# User's Guide for TOUGH2-CSM (TOUGH2-Carbon Sequestration Model) -

# Massively Parallel Simulation of Fully-Coupled Flow with Geomechanics

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# ABSTRACT

TOUGH2-CSM is a numerical simulation program for multi-dimensional, multiphase, multicomponent fluid flow and heat transfer in porous and fractured media with geomechanical effects. TOUGH2-CSM is based on the TOUGH2-MP code, the massively parallel version of TOUGH2, a general-purpose numerical simulation program for multi-dimensional, multiphase, multicomponent fluid flow and heat transfer in porous and fractured media. In TOUGH2-CSM, the TOUGH2 mass and energy conservation equations are augmented by a momentum balance equation that models geomechanical effects. This equation is derived by combining the geomechanical equations relating stresses and displacements to yield an equation for mean stress as a function of pore pressure and temperature. In addition, rock properties such as porosity and permeability are functions of effective stress, the difference between mean stress and pore pressure, from theories of poroelasticity and empirical correlations from the literature. The TOUGH2-CSM flow equations are solved numerically by the parallel code.

This report gives the user detailed information on how to run TOUGH2-CSM. There is a detailed description of the TOUGH2-CSM flow equations and input data, followed by several example problems. These example problems are described in detail and their input data are presented. TOUGH2-CSM is written in Fortran 90 and has been used primarily to model geological sequestration of $CO_2$ in deep saline aquifers, a primary option for reducing anthropogenic $CO_2$ emissions into the atmosphere.

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# 1. INTRODUCTION

TOUGH2-CSM is a numerical simulation program for multi-dimensional, multiphase, multicomponent fluid flow and heat transfer in porous and fractured media with geomechanical effects. It has been used to model geological sequestration of $CO_2$ in deep saline aquifers, a primary option for reducing anthropogenic $CO_2$ emissions into the atmosphere. Sequestration is achieved by trapping supercritical $CO_2$ in the aquifer pore spaces (either as a separate phase trapped beneath impermeable rock or through capillary forces where $CO_2$ is an immobile phase) and dissolution of $CO_2$ in the saline aqueous phase (which is dependent on pressure, temperature, and salinity). An additional sequestration mechanism, reaction of $CO_2$ with minerals present in the rock, requires a much longer time scale than the other ones and is not modeled by TOUGH2-CSM.

TOUGH2-CSM is based on the TOUGH2-MP (Zhang, 2008) code, the massively parallel version of TOUGH2 (Pruess, 1991), a general-purpose numerical simulation program for multi-dimensional, multiphase, multicomponent fluid flow and heat transfer in porous and fractured media. TOUGH2-CSM has two EOS (equation of state) modules from TOUGH2-MP, ECO2N and EOS2. The ECO2N (Pruess and Spycher, 2007) module calculates fluid properties for $H_2O$-NaCl-$CO_2$ mixtures accurate to within experimental error for pressure and salinity conditions of interest (10 °C $\leq T \leq$ 110 °C; $P \leq$ 600 bar; salinity up to full halite saturation) during $CO_2$ sequestration processes. Up to two phases, an aqueous and a $CO_2$-rich one, may be present as well as solid salt. The module does not distinguish between liquid and vapor $CO_2$-rich phases. These properties include the partitioning of $H_2O$ and $CO_2$ between the aqueous and a $CO_2$-rich phases, the partitioning of NaCl between the aqueous and the solid phases, and density, viscosity, and specific enthalpy of the aqueous, $CO_2$-rich, and solid phases. The EOS2 module (Pruess *et al.*, 1999) calculates properties of $H_2O$-$CO_2$ mixtures for higher temperatures, accurate in the range 0 °C $\leq T \leq$ 350 °C. As in ECO2N, up to two phases, an aqueous and a $CO_2$-rich one may be present and the module does not distinguish between liquid and vapor $CO_2$-rich phases.

In TOUGH2-CSM, the TOUGH2 mass and energy conservation equations are augmented by a momentum balance equation that models geomechanical effects. This equation is derived by combining the geomechanical equations relating stresses and displacements to yield an equation for mean stress as a function of pore pressure and temperature. In addition, rock properties such as porosity and permeability are functions of effective stress, the difference between mean stress and pore pressure, from theories of poroelasticity and empirical correlations from the literature.

This report provides a comprehensive description of the mathematical formulation, numerical methods used, and specifications for preparing input data for TOUGH2-CSM, along with illustrative sample problems. Section 2 covers the TOUGH2-CSM mathematical model including the derivation and discussion of the governing mass, momentum, and energy equations, their discretization and solution, and the above rock property correlations. Section 3 discusses features of the parallel code including grid partitioning, Jacobian matrix storage and solution, and communication between processors. Section 4 contains a detailed description of TOUGH2-CSM input data and input files. Section 5 discusses options for primary variable initialization, and Section 6 contains several examples problem.

# 2. MATHEMATICAL MODEL

## 2.1 TOUGH2-CSM Geomechanical Equations

The TOUGH2-CSM geomechanical equations are based on the classical theory of elasticity extended to multi-porosity non-isothermal media. In the theory of elasticity, the stress-strain behavior of an isothermal elastic material is described by Hooke's law:

$$\bar{\bar{\tau}} = 2G\bar{\bar{\epsilon}} + \lambda(tr\bar{\bar{\epsilon}})\bar{\bar{I}} \tag{2.1}$$

where $G$ is shear modulus and λ is the Lamé parameter. Hooke's law is extended to non-isothermal fluid-filled porous rocks by including a term dependent on pore pressure, $\alpha P$, where $\alpha$ is the Biot coefficient (Biot and Willis, 1957), and one dependent on temperature (Norris, 1992), $3\beta K\left(T - T_{ref}\right)$, where $T_{ref}$ is reference temperature for a thermally unstrained state, $K$ is bulk modulus, and $\beta$ is linear thermal expansion coefficient. Finally, for a multi-porosity medium, a common example of which is the double-porosity medium consisting of a network of fractures and rock matrix, the additional terms are summed over the multi-porosity continua yielding:

$$\bar{\bar{\tau}} - \left[\sum_j \left(\alpha_j P_j + 3\beta K\omega_j\left(T_j - T_{ref}\right)\right)\right]\bar{\bar{I}} = 2G\bar{\bar{\epsilon}} + \lambda(tr\bar{\bar{\epsilon}})\bar{\bar{I}} \tag{2.2}$$

where subscript $j$ refers to a multi-porosity continuum such as fracture or matrix and each temperature term is weighted by $\omega_j$, the multi-porosity continuum volume fraction. Expressions for the generalized Biot coefficients $\alpha_j$ for a double-porosity (fracture-matrix) medium have been presented by Wilson and Aifantis (1982):

$$\begin{aligned} \alpha_1 &= 1 - \frac{K}{K_*} \\ \alpha_2 &= \frac{K}{K_*}\left(1 - \frac{K_*}{K_S}\right) \end{aligned} \tag{2.3}$$

where $K_S$ is the solid modulus, $K_*$ is the modulus of the porous medium without the fractures, subscript 1 refers to the fractures, and subscript 2 to the matrix.

Two other fundamental relations in the theory of linear elasticity are the relation between strain tensor and the displacement vector $\bar{u}$:

$$\bar{\bar{\epsilon}} = \frac{1}{2}(\nabla\bar{u} + \nabla\bar{u}^t) \tag{2.4}$$

and the static equilibrium equation:

$$\nabla \cdot \bar{\bar{\tau}} + \bar{F}_b = 0 \tag{2.5}$$

where $\bar{F}_b$ is the body force. We combine Equations 2.2, 2.4, and 2.5 to obtain the thermo-multi-poroelastic Navier equation:

$$\nabla\left[\sum_j\left(\alpha_j P_j + 3\beta K\omega_j T_j\right)\right] + (\lambda + G)\nabla(\nabla \cdot \bar{u}) + G\nabla^2\bar{u} + \bar{F}_b = 0 \tag{2.6}$$

Equation 2.6 has two terms containing the displacement vector and taking the divergence of it results in an equation that has one term containing the divergence of the displacement vector:

$$\nabla^2\left[\sum_j\left(\alpha_j P_j + 3\beta K\omega_j T_j\right)\right] + (\lambda + 2G)\nabla^2(\nabla \cdot \bar{u}) + \nabla \cdot \bar{F}_b = 0 \tag{2.7}$$

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

$$\nabla \cdot \bar{u} = \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z} = \epsilon_{xx} + \epsilon_{yy} + \epsilon_{zz} = \epsilon_v \tag{2.8}$$

The trace of the stress tensor is an invariant, having the same value for any coordinate system. We obtain the following when we take the trace of Equation 2.2, Hooke's law for a thermo-multi-poroelastic medium:

$$K\epsilon_v = \tau_m - \sum_j\left(\alpha_j P_j + 3\beta K\omega_j\left(T_j - T_{ref}\right)\right) \tag{2.9}$$

where mean stress, $\tau_m$, is the average of the normal stress components. Finally, combining Equations 2.7-2.9 yields an equation relating mean stress, pore pressures, temperatures, and body force:

$$\nabla \cdot \left[\frac{3(1-\nu)}{1+\nu}\nabla\tau_m + \bar{F}_b - \frac{2(1-2\nu)}{1+\nu}\nabla\left[\sum_j\left(\alpha_j P_j + 3\beta K\omega_j T_j\right)\right]\right] = 0 \qquad (2.10)$$

Equations 2.9 and 2.10 are the governing geomechanical equations for TOUGH2-CSM, and mean stress and volumetric strain are the geomechanical variables associated with those equations. Equation 2.10 is a statement of momentum conservation in terms of mean stress and other variables and Equation 2.09 is a property relation, relating volumetric strain to mean stress and other variables.

## 2.2 TOUGH2-CSM Conservation Equations

The TOUGH2-CSM conservation equations are based on the TOUGH2 formulation (Pruess *et al.,* 1999) of mass and energy balance equations that describe fluid and heat flow in general multiphase, multicomponent, multi-porosity systems. Fluid advection is described with a multiphase extension of Darcy's law; in addition there is diffusive mass transport in all phases. Heat flow occurs by conduction and convection, the latter including sensible as well as latent heat effects. The description of thermodynamic conditions is based on the assumption of local equilibrium of all phases. Fluid and formation parameters can be arbitrary nonlinear functions of the primary thermodynamic variables. We modify this formulation to include geomechanics. In addition to the mass and energy balance equations, we solve a momentum balance equation for mean stress that was derived in the previous section (Equation 2.10), we add mean stress to the primary thermodynamic variables, and we add volumetric strain to the calculated properties. The conservation equations for mass, momentum, and energy can be written in differential form as:

$$\frac{\partial M^k}{\partial t} = \nabla \cdot \bar{F}^k + q^k \qquad (2.11)$$

where $M^k$ is conserved quantity $k$ per unit volume, $q^k$ is source or sink per unit volume, and $\bar{F}^k$ is flux. Mass per unit volume is a sum over phases:

$$M^k = \phi \sum_l S_l \rho_l X_l^k \tag{2.12}$$

where $\phi$ is porosity, $S$ is phase saturation, $\rho$ is mass density, and $X$ is mass fraction of component $k$. Energy per unit volume accounts for energy in rock and fluid and is the following:

$$M^{N+1} = (1-\phi) C_r \rho_r T + \phi \sum_l S_l \rho_l U_l \tag{2.13}$$

where $\rho_r$ is rock density, $C_r$ is rock specific heat, $T$ is temperature, and $U$ is phase specific internal energy, and $N$ is the number of mass components. Advective mass flux is a sum over phases:

$$F_{adv}^k = \sum_l F_l X_l^k \tag{2.14}$$

and phase flux $F_l$ is given by Darcy's law:

$$F_l = -k \frac{k_{rl} \rho_l}{\mu_l} \left( \nabla P + \nabla P_{c,l} - \rho_l \bar{g} \right) \tag{2.15}$$

where $k$ is absolute permeability, $k_r$ is phase relative permeability, $\mu$ is phase viscosity, $P$ is pore pressure, $P_c$ is phase capillary pressure, and $\bar{g}$ is gravitational acceleration. Capillary pressure is relative to a reference phase, which is the gaseous phase. The gas phase absolute permeability increases as pressure is lowered according to the Klinkenberg effect (Klinkenberg, 1941):

$$k = k_\infty \left( 1 + \frac{b}{P} \right) \; for \; l = g \tag{2.16}$$

where $b$ is the Klinkenberg constant and $k_\infty$ is infinite pressure permeability. Diffusive mass flux is given by:

$$F_{dif}^{k} = -\phi\tau_0 \sum_l \tau_l \rho_l d_l^k \nabla X_l^k \tag{2.17}$$

where $\tau_0$ is the porous medium dependent tortuosity factor, $\tau_l$ is the phase saturation dependent tortuosity factor, and $d_l^k$ is themolecular diffusion coefficient for component $k$ in phase $l$. Energy flux includes conductive and convective components:

$$F^{N+1} = -\lambda \nabla T + \sum_l h_l F_l \tag{2.18}$$

where $\lambda$ is thermal conductivity and $h_l$ is phase $l$ specific enthalpy.

The momentum balance equation (Equation 2.10) is a statement of momentum conservation and is written as the divergence of a momentum flux. The momentum accumulation term is small compared to momentum flux term and has been neglected in our formulation.

## 2.3 Discretization of Single-Porosity TOUGH2-CSM Conservation Equations

In this section, we restrict our discussion of discretized TOUGH2-CSM conservations equations to the single-porosity case. We discuss the multi-porosity case later when we describe multi-porosity flow models. For the single-porosity case, the summation in Equation 2.2 is over one porous continuum and the subscripts for that summation are omitted in what follows.

The TOUGH2-CSM mass, energy, and momentum balance equations are discretized in space using the integral finite difference method (Narasimhan and Witherspoon, 1976). In this method, the simulation domain is subdivided into grid blocks and the conservation equations (Equation 2.11) are integrated over grid block volume $V_n$ with flux terms expressed as an integral over grid block surface $\Gamma_n$ using the divergence theorem:

$$\frac{d}{dt}\int_{V_n} M^k dV = \int_{\Gamma_n} \bar{F}^k \cdot \hat{n} d\Gamma + \int_{V_n} q^k dV \tag{2.19}$$

Volume integrals are replaced with volume averages:

$$\int_{V_n} M^k dV = M_n^k V_n \tag{2.20}$$

and surface integrals with discrete sums over surface averaged segments:

$$\int_{\Gamma_n} \bar{F}^k \cdot \hat{n} d\Gamma = \sum_m A_{nm} F_{nm}^k \tag{2.21}$$

where subscript $n$ denotes an averaged quantity over volume $V_n$, $A_{nm}$ is the area of a surface segment common to volumes $V_n$ and $V_m$, and double subscript $mn$ denotes an averaged quantity over area $A_{nm}$. The definitions of the geometric parameters used in this discretization are illustrated in Figure 2.1.

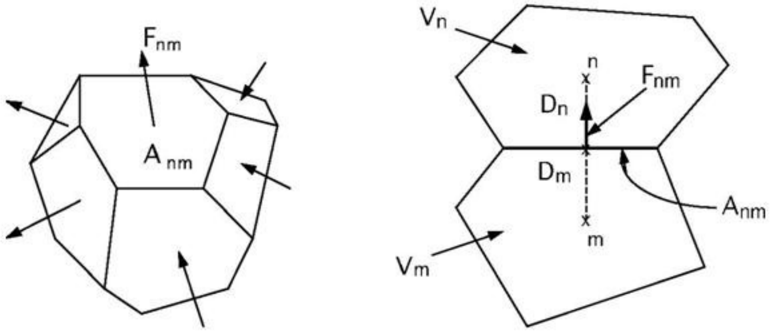


Figure 2.1. Parameter definitions for the integral finite difference method, adapted from Pruess et al. (1999).

Strictly speaking, the integrals in Equation 2.19 apply to fixed grid block geometry. Because volumetric strain is a variable in our geomechanical formulation, grid block volume as well as grid block distances and areas are no longer fixed. We introduce volumetric strain dependence into the volumes, areas, and distances that arise when the integrals in Equations 2.20 and 2.21 are evaluated. These dependencies are based on the definition of volumetric strain:

$$V_n(\epsilon_{v,n}) = V_{n,0}(1 - \epsilon_{v,n}) \tag{2.22}$$

where $V_{n,0}$ is grid block $n$ volume at zero strain and $\epsilon_{v,n}$ is grid block $n$ average volumetric strain. Changes in volumetric strain also cause changes in grid block areas and distances. We account for these by first defining analogs of Equation 2.22 for areas and distances ($A$ and $D$) in terms of average area and distance strains ($\epsilon_A$ and $\epsilon_D$):

$$A_{mn}(\epsilon_{A,mn}) = A_{mn,0}(1-\epsilon_{A,mn}) \tag{2.23}$$

and:

$$D_n(\epsilon_{D,n}) = D_{n,0}(1-\epsilon_{D,n}) \tag{2.24}$$

where $\epsilon_{A,mn}$ is the average of volumetric strains $\epsilon_{A,m}$ and $\epsilon_{A,n}$. Substituting Equation 2.22 into the volume integral (Equations 2.20) yields:

$$\int_{V_n} M^k dV = M_n^k V_{n,0}(1-\epsilon_{v,n}) \tag{2.25}$$

and substituting Equation 2.23 into the surface integral (Equations 2.21) yields

$$\int_{\Gamma_n} \bar{F}^k \cdot \hat{n} d\Gamma = \sum_m A_{mn,0}(1-\epsilon_{A,mn}) F_{nm}^k \tag{2.26}$$

Next, we relate area and distance strains to volumetric strain. Because our geomechanical formulation is in terms of volumetric strain only, we must make an assumption to do this. We assume either isotropic or uniaxial volumetric strain. For isotropic volumetric strain, area strain and volumetric strain are related by:

$$(1-\epsilon_v) \ = (1-\epsilon_A)^{\frac{3}{2}} \tag{2.27}$$

and since strains are small:

$$\epsilon_A \approx \frac{2\epsilon_v}{3} \tag{2.28}$$

Distance strain and volumetric strain are related by:

$$(1-\epsilon_v) = (1-\epsilon_D)^3 \tag{2.29}$$

and since strains are small:

$$\epsilon_D \approx \frac{\epsilon_v}{3} \tag{2.30}$$

For uniaxial volumetric strain, distance strain in the strain direction would be equal to volumetric strain and distance strain in other directions would be zero; area strain in the strain direction would be zero and area strain in the other directions would be equal to volumetric strain.

The integral finite difference approximation to the advective mass flux for component *k* (Equations 2.14 and 2.15) is the following:

$$A_{nm}F_{nm}^{k} = \sum_{l} -k_{nm}\left[\frac{k_{rl}\rho_l x_{lk}}{\mu_l}\right]_{nm}\left[\frac{P_n-P_m+P_{cl,n}-P_{cl,m}}{D_{n,0}(1-\epsilon_{D,n})+D_{m,0}(1-\epsilon_{D,m})}-\rho_{l,nm}g_{nm}\right]A_{mn,0}(1-\epsilon_{A,nm}) \tag{2.31}$$

where $g_{nm}$ is the component of gravitational acceleration pointing between grid block *m* and grid block *n*. The pressure and capillary pressure gradient terms in Equation 2.15 are approximated as their difference divided by grid block distances ($D_n$ and $D_m$) that depend on distance strain. Analogous expressions can be obtained for energy and diffusive mass fluxes as well.

Applying the integral finite difference method to the geomechanical equations yields an equation for grid block volumetric strain in terms of grid block mean stress, pore pressure, and temperature:

$$K\epsilon_{v,n} = \tau_{m,n} - \left(\alpha P_n + 3\beta K\left(T_n - T_{ref}\right)\right) \tag{2.32}$$

and a discrete sum of momentum fluxes over grid block surface segments:

$$\sum_m \left[\left(\frac{3(1-\nu)}{(1+\nu)}\right)_{nm} \frac{\tau_n-\tau_m}{D_{n,0}(1-\epsilon_{D,n})+D_{m,0}(1-\epsilon_{D,m})} + (\bar{F}_b\cdot\hat{n})_{nm} - \left(\frac{2(1-2\nu)}{(1+\nu)}\right)_{nm}\left(\alpha\frac{P_n-P_m}{D_{n,0}(1-\epsilon_{D,n})+D_{m,0}(1-\epsilon_{D,m})} + (3\beta K)_{nm}\frac{T_n-T_m}{D_{n,0}(1-\epsilon_{D,n})+D_{m,0}(1-\epsilon_{D,m})}\right)\right] A_{mn,0}(1-\epsilon_{A,nm}) = 0 \tag{2.33}$$

The TOUGH2-CSM conservation equations are assembled by using Equations 2.25 and 2.36 to approximate the volume and surface integrals in Equation 2.19, replacing the time derivative by the standard first order finite difference approximation, and evaluating the fluxes and source/sink terms fully implicitly. The resulting set of nonlinear of algebraic equations in residual form is:

$$[R_n^k]^{l+1} = \left[M_n^k(1-\epsilon_{v,n})\right]^{l+1} - \left[M_n^k(1-\epsilon_{v,n})\right]^{l} - \frac{\Delta t}{V_{n,0}}\left[\sum_m A_{nm,0}(1-\epsilon_{A,mn})F_{nm}^k + V_{n,0}(1-\epsilon_{v,n})q_n^k\right]^{l+1} = 0 \tag{2.34}$$

where *l* is time level. These equations, expressed in vector form as:

$$\bar{\mathrm{R}}(\bar{\mathrm{x}}^{l+1}) = 0 \tag{2.35}$$

where $\bar{\mathrm{x}}^{l+1}$ is the primary variable vector at time level *l+1*, are solved by the Newton-Raphson method. The Newton-Raphson method is an iterative procedure used to solve systems of non-linear equations. Denoting iteration number by subscript *p*, the following system of equations result from applying the Newton-Raphson method to Equation 2.34:

$$\bar{\bar{\mathrm{J}}}(\bar{\mathrm{x}}_p^{l+1})(\bar{\mathrm{x}}_{p+1}^{l+1} - \bar{\mathrm{x}}_p^{l+1}) = -\bar{\mathrm{R}}(\bar{\mathrm{x}}_p^{l+1}) \tag{2.36}$$

where the Jacobian matrix $\bar{\bar{\mathrm{J}}}(\bar{\mathrm{x}})$ is defined as:

$$\left[\bar{\bar{\mathrm{J}}}(\bar{\mathrm{x}})\right]_{ij} = \frac{\partial R_i(\bar{\mathrm{x}})}{\partial x_j} \tag{2.37}$$

The Jacobian matrix is evaluated by numerical differentiation:

$$\frac{\partial R_i(\bar{x})}{\partial x_j} \approx \frac{R_i\big(\bar{x}(\forall i \neq j), x_j + \epsilon_j\big) - R_i(\bar{x})}{\epsilon_j} \qquad (2.38)$$

where $\epsilon_j$ is the increment for primary variable $x_j$. The iteration is converged when all residuals $R_i$ are less than a prescribed tolerance, $\epsilon_{tol}$:

$$\left|\frac{R_i(\bar{x}_{p+1}^{l+1})}{M_i(\bar{x}_{p+1}^{l+1})}\right| \leq \epsilon_{tol} \qquad (2.39)$$

## 2.4 Multi-Porosity Flow Model

Flow in multi-porosity media is modeled using the MINC approach (Pruess and Narasimhan, 1985). The MINC approach is a generalization of the double-porosity concept, originally developed by Barenblatt *et al.,* (1960) and Warren and Root, (1963) among others, to multiple porous continua. The double-porosity approach is used to describe fluid flow in fractured reservoirs, an idealization of which is shown in Figure 2.2. 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 the fractures much faster than through the rock matrix. The double-porosity approach assumes that global fluid and heat flow occurs mostly though the fractures with a quasi-steady exchange between the fractures and matrix that is dependent on pressure and temperature differences between them.

For many systems, such as those with complex, multiphase flow or large matrix volumes, the assumption of quasi-steady exchange between the fractures and matrix is not a good one because the time scale associated with flow through the matrix is too large. We use the MINC approach to describe flow in these systems. In the MINC approach, flow within the matrix is described more accurately by subdividing the matrix into nested volumes, as shown in Figure 2.3, with flow occurring between adjacent nested matrix volumes as well as between the fractures and the outer matrix volume. Flow within the matrix is one-dimensional and transient and the MINC approach reduces to the double-porosity one if there is only one matrix subdivision.

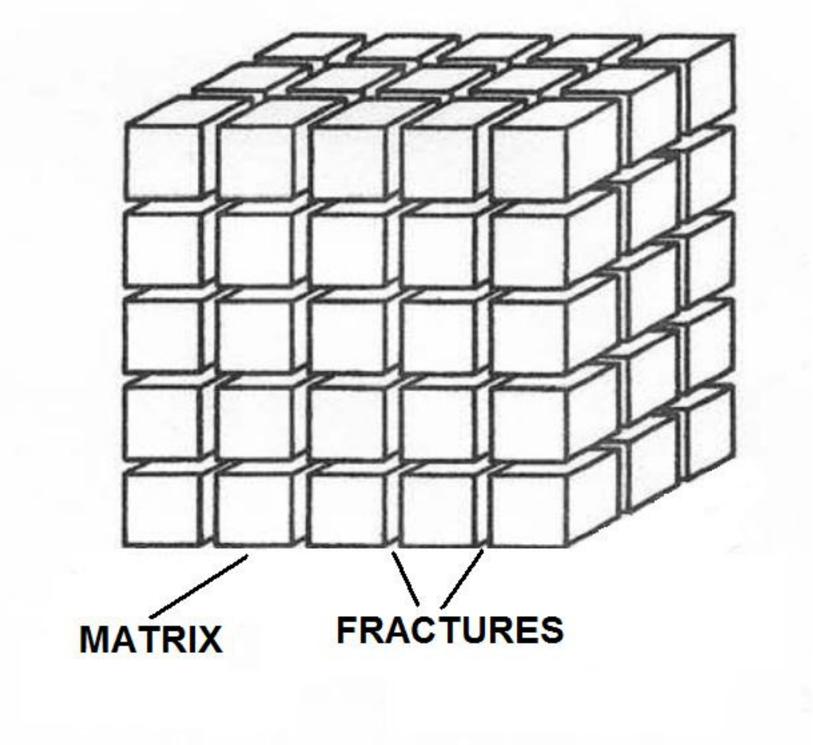


Figure 2.2. Idealized double porosity model of a fractured reservoir showing fractures and matrix blocks, adapted from Pruess et al. (1999).

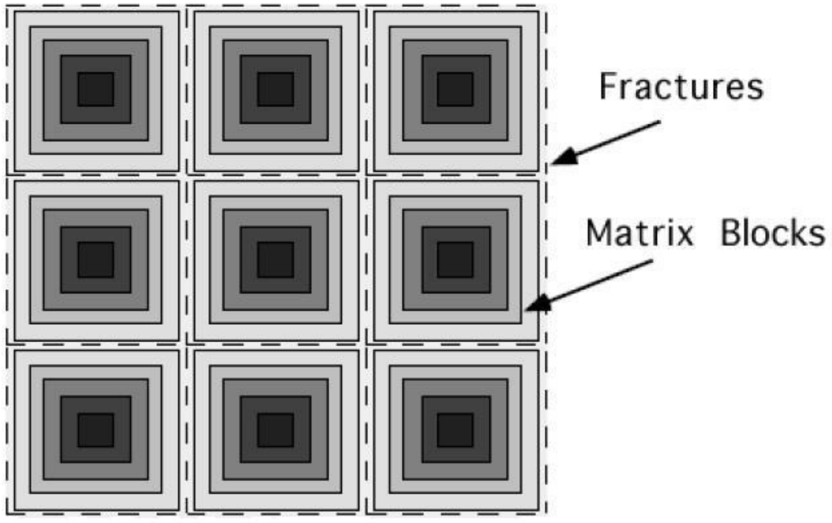


Figure 2.3. Idealized MINC grid showing fractures and nested matrix volumes, adapted from Pruess et al. (1999).

Consider a simulation domain discretized into $N_v$ grid blocks with $N_k$ components. When using the single-porosity approach, $N_k$ mass conservation equations, one momentum conservation equation, and one energy conservation equation are associated with each grid block for a total of $N_v(2 + N_k)$ equations for the entire simulation domain. When using the MINC approach with $N_\phi$ multi-porous continua in each grid block, $N_k$ mass conservation equations and one energy conservation equation are associated with each porous continuum, and one momentum equation is associated with the entire grid block for a total of $N_v(1 + N_\phi (1+N_k))$ equations for the entire simulation domain. The number of conservation equations for single-porosity and multi-porosity simulations are summarized in Table 2.1.

Table 2.1. Summary of conservation equations for single-porosity and multi-porosity simulations.

| Porosity | Number Grid Blocks | Porous Continua/ Grid Block | Mass and Energy Conservation Equations/GB | Momentum Conservation Equations/GB | Total Equations/ GB | Total Equations |
|---|---|---|---|---|---|---|
| Single | $N_v$ | 1 | $1+N_k$ | 1 | $2+N_k$ | $(2+N_k)N_v$ |
| Multi | $N_v$ | $N_\phi$ | $(1 + N_k) N_\phi$ | 1 | $(1+N_k) N_\phi+1$ | $((1+N_k) N_\phi+1)N_v$ |

The discretized multi-porosity TOUGH2-CSM conservation equations have a somewhat different form than the single porosity ones. When applying the integral finite difference method to the multi-porosity geomechanical equations, we integrate over a grid block volume as before. However, this integral encompasses all multi-porosity continua in the grid block volume. When applied to Equation 2.9 we obtain an equation for grid block volumetric strain in terms of grid block mean stress, and pore pressure and temperature of each multi-porosity continuum in the grid block:

$$K\epsilon_{v,n} = \tau_{m,n} - \sum_j \left(\alpha_j P_{j,n} + 3\beta K \omega_{j,n}\left(T_{j,n} - T_{ref}\right)\right) \qquad (2.40)$$

where the double subscript *j,n* denotes porous continuum *j* in grid block *n*. When applied to the momentum conservation equation (Equation 2.10) we obtain:

$$\sum_m \left[\left(\frac{3(1-\nu)}{(1+\nu)}\right)_{nm} \frac{\tau_n-\tau_m}{D_{n,0}(1-\epsilon_{D,n})+D_{m,0}(1-\epsilon_{D,m})} + (\bar{F}_b \cdot \hat{n})_{nm} - \left(\frac{2(1-2\nu)}{(1+\nu)}\right)_{nm} \sum_j \left(\alpha_j \frac{P_{j,n}-P_{j,m}}{D_{n,0}(1-\epsilon_{D,n})+D_{m,0}(1-\epsilon_{D,m})} + (3\beta K\omega_j)_{nm} \frac{T_{j,n}-T_{j,m}}{D_{n,0}(1-\epsilon_{D,n})+D_{m,0}(1-\epsilon_{D,m})}\right)\right] A_{mn,0}(1-\epsilon_{A,nm}) = 0 \qquad (2.41)$$

When applying the integral finite difference method to the multi-porosity mass and energy conservation equations, we integrate over a porous continuum volume rather than the entire grid block volume and obtain:

$$\left[M_{j,n}^k(1-\epsilon_{v,n})\right]^{l+1} - \left[M_{j,n}^k(1-\epsilon_{v,n})\right]^{l} - \frac{\Delta t}{V_{j,n,0}}\left[\sum\nolimits_m A_{nm,0}(1-\epsilon_{A,mn})F_{j,nm}^k + V_{j,n,0}(1-\epsilon_{v,n})q_{j,n}^k\right]^{l+1} = 0 \qquad (2.42)$$

where $V_{j,n,0}$ is zero strain volume of porous continuum *j* in grid block *n*.

## 2.5 Geomechanical Boundary Conditions

The momentum conservation equation (Equation 2.10) is the divergence of a momentum flux and applying the integral finite difference method to it yields an integral of momentum flux over the grid block surface that is approximated as a discrete sum over surface averaged segments. Grid block surface segments are common to another grid block or border the surroundings. The Equation 2.41 summation term as is applies to surface segments that are common to another grid block. For grid block surface segments that border the surroundings, we modify that term by applying the geomechanical boundary conditions.

