Internal Report
Sandia National Laboratories
Division 6413

August 1983

Trip Report: Workshop on the Computer Code "TOUGH" (Transport of Unsaturated Groundwater and Heat)

Paul Davis

Date: August 17 - 19, 1983

Location: Lawrence Berkeley Laboratory

Instructors: K. Pruess and T.N. Narasimham

Purpose: Learn the theory, formulation, and application of the "TOUGH" computer code.

Background: As part of Sandia's responsibility for developing risk assessment methodology to be used in tuff, we are evaluating computer codes which simulate unsaturated flow. TOUGH is one of the codes we are including in our evaluation.

Summary: The workshop began with lectures by T. N. Narasimham and K. Pruess. Dr. Narasimham detailed the historical development of equations used to simulate flow in the unsaturated zone and provided a general overview of the physics of unsaturated flow. Dr. Pruess explained the numerical implementation of the equations and the input needed to run the model. Also discussed were the various pre- and post-processors used with the model. The remainder of the workshop was spent performing various simulations set up by the the LBL staff to demonstrate the code's capabilities. The code appears to be promising if computer storage limitations can be overcome and simpler means of setting up complex 3-dimensional problems can be developed.

WORKSHOP OUTLINE

Historical Development of Unsaturated Flow Equations
by T. N. Narasimham

Steady-State Unsaturated Flow

In 1907, Edgar Buckingham extended Darcy's law to unsaturated flow. Realizing the forces involved in unsaturated flow (Figure 1),

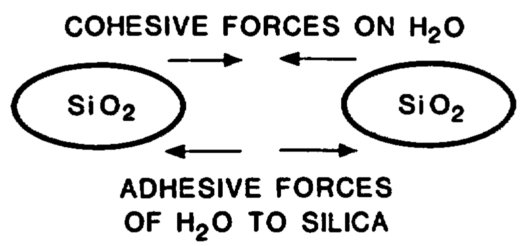

Figure 1. Forces Involved in Unsaturated Flow

Buckingham incorporated the concept of capillary pressure into Darcy's law. The capillary pressure is given by

$$P_c = P_a - P_w$$

where

P_c = capillary pressure

P_a = air phase pressure, which is assumed as equal to atmospheric pressure (P_{atm}) for the unsaturated zone

P_w = water phase pressure

because $P_a = P_{atm}$ = constant, P_c is negative.

By idealizing porous media as a bundle of disconnected capillary tubes, Buckingham proposed the following equation:

$$q = -K_{eff}(\psi)[\rho g \nabla z + \nabla \psi]$$

where

ψ = pressure head in the water phase, assuming $P_a = P_{atm}$ and P_a is the datum pressure (also = the "gage" pressure), or in other words,

$$\psi = \psi_w = \frac{P_w}{\rho g}$$

with P_w being less than atmospheric.

$K_{eff}(\psi)$ = the effective hydraulic conductivity of water as a function of the water phase pressure head

ρ_w = density of water

g = acceleration due to gravity

z = vertical position

This equation for steady-state unsaturated flow is known as the Darcy-Buckingham Law.

Transient Unsaturated Flow

L. A. Richards (in 1931) plugged the Darcy-Buckingham Law into the equation for transient ground-water flow to obtain an equation for transient unsaturated flow. In order to do this, he introduced the concept of "fluid mass capacity" for unsaturated flow.

This term is given by the equation:

$$m_{CA} = \frac{dM_w}{d\psi} = V\rho_w \quad S\eta\rho g\beta + \rho S \frac{d\eta}{d\psi} + \eta \frac{dS_w}{d\psi}$$

where

m_{CA} = fluid mass capacity

V = volume of a finite region

S = saturation

η = porosity

β = coefficient of compressibility of water

ρ = density of water at atmospheric pressure

Assuming that the first two terms of the right side of this equation are negligible for unsaturated flow, Richards derived the following equation for transient unsaturated flow.

$$\nabla \bullet \rho K_{eff}(\psi)[\rho g \nabla z + \nabla \psi] = \rho c(\psi) \frac{\partial \psi}{\partial t}$$

where

$$C(\psi) = \frac{d\theta}{d\psi} = \eta \frac{dS}{d\psi}$$

and

θ = volumetric moisture content

This equation has become known as Richards' Equation.

