See packet 2 for Enclosure

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LPDR- Wm-10 (2)
Wm-11 (2)
Wm-16 (2)

Sandia National Laboratories
Albuquerque, New Mexico 87185

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June 22, 1987

Neil M. Coleman
Hydrology Section
Geotechnical Branch
Division of Waste Management
U.S. Nuclear Regulatory Commission
7915 Eastern Avenue
Silver Spring, MD 20910

Dear Mr. Coleman:

Enclosed is a copy of the final draft of the "TOUGH User's Guide", NUREG/CR-4645, dated June 1987. The camera-ready copy, fiche of input and ouput sample problems to be placed in the back cover of the report, and other associated materials will be transmitted to the NRC publications department by Ms. Ruby Cochrell of organization 6400. If you have any questions, please call me at FTS-844-8164.

Sincerely,

Charlene Harlan

Charlene Harlan
Waste Management Systems
Division 6416

CPH:6416

Enclosures

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TOUGH USER'S GUIDE

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ABSTRACT

This document contains a technical description of the TOUGH computer program, which was developed at Lawrence Berkeley Laboratory for simulating the coupled transport of water, vapor, air and heat in porous and fractured media. The physical processes taken into account in TOUGH are discussed, and the governing equations actually solved by the simulator are stated in full detail. A brief overview is given of the mathematical and numerical methods, and the code architecture. The report provides detailed instructions for preparing input decks. Code applications are illustrated by means of six sample problems.

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ACKNOWLEDGEMENT

The development of the TOUGH simulator was made possible, in part, by support from the Office of Basic Energy Science, and by the Geothermal Technology Division of the U.S. Department of Energy, under Contract No. DE-AC03-76SF00098. Support for documentation of the program and preparation of the User's Guide was provided by Sandia National Laboratories and the Nuclear Regulatory Commission. M. Alavi, C. Doughty, Y. W. Tsang, and C. Liu of Lawrence Berkeley Laboratory assisted in testing and debugging the program. Sample Problem No. 6 (Heat Pipe) was developed by C. Doughty. Thanks are due to C. Doughty and Y. W. Tsang for a careful review of the User's Guide, and to D. Updegraff of Science Applications International Corp., Albuquerque, NM., for suggesting numerous improvements in the text. The manuscript was prepared by Leslie Fairbanks, with help from Carrie Joy, Diana Swantek and Mary Bodvarsson. The author is grateful to all these individuals and organizations for their support.

1. INTRODUCTION

TOUGH is a multi-dimensional numerical model for simulating the coupled transport of water, vapor, air and heat in porous and fractured media. It is a member of the MULKOM family of multi-phase, multi-component codes, which is being developed at Lawrence Berkeley Laboratory primarily for geothermal reservoir applications (Pruess, 1983). The acronym "TOUGH" stands for "transport of unsaturated groundwater and heat." TOUGH has so far been applied mostly to studies of high-level nuclear waste isolation in partially saturated geological media (Pruess and Wang, 1984; Pruess, Tsang, and Wang, 1985), but it should also be useful for a wider range of problems in heat and moisture transfer, and in the drying of porous materials.

This report gives a technical description of the TOUGH-code, including discussions of the physical processes modeled, governing mass- and energy-balance equations, mathematical and numerical methods, and code architecture. We also provide complete instructions for preparing input decks, and present a number of illustrative problems.

Most of the development of TOUGH was carried out on the CDC-7600 computer at Lawrence Berkeley Laboratory. Before distribution the program was transferred to the Cray X-MP at the National Magnetic Fusion Energy Computer Center, Lawrence Livermore National Laboratory. An effort was made to eliminate all non-standard FORTRAN, and to bring the coding as much as possible into compliance with the ANSI FORTRAN 77 language standard. We believe that the code should run with very minor modifications on any 64-bit mainframe computer with a FORTRAN 77 compiler.

2. PHYSICAL PROCESSES AND APPROXIMATIONS

The "conventional" description of unsaturated flow, as recently reviewed by Narasimhan (1982), was developed primarily by soil physicists. It assumes isothermal conditions and treats the gas phase as a passive spectator, which remains at constant pressure (1 bar) at all times. Liquid phase flows under gravity and capillary suction, as given by Richards' law (1931).

This approach has been extended to "weakly" non-isothermal systems (temperatures up to 50° C) by Philip and de Vries (1957), Sophocleous (1979), Milly (1982), and others. These authors consider moisture migration in the form of liquid or vapor. Vapor transport occurs only by molecular diffusion, and no overall movement of the gas phase is taken into account. The present status of "weakly" non-isothermal unsaturated flow has been reviewed by Walker, Sabey, and Hampton (1981), and Childs and Malstaff (1982).

The development of the TOUGH simulator was motivated by problems involving "strongly" heat-driven flow, for which the approaches mentioned above are not applicable. As temperatures approach or exceed the boiling point of water, vaporization will take place with associated increases in vapor partial pressure and strong forced convection of the gas phase. To describe these phenomena it is necessary to employ a multi-phase approach to fluid and heat flow, which fully accounts for the movement of gaseous and liquid phases, their transport of latent and sensible heat, and phase transitions between liquid and vapor. The gas phase will in general consist of a mixture of water vapor and air, and both these components must be kept track of separately.

The TOUGH simulator takes account of the following physical processes. Fluid flow in both liquid and gaseous phases occurs under pressure, viscous, and gravity forces according to Darcy's law, with interference between the phases represented by means of relative permeability functions. In addition we consider binary diffusion in the gas phase. However, no account is presently made of Knudsen diffusion, which will effectively enhance gas phase permeability under conditions when the mean free path of gas molecules becomes comparable to or larger than typical pore sizes (Knudsen, 1909; Klinkenberg, 1941; Hadley, 1982). This effect will become important for media with very small pores and/or at small gas pressures. Capillary and phase adsorption effects are taken into account for the liquid phase, but no allowance is made for vapor pressure lowering, which will become significant for very strong suction pressures (for example, a suction pressure of -14.5 MPa will cause approximately 10% reduction in vapor pressure). Also, no allowance is made for hysteresis in either capillary pressure or relative permeability. All thermophysical properties of liquid water and vapor are obtained within experimental accuracy from steam table equations (International Formulation Committee, 1967). Air is treated as an ideal gas, and additivity of partial pressures is assumed for air/vapor mixtures. Air dissolution in water is represented by Henry's law. However, because air solubility in water is very small, we felt justified in neglecting the temperature dependence of Henry's

constant. The value implemented in TOUGH, $K_H=10^{10}$ Pa, is accurate to within $\pm$ 10% in the temperature range from 40 ° C to 100 ° C (Loomis, 1928).

Heat transport occurs by means of conduction, with thermal conductivity dependent on water saturation, and convection and binary diffusion, which includes both sensible and latent heat.

The governing equations used in TOUGH, and their numerical implementation, are applicable to one-, two- or three-dimensional anisotropic porous or fractured media (see below). TOUGH does not perform stress calculations for the solid skeleton, but it allows for porosity changes in response to changes in pore pressure (compressibility) and temperature (expansivity).

3. GOVERNING EQUATIONS

The formulation used in TOUGH is analogous to the multi-phase treatment customarily employed in geothermal reservoir simulators. The basic mass- and energy-balance equations are written in integral form for an arbitrary flow domain V_n as follows (Pruess and Narasimhan, 1985):

$$\frac{d}{dt}\int_{V_n} M^{(\kappa)}dv = \int_{\Gamma_n} F^{(\kappa)} \cdot n \; d\Gamma + \int_{V_n} q^{(\kappa)} \; dv \tag{1}$$

($\kappa = 1$: water; $\kappa = 2$: air; $\kappa = 3$: heat)

The mass accumulation terms ($\kappa = 1,2$) are

$$M^{(\kappa)} = \phi \sum_{\beta=l,g} S_\beta \rho_\beta X_\beta^{(\kappa)} \tag{2}$$

where ϕ is porosity, S_β is saturation of phase β (= liquid, gas), ρ_β is density of phase β, and $X_\beta^{(\kappa)}$ is the mass fraction of component κ present in phase β. The heat accumulation term contains rock and fluid contributions

$$M^{(3)} = (1-\phi)\,\rho_R\, C_R T + \phi \sum_{\beta=l,g} S_\beta \rho_\beta u_\beta \tag{3}$$

where ρ_R is rock grain density, C_R is specific heat of the rock grains, T is temperature, and u_β is specific internal energy of phase β.

The mass flux terms contain a sum over phases

$$F^{(\kappa)} = \sum_{\beta=l,g} F_\beta^{(\kappa)} \tag{4}$$

where the flux in each phase is

$$F_\beta^{(\kappa)} = -k \frac{k_{r\beta}}{\mu_\beta} \rho_\beta X_\beta^{(\kappa)} (\nabla P_\beta - \rho_\beta g) - \delta_{\beta g} D_{va} \rho_\beta \nabla X_\beta^{(\kappa)} \tag{5}$$

Here k is absolute permeability, $k_{r\beta}$ is relative permeability of phase β, μ_β is viscosity of phase β, $P_\beta = P + P_{cap,\beta}$ is the pressure in phase β (sum of a reference phase pressure and capillary pressure), and g is gravitational acceleration. The last term in equation (5) contributes only to gas phase flow and represents a binary diffusive flux, with D_{va} the diffusion coefficient for vapor-air mixtures.

Heat flux contains conductive and convective components (no dispersion)

$$\mathbf{F}^{(3)} = - K\nabla T + \sum_{\substack{\beta = l,g \\ \kappa = 1,2}} h_\beta^{(\kappa)} \mathbf{F}_\beta^{(\kappa)} \tag{6}$$

Here K is heat conductivity of the rock-fluid mixture, and $h_\beta^{(\kappa)}$ is specific enthalpy of component κ in phase β.

The transport equations given above need to be complemented with constitutive relationships, which express all parameters as functions of a set of primary thermodynamic variables. The thermophysical properties of water substance are accurately represented by the steam table equations, as given by the International Formulation Committee (1967). Air is approximated as an ideal gas, and additivity of partial pressures is assumed for air and vapor, $P_g = P_v + P_a$. The viscosity of air-vapor mixtures is computed from a formulation given by Hirschfelder et al., (1954), but using steam table values for vapor viscosity instead of approximations from kinetic gas theory. Henry's law was assumed for solubility of air in liquid water:

$$P_a = K_H X_l^{(air)} \cdot \frac{M_{H_2O}}{M_{air}} \tag{7}$$

Here $K_H = 10^{10}$ Pa is Henry's constant, $X_l^{(air)}$ is the mass fraction of air in liquid water, and M_{H_2O}, M_{air} are the respective molecular weights.

Capillary pressures and relative permeabilities will usually depend on phase saturations, but more general relationships are possible (e.g. temperature dependence; however, TOUGH does not allow for hysteresis). A library of the most commonly used functional forms is provided in the TOUGH code, and can be selected by means of input data (see Appendices A and B). Additional capillary pressure and relative permeability functions may be used by adding FORTRAN code to the appropriate subroutines (see Appendix A).

The vapor-air diffusion coefficient is written as (Vargaftik, 1975; Walker et al., 1981)

$$D_{va} = \tau \phi S_g \frac{D_{va}^0}{P} \left(\frac{T + 273.15}{273.15} \right)^\theta \tag{8}$$

where τ is a tortuosity factor, which is dependent on pore geometry, and D_{va}^{0} and θ are material parameters which for air/vapor mixtures have values of $D_{va}^{0} = 2.13 \times 10^{-5}$ m^2/s (at standard conditions of P = 1 bar, T = 0 °C), and $\theta = 1.80$ (Vargaftik, 1975).

