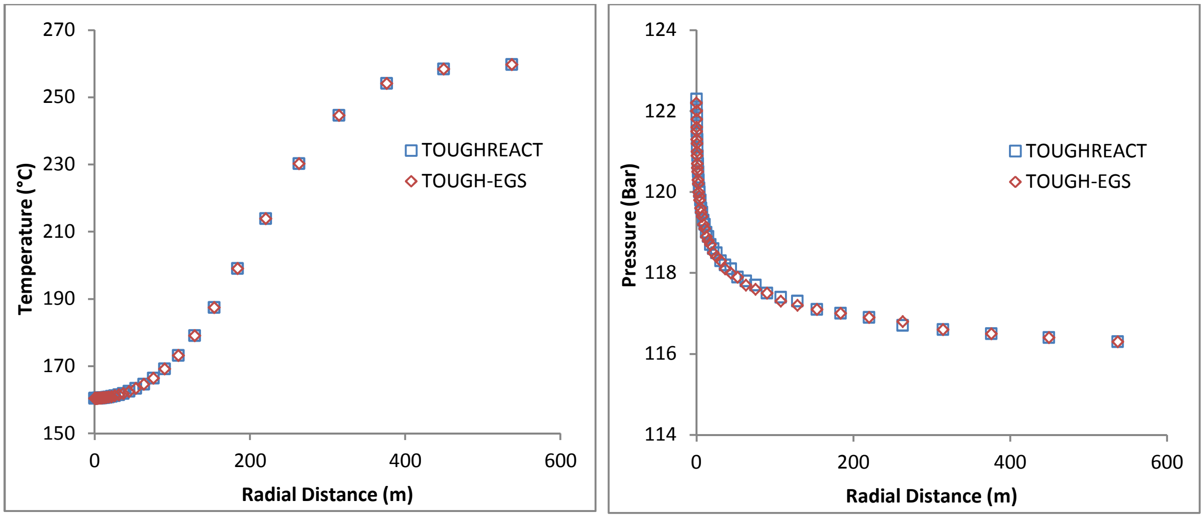


Figure 6-19 Pressure and temperature profile (1 year) between TOUGHREACT and TOUGH2-EGS

The change of abundance of minerals affects the reservoir performance by changing the porosity and permeability. The change of abundance of minerals is due to the chemical reaction among the species and rock minerals. The Figure 6-20 shows the *SiO2*(Amorphous) has the largest positive value, which means it is the most precipitated minerals, and calcite has the smallest negative values, which means calcite the most dissolved minerals. But the precipitation from SiO2 is much larger than dissolution of calcite, which explains the porosity and permeability decrease in Figure 6-17. We also compare the *SiO2*(Amorphous) volume fraction change between TOUGHREACT and TOUGH2-EGS.

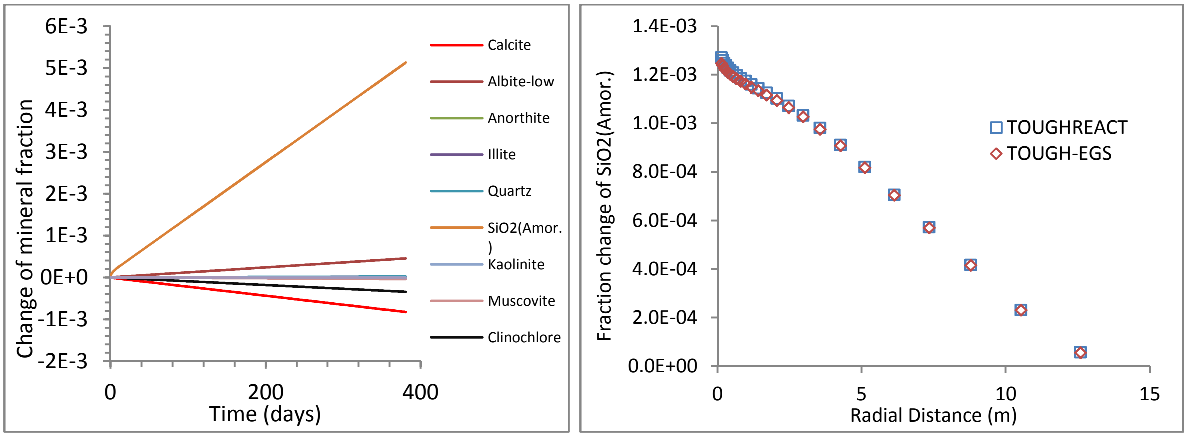


Figure 6-20 The volume fraction change of mineral (left – injection well, right – 1 year profile)

6.5 Heat sweep in a vertical fracture

In this example, we compared our simulator (TOUGH2-EGS) with a non-isothermal commercial reservoir simulator (STARS) of Computer Modeling Group (CMG).

6.5.1 Description

In many geothermal fields, there is evidence of rapid migration of injected fluids along preferential flow paths, presumably along fractures. The present problem is designed to study thermal interference along such paths, by modeling non-isothermal injection into and production from a single vertical fracture, as illustrated in Figure 6-21 (Pruess and Bodvarsson, 1984). The fracture is bounded by semi-infinite half-spaces of impermeable rock, which provide a conductive heat supply. Initial temperature is 300 °C throughout. Water at 100 °C temperature is injected at one side of the fracture at a constant rate of 3.75 kg/s, while production occurs at the other side against a specified wellbore pressure. Problem parameters are given in Table 6-5 for injecting at point I and producing at point P.

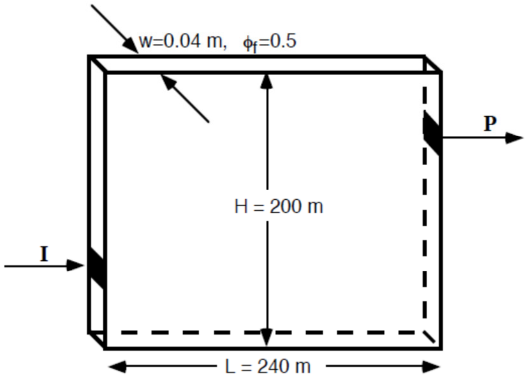


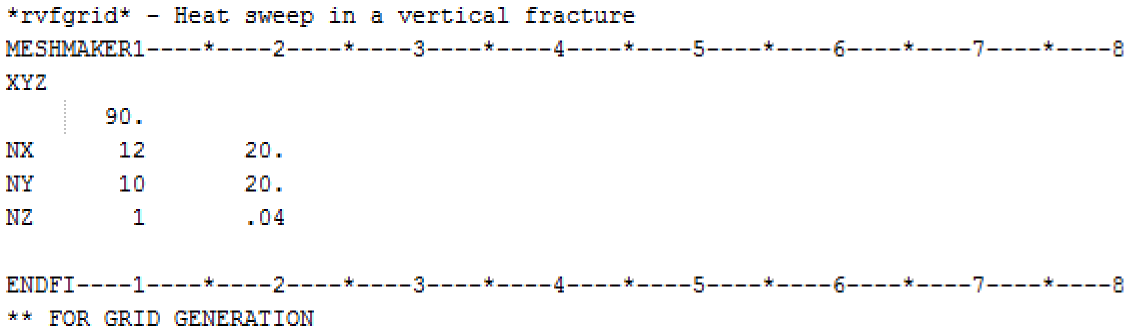
Figure 6-21 Schematic diagram of injection-production system in vertical fracture injection occurs at I, production at P. (Pruess et al.,1999)

Table 6-5 Input parameters used in simulation for the heat sweep in vertical fracture problem

Parameters	**Value**	**Unit**
Rock properties		
Rock grain density	2650	kg/m^3
Specific heat	1000	J/kg°C
Heat conductivity	2.1	W/m°C
Fracture		
Height	200	m
Length	240	m
Aperture	0.04	m
Permeability	200	Darcy
Porosity	50	%
Initial Conditions		
Pressure	10.0	MPa
Temperature	300	°C

6.5.2 *Numerical simulation setup*

We simulated this problem in three steps. The first step was to generate mesh data. In this problem, we consider the heat conduction from semi-infinite half space from the lateral connections. However, MESHM function generates data for the analytical solution for the connection from top and bottom of the model. Thus, the model was constructed by rotating the horizontal plane by 90°, as seen in Figure 6-22.

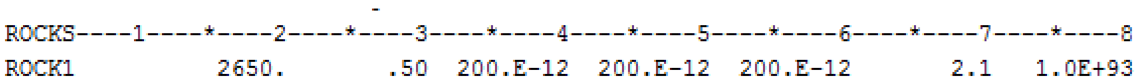


```
*rvfgrid* - Heat sweep in a vertical fracture
MESHMAKER1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
XYZ
       90.
NX      12       20.
NY      10       20.
NZ       1       .04

ENDFI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
** FOR GRID GENERATION
```

Figure 6-22 Mesh generation for the heat sweep in vertical fracture problem

Then, we initialized pressure in the model by running the model without sink and source term until the pressure reach gravity equilibrium. Then, the ‘SAVE’ file which is the results from the initialization was renamed to ‘INCON’ which would be used as the initial condition for the next runs. Here, the rock heat capacity is set as infinity so that the run was in isothermal mode, see Figure 6-23.



```
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
ROCK1          2650.        .50  200.E-12  200.E-12  200.E-12       2.1   1.0E+93
```

Figure 6-23 ROCKS data for model initialization

Finally, the source term was included at ‘00008’ element which is representing point I and the sink term was added at ‘0001p’ element which is representing point P in Figure 6-21. Two cases were run to demonstrate the effect of heat conduction from infinite impermeable layers. The two cases were achieved by switching MOP (15) option.

6.5.3 Results and comparison

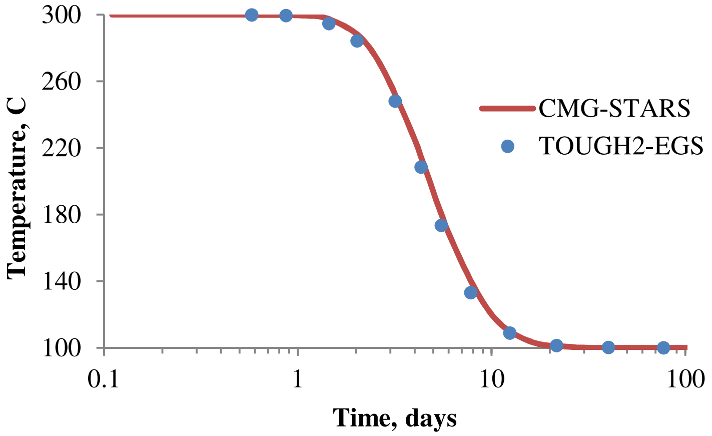


Figure 6-24 Comparison between CMG-STARS and TOUGH2-EGS results: production fluid temperature of the vertical sweep in a vertical fracture problem: no heat gain from surrounding rock

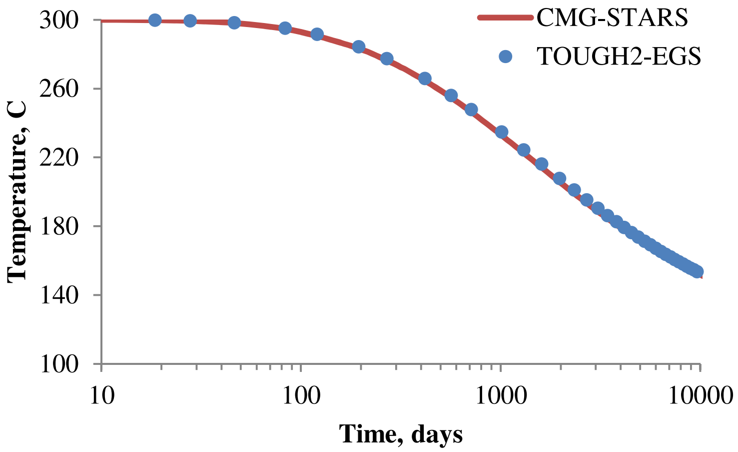


Figure 6-25 Comparison between CMG-STARS and TOUGH2-EGS results: production fluid temperature of the vertical sweep in a vertical fracture problem: with heat gain from surrounding rock

6.6 The Geyser Geothermal Field cases

6.6.1 Problem description

The Geysers is the site of the largest geothermal electricity generating operation in the world and has been in commercial production since 1960 (Mossop and Segall, 1997 and 1999; Rutqvist and Tsang, 2002a; Rutqvist et al., 2006a; Rutqvist et al., 2006b; Rutqvist and Oldenburg 2008; Rutqvist et al., 2010; Khan and Truschel 2010; Rutqvist 2011). It is a vapor-dominated geothermal reservoir system that is hydraulically confined by low permeability rock. As a result of high steam withdrawal rates, the reservoir pressure declined until the mid-1990s, when increasing water injection rates resulted in a stabilization of the steam reservoir pressure. Archival INSAR images were acquired from approximately monthly satellite passes over the region for a seven-year period, seven-year period, from 1992 to 1999, and the data is compared with displacement calculated from our model.