There are four terms that comprise the momentum flux: the body force, and the mean stress, pressure, and temperature difference terms. The body force term contains the dot product of the body force, which points in the direction of the gravitational vector, with the vector pointing between grid blocks n and m, as shown in Figure 2.1. We neglect this term for surface segments bordering the surroundings. For such a segment, the vector pointing between grid blocks n and m is arbitrary so we assume it is orthogonal to the gravitational vector. Surface segments bordering the surroundings generally have no fluid flowing through them (fluid loss to the surroundings is generally represented as a constant pressure sink), so there would be no pore pressure communication between a grid block and the surroundings. Consequently, we neglect the pressure difference term as well. Finally, we assume temperature and mean stress of the surroundings are the grid block's initial values.

We apply the above boundary conditions to the Equation 2.41 summation term and obtain the form for a surface segment bordering the surroundings:

$$\left[\left(\frac{3(1-\nu)}{(1+\nu)}\right)_n \frac{\tau_n-\tau_n^0}{2D_{n,0}(1-\epsilon_{D,n})} - \left(\frac{2(1-2\nu)}{(1+\nu)}\right)_n \sum_j \left(\left(3\beta K\omega_j\right)_n \frac{T_{j,n}-T_{j,n}^0}{2D_{n,0}(1-\epsilon_{D,n})}\right)\right] A_{mn,0}\left(1-\epsilon_{A,n}\right) \quad (2.43)$$

where superscript 0 refers to grid block initial value and $D_m$ is replaced by $D_n$.

## 2.6 Rock Property Correlations

We describe the dependence of permeability and porosity on effective stress and other quantities in this section. Effective stress was initially defined as the difference between average stress and pore pressure by Terzhagi (1936) and was generalized by Biot and Willis (1957) as:

$$\tau' = \tau_m - \alpha P \quad (2.44)$$

where $\alpha$ is the Biot or effective stress coefficient. Correlations have been developed for porosity as a function of effective stress and other quantities and permeability as a function of either porosity or effective stress. There are numerous examples of the above correlations, with each developed for a specific set of conditions. We describe those that have been incorporated into TOUGH2-CSM below.

We developed an expression for porosity starting with its definition. Porosity is the ratio of fluid volume to bulk volume, and since fluid volume plus solid volume equals bulk volume, porosity can be written as:

$$\phi = 1 - \frac{V_s}{V} \tag{2.45}$$

where *V* is bulk volume and $V_s$ solid volume. 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:

$$V_s(P, \tau') = V_{s,r}\left(1 + \frac{1-\phi_r}{K_s}(P - P_r) - \frac{1}{K_s}(\tau' - \tau_r')\right) \tag{2.46}$$

where subscript *r* refers to reference conditions. Equation 2.22 relates bulk volume to volumetric strain, and when combined with Equations 2.45 and 2.46 yield porosity as a function of pressure, temperature, and effective stress:

$$\phi = 1 - \frac{(1-\phi_r)\left(1+\frac{(1-\phi_r)}{K_s}(P-P_r)-\frac{1}{K_s}(\tau'-\tau_r')\right)}{\frac{(1-\epsilon_v)}{(1-\epsilon_{v,r})}} \tag{2.47}$$

An example of reference conditions for Equation 2.47 is the initial conditions for a simulation, where volumetric strain, porosity, mean stress, and pressure are specified.

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

$$\phi = \phi_1 + (\phi_0 - \phi_1)e^{-a\tau'} \tag{2.48}$$

where $\phi_0$ is zero effective stress porosity, $\phi_1$ is high effective stress porosity, and the exponent *a* is a parameter. They also presented an associated function for permeability in terms of porosity:

$$k = k_0 e^{c\left(\frac{\phi}{\phi_0}-1\right)} \tag{2.49}$$

For fractures, they defined an aperture width $b_i$ for direction *i* as:

$$b_i = b_{0,i} + \Delta b_i \left( e^{-d\sigma'} - e^{-d\sigma'_0} \right) \tag{2.50}$$

where subscript 0 refers to initial conditions, $\Delta b_i$ is the aperture change, and the exponent *d* is a parameter. Fracture porosity is correlated to changes in $b_i$ as:

$$\phi = \phi_0 \frac{b_1 + b_2 + b_3}{b_{1,0} + b_{2,0} + b_{3,0}} \tag{2.51}$$

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

$$k_i = k_{i,0} \frac{b_j^3 + b_k^3}{b_{i,0}^3 + b_{k,0}^3} \tag{2.52}$$

McKee et al. (1988) derived a relationship between porosity and effective stress from hydrostatic poroelasticity theory by assuming incompressible rock grains:

$$\phi = \phi_0 \frac{e^{-c_p\left(\tau' - \tau'_0\right)}}{1 - \phi_0\left(1 - e^{-c_p\left(\tau' - \tau'_0\right)}\right)} \tag{2.53}$$

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

$$k \propto \frac{\phi^3}{(1-\phi)^2} \tag{2.54}$$

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 and approximated permeability as:

$$k^n = Dln\frac{\tau^{','*}}{\tau'} \tag{2.55}$$

where exponential $n$ is 0.5, $D$ is a parameter, and $\tau^{','*}$ 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:

$$\frac{k-k_c}{k_0-k_c} = \left(\frac{\phi-\phi_c}{\phi_0-\phi_c}\right)^n \tag{2.56}$$

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

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

$$P_c = P_{c0}\frac{\sqrt{(k/\phi)_0}}{\sqrt{k/\phi}} \tag{2.57}$$

## 3. METHODOLOGY AND CODE ARCHITECTURE

The TOUGH2-CSM code is a parallel computer program. A parallel computer program solves a problem by subdividing it into a number of smaller ones, solving those smaller ones concurrently, and then assembling the overall solution from those of the subdivisions. Solving a problem in parallel is often faster than solving it serially. Amdahl's law gives a theoretical upper limit, *S*, for the speedup of a parallel program in which *A* is the fraction of the program's run time spent on non-parallelizable parts and *P* is the number of problem subdivisions (or processors):

$$S = \frac{1}{A + \frac{1-A}{P}} \qquad (3.1)$$

One deficiency in Amdahl's law is the assumption that the parallelizable part scales linearly with the number of problem subdivisions. Parallel programs often require problem subdivisions to communicate with each other, and the overhead associated with this communication could severely diminish the speedup factor as the number of problem subdivisions becomes large. In addition, the computational work needs to be evenly distributed among subdivisions in order for this speedup to occur.

For a typical TOUGH2-CSM simulation, most of the computation time is spent in three parts: updating thermophysical parameters, assembling the Jacobian matrix, and solving the algebraic equations, with the latter dominating for extremely large problems. The algebraic equations are solved in parallel using the AZTEC package (Tuminaro et al., 1999). AZTEC includes a number of Krylov iterative methods, such as conjugate gradient (CG), generalized minimum residual (GMRES) and stabilized biconjugate gradient (BiCGSTAB). In order to maximize computational speed and efficiency, a parallel simulation needs to distribute computational time uniformly for these three parts. In order to do that, a parallel scheme must take into account domain decomposition, grid block reordering, and efficient message exchange between processors. These important parallel computing strategies and implementation procedures are discussed below.

## 3.1 Grid Domain Partitioning and Grid Block Reordering

A successful parallel computing scheme requires an efficient and effective method for partitioning grids. Such a scheme would distribute grid blocks evenly to different processors and minimize the number of connections common to different processors. This distribution would balance computational work among the processors and minimize the time consumed in communication between processors.

In TOUGH2-CSM, the simulation domain is subdivided into grid blocks and communication between grid blocks occurs at the interfaces between them. This can be represented as a grid with each grid block as a node and grid block interfaces as connections. The grid configuration is arbitrary so the grid is said to be unstructured. From the connection information, an adjacency matrix can be constructed that is stored in a compressed storage format (CSR).

In the CSR format, the adjacency matrix of a global domain with *n* grid blocks and *m* connections is represented by two arrays, *xadj* and *adj*. The *xadj* array has a size of *n+1,* whereas the *adj* array has a size of *2m*. For grid block numbering starting from *1*, the adjacency list of grid block *i* is stored in array *adj,* starting at index *xadj(i)* and ending at index *xadj(i+1)-1*. Array *adj* stores adjacency lists in consecutive locations and array *xadj* points to the start of a grid block adjacency list. Figure 3.1 shows a 15 grid block domain including connections (as well as a partition among four processors) and Table 3.1 illustrates its corresponding CSR format arrays.

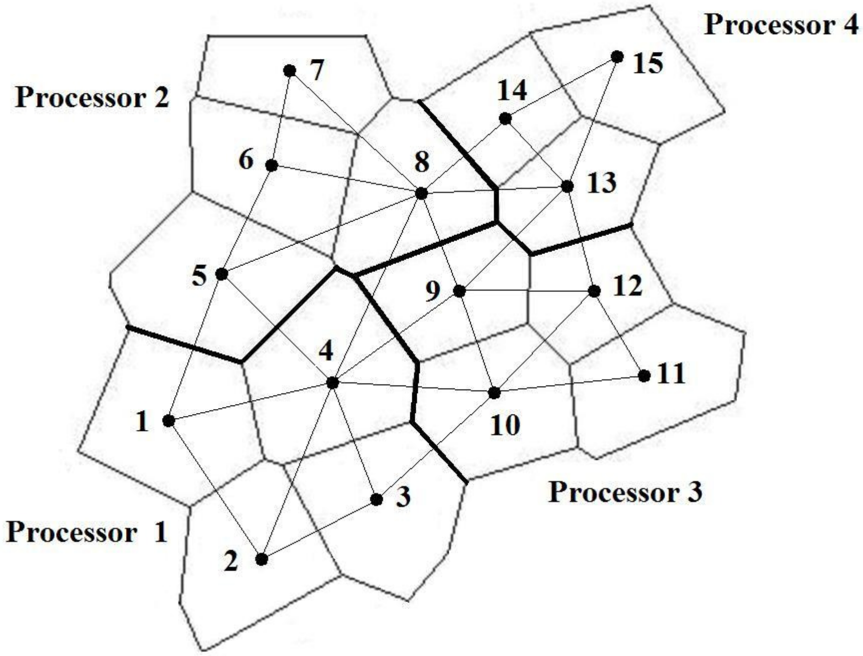


Figure 3.1. An unstructured grid containing fifteen grid blocks and showing partitions (bold lines) among four processors and connections between grid blocks (thin lines).

Table 3.1. Global *xadj* and *adj* arrays for grid in Figure 3.1.

| Grid block | *xadj* array | *adj* array |
|---|---|---|
| 1 | 1 | 2 |
| | | 4 |
| | | 5 |
| 2 | 4 | 1 |
| | | 3 |
| | | 4 |
| 3 | 7 | 2 |
| | | 4 |
| | | 10 |
| 4 | 10 | 1 |
| | | 2 |
| | | 3 |
| | | 5 |
| | | 8 |
| | | 9 |
| | | 10 |
| 5 | 17 | 1 |
| | | 4 |
| | | 6 |
| | | 8 |
| 6 | 21 | 5 |
| | | 8 |
| | | 7 |
| 7 | 24 | 6 |
| | | 8 |
| 8 | 26 | 4 |
| | | 5 |
| | | 6 |
| | | 7 |
| | | 9 |
| | | 13 |
| | | 14 |
| 9 | 33 | 4 |
| | | 8 |
| | | 10 |
| | | 12 |
| | | 13 |
| 10 | 38 | 3 |
| | | 4 |
| | | 9 |
| | | 11 |
| | | 12 |
| 11 | 43 | 10 |
| | | 12 |
| 12 | 45 | 9 |
| | | 10 |
| | | 11 |
| | | 13 |
| 13 | 49 | 9 |
| | | 8 |
| | | 12 |
| | | 14 |
| | | 15 |
| 14 | 54 | 8 |
| | | 13 |
| | | 15 |
| 15 | 57 | 13 |
| | | 14 |
| | 59 | |

Algorithms from the METIS software package (Karypsis and Kumar, 1998) are used to partition the grid. The package contains three algorithms: *K-way*, *VK-way*, and *Recursive*. *K-way* is used for partitioning a grid into a large number of partitions (more than 8). This algorithm seeks to minimize the number of edges that are common to different partitions. If a small number of partitions is desired, the *Recursive* partitioning method, a recursive bisection algorithm, should be used. *VK-way* is a modification to *K-way* and seeks to minimize the total number of edges that are common to different partitions. Both *K-way* and *VK-way* belong to multilevel partitioning algorithms.

Figure 3.1 shows a partitioning of the grid into four parts. Grid blocks are assigned to different processors through partitioning methods discussed above. Grid blocks assigned to a processor are referred to as the *update* set. The *update* set is further divided into two subsets: *internal* and *border*. The *internal* set consists of grid blocks with no connections to grid blocks that are assigned to another processor. The *border* set consists of grid blocks with at least one connection to a grid block that is assigned to another processor. Those grid blocks connected to the border set that are not assigned to the processor is called the *external* set. The *border* set requires information from the other processors during a simulation but the *internal* set does not. Table 3.2 summarizes the partitioning in Figure 3.1.

Table 3-2. Partitioning and grid block sets for Figure 3.1 grid.

| | Update | | External |
|---|---|---|---|
| | Internal | Border | |
| Processor 1 | 2 | 1, 3, 4 | 5, 8, 9, 10 |
| Processor 2 | 6, 7 | 5, 8 | 1, 4, 9, 13, 14 |
| Processor 3 | 11 | 9, 10, 12 | 3, 4, 8, 13 |
| Processor 4 | 15 | 13, 14 | 8, 9, 12 |

A processor's update and external sets have a local numbering.  The connection information for these sets is stored in similar CSR format arrays to the global arrays discussed above. Each processor stores only the rows of the Jacobian matrix that correspond to its *update* set. These rows form a sub matrix whose columns correspond to both the *update* set and the *external* set for the processor.

### 3.2 Organization of Input and Output Data

TOUGH2-CSM input data includes hydrogeologic parameters and constitutive relations of porous media and fluids, such as absolute and relative permeability, porosity, capillary pressure, thermophysical properties of fluids and rock, and initial and boundary conditions of the system. Other processing requirements include the specification of space-discretized geometric information (grid) and various program options (computational parameters and time-stepping information). For a large-scale, three-dimensional model, a computer memory on the order of gigabytes is generally required and the distribution of the memory to all processors is necessary for practical application of TOUGH2-CSM.

To efficiently use the memory of each processor (considering that each processor has a limited memory available), the input data files for the TOUGH2-CSM simulation are organized in sequential format. There are two large groups of data blocks within a TOUGH2-CSM mesh file: one with dimensions equal to the number of grid blocks; the other with dimensions equal to the number of connections (interfaces). Large data blocks are read one by one through a temporary full-sized array and then distributed to different processors. This method avoids storing all input data in a single processor (whose memory space may be too small) and greatly enhances the I/O efficiency. Other small-volume data, such as simulation control parameters, are duplicated onto all processors.

All data input and output are carried out through the master processor.  Time series outputs, however, are written out by the processors at which the specified grid blocks or connections for output are located.

### 3.3 Assembly and Solution of Linearized Equation Systems

In the TOUGH2-CSM formulation, the discretization in space using the integral finite difference method leads to a set of strongly coupled nonlinear algebraic equations, which are linearized by the Newton method. Within each Newton iteration step, the Jacobian matrix is first constructed by numerical differentiation. The resulting system of linear equations is then solved using an iterative linear solver with different preconditioning procedures. The following gives a brief discussion of assembling and solving the linearized equation systems with parallel simulation.

The discrete mass, momentum, and energy balance equations solved by the TOUGH2-CSM code can be written in a residual form as:

$$\bar{R}(\bar{x}^{l+1}) = 0 \tag{3.2}$$

where $\bar{x}^{l+1}$ is the primary variable vector at time level *l+1*. The Newton-Raphson method is an iterative procedure used to solve systems of non-linear equations. Denoting iteration number by subscript *p*, the following system of equations result from applying the Newton-Raphson method to Equation 3.2:

$$\bar{\bar{J}}(\bar{x}_p^{l+1})\left(\bar{x}_{p+1}^{l+1} - \bar{x}_p^{l+1}\right) = -\bar{R}(\bar{x}_p^{l+1}) \tag{3.3}$$

where the Jacobian matrix $\bar{\bar{J}}(\bar{x})$ is defined as:

$$\left[\bar{\bar{J}}(\bar{x})\right]_{ij} = \frac{\partial R_i(\bar{x})}{\partial x_j} \tag{3.4}$$

and $\bar{x}_p^{l+1}$ is the primary variable vector at time level *l+1* and iteration *p*.

The Jacobian matrix and the right-hand side of Equation 3.3 need to be recalculated for each Newton iteration, and that computational effort may be extensive for a large simulation. In the parallel code, the assembly of this linear equation system is shared by all processors, and each processor is responsible for computing the rows of the Jacobian matrix that correspond to grid blocks in the processor's *update* set. Computation of the elements in the Jacobian matrix is performed in two parts. The first part consists of the computations related to the individual grid blocks (accumulation and source/sink terms). Such calculations are carried out using the information stored on the current processor, without need of communication with other processors. The second part includes all the computations related to the connections or flow terms. Grid blocks in the *border* set need information from those in the *external* set, which requires communication with neighboring processors. Before performing these computations, an exchange of relevant information is required. For grid blocks in the *border* set, each processor sends their information to the relevant processors, which contain these grid blocks in their *external* set.

The Jacobian matrix for each processor's grid blocks is stored in the distributed variable block row (DVBR) format, a generalization of the VBR format. All matrix blocks are stored row-wise, with the diagonal blocks stored first in each block row. Scalar elements of each matrix block are stored in column major order. The data structure consists of a real-type vector and five integer-type vectors, forming the Jacobian matrix. Detailed explanation of the DVBR data format can be found in Tuminaro et al. (1999).

The linearized equation system arising at each Newton step is solved using an iterative linear solver from the AZTEC package. There are several different solvers and preconditioners from the package for users to select and the options include conjugate gradient, restarted generalized minimal residual, conjugate gradient squared, transposed-free quasi-minimal residual, and bi-conjugate gradient with stabilization methods. The work for solving the global linearized equation is shared by all processors, with each processor responsible for computing its own portion of the partitioned domain equations. To accomplish the parallel solution, communication between a pair of processors is required to exchange data between the neighboring grid partitions. Moreover, global communication is also required to compute the norms of vectors for checking the convergence.

During a parallel simulation, the time-step size is automatically adjusted (increased or reduced), depending on the convergence rate of the Newton method. In the TOUGH2-CSM code, time-step size is calculated at the master processor after collecting necessary data from all processors. The convergence rates may be different in different processors. Only when all processors reach stopping criteria will the time march to the next time step.

### 3.4 Communication between Processors

Communication between processors working on grid block connections that cross partition boundaries is an essential component of the parallel algorithm. Moreover, global communication is also required to compute norms of vectors, contributed by all processors, for checking the convergence. In addition to the communication taking place inside the linear solver routine to solve the linear equation system, communication between neighboring processors is necessary to calculate the Jacobian matrix. A subroutine is used to manage data exchange between processors. When the subroutine is called by a processor, an exchange of vector elements corresponding to the processor's *external* set is performed. More discussion on the prototype scheme used for data exchange is given in Elmroth et al. (2001). In addition, non-blocking communication was introduced to the Aztec package and Newton iterations (Zhang and Wu, 2006) to further improve them.

### 3.5 Updating Thermophysical Properties

The thermophysical properties of fluid mixtures (secondary variables) needed for assembling the governing conservation equations are calculated at the end of each Newton iteration step based on the updated set of primary variables. At the same time, the phase conditions are identified for all grid blocks, the appearance or disappearance of phases is recognized, and primary variables are switched and properly re-initialized in response to a change of phase. All these tasks must be done grid block by grid block for the entire simulation domain. The computational work for these tasks is readily parallelized by each processor handling its corresponding sub domain. A tiny overlapping of computation is needed for the grid blocks at the neighboring sub domain border to avoid communication for secondary variables.

### 3.6 Program Structure and Flow Chart

In TOUGH2-CSM, dynamic memory allocation, modules, array operations, matrix manipulation, and other FORTRAN 90 features are implemented in the parallel code. In particular, the message-passing interface (MPI) library of Message Passing Forum (1994) is used for message passing.

In summary, all data input and output are carried out through the master processor. The most time-consuming computations (assembling the Jacobian matrix, updating thermophysical parameters, solving linear equation systems.) are distributed to all processors involved. The memory requirements are also distributed to all processors. Distributing both computing and memory requirements is essential for solving large-scale problems and obtaining better parallel performance. Figure 3.2 shows an abbreviated program flow chart.

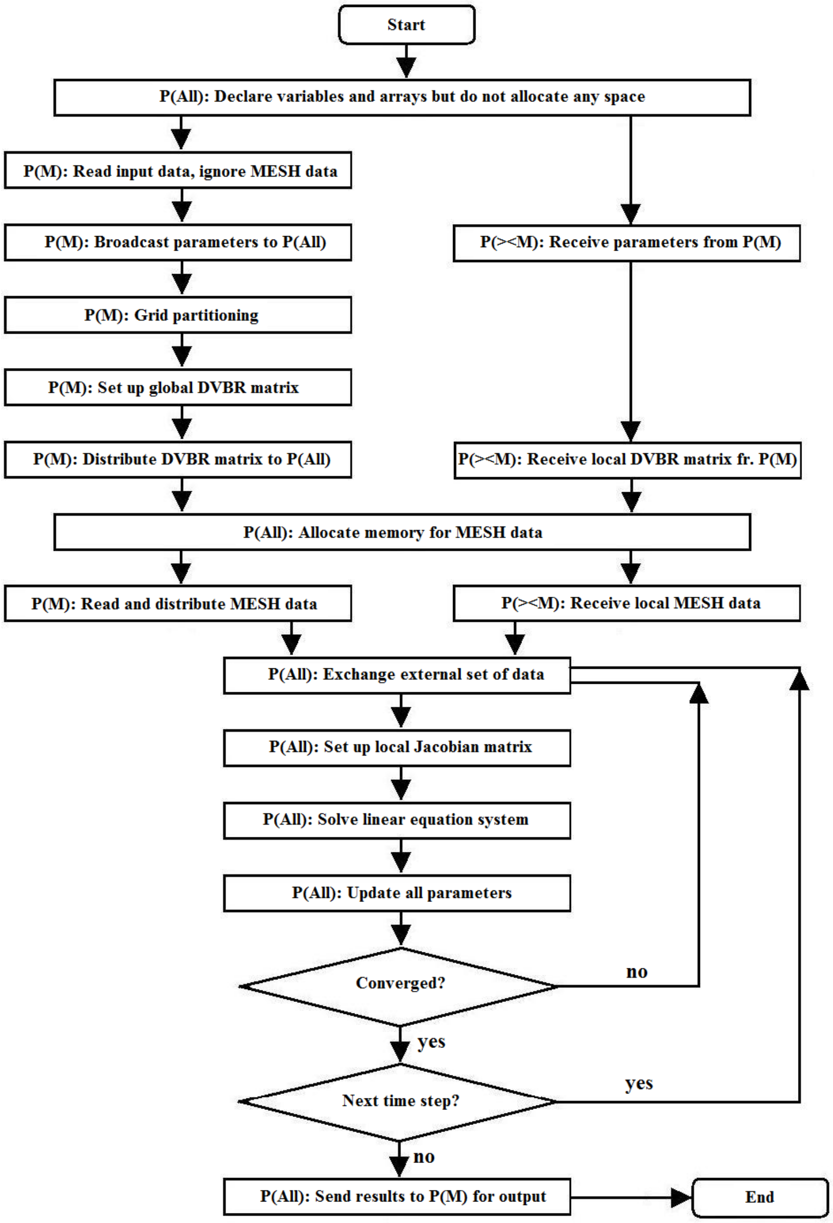

Start
P(All): Declare variables and arrays but do not allocate any space
P(M): Read input data, ignore MESH data
P(M): Broadcast parameters to P(All)
P(><M): Receive parameters from P(M)
P(M): Grid partitioning
P(M): Set up global DVBR matrix
P(M): Distribute DVBR matrix to P(All)
P(><M): Receive local DVBR matrix fr. P(M)
P(All): Allocate memory for MESH data
P(M): Read and distribute MESH data
P(><M): Receive local MESH data
P(All): Exchange external set of data
P(All): Set up local Jacobian matrix
P(All): Solve linear equation system
P(All): Update all parameters
Converged?
no
yes
Next time step?
yes
no
P(All): Send results to P(M) for output
End

Figure 3.2. TOUGH2-CSM flow chart. P(M) stand for master processor, P(><M) stands for the others, and P(All) stands for all processors

Table 4-1. TOUGH2-CSM input data blocks[§]

| KEYWORD | FUNCTION |
|---|---|
| TITLE<br>(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. |
| MULTI | Optional; specifies number of fluid components and balance equations/ grid block; applicable only for certain fluid property (EOS) modules. |
| START | Optional; one data record for more flexible initialization. |
| PARAM | Computational 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. |
| GRMOD | Optional; setting individual properties for specific grid blocks. |
| NOVER<br>(optional) | Optional; if present, suppresses printout of version numbers and dates of the program units executed in a TOUGH2-CSM run. |
| TIMBC | Optional; introducing a table for time-dependent pressure boundary. |
| RTSOL | Optional; provide linear solver parameters. |
| FOFT | Optional; list of grid blocks for time-dependent output. |
| GOFT | Optional; list of source/sink grid blocks for time-dependent output. |
| COFT | Optional; list of connections for time-dependent output. |
| DIFFU | Optional; introduce diffusion coefficients. |
| SELEC | Optional, provide parameters for requirements by specific modules. |
| ENDCY<br>(last record) | Record to close TOUGH2-CSM input file and initiate the simulation. |
| ENDFI | Alternative to “ENDCY” for closing TOUGH2-CSM input file; 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 INFILE file.

# 4. DESCRIPTION OF INPUT FILES

## 4.1 Preparation of Input Data

Input for TOUGH2-CSM is provided through a file named INFILE or separate additional files (e.g. MESH, GENER, INCON, INCNST), organized into a number of data blocks, labeled by five-character keywords (Table 4-1). The parallel program may also receive additional data input through optional input files (See Section 4.4 for details). A summary of input data keywords is shown in Figure 4.1.

## 4.2 Input File Format

This section presents the data input formats for TOUGH2-CSM.

**TITLE** is the first record of the input file, containing a header of up to 80 characters, to be printed on the 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 organized by keywords. Detailed instructions for preparing MESHMaker input are given in Section 4.3.

Record MESHM.1

Format(A5)
WORD

WORD enter one of several keywords, such as RZ2D, RZ2DL, XYZ, MINC, to generate different kinds of computational meshes. Additonal data described in given in Section 4.3 will be required.

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

**ENDFI** is a keyword that can be used to close a TOUGH2-CSM 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 different reservoir domains.

Record ROCKS.1

Format (A5, I5, 7E10.4)
MAT, NAD, DROK, POR, (PER (I), I = 1,3), CWET, SPHT

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 a record 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." Option "START" is necessary for using default porosity. Default porosity may be overridden in GRMOD section.

PER(I) I = 1, 2, and 3; default absolute permeability along the three principal axes, as specified by ISOT in block CONNE. Default permeability may be overridden in GRMOD section.

CWET formation heat conductivity under fully liquid-saturated conditions (W/m ˚C).

SPHT rock grain specific heat (J/kg ˚C). Domains with SPHT > $10^4$ 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.

Record ROCKS.1.1 (optional, NAD ≥ 1 only)

Format (5E10.4)
COM, EXPAN, CDRY, TORTX, GK

COM pore compressiblity ($Pa^{-1}$), used for porosity correlations requiring this parameter. Set to zero otherwise.

EXPAN linear thermal expansion coefficient (1/ ˚C). Set to zero for constant temperature simulation or if not used.

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 permeability according to the relationship $k_{gas} = k_{liq} * (1 + b/P)$.

Record ROCKS.1.2 (optional, NAD ≥ 2 only)

Format (I5, 5X,7E10.4)
IRP, (RP(I), I= 1,7)

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 ROCKS.1.3 (optional, NAD ≥ 2 only)

Format (I5, 5X,7E10.4)
ICP, (CP(I), I = 1,7)

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).

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

Format (2I5,5E10.4)
IRPOPT, IRKOPT, POIRAT, YOUNGM, CBIOT, TREF, SOLMOD

IPOPT Option for porosity variation with primary variables. See Appendix D.

IKOPT Option for permeability variation with primary variables. See Appendix E.

POIRAT Poisson's ratio.

YOUNGM Young's modulus, Pa.

CBIOT Biot coefficient.

TREF Reference temperature, °C, used in non-isothermal Hooke's law.

SOLMOD Inverse of rock grain modulus, Pa, zero signifies incompressible rock.

Record ROCKS.1.5 (optional, NAD≥3 only)

Format (8E10.4)
(RCKPAR(I), I=1,8)

RCKPAR(I) I=1-8, parameters for porosity and permeability variation options.

Repeat records 1.1-1.5 for each reservoir domains.

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

**MULTI** permits the user to select the number and nature of balance equations that will be solved. The keyword MULTI is followed by a single data record.

Record MULTI. 1

Format (5I5)
NK, NEQ, NPH, NB, ISTCAL

NK number of mass components.

NEQ number of balance equations per grid block. For NEQ = NK, only NK mass balances and no energy or momentum equations will be solved. For NEQ =NK + 1, NK mass balances and either one energy equation or one momentum equation will be solved (see ISTCAL below). For NEQ =NK + 2, NK mass balances, one energy equation, and one momentum equation will be solved.

NPH number of phases that can be present.

NB number of secondary parameters in the PAR-array other than component mass fractions (NB = 6 for no diffusion; NB=8 for diffusion).

ISTCAL flag which shows whether the momentum equation (ISTCAL=1) or energy balance equation (ISTCAL=0) will be solved for NEQ =NK + 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.

<u>Record PARAM.1</u>

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

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

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. The value 9999 is interpreted as infinity.

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-CSM run.

MOP(1) if unequal 0, a short printout for non-convergent iterations will be generated in the OUTPUT file.

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). This additional printout appears in the processor DEGUBxx files.

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).

= 1: Jacobian matrix and right hand side.

= 2: Jacobian matrix and right hand side, and primary variables and primary variable increments.

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 $t_i$ and generation rates $q_i$ 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 $q_i$ during the time interval $[t_i, t_{i+1}]$, and changes to $q_{i+1}$ at $t_{i+1}$. Actual rate used during a time step that ends at time t, with $t_i \leq t \leq t_{i+1}$, 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(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) chooses scaling-option for preconditioning the Jacobian matrix (MA28 only).

= 0: no scaling.

= 7: scaling.

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(21) allows one more iteration if solution converges with 1 Newton iteration

= 0: one more iteration not needed

= 1: perform one more iteration

MOP(22) used by dispersion module T2DM.

MOP(23) used by dispersion module T2DM.

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 $\phi\tau_0\tau_\beta$ for vapor diffusion.

Record PARAM.2

Format (4E10.4, A5, 5X,3E10.4)
TSTART, TIMAX, DELTEN, DELTMX, ELST, GF, REDLT, SCALE

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.

Format (8E10.4)
(DLT(I), I = 1, 100)

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

Format (6E10.4)
RE1, RE2, U, WUP, WNR, DFAC

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

RE2 convergence criterion for absolute error (default= 1).

U pivoting parameter for linear equation solution with the MA28 direct solver. U must be in the range $0 \leq U < 1$, and the default is U = 0.1. Increased value for U will make criterion for pivot selection more stringent, resulting in better numerical stability at the expense of increased computing time for matrix decomposition.

WUP upstream weighting factor for mobilities 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 is 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 ≈ $10^{-8}$).

Record PARAM.4 introduces a set of primary variables which are used as default initial conditions for all grid blocks that are not assigned by means of data blocks INDOM or INCON or in the GRMOD section. Option START is necessary to use default INCON.

Format (4E20.14)
DEP(I), I = 1, NK+1

The number of these primary variables, NK+1, is normally assigned internally in the EOS module. These primary variables do not include mean stress. 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. l

Format(A5)
MAT

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

Record INDOM.2

Format(4E20.13)
Xl, X2, X3, X4

A set of primary 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.