Heat conductivity can depend on liquid saturation according to one of the following two relationships (Somerton et al., 1973, 1974)

$$K(S_l) = K(S_l = 0) + \begin{cases} \sqrt{S_l} \cdot (K(S_l = 1) - K(S_l = 0)) & (9a) \\ S_l \cdot (K(S_l = 1) - K(S_l = 0)) & (9b) \end{cases}$$

4. MATHEMATICAL AND NUMERICAL METHODS

The continuum Equations (1) are discretized in space using the "integral finite difference" method (Edwards, 1972; Narasimhan and Witherspoon, 1976). Introducing appropriate volume averages, we have

$$\int_{V_n} M dv = V_n M_n \tag{10}$$

Here M is a volume-normalized extensive quantity, and M_n is the average value of M over V_n. Surface integrals are approximated as a discrete sum of averages over surface segments A_{nm} :

$$\int_{\Gamma_n} \mathbf{F} \cdot \mathbf{n} \, d\Gamma = \sum_m A_{nm} F_{nm} \tag{11}$$

Time is discretized fully implicitly as a first order finite difference, to obtain the numerical stability needed for an efficient calculation of multi-phase flow. Equations (1) reduce to the following set of coupled algebraic equations:

$$R_n^{(\kappa)k+1} \equiv M_n^{(\kappa)k+1} - M_n^{(\kappa)k} - \frac{\Delta t}{V_n} \left\{ \sum_m A_{nm} F_{nm}^{(\kappa)k+1} + V_n \, q_n^{(\kappa)k+1} \right\} = 0 \tag{12}$$

Here k labels the time step, $\Delta t = t^{k+1} - t^k$. For a flow system which is discretized into N grid blocks, Equations (12) represent a set of 3N algebraic equations. These are strongly coupled because of interdependence of mass and heat flow. They are highly non-linear, because of order-of-magnitude changes in parameters during phase transitions, and because of non-linear material properties (chiefly relative permeabilities and capillary pressures). Because of these features of the equation system, TOUGH performs a completely simultaneous solution of the discretized mass- and energy-balance equations, taking all coupling terms into account. To handle the non-linearities we perform Newton/Raphson iteration. The unknowns in Equations (12) are the 3N independent "primary" variables, which completely define the thermodynamic state of the flow system at time level t^{k+1}. For each volume element (grid block) there are three primary variables, the choice of which depends upon the phase composition (see Table 1).

Table 1
Primary Thermodynamic Variables

Phase composition	variable #1	variable #2	variable #3
single phase	P-pressure (Pa)	T-temperature (° C)	X-air mass fraction
two-phase	P-pressure (Pa)	S_g-gas saturation	T-temperature (° C)

Denoting these primary variables collectively as (x_i; i=1, ..., 3N), the Newton/Raphson iteration process can be written as follows. Demanding that the residuals $R_n^{(\kappa)k+1}$ in Equations (12) vanish at iteration index p + 1, and expanding to first order in terms of the residuals at iteration index p, we have

$$R_n^{(\kappa)k+1}(x_{i,p+1}) \approx R_n^{(\kappa)k+1}(x_{i,p}) + \sum_i \frac{\partial R_n^{(\kappa)k+1}}{\partial x_i} \Big|_p (x_{i,p+1} - x_{i,p}) = 0 \quad (13)$$

Equations (13) represent a set of 3N coupled linear equations for the $x_{i,p+1}$. These are solved with an efficient direct solver, which uses sparse storage techniques, requiring only the storage of non-zero members of the coefficient matrix (Duff, 1977). Iteration is continued until the residuals are reduced to a small fraction of the accumulation terms (for all n, κ).

$$\left| \frac{R_{n,p+1}^{(\kappa)k+1}}{M_{n,p+1}^{(\kappa)k+1}} \right| \leq \epsilon_1 . \quad (14)$$

The default (relative) convergence criterion is $\epsilon_1 = 10^{-5}$. When the accumulation terms are smaller than ϵ_2, $|M_n^{(\kappa)}| < \epsilon_2$, we impose an absolute convergence criterion: $|R_n^{(\kappa)}| \leq \epsilon_1 \cdot \epsilon_2$. The cutoff ϵ_2 can be set by the user (default: ϵ_2=1). Convergence is usually attained in 3-4 iterations. If convergence can not be achieved within a certain number of iterations (default 8), the time step size Δt is reduced and a new iteration process is started. All derivatives $\partial R_n / \partial x_i$ needed in the coefficient matrix are obtained by numerical differentiation.

It is appropriate to add some comments about our space discretization technique. As an example let us consider a discretized version of the mass flux term, Equation (5).

$$F_{\beta,nm}^{(\kappa)} = -\, k_{nm} \left(\frac{k_{r\beta}\, \rho_\beta}{\mu_\beta} \right)_{nm} (X_\beta^{(\kappa)})_{nm} \cdot \left[\frac{P_{\beta,n} - P_{\beta,m}}{D_{nm}} - \rho_{\beta,nm}\, g_{nm} \right] - \delta_{\beta g} (D_{va})_{nm}\, (\rho_\beta)_{nm}\, \frac{X_{\beta,n}^{(\kappa)} - X_{\beta,m}^{(\kappa)}}{D_{nm}} \qquad (15)$$

The subscripts (nm) indicate that the respective quantities are to be evaluated at the interface between volume elements n and m, based on average values within V_n and V_m. As has been discussed elsewhere (e.g. Pruess and Narasimhan, 1985), this requires different weighting procedures for different parameters, such as harmonic weighting, spatial interpolation, and upstream weighting.

The entire geometric information of the space discretization in Equations (12) is provided in the form of a list of grid block volumes V_n, interface areas A_{nm}, nodal distances D_{nm}, and components g_{nm} of gravitational acceleration along nodal lines. There is no reference whatsoever to a global system of coordinates, or to the dimensionality of a particular flow problem. The discretized equations are in fact valid for arbitrary irregular discretizations in one, two or three dimensions, and for porous as well as for fractured media. This flexibility should be used with caution, however, because the accuracy of solutions depends upon the accuracy with which the various interface parameters in equations such as (15) can be expressed in terms of average conditions in grid blocks. A necessary condition for this to be possible is that there exists approximate thermodynamic equilibrium in (almost) all grid blocks at (almost) all times (Pruess and Narasimhan, 1985). For systems of regular grid blocks referenced to global coordinates (such as r - z, x - y - z), Equations (12) reduce to a conventional finite difference formulation (e.g. Peaceman, 1977).

5. TREATMENT OF SINKS AND SOURCES, AND BOUNDARY CONDITIONS

TOUGH provides various options for specifying injection or withdrawal of heat and fluids, which are discussed in Section 7. In the simplest case, source rates are specified as constants, or as a table of time-dependent values. TOUGH also provides an option to produce a well based on a deliverability model, by prescribing a wellbore pressure P_{wb} and a productivity index PI (Coats, 1977). Production rate in phase β is

$$q_\beta = \frac{k_{r\beta}}{\mu_\beta} \rho_\beta \cdot PI \cdot (P_\beta - P_{wb}) \tag{16}$$

For wells on deliverability which are completed in more than one layer, the flowing wellbore pressure P_{wb} can be corrected to approximately account for gravity effects. Assume that the open interval extends from layer $l=1$ at the bottom to $l=L$ at the top. The flowing wellbore pressure in layer l, P_{wbl}, is obtained from the wellbore pressure in layer $l+1$ immediately above it by means of the following recursion formula

$$P_{wbl} = P_{wbl+1} + \frac{g}{2}\left(\rho_l^f \Delta z_l + \rho_{l+1}^f \Delta z_{l+1}\right) \tag{17}$$

Here, Δz_l denotes the layer thickness, and ρ_l^f is the flowing density in the tubing opposite layer l. Flowing densities are computed using a procedure given by Coats (private communication, 1982). If wellbore pressure were zero, we would obtain the following volumetric production rate of phase β from layer l :

$$r_{l,\beta} = \left(\frac{k_{r\beta}}{\mu_\beta}\right)_l (PI)_l \; P_{l,\beta} \tag{18}$$

The total volumetric flow rate of phase β opposite layer l is , for zero wellbore pressure

$$r_{l,\beta}^T = \sum_{m=1}^{l} r_{m,\beta} \tag{19}$$

From this we obtain the following approximate expression for flowing density opposite layer l:

$$\rho_l^f = \frac{\sum_{\beta=l,g} \rho_{l,\beta} \, r_{l,\beta}^T}{\sum_{\beta=l,g} r_{l,\beta}^T} \tag{20}$$

Boundary conditions are specified, generally speaking, by means of appropriately chosen volume elements, flow connections, and sinks and sources. The simplest boundary conditions to implement are "no flux"; these are realized simply by not introducing "no flux" areas into the list of geometric parameters where no crossflow is desired. More general flux (Neumann) boundary conditions can be prescribed by introducing sinks or sources of appropriate strengths into the elements adjacent to the boundary. Dirichlet-type boundary conditions, such as constant pressures or temperatures, can be conveniently specified by introducing appropriate boundary elements and connections (a "connection" consists of an interface area, and a pair of distances of adjacent nodes from the interface). Assigning very large volumes to such boundary elements will ensure that their thermodynamic state remains unchanged in a simulation. It is also possible to fix temperature and to allow pressure to vary. This can be done by means of assigning a very large heat capacity to an element with "normal" volume. The only feature distinguishing boundary elements from the "normal" grid blocks forming the flow domain is their large volume (and/or heat capacity); in the calculations they are treated on an equal footing with all other elements.

6. OVERVIEW OF PROGRAM STRUCTURE AND EXECUTION

The subroutines contained in the TOUGH-program can be grouped according to their functions as summarized in Table 2. Figure 1 gives an abbreviated overview of the computational procedure (flow chart).