The combined effects of steam production and water injection in 44 years and their influences on the ground deformation will be analyzed. Based on the work by Rutqvist and Oldenburg, 2008 and Rutqvist et al. 2010, a cross-axis (NE-SW) two-dimensional model grid of the Geysers Geothermal Field was established. Permeability, temperature, and boundary conditions are shown in Figure 6-26. The initial thermal and hydrological conditions (vertical distributions of temperature, pressure and liquid saturation) are typically established through steady-state multi-phase flow simulations. According to previous studies, the adopted rock-mass bulk modulus is 3 GPa and the linear thermal expansion coefficient is 3×10^{-5} $°C^{-1}$. Pore compressibility and the reservoir Poisson's ratio of the reservoir is 1.0×10^{-10} Pa^{-1} and 0.25, respectively. The injection well is about 217.5 m away from the production well. The steam-production and water-injection rate used in the model is estimated from the field-wide production and injection data (Mossop and Segall 1997; Majer and Peterson 2007; Khan and Truschel 2010; Sanyal and Enedy, 2011).

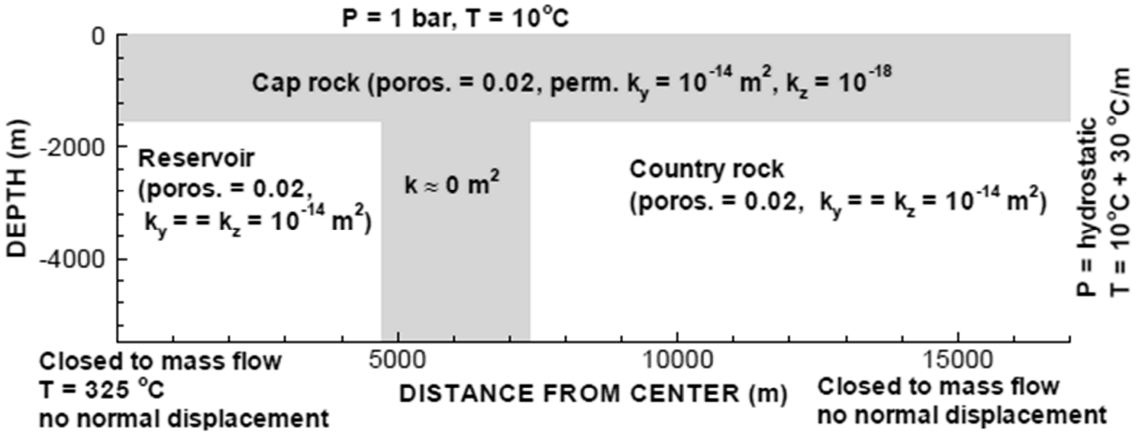


Figure 6-26. Half-symmetric model domain with hydraulic properties and boundary conditions (Rutqvist and Oldenburg, 2008).

6.6.2 Change of pressure and temperature after 44 years

Figure 6-27 shows calculated liquid saturation and changes in fluid pressure and temperature after 44 years of production and injection. Figure 6-27a shows the injection caused formation of a wet zone that extends towards 1,000m. Figure 6-27b demonstrates pressure decrement is about 2×106 Pa after steam production and water injection. Figure 6-27c indicates a local cooling effect and the maximum temperature decrement is about 50°C. All the results are almost the same as the results from Rutqvist and Oldenburg (2008).

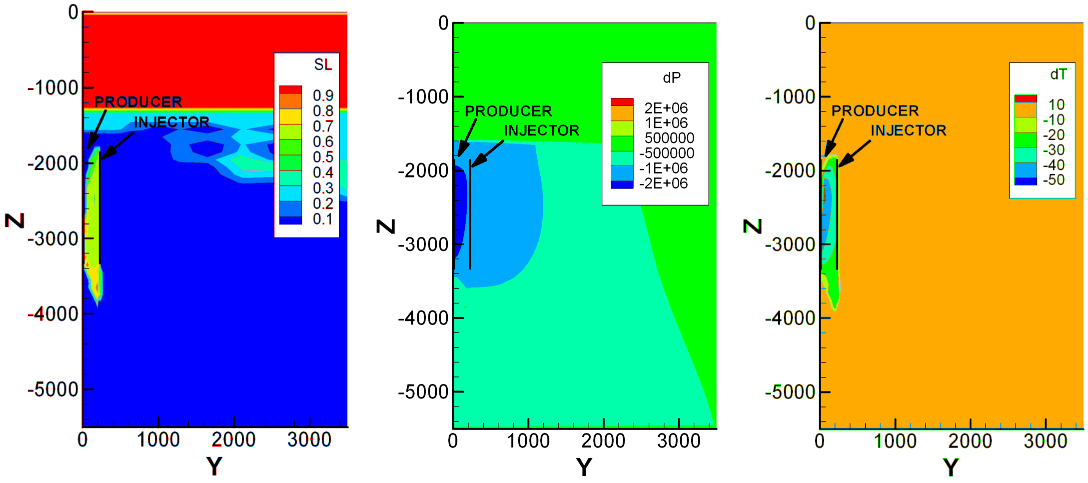


Figure 6-27. Simulated profile of liquid saturation (a), changes in fluid pressure (b), changes in temperature(c) after 44 years of production and injection.

6.6.3 Changes in stress and volumetric strain

Figure 6-28a and 6-29b display changes in mean total stress and volumetric strain, respectively. The mean total stress change in the rock mass depends on the production-induced depletion and injection-induced cooling. The change in mean total stress is about 0.5-1.5 MPa and the volumetric strain is about 0.0001-0.0004. Figure 6-29 shows the change of simulated ground displacement with time and the comparison with INSAR data and results from TOUGH2-FLAC (Rutqvist, 2011). Figure 6-30 shows the change of displacement along the cross-section of the model and the comparison with observed and known simulated results. It can be seen from these two figures that there is good agreement between simulated ground displacement and INSAR data.

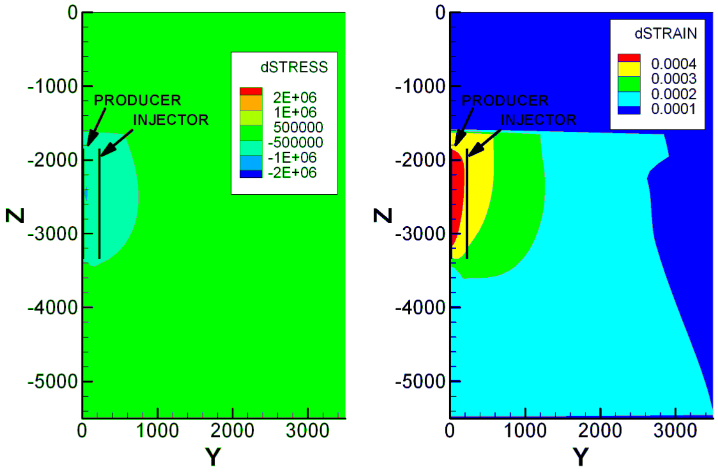


Figure 6-28 Simulated profile of stress (a) and strain (b) after 44 years of production and injection

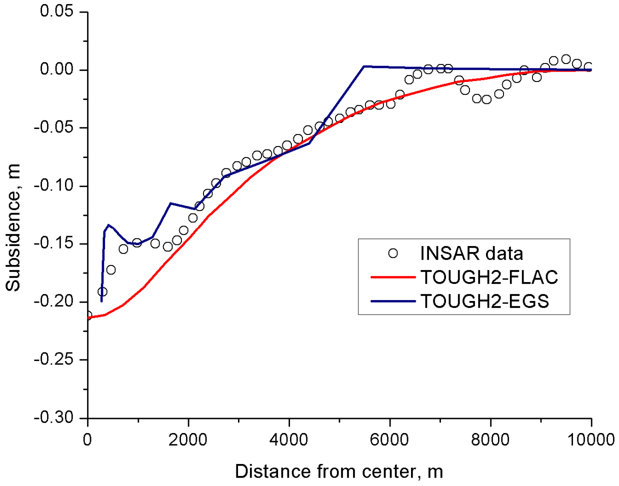


Figure 6-29 Subsidence profile comparison between INSAR data, TOUGH2-FLAC, and TOUGH2-EGS simulation results after 44 years of production and injection.

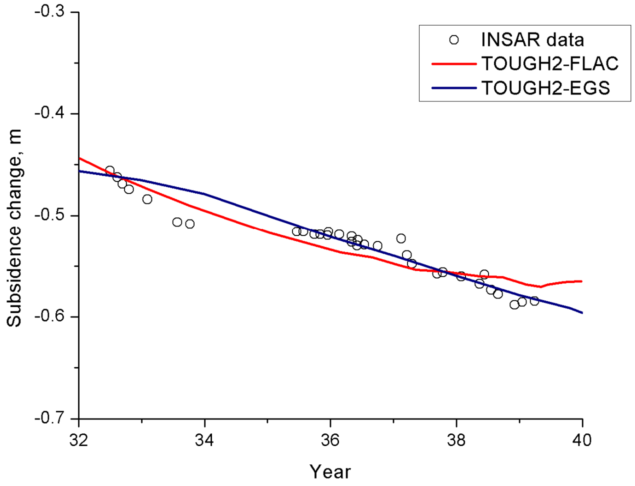


Figure 6-30 Subsidence profile comparison between INSAR data, TOUGH2-FLAC, and TOUGH2-EGS simulation results from year 32 to 40 (1992 -2000).

6.7 THMC effects on the injection wells

In the application example, we present one prototypical EGS reservoir to simulate THMC process of the vicinity of the injection well. In order to show the geomechanical and geochemical effects and other influencing factors, there are couple simulations runs performed, including THM without chemical reactions effects and THMC with different injection temperature and chemical concentrations.

6.7.1 *Problem Description*

As shown in Figure 6-31, the fractured reservoir is overlain by the caprock and the injection well is in the middle of the simulated area. The mesh is generated with radial dimensions and logarithmic distribution in radial direction to capture the subtle effects around the wellbore. We are going to simulate the injection well and its vicinity reservoir for continuous two years injection.

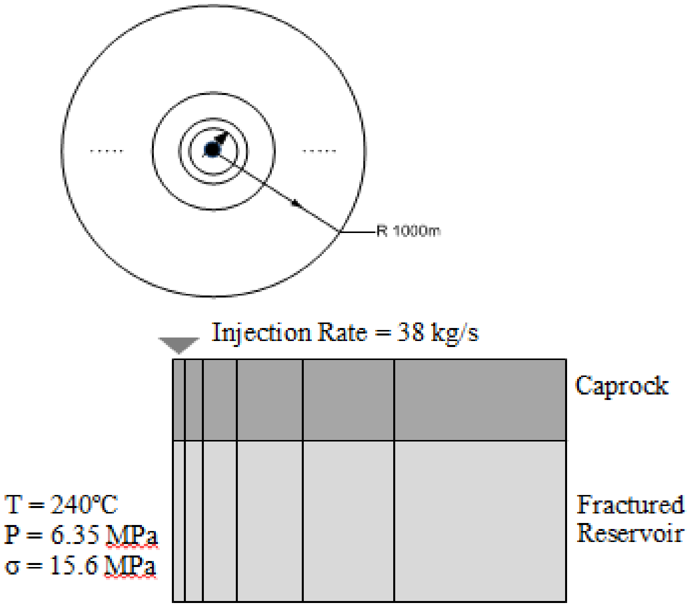


Figure 6-31 Injection well sketch for THMC simulation

The reservoir hydraulic properties, including porosity and permeability, are considered dynamically changed due to mechanical and chemical effects. The Equation 2.49 described the correlation between stress and porosity for sedimentary rock, and it is used in the simulation. The Carman-Kozeny correlation as Equation 2.55 is used for the permeability correlation with porosity.