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

Format (A5, 10X, E15.8)
ELEM, PORX

ELEM five-character code name of a grid block. Grid blocks are ordered in some sequence and this character code is the grid block number expressed in base 62 with leading zeroes to make it five characters long. The base 62 digits are the numerals 0-9, the uppercase letters A-Z, and the lower case letters a-z. The number of these character codes is 916,132,832.

PORX porosity

Record INCON.2 specifies primary variables.

Format (4E20.14)
Xl, X2, X3, X4

A set of 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. Different sets of primary variables are used for different EOS modules.

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 restart run from a previous TOUGH2-CSM simulation.

**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

Format(A5)
EOFT(I)

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

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

Format(A10)
ECOFT(I)

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

Format(A5)
EGOFT(I)

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**SION (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-CSM run.

**DIFFU**SION (optional; needed only for NB≥8) introduces diffusion coefficients.

Record DIFFU.1

Format(8E10.4)
FDDIAG(I,1), I=1,NPH

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

Record DIFFU.2

Format(8E10.4)
FDDIAG(I,2), I=1,NPH

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**TION (optional) introduces a number of integer and floating point parameters that are used for different purposes in different TOUGH2-CSM modules.

Record SELEC.1

Format(16I5)
IE(I), I=1,16

IE(1) 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

Format(8E10.4)
FE(I), I=1,IE(1)*8
provide as many records with floating point numbers as specified in IE(1), up to a maximum of 64 records.

**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

Format (I5,5X,7E10.4)
IRP, (RP(I), I = 1, 7)

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

Format (I5,5X,7E10.4)
ICP, (CP(I), I = 1, 7)

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.

Record TIMES.1

Format (2I5,2E10.4)
ITI, ITE, DELAF, TINTER

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.

Record TIMES.2, TIMES.3, etc.

Format (8E10.4)
(TIS(I), I = l, ITI)

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

**ELEME** introduces element (grid block) information.

Record ELEME.1

Format (A5,10X,A5,6E10.4,9X,I1)
ELEM, MATR, VOLX, AHTX, PMX, X, Y, Z, ISPOR

ELEM five-character code name of a grid block. Grid blocks have an ordering and this character code is the grid block number expressed in base 62 with leading zeroes to make it five characters long. The base 62 digits are the numerals 0-9, the uppercase letters A-Z, and the lower case letters a-z. The number of these character codes is 916,132,832.

MATR 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 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-CSM 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.

ISPOR flag for MINC preprocessor. See Section 4.5 for further details.

= 0: primary grid block may be subdivided into MINC blocks by MINC preprocessor

= 1: primary grid block may not be subdivided into MINC blocks by MINC preprocessor

Default value is zero. The MESH file may be edited to inset values of one where needed.

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

Format (A5,A5,15X,I5,5E10.4)
ELEM1, ELEM2, ISOT, D1, D2, AREAX, BETAX, SIGX

ELEM1 five-character code name of the first grid block.

ELEM2 five-character code name of the second grid block.

ISOT set equal to 1, 2, or 3 to specify absolute permeability (PER(ISOT)) for the connection between grid blocks ELEM1 and ELEM2, where PER is initially read in block ROCKS. This allows assignment of different permeabilities for different directions. Values of 4 or greater signify an intra block connection for MINC media. MINC subdivisions are numbered consecutively, starting from 1 (fracture) to NMINC, the number of MINC media (2 for fracture- matrix). These intra block connections are between consecutive MINC media (fracture-matrix is MINC medium 1 to 2). ISOT is set to two plus the larger MINC medium number (4 for fracture-matrix connections). The absolute permeability for these connections is the average of the three permeabilities for the larger MINC medium number. Negative ISOT values signify connections needed for the Jacobian matrix but have no fluid flow associated with them. These connections are needed for MINC media. See Section 4.5 for more details.

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

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

where $\sigma_0$ = 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.

<u>Record CONNE.2</u> 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-CSM.

**GRMOD** sets 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 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

Format (A5, 5X,5I10)
TYPE, NUMI, NUMJ, NUMK, KJI0, JMINC

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

Format (A5, I5,6(I10),E10.4)
PROP, ISOT, I1, I2, J1, J2, K1, K2, VALUE

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.

<u>Record GRMOD.2.2</u>

Format (A5, 5X,6(I10),E10.4)
PROP, I1, I2, J1, J2, K1, K2, VALUE

PROP Property identifier, options are:
MFCO2 - mass fraction CO$_2$;
MFSLT - mass fraction NaCl;
POROS - porosity;
PRESS - pressure, Pa;
PVAR2 - primary variable position 2;
PVAR3 - primary variable position 3;
TEMPR - temperature, °C;

STRES - mean stress, Pa.

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.2.3

Format (A5, 5X,6(I10),I10)
PROP, I1, I2, J1, J2, K1, K2, IVALUE

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.

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.

IVALUE Property value.

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 and/or sources.

Record GENER.1

Format (A5, A5, 15X, I5, 5X, A4, A1, 3E10.4)
ELEM, SNAM, LTAB, TYPE, ITAB, GX, EX, HX

ELEM code name of the element containing the sink/source.

SNAM code name of the sink/source. This code name is arbitrary and contains five characters.

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 sinks and sources. 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 source or sink

WATE component 1 (water), injection only

COM1 component 1 (water), injection only

COM2 component 2, injection only

COM3 component 3, injection only

COMn component N, injection only

MASS mass production rate specified.

DELV - well on deliverability, i.e., production occurs against specified bottomhole pressure. If the well is completed in more than one layer, the 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 stress at a specified elevation and temperature, used only for mean 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 stress (Pa); 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; for reference stress calculation, EX is reference temperature; for heat loss against a specified temperature, EX is specified temperature.

HG thickness of layer (m; wells on deliverability with specified bottomhole pressure only). For reference stress calculation, HG is reference elevation (m).

Record GENER.l.l (optional, LTAB > l only)

Format (4E14.7)
Fl(L), L=l, LTAB

F1 generation times

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

Format (4E14.7)
F2(L), L=1, LTAB

F2 generation rates.

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

Format (4E14.7)
F3(L), L=1, LTAB

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-CSM input file and initiates the simulation.

**Note on closure of blocks CONNE, GENER, INCON, and INCNST**

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, SAVE, or SAVEST which have been generated by a previous TOUGH2-CSM run. These files are written exactly according to the specifications of data blocks ELEME and CONNE (file MESH), GENER (file GENER), INCON (file SAVE), and INCNST (file SAVEST), except that the CONNE, GENER, INCON, and INCNST data terminate on a record with "+++" in columns 1-3, followed by some cross-referencing and restart information.

TOUGH2-CSM will accept this type of input, and in this case there is no blank record at the end of indicated data block.

# TOUGH2-CSM INPUT FORMATS

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

| | |
|---|---|
| **TITLE** | |

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

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| **ROCK** | | | | | | | | |
| MAT | NAD | DROK | POR | PERM(1) | PERM(2) | PERM(3) | CWET | SPHT |
| COM | | EXPAN | CDRY | TORTX | GK | | | |
| IRP | | RP(1) | RP(2) | RP(3) | RP(4) | RP(5) | RP(6) | RP(7) |
| ICP | | CP(1) | CP(2) | CP(3) | CP(4) | CP(5) | CP(6) | CP(7) |
| IPOPT | IKOPT | POIRAT | YOUNGM | CBIOT | TREF | SOLMOD | | |
| RCKPAR(1) | | RCKPAR(2) | RCKPAR(3) | RCKPAR(4) | RCKPAR(5) | RCKPAR(6) | RCKPAR(7) | RCKPAR(8) |

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

| | | | | | |
|---|---|---|---|---|---|
| **MULTI** | | | | | |
| NK | NEQ | NPH | NB | ISTCAL | |
| **START** | | | | | |

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

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **PARAM** | | | | | | | | | |
| (1) | (2) | MCYC | MSEC | MCYPR | MOP(I),I=1,24 | | TEXP | BE | |
| TSTART | TIMAX | DELTEN/NDLT | DELTMX | ELST | | GF | REDLT | SCALE | |
| DLT(1) | DLT(2) | DLT(3) | … | … | … | … | … | | |
| … | … | … | … | … | … | DLT(M) | M≤8*NDLT | | |
| RE1 | RE2 | U | WUP | WNR | DFAC | | | | |
| DEP(1) | DEP(2) | DEP(3) | DEP(4) | | | | | | |

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

| | | | |
|---|---|---|---|
| **INDOM** | | | |
| MAT | | | |
| X1 | X2 | X3 | X4 |

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

| | | | |
|---|---|---|---|
| **INCON** | | | |
| ELEM | | PORX | |
| X1 | X2 | X3 | X4 |

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

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| **RCAP** | | | | | | | | |
| IRP | | RP(1) | RP(2) | RP(3) | RP(4) | RP(5) | RP(6) | RP(7) |
| ICP | | CP(1) | CP(2) | CP(3) | CP(4) | CP(5) | CP(6) | CP(7) |

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

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| **ELEM** | | | | | | | | |
| ELEM | | MATR | VOLX | AHTX | PMX | X | Y | Z |

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

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| **CONN** | | | | | | | | |
| ELEM | ELEM2 | | ISO | D1 | D2 | AREAX | BETAX | SIG |

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

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **GENER** | | | | | | | | | |
| ELEM | SNAM | | LTA | | TYPE | GX | EX | HX | |
| F1(1) | F1(2) | F1(3) | … | F1(LTAB) | | | | | |
| F2(1) | F2(2) | F2(3) | … | F2(LTAB) | | | | | |
| F3(1) | F3(2) | F3(3) | … | F3(LTAB) | | | | | |

Figure 4.1. TOUGH2-CSM keyword format.

| TOUGH2-CSM INPUT FORMATS (continued) | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| - - - - * - - - - 1 - - - - * - - - - 2 - - - - * - - - - 3 - - - - * - - - - 4 - - - - * - - - - 5 - - - - * - - - - 6 - - - - * - - - - 7 - - - - * - - - - 8 | | | | | | | | | | | | | | | |
| **GRMOD** | | | | | | | | | | | | | | | |
| **COEFS** | | NUMI | | NUMJ | | NUMK | | KJI0 | | JMINC | | | | | |
| PROP | IDIR | I1 | | I2 | | J1 | | J2 | | K1 | | K2 | | VALUE | |
| PROP | | I1 | | I2 | | J1 | | J2 | | K1 | | K2 | | VALUE | |
| PROP | | I1 | | I2 | | J1 | | J2 | | K1 | | K2 | | IVALUE | |
| | | | | | | | | | | | | | | | |
| - - - - * - - - - 1 - - - - * - - - - 2 - - - - * - - - - 3 - - - - * - - - - 4 - - - - * - - - - 5 - - - - * - - - - 6 - - - - * - - - - 7 - - - - * - - - - 8 | | | | | | | | | | | | | | | |
| **DIFFU** | | | | | | | | | | | | | | | |
| FDDIAG(1,1) | | FDDIAG(2,1) | | … | | FDDIAG(NPH,1) | | | | | | | | | |
| FDDIAG(1,2) | | FDDIAG(2,2) | | … | | FDDIAG(NPH,2 | | | | | | | | | |
| - - - - * - - - - 1 - - - - * - - - - 2 - - - - * - - - - 3 - - - - * - - - - 4 - - - - * - - - - 5 - - - - * - - - - 6 - - - - * - - - - 7 - - - - * - - - - 8 | | | | | | | | | | | | | | | |
| **SELEC** | | | | | | | | | | | | | | | |
| IE(1) | IE(1) | IE(1) | IE(1) | IE(1) | IE(1) | IE(1) | IE(1) | IE(1) | IE(1) | IE(1) | IE(1) | IE(1) | IE(1) | IE(1) | IE(1) |
| FE(1) | | FE(1) | | FE(1) | | FE(1) | | FE(1) | | FE(1) | | FE(1) | | FE(1) | |
| FE(1) | | FE(1) | | FE(1) | | … | | | | | | | | FE(8*IE(1)) | |
| - - - - * - - - - 1 - - - - * - - - - 2 - - - - * - - - - 3 - - - - * - - - - 4 - - - - * - - - - 5 - - - - * - - - - 6 - - - - * - - - - 7 - - - - * - - - - 8 | | | | | | | | | | | | | | | |
| **TIMES** | | | | | | | | | | | | | | | |
| ITI | ITE | DELAF | | TINTER | | | | | | | | | | | |
| TIS(1) | | TIS(2) | | … | | | | | | | | | | TIS(ITI) | |
| - - - - * - - - - 1 - - - - * - - - - 2 - - - - * - - - - 3 - - - - * - - - - 4 - - - - * - - - - 5 - - - - * - - - - 6 - - - - * - - - - 7 - - - - * - - - - 8 | | | | | | | | | | | | | | | |
| **FOFT** | | | | | | | | | | | | | | | |
| EOFT | | | | | | | | | | | | | | | |
| | | | | | | | | | | | | | | | |
| **COFT** | | | | | | | | | | | | | | | |
| ECOFT | | | | | | | | | | | | | | | |
| | | | | | | | | | | | | | | | |
| **GOFT** | | | | | | | | | | | | | | | |
| EGOFT | | | | | | | | | | | | | | | |
| | | | | | | | | | | | | | | | |
| **NOVER** | | | | | | | | | | | | | | | |
| **ENDFI** | | | | | | | | | | | | | | | |
| **ENDCY** | | | | | | | | | | | | | | | |

(1)=NOITE
(2)=KDATA
(3)=ITAB

Figure 4.1. TOUGH2-CSM keyword format, continued.

## 4.3 Input Formats for MESHMAKER

The MESHMaker module performs internal mesh generation and processing. This module has not been parallelized and is run on the master processor only. 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. The output for MESHMaker is a text file containing first record ELEM, then volume element data, a blank line, followed by record CONNE, then connection data, and finally a blank line.

There are three submodules 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 subpartition 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 text file MESH. The MINC processing operates on the data in file MESH and outputs a text file called MINC, 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. A summary of the MESHMaker keywords is shown in Figure 4.2.  We shall now separately describe the preparation of input data for the three MESHMaker submodules.

## MESHMAKER - Two-dimensional R-Z Grids

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

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| **MESHM** | | | | | | | | |
| **RZ2D** | | | | | | | | |
| **RADII** | | | | | | | | |
| NRAD | | | | | | | | |
| RC(1) | | RC(2) | RC(3) | … | | | | RC(NRAD) |
| **EQUID** | | | | | | | | |
| NEQU | | DR | | | | | | |
| **LOGA** | | | | | | | | |
| NLOG | | RLOG | DR | | | | | |
| **LAYER** | | | | | | | | |
| NLAY | | | | | | | | |
| H(1) | | H(2) | … | | | | | H(NLAY) |
| | | | | | | | | |

## MESHMAKER - Rectilinear Grids

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

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| **MESHM** | | | | | | | | |
| **XYZ** | | | | | | | | |
| DEG | | | | | | | | |
| **NX** | NO1 | DEL | | | | | | |
| DX(1) | | DX(2) | … | | | | | DX(NO1) |
| **NX** | NO2 | DEL | | | | | | |
| DX(NO1+1) | | DX(NO1+2) | … | | | | | DX(NO1+NO2) |
| **NY** | NO | DEL | | | | | | |
| DY(1) | | DY(2) | … | | | | | DY(NO) |
| **NZ** | NO | DEL | | | | | | |
| DZ(1) | | DZ(2) | … | | | | | DZ(NO) |
| | | | | | | | | |

## MESHMAKER - MINC Processing for Fractured Media

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

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **MESHM** | | | | | | | | | |
| **MINC** | | | | | | | | | |
| **PART** | | | | | | | | | |
| NRAD | | | | | | | | | |
| PART | | TYPE | | DUAL | | | | | |
| J | NVOL | WHER | PAR(1) | | PAR(2) | PAR(3) | PAR(4) | PAR(5) | PAR(6) | PAR(7) |
| VOL(1) | | | VOL(2) | | … | | | | | VOL(NVOL) |
| | | | | | | | | | |

Figure 4.2. MESHMaker keyword format.

### 4.3.1 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 gridblocks 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 grid blocks, the two meshes for RZ2D and RZ2DL are identical. Assignment of inactive grid blocks 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 (gridblock boundaries) in the radial direction.

Record RADII.l

Format(I5)
NRAD

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.

Format(8E10.4)
RC(I), I = 1, NRAD

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

**EQUID**istant introduces data on a set of equal radial increments.

Record EQUID. L

Format(I5, 5X, E10.4)
NEQU, DR

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.

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

Record LOGAR. 1

Format(A5, 5X, 2E10.4)
NLOG, RLOG, DR

NLOG number of additional interface radii desired.
RLOG desired radius of the last (largest) of these radii.
DR reference radial increment: the first ΔR generated will be equal to f • DR, with f internally 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

Format(I5)
NLAY

NLAY number of horizontal grid layers.

Record LAYER.2

Format(8E10.4)
H(I), I = 1, NLAY

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 nonzero 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).

### 4.3.2 Generation of Rectilinear Grids

**XYZ** invokes generation of a Cartesian (rectilinear) mesh.

Record XYZ.1

Format(E10.4)
DEG

DEG angle (in degrees) between the Y-axis and the horizontal. If gravitational acceleration (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

Format(A2, 3X, I5, E10.4)
NTYPE, NO, DEL

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)

Format(8E10.4)
DEL(I), I = 1, NO

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.

### 4.3.3 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. The output from MINC processing is a text file named MINC. This file is renamed MESH when used to simulate fractured or multi-porosity media.

**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.

Format(2A5, 5X, A5)
PART, TYPE, DUAL

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 the 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

Format (2I3, A4, 7E10.4)
J, NVOL, WHERE, (PAR(I), I = 1, 7)

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, 7 holds parameters for fracture spacing (see above).

Record PART.2.1, 2.2, etc.

Format (8E10.4)
(VOL(I), I = 1, NVOL)

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.

## 4.4 Special Input Requirements for TOUGH2-CSM

In some cases, TOUGH2-CSM needs to be run in batch mode. To run a job in batch mode, the user submits a job to a computer and the computer schedules the job in a queue. When the requested number of processors is available, the job will be run. In batch running mode, all data are provided in input files, since run-time communication is not feasible. For both batch and interactive mode, the input files for the parallel run include:

### MESH AND MINC FILES

The purpose of replacing file MESH (or blocks ELEME and CONNE in an input file) with MESHA and MESHB is to reduce the memory requirement for the master processor and to enhance I/O efficiency. Both MESHA and MESHB are binary files. These two files contain all information provided by file MESH. There are two groups of large data blocks within a TOUGH2-CSM mesh file: one with dimensions equal to the number of grid blocks, the other with dimensions equal to the number of connections (interfaces).

### INFILE

This file is in the same data format as a TOUGH2-CSM input file, as discussed in Section 4.2. In this input file, data are organized in blocks that are defined by five-character keywords typed in Columns 1-5. The first record must be a problem title of up to 80 characters. The last record usually is ENDCY. Data records beyond ENDCY will be ignored. The most important data blocks include ROCKS, MULTI, PARAM, ELEME, CONNE, INCON, GENER, and GRMOD. All input data in INFILE are in fixed format and standard metric (SI) units. Detailed information about this file format can be found in Section 4.2

The blocks of ELEME, CONNE, GENER and INCON can be extremely large. It is good practice to provide these blocks through separate data files. An alternative input for ELEME and CONNE blocks is through the MESH file or through two binary files: MESHA and MESHB. The two binary files are intermediate files which are created by TOUGH2-CSM during its first run for a model. If MESHA and MESHB exist in the working folder, the code will ignore MESH file and read information directly from these two files. If the mesh is changed, MESHA and MESHB must be deleted from the working folder to make the changes take effect. The two files have completely different data formats from the ELEME and CONNE blocks. The detailed format information is given in the following.

**MESHA, MESHB**

The purpose of replacing file MESH (or blocks ELEME and CONNE in an input file) with MESHA and MESHB is to reduce the memory requirement for the master processor and to enhance I/O efficiency. Both MESHA and MESHB are binary files. These two files contain all information provided by file MESH. There are two groups of large data blocks within a TOUGH2-CSM mesh file: one with dimensions equal to the number of grid blocks, the other with dimensions equal to the number of connections (interfaces). To read and use computer memory efficiently, the input data are organized in sequential and binary format. Large data blocks are read one by one through a temporary full-size array and then distributed to processors one by one. This method avoids storing all input data in one single processor and enhances the I/O efficiency and total storage capacity.

The file MESHA is written (to file unit 20 that was opened as an unformatted file) in the following sequence:

```
write(20) NEL,NCON
write(20) (EVOL(iI),iI=1,NEL)
write(20) (AHT(iI),iI=1,NEL)
write(20) (PMX(iI),iI=1,NEL)
write(20) (GCOORD(iI,1),iI=1,NEL)
write(20) (GCOORD (iI,2),iI=1,NEL)
write(20) (GCOORD (iI,3),iI=1,NEL)
write(20) (IMINC(iI),iI=1,NEL)
write(20) (DEL1(iI), iI=1,NCON)
write(20) (DEL2(iI), iI=1,NCON)
write(20) (AREA(iI), iI=1,NCON)
write(20) (BETA(iI), iI=1,NCON)
write(20) (SIG(iI), iI=1,NCON)
write(20) (ISOX(iI),iI=1,NCON)
write(20)(ELEM1(iI), iI=1,NCON)
write(20)(ELEM2(iI), iI=1,NCON)
```

where

NEL total gridblock number, in 8-byte integer.

NCON total connection number, in 8-byte integer.

EVOL element volume (m$^3$), in 8-byte real

AHT interface area (m$^2$) for heat exchange with semi-infinite confining beds, in 8-byte real.

PMX permeability modifier, in 8-byte real.

GCOORD cartesian coordinates (X=1,Y=2,Z=3) of gridblock center, in 8-byte real.

IMINC MINC continuum number, in 8-byte integer.

DEL1, DEL2 distance (m) from first and second element, respectively, to their common interface, in 8-byte real.

AREA interface area (m$^2$), in 8-byte real.

BETA cosine of the angle between the gravitational acceleration vector and the line between two elements, in 8-byte real.

SIG "radiant emittance" factor for radiative heat transfer, in 8-byte real.

ISOX specify absolute permeability for the connection, in 4-byte integer.

ELEM1 code name for the first element of a connection, in 5 characters.

ELEM2 code name for the second element of a conection, in 5 characters.

The file MESHB is written (to file unit 30, unformatted) in the following sequence:

```
write(30) NCON,NEL
write(30) (ELEM(iI),iI=1,NEL)
write(30) (MA12(iI),iI=1,NEL)
write(30) (NEX1(iI),iI=1,NCON)
write(30) (NEX2(iI),iI=1,NCON)
```

where

ELEM code name of the element, in 5 characters.

MA12 material identifier of the element, in 5 characters.

NEX1, NEX2 first and second element number of the connection, in 4-byte integer.

MESHA and MESHB can also be created directly from MESH file through a preprocessing program. For extremely large problems, generation of MESHA and MESHB is the bottleneck of memory requirement for a simulation using TOUGH2-CSM. By using a preprocessing program, the bottleneck for memory requirement can be avoided.

**PARAL.prm**

PARAL.prm is an optional file providing TOUGH2-CSM some parameters. If this file does not exist in the working folder, the code will take default parameters. These parameters are needed if a user wants to try different options with the parallel linear solver, partitioning algorithms, and main program. The following is an example of the file.

```
1008680, 4000000, 0
AZ_solver AZ_bicgstab
AZ_scaling AZ_BJacobi
AZ_precond AZ_dom_decomp
AZ_tol 1.0e-6
AZ_overlap 0
AZ_max_iter 250
```

```
AZ_conv AZ_rhs
AZ_subdomain_solve AZ_ilut
AZ_output AZ_none
EE_partitioner METIS_Kway
EE_output 100
END OF INPUTS
```

The three numbers at first line are:

MNEL: Estimated total gridblocks, must be larger than model gridblock number.

MCON: Estimated total connections, must be larger than model connection number.

PartReady: A parameter to inform the program that domain partitioning was done by a preprocessing program or will be done inside TOUGH2-CSM. If PartReady=0, the parallel code will perform domain partitioning during running the code. If PartReady>0, the code will not perform domain partitioning and partition data will be read directly from file “part.dat” at the working directory. Default PartReady=0.

The default values of MNEL and NCON are 500,000 and 2,300,000. The two parameters are required only in generating MESHA and MESHB and when a model has more than 500,000 gridblocks or 2,300,000 connections.

From the second line and below, each line provides a parameter. These parameters give options or parameters for running the Aztec and METIS packages, and SAVE and SAVEST file output frequency control. The parameters can be in any order. If one parameter is not present, its default value will be used. Each line in the file consists of two terms. The first term is parameter’s name and the second term is its value. Detailed content of the parameters is discussed below.

AZ_solver specifies solution algorithm, available solvers:

AZ_cg conjugate gradient (only applicable to symmetric positive definite matrices).

AZ_gmres restarted generalized minimal residual.

AZ_cgs conjugate gradient squared.

AZ_tfqmr transpose-free quasi-minimal residual.

AZ_bicgstab bi-conjugate gradient with stabilization.

AZ_lu sparse direct solver (single processor only).

AZ_scaling specifies scaling algorithm, user can select from:

AZ_none no scaling.

AZ_Jacobi point Jacobi scaling.

AZ_BJacobi block Jacobi scaling where the block size corresponds to the VBR blocks.

Az_row_sum scale each row so the magnitude of its elements sum to 1.

AZ_sym_diag symmetric scaling so diagonal elements are 1.

AZ_sym_row_sum symmetric scaling using the matrix row sums.

AZ_precond specifies preconditioner. Available selections include:

AZ_none no preconditioning.

AZ_Jacobi k step Jacobi (or block Jacobi for DVBR matrices).

AZ_Neumann Neumann series polynomial.

AZ_ls least-squares polynomial.

AZ_sym_GS non-overlapping domain decomposition (additive Schwarz) k step symmetric Gauss-Seidel.

AZ_dom_decomp domain decomposition preconditioner (additive Schwarz).

AZ_tolspecifies tolerance value used in conjunction with convergence tests.

AZ_type_overlap determines how overlapping subdomain results are combined when different processors have computed different values for the same unknown. Available selections include:

- AZ_standard the resulting value of an unknown is determined by the processor owning that unknown.
- AZ_symmetric average the results obtained from different processors corresponding to the same unknown.

AZ_overlap determines the submatrices factored with the domain decomposition algorithms.

AZ_max_iter maximum number of iterations.

AZ_conv determines the residual expression used in convergence check and printing. Available selections include: AZ_r0, AZ_rhs, AZ_Anorm, AZ_noscaled, AZ_sol, AZ_weighted.

AZ_subdomain_solve specifies the solver to use on each subdomain when AZ_precond is set to AZ_dom_decomp, available selections include: AZ_lu, AZ_ilut, AZ_ilu, AZ_rilu, AZ_bilu, and AZ_icc.

AZ_reorder determines whether RCM reordering will be done in conjunction with domain decomposition incomplete factorizations, 1 yes; 0 no.

AZ_pre_calc indicates whether to use factorization information from previous calls to AZ_solve, three selections: AZ_calc, AZ_recalc, and AZ_reuse.

AZ_output specifies information to be printed, available selections: AZ_all, AZ_none, AZ_warnings, AZ_last, and >0.

EE_partitioner specifies the partitioner to be used, user can select partitioners from:

METIS_Kway uses the multilevel k-way partitioning algorithm. The objective of this partitioning method is to minimize the edgecut. It should be used to partition a graph into a large number of partitions (greater than 8).

METIS_Vkway uses the multilevel k-way partitioning algorithm. The objective of this partitioning method is to minimize the total communication volume.

METIS_Recursive uses multilevel recursive bisection. The objective of this partitioning method is to minimize the edgecut, this function should be used to partition a graph into a small number of partitions (less than 8).

EE_output Output control for solution results. The SAVE file will be written every EE_output time steps. If EE_output=0, no SAVE file will be written out until last time step. A special value of 666888 for this parameter will evoke debugging run, which will produce more informative output.

More options or parameters for the Aztec parallel linear equation solver can be specified. For further discussion, readers may refer to Tuminaro et al. (1999). Table 4-2 presents the default values used in TOUGH2-CSM

Table 4-2. Default values of the options and parameters

| Parameters or options | Values |
|---|---|
| AZ_solver | AZ_bicgstab |
| AZ_scaling | AZ_Bjacobi |
| AZ_pecond | AZ_dom_decomp |
| AZ_tol | $1x10^{-6}$ |
| AZ_type_overlap | AZ_standard |
| AZ_max_iter | 500 |
| AZ_conv | AZ_r0 |
| AZ_subdomain_solve | AZ_ilut |
| AZ_reorder | 1 |
| AZ_pre_calc | AZ_calc |
| AZ_output | AZ_none |
| EE_partitioner | METIS_Kway |
| EE_output | 200 |

## INCON

During initialization of a TOUGH2-CSM run, all grid blocks are first assigned to the default thermodynamic conditions specified in data block PARAM in file INFILE. The default initial conditions may be superseded by thermodynamic conditions assigned to individual grid blocks in disk file INCON.

The INCON file is set up either by the user or generated by a previous TOUGH2-CSM run through an output file SAVE (compatible with formats of file or data block INCON for initializing a continuation run). The INCON file can be obtained by simply renaming SAVE file to INCON. If the INCON file is set up by the user the grid blocks must be entered sequentially. Thermodynamic conditions specified in INCON or data block PARAM are overwritten by those specified in the GRMOD section of the INFILE. These thermodynamic conditions do not include mean stress, which is discussed below.

## INCNST FILE

Mean stress can be initialized in three ways: specification in the GRMOD section of the INFILE, assigned to individual grid blocks using the INCNST file, a companion file to INCON, or calculated from a reference mean stress and temperature at a given elevation using the RSTR option in the GENER section.

The INCNST file is set up either by the user or generated by a previous TOUGH2-CSM run through an output file SAVEST (a companion file to SAVE and compatible with formats of file INCNST for initializing a continuation run). The INCNST file can be obtained by simply renaming SAVEST file to INCNST. If the INCNST file is set up by the user the grid blocks must be entered sequentially. Thermodynamic conditions specified in INCNST are overwritten by those specified in the GRMOD section of the INFILE.

Use of the RSTR option in the GENER section is described elsewhere.

**GENER**

The format of file GENER is the same as the block format described in Section 4.2.

**part.dat**

If parameter “PartReady” in “PARAL.prm” has a value larger than 0, the parallel code will read file “part.dat” from working directory during run-time. The file contains domain-partitioning results. It is read by the following code:

```
        open (unit=50,file='part.dat',form='formatted',status='old')
        read(50,133) nparts,edgecut,NEL
        read(50,144) (part(iI),iI=1,NEL) 133 format(3I10)
  133   format(3I10)
  144   format(10I8)
```

where

nparts number of portions, equal to the number of processors used, that the domain has been partitioned into.

edgecut number of cut edges.

nel total number of gridblocks in the simulation domain.

part partition for each gridblock, an integer value indicating the processor associated with each gridblock.

The file “part.dat” can be generated by the user through a preprocessing program.

## 4.5 MINC File Configuration

In Section 4.3.3, the MINC preprocessor data requirements are described. A MESH file (or blocks ELEME and CONNE in an input file) containing primary grid information is input to the preprocessor and the output from the preprocessor is a file called MINC, a form of MESH file, that contains grid block and connection information for the fractured or multi-porosity grid created from the primary one. Subdivision of a primary grid into a MINC one with three subdivisions (NMINC=3) is illustrated in Figure 4.3.

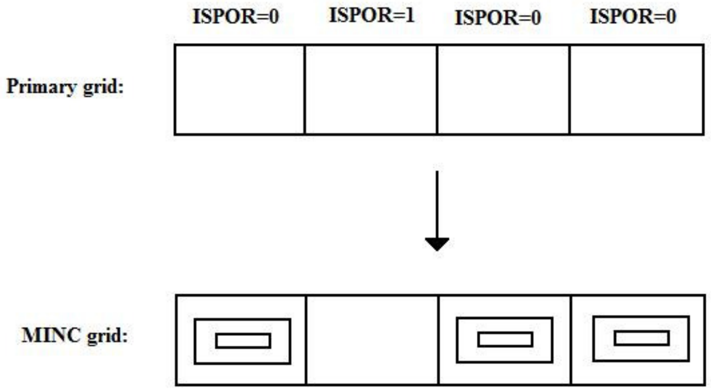


Figure 4.3: Subdivision of primary grid into a MINC one with NMINC=3 and one grid block that is not subdivided (ISPOR=1).