Table 2
TOUGH Program Structure

Function	Subroutine(s)
data input	INPUT, REAFIL
printout of input data	INDATA
driver for execution	CYCIT
thermophysical properties and phase diagnostic	EOS (and satellite programs)
assembling of equations	MULTI
production, injection	QU
data interpolation	FINDER, FINDL, HINTER, QINTER
scaling of equations	MC19A
solution of equations	LINEQ (with satellite package "MA28")
conclusion of converged time steps	CONVER
output of results	WRIFI, OUT, BALLA

The initialization of a simulation run is accomplished by the subroutines INPUT and REAFIL in a flexible way. Most of the necessary data are supplied from disk files, which can be either directly provided by the user, or which will be generated internally from input data. The initialization stage can generate simple regular computational grids in one, two, or three dimensions. If desired, a printout of input data can be provided (subroutine INDATA). The iterative sequence for time stepping is controlled by CYCIT. On the first time step, all thermophysical parameters are initialized (subroutine EOS), and then time step counter KCYC, iteration counter ITER, and convergence flag KON are defined. The iteration counter is incremented, and the accumulation- and flow-terms for

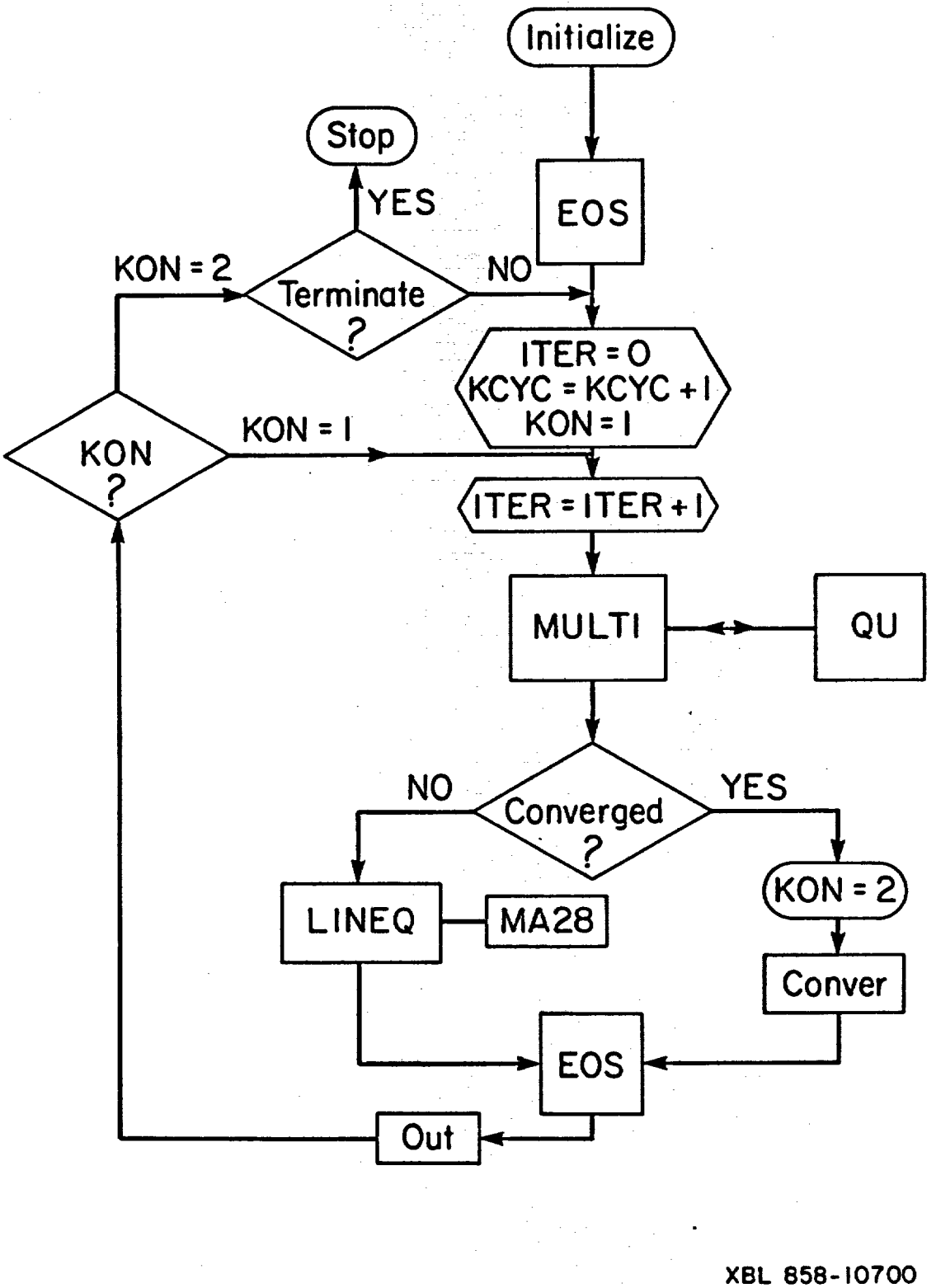


Figure 1. Simplified flow chart of TOUGH.

all equations are assembled (subroutine MULTI). If sinks or sources are present, MULTI calls subroutine QU to compute their contributions. MULTI also computes all residuals, as well as element index (NER) and equation index (KER) of the largest residual. If convergence is achieved (KON=2), CONVER is called to update the primary variables. Otherwise, LINEQ is called to solve Eqs. (13) and to compute new values for the primary variables. LINEQ calls the subroutine package MA28, which performs a sparse version of LU-decomposition with partial pivoting and back substitution (Duff, 1977). Informative messages generated by MA28 are written onto a disk file called LINEQ. Subsequently, EOS finds all thermophysical parameters pertaining to the latest primary variables. Printed output can be generated at user-specified time steps or simulation times either for each iteration or after convergence (subroutine OUT). Depending upon the value of the convergence flag KON, the program will then proceed to the next iteration (KON=1) or to the next time step (KON=2). If anything goes wrong -- failure in solving the linear equations, failure in computing thermophysical parameters, failure to converge within a given maximum number of iterations -- the time step will be repeated with a reduced time increment Δt.

In certain cases a calculation will progress in time with convergence achieved on the first iteration (ITER = 1). This occurs when the time step is chosen so small, or the simulated problem is so close to steady state, that the convergence tolerances (see Chapter 4) are satisfied without any changes in primary variables. Misleading results may be obtained if a time period over which significant changes in thermodynamic conditions would occur is simulated by means of many very small time steps, each of which gives convergence on ITER = 1. This pitfall can be avoided by specifying automatic time step adjustment (via parameter MOP(16), see page 23).

The simulation proceeds until it terminates for one of several termination criteria (number of time steps, machine time, simulation time). At that time, a disk file called SAVE is written; this file allows for restarting the problem in a simple way (see below).

The major arrays used by TOUGH, and their dimensions in dependence upon problem size (number of grid blocks and connections, dimensionality), are described in full detail in comment cards in the MAIN program.

7. PREPARATION OF INPUT DECKS

7.1 Data Blocks

The types of data needed to characterize a flow system are summarized in Table 3. The input of TOUGH is organized into "blocks" which correspond to the data groups given in Table 3. There is no special data block for boundary conditions; these have to be specified through appropriately chosen elements, interfaces, initial conditions, and sinks/sources. An overview of the most general input structure is given in Table 4.

The first data card must be the TITLE-card. The last data card must be the ENDCY-card, with ENDCY typed in columns 1-5. The data blocks between TITLE and ENDCY can be provided in arbitrary order, except that block ELEME must precede block CONNE. The blocks ELEME and CONNE must either be both provided through the input deck, or both through a disk file called MESH. The block GENER can be omitted if there are no sinks or sources in the problem. If block START is present, consisting of one data card with START typed in columns 1-5, the block INCON can be incomplete, with elements in arbitrary order, or it can be absent altogether. Elements for which no initial conditions are specified in INCON will then be assigned default initial conditions as given in block PARAM, and default porosities as given in block ROCKS. If START is not present, INCON must contain information for all elements, in exactly the same order as the elements are listed in block ELEME.

During initialization, TOUGH can write the following disk files from information provided through input data blocks:

- a file MESH, consisting of blocks ELEME and CONNE;
- a file GENER, consisting of the block GENER;
- a file INCON, consisting of the block INCON.

The initialization of the actual program variables for data on geometry, generation, and intial conditions will always be made from the disk files MESH, GENER, and INCON. When no data blocks ELEME and CONNE, GENER, and INCON are present in the input deck, TOUGH will attempt to read data for flow geometry, generation, and initial conditions from pre-existing disk files MESH, GENER, and INCON, respectively. Geometry data have to be specified for each TOUGH run either in the input deck, or on a disk file called MESH. If no data blocks GENER and INCON are provided in the input deck, and if no disk files GENER and INCON are present, defaults will take effect (no generation; default initial conditions as specified in block PARAM). If a user intends to use these defaults, (s)he has to make sure that at execution time no disk files INCON or GENER are present from a previous run (or perhaps from a different problem). A safe way to use default GENER and INCON is to specify "dummy" data blocks in the input deck, consisting of just the identifier GENER or INCON, followed by one blank line.

Table 3

Data Groups for a Simulation Problem

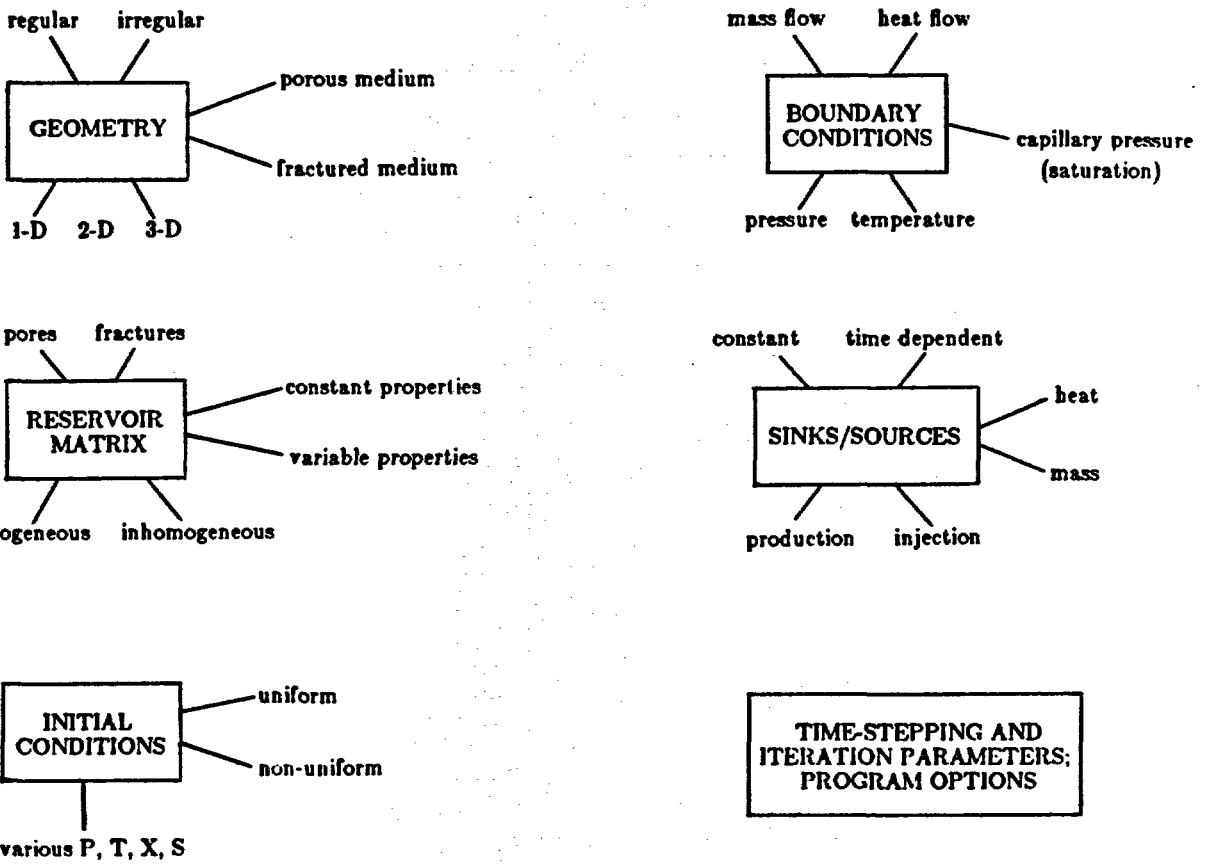


Table 4
Input Data Blocks[1]

Block	Description
TITLE (first card)	One data card containing a problem title for identifying output.
ROCKS	Material parameters for the various reservoir domains.
PARAM	Computational parameters (time stepping information, program options).
RPCAP	Parameters for relative permeability and capillary pressure functions.
TIMES (optional)	List of (physical) times at which printout is to be generated.
*ELEME	List of grid elements. } MESH - information
*CONNE	List of interfaces (connections). } MESH - information
*GENER (optional)	List of mass or heat sinks/sources.
*INCON (optional)	List of initial conditions and (optional) restart information.
START (optional)	One data card allowing a more flexible initialization.
ENDCY (last card)	One card closing the TOUGH input deck.