The reservoir and material properties used in the simulation are referred to the Table 6-6. The reservoir and injection water chemical data in this simulation are same as the example 4 as Table 6-4.

Table 6-6 Reservoir and material properties

Properties	Values
Young's Modulus *(GPa)*	14.4
Poisson's ratio *(dimensionless)*	0.20
Permeability *(m^2)*	5.37×10^{-14}
Porosity *(dimensionless)*	0.1
Pore compressibility*(Pa^{-1})*	5×10^{-7}
Linear thermal expansion coefficient *($^{o}C^{-1}$)*	4.14×10^{-6}
Rock grain specific heat *(J/kg ºC)*	1000
Rock grain density *(kg/m^3)*	2750
Formation thermal conductivity *(W/m ºC)*	2.4
Biot's coefficient *(dimensionless)*	1.0
Initial mean normal stress *(MPa)*	15.6
High stress residual porosity *(dimensionless)*	0.8
Exponent parameter a of Equation 2.49 *(Pa^{-1})*	2×10^{-7}

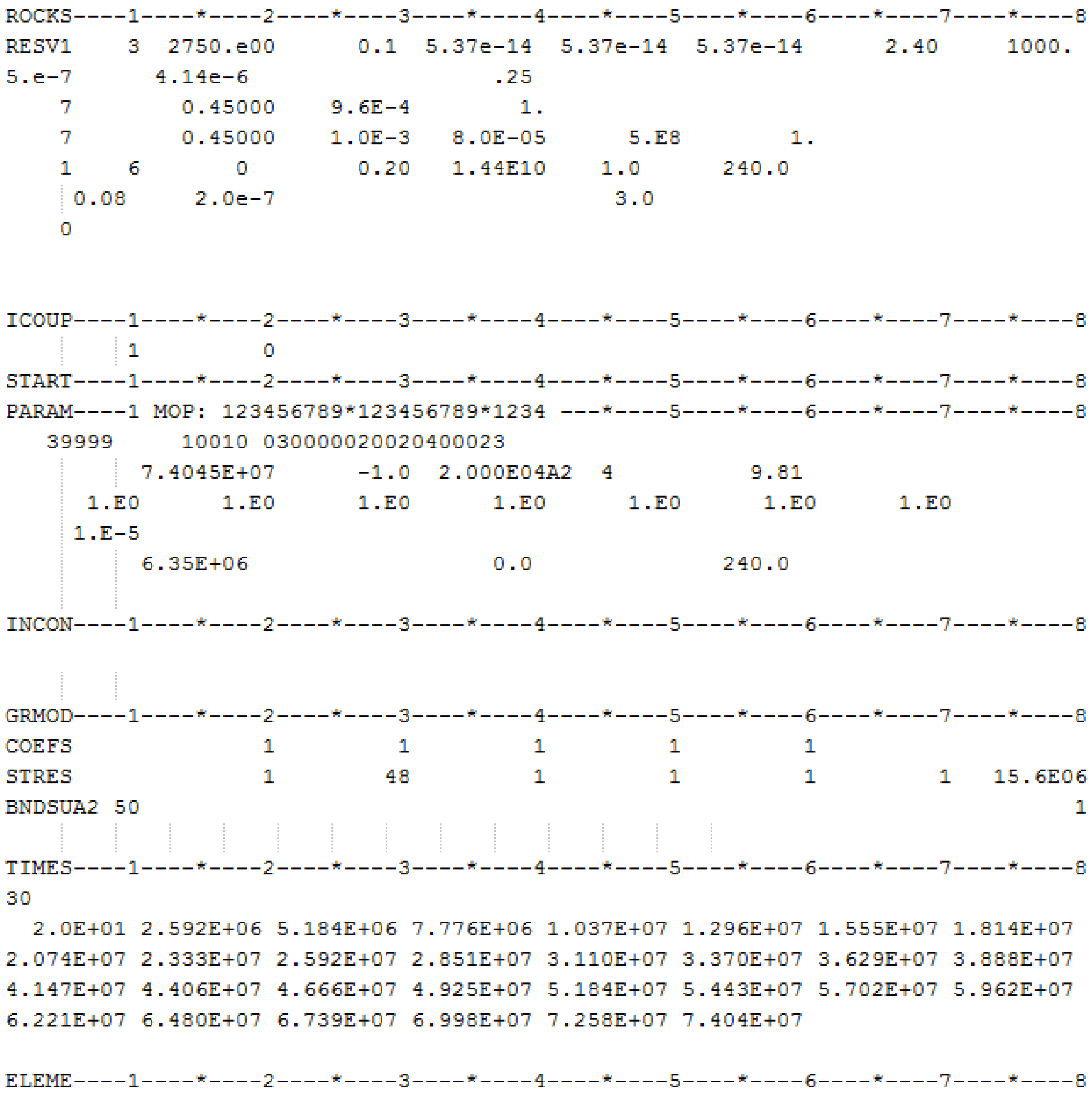
6.7.2 Simulation Setup

There are four simulation runs performed and the Table 6-7 shows the abstract information of each simulation.

Table 6-7 Simulation runs configuration

Simulation Run	Coupling	T of Injection water (°C)	Aqueous SiO2 Concentration of Injection water (ppm)	Comments
Run 1	THM	150	N/A	Without chemical coupling
Run 2	THMC	150	700	THMC base case
Run 3	THMC	100	700	Reduced Temperature

In the first run, the chemical reaction is not coupled in the simulation. The second run involves both mechanical and chemical effects. The third run reduces the injection temperature from 150°C to 100°C for THMC simulation. See the Figure 6-32 for the sample main input file for the THM simulation run.



```
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
RESV1    3  2750.e00      0.1  5.37e-14  5.37e-14  5.37e-14      2.40     1000.
5.e-7      4.14e-6                  .25
    7        0.45000    9.6E-4        1.
    7        0.45000    1.0E-3   8.0E-05      5.E8        1.
    1    6       0        0.20   1.44E10    1.0      240.0
     0.08     2.0e-7                 3.0
    0


ICOUP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
         1         0
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
PARAM----1 MOP: 123456789*123456789*1234 ---*----5----*----6----*----7----*----8
   39999     10010 030000020020400023
          7.4045E+07      -1.0  2.000E04A2  4          9.81
      1.E0      1.E0      1.E0      1.E0      1.E0      1.E0      1.E0
     1.E-5
          6.35E+06                  0.0              240.0

INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8


GRMOD----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
COEFS              1         1         1         1         1
STRES              1        48         1         1         1         1   15.6E06
BNDSUA2 50                                                                     1

TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
30
  2.0E+01 2.592E+06 5.184E+06 7.776E+06 1.037E+07 1.296E+07 1.555E+07 1.814E+07
2.074E+07 2.333E+07 2.592E+07 2.851E+07 3.110E+07 3.370E+07 3.629E+07 3.888E+07
4.147E+07 4.406E+07 4.666E+07 4.925E+07 5.184E+07 5.443E+07 5.702E+07 5.962E+07
6.221E+07 6.480E+07 6.739E+07 6.998E+07 7.258E+07 7.404E+07

ELEME----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
```

Figure 6-32 The main input file for THM simulation

The THMC simulation requires the following setting:

(1) Set ICOUP keyword to both 1 and 1 in the main input file

(2) Set the IPORERM flag, which will be used to correlated the porosity change, due to both mechanical and chemical effects, with permeability

(3) Prepare another three input files, solute.inp, chemical.inp and thermodynamic database file as example 4.

6.7.3 Simulation Results

The simulation results from the above four runs are presented at time 30 days, 0.5 year, 1 year, 1.5 years and 2 years, and the evolution of the reservoir properties can be well observed.

6.7.3.1 Simulation Run1 - THM effects

The Figure 6-33 shows the low temperature, 150 °C, propagation to the reservoir with 240°C from the injection well.

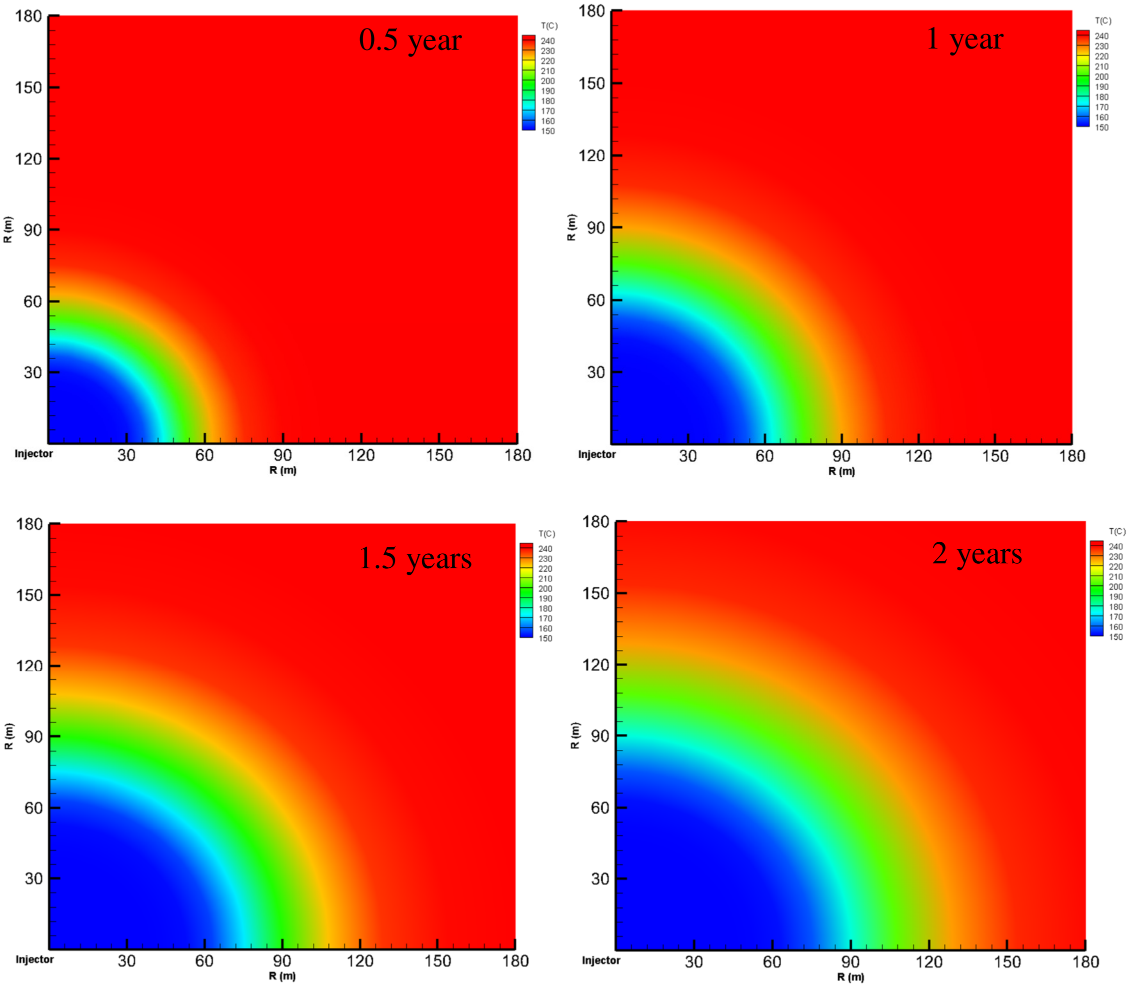


Figure 6-33 The injection water temperature propagation

The mean effective stress is subjected to change due to the pore pressure and temperature change, as shown in the Figure 6-34 for the mean effective stress evolution. The mean effective stress decrease due to the injection effects and the low effective stress propagates to the reservoir as the injection keeps going. After two years injection, the low effective stress reaches about 150m from the injector.

