

INTEGRATION OF POROELASTICITY INTO TOUGH2

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ABSTRACT

This paper describes the addition of integrated stress analysis into the TOUGH2 code. The goal is to provide a fully coupled analysis capability that takes advantage of the present flow and heat transfer analysis in TOUGH2 and extends this in a consistent manner to incorporate stress. The stress analysis is performed using the dual of the TOUGH2 mesh for the finite element stress analysis. This leads to an elegant and efficient coupling, that minimizes changes to the TOUGH2 code, while adding new stress solution capability.

BACKGROUND

TOUGH2 is a program for calculation of multi-phase, multi-component, non-isothermal flow in porous media (Pruess, 1999). It uses a modified dual-permeability approach (MINC) to represent flow in fractured media. Some of the strengths of the code include:

- Use of the integral finite difference approach, which can accommodate general geometry (with the constraint that the mesh be Voronoi).
- Implementation of several equation-of-state modules to represent different fluid mixtures.
- Continual development to add new capability such as multiple volatile organic compounds (TMVOC) and chemical reactions (TOUGHREACT).

One physical phenomenon that is not included in TOUGH2 is deformation and stress. For some problems, stress coupling can be important. For example, the heated rock around a nuclear waste cask expands which can close fractures in the heated region (Rutqvist and Tsang, 2003a). Alternately, cooling due to injection of cold water in geothermal reservoirs can lead to opening of fractures and increased injection rates (Ito, 2002). In conventional rock mechanics, water flow into tunnels can be a

function of the stress around the tunnel. It is a logical extension of TOUGH2 to consider how to add stress coupling.

DUAL MESHES

Dual meshes are alternate representations of the same geometry (George and Borouchaki, 1998). An example is shown in Figure 1, which illustrates a Delaunay mesh and its dual, the Voronoi mesh. The Voronoi mesh corresponds to the TOUGH2 mesh, with a node interior to the volume.

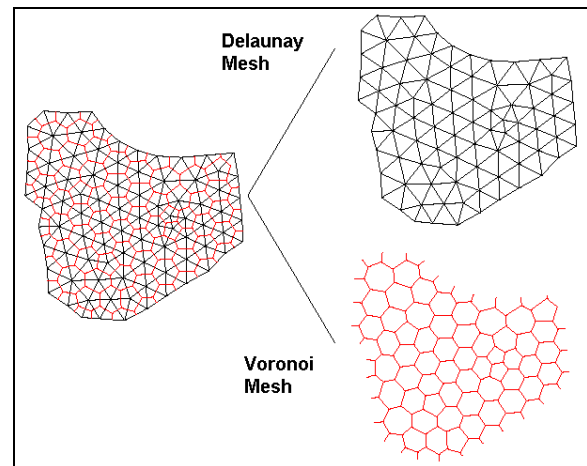


Figure 1: An example of two dual meshes, a Delaunay mesh and a Voronoi mesh (figure from Cosmi and Marino, 2002)

The two meshes are shown in greater detail in Figure 2. In the Voronoi (TOUGH2) mesh, the center point is the point used for spatial discretization with the associated volume, while the Delaunay mesh corresponds to a finite element triangulation of the area.

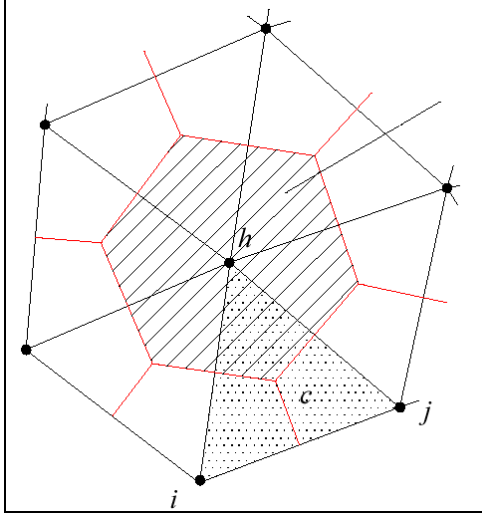


Figure 2: Detail of a Delaunay and Voronoi mesh (figure from Cosmi and Marino, 2002)

Each Voronoi cell is associated with a point, P_i . A cell, V_i , is the locus of the points closer to P_i than any other point in the volume. This gives a volume around each node in the Voronoi mesh. The Voronoi mesh can be visualized as being formed by perpendicular bisection of a triangular mesh, as long as the triangulation is Delaunay.