[1]Blocks labeled with a star * can be provided as disk files, in which case they would be omitted from the input deck.

The format for data blocks ELEME, CONNE, GENER, and INCON is basically the same when these data are provided as disk files as when they are provided as part of the input deck. However, specification of these data as part of the input deck rather than as disk files offers some added conveniences, which are useful when a new simulation problem is initiated. For example, a sequence of identical items (volume elements, connections, sinks or sources) can be specified on a single data card. Also, indices needed for cross-referencing elements, interfaces, and sources will be generated by TOUGH rather than having them provided by the user. Disk files written by TOUGH can be merged into an input deck without any changes, keeping the cross-referencing information (see note at end of Chapter 7; for example, disk file MESH can be directly used as input data blocks ELEME and CONNE).

At the completion of a run, the results needed for a subsequent continuation (restarting) of the problem are written onto a file SAVE. This file is compatible with INCON format specifications, and can be provided for a subsequent run either as a disk file (to be named "INCON"), or as part of the input deck.

We expect the user to initiate a problem with ELEME, CONNE, GENER, and INCON as part of the input deck, using the START-option for flexibility and convenience. Typically, the user will want to run only a few time steps initially, examine the results, and then restart the problem with time steps chosen manually or automatically to give an optimum compromise between accuracy and efficiency. The file SAVE of a completed run must be provided as disk file INCON or input data block INCON for a continuation run. Apart from initial conditions, file SAVE also transmits information on simulation times and time steps for a restart. Further discussion on restarting a problem is given on page 38.

As was discussed above, all geometric data defining the flow domain and its discretization have to be provided as input to TOUGH in the form of lists of grid block volumes V_n, interface areas A_{nm}, nodal distances D_{nm}, and cosines β_{nm} of the angles between nodal lines and the vertical. For all but the most trivial flow geometries, generation of these data will require a separate step of geometric preprocessing prior to the actual simulation. For the most commonly used cylindrical or linear flow geometries, we have written simple FORTRAN programs to carry out the elementary geometric calculations involved, and to generate a MESH-file compatible with TOUGH input specifications. More elaborate grid generators are available for irregular geometries ("OGRE", Weres and Schroeder, 1978) and for fractured porous media ("GMINC", Pruess, 1983). Illustrative examples for a variety of flow problems have been given by Narasimhan (1982).

7.2 TOUGH–Input Formats

The input data to be provided for a TOUGH simulation are summarized in Figure 2. The blocks ROCKS, ELEME, CONNE, GENER, and INCON can have a variable number of cards, depending upon how many items the user wishes to specify. The end of these variable-length blocks is indicated with a blank card. (For CONNE, GENER, and INCON it is possible to have, instead of the blank card, a card with "+++" typed in columns 1-3, followed by some element and source cross-referencing information in the case of CONNE and GENER, and followed by restart-information in the case of INCON; see below.)

We shall now explain the cards and variables in detail. Clarifying examples will be given in Section 9.

All input and output of TOUGH is in standard metric units.

TITLE — is the first card of the deck, containing a header of up to 80 characters, to be printed on output. This can be used to identify a problem. If no title is desired, leave this card blank.

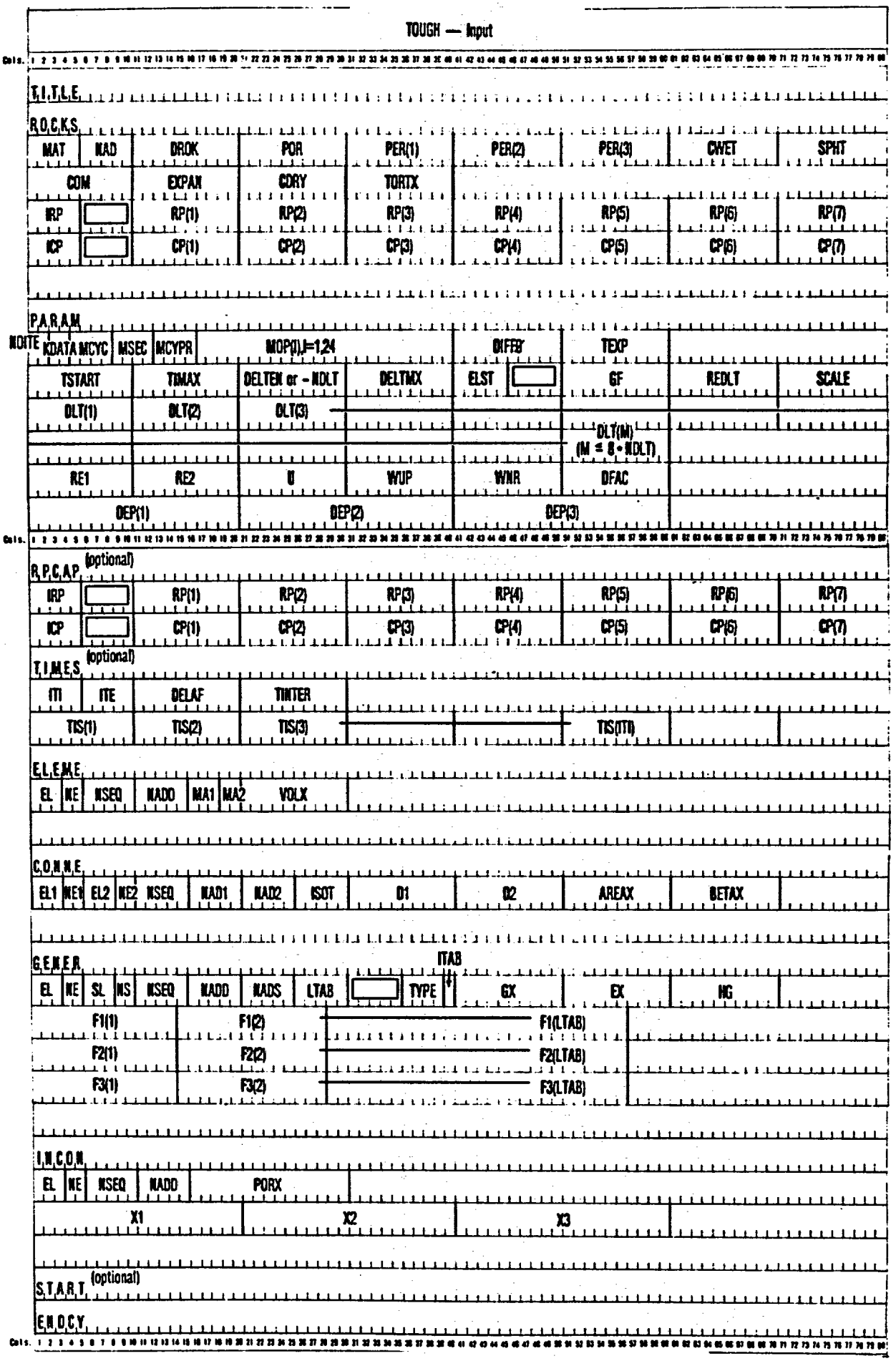


Figure 2. TOUGH input formats.

XBL 838-2169 A

ROCKS introduces material parameters for up to 27 different reservoir domains.

Card 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);
$\geq$1: will read another data card to override defaults.
$\geq$2: will read two additional cards after the default override card with parameters for relative permeability and capillary pressure functions.

DROK rock grain density (kg/m^3).

POR default porosity (void fraction) for all elements belonging to domain "MAT" for which no other porosity has been specified in block INCON. Option "START" is necessary for using default porosity.

PER(I), I = 1,3 absolute permeabilities along the three principal axes, as specified by ISOT in block CONNE.

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

SPHT rock grain specific heat ($J/kg \cdot C$). Domains with SPHT > $10^4 J/kg \cdot C$ will not be included in global material balances. This provision is useful for boundary nodes, which are given very large volumes so that their thermodynamic state remains constant. Because of the large volume, inclusion of such nodes in global material balances would make them useless.

Card ROCKS.1.1 (optional, NAD $\geq$1 only)

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

COM compressiblity (m^2/N), $\frac{1}{\phi}\left(\frac{\partial \phi}{\partial P}\right)_T$ (default is 0)

EXPAN expansivity ($1/^\circ C$), $\frac{1}{\phi}\left(\frac{\partial \phi}{\partial T}\right)_P$ (default is 0)

CDRY	formation heat conductivity under desaturated conditions (W/m * C).	(default is CWET)
TORTX	tortuosity factor for binary diffusion	(default is 0; i.e., binary diffusion turned off)

Card ROCKS.1.2 (optional, NAD $\geq$ 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 A).

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

Card ROCKS.1.3 (optional, NAD $\geq$ 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 B).

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

Repeat cards 1, 1.1, 1.2, and 1.3 for up to 27 reservoir domains.

Card ROCKS.2 A blank card closes the ROCKS data block.

START (optional)

A card with START typed in columns 1-5 allows a more flexible initialization.

PARAM introduces computation parameters.

Card PARAM.1

Format (2I2, 3I4, 24I1, 2E10.4).
NOITE, KDATA, MCYC, MSEC, MCYPR, (MOP(I), I = 1, 24), DIFF0, TEXP

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

KDATA specifies amount of printout (default = 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 iteration (not just after convergence).

MCYC maximum number of time steps to be calculated.

MSEC maximum duration, in machine 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.

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

MOP(2) through MOP(6) generate additional printout in various subroutines, if set $\neq$ 0. This feature should never be needed in "normal" applications, but it may be convenient when a user suspects a bug and wishes to examine the inner workings of the code. The amount of printout increases with MOP(I) (consult source code listings for details).

MOP(2) CYCIT (main subroutine).

MOP(3) MULTI (flow- and accumulation-terms).

MOP(4) QU (sinks/sources).

MOP(5) EOS (equation of state).

MOP(6) LINEQ (linear equations).

MOP(7) if unequal 0, a printout of input data will be provided.

Calculational choices are as follows:

MOP(9) determines the composition of produced fluid with the MASS option (page 35). The relative amounts of phases are determined:

0: according to relative mobilities in the source element.

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

MOP(10) chooses the interpolation formula for heat conductivity 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 mobilities at interfaces.

0: mobilities are upstream weighted with WUP (default is WUP = 1).

1: mobilities are averaged between adjacent elements.

MOP(12) determines interpolation procedure for time-dependent generation data.

0: triple linear interpolation.

1: step function option.

MOP(14) determines handling of pivot failures in matrix decomposition.

0: perform new matrix decomposition when encountering a pivot failure.

$\neq$0: ignore pivot failures.

MOP(16) provides automatic time step control. Time step size will be doubled, if convergence occurs within ITER $\leq$ MOP(16) iterations.

MOP(17) permits to choose a scaling-option for preconditioning the Jacobian matrix.

0: perform scaling.

$\neq$0: do not perform scaling.

DIFF0 strength parameter for diffusive vapor flux at standard conditions of T = 0 °C, P = 1 bar.
(for free gas, DIFF0 = $2.13 \times 10^{-5} m^2/s$)

TEXP parameter for temperature dependence of binary diffusion. (default = 1.80)

Card PARAM.2

Format (4E10.4, A5, 5X,3E10.4)

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

TSTART starting time of simulation in seconds.