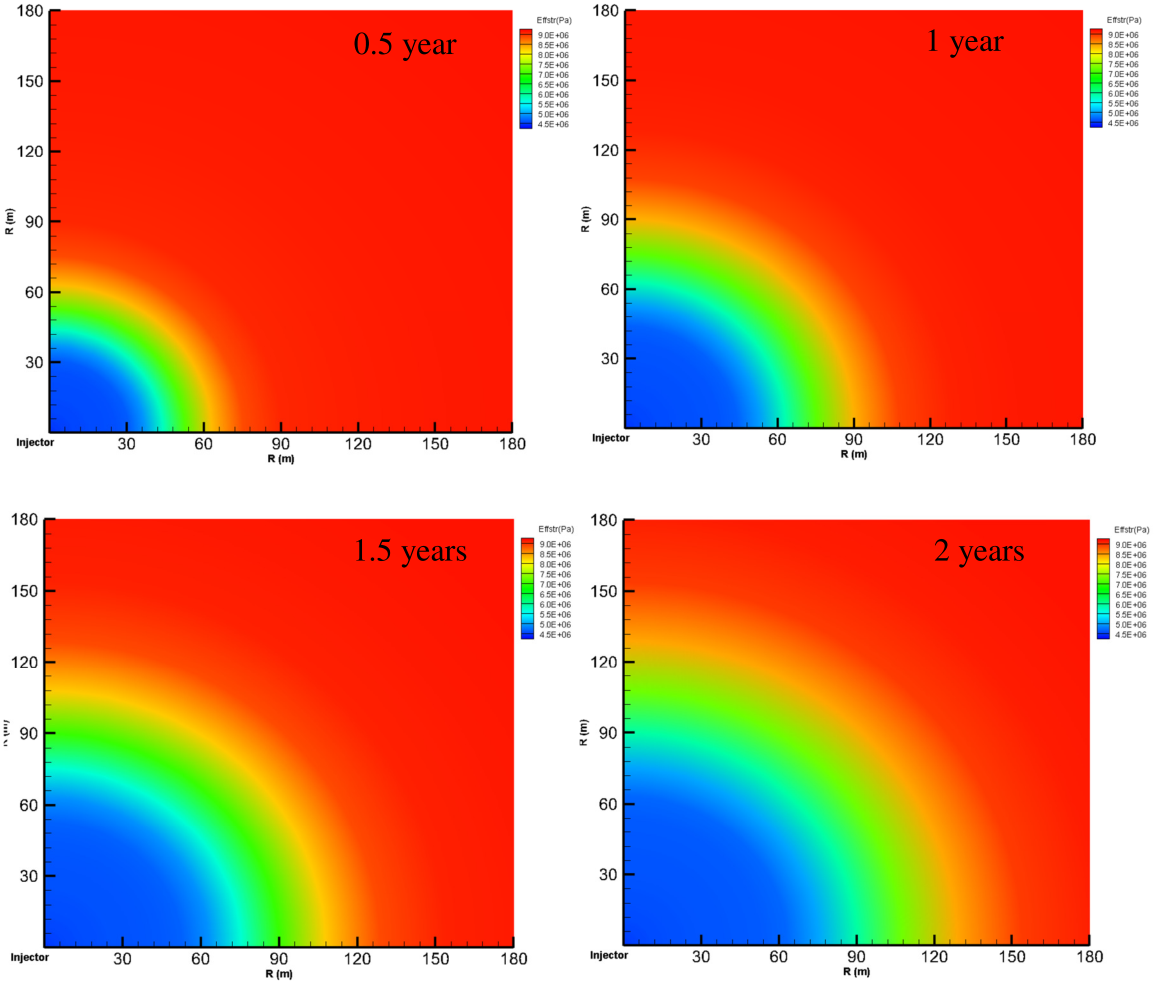


Figure 6-34 Effective mean stress evolution

The simulation also includes the porosity and permeability change due to the stress effects, and the updated porosity and permeability also feedback to affect the flow at each time step. The Figure 6-35 presents the porosity and permeability enhancement due to decrease of effective stress after 2 years injection. The porosity increases from 0.1 to 0.13 and the permeability is enhanced from initial 5.37×10-14 m2 to 1.37×10-13 m2.

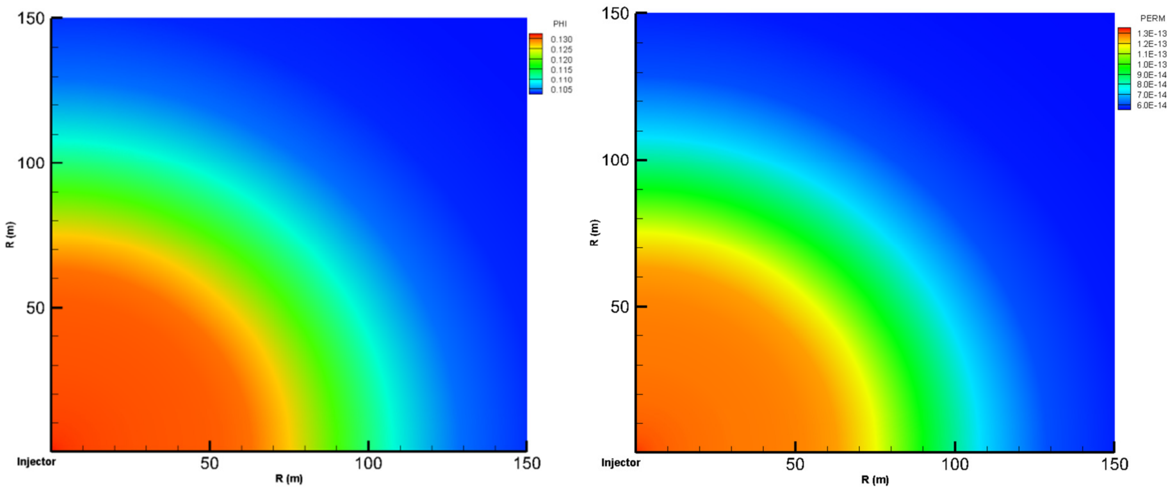


Figure 6-35 The porosity(left) and permeability(right) profile after 2 years injection

6.7.3.2 Simulation Run2 –THMC effects

Besides the mechanical effects in the run1, the chemical reaction is included in the run2. The chemical system is same as example 4 therefore we can expect the precipitation effects around the injector. The Figure 6-36 shows the precipitation effects of amorphous SiO2.

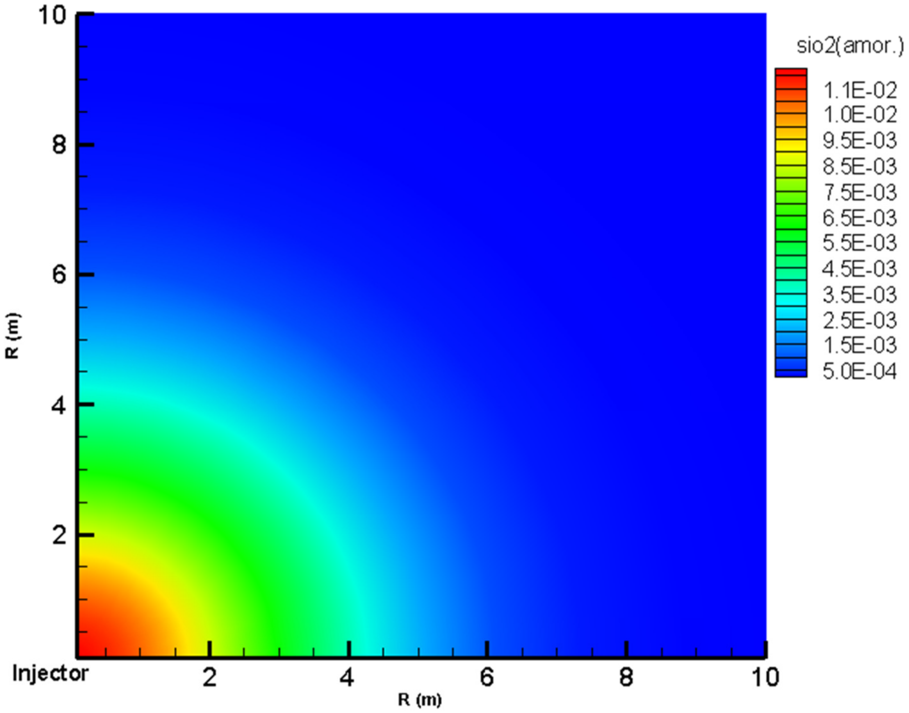


Figure 6-36 The volume fraction change of amorphous SiO2

The volume fraction change of amorphous SiO2 shows that the chemical precipitation concentrates around the wellbore and only reaches 6 meters after two years injection. The closer to the injector, the higher precipitation effects is observed. The chemical effects can be confirmed from the porosity and permeability profile figure as follow.

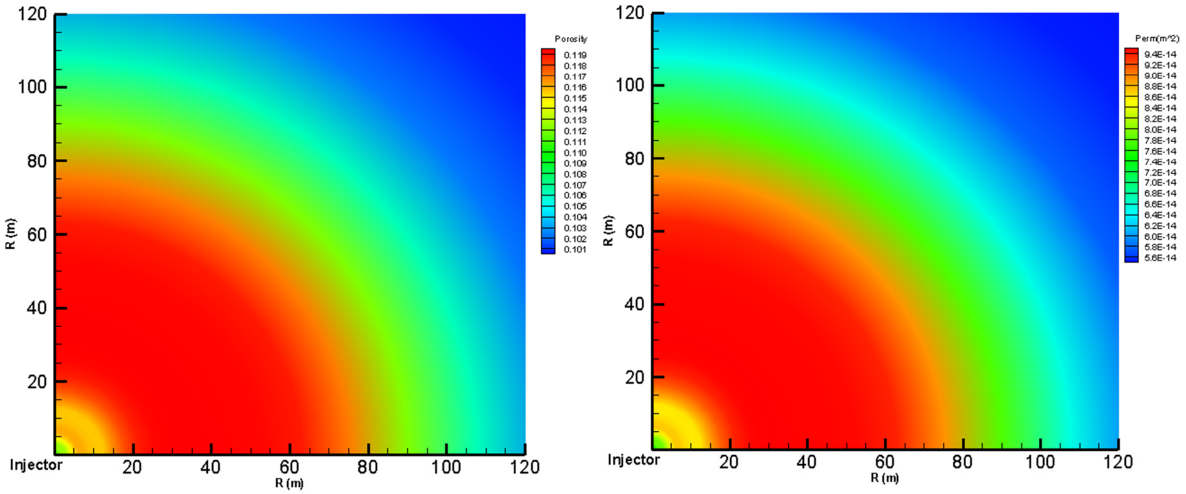


Figure 6-37 The porosity (left) and permeability(right) profile due to THMC effects after 2 years injection

The above figure shows that the highest porosity and permeability is not around wellbore, but some distance from the injector, from 20m to 80m. It is because the mechanical enhanced effects are offset by the chemical precipitation. It also explains that the highest porosity and permeability in the THMC simulation run is lower than THM run.

6.7.3.3 Simulation Run3 – THMC with lower injection temperature

If the injection temperature is lower, the effective stress will decrease more from the governing geomechanical equation. On the other hand, the lower temperature will enhance the chemical precipitation effects. See the Figure 6-38 and 6-39 for the comparisons of effective stress and SiO2 precipitation profile.