Grid blocks with ISPOR=0 are subdivided into three MINC blocks, and those with ISPOR=1 are not subdivided. MINC block numbering is shown in Figure 4.4 with the numbering starting at the outermost block.

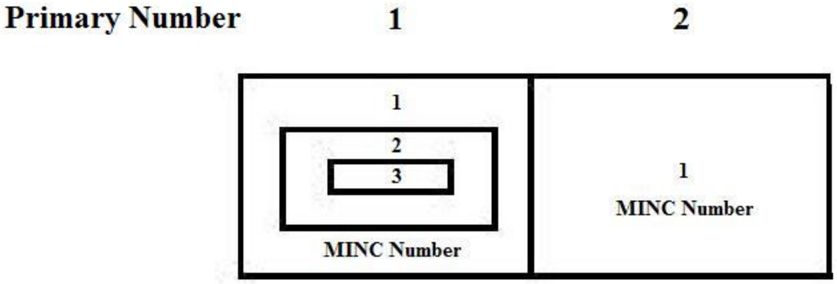


Figure 4.4. Primary and MINC numbering for the two leftmost grid blocks in Figure 4.3. The MINC numbering of the rest of those in Figure 4.1 is identical to the left one shown.

Adjacent MINC subdivisions within a primary grid block are connected. For primary grid block 1 in Figure 4.2, for example, MINC blocks 1 and 2, and 2 and 3, are connected. These connections are written to the MINC file with ISOT equals 2 plus the connection's larger MINC subdivision number, or 4 and 5, respectively. Connections between primary grid block pairs give rise to connections in the MINC file as well. For the configuration shown in Figure 4.5,

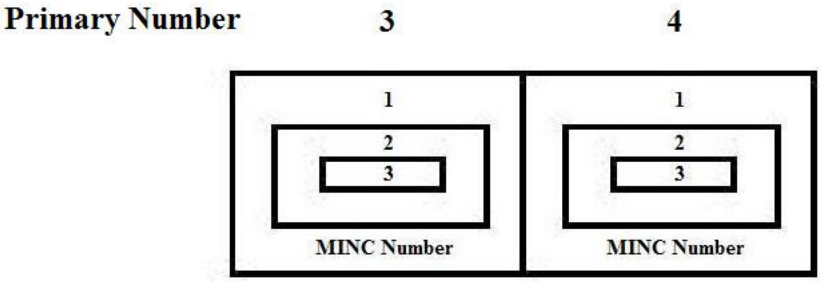


Figure 4.5. Primary and MINC numbering for the two rightmost grid blocks in Figure 4.3.

MINC subdivisions 1 are connected (dual porosity model) or like MINC subdivisions are connected (dual permeability model). These connections are written to the MINC file with ISOT specifying absolute permeability (PER(ISOT)) for the direction associated with the connection. For the configuration shown in Figure 4.2, MINC subdivisions 1 are connected (dual porosity model) or MINC subdivision1 of primary grid block 2 is connected to each MINC subdivision of primary grid block 1 (dual permeability model) . These flow connections are written to the MINC file with ISOT specifying absolute permeability (PER(ISOT)) for the direction associated with the connection.

Additional connections are written to the MINC file due to the presence of volumetric strain in Equations 2.41 and 2.42. Volumetric strain (as well as mean stress) is only assigned to primary grid blocks and depends on MINC subdivision pressures and temperatures from Equation 2.40. Connection terms contain volumetric strain from both primary grid blocks and accumulation terms contain volumetric strain from the primary grid block. Consequently, the Jacobian matrix needs connections between a MINC subdivision and every other MINC subdivision in the primary grid block, and between a MINC subdivision and every other MINC subdivision in the other primary grid blocks connected to its primary grid block. These connections that have not previously been written to the MINC file are written to it with negative ISOT (the magnitude being unimportant). Two examples of these connections are: between MINC subdivisions 1 and 3 in primary grid block 1 in Figure 4.2; and between primary grid block 2, MINC subdivision 3 and primary grid block 3, MINC subdivision 2 in Figure 4.3.

### 4.6 Output from TOUGH2-CSM

TOUGH2-CSM produces a variety of output, most of which can be controlled by the user. Information written in the initialization phase on 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, the parallel program can optionally generate a brief message for Newtonian iterations and time steps. At the end, a summary of subroutines used and parallel computation information are provided. In TOUGH2-CSM, standard output at user-specified simulation times or time steps is generated by a subroutine called FINALOUT, contained in the EOS module. The output files in TOUGH2-CSM are named OUTPUT and OUTPUT_DATA. The first file provides problem initialization, time-stepping, and parallel computing information, and the second file gives a complete report of grid block thermodynamic state variables and other important parameters. Grid block output from each processor is assembled into one for the global grid.

```
EEE
EEE
EEE  Number of processors =            8
EEE Time perform model computaion  =    36.9248681068420
EEE   of which spent in lin. solv. =    25.6461408138275
EEE   and spent on other           =    11.2787272930145
EEE
EEE Total number of time steps =           49
EEE Average time in Aztec per time step =   0.523390628853623
EEE Average time spent on other per time step =   0.230178108020705
EEE
EEE Total number Newton steps =          110
EEE Average number of Newton steps per time step   2.24489795918367
EEE Average time per Newton step =   0.233146734671159
EEE Average time spent on other per Newton st =   0.102533884481950
EEE
EEE Total number of iter in Aztec =         6686
EEE Average number of iter per call to Aztec   60.7818181818182
EEE Average time per iter in Aztec =   3.835797309875488E-003
EEE
EEE Partitioning algorithm used: METIS_Kway
EEE Number of edges cut =         2411
EEE
EEE Average number elements per proc =    2050.00000000000
EEE Maximum number elements at any proc =         2085
EEE Minimum number elements at any proc =         1990
EEE Allocated LNEL =         2727
EEE Average number connections per proc =    6196.37500000000
EEE Minimum number connections at any proc =         6048
EEE Maximum number connections at any proc =         6404
EEE Allocated LMNCON =         6404
EEE
EEE Average number of neighbors per proc =    4.25000000000000
EEE Maximum number of neighbors at any proc =            6
EEE Minimum number of neighbors at any proc =            3
EEE
EEE Average number of external elem. per proc =    521.500000000000
EEE Maximum number of external elem. per proc =          651
EEE Minimum number of external elem. per proc =          404
EEE
EEE Maximum size for local matrix (in Kbyte) =    1193.00000000000
EEE Maximum size data in matvec (in Kbyte) =    1305.00000000000
EEE
EEE  ====
EEE
EEE Linear Solver Used: BICGSTAB
EEE Scaling method: No Scaling
EEE Preconditioner: Domain Decomposition
EEE    with overlap type: Standard
EEE    and size of overlap:           0
EEE    and subdomain solver: ILUT
EEE    without RCM reordering
EEE Residual norm: ||r||2 / ||b||2
EEE Max. number of iterations:         250
EEE Tolerance:  1.000000000000000E-006
EEE  ============================================
EEE
EEE
```

Figure 4-1 Example for output of parallel computing information

The parallel computing information is written out near the end of OUTPUT file. Figure 4-1 shows an example of a portion of the output. The output provides detailed information of the number of processors used, timing for tasks, code performance for each time step, Newton iteration, and linear iteration, algorithm used for domain partitioning, and domain decomposition results. At the end of the list in Figure 4-1, linear solver, preconditioner, and options and parameters selected for solving the linear equations are presented. This information is very important for evaluating the parallel code performance.

Some informative output generated by other than master processor is written to fort.36. The user may get additional information for the program run from this file. Other output files include SAVE, SAVEST, and FOFT_P.xxx. The SAVE contains primary variables for a restart run, and has the same format as INCON; the SAVEST contains primary variables related to mean stress calculation for a restart run, and has the same format as INCNST.  The requested time-dependent data for gridblocks (identified with FOFT), connections (COFT), and source/sinks (GOFT) are written out to file FOFT_P.xxx. The extension name xxx is a number indicating the processor number by which the file is written. TOUGH2-CSM can generate multiple time-dependent data output from different processors.

# 5. PRIMARY VARIABLE INITIALIZATION

Primary variables are initialized at the start of a simulation. These variables, for the ECO2N fluid property module, are pressure, $CO_2$ mass fraction or saturation, salt mass fraction or solid salt saturation, temperature, and mean stress. Primary variables besides mean stress can be initialized in record PARAM.4 for the entire simulation domain, in record INDOM for each material region, or in GRMOD for selected grid block intervals. Mean stress can be initialized as well in GRMOD for selected grid block intervals. For these initialization modes, primary variable values are arbitrary.

In many instances, it is desirable for the simulation initialization to be hydrostatically stable such that if the system were isolated, the primary variables would not change over time. Assignment by value of primary variables results in a hydrostatically stable system only in a limited number of cases, for example, initializing as constant pressure and mean stress in a system without gravity. In what follows, the procedure for initialization of a hydrostatically stable system with gravity present is described.

## 5.1 Hydrostatic Stability

In a hydrostatically stable system, the primary variables would not change over time if the system were isolated. Primary variable change in an isolated system would result from mass, energy, or momentum, fluxes in the system, and a hydrostatically stable system would require these fluxes to be zero throughout the simulation domain. The condition for zero mass flux is zero fluid flow potential. For phase *l*:

$$\nabla P + \nabla P_{c,l} - \rho_l \bar{g} = 0 \qquad (5.1)$$

If diffusion is included then concentration gradients would be zero as well. The condition for zero energy flux is zero temperature gradient.

$$\nabla T = 0 \qquad (5.2)$$

The condition for zero momentum flux is obtained from the momentum equation (Equation 2.10):

$$\frac{3(1-\nu)}{1+\nu}\nabla\tau_m + \bar{F}_b - \frac{2(1-2\nu)}{1+\nu}\nabla[\alpha P + 3\beta K T] = 0 \tag{5.3}$$

For multiple porosity systems, we assume primary variables of MINC subdivisions are all identical.

### 5.2 TOUGH2-CSM Implementation

We generate a set of hydrostatically stable primary variables by running a TOUGH2-CSM simulation with the INFILE modified. We do not solve for mean stress. If we originally intended to solve for it, we set ISTCAL in the MULTI section to zero and NEQ to one less. We remove the contents of the GENER Section and replace them with a deliverability well (DELV option) that produces fluid against a reference pressure in a reference grid block. We assign pressures to all grid blocks, corrected for depth, that are higher than the reference pressure. We run this simulation, where fluid is produced through the deliverability well, until equilibrium at which flow potential satisfies Equation 5.1 and temperature and concentration gradients (if we are solving the energy equation and if there is diffusion, respectively) are zero. The SAVE file from this simulation contains the equilibrated primary variables and is used for primary variable initialization in out actual simulation by renaming it INCON and replacing the bottom three lines with a blank one. We restore the original contents of the GENER Section and if mean stress is solved for, we set ISTCAL in the MULTI section to one and NEQ to the original value. Mean stress initialization is calculateded in TOUGH2-CSM by solving Equation 5.3 with a reference mean stress (and temperature) specified at a reference elevation. This data are input using the RSTR option in the GRMOD Section. In this mean stress initialization, other primary variables are considered to be constant and would be specified in the INCON file.

# 6. SAMPLE PROBLEMS

Five sample problems are included with the TOUGH2-CSM user's manual. These problems may be used as benchmarks for testing the code's performance on their computers and the input data files can be used as templates to facilitate preparation of input data for new simulations. The first two problems, simulation of one-dimensional consolidation of a double-porosity medium and simulation of the Mandel-Cryer effect, are compared with analytical solutions. The rest are comparisons of TOUGH2-CSM to published simulations. The third, simulation of $CO_2$ injection into a layered aquifer, is run without solving the momentum equation. The fourth, In Salah Gas Project simulation, is a simulation of $CO_2$ injection into a depleted gas field and features a match of simulated surface uplift. Finally, the fifth is a simulation of deformation and fluid circulation in a volcanic caldera structure in which the mass, momentum, and energy equations are solved. This problem uses the EOS2 fluid property module; the others use the ECO2N module.

## 6.1 One-Dimensional Consolidation of Double-Porosity Medium

### 6.1.1 Problem Description

In this one-dimensional consolidation problem, a z-direction stress is applied to the top of a fluid-filled double-porosity (fracture and matrix) rock column, instantaneously inducing a deformation and a pore pressure increase. Fluid then is allowed to drain out of the column top and the pore pressure increase dissipates. An analytical solution to this problem was presented by Wilson and Aifantis (1982). In their analysis, strain is uniaxial and z-direction stress is constant throughout the process.

We simulated this problem is two steps. The first step was the load application to produce the pore pressure increase. We started from an unstrained state where pore pressures (fracture and matrix) and mean stress were both equal ($\tau_{m,0} = P_{1,0} = P_{2,0}$) and imposed a greater mean stress at the column top ($\tau_{m,1}$) that induced a pore pressure increase ($P_{j,1}$) in the column after the system equilibrated. For uniaxial deformation in an isothermal, double-porosity system, mean stress, z-direction stress, and pore pressures are related by:

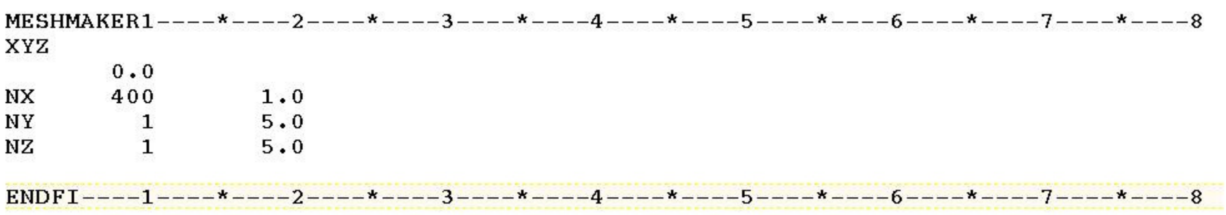
$$\tau_m = \frac{1}{3}\frac{(1+\nu)}{(1-\nu)}\left(\tau_{zz} - \sum_j \alpha_j P_j\right) + \sum_j \alpha_j P_j \qquad (6.1)$$

Using Equation 6.1, we calculated the constant z-direction stress ($\tau_{zz,0}$) from the imposed mean stress ($\tau_{m,1}$) and the equilibrated pore pressures ($P_{j,1}$).

The second step was simulation of fluid drainage. The column was initially at the above equilibrated state. We set the pore pressures at the column top to the initial pore pressures ($P_{j,0}$). We also set the mean stress at the column top to that calculated from Equation 6.1 using the constant z-direction stress ($\tau_{zz,0}$) and the initial pore pressures. Fluid then drained out of the column top as the pore pressures in the column returned to the initial values.

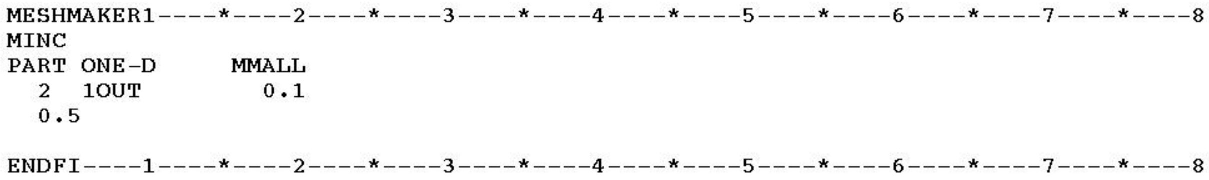
### 6.1.2 TOUGH2-CSM Simulation Details

Our simulation domain is one-dimensional and 400 m long. We discretized this domain into a uniform primary grid containing 400 grid blocks. We created the grid's MESH file by running TOUGH2-CSM with the INFILE shown in Figure 6.1. Using this MESH file as input, we then ran TOUGH2-CSM with the INFILE shown in Figure 6.2 to generate the MINC file for the double porosity grid. Each grid block of the primary grid is subdivided into two porous continua, fracture and matrix, with the same volume. The MINC grid is dual permeability; each primary grid connection spawns a fracture-fracture and a matrix-matrix connection, and there is a fracture-matrix connection for each primary grid block. We renamed this MINC file MESH in order to run the double porosity simulation.



```
MESHMAKER1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
XYZ
       0.0
NX     400       1.0
NY       1       5.0
NZ       1       5.0

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

Figure 6.1. INFILE for primary grid generation.

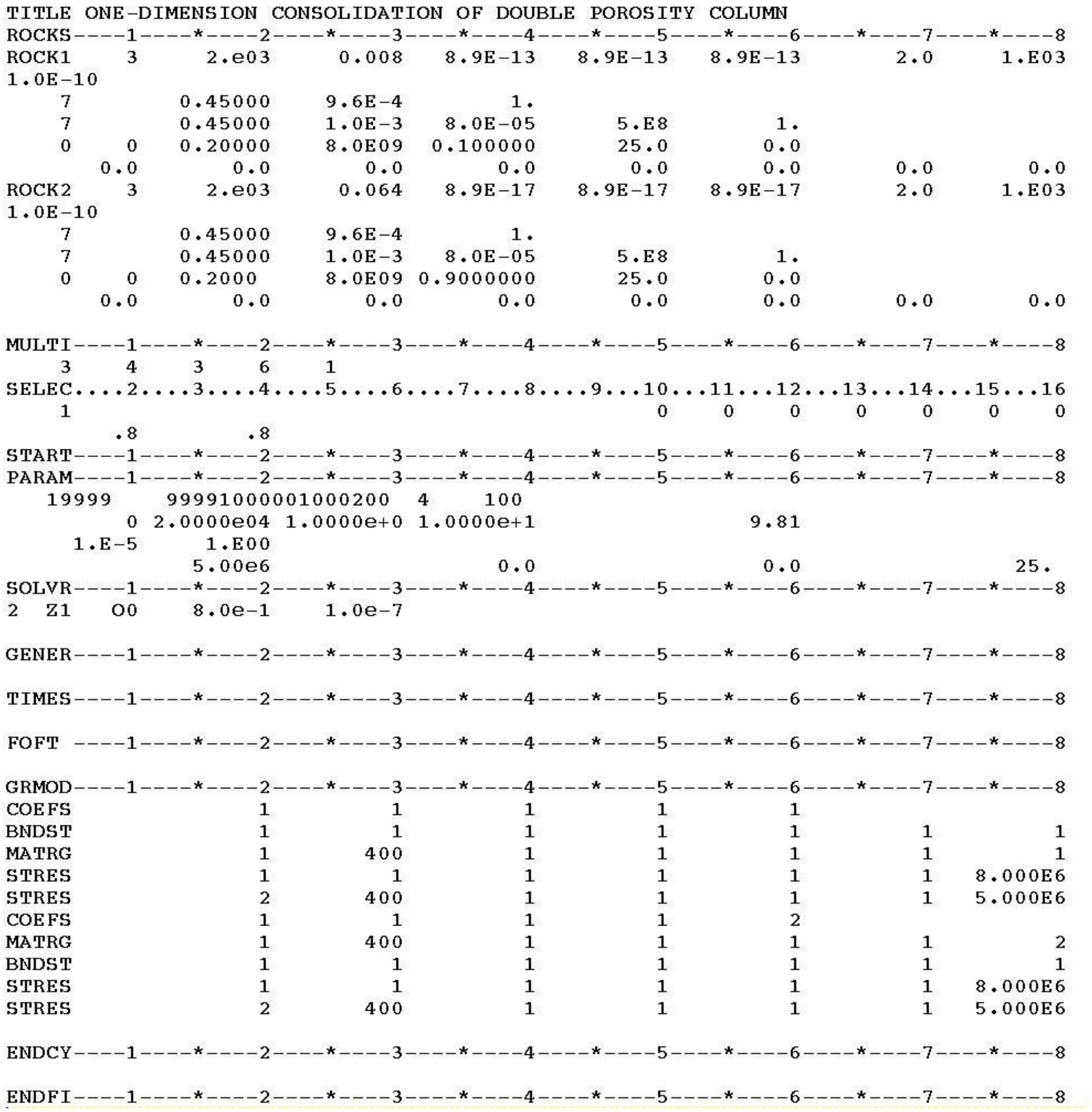


```
MESHMAKER1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
MINC
PART ONE-D      MMALL
  2  1OUT         0.1
  0.5

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

Figure 6.2 INFILE for MINC grid generation.

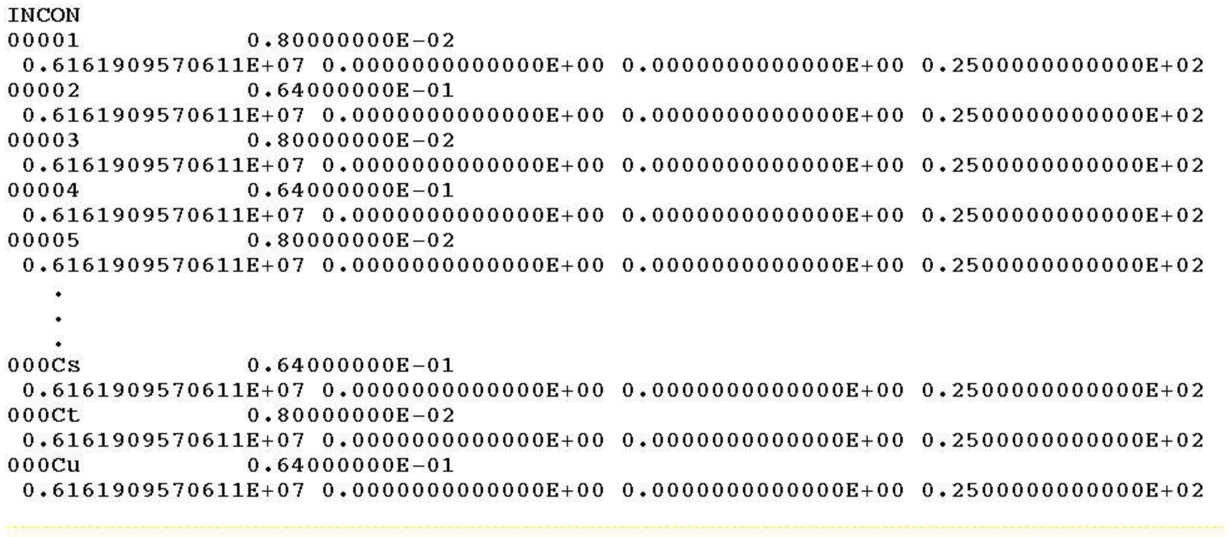
We next simulated the load application. The INFILE is shown in Figures 6.3. Material domain properties are entered in the ROCKS section with domain 1, ROCK1, being the fractures and domain 2, ROCK2, the matrix. The MULTI section contains the number of primary variables and the flag indicating that mean stress is a primary variable, (NEQ=4 and ISTCAL=1, respectively, in Figure 4.1). The GENER section is empty since there are no sources or sinks. Properties are assigned to grid block ranges in the GRMOD section with the first COEFS record specifying fracture grid blocks (JMINC=1) and the second matrix grid blocks (JMINC=2). Material region is assigned using the MATRG keyword, mean stress is assigned using the STRES keyword with mean stress at the top (grid block 1) at 8•$10^6$ Pa and the rest at 5•$10^5$ Pa. The external force is applied to the system top so the top fracture and matrix grid blocks are connected to the surroundings using the BNDST keyword with a value of one.

Finally, we simulated fluid drainage. The load application simulation output a SAVE file that was renamed INCON and the bottom three lines were replaced with a blank line. The INCON file, shown in Figure 6.4, contains porosity and primary variables (except mean stress) for all grid blocks, including the equilibrated pore pressures, and a blank line at the bottom. These primary variables are initial values for the fluid drainage simulation. The INFILE for the fluid drainage simulation is shown in Figure 6.5. Grid blocks *00001* and *00002* (fracture and matrix the top grid block) contain deliverability wells at the initial pore pressure through which the system drained. Mean stress is initialized in the GRMOD section with those top grid blocks set to the value calculated from Equation 6.1 using the applied z-direction stress and the initial pore pressure (7.4•$10^6$ Pa). The rest are initialized with the uniform mean stress from the end of the load application simulation (8•$10^5$ Pa). Comparison of simulated fracture pressure with the analytical solution is shown in Figure 6.6, with excellent agreement.



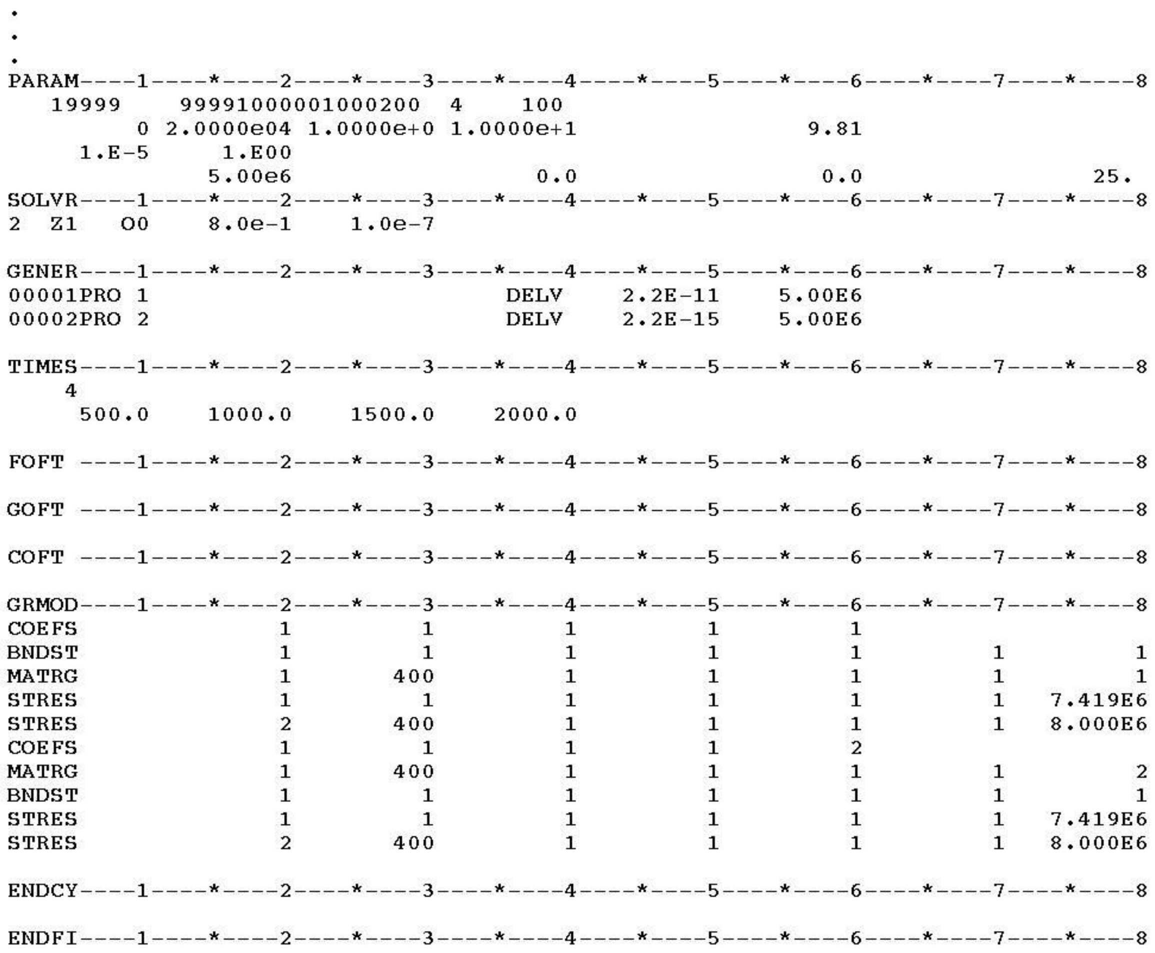
```
TITLE ONE-DIMENSION CONSOLIDATION OF DOUBLE POROSITY COLUMN
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
ROCK1    3     2.e03     0.008   8.9E-13   8.9E-13   8.9E-13       2.0     1.E03
1.0E-10
    7        0.45000    9.6E-4        1.
    7        0.45000    1.0E-3   8.0E-05      5.E8        1.
    0    0   0.20000    8.0E09  0.100000      25.0       0.0
       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0
ROCK2    3     2.e03     0.064   8.9E-17   8.9E-17   8.9E-17       2.0     1.E03
1.0E-10
    7        0.45000    9.6E-4        1.
    7        0.45000    1.0E-3   8.0E-05      5.E8        1.
    0    0   0.2000     8.0E09 0.9000000      25.0       0.0
       0.0       0.0       0.0       0.0       0.0       0.0       0.0       0.0

MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    3    4    3    6    1
SELEC....2....3....4....5....6....7....8....9...10...11...12...13...14...15...16
    1                                            0    0    0    0    0    0    0
        .8        .8
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   19999     99991000001000200 4    100
         0 2.0000e04 1.0000e+0 1.0000e+1                    9.81
     1.E-5     1.E00
              5.00e6                 0.0                 0.0                25.
SOLVR----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
2  Z1   O0    8.0e-1    1.0e-7

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

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

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

GRMOD----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
COEFS              1         1         1         1         1
BNDST              1         1         1         1         1         1         1
MATRG              1       400         1         1         1         1         1
STRES              1         1         1         1         1         1   8.000E6
STRES              2       400         1         1         1         1   5.000E6
COEFS              1         1         1         1         2
MATRG              1       400         1         1         1         1         2
BNDST              1         1         1         1         1         1         1
STRES              1         1         1         1         1         1   8.000E6
STRES              2       400         1         1         1         1   5.000E6

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

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

Figure 6.3. INFILE for load application simulation.



```
INCON
00001           0.80000000E-02
 0.6161909570611E+07 0.0000000000000E+00 0.0000000000000E+00 0.2500000000000E+02
00002           0.64000000E-01
 0.6161909570611E+07 0.0000000000000E+00 0.0000000000000E+00 0.2500000000000E+02
00003           0.80000000E-02
 0.6161909570611E+07 0.0000000000000E+00 0.0000000000000E+00 0.2500000000000E+02
00004           0.64000000E-01
 0.6161909570611E+07 0.0000000000000E+00 0.0000000000000E+00 0.2500000000000E+02
00005           0.80000000E-02
 0.6161909570611E+07 0.0000000000000E+00 0.0000000000000E+00 0.2500000000000E+02
   .
   .
   .
000Cs           0.64000000E-01
 0.6161909570611E+07 0.0000000000000E+00 0.0000000000000E+00 0.2500000000000E+02
000Ct           0.80000000E-02
 0.6161909570611E+07 0.0000000000000E+00 0.0000000000000E+00 0.2500000000000E+02
000Cu           0.64000000E-01
 0.6161909570611E+07 0.0000000000000E+00 0.0000000000000E+00 0.2500000000000E+02
```

Figure 6.4. INCON file containing initial primary variables (except mean stress) and porosity.



```
.
.
.
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   19999    99991000001000200  4    100
         0 2.0000e04 1.0000e+0 1.0000e+1                9.81
     1.E-5    1.E00
              5.00e6                 0.0                 0.0                25.
SOLVR----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
2  Z1   O0    8.0e-1    1.0e-7

GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
00001PRO 1                         DELV    2.2E-11    5.00E6
00002PRO 2                         DELV    2.2E-15    5.00E6

TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    4
     500.0     1000.0     1500.0     2000.0

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

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

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

GRMOD----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
COEFS              1         1         1         1         1
BNDST              1         1         1         1         1         1         1
MATRG              1       400         1         1         1         1         1
STRES              1         1         1         1         1         1   7.419E6
STRES              2       400         1         1         1         1   8.000E6
COEFS              1         1         1         1         2
MATRG              1       400         1         1         1         1         2
BNDST              1         1         1         1         1         1         1
STRES              1         1         1         1         1         1   7.419E6
STRES              2       400         1         1         1         1   8.000E6

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

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

Figure 6.5. INFILE for fluid drainage simulation.  Portion above PARAM keyword is identical to that in Figure 6.3.