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 cards with time step information. Note that - NDLT must be provided as a real number, with decimal point.

DELTMX upper limit for time step size (s). (default = ∞)

ELST set equal to the name of one element to obtain a short printout after each time step.

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).

Card 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 cards is optional for DELTEN = -NDLT, a negative integer: Up to 13 cards can be read, each containing 8 time step sizes. 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 (except for automatic time step reductions when problems are encountered, or time step increases when automatic time step control is chosen with MOP(16) $\neq$0)

Card PARAM.3

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

RE1 convergence criterion for relative error (parameter ϵ_1 in Eq. (14); default = 1.E-5).

RE2 convergence criterion for absolute error (parameter ϵ_2 [page 8]; default = 1).

U pivoting parameter for linear equation solution (default = 0.1). $0 \leq U < 1$; 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). $0 \leq WUP \leq 1$.

WNR weighting factor for increments in Newton/Raphson - iteration (default = 1.0 is recommended). $0 < WNR \leq 1$.

DFAC increment factor for numerically computing derivatives (default = 1.E-8).

Card PARAM.4

Format (3E20.14)
DEP(I), I = 1,3

This card holds a set of primary variables which are used as default initial conditions for all elements not specified in block "INCON," if option "START" is selected.

DEP(1) pressure (Pa)

DEP(2) ≥ 1.5: temperature (°C; single-phase points).
< 1.5: gas saturation (two-phase points).

DEP(3) ≥ 1.5: temperature (°C; two-phase points).
< 1.5: air mass fraction (single phase points).

Note: A special feature is available for initializing two-phase conditions with only water present (no air), such as arise in geothermal problems. In this case one may set DEP(1) = temperature (°C); DEP(2) = vapor saturation; DEP(3) = 0 (or blank). The condition that DEP(1) $\leq$ 374.15 (critical point of water) serves as a flag to indicate that DEP(1) "means" temperature rather than pressure.

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 cards ROCKS.1.2 and ROCKS.1.3. A catalog of relative permeability and capillary pressure functions is presented in Appendix A and Appendix B, respectively.

Card 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 A).

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

Card 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 B).

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

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

Card TIMES.1

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

ITI number of times provided on cards TIMES.2, TIMES.3, etc., below (ITI $\leq$ 100).

ITE total number of times desired (ITI $\leq$ ITE $\leq$ 100; default is ITE = ITI).

DELAF maximum time step size after any of the prescribed times have been reached (default is ∞).

TINTER time increment for times with index ITI, ITI+1, ..., ITE.

Card TIMES.2, TIMES.3, etc.

Format (8E10.4)
(TIS(I), I = 1, ITI)

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

ELEME introduces element information.

Card ELEME.1

Format (A3, I2, 2I5, A3, A2, E10.4)
EL, NE, NSEQ, NADD, MA1, MA2, VOLX

EL, NE 5-character code name of an element. The first three characters are arbitrary, the last two characters must be numbers.

NSEQ number of additional elements having the same volume and belonging to the same reservoir domain.

NADD increment between the code numbers of two successive elements. (Note: the maximum permissible code number NE + NSEQ * NADD is $\leq$ 99.).

MA1, MA2 a five character material identifier corresponding to one of the reservoir domains as specified in block ROCKS. If the first three characters are blanks, the last two characters must be numbers in which case they would indicate the sequence number of the domain as entered in ROCKS.

VOLX element volume (m^3).

Repeat card ELEME.1 for the number of elements desired.

Card ELEME.2 A blank card closes the ELEME data block.

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

Card CONNE.1

Format (A3, I2, A3, I2, 4I5, 4E10.4)
EL1, NE1, EL2, NE2, NSEQ, NAD1, NAD2, ISOT, D1, D2, AREAX, BETAX

EL1, NE1 code name of the first element.

EL2, NE2 code name of the second element.

NSEQ number of additional connections in the sequence.

NAD1 increment of the code number of the first element between two successive connections.

NAD2 increment of the code number of the second element between two successive connections.

ISOT set equal to 1, 2, or 3; specifies absolute permeability to be PER(ISOT) for the materials in elements (EL1, NE1) and (EL2, NE2), where PER is read in block ROCKS. This allows assignment of different permeabilities, e.g., in the horizontal and vertical direction.

D1, D2 — distance (m) from center of 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.

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

Card CONNE.2 A blank card closes the CONNE data block.
(For an alternative, see note at the end of Chapter 7).

GENER — introduces sinks and/or sources.

Card GENER.1

Format (A3, I2, A3, I2, 4I5, 5X,A4, A1,3E10.4)
EL, NE, SL, NS, NSEQ, NADD, NADS, LTAB, TYPE, ITAB, GX, EX, HG

EL, NE — code name of the element containing the sink/source.

SL, NS — code name of the sink/source. The first three characters are arbitrary, the last two characters must be numbers.

NSEQ — number of additional sinks/sources with the same injection/production rate (not applicable for TYPE = DELV).

NADD — increment between the code numbers of two successive elements with identical sink/source.

NADS — increment between the code numbers of two successive sinks/sources.

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

HEAT - heat sink/source.

COM1, WATE - component 1 (water). injection only

COM2, AIR - component 2 (air). injection only

MASS - mass production rate specified.

DELV - well on deliverability, i.e. production occurs against specified wellbore pressure. If well is completed in more than one layer, bottommost layer must be specified first, with number of layers given in LTAB. Subsequent layers must be given sequentially for a total number of LTAB layers.

ITAB — if set unequal to 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 COM1, WATE, COM2, AIR, and MASS; it is energy rate (J/s) for a HEAT sink/source. For wells on deliverability, GX is productivity index PI (m^3).

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

HG — thickness of layer (m; wells on deliverability only).

Card GENER.1.1 (optional, LTAB>1 only)

Format (4E14.7)
F1(L), L=1, LTAB

F1 — generation times.

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

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

F2 generation rates.

Card 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 cards GENER.1, 1.1, 1.2, and 1.3 for up to 100 sinks/sources.

Card GENER.2 A blank card closes the GENER data block.
(For an alternative, see note at the end of Chapter 7).

INCON introduces initial conditions.

Card INCON.1

Format (A3, I2, 2I5, E15.9)
EL, NE, NSEQ, NADD, PORX

EL, NE code name of element.

NSEQ number of additional elements with the same initial conditions.

NADD increment between the code numbers of two successive elements with identical initial conditions.

PORX porosity (void fraction); if zero or blank, porosity will be taken as specified in block ROCKS if option START is used.

Card INCON.2

Format (3E20.14)
X1, X2, X3

Set of primary variables for the element specified in card INCON.1.

X1 pressure (Pa)

X2 $\geq$ 1.5: temperature (° C; single-phase points).
$<$ 1.5: gas saturation (two-phase points).

X3 $\geq$ 1.5: temperature (° C; two-phase points).
$<$ 1.5: air mass fraction (single phase points).

(Two-phase conditions without air present can be initialized as X1-temperature, X2-vapor saturation, X3-0; see note on page 26).

Card INCON.3 A blank card closes the INCON data block.
(For an alternative, see note below).

ENDCY closes the TOUGH data deck and initiates the simulation.

Note on closure of blocks CONNE, GENER, and INCON

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

8. OUTPUT FROM TOUGH

TOUGH can produce a variety of printed output, most of which is controllable by the user. Standard output at specified time steps or simulation times consists of some time stepping information, and a complete element-by-element report of thermodynamic state variables and other important parameters. Additional optional output is available on mass and heat flow rates and velocities, and on changes in thermodynamic state variables during a time step. Actual examples of TOUGH-output are reproduced in Section 9. Here we shall describe the meaning of those output parameters which are not self-explanatory.

TOTAL TIME	simulation time in seconds
KCYC	total number of time steps
ITER	iteration number for current time step
ITERC	total cumulative number of Newton/Raphson iterations
DX1M, DX2M, DX3M	maximum change in first, second, and third primary variable in present time step
MAX.RES.	maximum (relative) residual in any of the mass- and energy-balance equations (see Eq. (13))
@ELEM	code name of element for which maximum residual is encountered
@EQ.	equation number of maximum residual (1-water mass balance, 2-air mass balance, 3-heat balance)
DELTEX	time step size in seconds
ELEM.	code name of element
INDEX	internal indexing number of element
P	pressure in Pa
T	temperature in °C
SG	gas saturation, fraction
SL	liquid saturation, fraction

XAIRG	mass fraction of air in gas phase
XAIRL	mass fraction of air in liquid phase
PSAT	saturated vapor pressure in Pa
PCAP	capillary pressure in Pa
DG	gas phase density in kg/m^3
DL	liquid phase density in kg/m^3
ELEM1 ELEM2	code name of first and second element, respectively, in a flow connection
INDEX	internal indexing number of connection
*FLOH	total rate of heat flow in W
FLOH/FLOF	ratio of heat and fluid flow rates in J/kg
*FLOF	fluid flow rate in kg/s
*FLO(GAS)	gas phase flow rate in kg/s
*FLO(LIQ.)	liquid phase flow rate in kg/s
*VEL(GAS)	(pore) velocity of gas flow in m/s
*VEL(LIQ.)	(pore) velocity of liquid flow in m/s
X1 X2 X3	first, second and third thermodynamic variable, respectively
DX1 DX2 DX3	changes in first, second and third thermodynamic variable, respectively, during time step
K(GAS)	gas phase relative permeability
K(LIQ.)	liquid phase relative permeability
H(GAS)	gas phase specific enthalpy in J/kg

* positive if flow is from ELEM2 into ELEM1

H(LIQ.)	liquid phase specific enthalpy in J/kg
SOURCE	code name of sink/source
GENERATION RATE	sink (>0) or source (<0) rate; in kg/s for mass sinks/sources, in W for heat sinks/sources
ENTHALPY	flowing specific enthalpy for mass sinks/sources in J/kg
FF(GAS) FF(LIQ.)	mass fraction of flow in gas and liquid phases, respectively (mass production wells only)
P(WB)	flowing wellbore pressure in Pa (production wells on deliverability only)

Additional printout can be generated when parameters MOP(1) through MOP(7) are set to non-zero values, or when an element code name is specified in variable ELST (see Section 7). For MOP(1) $\neq$ 0 a one-line printout will be generated for each non-convergent Newton/Raphson iteration. This gives information on current time step size (DELTEX), and the maximum (relative) residual encountered at that iteration. The element code name and equation number for which the maximum residual is encountered are also given. This information is useful for identifying convergence "hang-ups". When an element code name is specified in variable ELST, a one-line printout is generated after convergence is achieved. This gives simulation time (ST) and time step size (DT) in seconds, the increment in first and second primary variable (DX1, DX2), and temperature, pressure and gas saturation (P, T, S) for element ELST. When parameters MOP(2) through MOP(6) are set unequal to zero, additional printout will be generated in various subroutines (see Section 7). This feature would normally only be used if some difficulty is encountered in a simulation, and it is desired to look more closely into the inner workings of the code. An exception is parameter MOP(5), which we usually set equal to 3 to obtain a one-line informative message for each phase transition.