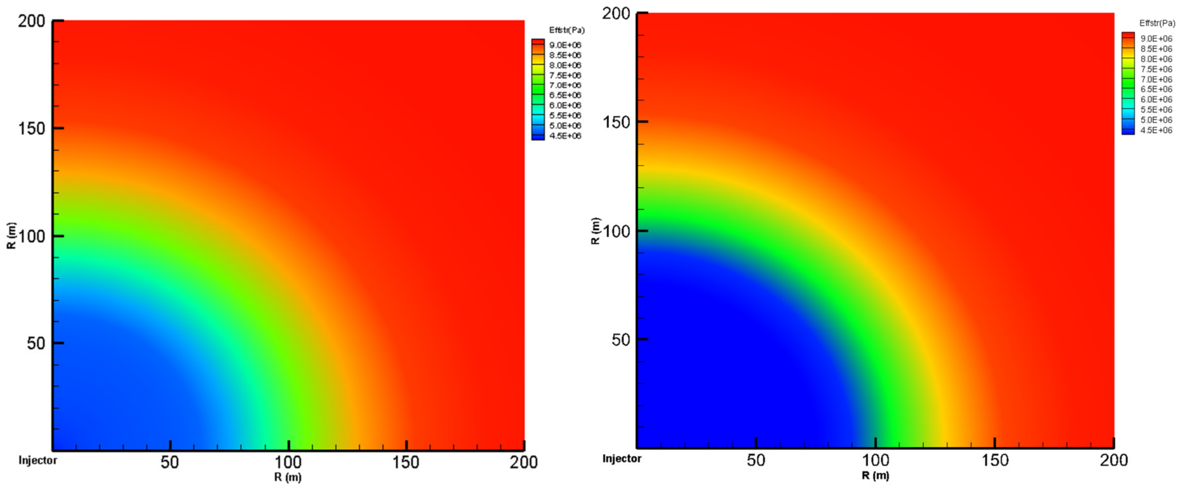


Figure 6-38 Effective stress profile for 150 °C (left) and 100 °C (right) of injection water after 2 years injection

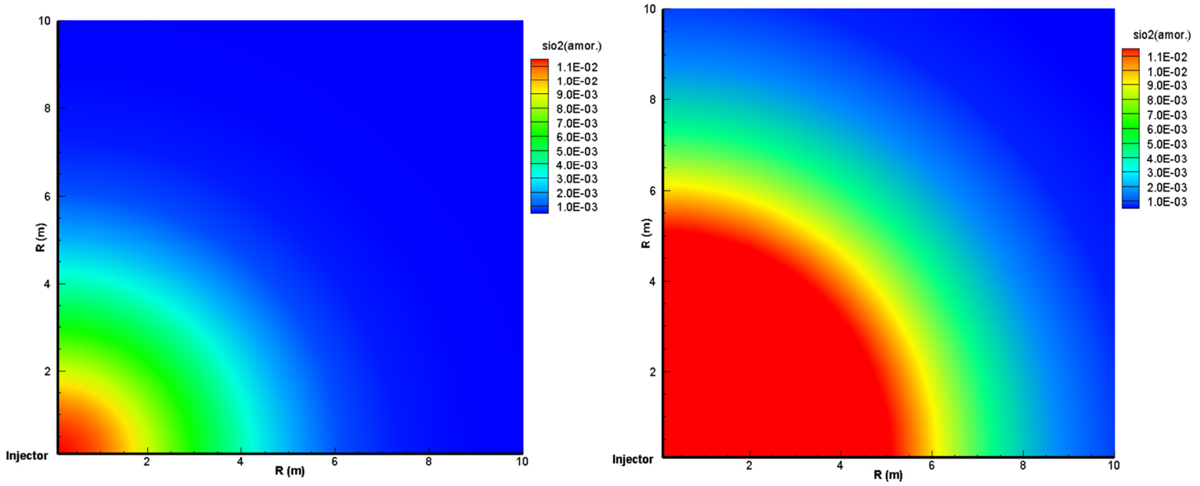


Figure 6-39 SiO2 precipitation profile for 150 °C (left) and 100 °C(right) of injection water after 2 years injection

The lower temperature leads to more decrease of mean effective stress but increase of chemical precipitation. Therefore the lower temperature has the opposite effects on the reservoir porosity and permeability change. See the Figure 6-40 and 6-41 for the porosity and permeability comparisons. Xiong et al. (2013) gave the detailed analysis on the temperature impacts on the mechanical and chemical effects.

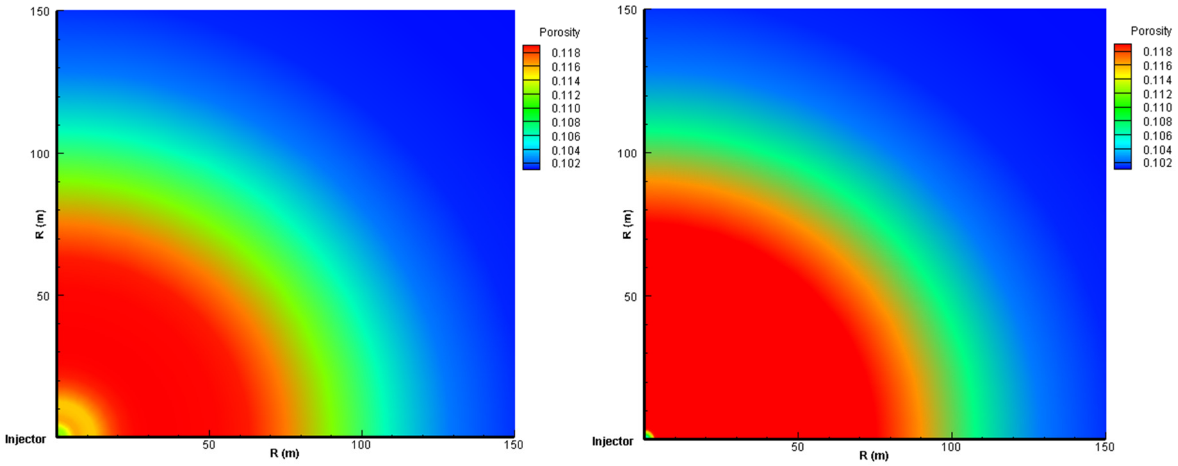


Figure 6-40 Porosity profile under THMC effects for 150 °C (left) and 100 °C(right) of injection water after 2 years injection

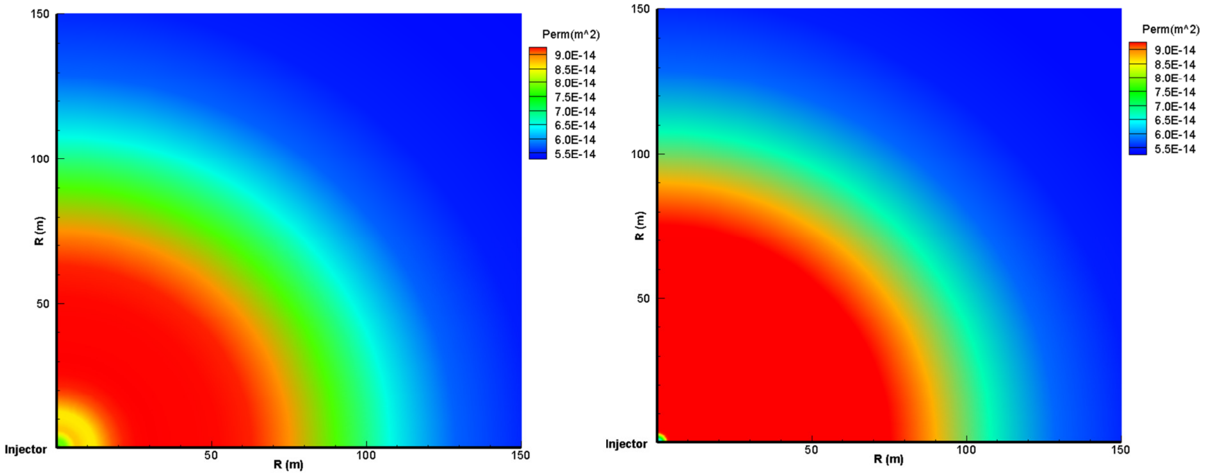


Figure 6-41 Permeability profile under THMC effects for 150 °C (left) and 100 °C (right) of water after 2 years injection

6.8 Effects of cold water injection in fractured reservoirs

Production in some geothermal reservoirs, water injection is required to replace steam or water production from the reservoirs. Number of reports indicates that cold water injection could achieve increasing water injectivity due to stress change around the injector. In this example, we demonstrated how to incorporate stress induced-permeability enhancement during cold water injection.

6.8.1 *Description*

In this example, a 2-D radial grid model represents a geothermal reservoir. The reservoir formation is fractured rock with low matrix permeability (Figure 6-42). Multiple continuum (MINC) was used to represent the formation. The reservoir is overlain by a caprock layer, modeled by porous media (single porosity). Constant pressure and temperature was imposed at the top of the model.

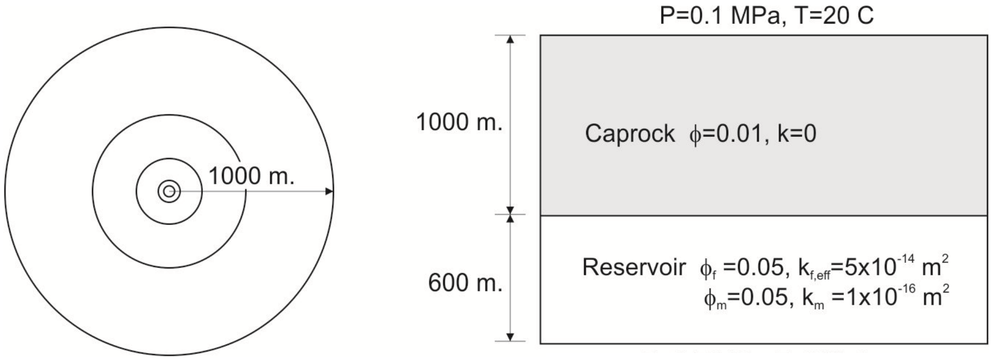


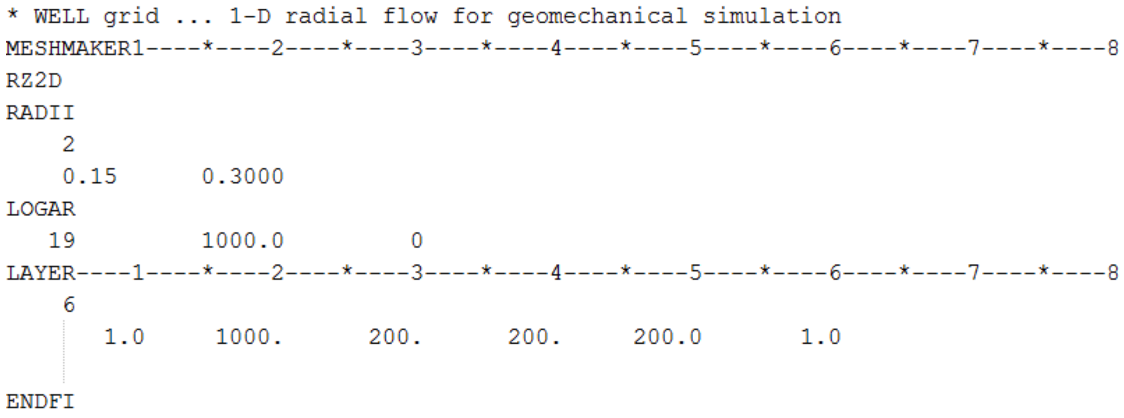
Figure 6-42 Model configuration

Table 6-8 Input parameters

Properties	**Values**
Young’s Modulus *(GPa)*	14.4
Poisson’s ratio *(dimensionless)*	0.20
Pore compressibility *(Pa^{-1})*	1×10^{-10}
Thermal expansion coefficient *($^oC^{-1}$)*	3.0×10^{-5}
Rock grain specific heat *(J/kg ºC)*	1000
Rock grain density *(kg/m^3)*	2750
Formation thermal conductivity *(W/m ºC)*	2.5