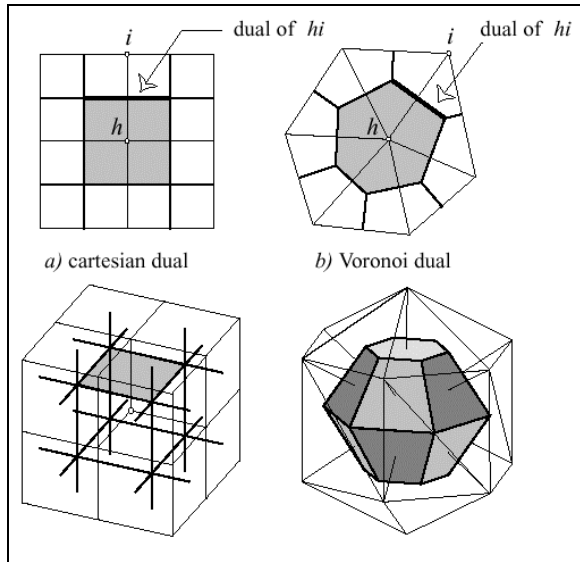


Figure 3: Duals for different meshes (figure from Tonti, 2002)

Triangular Delaunay and the corresponding Voronoi meshes are not the only approaches to dual meshes. The dual of a regular rectangular mesh is a shifted rectangle, Figure 3a. Various 3D duals based on tetrahedral are also illustrated in Figure 3, b and c.

With respect to TOUGH2, the importance of Voronoi and rectangular meshes is that they satisfy the convergence criteria for the integrated finite

difference approach. With respect to the stress analysis, the dual of the Voronoi mesh (the Delaunay mesh) is a natural approach for use in finite elements.

This is the approach used in the development of stress in TOUGH2. The Voronoi mesh (integrated finite difference mesh) is used for the flow analysis in TOUGH2, and the Delaunay mesh (finite element mesh) is used for the finite element calculation of stress. The points at the “center” of the TOUGH2 cells become the nodes for the stress finite element analysis. Changes to the present TOUGH2 flow analysis are minimal. The stress analysis is added as a natural extension to the present capability. State variables for the flow analysis (such as pressure and temperature) continue to be represented at the centers of their corresponding TOUGH2 volumes, while displacements are added as unknowns and used to solve the stress problem.

IMPLEMENTATION

Approach

A primary goal of the implementation of poroelasticity in TOUGH2 is to minimize changes to the TOUGH2 code. This has been accomplished in two ways.

First, the poroelastic calculations are performed as much as possible across an interface between the standard FORTRAN code used for TOUGH2 and the C++ code used for the finite element analysis. This barrier provides a clear break between the different functions of the code. To speed development, the finite element analysis is based on the Geocrack3D code (Hardeman et al., 1999).

On the TOUGH2 side, the changes to implement poroelasticity have been added as tasks that are performed after the standard TOUGH2 solution procedures. For example, the addition of the poroelastic coefficients to the Jacobian matrix are only calculated and added after the standard code for calculation of the Jacobian. The stress coefficients are appended to the Jacobian and then the standard solvers are used to calculate the result. The Jacobian is shown below:

$$\begin{bmatrix} J_{FF} & J_{FS} \\ J_{SF} & J_{SS} \end{bmatrix} \begin{Bmatrix} p_F \\ u_S \end{Bmatrix} = \begin{Bmatrix} R_F \\ R_S \end{Bmatrix}$$

where the unknowns have been divided into the primary variables for the flow solution p_F and the displacements for the stress solution u_S . In the Jacobian, the J_{FF} coefficients are the standard terms in TOUGH2, the J_{SS} coefficients are the finite

element stress solution terms, and J_{SF} and J_{FS} are the coupling terms between the two solutions.

Mesh Generation

In order to minimize the task of performing a stress analysis, the coordinates of the TOUGH2 cells (the Voronoï mesh) are read and used to create the finite element mesh (the Delaunay mesh) automatically. This is done in a small translation program. At the present time, the TOUGH2 mesh must be a Cartesian (rectangular) grid. This simplifies the generation of the corresponding finite element mesh. In addition, the program that performs the mesh translation also is used to define the material properties and boundary conditions for the finite element stress model.