9. SAMPLE PROBLEMS

In this section we present a number of sample problems, with varying levels of detail on problem specifications, preparation of input decks, and computed output. The sample problems are summarized in Table 5; they were chosen to satisfy several objectives. Some problems were selected to illustrate user options and code performance, and to aid in code verification when TOUGH is implemented on a different computer system, or to provide a check on numerical accuracy by comparison with known analytical or numerical solutions. Other problems emphasize applications to nuclear waste isolation, and illustrate the various physical phenomena that can be modeled with TOUGH. We have attempted to cover a reasonably broad range of problems, but we have not endeavored to be "complete". For example, although TOUGH can handle three-dimensional flow, there is no 3-D example in this section for the simple reason that we lacked definition of an appropriate meaningful problem. A user wishing to simulate a 3-D problem can do so simply by providing appropriate volume and interface parameters in blocks ELEME and CONNE. There are no special parameters or switches to "tell" TOUGH about the dimensionality of a flow problem.

In keeping with the tutorial nature of the sample problems, we have generally chosen simple and schematic problem specifications. Readers interested in applying TOUGH to the complex conditions encountered at a "real" site are referred to the recent simulation study by Rulon et al. (1986) for the hydrology of Yucca Mountain, Nevada.

Table 5
Summary of Sample Problems

	Problem Title	Dimensions	Features	Issues
1	code demonstration	1-D,"small"	flow, production, injection	phase transitions, component (dis)appearances
2	infiltration	1-D,linear	isothermal	code verification against known semi-analytical solution (Philip, 1955; Ross et al., 1982)
3	infiltration	2-D,vertical	two-dimensional fronts, gravity effects	code verification
4	flow to a geothermal well	1-D,radial	water and steam only, no air	propagating boiling front; code verification against known semi-analytical and numerical solutions (Garg, 1978)
5	waste package	1-D,radial 2-D,radial	strongly heat driven flow in a partially saturated porous or fractured medium	exploration of possible thermohydrological conditions near high-level waste packages
6	heat pipe	1-D,linear	liquid-gas counter-flow with very strong binary diffusion	code verification against known semi-analytical solution (Udell and Fitch, 1985)

9.1 Problem No. 1 – Code Demonstration

This problem consists of a number of one- and two-element sub-problems, which are entirely independent of each other (no flow connections between sub-problems), except that being run together they all must go through the same sequence of time steps. Problem specifications were chosen in such a way that phase transitions and component (dis-) appearances will take place. This engages some subtle numerical procedures which will make the calculated results useful for checking on proper code implementation. Table 6 summarizes the main features of the various sub-problems, and Table 7 gives a summary of the generation options used. Figure 3 shows the TOUGH input deck, and Figures 4a-d show the disk files MESH, GENER, INCON, and SAVE generated by TOUGH. Figure 5 reproduces some of the printed output.

If it were desired to restart this problem after the four time steps specified in the input deck (Figure 3), the only change necessary in that input deck would be to replace data block "INCON" with the file "SAVE" (Figure 4d). For restarting the "START" option is not needed (but its presence does not cause trouble, the only effect being somewhat increased computational work on initialization). Alternatively, a restart can be accomplished by deleting data block "INCON" from the input deck, and providing a disk file "INCON" with contents identical to file "SAVE" at execution time.

Table 6
Summary of Problem No. 1 Features

Connection or Element	Process	Features
(F1, F2)	flow from single phase liquid (no air) into single phase gas (no vapor)	phase transitions from liquid to two-phase, gas to two-phase; appearance of water component
(F3, F4)	flow from hot two-phase conditions into cold two-phase conditions	vaporization and condensation; phase transitions from two-phase to liquid and gas
(F5, F6)	flow of air into single phase liquid	phase transition from liquid to two-phase; appearance of air component
F7	injection of air into cold liquid	phase transition from liquid to two-phase; appearance of air component
F8	production of fluid from single phase liquid	phase transition from liquid to two-phase; vaporization
F9	injection of heat into two-phase fluid	phase transition from two-phase to gas; vaporization
F10	withdrawal of heat from single phase vapor	phase transition from gas to two-phase; condensation
sho 1-sho 12	fluid production and injection	demonstration of generation options (see Table 7)

Table 7
Generation Options in Problem No.1

Element	Generation Option
sho 1	fluid production with specified enthalpy
sho 2	unknown (gives an informative diagnostic)
sho 3-sho 5	fluid production with time-dependent rate; sequential specification feature
sho 6-sho 8	fluid production with time-dependent rate and enthalpy; sequential specification feature
sho 9	well feed on deliverability against specified bottomhole pressure
sho 10	water injection with time-dependent rate and enthalpy
sho 11 - sho 12	well on deliverability with two source blocks (feeds); specified bottomhole pressure at top source block; gravity correction for bottomhole pressure at bottom source block

```
*SAM1* CODE DEMONSTRATION: PHASE TRANSITIONS, COMPONENT (DIS-)APPEARANCES
ROCKS
TRANS     2650.      .50              1.E-14                              2.10      1000.
SHOME   2   2650.      .50    1.e-14                                    2.10      1000.
                              1.8       .1
    3           .40       .10
    1          1.e5        .2        1.

START
PARAM
   2   4       11000301000000000000000000
                 -1.                      F   1
       1.E2       5.E3
                 45.E5                    .5                 250.
RPCAP
    3     .30        .05
    1                1.
TIMES
    1   3                    2.E3
      1.E3
ELEME
F   1    9    1TRANS        10.
sho 1    9    1SHOME        10.
sho11    1    1SHOME       1.e4

CONNE
F   1F   2                     1        5.        5.        1.
F   3F   4                     1        5.        5.        1.
F   5F   6                     1        5.        5.        1.

INCON
F   1
                  1.E5                  20.                  1.
F   2
                  1.E6                 170.                  0.
F   3
                  1.E5                 .001                 99.5
F   4
                 99.E5                 .999                 310.
F   5
                  1.E6                 100.                  0.
F   6
                 10.E6                 100.                  1.
F   7
                  1.E5                  20.                  0.
F   8
                  1.E7                 300.                  0.
F   9
                  1.E5                  .99                  90.
F  10
                 40.E5                 280.                  0.
sho11
                 50.e5                 240.
sho12
                 40.e5                 100.

GENER
F   7AIR                                    AIR       5.E-3    9.882E4
F   8WEL                                    MASS     -1.5E-2
F   9HOT                                    HEAT       2.E6
F  10COL                                    HEAT      -5.E5
sho 1p   1                                  MASS1       -1.       1.e6
sho 2p   2                                  FUNY        -1.
sho 3p   3   2    1    1    4              MASS
              0.             1.e2              2.e2              4.e3
            -0.1             -0.2              -0.3              -1.1
sho 6p   6   2    1    0    4              MASS1
              0.             1.e2              2.e2              4.e3
            -0.1             -0.2              -0.3              -1.1
            1.e6             2.e6              3.e6             1.1e7
sho 9p   9                      1           DELV     1.e-12       1.e6
sho10p  10                      4           WATE1
              0.             1.e2              2.e2              3.e3
            1.1              1.0               0.9               0.1
          1.e6             1.2e6             1.4e6             3.0e6
sho11we100                      2           DELV     1.e-12                 1.e2
sho12we100                                  DELV     2.e-12       1.e6      1.e2

ENDCY
```

Figure 3. TOUGH input deck for Sample Problem 1.

(a) File MESH.

```
ELEME
F   1                1 1.000e+01
F   2                1 1.000e+01
F   3                1 1.000e+01
F   4                1 1.000e+01
F   5                1 1.000e+01
F   6                1 1.000e+01
F   7                1 1.000e+01
F   8                1 1.000e+01
F   9                1 1.000e+01
F  10                1 1.000e+01
sho 1                2 1.000e+01
sho 2                2 1.000e+01
sho 3                2 1.000e+01
sho 4                2 1.000e+01
sho 5                2 1.000e+01
sho 6                2 1.000e+01
sho 7                2 1.000e+01
sho 8                2 1.000e+01
sho 9                2 1.000e+01
sho10                2 1.000e+01
sho11                2 1.000e+04
sho12                2 1.000e+04

CONNE
F   1F   2                    1 5.000e+00 5.000e+00 1.000e+00 0.
F   3F   4                    1 5.000e+00 5.000e+00 1.000e+00 0.
F   5F   6                    1 5.000e+00 5.000e+00 1.000e+00 0.
+++
   1   2   3   4   5   6
```

(b) File INCON.

```
INCON
F   1            0.
 1.000000000000e+05 2.000000000000e+01 1.000000000000e+00
F   2            0.
 1.000000000000e+06 1.700000000000e+02 0.
F   3            0.
 1.000000000000e+05 1.000000000000e-03 9.950000000000e+01
F   4            0.
 9.900000000000e+06 9.990000000000e-01 3.100000000000e+02
F   5            0.
 1.000000000000e+06 1.000000000000e+02 0.
F   6            0.
 1.000000000000e+07 1.000000000000e+02 1.000000000000e+00
F   7            0.
 1.000000000000e+05 2.000000000000e+01 0.
F   8            0.
 1.000000000000e+07 3.000000000000e+02 0.
F   9            0.
 1.000000000000e+05 9.900000000000e-01 9.000000000000e+01
F  10            0.
 4.000000000000e+06 2.800000000000e+02 0.
sho11            0.
 5.000000000000e+06 2.400000000000e+02 0.
sho12            0.
 4.000000000000e+06 1.000000000000e+02 0.
```

Figure 4. Disk files generated for Problem 1.

(c) File GENER.

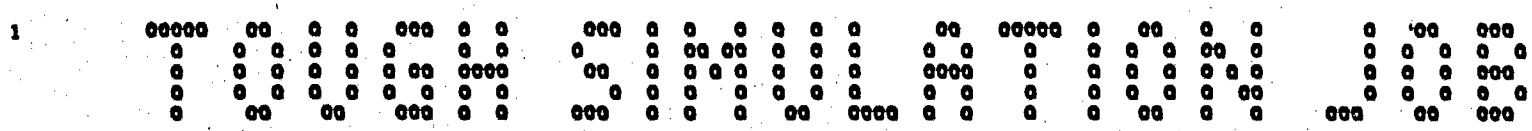
```
GENER
F   7AIR 0                    0     AIR   5.000e-03 9.882e+04 0.000
F   8WEL 0                    0     MASS -1.500e-02 0.000     0.000
F   9HOT 0                    0     HEAT  2.000e+06 0.000     0.000
F  10COL 0                    0     HEAT   .000e+05 0.000     0.000
sho 1p   1                    0     MASS1 -1.00     1.000e+06 0.000
sho 2p   2                    0     FUNY  -1.00     0.000     0.000
sho 3p   3                    4     MASS  0.000     0.000     0.000
 0.             1.0000000e+02 2.0000000e+02 4.0000000e+03
-1.0000000e-01-2.0000000e-01-3.0000000e-01-1.1000000e+00
sho 4p   4                    4     MASS  0.000     0.000     0.000
 0.             1.0000000e+02 2.0000000e+02 4.0000000e+03
-1.0000000e-01-2.0000000e-01-3.0000000e-01-1.1000000e+00
sho 5p   5                    4     MASS  0.000     0.000     0.000
 0.             1.0000000e+02 2.0000000e+02 4.0000000e+03
-1.0000000e-01-2.0000000e-01-3.0000000e-01-1.1000000e+00
sho 6p   6                    4     MASS1 0.000     0.000     0.000
 0.             1.0000000e+02 2.0000000e+02 4.0000000e+03
-1.0000000e-01-2.0000000e-01-3.0000000e-01-1.1000000e+00
 1.0000000e+06 2.0000000e+06 3.0000000e+06 1.1000000e+07
sho 7p   6                    4     MASS1 0.000     0.000     0.000
 0.             1.0000000e+02 2.0000000e+02 4.0000000e+03
-1.0000000e-01-2.0000000e-01-3.0000000e-01-1.1000000e+00
 1.0000000e+06 2.0000000e+06 3.0000000e+06 1.1000000e+07
sho 8p   6                    4     MASS1 0.000     0.000     0.000
 0.             1.0000000e+02 2.0000000e+02 4.0000000e+03
-1.0000000e-01-2.0000000e-01-3.0000000e-01-1.1000000e+00
 1.0000000e+06 2.0000000e+06 3.0000000e+06 1.1000000e+07
sho 9p   9                    1     DELV  1.000e-12 1.000e+06 0.000
sho10p  10                    4     WATE1 0.000     0.000     0.000
 0.             1.0000000e+02 2.0000000e+02 3.0000000e+03
 1.1000000e+00 1.0000000e+00 9.0000000e-01 1.0000000e-01
 1.0000000e+06 1.2000000e+06 1.4000000e+06 3.0000000e+06
sho11wel 0                    2     DELV  1.000e-12 0.000       100.
sho12wel 0                    0     DELV  2.000e-12 1.000e+06  100.
+++
   7   8   9  10  11  13  14  15  16  17  18  19  20  21  22
```

Figure 4. Disk files generated for Problem 1 (continued).