6.8.2 Numerical simulation setup

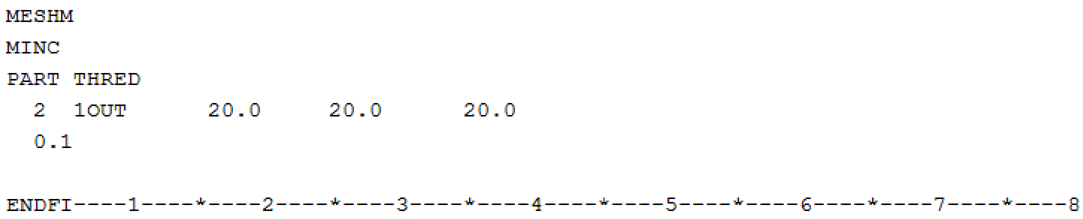
We first generated the mesh data. In this problem, the primary mesh was constructed as a 2-D radial grid system where the mesh was logarithmically distributed in radial direction (Figure 6-43). This process generated mesh data in “MESH” file. Then, the reservoir layers were subdivided into fracture and matrix mesh, where fracture volume is 10% of the primary mesh volume (Figure 6-44). Noted that, the caprock layer was not refined and the volume was the same as the primary mesh. The combined model of single- and multiple-porosity was achieved by specifying the refinement flag at the end of mesh data (Figure 6-45); only the elements with the flag of “0” is refined to fracture and matrix elements. This process generated mesh data in “MINC” file.



```
* WELL grid ... 1-D radial flow for geomechanical simulation
MESHMAKER1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
RZ2D
RADII
    2
    0.15      0.3000
LOGAR
   19        1000.0         0
LAYER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    6
       1.0     1000.      200.      200.     200.0       1.0

ENDFI
```

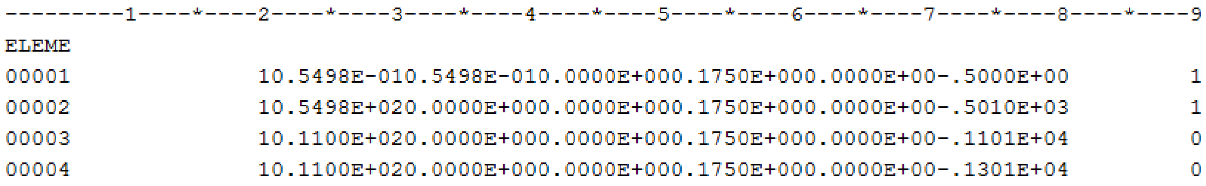
Figure 6-43 Primary mesh generation input



```
MESHM
MINC
PART THRED
  2  1OUT      20.0     20.0      20.0
  0.1

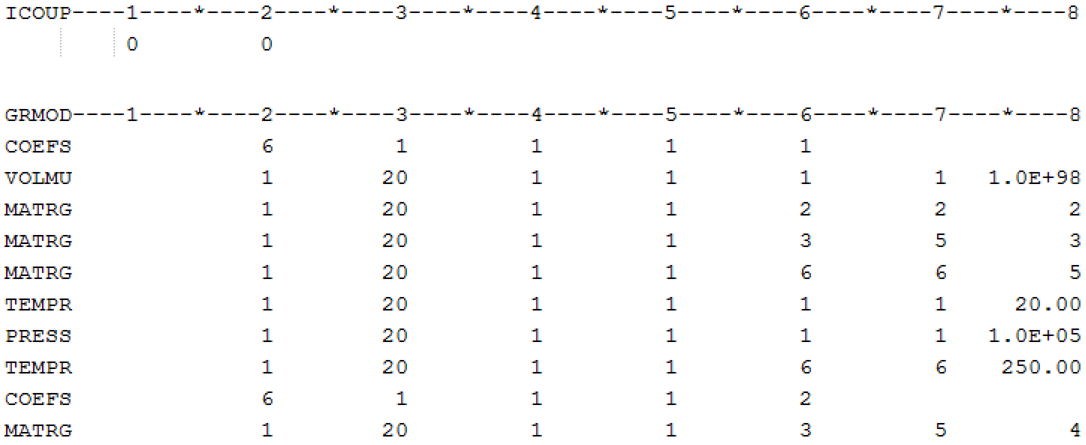
ENDFI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
```

Figure 6-44 Input for mesh division from primary mesh to double porosity mesh



```
---------1----*----2----*----3----*----4----*----5----*----6----*----7----*----8----*----9
ELEME
00001              10.5498E-010.5498E-010.0000E+000.1750E+000.0000E+00-.5000E+00         1
00002              10.5498E+020.0000E+000.0000E+000.1750E+000.0000E+00-.5010E+03         1
00003              10.1100E+020.0000E+000.0000E+000.1750E+000.0000E+00-.1101E+04         0
00004              10.1100E+020.0000E+000.0000E+000.1750E+000.0000E+00-.1301E+04         0
```

Figure 6-45 Primary mesh data as input for double porosity mesh

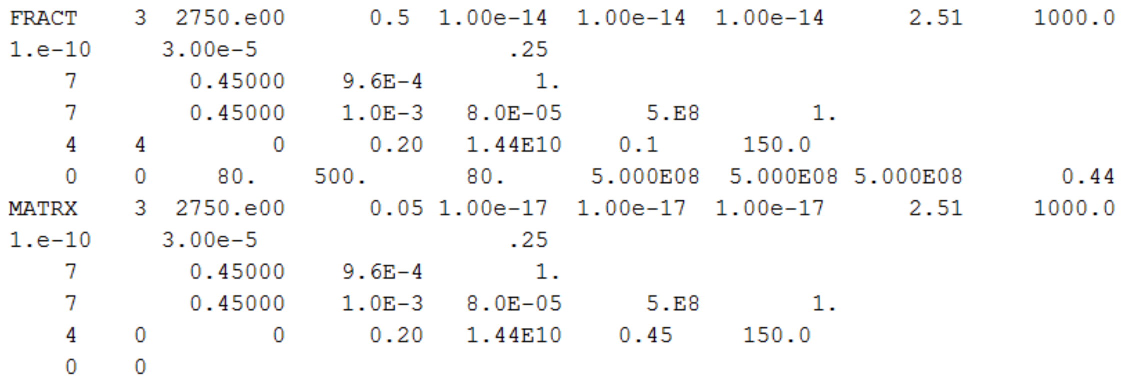


```
ICOUP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
         0         0

GRMOD----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
COEFS              6         1         1         1         1
VOLMU              1        20         1         1         1         1   1.0E+98
MATRG              1        20         1         1         2         2         2
MATRG              1        20         1         1         3         5         3
MATRG              1        20         1         1         6         6         5
TEMPR              1        20         1         1         1         1     20.00
PRESS              1        20         1         1         1         1   1.0E+05
TEMPR              1        20         1         1         6         6    250.00
COEFS              6         1         1         1         2
MATRG              1        20         1         1         3         5         4
```

Figure 6-46 ICOUP and GRMOD data for reservoir initialization

Then, the model was initialized by imposing constant temperature of 250 °C at the bottom layer and constant pressure of 0.1MPa and temperature of 20 °C at the top layer, which represents surface condition. We used "GRMOD" keyword to assign the specific condition including pressure, temperature, rock unit, and boundary flag (Figure 6-46). The model was run without stress and chemical reaction calculations, indicated under "ICOUP" keyword (Figure 6-46), until it reached thermodynamics equilibrium. Then, the 'SAVE' file which is the results from the initialization was renamed to 'INCON' which would be used as the initial condition for the next runs.



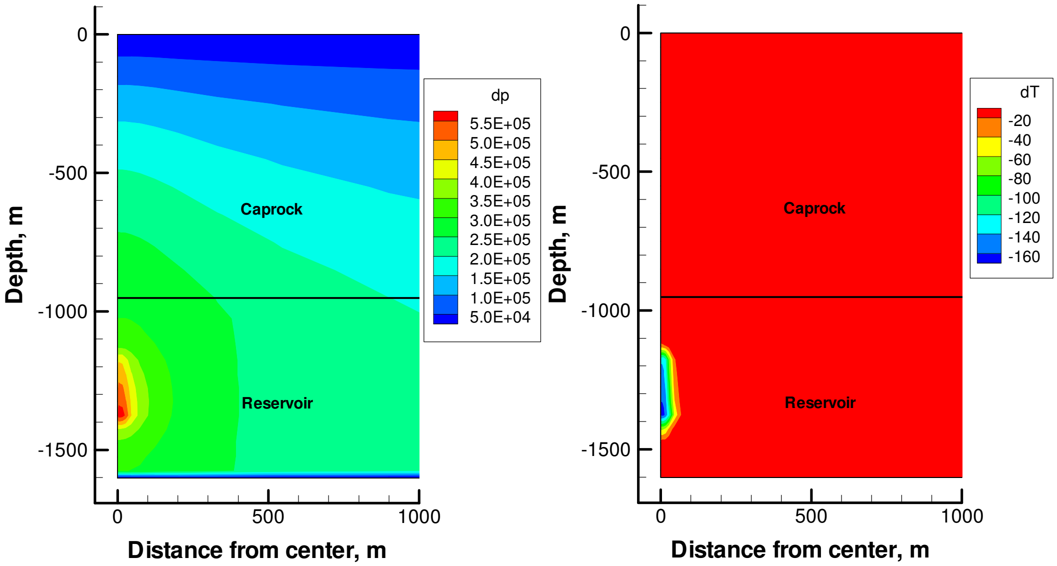
```
FRACT    3  2750.e00       0.5 1.00e-14  1.00e-14  1.00e-14      2.51     1000.0
1.e-10     3.00e-5                  .25
    7        0.45000    9.6E-4        1.
    7        0.45000    1.0E-3   8.0E-05      5.E8        1.
    4    4         0      0.20   1.44E10    0.1      150.0
    0    0     80.    500.       80.      5.000E08  5.000E08 5.000E08       0.44
MATRX    3  2750.e00      0.05 1.00e-17  1.00e-17  1.00e-17      2.51     1000.0
1.e-10     3.00e-5                  .25
    7        0.45000    9.6E-4        1.
    7        0.45000    1.0E-3   8.0E-05      5.E8        1.
    4    0         0      0.20   1.44E10    0.45     150.0
    0    0
```

Figure 6-47 ROCKS data for fracture and matrix continuum

The permeability enhancement around the injector is arguably dominated by that of fractures. Thus, the fracture permeability was set as stress sensitive permeability using Ostensen (1986) correlation (Eq. 2.56) while the matrix permeability was constant. Detailed fractures and matrix rock parameters are shown in Figure 6-47. Cold water was injected into the reservoirs for 2 years.

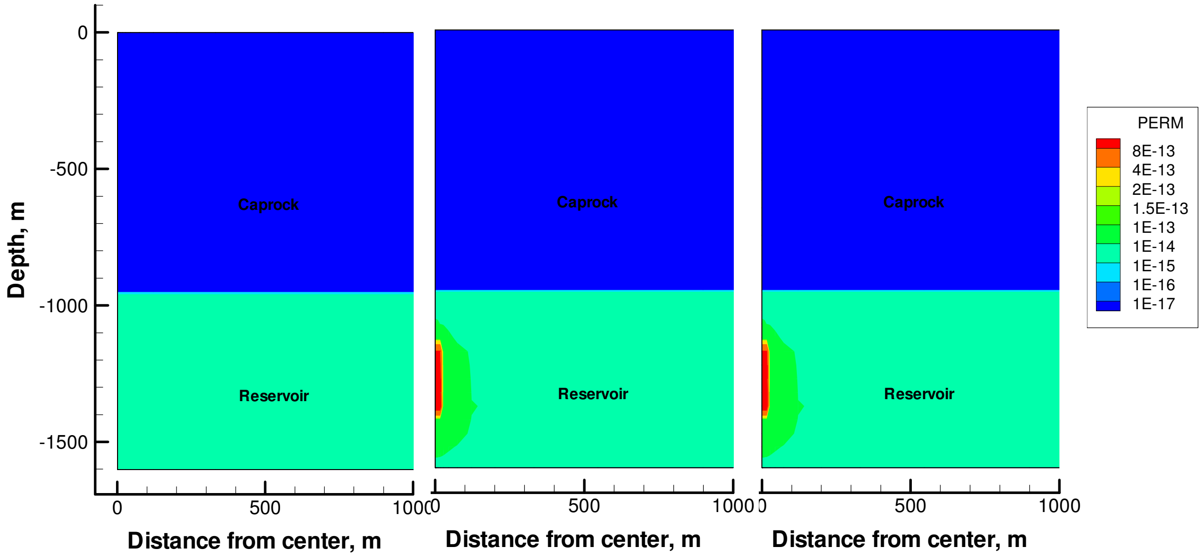
6.8.3 Simulation Results

After two years of a constant rate cold-water injection, the pressure propagated deep into the reservoir (Figure 6-48a) while the temperature change occurred around the injector (Figure 6-48b). As a result, the effective stress was reduced and the permeability was increased (Figure 6-49). Two additional simulations were run to investigate the effect of pressure- and temperature-induced permeability enhancement. Pressure-induced permeability was minimal while the temperature-induced stress dominated the overall permeability enhancement. Figure 6-49 shows permeability profile after two years of injection; and Figure 6-50 shows the bottom hole pressure profile where the pressure decreased in the case of temperature and combined pressure temperature induced permeability because the permeability increase caused reduction in required pressure.