Finite Element Formulation for Poroelasticity

The implementation of stress follows that given by Lewis and Schrefler, 1987. The solid phase is assumed to be a porous skeleton surrounded by one or more fluids. The major deformation of the porous skeleton is governed by the effective stress σ' :

$$\sigma = \sigma' - \mathbf{m}p$$

where σ is the total stress, \mathbf{m} is a vector with coefficients equal to unity for the normal stress components and zero for shear stress components, and p is the pressure.

Equilibrium is given by:

$$\sigma_{ij,j} + b_i = 0$$

The finite element form is obtained using the weak form of the equilibrium equation:

$$\int_V \sigma_{ij} \delta \varepsilon_{ij} dV = \int_V b_i \delta u_i dV + \int_S t_i \delta u_i dS$$

The constitutive equation relating stress to strain is:

$$\sigma = \mathbf{D}(\varepsilon - \varepsilon_p - \varepsilon_T)$$

where,

$$\varepsilon_p = -\mathbf{m} \left(\frac{1}{3K_s} \right) \Delta p$$

$$\varepsilon_T = \mathbf{m} \alpha \Delta T$$

and \mathbf{D} is the elastic material matrix, ε is the total strain increment, ε_p is the volumetric strain caused by uniform compression of the solid particles of the skeleton by the change of pressure of the pore fluid, K_s is the bulk modulus of the solid phase, ε_T is the thermal strain increment, and α is the thermal expansion coefficient of the skeleton.

Using shape functions to approximate the solution and the weighting functions, we obtain:

$$\left(\int_V \mathbf{B}^T \mathbf{D} \mathbf{B} dV \right) \mathbf{u} = \beta \int_V \mathbf{B}^T \mathbf{m} \Delta p dV + 3K_s \alpha \int_V \mathbf{B}^T \mathbf{m} \Delta T dV + \int_V \mathbf{N}^T \mathbf{b} dV + \int_S \mathbf{N}^T \mathbf{t} dS - \left(\int_V \mathbf{B}^T \mathbf{D} \mathbf{B}_u dV \right) \mathbf{u}_u$$

where β is the Biot-Willis coefficient, and the subscript u refers to the known essential boundary conditions.

TERZAGHI VERIFICATION PROBLEM

The first verification problem to test the coupled analysis is the solution of the Terzaghi consolidation problem, Figure 4. In this test, a constant stress is applied suddenly on the surface of a fluid-saturated sample. The piston applying the load is permeable, such that the top boundary is drained. Following an initial step displacement, the sample consolidates gradually as fluid flows out the top drain.

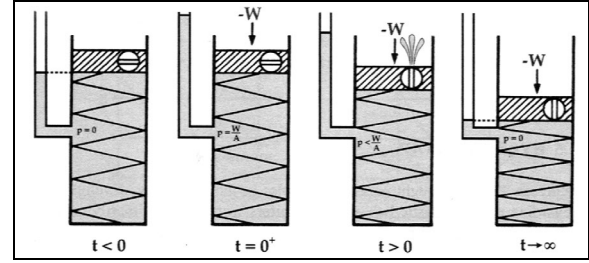


Figure 4: Schematic of uniaxially constrained soil consolidation (after Wang, 2000)

Because the vertical stress is independent of time, the pore pressure is uncoupled from the stress and satisfies the homogeneous diffusion equation. The solution is (Wang, 2000),

$$p(z, t) = \frac{4\gamma\sigma_0}{\pi} \sum_{m=0}^{\infty} \frac{1}{2m+1} \exp\left[-\frac{(2m+1)^2 \pi^2 ct}{4L^2}\right] \sin\left[\frac{(2m+1)\pi z}{2L}\right]$$

A plot of this solution is shown in Figure 5. Initially, the pressure in the fluid is zero. When the load is applied, the pressure instantly reaches a value (4.14E5 Pa) that is the portion of the load carried by the fluid. Then, as time increases, the fluid is drained and the pressure is reduced. At long times, the pressure will approach zero and all the load is carried by the porous media and not the fluid. As can be seen, the comparison between the analytic and calculated pressures is very good.

The additional displacement during drainage is shown in Figure 6. As can be seen, initially the drainage displacement is only near the top. However,

as more fluid is drained, this displacement becomes larger. Again, the comparison between the analytic and calculated displacements is very good.