(d) File SAVE.

```
INCON -- INITIAL CONDITIONS FOR   22 ELEMENTS AT TIME  1.875000e+03
F   1             5.00000000e-01
 1.0266379604009e+05 9.9846400241964e-01 2.0359769934755e+01
F   2             5.00000000e-01
 7.9164034812709e+05 1.6079600502834e-03 1.6998002625104e+02
F   3             5.00000000e-01
 7.8016254317516e+06 1.0104286782484e+02 1.1942096433908e-05
F   4             5.00000000e-01
 9.5671037097371e+06 3.0918987989178e+02 3.2324161456927e-03
F   5             5.00000000e-01
 9.6372597201536e+06 2.5050114668019e-03 1.0030689715561e+02
F   6             5.00000000e-01
 9.8167022857770e+06 9.9933228112498e+01 9.9999999999999e-01
F   7             5.00000000e-01
 9.7036723286668e+06 2.7358354669631e-03 2.0092427319425e+01
F   8             5.00000000e-01
 8.5383096488538e+06 5.0808252264588e-03 2.9954955076665e+02
F   9             5.00000000e-01
 2.8711181800645e+06 3.6384474005122e+02 2.7417514274476e-02
F  10             5.00000000e-01
 2.0914735538840e+06 9.9098637309143e-01 2.1464668621903e+02
sho 1             5.00000000e-01
 4.5791562829086e+06 9.8291809144394e-01 2.5473853079520e+02
sho 2             5.00000000e-01
 4.5000000000000e+06 5.0000000000000e-01 2.5000000000000e+02
sho 3             5.00000000e-01
 1.0062410143469e+06 7.2185920098922e-01 1.8014561072662e+02
sho 4             5.00000000e-01
 1.0062410143469e+06 7.2185920098922e-01 1.8014561072662e+02
sho 5             5.00000000e-01
 1.0062410143469e+06 7.2185920098922e-01 1.8014561072662e+02
sho 6             5.00000000e-01
 3.4651801590417e+05 7.4141817630309e-01 9.7730684977936e+01
sho 7             5.00000000e-01
 3.4651801590417e+05 7.4141817630309e-01 9.7730684977936e+01
sho 8             5.00000000e-01
 3.4651801590417e+05 7.4141817630309e-01 9.7730684977936e+01
sho 9             5.00000000e-01
 1.2930616375166e+06 6.9357943554391e-01 1.9135077987013e+02
sho10             5.00000000e-01
 8.6397793754372e+06 1.0764756348147e-01 2.7964939186539e+02
sho11             5.00000000e-01
 3.3331150816777e+06 3.4824202657335e-03 2.3974962306756e+02
sho12             5.00000000e-01
 1.1134385711348e+06 9.9879394373028e+01 6.5780654668558e-26
+++
    4   22    2 0.              1.87500000e+03
```

Figure 4. Disk files generated for Problem 1 (continued).



TOUGH IS A PROGRAM FOR TWO-PHASE TWO-COMPONENT FLOW OF WATER AND AIR, INCLUDING HEAT FLOW.
IT WAS DEVELOPED BY K. PRUESS AT LAWRENCE BERKELEY LABORATORY.

****
****

SUMMARY OF OPTIONAL FILES

file *MESH* exists --- open as an old file
file *INCON* exists --- open as an old file
file *GENER* exists --- open as an old file
file *SAVE* does not exist --- open as a new file
file *LINEQ* exists --- open as an old file

****
****

PROBLEM TITLE: *SAM1* CODE DEMONSTRATION: PHASE TRANSITIONS, COMPONENT (DIS-)APPEARANCES

DOMAIN NO. 1 MATERIAL NAME -- TRANS
DOMAIN NO. 2 MATERIAL NAME -- SHOME
write file *MESH* from INPUT data
write file *INCON* from INPUT data
write file *GENER* from INPUT data

IGNORE UNKNOWN GENERATION OPTION *FUNY* AT ELEMENT *sho 2* SOURCE *p 2*
MESH HAS 22 ELEMENTS AND 3 CONNECTIONS (INTERFACES) BETWEEN THEM
GENER HAS 15 SINKS/SOURCES

Figure 5. Printed output for Problem 1.

```
1********** VOLUME- AND MASS-BALANCES **********************************************************************************************

 ********** [KCYC,ITER] = [   0,  0] *****                                THE TIME IS  0.          SECONDS, OR  0.          DAYS

 PHASE VOLUMES IN PLACE
 GAS  4.99500e+01 M**3;   LIQUID  1.00500e+04 M**3

 MASS IN PLACE
 GAS  1.42631e+03 KG;     LIQUID  8.91951e+06 KG;    AIR  5.63633e+02 KG;    VAPOR  8.64358e+02 KG;   LIQUID WATER  8.91951e+06 KG

 ************************************************************************************************************************************

 NO CONVERGENCE AT [   1,  1] --- DELTEX =  1.00000e+02   MAX. RES. =  3.93495e+00  AT ELEMENT *sho 9*  EQUATION   2
 $$$$$$$$$$$$$ LIQUID PHASE EVOLVES AT ELEMENT *F   1*  $$$$$   PS=  1.20568e+04  PSAT=  2.33989e+03
 $$$$$$$$$$$$$$$$ GAS PHASE EVOLVES AT ELEMENT *F   5*  $$$$$   XAIR=  6.79617e-04  PX=  2.40507e+06  PG=  4.32668e+06
 $$$$$$$$$$$$$$$$ GAS PHASE EVOLVES AT ELEMENT *F   7*  $$$$$   XAIR=  1.00168e-04  PX=  3.22602e+05  PG=  6.24952e+05
 NO CONVERGENCE AT [   1,  2] --- DELTEX =  1.00000e+02   MAX. RES. =  8.63094e-01  AT ELEMENT *sho 9*  EQUATION   2
 NO CONVERGENCE AT [   1,  3] --- DELTEX =  1.00000e+02   MAX. RES. =  8.10495e-03  AT ELEMENT *sho 9*  EQUATION   2
 F   1(   1,  4) ST =  1.00000e+02 DT =  1.00000e+02 DX1=  2.34670e+03 DX2= -1.90001e+01 T =  20.006 P =   102347. S =  9.99928e-01
```

Figure 5. Printed output for Problem 1 (continued).

1*SAM1* CODE DEMONSTRATION: PHASE TRANSITIONS, COMPONENT (DIS-)APPEARANCES

OUTPUT DATA AFTER (1, 4)-2-TIME STEPS THE TIME IS 1.15741e-03 DAYS

000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000

TOTAL TIME	KCYC	ITER	ITERC	KON	DX1M	DX2M	DX3M	MAX. RES.	NER	KER	DELTEX
1.00000e+02	1	4	4	2	1.64382e+06	9.99996e+01	1.00055e+02	1.15832e-06	19	2	1.00000e+02

000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000

0ELEM.	INDEX	P (PA)	T (DEG-C)	SG	SL	XAIRG	XAIRL	PSAT (PA)	PCAP (PA)	DG (KG/M**3)	DL (KG/M**3)
F 1	1	1.0235e+05	2.0006e+01	9.9993e-01	7.1501e-05	9.8565e-01	1.6090e-05	2.3375e+03	0.	1.2056e+00	9.9832e+02
F 2	2	8.4410e+05	1.6999e+02	0.	1.0000e+00	0.	0.	7.9179e+05	0.	0.	8.9734e+02
F 3	3	1.0570e+05	9.9591e+01	6.5930e-04	9.9934e-01	8.4732e-02	9.3976e-07	9.9856e+04	0.	6.4420e-01	9.5842e+02
F 4	4	9.8861e+06	3.0990e+02	9.9927e-01	7.3379e-04	3.2624e-03	4.7995e-06	9.8562e+06	0.	5.4629e+01	6.9093e+02
F 5	5	2.6438e+06	1.0005e+02	3.7348e-04	9.9963e-01	9.7538e-01	4.0896e-04	1.0152e+05	0.	2.4327e+01	9.5931e+02
F 6	6	9.9566e+06	9.9984e+01	1.0000e+00	0.	1.0000e+00	0.	1.0127e+05	0.	9.2947e+01	0.
F 7	7	6.1870e+05	2.0005e+01	1.3587e-04	9.9986e-01	9.9764e-01	9.9161e-05	2.3373e+03	0.	7.3409e+00	9.9856e+02
F 8	8	9.8110e+06	2.9995e+02	0.	1.0000e+00	0.	0.	8.5865e+06	0.	0.	7.1508e+02
F 9	9	1.5045e+05	1.0465e+02	9.9017e-01	9.8254e-03	2.9150e-01	5.0023e-06	1.1936e+05	0.	9.8338e-01	9.5473e+02
F 10	10	3.9597e+06	2.7628e+02	1.0000e+00	0.	0.	0.	6.0674e+06	0.	1.8037e+01	0.
sho 1	11	4.4873e+06	2.5017e+02	5.2552e-01	4.7448e-01	1.4193e-01	8.0138e-05	3.9892e+06	-6.5690e+04	2.3361e+01	7.9951e+02
sho 2	12	4.5000e+06	2.5000e+02	5.0000e-01	5.0000e-01	1.4824e-01	8.4045e-05	3.9776e+06	-6.2500e+04	2.3463e+01	7.9979e+02
sho 3	13	4.3239e+06	2.4902e+02	5.0401e-01	4.9599e-01	1.2259e-01	6.6207e-05	3.9124e+06	-6.3001e+04	2.2393e+01	8.0110e+02
sho 4	14	4.3239e+06	2.4902e+02	5.0401e-01	4.9599e-01	1.2259e-01	6.6207e-05	3.9124e+06	-6.3001e+04	2.2393e+01	8.0110e+02
sho 5	15	4.3239e+06	2.4902e+02	5.0401e-01	4.9599e-01	1.2259e-01	6.6207e-05	3.9124e+06	-6.3001e+04	2.2393e+01	8.0110e+02
sho 6	16	4.4764e+06	2.4971e+02	5.0405e-01	4.9595e-01	1.4790e-01	8.3349e-05	3.9583e+06	-6.3006e+04	2.3337e+01	8.0021e+02
sho 7	17	4.4764e+06	2.4971e+02	5.0405e-01	4.9595e-01	1.4790e-01	8.3349e-05	3.9583e+06	-6.3006e+04	2.3337e+01	8.0021e+02
sho 8	18	4.4764e+06	2.4971e+02	5.0405e-01	4.9595e-01	1.4790e-01	8.3349e-05	3.9583e+06	-6.3006e+04	2.3337e+01	8.0021e+02
sho 9	19	3.2791e+06	2.3713e+02	5.5068e-01	4.4932e-01	4.0001e-02	1.5639e-05	3.1819e+06	-6.8834e+04	1.6588e+01	8.1772e+02
sho10	20	4.5462e+06	2.5026e+02	4.7289e-01	5.2711e-01	1.5456e-01	8.8714e-05	3.9948e+06	-5.9111e+04	2.3744e+01	7.9945e+02
sho11	21	4.5429e+06	2.3994e+02	0.	1.0000e+00	0.	0.	3.3441e+06	0.	0.	8.1498e+02
sho12	22	3.2957e+06	9.9971e+01	0.	1.0000e+00	0.	0.	1.0122e+05	0.	0.	9.5968e+02

000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000000

Figure 5. Printed output for Problem 1 (continued).