<u>Problems Associated with Nonisothermal Unsaturated Flow</u>

<u>Water in the vapor phase</u> -- The presence of heat in the unsaturated zone could result in liquid water being transformed into vapor. Most existing unsaturated flow codes treat only the liquid water phase. Therefore, to enable a code to simulate coupled heat and unsaturated flow, the energy equations and an equation for the vapor phase of water need to be included.

<u>Air phase</u> -- Heating of the water in the unsaturated zone also could cause dissolved air to come out of the liquid water. Thus, in addition to the equations mentioned above, an equation for the air phase is required. From my point of view, the air phase equation may be more important in simulating the infiltration of surface water and the subsequent displacement of air.

Convective Cell Formation -- Several investigators have postulated the formation of a convective cell around the canisters of a repository located in the unsaturated zone. The idea is that the heat from the canisters would vaporize the water in the rock matrix. This vapor would then move away from the canisters until it reached a point that was cool enough for condensation to occur. Upon condensation, the liquid water would move back toward the canisters under a moisture gradient. The formation of such a convective cell could have a significant effect on the distribution of heat and radionuclides near a repository. To simulate this postulated phenomena, equations for energy, liquid water, and vapor water will be necessary components of an unsaturated flow code.

Existence of Data -- As pointed out by K. Pruess, another major problem with simulating flow in the unsaturated zone is the lack of data describing such flow. Very few (if any) lab or field experiments of nonisothermal unsaturated flow have been conducted. Particularly lacking are data describing hydraulic conductivity as a function of moisture content or degree of saturation. It should be pointed out that this is also true for isothermal unsaturated flow in fractured rock such as the tuff at the Nevada Test Site.

Numerical Methodology and Code Structure
by K. Pruess*

Development of the TOUGH code

TOUGH is a code that has evolved from a long history of work at LBL dealing with evaluation of geothermal reservoirs. My understanding is that TOUGH is a streamlined version of MULKOM, LBL's multicomponent, multiphase, code designed to handle nonisothermal flow in the unsaturated zone. MULKOM came about after LBL realized a need for a multicomponent capability in their geothermal work. Instead of modifying their existing single component code, SHAFT79, they developed MULKOM.

---

*Dr. Pruess provided handouts that cover each of his lectures. These handouts are available from me upon request. The following discussion gives a general description of the lectures along with points I feel should be emphasized.

Code Description

1. Equations Solved

   - <u>Conservation Equations</u>
     Water Phase
     Air Phase
     Vapor Phase

   - <u>Energy Equations</u>
     Heat Transfer

2. Solution Technique
   - Integrated Finite Difference

The integrated finite-differences method (IFDM) for solving ground-water flow equations differs from the finite-difference method in that it can handle complex geometries. Actually, for a regular grid, the IFDM reduces to first-order finite difference. IFDM differs from finite-element methods in the way it computes spatial gradients. From a user's point of view, the most notable difference between IFDM and either finite-difference or finite-element is the need to specify the volumes, interface areas, nodal distances and the components of gravitational acceleration along nodal lines. This requires a preprocessor for all but the simplest grids.

Sample Problems

1-D Linear Isothermal Infiltration

This problem was taken from the set of benchmarking problems published by Ross and others (1982). A diagram of the problem, its resulting moisture profile, the conceptual TOUGH setup, and the actual TOUGH setup are shown in Figure 2.

The imaginary ring and its associated elements were needed to take up the gas flux as the water infiltrates. Using the above setup and parameters specified in Ross and others (1982), the TOUGH code reproduced the analytically obtained moisture content vs distance curve. After running this initial problem, several parameters were changed in order to allow the participants to get used to the model input and output.

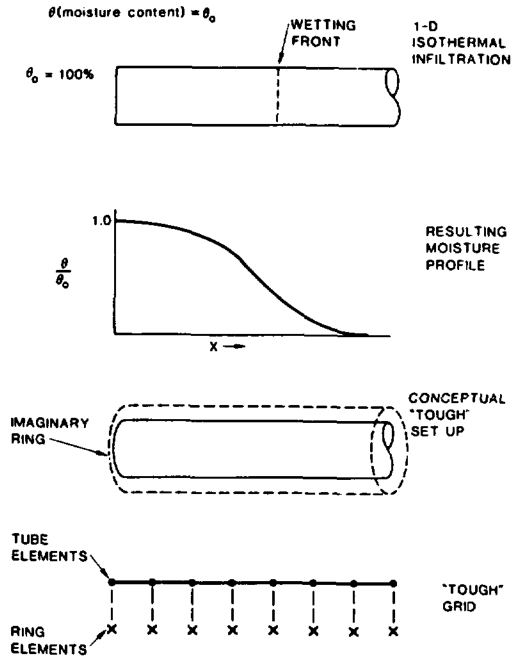

Figure 2. Linear Isothermal Infiltration Problems

The following is a list of the remaining problems that were set up by the LBL staff and run by the workshop participants.