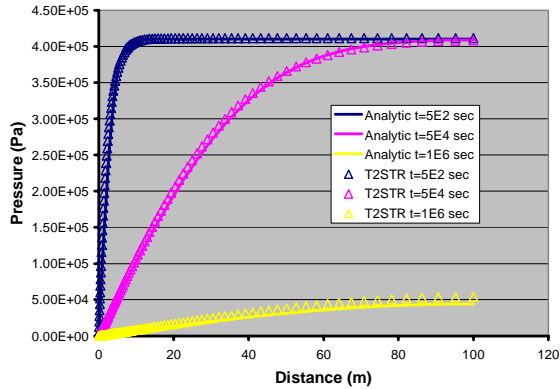


Figure 5: Pressures in column for times following the step load

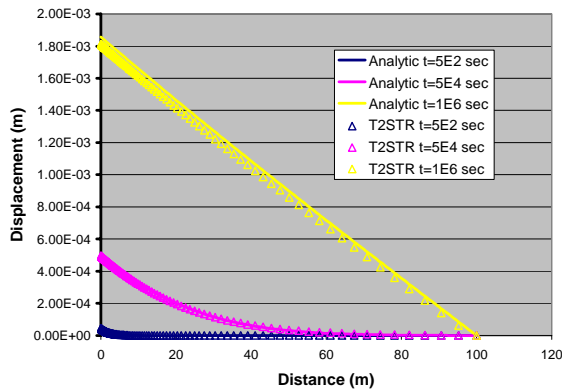


Figure 6: Drainage displacement

EXAMPLE PROBLEMS

LBNL 1-D Geothermal Problem

LBNL (Rutqvist, 2003b) provided a first comparison problem. This problem is a one-dimensional column extending 1500 meters (Figure 7). At the bottom of the model there is a 200 meter thick reservoir overlaid by a 100 meter thick cap rock.

Initial conditions are established by running a steady state analysis with fixed atmospheric pressure and temperature of 10°C on the ground surface and 240°C at the bottom of the model. Then a constant pressure injection was conducted just below the caprock. The injection pressure was set to 20 MPa and the temperature of injection fluid was set to 30°C. In the initial problem, water leakage was simulated by adding one extra column of inactive elements at a connection distance of 5 km. Since the water leakage is a somewhat artificial geometry, the problem was further simplified to model only the column with fixed boundary conditions at the top and bottom during injection.

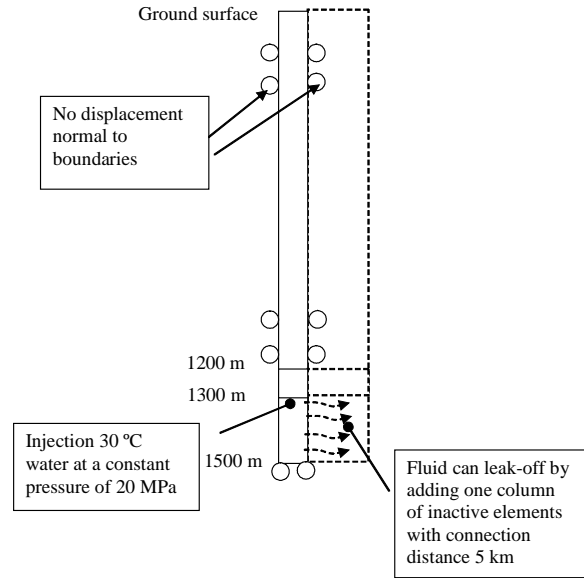


Figure 7: Model domain

The resulting temperature profile is shown in Figure 8 and the corresponding displacement at the surface is shown in Figure 9.