(a) (b)

Figure 6-48 Simulation results after 2 years of injection: (a) Pressure and (b) Temperature changes. The pressure change propagates away from the injector while the temperature change occurs around the injector.



(a) (b) (c)

Figure 6-49 Permeability profiles after 2 years of injection, where the stress change was induced by: (a) Pressure, (b) Temperature, and (c) Pressure and temperature changes. The temperature-induced stress significantly affects the permeability enhancement while the pressure-induced stress has minimal effect on permeability around the injector.

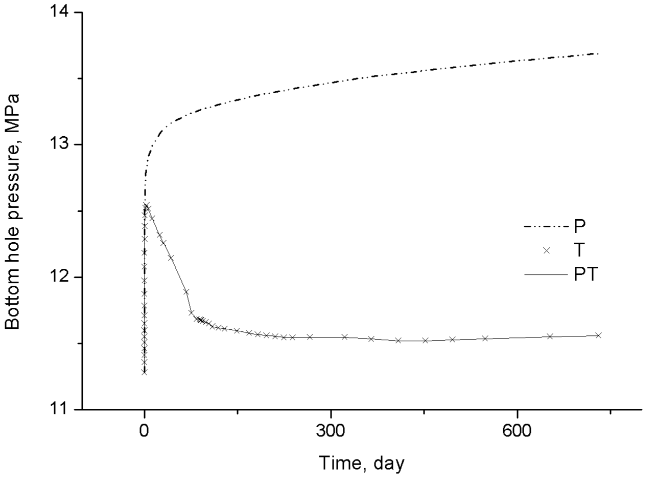


Figure 6-50 The injector bottomhole pressure profiles, where the stress change was induced by: Pressure (p), Temperature (T), and Pressure and temperature changes (PT). The bottomhole pressure is decreased in both (T) and (PT) cases because the permeability enhancement around the injector.

7 CONCLUSIONS

We present a fully-coupled fluid flow and geomechanics, and sequentially coupled reactive geochemistry simulator (TOUGH2-EGS) for simulating multiphase flow, heat transfer, rock deformation, and chemical reactions in porous and fractured media. The fluid and heat flow formulation is based on the framework of TOUGH2/EOS3. 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 when needed. Primary variables in TOUGH2-EGS are pressure, air mass fraction (or gas saturation), 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 chemical reaction module of TOUGHREACT framework is implemented into the THM model.

Our geomechanical and geochemical models are verified against analytical solutions and other numerical simulators in several test cases. The one-dimensional consolidation in porous media (example 1), one-dimensional heat conduction in deformation media (example 2), two-dimensional Mandel's problem (example 3) are verified against analytical solutions. The mineral precipitation case (example 4) and heat sweep case (example 5) are verified against two reservoir simulators: CMG-STAR and TOUGHREACT. The Geyser field case (example 6) demonstrates the field scale application capabilities of TOUGH2-EGS, and the THMC simulation for injection well (example 7) shows the coupling process for both geomechanical and geochemical effects. The last example (example 8) illustrates the simulations of the multi porosity systems of a fractured reservoir with TOUGH2-EGS.

Compared with other numerical modeling codes for geotechnical analysis of soil, rock, and structural support, such as FLAC3D and ECLIPSE, 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 geothermal reservoirs for analyzing multiphase fluid, heat flow, rock deformation and chemical reactions.

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NOMENCLATURE

A_j	Cross area of grid j, m^2.
A_{ij}	Cross area between grid i and j, m^2.
C_R	Heat conductivity, $W K^{-1} m^{-1}$.
C_{ϕ}	Pore compressibility, Pa^{-1}.
c_s	Specific heat capacity of rock, $Jkg^{-1}°C^{-1}$.
c_t	Bulk total compressibility, Pa^{-1}.
D_T	Thermal diffusivity, m^2s^{-1}.
E	Young modulus, Pa.
F	Body force per area, Pa.
F^{κ}	Mass or energy flux terms due to advective processes, W m^{-1}.
F_l	l-direction body force (gravity), Pa m^{-1}.
g	Gravitational acceleration constant, m s^{-2}.
h	Total column height, m.
h_{β}	Specific enthalpy in phase β, J kg^{-1}.
k	Absolute permeability, m^2.
k_T	Heat conductivity of rock $Wm^{-1}°C^{-1}$.
K	Bulk modulus, Pa.
$k_{r\beta}$	Relative permeability to phase.

M	Biot’s modulus, Pa.
M^{κ}	Accumulation terms of the components and energy, kg m^{-3}.
M_n^{κ}	Accumulation terms of the components and energy of grid n, kg m^{-3}.
$\boldsymbol{n}$	Normal vector on surface element, dimensionless.
t	Time, s.
T	Temperature, °C or K.
T_{ref}	Reference temperature, °C or K.
u_{β}	Darcy velocity in phase, m s^{-1}.
U_{β}	Internal energy of phase per unit mass, J kg^{-1}.
V_n	Volume of the nth grid cell, m^3.
P	Pressure. Pa.
P_0	Incremental pressure due to load, Pa.
P_c	Capillary pressure. Pa.
P_{c0}	Reference capillary pressure. Pa.
P_{β}	Fluid pressure of phase , Pa.
q^{κ}	Source/sink terms for mass or energy components, kg $m^{-3}s^{-1}$.
q_n^{κ}	Source/sink terms for mass or energy components of grid *n*, kg $m^{-3}s^{-1}$.
R_n^{κ}	Residual of component κ for grid block n, kg s^{-1}.
R_n^4	Residual of stress for grid block n, Pa m^{-2}.

S	Storage coefficient, Pa^{-1}.
S_l	Saturation of liquid phase, dimensionless.
S_β	Saturation of phase, dimensionless.
T_b	Constant temperature boundary, °C.
T_i	Initial temperature, °C.
w	Vertical displacement of the upper surface, m.
x^t	Primary variables at time t, pressure, temperature, air fraction, or stress.
X_β^κ	Mass fraction of component in fluid phase, dimensionless.
V_b	Bulk volume, m^3.
z	Distance along-column coordinate, m.

Greek Letters

α	Biot's coefficient, dimensionless.
α_P	Biot's coefficient, dimensionless.
α_T	Biot's coefficient, dimensionless.
β	Linear thermal expansion coefficient, °C^{-1}.
μ_β	Viscosity, Pa.s.
μ_f	Fluid viscosity, Pa.s..
ϕ	Porosity, dimensionless.
λ	Thermal conductivity, $W\,K^{-1}\,m^{-1}$.

λ_s	Lame’s constant, Pa.
ε_{ll}	Strain components, l=x, y, z, dimensionless.
ε_{ls}	Strain components, ls=xy, yz, zx, dimensionless.
ε_{il}	Strain components, j=x, y, z, l=x, y, z, dimensionless.
ε_v	Volumetric strain, dimensionless.
$\overline{\overline{\varepsilon}}$	Strain tensor, dimensionless.
$\overline{u}$	Displacement vector, m.
u_l	Displacement component, l=x, y, z, m.
ν	Poisson’s ratio of rock, dimensionless.
ν_u	Undrained Poisson’s ratio of rock, dimensionless.
σ'	Effective stress, Pa.
σ_{ex}	External load per area at the top column, Pa.
ρ_{tot}	Density of rock, kg m^{-3}.
ρ_R	Density of rock grain. kg m^{-3}.
ρ_β	Density of phase, kg m^{-3}.
Γ	Perimeter of the cross-section, m.
Γ_n	Area of closed surface, m^2.

APPENDIX A. POROSITY-STRESS CORELATION OPTIONS

IRPOPT=0 Constant porosity

IRPOPT=1 Equation 2.49 from Rutqvist et al. (2002b), usually used with IRKOPT =1

RCKPAR(1) = ϕ_r

RCKPAR(2) = a

IRPOPT= 2 Equation 2.52 from Rutqvist et al. (2002), usually used with IRKOPT=2

RCKPAR(1) = $b_{1,0}$

RCKPAR(2) = $\Delta b_{1,0}$

RCKPAR(3) = $b_{2,0}$

RCKPAR(4) = $\Delta b_{2,0}$

RCKPAR(5) = $b_{3,0}$

RCKPAR(6) = Δb_3

RCKPAR(7) = d

IRPOPT = 3 Equation 2.54 from McKee et al. (1988).

IRPOPT = 4 Slightly compressible rock and thermal expansion.

$$\phi = \phi_0 \left(1 + c_p \left(P - P_{ref}\right) + 3\beta \left(T - T_{ref}\right)\right)$$

c_p is pore compressibility and β is linear thermal expansion coefficient

RCKPAR(1) = P_{ref}

RCKPAR(2) = T_{ref}

IRPOPT = 5 Equation 2.61

APPENDIX B. PERMEABILITY-STRESS CORELATION OPTIONS

IRKOPT = 0 Constant permeability

IRKOPT = 1 Equation 2.49 from Rutqvist et al. (2002), usually used with IRPOPT =1

RCKPAR(5) = c

IRKOPT = 2 Equation 2.52 from Rutqvist et al. (2002), usually used with IRPOPT=2

RCKPAR(1) = $b_{1,0}$

RCKPAR(2) = $\Delta b_{1,0}$

RCKPAR(3) = $b_{2,0}$

RCKPAR(4) = $\Delta b_{2,0}$

RCKPAR(5) = $b_{3,0}$

RCKPAR(6) = Δb_3

RCKPAR(7) = d

IRKOPT = 3 Equation 2.55, Carman-Kozeny equation

IRKOPT = 4 Equation 2.56 from Ostensen (1986)

RCKPAR(5) = x-direction σ'^*

RCKPAR(6) = y-direction σ'^*

RCKPAR(7) = z-direction σ'^*

RCKPAR(8) = n

IRKOPT = 5 Equation 2.57, Verma and Pruess (1988)

RCKPAR(6) = k_r/k_0

RCKPAR(7) = ϕ_r/ϕ_0

RCKPAR(8) = n

APPENDIX C. RELATIVE PERMEABILITY FUNCTIONS

IRP = 1 Linear functions

k_{rl} increases linearly from 0 to 1 in the range

RP(1) $\leq S_l \leq$ RP(3);

k_{rg} increases linearly from 0 to 1 in the range

RP(2) $\leq S_g \leq$ RP(4)

Restrictions: RP(3) > RP(1); RP(4) > RP(2).

IRP = 2 $k_{rl} = S_l$**RP(1)

k_{rg} = 1.