Problem No.	Description
2	2-D vertical isothermal infiltrations
3	1-D radial flow to a geothermal well
4	2-D vertical flow to a well intercepting a fracture
5	1-D radial flow in the vicinity of a hot waste package

In addition to these problems, the workshop participants changed the waste package problem from 1-D radial flow to 3-D flow. A diagram of this problem is shown in Figure 3. Only one-fourth of the system needs to be simulated because of symmetry.

This problem was perhaps more instructive than the problems the LBL staff had set up for us to run. The main reason for this is that several unexpected problems were encountered in attempting to run this problem. The problems and their resolutions are listed below in the order they were encountered.

1. Although the grid setup was only 6 by 5 by 8, the dimensions of several arrays needed to be increased in order to solve the problem. With these new array dimensions, a substantial amount of computer storage was required to run this relatively small problem.

2. After recompiling the newly dimensioned code, the first run failed to come to a solution due to an attempt by the code to take the fourth root of a negative number. This happened in a subroutine used to calculate capillary pressure as a function of liquid saturation according to a function described by Milly. By using a linear function instead of Milly's, this problem was avoided.

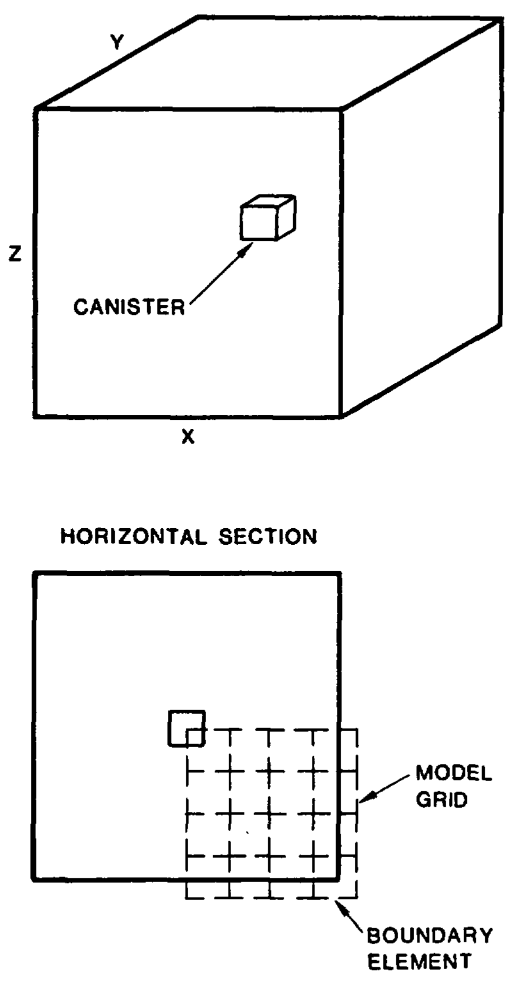

Figure 3. Conceptual Model of the 3-D Flow Problem

3. The most serious problem we encountered was a failure of the matrix decomposition. This happens when the offdiagonal terms of the matrix are too large. These terms are the form $\Delta t/v(F)$. Therefore, by reducing Δt (the time step), the matrix can be decomposed. However, if Δt is too small, the values of the primary variables will change very little and the code will achieve convergence prior to the calculation of the secondary variables. In other words, you will reach a "false" solution. We tried to run this same 3-D problem without heat and were forced to add heat for the initial time step to cause enough changes in the primary variables. For subsequent time steps, the heat was dropped and Δt was increased each time step until a steady-state solution was achieved.

Future Nuclear Regulatory Commission (NRC) and Sandia Work with TOUGH

On Friday, August 19, Peter Ornstein and myself met with Karsten Pruess to discuss future development and use of TOUGH. It was agreed that the next stage was for NRC to fund the documentation of TOUGH through a Sandia contract. Dr. Pruess believed that this documentation could not begin for at least 5 weeks. The context and format of the documentation were discussed, but no final decisions were reached. As for the use of the code, LBL will send a copy to Sandia as soon as they receive NRC approval.