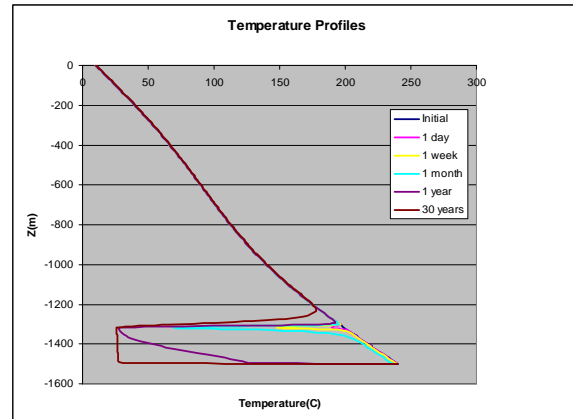


Figure 8: Temperature profiles

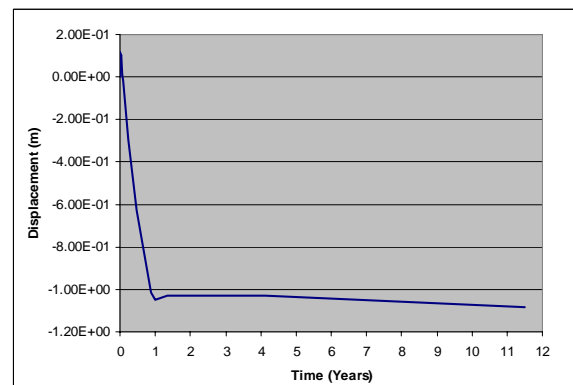


Figure 9: Time evolution of surface displacement

LBNL 2-D Geothermal Problem

The 1D problem was extended to 2D. The calculation used a horizontal distance of 400 m. The mesh for this analysis is shown in Figure 10. The well injection is just beneath the cap rock, shown in green in Figure 10.

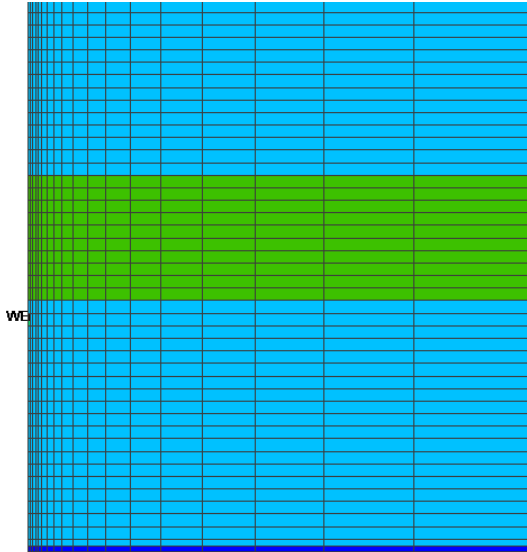


Figure 10: Detail showing 2D model with cap rock and injection well

Results for the temperature and horizontal stress are shown in Figure 11 and Figure 12. As can be seen in Figure 11, the injection cools the rock in the vicinity of the well below the caprock. Cooling of the rock causes thermal contraction which reduces the horizontal stress (Figure 12).

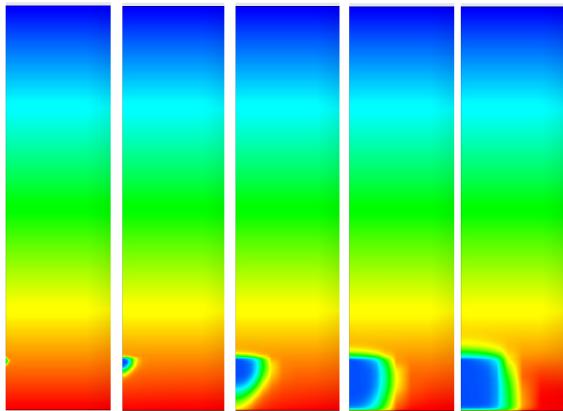


Figure 11: Evolution of temperature

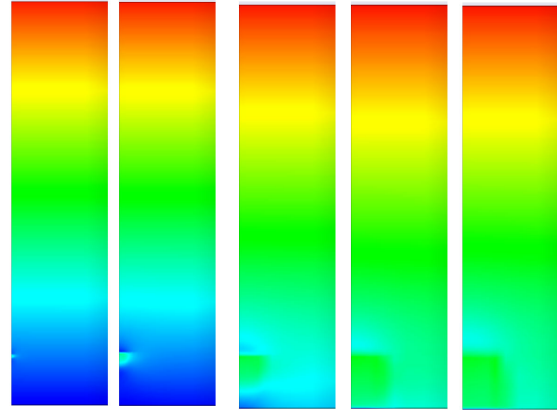


Figure 12: Evolution of horizontal stress (all stresses are negative, with blue indicating the most negative stress)

FUTURE WORK

Future work will consist of both extending the model and applying the model to the Coso site. Model development will include the coupling of flow to stress. This will be done both by making the permeability a function of stress and by adding a stress dependence to the flow on fractures in the MINC model.

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