IRP = 3 Corey's curves (1954)

$$k_{rl} = \hat{S}^4$$

$$k_{rg} = \frac{\left(1-\hat{S}\right)^2}{\left(1-\hat{S}^2\right)}$$

where $$\hat{S} = \frac{\left(S_l - S_{lr}\right)}{\left(1 - S_{lr} - S_{gr}\right)}$$

with S_{lr} = RP(1); S_{gr} = RP(2)

Restrictions: RP(1) + RP(2) < 1

IRP = 4 Grant's curves (Grant, 1977)

$$k_{rl} = \hat{S}^4$$

$$k_{rg} = 1 - k_{rl}$$

where $\hat{S} = \frac{(S_l - S_{lr})}{(1 - S_{lr} - S_{gr})}$

with S_{lr} = RP(1); S_{gr} = RP(2)

Restrictions: RP(1) + RP(2) < 1

IRP = 5 All phases perfectly mobile

$k_{rg} = k_{rl} = 1$ for all saturations; no parameters

IRP = 6 Functions of Fatt and Klikoff (1959)

$$k_{rl} = \left(S^*\right)^3$$

$$k_{rg} = \left(1 - S^*\right)^3$$

where $S^* = \frac{(S_l - S_{lr})}{(1 - S_{lr})}$

with S_{lr} = RP(1).

Restriction: RP(1) < 1.

IRP = 7 van Genuchten-Mualem model (Mualem, 1976; van Genuchten, 1980)

$$k_{rl} = \begin{cases} \sqrt{S^*}\left\{1 - \left(1 - [S^*]^{1/\lambda}\right)^{\lambda}\right\}^2 & if S_l < S_{ls} \\ 1 & if S_l \geq S_{ls} \end{cases}$$

Gas relative permeability can be chosen as one of the following three forms, the second of which is due to Corey (1954)

$$k_{rg} = \begin{cases} 1 - k_{rl} \; if \; S_{gr} = 0 \; and \; RP(4) = RP(5) = 0 \\ \left(1 - \hat{S}\right)^2 \left(1 - \hat{S}^2\right) \; if \; S_{gr} > 0 \; and \; RP(4) > 0 \; and \; RP(5) = 0 \\ (1 - S^*)^2 (1 - S^{*\frac{2+\gamma}{\gamma}}, r = \dfrac{\lambda}{1-\lambda} \; if \; S_{gr} = 0 \; and \; RP(5) > 0 \end{cases}$$

subject to the restriction $0 \le k_{rl}, k_{rg} \le 1$

Here, $S^* = \dfrac{(S_l - S_{lr})}{(S_{ls} - S_{lr})}$, $\hat{S} = \dfrac{(S_l - S_{lr})}{(1 - S_{lr} - S_{gr})}$

Parameters: RP(1) = λ

RP(2) = S_{lr}

RP(3) = S_{ls}

RP(4) = S_{gr}

RP(5) = switching parameter

Notation: Parameter λ is m in van Genuchten's notation, with m = 1 - 1/n;
Parameter n is often written as β.

IRP = 8 Function of Verma et al. (1985)

$$k_{rl} = \hat{S}^3$$

$$k_{rg} = A + B\hat{S} + C\hat{S}^2$$

where $$\hat{S} = \frac{(S_l - S_{lr})}{(S_{ls} - S_{lr})}$$

Parameters as measured by Verma et al. (1985) for steam-water flow in an unconsolidated sand:

S_{lr} = RP(1) = 0.2

S_{ls} = RP(2) = 0.895

A = RP(3) = 1.259

B = RP(4) = -1.7615

C = RP(5) = 0.5089

IRP = 9, 10 ECM function (Pruess and Tsang, 1994)

These two options are the original effective continuum model (ECM), which use a threshold liquid saturation concept, defined as

$$S_{th} = \phi_m/(\phi_m + \phi_f)$$

where both ϕ_m and ϕ_f are void fractions or porosities for matrix and fractures respectively, defined in terms of the bulk volume of formation.

The only difference between IRP = 9 and = 10 is that option of IRP = 9 handles isotropic permeability cases and IRP = 10 handles anisotropic permeability scenarios. In general, the two ECM relative permeability functions need (1) matrix continuum and fracture continuum permeability and (2) a special capillary function (defined in ICP = 8 in Appendix D).

It is assumed that PER(i) and PERF(i), input in ROCKS, are absolute continuum permeability of matrix and fractures (i = 1, 2, 3), respectively, along the three principal axes or directions, as defined in CONNE. See the following table for parameter definition.

Table C-1. Definition of parameters for with ECM functions for IRP=10

IRP=	9	for ECM option in isotropic fracture systems.
IRP=	10	for ECM option in anisotropic fracture systems.
RP(1)=	M_m	of van Genuchten's function for matrix.
RP(2)=	S_{lr}	residual liquid saturation in matrix.
RP(3)=	M_f	of van Genuchten's function for fractures.
RP(4)=	S_{lr}	residual liquid saturation in fractures.
RP(5)=	k_f/k_m	ratio of fracture and matrix permeabilities, used only for isotropic properties of fracture-matrix systems.
RP(6)=	S_{th}	threshold liquid saturation.
RP(7)=	$1-\phi_f$	f is fracture porosity.

IRP = 11 Generalized ECM function (Wu et al. 1996; Wu 2000)

This is a generalized ECM formulation, which relies only on thermodynamic equilibrium assumption for fracture and matrix systems (Wu, 2000). The generalized ECM relative permeability functions need (1) matrix continuum and fracture continuum permeability and (2) a special capillary function (defined in ICP = 9 in Appendix D). It is assumed that PER(i) and PERF(i), input in ROCKS, are absolute continuum permeability of matrix and fractures (i = 1, 2, 3), respectively, along the three principal axes or directions, as defined in CONNE. The following table defines the parameters for the ECM relative permeability function.

Table C-2. Definition of parameters for with ECM functions for IPR =11

IRP=	11	For generalized ECM option.
RP(1)=	M_m	Of van Genuchten's function for matrix.
RP(2)=	S_{lr}	Residual liquid saturation in matrix.
RP(3)=	M_f	Of van Genuchten's function for fractures.
RP(4)=	Slr	Residual liquid saturation in fractures.
RP(5)=	> 0 krg = 1.0 - krl <0 using Corey's function for krg.	
RP(6)=	S_{gr}	Residual gas saturation in matrix.
RP(7)=	ϕf	Fracture continuum porosity.

IRP = 12 Generalized Power Law

$$k_{rl} = \left(\frac{S_l - S_{l,min}}{S_{l,max - s_{l,min}}}\right)^{n_1}$$

$$k_{rg} = \left(\frac{S_g - S_{g,min}}{S_{g,max - s_{g,min}}}\right)^{n_g}$$

with $S_{l,min}$ = RP(1), Sl,max = RP(2), n1 =RP(3), Sg,min=RP(4), Sg,max = RP(5), ng=RP(6)

APPENDIX D. CAPILLARY PRESSURE FUNCTIONS

ICP = 1 Linear function

$$P_{cap} = \begin{cases} -CP(1) & for\ S_l \leq CP(2) \\ 0 & for\ S_l \leq CP(2) \\ -CP(1)\frac{CP(3) - S_L}{CP(3) - CP(2)} & for\ CP(2) < S_l < CP(3) \end{cases}$$

Restriction: CP(3) > CP(2).

ICP = 2 Function of Pickens et al. (1979)

$$P_{cap} = -P_0 \left\{ ln \left[\frac{A}{B} \left(1 + \sqrt{1 - \frac{B^2}{A^2}} \right) \right] \right\}^{\frac{1}{x}}$$

with

$A = (1 + S_l/S_{l0})(S_{l0} - S_{lr})/(S_{l0} + S_{lr})$

$B = 1 - S_l/S_{l0}$

where

$P_0 = CP(1)$ $S_{lr} = CP(2)$ $S_{l0} = CP(3)$ $x = CP(4)$

Restrictions: $0 < CP(2) < 1 \leq CP(3)$; $CP(4) \neq 0$

ICP = 3 TRUST capillary pressure (Narasimhan et al., 1978)

$$P_{cap} = \begin{cases} -P_e - P_0 \left(\frac{1 - S_l}{S_l - S_{lr}} \right)^{\frac{1}{\eta}} & for\ S_l < 1 \\ 0 & for\ S_l < 1 \end{cases}$$

where

$P_0 = CP(1)$ $S_{lr} = CP(2)$ □ $\eta = CP(3)$ $P_e = CP(4)$

Restrictions: $CP(2) \geq 0$; $CP(3) \neq 0$

ICP = 4 Milly’s function (Milly, 1982)

$$P_{cap} = -97.783 \text{ x } 10^A$$

With

$$A = 2.26 \left(\frac{0.371}{S_l - S_{lr}} - 1 \right)^{1/4}$$

where $S_{lr} = CP(1)$

Restriction: CP(1) $\geq$ 0.

ICP = 6 Leverett's function (Leverett, 1941; Udell and Fitch, 1985)

$$P_{cap} = -P_0 \sigma(T) f(S_l)$$

with

$\sigma(T)$ - surface tension of water (supplied internally in TOUGH2-EGS)

$f(S_l) = 1.417 (1 - S^*) - 2.120 (1 - S^*)^2 + 1.263 (1 - S^*)^3$

where

$S^* = (S_l - S_{lr})/(1 - S_{lr})$

Parameters: P_0 = CP(1) S_{lr} = CP(2)

Restriction: $0 \leq$ CP(2) < 1

ICP = 7 van Genuchten function (van Genuchten, 1980)

$$P_{cap} = -P_0 \left[\left(S^* \right)^{-\frac{1}{\lambda}} - 1 \right]^{1-\lambda}$$

subject to the restriction

$$-P_{\max} \leq P_{cap} \leq 0$$

Here,

$$S^* = \left(S_l - S_{lr} \right) / \left(S_{ls} - S_{lr} \right)$$

Parameters: CP(1) = $\lambda = 1 - 1/n$

CP(2) = S_{lr} (should be chosen smaller than the corresponding parameter in the relative permeability function; see note below.)

$CP(3) = 1/P_0$

$CP(4) = P_{max}$

$CP(5) = S_{ls}$

$CP(6) = \gamma$

Notation: Parameter λ is m in van Genuchten's notation, with $m = 1 - 1/n$; parameter n is often written as β.

Note on parameter choices: In van Genuchten's derivation (1980), the parameter S_{lr} for irreducible water saturation is the same in the relative permeability and capillary pressure functions. As a consequence, for $S_l \rightarrow S_{lr}$ we have $k_{rl} \rightarrow 0$ and $P_{cap} \rightarrow -\infty$, which is unphysical because it implies that the radii of capillary menisci go to zero as liquid phase is becoming immobile (discontinuous). In reality, no special capillary pressure effects are expected when liquid phase becomes discontinuous. Accordingly, we recommend to always choose a smaller S_{lr} for the capillary pressure as compared to the relative permeability function.

ICP = 8 ECM function (Pruess and Tsang, 1994)

This ECM capillary function should be used with Option IRP=9 or 10 of ECM relative permeability functions. Table D-1 lists the definition of the related parameters.

Table D-1. Definition of parameters for ICP=8 with ECM capillary pressure functions

ICP=	8	For effective continuum approach option.
CP(1)=	M	Of van Genuchten's function for matrix.
CP(3)=	S_{lr}	Residual liquid saturation in matrix.
CP(2)=	α	With units Pa^{-1}, van Genuchten's parameter for matrix.
CP(4)=	P_{cmax}	Maximum capillary pressure allowed.
CP(5)=	S_s	Satiated saturation in matrix.

CP(6)=	S_{th}	Threshold liquid saturation.
CP(7)=	δ	Parameter used to considering air entry effects.

ICP = 9 Generalized ECM function (Wu et al. 1996, Wu 2000)

The generalized ECM capillary function should be used only with Option IRP=11 of generalized ECM relative permeability functions. Table D-2 lists the definition of the related parameters.

Table D-2. Definition of parameters for ICP=9 with ECM capillary pressure functions

ICP=	9	For ECM option.
CP(1)=	M_m	Of van Genuchten's m for matrix.
CP(3)=	S_{lr}	Residual liquid saturation in matrix.
CP(2)=	α_m	With units Pa^{-1}, van Genuchten's parameter for matrix.
CP(4)=	P_{cmax}	Maximum capillary pressure allowed.
CP(5)=	S_{lr}	Residual liquid saturation in fractures.
CP(6)=	M_f	Of van Genuchten's m for fractures.
CP(7)=	α_f	With units Pa^{-1}, van Genuchten's parameter for fractures.