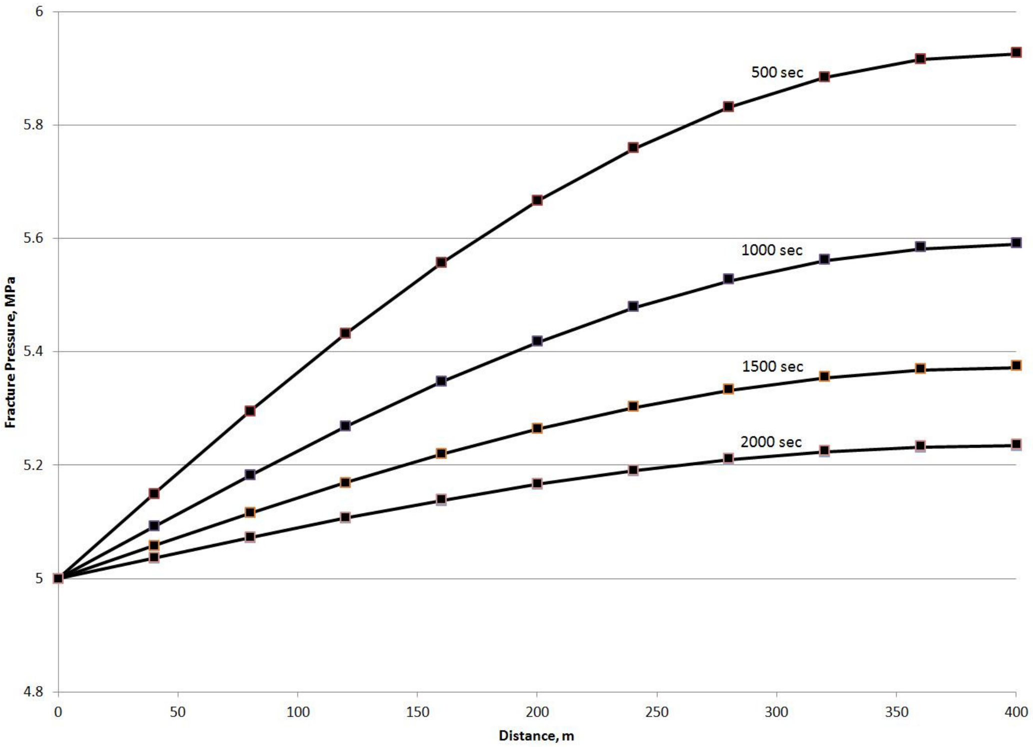


Figure 6.6. Comparison of fracture pressure analytical solution (solid lines) to simulation (points) for one-dimensional consolidation of double-porosity column

## 6.2 Mandel-Cryer Effect

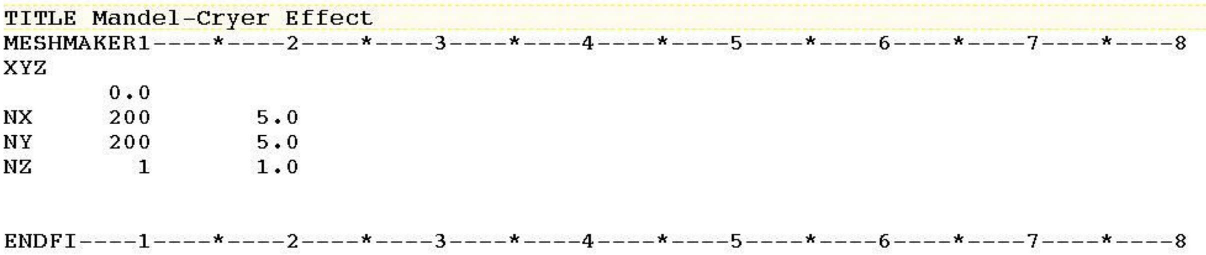
### 6.2.1 Problem Description

A constant compressive force is applied to the top of a fluid-filled poroelastic material, inducing an instantaneous uniform pore pressure increase and compression. 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.

We simulated this problem is two steps. The first step was to simulate the application of force that induced the pore pressure increase. We started from an unstrained state where pore pressure and mean stress are both equal ($\tau_{m,0} = P_0$), imposed a greater mean stress ($\tau_{m,1}$) at the top to produce a pore pressure increase, and let the system equilibrate (to pore pressure $P_1$). We next simulated fluid drainage. The system was initially at the above equilibrated state, mean stress $\tau_{m,1}$ and pore pressure $P_1$, and we imposed the initial pore pressure on the lateral boundaries to allow the system to drain.

### 6.2.2 TOUGH2-CSM Simulation Details

Our simulation domain is two-dimensional and 1000 m square. We discretized this domain into a uniform a 200 x 200 xy-grid with 5 m square grid blocks. We created the grid's MESH file by running TOUGH2-CSM with the INFILE shown in Figure 6.7.

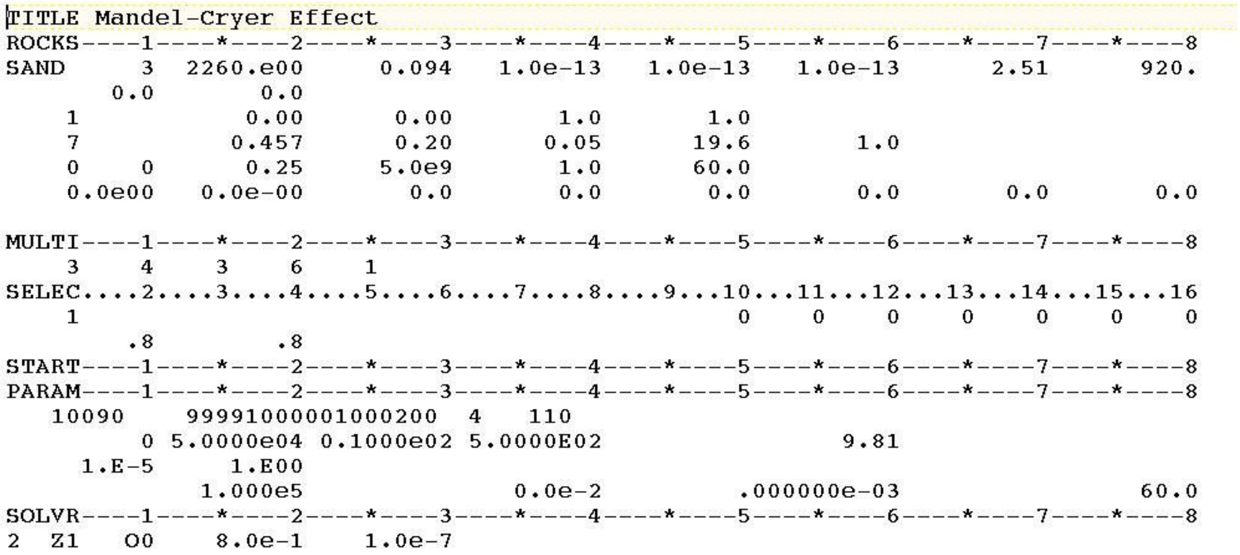


```
TITLE Mandel-Cryer Effect
MESHMAKER1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
XYZ
       0.0
NX     200       5.0
NY     200       5.0
NZ       1       1.0

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

Figure 6.7. INFILE for grid generation.

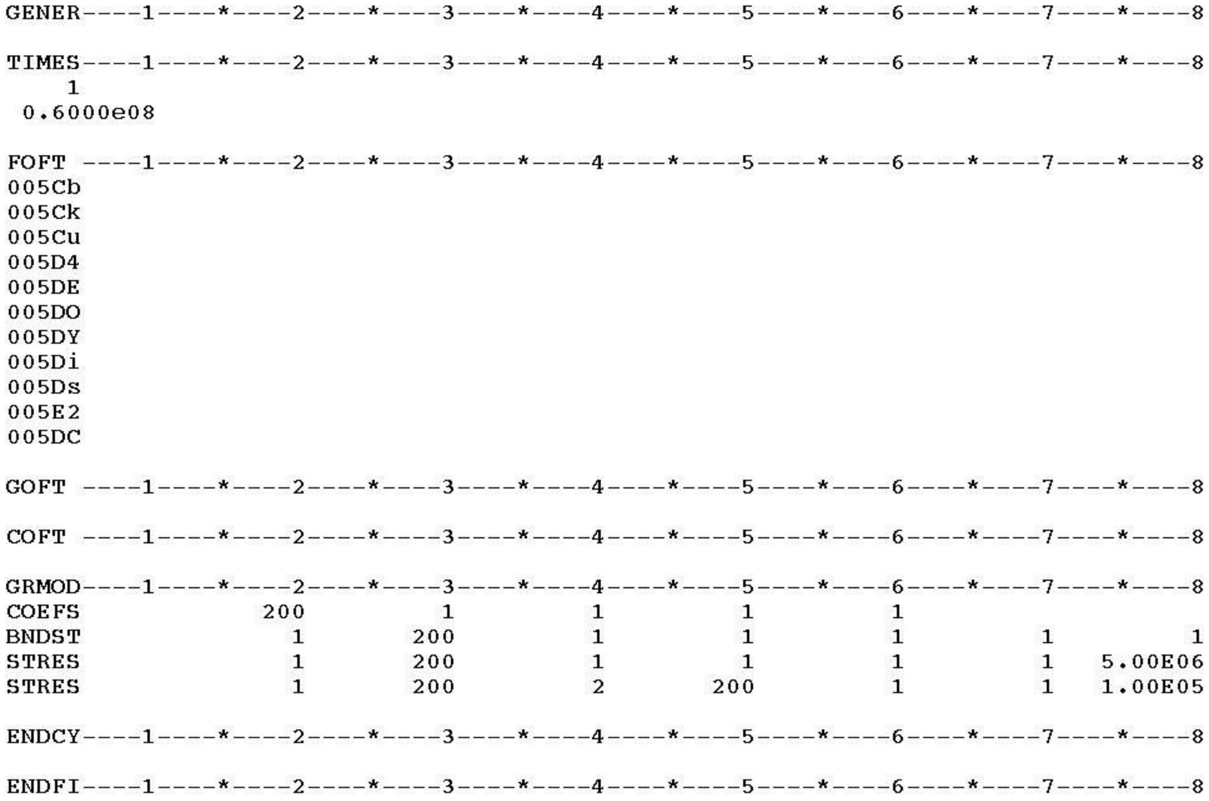
We next simulated the load application. The INFILE is shown in Figures 6.8a and 6.8b. Figure 6.8a shows the beginning of INFILE, starting with the ROCKS section and ending with the SOLVR section. Material domain properties are entered in the ROCKS section. The material domain is named SAND, porosity is 0.094, the three directional permeabilities are $10^{-13}$ $m^2$, and porosity and permeability are constant. The MULTI section contains the number of primary variables and the flag indicating that mean stress is a primary variable (NEQ=4 and ISTCAL=1, respectively, in Figure 4.1). Figure 6.8b shows the end of INFILE. There GENER section is empty since there are no sources or sinks. The GRMOD section contains initial mean stress, $5•10^6$ Pa for the top layer and $10^5$ Pa for the rest. The external force is applied to the system top so the top row of grid blocks is connected to the surroundings using the BNDST keyword with a value of one. The load application simulation was run until the system equilibrated.

Finally, we simulated fluid drainage. The load application simulation outputted a SAVE and a SAVEST file. The bottom three lines of those files were replaced with a blank line and they were renamed INCON and INCNST, respectively. The top of the INCNST file is shown in Figure 6.9. The INCON and INCNST files contain initial primary and other variables for the fluid drainage simulation. The GENER section of the INFILE for the fluid drainage simulation is shown in Figure 6.10. Each grid block in the two columns on either side of the grid contains a deliverability well at the initial system pressure ($10^5$ Pa) through which the system drained. The fluid drainage simulation was for 50,000 seconds. We compared pressure at the middle of the system with the analytical solution, shown in Figure 6.11. The simulated results (grid block *005DC*) exhibit the pore pressure maximum characteristic of the Mandel-Cryer effect and lie extremely close to the analytical solution.



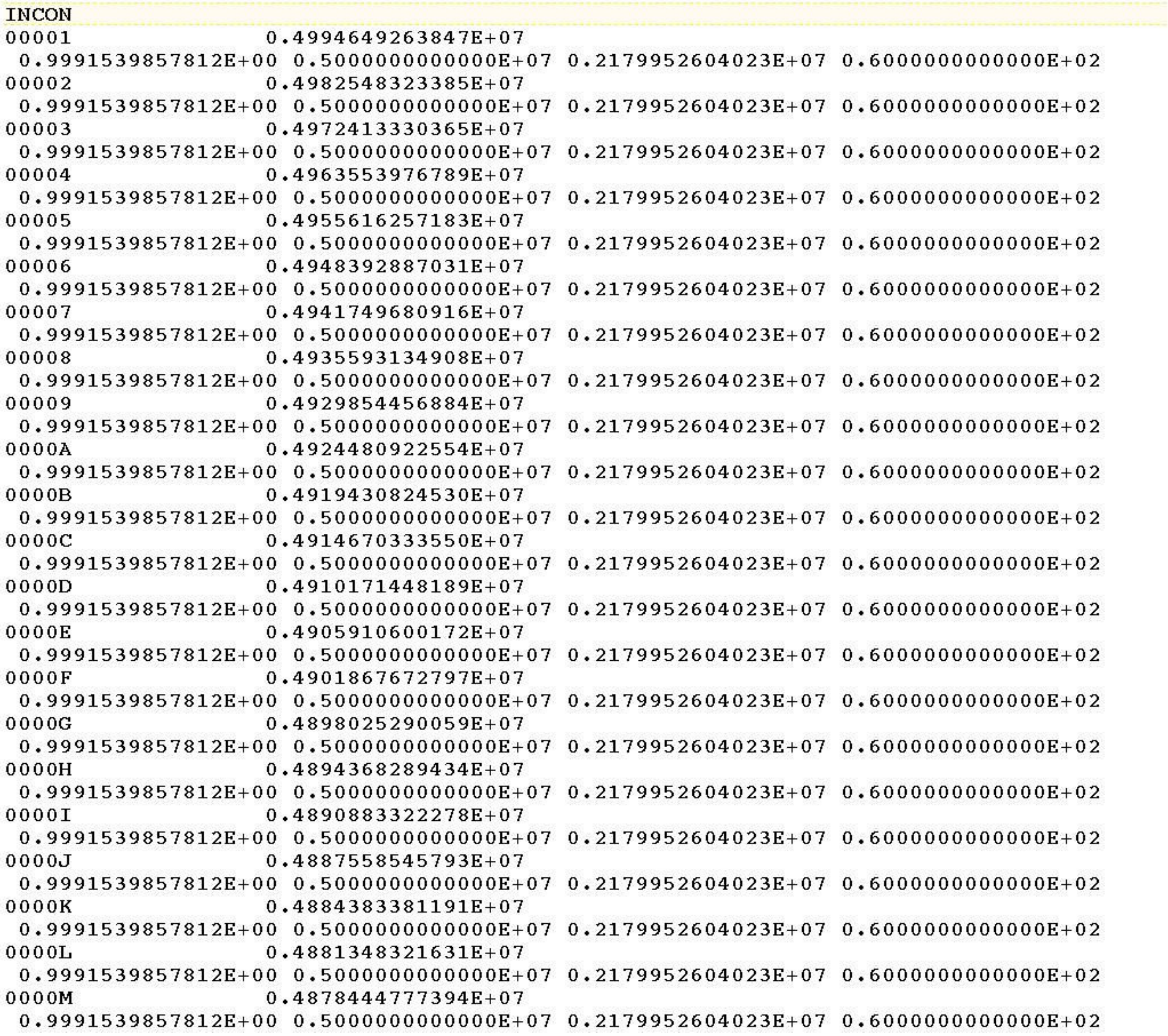
```
TITLE Mandel-Cryer Effect
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
SAND     3  2260.e00     0.094   1.0e-13   1.0e-13   1.0e-13      2.51      920.
       0.0       0.0
    1           0.00      0.00       1.0       1.0
    7          0.457      0.20      0.05      19.6       1.0
    0    0      0.25     5.0e9       1.0      60.0
    0.0e00   0.0e-00       0.0       0.0       0.0       0.0       0.0       0.0

MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    3    4    3    6    1
SELEC....2....3....4....5....6....7....8....9...10...11...12...13...14...15...16
    1                                            0    0    0    0    0    0    0
        .8        .8
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   10090    99991000001000200  4   110
         0 5.0000e04 0.1000e02 5.0000E02                   9.81
     1.E-5     1.E00
             1.000e5                0.0e-2       .000000e-03                  60.0
SOLVR----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
2  Z1   O0    8.0e-1    1.0e-7
```

Figure 6.8a. Beginning of INFILE.



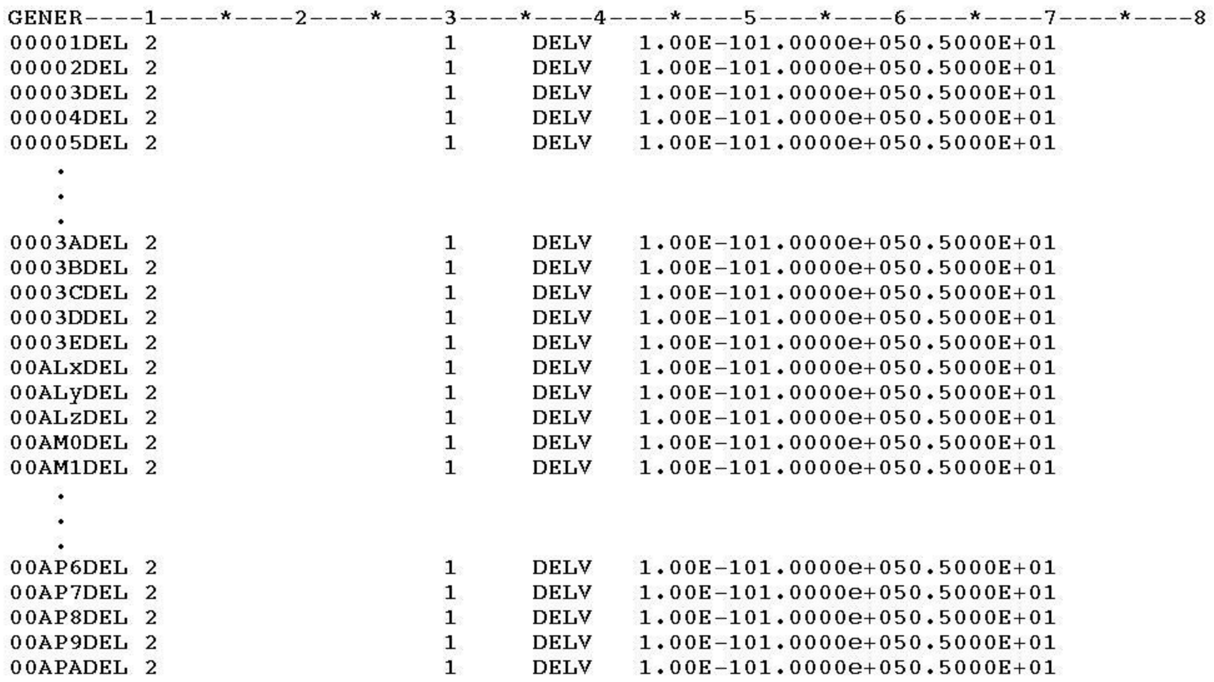
```
GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8

TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    1
 0.6000e08

FOFT ----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
005Cb
005Ck
005Cu
005D4
005DE
005DO
005DY
005Di
005Ds
005E2
005DC

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

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

GRMOD----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
COEFS              200         1         1         1         1
BNDST                1       200         1         1         1         1         1
STRES                1       200         1         1         1         1   5.00E06
STRES                1       200         2       200         1         1   1.00E05

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

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

Figure 6.8b. End of INFILE.



```
INCON
00001              0.4994649263847E+07
 0.9991539857812E+00 0.5000000000000E+07 0.2179952604023E+07 0.6000000000000E+02
00002              0.4982548323385E+07
 0.9991539857812E+00 0.5000000000000E+07 0.2179952604023E+07 0.6000000000000E+02
00003              0.4972413330365E+07
 0.9991539857812E+00 0.5000000000000E+07 0.2179952604023E+07 0.6000000000000E+02
00004              0.4963553976789E+07
 0.9991539857812E+00 0.5000000000000E+07 0.2179952604023E+07 0.6000000000000E+02
00005              0.4955616257183E+07
 0.9991539857812E+00 0.5000000000000E+07 0.2179952604023E+07 0.6000000000000E+02
00006              0.4948392887031E+07
 0.9991539857812E+00 0.5000000000000E+07 0.2179952604023E+07 0.6000000000000E+02
00007              0.4941749680916E+07
 0.9991539857812E+00 0.5000000000000E+07 0.2179952604023E+07 0.6000000000000E+02
00008              0.4935593134908E+07
 0.9991539857812E+00 0.5000000000000E+07 0.2179952604023E+07 0.6000000000000E+02
00009              0.4929854456884E+07
 0.9991539857812E+00 0.5000000000000E+07 0.2179952604023E+07 0.6000000000000E+02
0000A              0.4924480922554E+07
 0.9991539857812E+00 0.5000000000000E+07 0.2179952604023E+07 0.6000000000000E+02
0000B              0.4919430824530E+07
 0.9991539857812E+00 0.5000000000000E+07 0.2179952604023E+07 0.6000000000000E+02
0000C              0.4914670333550E+07
 0.9991539857812E+00 0.5000000000000E+07 0.2179952604023E+07 0.6000000000000E+02
0000D              0.4910171448189E+07
 0.9991539857812E+00 0.5000000000000E+07 0.2179952604023E+07 0.6000000000000E+02
0000E              0.4905910600172E+07
 0.9991539857812E+00 0.5000000000000E+07 0.2179952604023E+07 0.6000000000000E+02
0000F              0.4901867672797E+07
 0.9991539857812E+00 0.5000000000000E+07 0.2179952604023E+07 0.6000000000000E+02
0000G              0.4898025290059E+07
 0.9991539857812E+00 0.5000000000000E+07 0.2179952604023E+07 0.6000000000000E+02
0000H              0.4894368289434E+07
 0.9991539857812E+00 0.5000000000000E+07 0.2179952604023E+07 0.6000000000000E+02
0000I              0.4890883322278E+07
 0.9991539857812E+00 0.5000000000000E+07 0.2179952604023E+07 0.6000000000000E+02
0000J              0.4887558545793E+07
 0.9991539857812E+00 0.5000000000000E+07 0.2179952604023E+07 0.6000000000000E+02
0000K              0.4884383381191E+07
 0.9991539857812E+00 0.5000000000000E+07 0.2179952604023E+07 0.6000000000000E+02
0000L              0.4881348321631E+07
 0.9991539857812E+00 0.5000000000000E+07 0.2179952604023E+07 0.6000000000000E+02
0000M              0.4878444777394E+07
 0.9991539857812E+00 0.5000000000000E+07 0.2179952604023E+07 0.6000000000000E+02
```

Figure 6.9. Top of INCNST file.



```
GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
00001DEL 2                   1     DELV   1.00E-101.0000e+050.5000E+01
00002DEL 2                   1     DELV   1.00E-101.0000e+050.5000E+01
00003DEL 2                   1     DELV   1.00E-101.0000e+050.5000E+01
00004DEL 2                   1     DELV   1.00E-101.0000e+050.5000E+01
00005DEL 2                   1     DELV   1.00E-101.0000e+050.5000E+01
    .
    .
    .
0003ADEL 2                   1     DELV   1.00E-101.0000e+050.5000E+01
0003BDEL 2                   1     DELV   1.00E-101.0000e+050.5000E+01
0003CDEL 2                   1     DELV   1.00E-101.0000e+050.5000E+01
0003DDEL 2                   1     DELV   1.00E-101.0000e+050.5000E+01
0003EDEL 2                   1     DELV   1.00E-101.0000e+050.5000E+01
00ALxDEL 2                   1     DELV   1.00E-101.0000e+050.5000E+01
00ALyDEL 2                   1     DELV   1.00E-101.0000e+050.5000E+01
00ALzDEL 2                   1     DELV   1.00E-101.0000e+050.5000E+01
00AM0DEL 2                   1     DELV   1.00E-101.0000e+050.5000E+01
00AM1DEL 2                   1     DELV   1.00E-101.0000e+050.5000E+01
    .
    .
    .
00AP6DEL 2                   1     DELV   1.00E-101.0000e+050.5000E+01
00AP7DEL 2                   1     DELV   1.00E-101.0000e+050.5000E+01
00AP8DEL 2                   1     DELV   1.00E-101.0000e+050.5000E+01
00AP9DEL 2                   1     DELV   1.00E-101.0000e+050.5000E+01
00APADEL 2                   1     DELV   1.00E-101.0000e+050.5000E+01
```

Figure 6.10. GENER Section of INFILE.

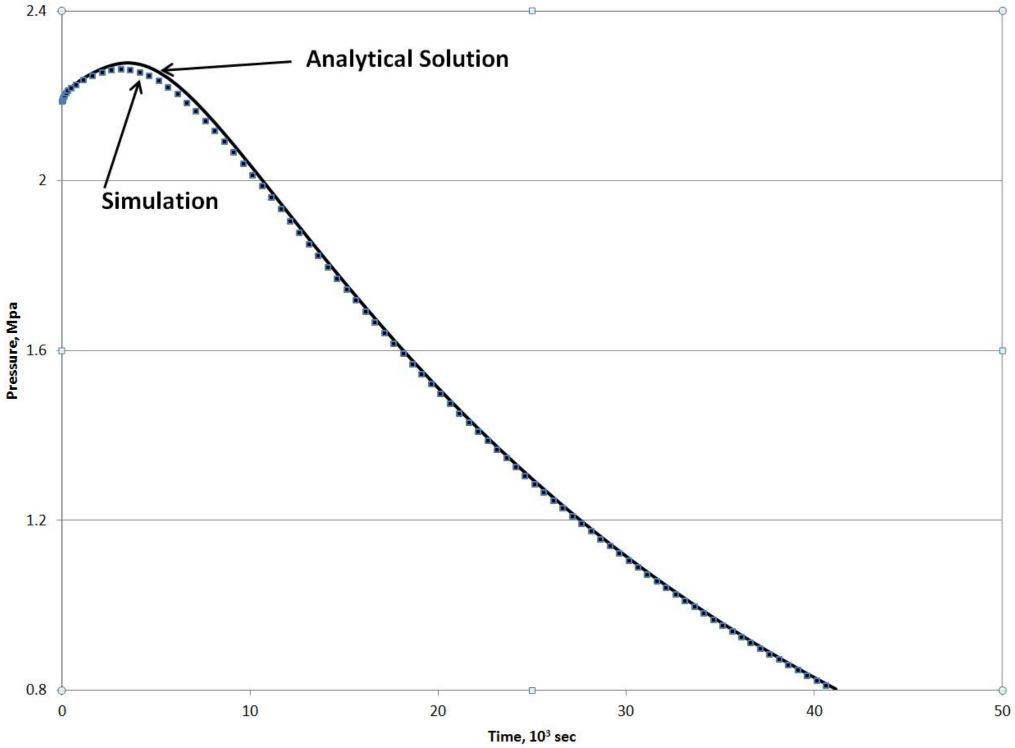


Figure 6.11. Comparison Mandel-Cryer effect analytical solution to simulation for pore pressure at system center.

## 6.3 $CO_2$ Injection into a Layered Saline Aquifer

### 6.3.1 Problem Description

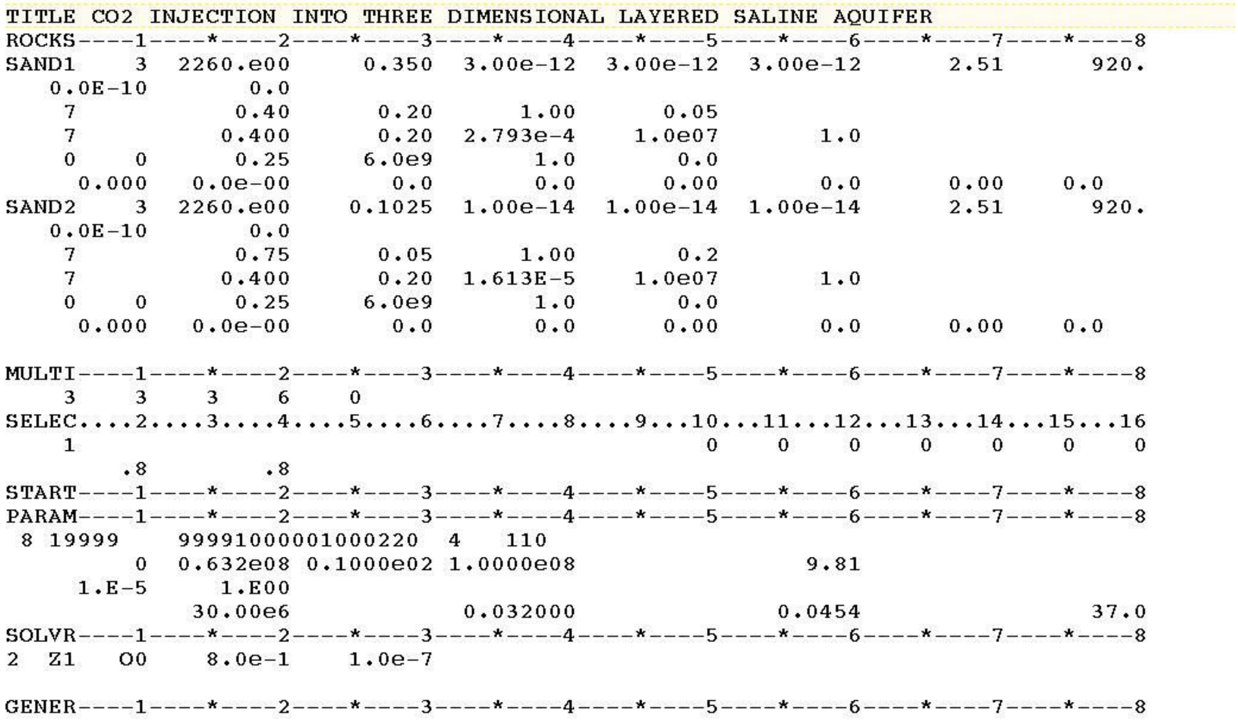
This three-dimensional model of $CO_2$ injection in a layered saline aquifer (Zhang et al., 2011) is based on the first industrial scale $CO_2$ storage project at the Sleipner Vest field in the North Sea and investigates $CO_2$ migration in heterogeneous reservoirs with alternating sand-shale zones. The simulation domain is a quarter symmetry element 6000 m x 6000 m x 184 m. There are four alternating sand-shale zones with the sand 30 m thick and the shale 3 m thick. Below those alternating sand-shale zones is a 52 m thick sand zone. A 50 m long horizontal well in the y-direction is located at the origin, 30 m below the bottom shale layer. The outer boundaries are maintained at hydrostatic pressure and the $CO_2$ injection rate is 7.925 kg/s. Initial pressure at the well is 110 bars, initial temperature is 37 °C, and initial $CO_2$ and salt mass fractions are $4.541 \times 10^{-4}$ and 0.032, respectively.

### 6.3.2 TOUGH2-CSM Simulation Details

We built our grid by discretizing the z-direction into 100 layers. All layers are 1 m thick except the bottom layer, which is 4 m thick, and the top three 30 m thick sand zones are discretized into 10 m thick layers. There are 69 subdivisions in the x- and y-directions. The first ten are 10 m wide, followed by 59 at 100 m. The resulting grid is 69 x 69 x 100 with 476,100 grid blocks.

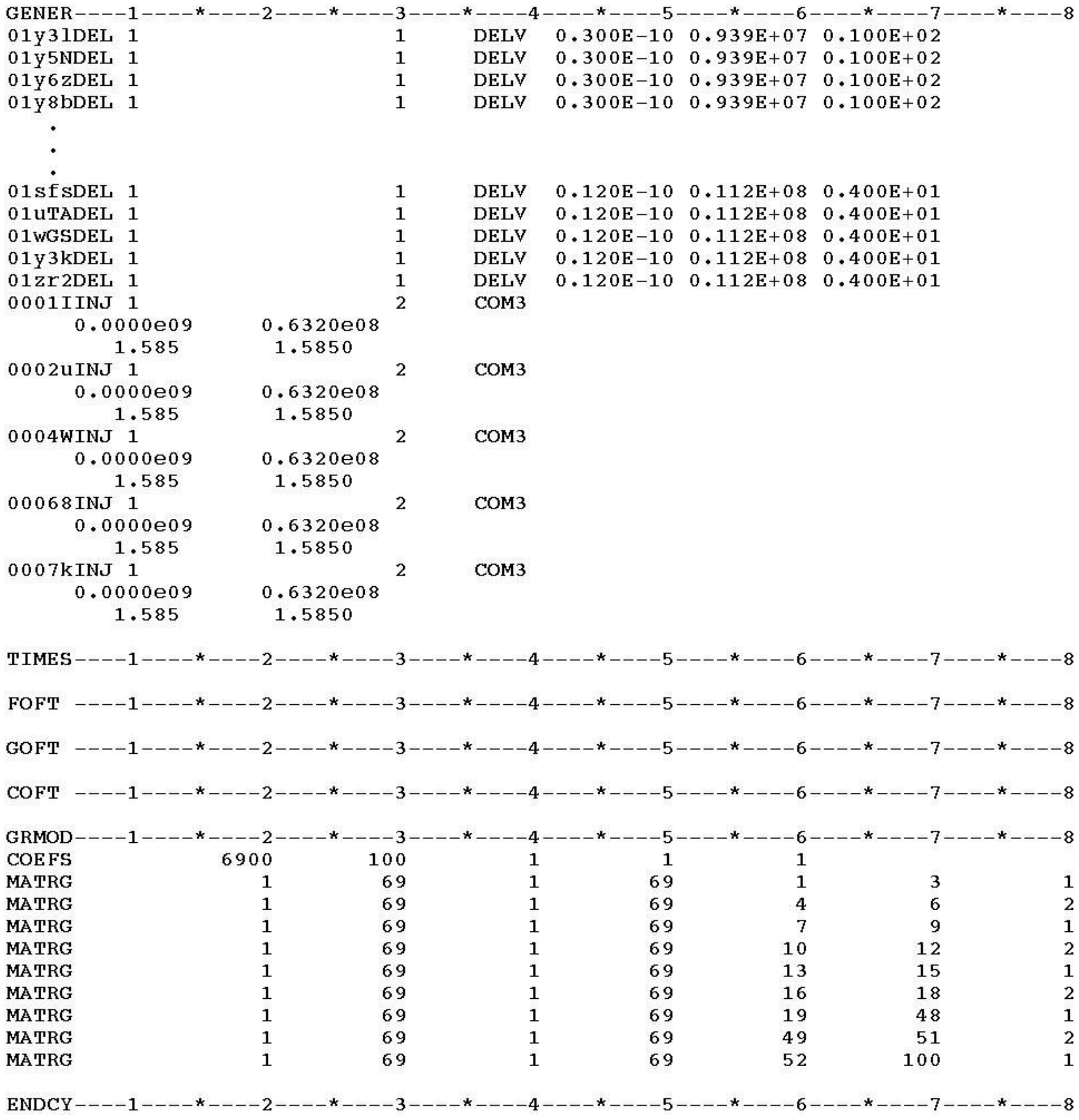
Figure 6.12a shows the beginning of the INFILE. Material SAND1 is the sand and material SAND2 is the shale. We ran this simulation without solving the momentum equation, so the stress calculation flag (ISTRC in Figure 4.1) in the MULTI Section is zero and the number of equations per grid block (NEQ in Figure 4.1) is three. Figure 6.12b show the end of the INFILE. The GENER Section contains deliverability wells at hydrostatic pressure located on the outer boundaries and the five injectors comprising the horizontal well. Primary variables initialized in the PARAM section were overwritten by those from file INCON, obtained by hydrostatic initialization of the system using the method described in Section 5.2. The sand and shale material regions are set in the GRMOD section. Figure 6.13 shows the $CO_2$ saturation profile at

150 m in the x-direction. This profile is similar to one reported in the reference with a different grid.



```
TITLE CO2 INJECTION INTO THREE DIMENSIONAL LAYERED SALINE AQUIFER
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
SAND1    3  2260.e00     0.350  3.00e-12  3.00e-12  3.00e-12      2.51      920.
   0.0E-10       0.0
    7           0.40      0.20      1.00      0.05
    7          0.400      0.20  2.793e-4    1.0e07       1.0
    0    0      0.25     6.0e9       1.0       0.0
     0.000   0.0e-00       0.0       0.0      0.00       0.0      0.00       0.0
SAND2    3  2260.e00    0.1025  1.00e-14  1.00e-14  1.00e-14      2.51      920.
   0.0E-10       0.0
    7           0.75      0.05      1.00       0.2
    7          0.400      0.20  1.613E-5    1.0e07       1.0
    0    0      0.25     6.0e9       1.0       0.0
     0.000   0.0e-00       0.0       0.0      0.00       0.0      0.00       0.0

MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    3    3    3    6    0
SELEC....2....3....4....5....6....7....8....9...10...11...12...13...14...15...16
    1                                            0    0    0    0    0    0    0
        .8        .8
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
 8 19999    99991000001000220  4   110
         0  0.632e08 0.1000e02 1.0000e08                    9.81
     1.E-5     1.E00
             30.00e6            0.032000                  0.0454                37.0
SOLVR----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
2  Z1   O0    8.0e-1    1.0e-7

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

Figure 6.12a. Beginning of INFILE.



```
GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
01y3lDEL 1                   1     DELV  0.300E-10 0.939E+07 0.100E+02
01y5NDEL 1                   1     DELV  0.300E-10 0.939E+07 0.100E+02
01y6zDEL 1                   1     DELV  0.300E-10 0.939E+07 0.100E+02
01y8bDEL 1                   1     DELV  0.300E-10 0.939E+07 0.100E+02
   .
   .
   .
01sfsDEL 1                   1     DELV  0.120E-10 0.112E+08 0.400E+01
01uTADEL 1                   1     DELV  0.120E-10 0.112E+08 0.400E+01
01wGSDEL 1                   1     DELV  0.120E-10 0.112E+08 0.400E+01
01y3kDEL 1                   1     DELV  0.120E-10 0.112E+08 0.400E+01
01zr2DEL 1                   1     DELV  0.120E-10 0.112E+08 0.400E+01
0001IINJ 1                   2     COM3
     0.0000e09     0.6320e08
        1.585       1.5850
0002uINJ 1                   2     COM3
     0.0000e09     0.6320e08
        1.585       1.5850
0004WINJ 1                   2     COM3
     0.0000e09     0.6320e08
        1.585       1.5850
00068INJ 1                   2     COM3
     0.0000e09     0.6320e08
        1.585       1.5850
0007kINJ 1                   2     COM3
     0.0000e09     0.6320e08
        1.585       1.5850

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

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

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

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

GRMOD----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
COEFS           6900       100         1         1         1
MATRG              1        69         1        69         1         3         1
MATRG              1        69         1        69         4         6         2
MATRG              1        69         1        69         7         9         1
MATRG              1        69         1        69        10        12         2
MATRG              1        69         1        69        13        15         1
MATRG              1        69         1        69        16        18         2
MATRG              1        69         1        69        19        48         1
MATRG              1        69         1        69        49        51         2
MATRG              1        69         1        69        52       100         1

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

Figure 6.12b. End of INFILE.

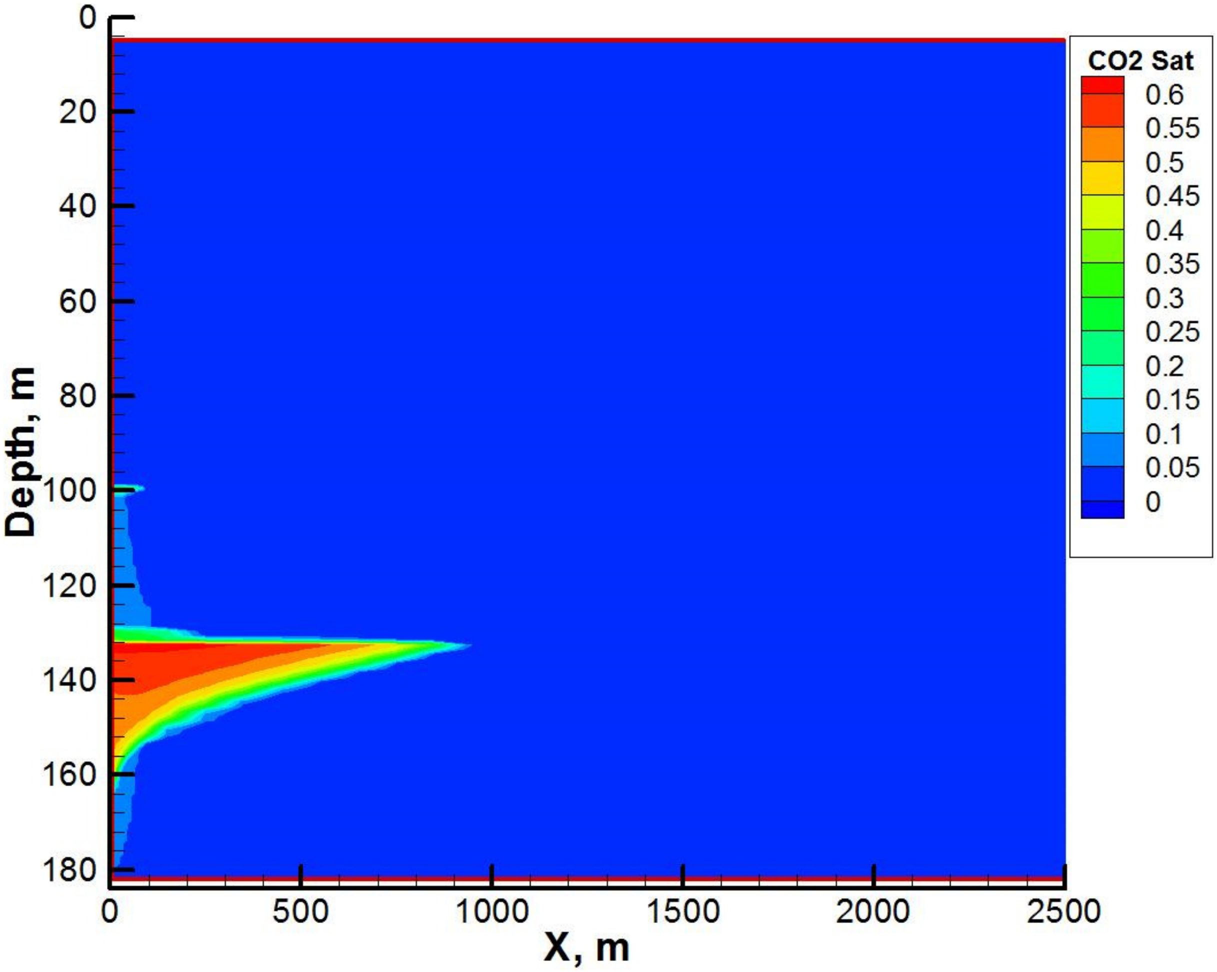


Figure 6.13. CO$_2$ saturation after 2 years injection, y=5.0 m.

## 6.4 In Salah Gas Project Simulation

### 6.4.1 Problem Description

The In Salah Gas Project, located in central Algeria, is a $CO_2$ storage project. Natural gas produced nearby is high in $CO_2$ and this $CO_2$ is injected back into the water leg of a depleting gas field for geological storage. Surface uplift from $CO_2$ injection has been measured by satellite-based inferrometry and Rutqvist et al. (2010) did a reservoir-geomechanical analysis of In Salah $CO_2$ injection and surface uplift using the TOUGH2-FLAC numerical simulator in order to determine if the uplift can be explained by pressure changes and deformation in the injection zone only. The TOUGH2-FLAC numerical simulator is a linkage of two existing well established codes, TOUGH2 (Pruess, 1991) that solves non-isothermal, multiphase, multi-component, fluid flow problems in complex geological systems and FLAC3D (Itasca, 1997), developed for rock and soil mechanics that can handle coupled thermomechanical and hydromechanical processes for single-phase fluid flow.

The simulated domain was 10x10x4 km with one 1.5 km horizontal injection well at 1810 m depth and in the domain center. The domain consisted of four geological layers. The reservoir initially contained water and the initial temperature and pressure at the injection well were 90 °C and 17.9 MPa, respectively. The lateral reservoir boundaries were maintained at hydrostatic pressure and $CO_2$ was injected at 9.734 kg/sec for three years.

$CO_2$ injection causes surface uplift, a change in reservoir height. Reservoir height is the sum of grid block height over a z-direction column of grid blocks. Defining linear strain, $\epsilon_z$, as:

$$\Delta z_l = \Delta z_{l,0}(1 - \epsilon_z) \tag{6.2}$$

where $\Delta z_l$ is grid block height, we can write surface uplift, $\Delta z_{uplift}$, as:

$$\Delta z_{uplift} = \sum_l (\Delta z_l - \Delta z_{l,i}) = \sum_l \Delta z_{l,i} \left(\frac{\epsilon_{z,i} - \epsilon_z}{1 - \epsilon_{z,i}}\right) \tag{6.3}$$

where the sum over index *l* refers to a z-direction column of grid blocks and the subscript *i* refers to initial conditions. Finally, we express linear strain in terms of volumetric strain by assuming isotropic strain:

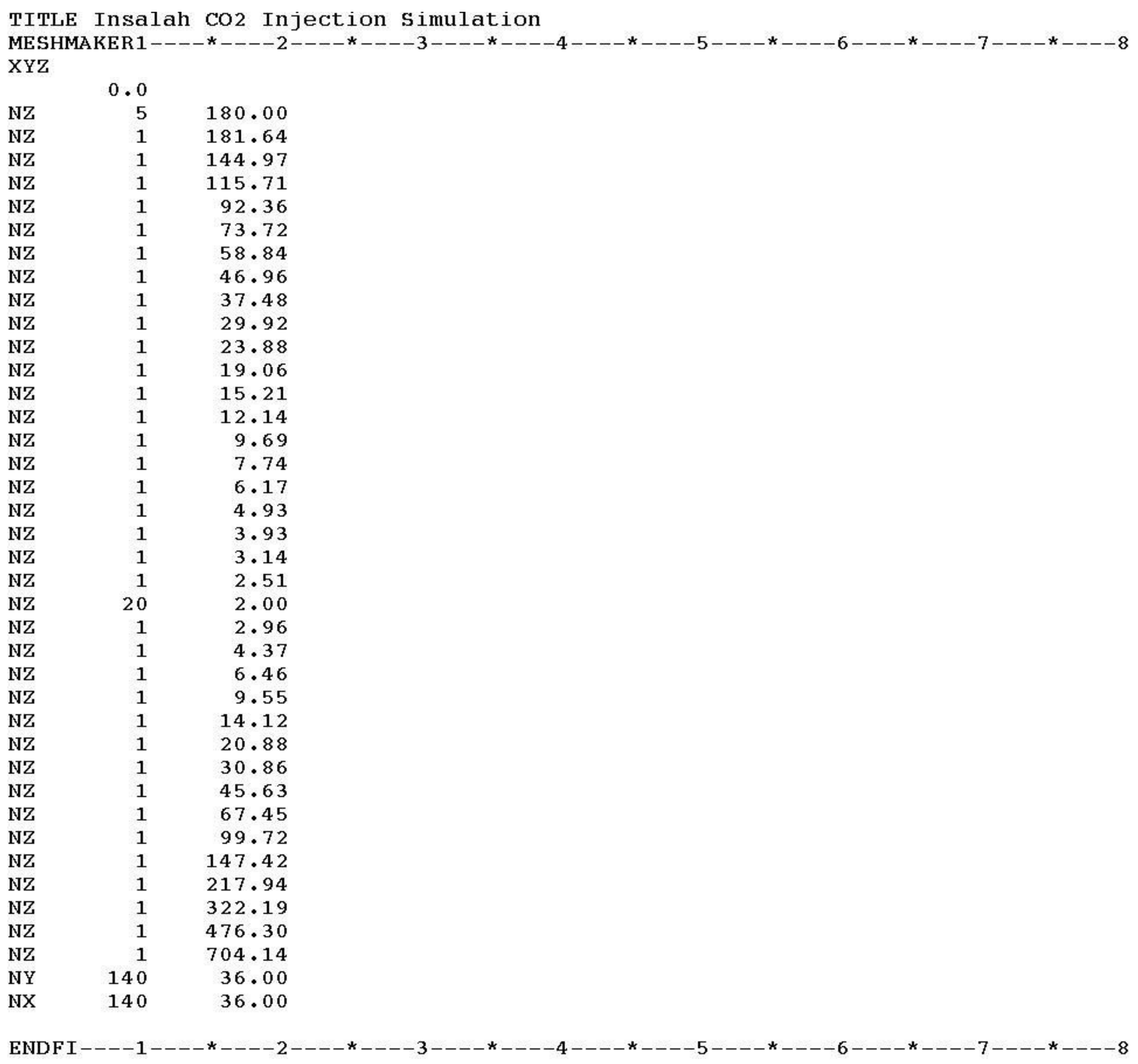
$$\epsilon_z = \frac{\epsilon_v}{3} \tag{6.4}$$

We use Equations 6.3 and 6.4 to calculate surface uplift.

### 6.4.2 TOUGH2-CSM Simulation Details

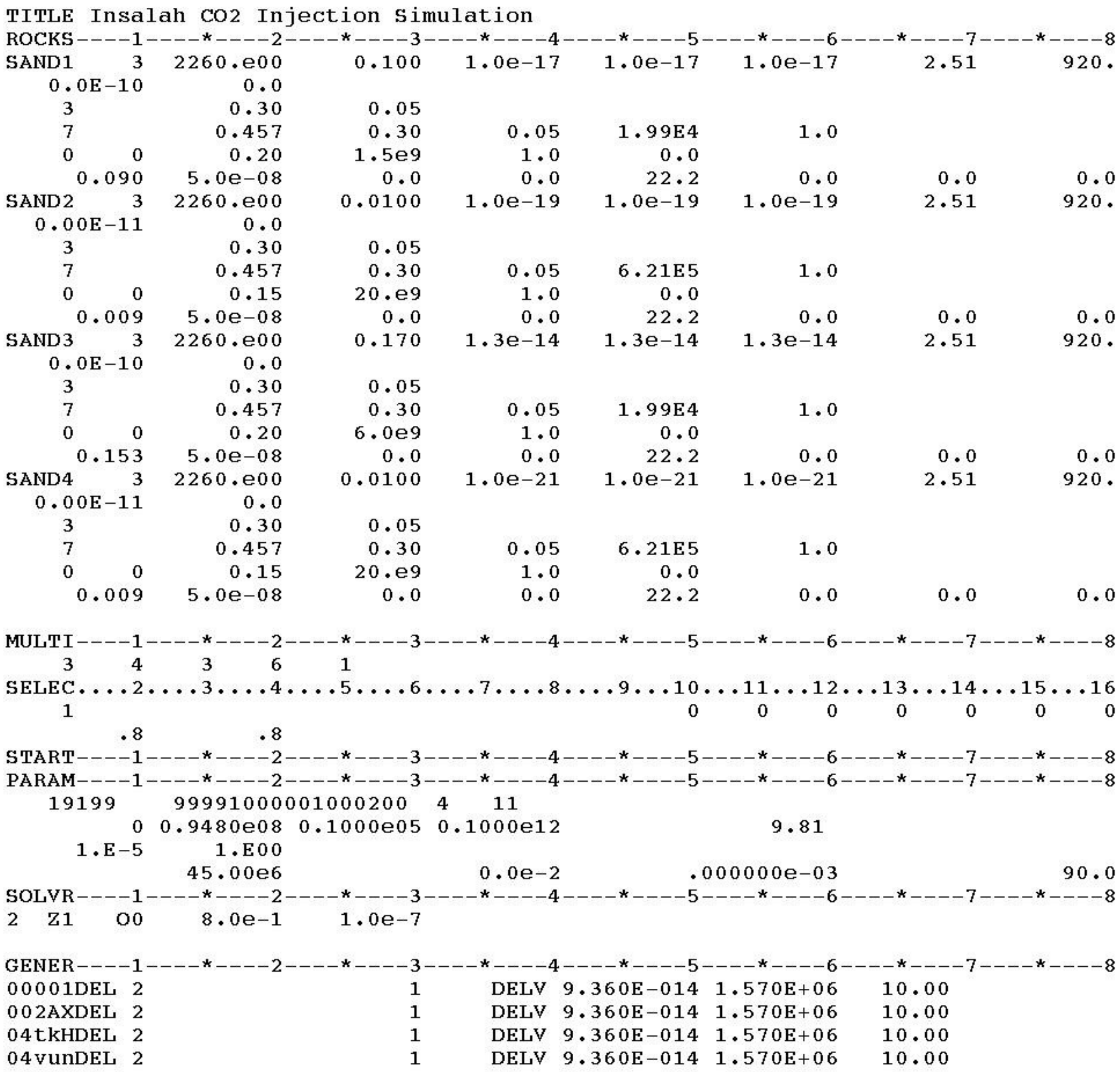
We ran TOUGH2-CSM on a cluster computer to demonstrate our parallel code's ability to simulate larger problems. Our cluster computer contains 16 nodes; each node has 24 GB of memory and two Intel® 5620 2.4GHZ 4-core processors. Our simulation domain is a 5 x 5 x 4 km quarter symmetry element of the system discretized into a 140 x 140 x 60 grid (1,176,000 grid blocks). The areal grid is uniform and the INFILE used to generate the grid is shown in Figure 6.14. The aquifer region is subdivided into ten 2 m layers and layer thickness gradually increased away from there.

We first ran a simulation to generate a primary variable set at hydrostatic equilibrium. The top of the INFILE used to run this simulation is shown in Figure 6.15. The material regions defined in the ROCKS Section, SAND1, SAND2, SAND3, and SAND4, correspond, respectively, to the four geological layers described in the reference, Shallow Overburden, Caprock, Injection Zone, and Base. We ran this simulation without solving the momentum equation, so the stress calculation flag (ISTRC in Figure 4.1) in the MULTI Section is zero and the number of equations per grid block (NEQ in Figure 4.1) is three. The GENER Section consists only of deliverability wells at a reference pressure (1.57 MPa) located along the top layer (cells *00001*, *002AX*, *04tkH*, and *04vun*). We assigned material region 3 (Injection Zone) to all grid blocks and ran the simulation until the system equilibrated. The extra deliverability wells (more than one) and uniform material region assignment were done to speed up system equilibration. The material regions other than Injection Zone have low permeability and would take an excessively long time to equilibrate.



```
TITLE Insalah CO2 Injection Simulation
MESHMAKER1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
XYZ
       0.0
NZ       5    180.00
NZ       1    181.64
NZ       1    144.97
NZ       1    115.71
NZ       1     92.36
NZ       1     73.72
NZ       1     58.84
NZ       1     46.96
NZ       1     37.48
NZ       1     29.92
NZ       1     23.88
NZ       1     19.06
NZ       1     15.21
NZ       1     12.14
NZ       1      9.69
NZ       1      7.74
NZ       1      6.17
NZ       1      4.93
NZ       1      3.93
NZ       1      3.14
NZ       1      2.51
NZ      20      2.00
NZ       1      2.96
NZ       1      4.37
NZ       1      6.46
NZ       1      9.55
NZ       1     14.12
NZ       1     20.88
NZ       1     30.86
NZ       1     45.63
NZ       1     67.45
NZ       1     99.72
NZ       1    147.42
NZ       1    217.94
NZ       1    322.19
NZ       1    476.30
NZ       1    704.14
NY     140     36.00
NX     140     36.00

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

Figure 6.14. INFILE for grid generation.

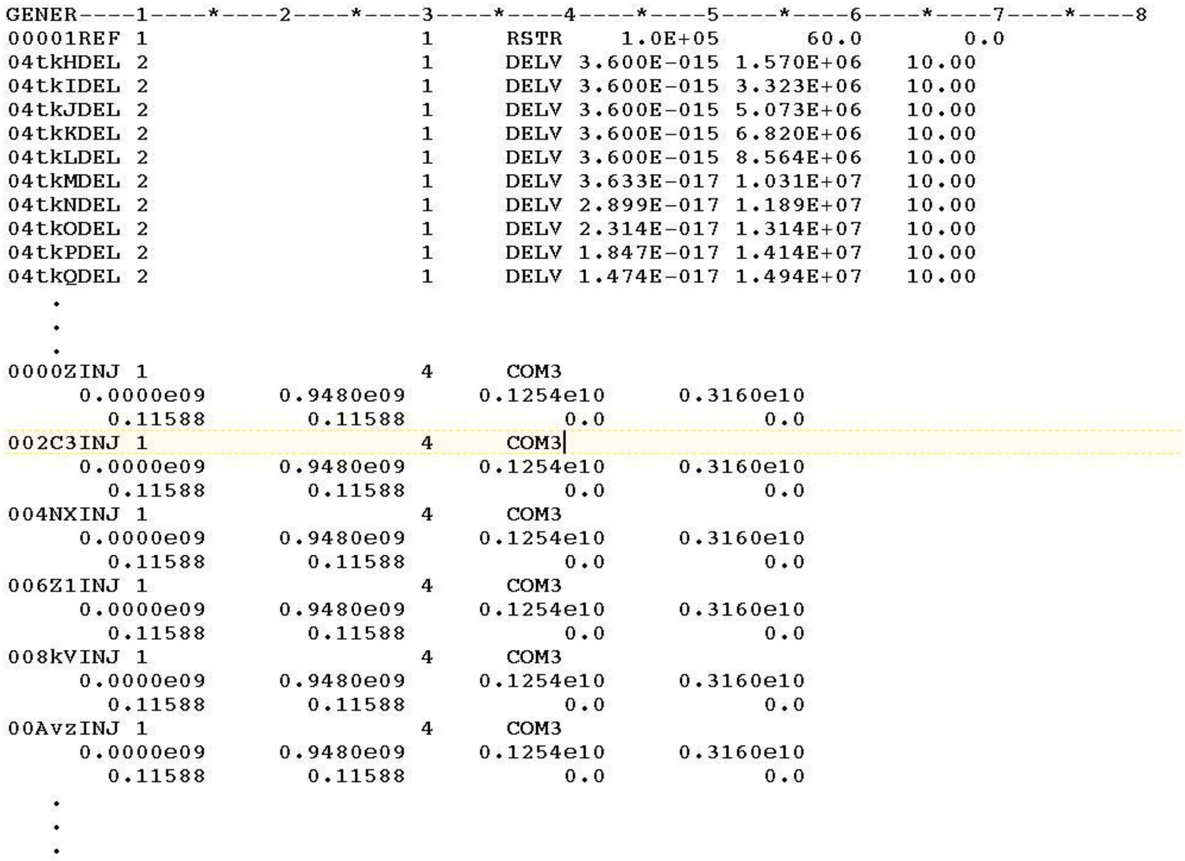


```
TITLE Insalah CO2 Injection Simulation
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
SAND1    3  2260.e00     0.100   1.0e-17   1.0e-17   1.0e-17      2.51      920.
   0.0E-10       0.0
    3           0.30      0.05
    7          0.457      0.30      0.05    1.99E4       1.0
    0    0      0.20     1.5e9       1.0       0.0
     0.090   5.0e-08       0.0       0.0      22.2       0.0       0.0       0.0
SAND2    3  2260.e00    0.0100   1.0e-19   1.0e-19   1.0e-19      2.51      920.
  0.00E-11       0.0
    3           0.30      0.05
    7          0.457      0.30      0.05    6.21E5       1.0
    0    0      0.15     20.e9       1.0       0.0
     0.009   5.0e-08       0.0       0.0      22.2       0.0       0.0       0.0
SAND3    3  2260.e00     0.170   1.3e-14   1.3e-14   1.3e-14      2.51      920.
   0.0E-10       0.0
    3           0.30      0.05
    7          0.457      0.30      0.05    1.99E4       1.0
    0    0      0.20     6.0e9       1.0       0.0
     0.153   5.0e-08       0.0       0.0      22.2       0.0       0.0       0.0
SAND4    3  2260.e00    0.0100   1.0e-21   1.0e-21   1.0e-21      2.51      920.
  0.00E-11       0.0
    3           0.30      0.05
    7          0.457      0.30      0.05    6.21E5       1.0
    0    0      0.15     20.e9       1.0       0.0
     0.009   5.0e-08       0.0       0.0      22.2       0.0       0.0       0.0

MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    3    4    3    6    1
SELEC....2....3....4....5....6....7....8....9...10...11...12...13...14...15...16
    1                                            0    0    0    0    0    0    0
        .8        .8
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   19199    99991000001000200  4   11
        0 0.9480e08 0.1000e05 0.1000e12                9.81
     1.E-5     1.E00
          45.00e6             0.0e-2          .000000e-03                 90.0
SOLVR----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
2  Z1   O0    8.0e-1    1.0e-7

GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
00001DEL 2                   1     DELV 9.360E-014 1.570E+06   10.00
002AXDEL 2                   1     DELV 9.360E-014 1.570E+06   10.00
04tkHDEL 2                   1     DELV 9.360E-014 1.570E+06   10.00
04vunDEL 2                   1     DELV 9.360E-014 1.570E+06   10.00
```

Figure 6.15. Top of INFILE for generation of primary variables at hydrostatic equilibrium.

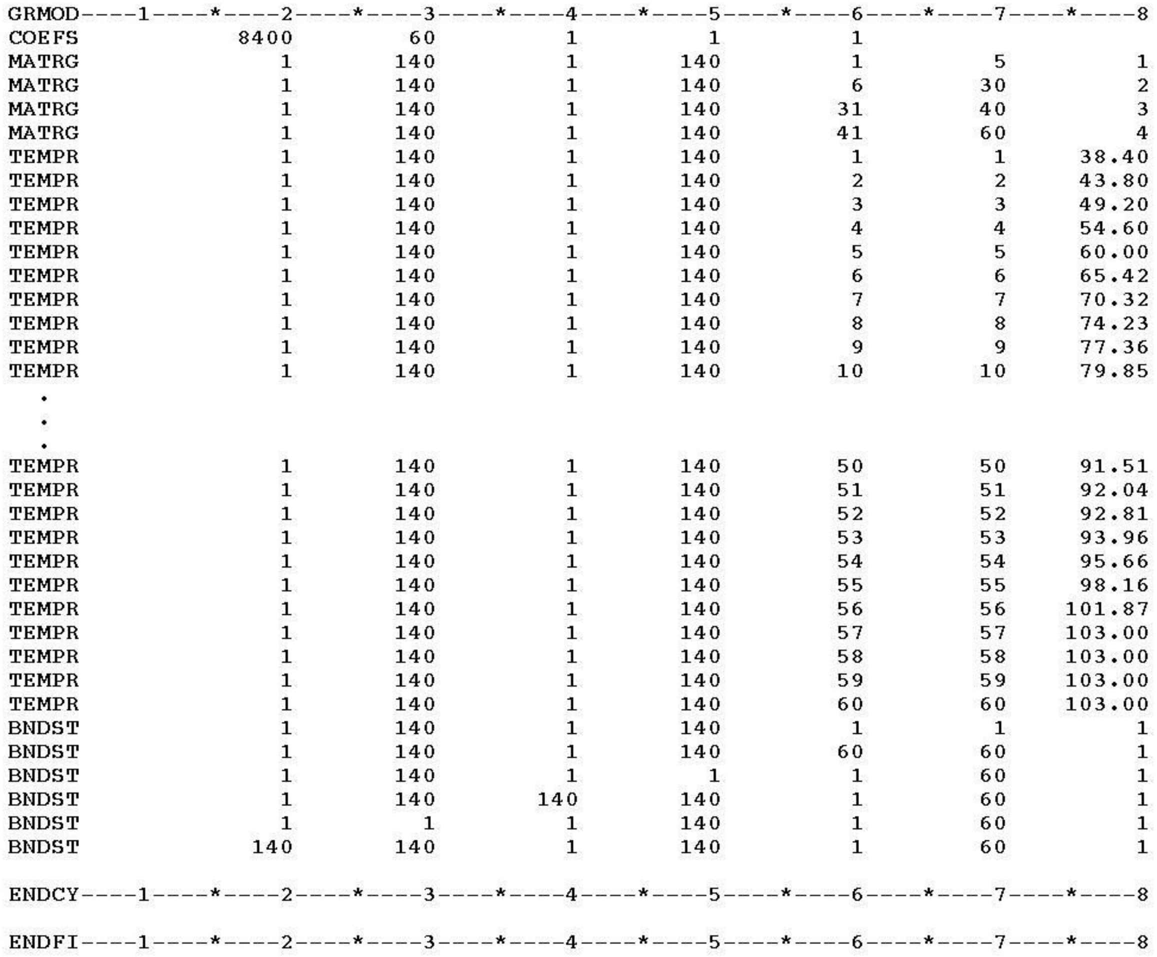
Finally, we simulated $CO_2$ injection. The previous simulation outputted a SAVE file that contained primary variables at hydrostatic equilibrium. The bottom three lines were replaced by a blank line and the file was renamed INCON. Figure 6.16 shows part of the GENER Section. The RSTR keyword is used to specify a reference mean stress at a reference elevation in order to initialize mean stress. Deliverability wells (DELV) at hydrostatic pressure are placed in grid blocks on the outer boundary to approximate the constant pressure boundary condition there. The horizontal well is located in an x-direction row of grid blocks starting at grid block *0000Z* and equal amounts of $CO_2$ are injected into each one. The total x-direction length of these grid blocks is approximately the well length. Figure 6.17 shows the rest of INFILE, namely the GRMOD Section. The material regions (MATRG) are set for layers corresponding to the four geological zones described above. Temperature does not vary with time, since the energy equation is not solved, but varies by layer and is set for each using the TEMPR record. The BNDST keyword specifies grid blocks connected to the surroundings, those on the lateral outer faces and top and bottom of the Cartesian grid.

The simulation was run for three years. Figure 6.18 shows surface uplift after three years of $CO_2$ injection and Figure 6.19 is a comparison of vertical displacement (surface uplift) versus depth at the well for TOUGH2-CSM and the reference. The two profiles are close to each other. The grid used in the reference is much coarser than the TOUGH2-CSM grid, consisting of about ten thousand grid blocks.



```
GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
00001REF 1                   1     RSTR    1.0E+05      60.0       0.0
04tkHDEL 2                   1     DELV 3.600E-015 1.570E+06   10.00
04tkIDEL 2                   1     DELV 3.600E-015 3.323E+06   10.00
04tkJDEL 2                   1     DELV 3.600E-015 5.073E+06   10.00
04tkKDEL 2                   1     DELV 3.600E-015 6.820E+06   10.00
04tkLDEL 2                   1     DELV 3.600E-015 8.564E+06   10.00
04tkMDEL 2                   1     DELV 3.633E-017 1.031E+07   10.00
04tkNDEL 2                   1     DELV 2.899E-017 1.189E+07   10.00
04tkODEL 2                   1     DELV 2.314E-017 1.314E+07   10.00
04tkPDEL 2                   1     DELV 1.847E-017 1.414E+07   10.00
04tkQDEL 2                   1     DELV 1.474E-017 1.494E+07   10.00
   .
   .
   .
0000ZINJ 1                   4     COM3
     0.0000e09     0.9480e09     0.1254e10     0.3160e10
       0.11588       0.11588           0.0           0.0
002C3INJ 1                   4     COM3
     0.0000e09     0.9480e09     0.1254e10     0.3160e10
       0.11588       0.11588           0.0           0.0
004NXINJ 1                   4     COM3
     0.0000e09     0.9480e09     0.1254e10     0.3160e10
       0.11588       0.11588           0.0           0.0
006Z1INJ 1                   4     COM3
     0.0000e09     0.9480e09     0.1254e10     0.3160e10
       0.11588       0.11588           0.0           0.0
008kVINJ 1                   4     COM3
     0.0000e09     0.9480e09     0.1254e10     0.3160e10
       0.11588       0.11588           0.0           0.0
00AvzINJ 1                   4     COM3
     0.0000e09     0.9480e09     0.1254e10     0.3160e10
       0.11588       0.11588           0.0           0.0
   .
   .
   .
```

Figure 6.16. GENER section for INFILE.



```
GRMOD----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
COEFS           8400        60         1         1         1
MATRG              1       140         1       140         1         5         1
MATRG              1       140         1       140         6        30         2
MATRG              1       140         1       140        31        40         3
MATRG              1       140         1       140        41        60         4
TEMPR              1       140         1       140         1         1     38.40
TEMPR              1       140         1       140         2         2     43.80
TEMPR              1       140         1       140         3         3     49.20
TEMPR              1       140         1       140         4         4     54.60
TEMPR              1       140         1       140         5         5     60.00
TEMPR              1       140         1       140         6         6     65.42
TEMPR              1       140         1       140         7         7     70.32
TEMPR              1       140         1       140         8         8     74.23
TEMPR              1       140         1       140         9         9     77.36
TEMPR              1       140         1       140        10        10     79.85
  .
  .
  .
TEMPR              1       140         1       140        50        50     91.51
TEMPR              1       140         1       140        51        51     92.04
TEMPR              1       140         1       140        52        52     92.81
TEMPR              1       140         1       140        53        53     93.96
TEMPR              1       140         1       140        54        54     95.66
TEMPR              1       140         1       140        55        55     98.16
TEMPR              1       140         1       140        56        56    101.87
TEMPR              1       140         1       140        57        57    103.00
TEMPR              1       140         1       140        58        58    103.00
TEMPR              1       140         1       140        59        59    103.00
TEMPR              1       140         1       140        60        60    103.00
BNDST              1       140         1       140         1         1         1
BNDST              1       140         1       140        60        60         1
BNDST              1       140         1         1         1        60         1
BNDST              1       140       140       140         1        60         1
BNDST              1         1         1       140         1        60         1
BNDST            140       140         1       140         1        60         1

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

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

Figure 6.17. End of INFILE.

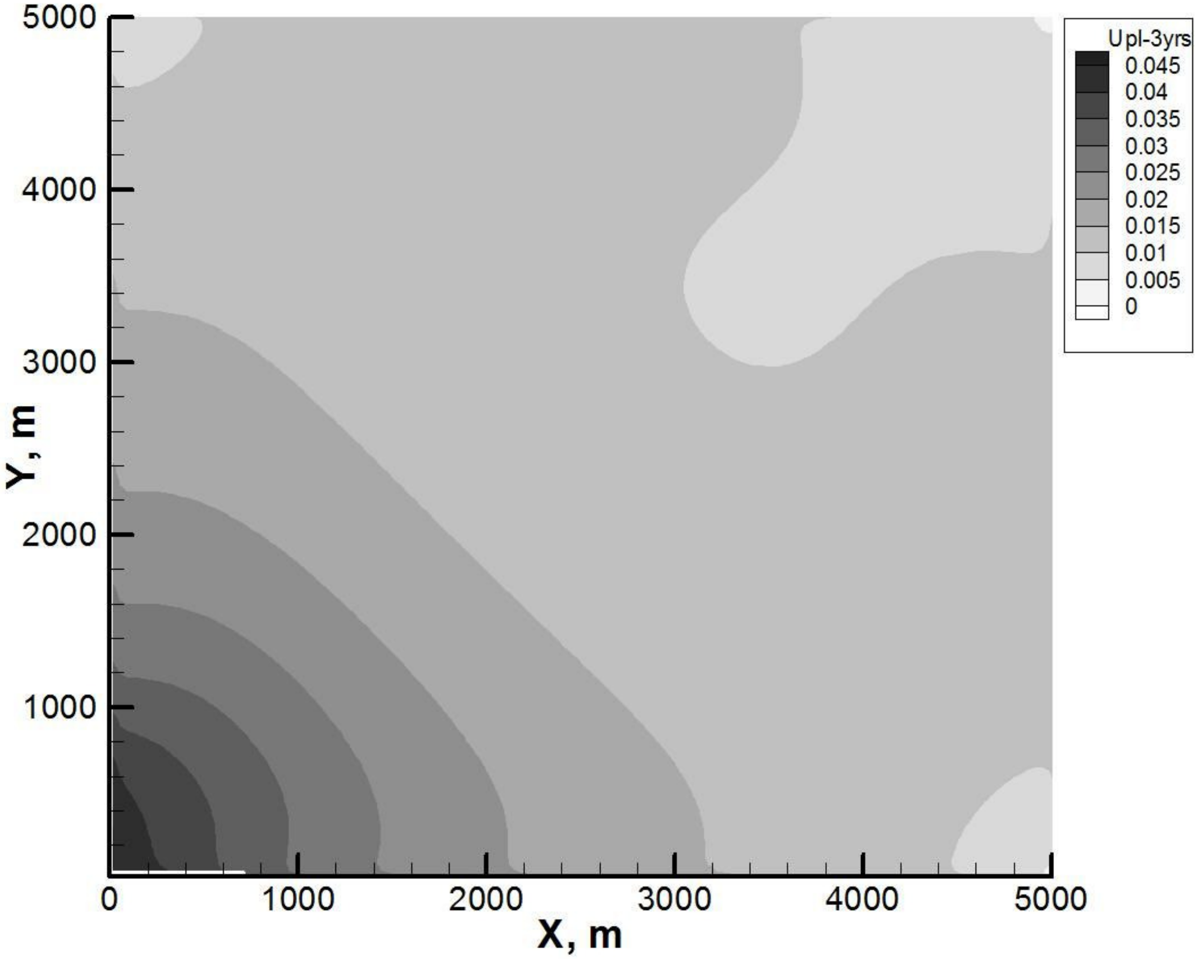


Figure 6.18. Surface uplift after three years of injection.

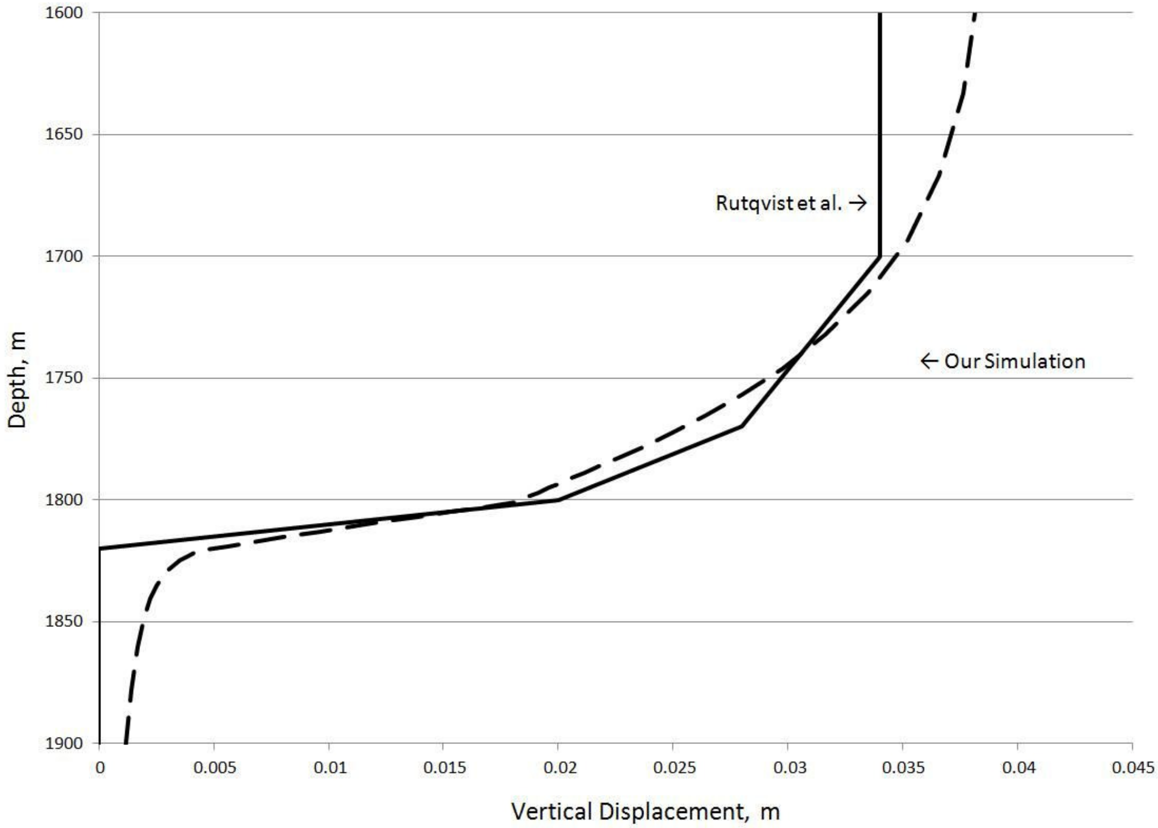


Figure 6.19. Match of surface uplift at well.

## 6.5 Ground Deformation and Heat Flow in Caldera Structure

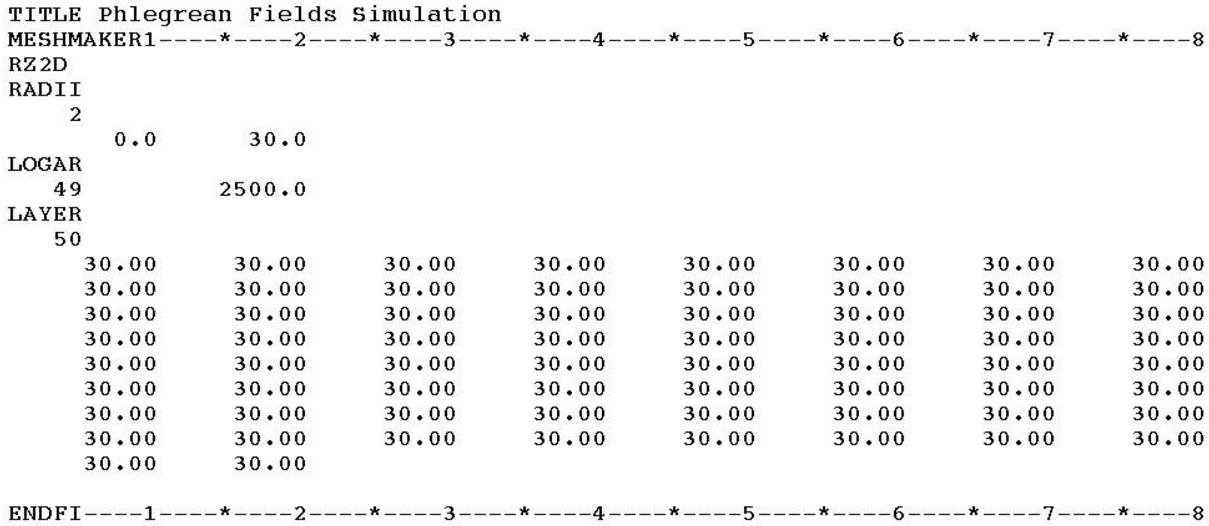
### 6.5.1 Problem Description

The Phlegrean Fields caldera, located near Naples, Italy, undergoes periodic episodes of volcanic unrest that includes seismic activity and slow ground movement. This unrest is believed to be caused by pressurization of the magma chamber and hot fluid migration. The caldera has been slowly subsiding with periodic short-lived minor uplifts after two major episodes of unrest during 1969-1972 and 1982-1984. Todesco et al. (2003a,b) hypothesized that the recent activity was associated with periods of more intense magmatic degassing that would cause larger amounts of fluid to enter the caldera, accompanied by ground deformation, increased pore pressure, and higher temperatures. To verify this they modeled hydrothermal fluid flow and porous medium deformation in a cylindrical system using the coupled TOUGH2-FLAC simulator, with fluid components water and carbon dioxide and the system heated by an influx of hot fluids from the bottom. Heat and fluid transport simulations were first done to match current conditions that were deduced from geochemical data, yielding injection rates of 3,000 t/day of water and 1500 t/d of $CO_2$ at 350 °C for 4,000 years. These results served as initial conditions for the periods of enhanced degassing, simulated by increasing the fluid influx for a given amount of time. The system top was at atmospheric pressure and ambient temperature (20 °C); the outer radial boundary and the rest of the bottom were impermeable and adiabatic.

### 6.5.2 TOUGH2-CSM Simulation Details

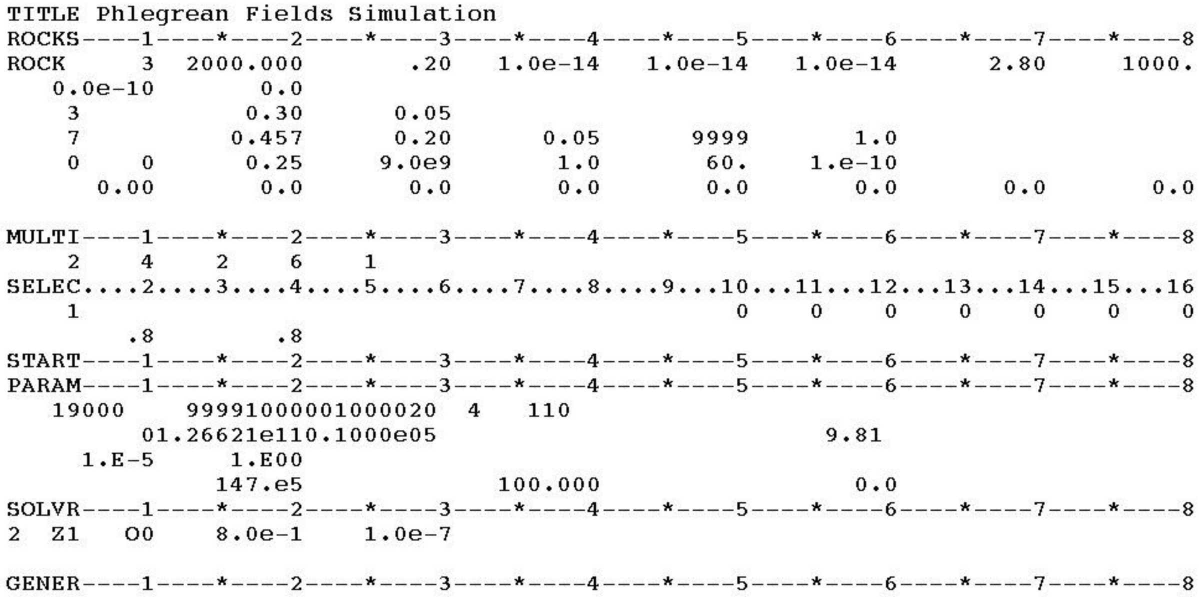
The simulation domain was 2,500 m in radius and 1,500 m in height. The r-z grid was 50 x 50, grid block height was constant, and grid block radial thickness varied logarithmically with the innermost grid blocks 30 m wide. The INFILE for grid generation is shown in Figure 6.20.

Figure 6.21 shows the beginning of the INFILE for the simulations. The MULTI record shows two for the number of components (NK in Figure 4.1), since fluid property module EOS2 contains only water and $CO_2$. The number of primary variables is four and the momentum calculation flag is one. The energy and momentum conservation equations are solved along with the two mass conservation equations.



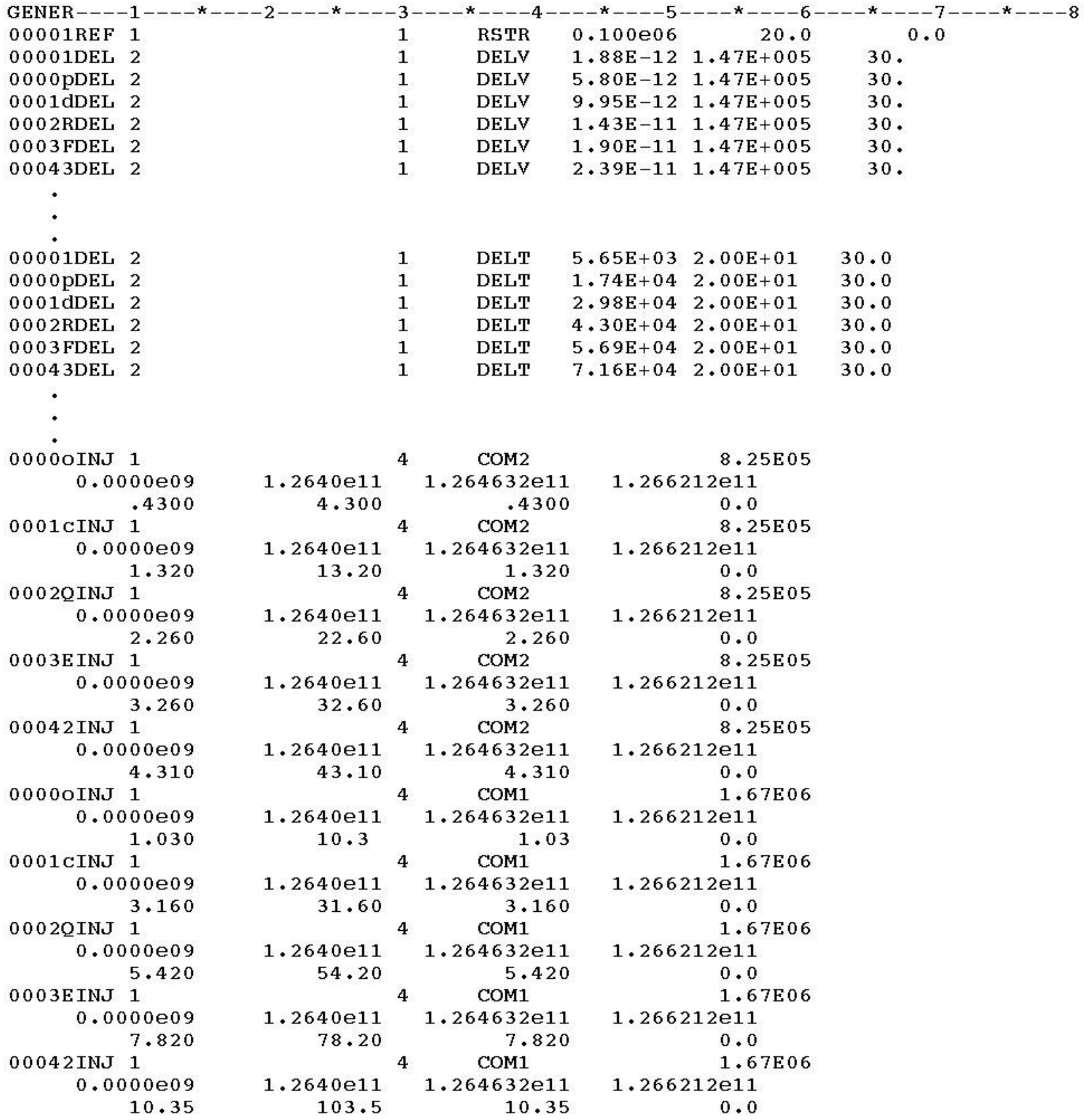
```
TITLE Phlegrean Fields Simulation
MESHMAKER1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
RZ2D
RADII
    2
       0.0      30.0
LOGAR
   49               2500.0
LAYER
   50
     30.00     30.00     30.00     30.00     30.00     30.00     30.00     30.00
     30.00     30.00     30.00     30.00     30.00     30.00     30.00     30.00
     30.00     30.00     30.00     30.00     30.00     30.00     30.00     30.00
     30.00     30.00     30.00     30.00     30.00     30.00     30.00     30.00
     30.00     30.00     30.00     30.00     30.00     30.00     30.00     30.00
     30.00     30.00     30.00     30.00     30.00     30.00     30.00     30.00
     30.00     30.00     30.00     30.00     30.00     30.00     30.00     30.00
     30.00     30.00     30.00     30.00     30.00     30.00     30.00     30.00
     30.00     30.00

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

Figure 20. INFILE for grid generation.



```
TITLE Phlegrean Fields Simulation
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
ROCK     3  2000.000       .20   1.0e-14   1.0e-14   1.0e-14      2.80     1000.
   0.0e-10       0.0
    3             0.30      0.05
    7            0.457      0.20      0.05      9999       1.0
    0    0        0.25     9.0e9       1.0       60.    1.e-10
      0.00       0.0       0.0       0.0       0.0       0.0       0.0       0.0

MULTI----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    2    4    2    6    1
SELEC....2....3....4....5....6....7....8....9...10...11...12...13...14...15...16
    1                                            0    0    0    0    0    0    0
        .8        .8
START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
   19000    99991000001000020  4   110
         01.26621e110.1000e05                          9.81
     1.E-5     1.E00
              147.e5              100.000                 0.0
SOLVR----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
2  Z1   O0    8.0e-1    1.0e-7

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

Figure 21. Beginning of INFILE for simulations.



```
GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
00001REF 1                    1    RSTR    0.100e06      20.0       0.0
00001DEL 2                    1    DELV    1.88E-12 1.47E+005    30.
0000pDEL 2                    1    DELV    5.80E-12 1.47E+005    30.
0001dDEL 2                    1    DELV    9.95E-12 1.47E+005    30.
0002RDEL 2                    1    DELV    1.43E-11 1.47E+005    30.
0003FDEL 2                    1    DELV    1.90E-11 1.47E+005    30.
00043DEL 2                    1    DELV    2.39E-11 1.47E+005    30.
    .
    .
    .
00001DEL 2                    1    DELT    5.65E+03 2.00E+01   30.0
0000pDEL 2                    1    DELT    1.74E+04 2.00E+01   30.0
0001dDEL 2                    1    DELT    2.98E+04 2.00E+01   30.0
0002RDEL 2                    1    DELT    4.30E+04 2.00E+01   30.0
0003FDEL 2                    1    DELT    5.69E+04 2.00E+01   30.0
00043DEL 2                    1    DELT    7.16E+04 2.00E+01   30.0
    .
    .
    .
0000oINJ 1                    4    COM2               8.25E05
     0.0000e09     1.2640e11   1.264632e11   1.266212e11
         .4300         4.300         .4300           0.0
0001cINJ 1                    4    COM2               8.25E05
     0.0000e09     1.2640e11   1.264632e11   1.266212e11
         1.320         13.20         1.320           0.0
0002QINJ 1                    4    COM2               8.25E05
     0.0000e09     1.2640e11   1.264632e11   1.266212e11
         2.260         22.60         2.260           0.0
0003EINJ 1                    4    COM2               8.25E05
     0.0000e09     1.2640e11   1.264632e11   1.266212e11
         3.260         32.60         3.260           0.0
00042INJ 1                    4    COM2               8.25E05
     0.0000e09     1.2640e11   1.264632e11   1.266212e11
         4.310         43.10         4.310           0.0
0000oINJ 1                    4    COM1               1.67E06
     0.0000e09     1.2640e11   1.264632e11   1.266212e11
         1.030         10.3           1.03           0.0
0001cINJ 1                    4    COM1               1.67E06
     0.0000e09     1.2640e11   1.264632e11   1.266212e11
         3.160         31.60         3.160           0.0
0002QINJ 1                    4    COM1               1.67E06
     0.0000e09     1.2640e11   1.264632e11   1.266212e11
         5.420         54.20         5.420           0.0
0003EINJ 1                    4    COM1               1.67E06
     0.0000e09     1.2640e11   1.264632e11   1.266212e11
         7.820         78.20         7.820           0.0
00042INJ 1                    4    COM1               1.67E06
     0.0000e09     1.2640e11   1.264632e11   1.266212e11
         10.35         103.5         10.35           0.0
```

Figure 6.22. GRMOD section for INFILE.

Figure 6.22 shows the GENER section of the INFILE. A reference mean stress at a reference elevation is specified for mean stress initialization. Below that are fifty deliverability wells producing fluid to ambient pressure, followed by fifty wells producing heat to ambient temperature, with one of each in the top row of grid blocks. Those are followed by five wells injecting $CO_2$ and five wells injecting water, with one of each in the five innermost grid blocks in the bottom row of the grid. The injected fluid enthalpy corresponds to the injection temperature of 350 °C and the well rates are selected such that the influx per unit surface area is constant.

We first ran a simulation to generate primary variables in hydrostatic equilibrium. We deactivated the momentum conservation equation by setting ISTCAL in the MULTI record to zero, set the number of primary variables to three, removed the $CO_2$ and water injectors from the GRMOD section, and ran the simulation until the system equilibrated. The simulation output a SAVE file that was renamed INCON and the bottom three lines replaced by blank one.

We then ran the actual simulation with the GRMOD section shown in Figure 6.22 and primary variables input using the above INCON file. Figure 6.23a shows the TOUGH2-CSM temperature profiles at 4,000 years and Figure 6.23b shows the published results; they are similar. Gas saturation profiles are shown in Figures 6.24a and 6.24b, and are also similar. Fluid injection rates were increased by a factor of ten for the next two years and surface uplift was calculated over this time interval using Equations 6.3 and 6.4. Figures 6.25a and 6.25b show surface uplift. The maximum value and the rate of decline of both profiles agree with each other.

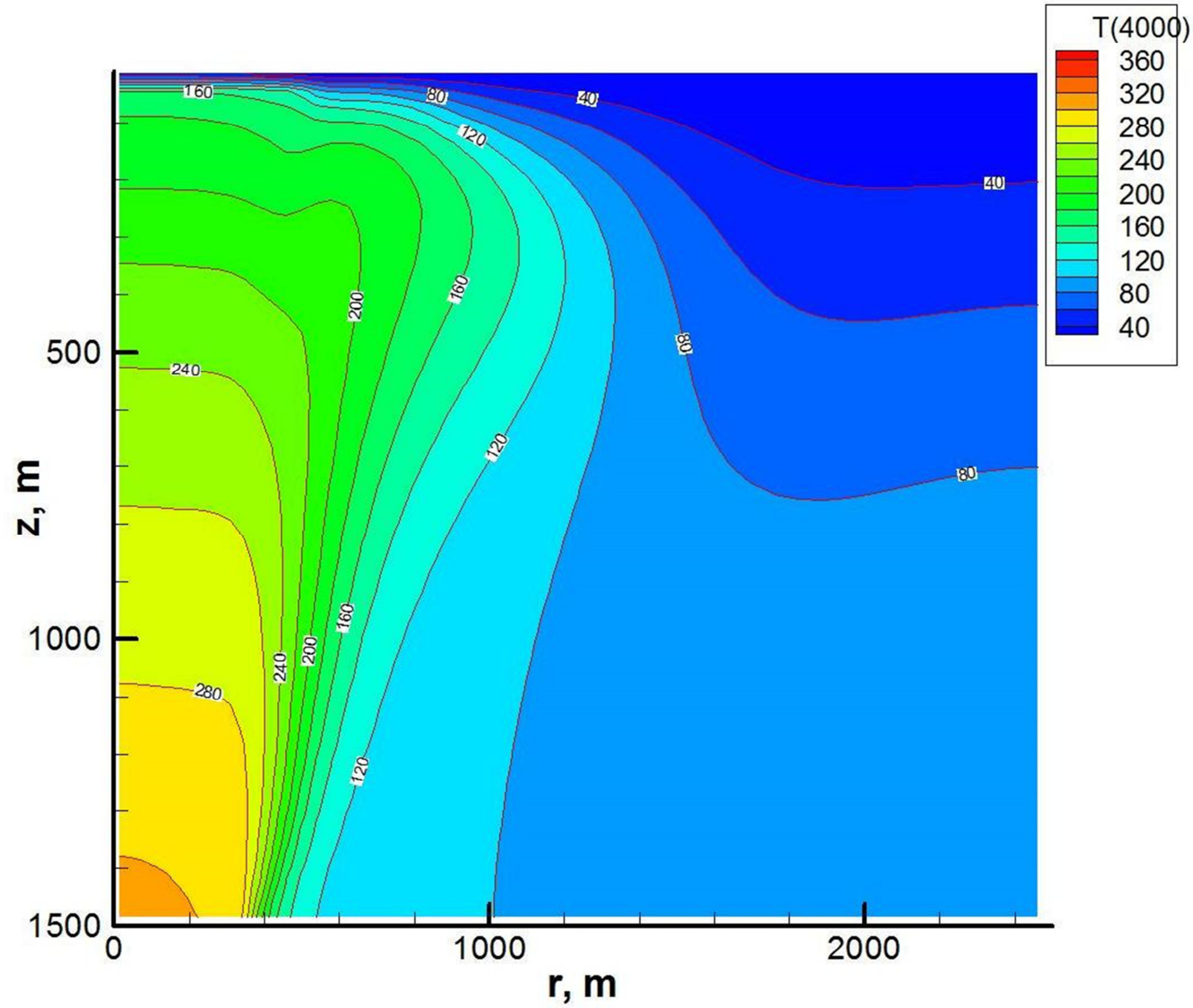


Figure 6.23a: Temperature profile after 4000 years injection.

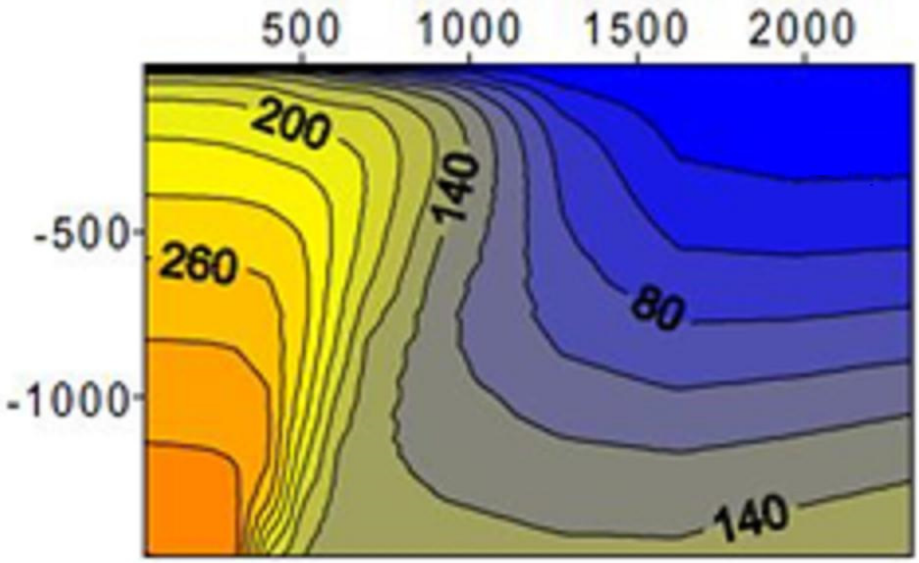


Figure 6.23b: Temperature profile after 4000 years injection Todesco et al. (2003a).

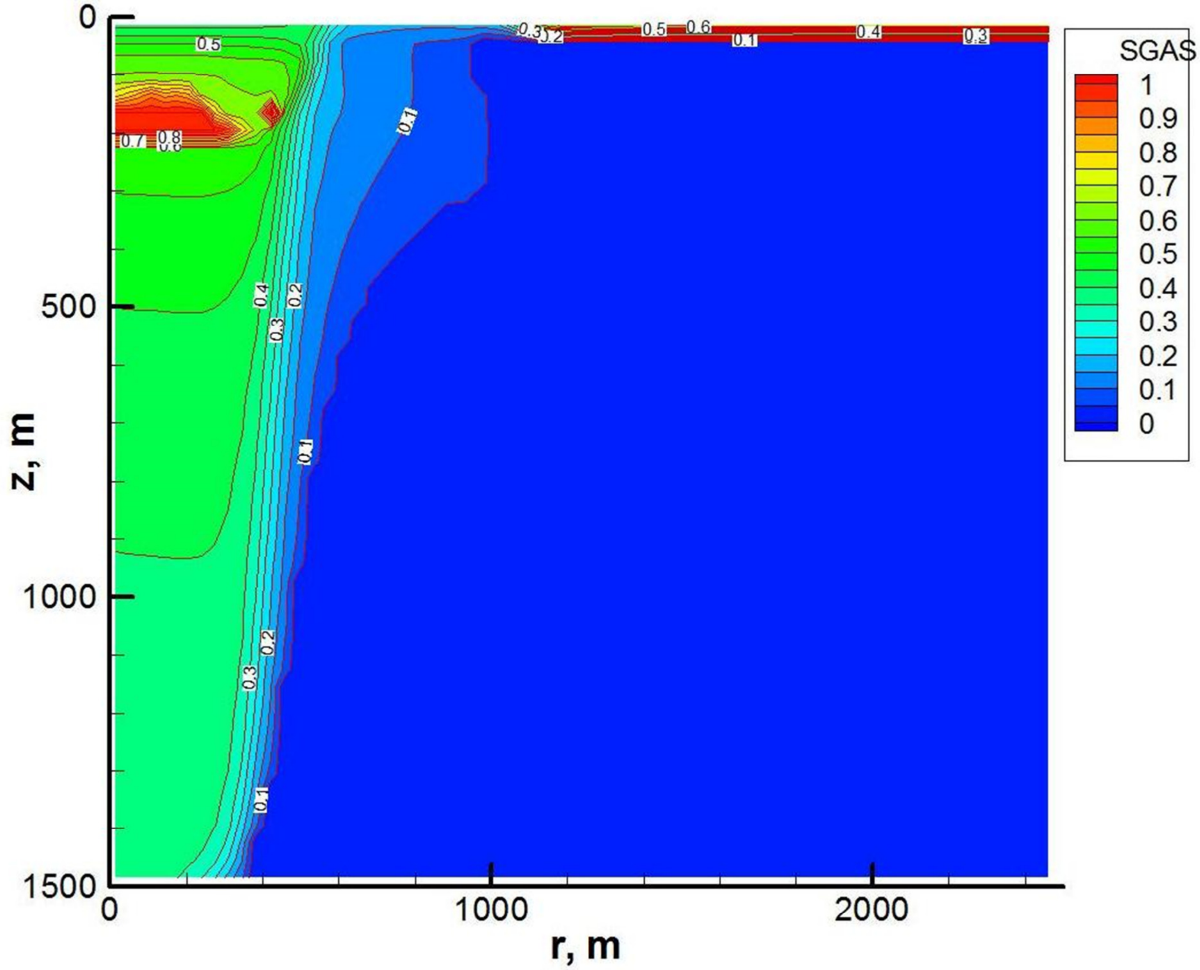


Figure 6.24a: $CO_2$ saturation profile after 4000 years injection.

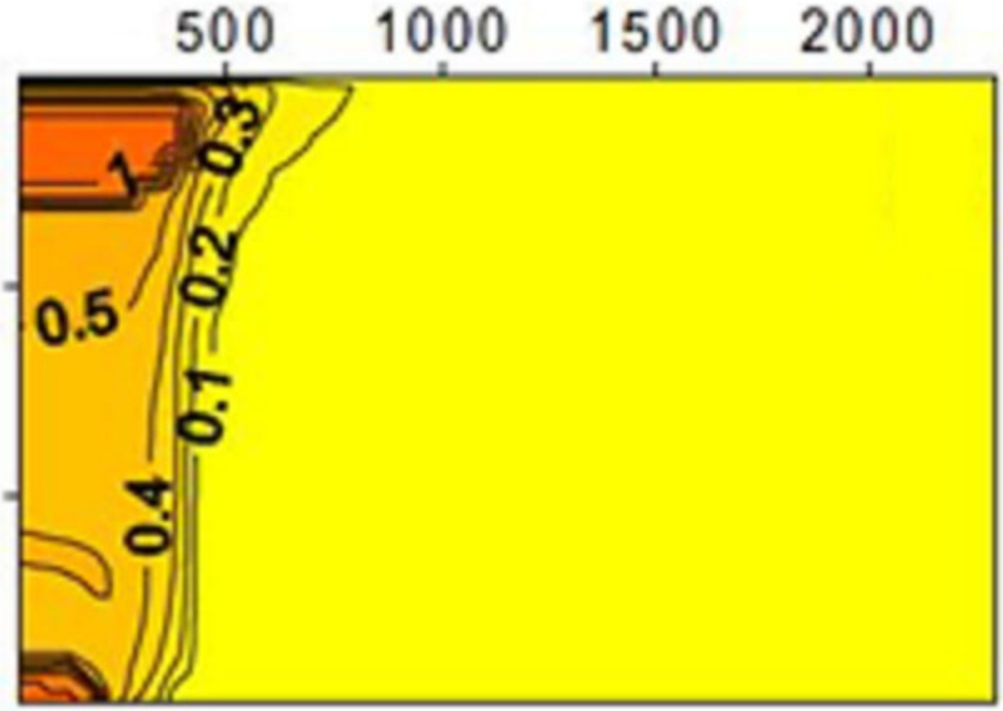


Figure 6.24b: $CO_2$ saturation profile after 4000 years injection Todesco et al. (2003a).

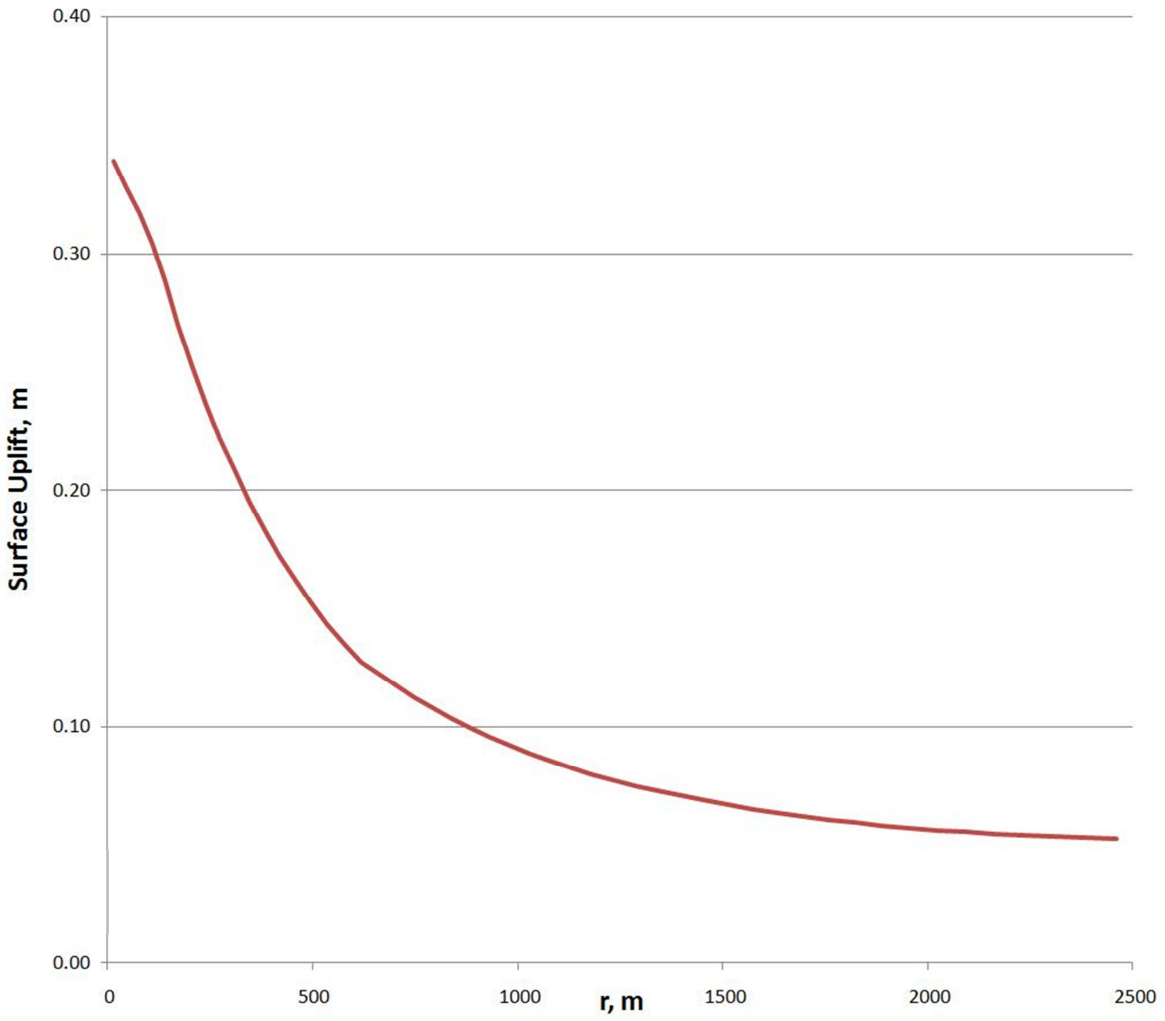


Figure 6.25a: Surface uplift after two years of higher injection rates (10 times).

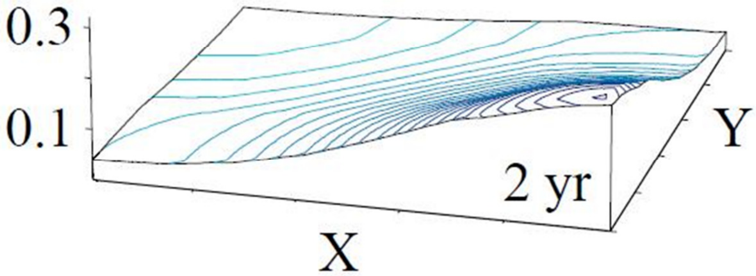


Figure 6.25b: Surface uplift after two years of higher injection rates (10 times) from Todesco et al. (2003a).

# 7. CONCLUSIONS

We developed a massively parallel reservoir simulator, called TOUGH2-CSM, for modeling thermal-hydrological-mechanical processes in fractured and porous media brine aquifers. The starting point for TOUGH2-CSM is the massively parallel TOUGH2-MP code and formulation. We derived, from the fundamental equations describing deformation of porous and fractured elastic media, a momentum conservation equation relating mean stress, pressure, and temperature, and incorporated it alongside the mass and energy conservation equations from the TOUGH2-MP formulation. In addition, rock properties, namely permeability and porosity, are functions effective stress and other variables that are obtained from the literature.

We presented detailed instructions for running TOUGH2-CSM. We described in detail the information contained in the input files needed to run a TOUGH2-CSM simulation and the outputs from such as simulation. We illustrated the simulator performance using several example problems that are described in detail, including a one-dimensional consolidation problem of a double porosity column, a two-dimensional simulation of the Mandel-Cryer effect, $CO_2$ injection into a layered saline aquifer, injection into the water leg of a depleting gas field, and a injection of hot fluid into a model of a caldera structure. These example problems provided good matches of analytical solutions and published results and illustrated TOUGH2-CSM simulation capabilities including its capacity to simulate geomechanical and thermal effects, multiple porosity media, and the parallel code's ability to solve large problems.

## ACKNOWLEDGEMENT

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# REFERENCES

Abousleiman Y., A. H. D. Cheng, L. Cui, E. Detournay, J. C. Roegiers, Mandel's problem revisited, *Géotechnique*, 46,187–95, 1996.

Barenblatt, G.E., Zheltov, I.P. & Kochina, I.N.: Basic concepts in the theory of seepage of homogenous liquids in fractured rocks. *J. Appl. Math. (USSR)* 24;5 (1960), pp.1286-1303.

Biot, M.A. & Willis, D.G.: The elastic coefficients of the theory of consolidation. *J. Appl. Mech.* 24 (1957), pp. 594–601.

Corey, A.T., The Interrelation Between Gas and Oil Relative Permeabilities, *Producers Monthly*, 38-41, November 1954. NNA.19900720.0036

Davies, J.P. & Davies, D.K.: Stress-dependent permeability: characterization and modelling. *SPE Journal* 6:2 (2001), pp. 224-235.

Elmroth, E., C. Ding, and Y. S. Wu, High Performance Computations for Large-Scale Simulations of Subsurface Multiphase Fluid and Heat Flow, *The Journal of Supercomputing,* 18(3), pp. 233-256, 2001.

Fatt, I. and W.A. Klikoff. Effect of Fractional Wettability on Multiphase Flow Through Porous Media, *AIME Transactions*, 216, 246, 1959. NNA.19900917.0129

Gutierrez, M. & Lewis, R.W.: Petroleum reservoir simulation coupling fluid flow and geomechanics. *SPE Reservoir Evaluation & Engineering,* June 2001, pp. 164-172.

Itasca Consulting Group, Inc.: FLAC3D manual: fast Lagrangian analysis of continua in three dimensions-version 2.0, Itasca Consulting Group, Inc, Minnesota, 1997.

Karypsis, G. and V. Kumar, METIS. A Software Package for Partitioning Unstructured Graphs, Partitioning Meshes, and Computing Fill-Reducing Orderings of Sparse Matrices*,* V4.0. Technical Report, Department of Computer Science, University of Minnesota, 1998.

Klinkenberg, L.J. The Permeability of Porous Media to Liquids and Gases, in API Drilling and Production Practice, pp. 200–213, 1941.

Lam, S.T., A. Hunsbedt, P. Kruger and K. Pruess. Analysis of the Stanford Geothermal Reservoir Model Experiments Using the LBL Reservoir Simulator, Geothermics, 17 (4), 595 - 605, LBL-25957, 1988.

Leverett, M.C., Capillary Behavior in Porous Solids, *Trans. Soc. Pet. Eng. AIME*, 142, 152-169, 1941.

Mandel, J.: Consolidation des sols (etude mathematique). *Geotechnique* (1953) pp. 3287–3299.

McKee, C.R., Bumb, A.C. & Koenig, R.A.: Stress-dependent permeability and porosity of coal and other geologic formations. *SPE Formation Evaluation*, 3:1 (1988), pp. 81-91.

Message Passing Forum, A Message-Passing Interface Standard, *International Journal of Supercomputing Applications and High performance Computing,* 8(3-4), 1994.

Milly, P.C.D., Moisture and Heat Transport in Hysteretic, Inhomogeneous Porous Media: A Matric-Head Based Formulation and a Numerical Model, *Water Resour. Res.*, Vol. 18, No. 3, pp. 489 - 498, 1982.

Mualem, Y., A New Model for Predicting the Hydraulic Conductivity of Unsaturated Porous Media, *Water Resour. Res.*, Vol. 12(3), pp. 513 - 522, 1976. NNA.19881228.0005

Narasimhan, T. N. and P. A. Witherspoon, An Integrated Finite Difference Method for Analyzing Fluid Flow in Porous Media, *Water Resources Research*, 12(1), pp. 57-64, 1976.

Narasimhan, T.N., P.A. Witherspoon and A.L. Edwards. Numerical Model for Saturated-Unsaturated Flow in Deformable Porous Media, Part 2: The Algorithm, *Water Resour. Res.*, 14 (2), 255-261, 1978.

Norris, A.: On the correspondence between poroelasticity and thermoelasticity. *J Appl Phys* 71 (1992), pp.1138-1141.

Ostensen, R.W.: The effect of stress-dependent permeability on gas production and well testing. *SPE Form. Eval.* 1:3 (1986), pp. 227–235.

Pickens, J.F., R.W. Gillham and D.R. Cameron. Finite Element Analysis of the Transport of Water and Solutes in Tile-Drained Soils, *J. of Hydrology*, 40, 243-264, 1979.

Pruess, K., GMINC – A Mesh Generator for Flow Simulations in Fractured Reservoirs, Report LBL-15227, Berkeley, California: Lawrence Berkeley National Laboratory, 1983.

Pruess, K., TOUGH2 – A general-purpose numerical simulator for multiphase fluid and heart flow, Lawrence Berkeley Laboratory Report LBNL-29400, Berkeley, CA, 1991.

Pruess, K., and T. N. Narasimhan, A Practical Method for Modeling Fluid and Heat Flow in Fractured Porous Media, *Soc. Pet. Eng. J., 25,* pp. 14-26, 1985.

Pruess, K, C. Oldenburg, and G. Moridis, TOUGH2 User's Guide*,* V2.0. Lawrence Berkeley National Laboratory Report LBNL-43134, Berkeley, CA, 1999.

Pruess K. and N. Spycher, ECO2N – A Fluid Property Module for the TOUGH2 Code for Studies of CO2 Storage in Saline Aquifers, *Energy Conversion and Management,* 48(6), 1761–1767, 2007.

Pruess, K., and Y. Tsang, 1994, Thermal Modeling for a Potential High-Level Nuclear Waste Repository at Yucca Mountain, Nevada, Lawrence Berkeley Laboratory Report, LBL-35381, UC-600, Lawrence Berkeley National Laboratories, Berkeley, CA

Rutqvist, J. & Tsang, C.F.: A study of caprock hydromechanical changes associated with CO2-injection into a brine formation. *Environ. Geol.* 42 (2002), pp. 296–305.

Rutqvist, J., Vasco, D.W. & Myer L.: Coupled reservoir-geomechanical analysis of $CO_2$ injection and ground deformations at In Salah Algeria. *Int. J. of Greenhouse Gas Control*, 4 (2010), pp. 225–230.

Terzaghi, K.: The shearing resistance of saturated soils and the angle between the planes of shear. *Proceedings of international conference on soil mechanics and foundation engineering,* Harvard University Press, Cambridge, MA, USA, 1936, pp. 54-56.

Todesco M, Rutqvist J, Chiodini G, Pruess K, Oldenburg C. Modeling of recent volcanic episodes at Phlegrean fields (Italy). Geochemical variations and ground deformation. Proceedings TOUGH Symposium 2003, Lawrence Berkeley National Laboratory, May 12–14, 2003.

Todesco M, Rutqvist J, Pruess K, Oldenburg C. SGP-TR-173, multiphase fluid circulation and ground deformation: a new perspective on bradyseismic activity at the Phlegrean fields (Italy). Proceedings Twenty Eighth Workshop on Geothermal Reservoir Engineering, Stanford University, January 27-29, 2003.

Tuminaro, R. S., M. Heroux, S. A. Hutchinson, and J. N. Shadid, Official Aztec user's guide, Ver 2.1, Massively Parallel Computing Research Laboratory, Sandia National Laboratories, Albuquerque, NM, 1999.

Udell, K.S. and J.S. Fitch. Heat and Mass Transfer in Capillary Porous Media Considering Evaporation, Condensation, and Non-Condensible Gas Effects, paper presented at 23rd ASME/AIChE National Heat Transfer Conference, Denver, CO, 1985.

Van Genuchten, M.Th. A Closed-Form Equation for Predicting the Hydraulic Conductivity of Unsaturated Soils, *Soil Sci. Soc.* , Vol. 44, pp. 892 - 898, 1980. NNA.19911009.0008

Verma, A., & Pruess, K.: Thermohydrological conditions and silica redistribution near high-level nuclear wastes emplaced in saturated geological formations. *J. Geophys. Res.*, 93 (1988), pp. 1159-1173.

Verma, A.K., K. Pruess, C.F. Tsang and P.A. Witherspoon. A Study of Two-Phase Concurrent Flow of Steam and Water in an Unconsolidated Porous Medium, Proc. 23rd National Heat Transfer Conference, Am. Society of Mechanical Engineers, Denver, CO, 135–143, 1985.

NNA.19890713.0198

Warren, J.E. & Root, P.J.: The Behavior of Naturally Fractured Reservoirs. *Society of Petroleum Engineers Journal, Transactions AIME*, 228, September 1963, pp. 245-255.

Wilson, R.K. & Aifantis, E.C.: On the theory of consolidation with double porosity. *Int. J. Eng. Sci.,* 20:9 (1982), pp. 1009-1035.

Wu, Y. S., USERS MANUAL (UM) for TOUGH2*,* Version 1.4, STN:10007-1.4-01, Research Report, Earth Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA, 2000.

Wu, Y. S., C. F. Ahlers, P. Fraser, A. Simmons, and K. Pruess, *Software Qualification of Selected TOUGH2 Modules*, Research Report, Earth Sciences Division, Lawrence Berkeley National Laboratory, LBL-39490, UC-800, October, 1996.

Zhang K., Y.-S. Wu, K. Pruess, *User's guide for TOUGH2-MP - a massively parallel version of the TOUGH2 code,* Lawrence Berkeley National Laboratory Report LBNL-315E, 2008.

Zhang K. and YS Wu, 2006, Enhancing Scalability and Efficiency of the TOUGH2_MP for Linux Clusters, Proceedings of TOUGH symposium 2006, Berkeley, CA.

Zhang K., Moridis M., and Pruess, K. TOUGH+CO2: A multiphase fluid flow simulator for CO2 geologic sequestration in saline aquifers, Computers & Geosciences 37 (2011) 714–723.

## APPENDIX B. RELATIVE PERMEABILITY FUNCTIONS

IRP = 1 Linear functions

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

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

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

RP(2) $\leq$ Sg $\leq$ 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 $\hat{S} = \frac{(S_l - S_{lr})}{(1 - S_{lr} - S_{gr})}$

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

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

IRP = 4 **Grant's curves**

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

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

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)**

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

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

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)**

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

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

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

subject to the restriction $0 \leq k_{rl}, k_{rg} \leq 1$

Here, $S^* = \frac{(S_l - S_{lr})}{(1 - S_{lr})}$, $\hat{S} = \frac{(S_l - S_{lr})}{(1 - S_{lr} - S_{gr})}$

Parameters: RP(1) = λ

RP(2) = $S_{lr}$

RP(3) = $S_{ls}$

RP(4) = $S_{gr}$

RP(5) = switching parameter

Notation: Parameter $\lambda$ is m in van Genuchten's notation, with m = 1-1/n;

parameter n is often written as $\beta$.

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

$$S_{th} = \frac{\phi_m}{\phi_m + \phi_f}$$

where both $\phi_m$ and $\phi_f$ 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 VI). 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 Table B.1 for parameter definition.

**Table B.1. Definition of parameters for IRP=9 and 10 with ECM relative permeability functions.**

| | | |
|---|---|---|
| IRP= | 9 | for ECM option in isotropic fracture systems. |
| IRP= | 10 | for ECM option in anisotropic fracture systems. |
| RP(1)= | M | of van Genuchten's function for matrix. |
| RP(2)= | $S_{lr}$ | residual liquid saturation in matrix. |
| RP(3)= | M | 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)= | $1- \phi_f$ | $\phi_f$ 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 VI). 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. Table B.2 defines the parameters for the ECM relative permeability function.

**Table B.2 Definition of parameters for IRP=11 with generalized ECM relative permeability functions.**

| | | |
|---|---|---|
| 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)= | $S_{lr}$ | Residual liquid saturation in fractures. |
| RP(5)= | | > 0 krg = 1.0 - krl<br>< 0 using Corey's function for krg. |
| RP(6)= | $S_{gr}$ | Residual gas saturation in matrix. |
| RP(7)= | $\phi_f$ | Fracture continuum porosity. |

IRP = 12 **Generalized Power Law**

$$k_{rl} = \left(\frac{S_l - S_{l,min}}{S_{l,max} - S_{l,min}}\right)^{n_l}$$

$$k_{rg} = \left(\frac{S_g - S_{g,min}}{S_{g,max} - S_{g,min}}\right)^{n_g}$$

with $S_{l,min}$ = RP(1) $S_{l,max}$ = RP(2) $n_l$ = RP(3) $S_{g,min}$ = RP(4)

$S_{g,max}$ = RP(5) $n_g$ = RP(6)

subject to the restriction $0 \leq k_{rl}, k_{rg} \leq 1$

## APPENDIX C. CAPILLARY PRESSURE FUNCTIONS

ICP = 1 **Linear function**

$$P_{cap} = \begin{Bmatrix} -\mathrm{CP}(1) & \text{for } S_l \leq \mathrm{CP}(2) \\ 0 & \text{for } S_l \leq \mathrm{CP}(2) \\ -\mathrm{CP}(1)\,\frac{\mathrm{CP}(3)-S_L}{\mathrm{CP}(3)-\mathrm{CP}(2)} & \text{for } \mathrm{CP}(2) < S_l < CP(3) \end{Bmatrix}$$

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

$P_0 = \mathrm{CP}(1)$ $S_{lr} = \mathrm{CP}(2)$ $S_{l0} = \mathrm{CP}(3)$ $x = \mathrm{CP}(4)$

Restrictions: $0 < \mathrm{CP}(2) < 1 \leq \mathrm{CP}(3)$; $\mathrm{CP}(4) \neq 0$

ICP = 3 **TRUST capillary pressure (Narasimhan et al., 1978)**

$$P_{cap} = \begin{Bmatrix} -P_e - P_0 \left[\frac{1-S_l}{S_l - S_{lr}}\right]^{\frac{1}{\eta}} & \text{for } S_l < 1 \\ 0 & \text{for } S_l < 1 \end{Bmatrix}$$

where

$P_0 = \mathrm{CP}(1)$ $S_{lr} = \mathrm{CP}(2)$ $\eta = \mathrm{CP}(3)$ $P_e = \mathrm{CP}(4)$

Restrictions: $\mathrm{CP}(2) \geq 0$; $\mathrm{CP}(3) \neq 0$

ICP = 4 **Milly's function (Milly, 1982)**

$$P_{cap} = -97.783 \cdot 10^{A}$$

with

$$A = 2.26\left(\frac{0.371}{S_l - S_{lr}} - 1\right)^{\frac{1}{4}}$$

where $S_{lr}$ = CP(1)

Restriction: CP(1) ≥ 0.

ICP = 6 **Leverett's function (Leverett, 1941; Udell and Fitch, 1985)**

$$P_{cap} = -P_0 \cdot \sigma(T) \cdot f(S_l)$$

with

σ(T) - surface tension of water (supplied internally in TOUGH2-CSM)

$f(S_l) = 1.417\ (1 - S^*) - 2.120\ (1 - S^*)^2 + 1.263\ (1 - S^*)^3$

where

$S^* = (S_l - S_{lr})/(1 - S_{lr})$

Parameters: P0 = CP(1) $S_{lr}$ = CP(2)

Restriction: 0 ≤ CP(2) < 1

ICP = 7 **van Genuchten function** (van Genuchten, 1980)

$$P_{cap} = -P_0\left([S^*]^{-\frac{1}{\lambda}} - 1\right)^{1-\lambda}$$

subject to the restriction

$$- P_{max} < P_{cap} \leq 0$$

Here,

$$S^* = (S_l - S_{lr})/(1 - S_{lr})$$

Parameters: CP(1)= $\lambda = 1 - \frac{1}{n}$

CP(2)=$S_{lr}$ (should be chosen smaller than the corresponding parameter in the relative permeability function;

see note below.)

$CP(3)=1/P_0$

$CP(4)=P_{max}$

$CP(5) = S_{ls}$

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 be coming immobile (discontinuous). In reality, no special capillary pressure effects are expected when liquid phase becomes discontinuous. Accordingly, we recommend always choosing a smaller $S_{lr}$ for the capillary pressure 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 C.1 lists the definition of the related parameters.

**Table C.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)= | $\alpha$ | 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)= | $\delta$ | 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 C.2 lists the definition of the related parameters.

**Table C.2 Definition of parameters for ICP = 8 with the generalized 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)= | $\alpha_m$ | 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)= | $\alpha_f$ | With units $Pa^{-1}$, van Genuchten's parameter for fractures. |

## APPENDIX D. POROSITY VARIATION OPTIONS

IPOPT = 0: Constant porosity

IPOPT = 1 Equation 2.48, from Rutqvist et al. (2002), usually used with IKOPT=1

RCKPAR(1) = $\phi_1$

RCKPAR(2) = a

IPOPT = 2 Equation 2.51, from Rutqvist et al. (2002) , usually used with IKOPT=2

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

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

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

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

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

RCKPAR(6) = $\Delta b_{0,3}$

RCKPAR(7) = d

IPOPT = 3 Equation 2.53, from McKee et al. (1988)

COM = $c_p$

IPOPT = 4 Slightly compressible rock with thermal expansion, given by

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

COM = $c_p$

EXPAN = $c_t$

RCKPAR(1) = $P_{ref}$

RCKPAR(2) = $T_{ref}$

IPOPT = 5 Equation 2.47

SOLMOD = $K_s$

## APPENDIX E. PERMEABILITY VARIATION OPTIONS

IKOPT = 0: Constant permeability

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

RCKPAR(5) = c

IKOPT = 2 Equation 2.51, from Rutqvist et al. (2002) , usually used with IPOPT=2

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

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

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

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

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

RCKPAR(6) = $\Delta b_{0,3}$

RCKPAR(7) = d

IKOPT = 3 Equation 2.54, Carman-Kozeny equation

IKOPT = 4 Equation 2.55, from Ostensen (1986)

RCKPAR(5) = x-direction $\tau^{\prime,*}$

RCKPAR(6) = y-direction $\tau^{\prime,*}$

RCKPAR(7) = z-direction $\tau^{\prime,*}$

RCKPAR(8) = n

IKOPT = 5 Equation 2.56, Verma and Pruess (1988)

RCKPAR(6) = $k_r/k_0$

RCKPAR(7) = $\phi_r/\phi_0$

RCKPAR(8) = n