1 *SAM1* CODE DEMONSTRATION: PHASE TRANSITIONS, COMPONENT (DIS-)APPEARANCES

KCYC = 1 - ITER = 4 - TIME = 1.ØØØØØe+Ø2

ØELEMENT	SOURCE	INDEX	GENERATION RATE (KG/S) OR (W)	ENTHALPY (J/KG)	FF(GAS)	FF(LIQ.)	P(WB) (PA)
F 7	AIR Ø	1	5.ØØØØØe-Ø3	9.882ØØe+Ø4			
F 8	WEL Ø	2	-1.5ØØØØe-Ø2	1.34329e+Ø6	Ø.	1.ØØØØØe+ØØ	
F 9	HOT Ø	3	2.ØØØØØe+Ø6	Ø.			
F 1Ø	COL Ø	4	-5.ØØØØØe+Ø5	Ø.	Ø.	Ø.	
sho 1	p 1	5	-1.ØØØØØe+ØØ	1.ØØØØØe+Ø6	Ø.	Ø.	
sho 3	p 3	6	-1.5ØØØØe-Ø1	2.47935e+Ø6	9.86745e-Ø1	1.32549e-Ø2	
sho 4	p 4	7	-1.5ØØØØe-Ø1	2.47935e+Ø6	9.86745e-Ø1	1.32549e-Ø2	
sho 5	p 5	8	-1.5ØØØØe-Ø1	2.47935e+Ø6	9.86745e-Ø1	1.32549e-Ø2	
sho 6	p 6	9	-1.5ØØØØe-Ø1	1.5ØØØØe+Ø6	Ø.	Ø.	
sho 7	p 6	1Ø	-1.5ØØØØe-Ø1	1.5ØØØØe+Ø6	Ø.	Ø.	
sho 8	p 6	11	-1.5ØØØØe-Ø1	1.5ØØØØe+Ø6	Ø.	Ø.	
sho 9	p 9	12	-1.75346e+ØØ	2.7Ø16Øe+Ø6	9.99134e-Ø1	8.65948e-Ø4	1.ØØØØØe+Ø6
sho1Ø	p 1Ø	13	1.Ø5ØØØe+ØØ	1.1ØØØØe+Ø6			
sho11	wel Ø	14	-1.94977e+Ø1	1.Ø3741e+Ø6	Ø.	1.ØØØØØe+ØØ	1.87Ø52e+Ø6
sho12	wel Ø	15	-1.57535e+Ø1	4.21338e+Ø5	Ø.	1.ØØØØØe+ØØ	1.ØØØØØe+Ø6

***** SOURCE $wel Ø$ RATE =-3.52512e+Ø1 KG/S FLOWING ENTHALPY = 7.62Ø92e+Ø5 J/KG *****

ØØ

Figure 5. Printed output for Problem 1 (continued).

1•SAM1• CODE DEMONSTRATION: PHASE TRANSITIONS, COMPONENT (DIS-)APPEARANCES

OUTPUT DATA AFTER (4, 4)-2-TIME STEPS THE TIME IS 2.17014e-02 DAYS

TOTAL TIME	KCYC	ITER	ITERC	KON	DX1M	DX2M	DX3M	MAX. RES.	NER	KER	DELTEX
1.87500e+03	4	4	22	2	1.70340e+06	5.62317e+01	6.63895e+01	2.60365e-06	13	2	3.75000e+02

ELEM.	INDEX	P (PA)	T (DEG-C)	SG	SL	XAIRG	XAIRL	PSAT (PA)	PCAP (PA)	DG (KG/M**3)	DL (KG/M**3)
F 1	1	1.0266e+05	2.0360e+01	9.9846e-01	1.5360e-03	9.8538e-01	1.6133e-05	2.3891e+03	0.	1.2077e+00	9.9825e+02
F 2	2	7.9164e+05	1.6998e+02	1.6080e-03	9.9839e-01	6.3954e-14	5.3942e-18	7.9164e+05	0.	4.1209e+00	8.9732e+02
F 3	3	7.8016e+06	1.0104e+02	0.	1.0000e+00	0.	1.1942e-05	1.0516e+05	0.	0.	9.6105e+02
F 4	4	9.5671e+06	3.0919e+02	1.0000e+00	0.	3.2324e-03	0.	9.7614e+06	0.	5.1834e+01	0.
F 5	5	9.6373e+06	1.0031e+02	2.5050e-03	9.9749e-01	9.9326e-01	1.5332e-03	1.0244e+05	0.	8.9536e+01	9.6244e+02
F 6	6	9.8167e+06	9.9933e+01	1.0000e+00	0.	1.0000e+00	0.	1.0108e+05	0.	9.1653e+01	0.
F 7	7	9.7037e+06	2.0092e+01	2.7358e-03	9.9726e-01	9.9985e-01	1.5599e-03	2.3500e+03	0.	1.1525e+02	1.0026e+03
F 8	8	8.5383e+06	2.9955e+02	5.0808e-03	9.9492e-01	6.3256e-14	7.6718e-17	8.5383e+06	0.	4.5849e+01	7.1315e+02
F 9	9	2.8711e+06	3.6384e+02	1.0000e+00	0.	2.7418e-02	0.	1.9560e+07	0.	1.0354e+01	0.
F 10	10	2.0915e+06	2.1465e+02	9.9099e-01	9.0136e-03	1.8298e-12	4.3274e-16	2.0915e+06	0.	1.0497e+01	8.4710e+02
sho 1	11	4.5792e+06	2.5474e+02	9.8292e-01	1.7082e-02	7.6742e-02	4.3960e-05	4.3059e+06	-1.0000e+05	2.3494e+01	7.9240e+02
sho 2	12	4.5000e+06	2.5000e+02	5.0000e-01	5.0000e-01	1.4824e-01	8.4045e-05	3.9776e+06	-6.2500e+04	2.3463e+01	7.9979e+02
sho 3	13	1.0062e+06	1.8015e+02	7.2186e-01	2.7814e-01	3.1892e-04	3.4576e-08	1.0060e+06	-9.0232e+04	5.1781e+00	8.8675e+02
sho 4	14	1.0062e+06	1.8015e+02	7.2186e-01	2.7814e-01	3.1892e-04	3.4576e-08	1.0060e+06	-9.0232e+04	5.1781e+00	8.8675e+02
sho 5	15	1.0062e+06	1.8015e+02	7.2186e-01	2.7814e-01	3.1892e-04	3.4576e-08	1.0060e+06	-9.0232e+04	5.1781e+00	8.8675e+02
sho 6	16	3.4652e+05	9.7731e+01	7.4142e-01	2.5858e-01	8.1106e-01	4.0725e-05	9.3387e+04	-9.2677e+04	2.9312e+00	9.5987e+02
sho 7	17	3.4652e+05	9.7731e+01	7.4142e-01	2.5858e-01	8.1106e-01	4.0725e-05	9.3387e+04	-9.2677e+04	2.9312e+00	9.5987e+02
sho 8	18	3.4652e+05	9.7731e+01	7.4142e-01	2.5858e-01	8.1106e-01	4.0725e-05	9.3387e+04	-9.2677e+04	2.9312e+00	9.5987e+02
sho 9	19	1.2931e+06	1.9136e+02	6.9358e-01	3.0642e-01	3.8194e-04	5.3951e-08	1.2927e+06	-8.6697e+04	6.5839e+00	8.7453e+02
sho10	20	8.6398e+06	2.7965e+02	1.0765e-01	8.9235e-01	3.0083e-01	3.6251e-04	6.3863e+06	-1.3456e+04	4.7201e+01	7.5486e+02
sho11	21	3.3331e+06	2.3975e+02	3.4824e-03	9.9652e-01	3.0320e-14	1.1987e-17	3.3331e+06	-4.3530e+02	1.6689e+01	8.1397e+02
sho12	22	1.1134e+06	9.9879e+01	0.	1.0000e+00	0.	6.5781e-26	1.0089e+05	0.	0.	9.5870e+02

Figure 5. Printed output for Problem 1 (continued).

9.2 Problem No. 2 – 1-D Infiltration

Here we consider infiltration into a semi-infinite tube of partially saturated soil. Philip (1955) obtained a semi-analytical solution for this problem, using a similarity transformation method. Detailed specifications were given in a report by Ross et al., (1982), who proposed this problem as a benchmark case for numerical simulators.

The TOUGH input deck is shown in Figure 6. The infiltration boundary is represented by means of a very large element (LB0), whose nodal distance we set to a small non-zero value, to avoid relative permeability at the boundary to be taken from the downstream element F1. The solution obtained by Philip (1955) treats the gas phase as a passive spectator at constant pressure. We enforce this approximation by placing around the soil tube a ring of very large volume, which we assign a pressure of P = 1 bar. Figure 7 shows that the simulated results agree well with the semi-analytical solution (plotted from the data given by Ross et al., 1982).

```
*SAM2* PROBLEM 4.1 OF ROSS ET AL. (1982)  ...  1-D INFILTRATION AFTER PHILIP
ROCKS
TUBES      2385.      .45          1.2E-14                          1.045  1030.
BOUND   -  2650.      .45          1.2E-14                          1.045  10000.
RING     2     2650.        .45   1.2e-14                          1.045      1.e4

    1             .333        -.1        1.        0.
    1               0.        .333       1.

PARAM
   2  20 600   1000000000000000
              9504.0         -1.            F   1
       1.E1       9.E1       2.E2       1.E3
     1.E-5      1.E-5                                      1.E-7
                  1.E5                     .56 20.
START
RPCAP
    1             .333        -.1        1.        0.
    1       9.79020E3         .333       1.
TIMES
    3             1.E3
    8.64E2    5.184E3    9.504E3
ELEME
LB  0           BOUND      1.E50
F   1   39     1TUBES      5.E-3
R   1   39     1RING       1.E50

CONNE
LB  0F   1                        1    1.e-10   .0025       1.       0.
F   1F   2   38    1    1    1    1    .0025    .0025       1.       0.
F   1R   1   39    1    1    1    1    .0025    .0          10.      0.

INCON
LB  0
                  1.e5                    20.
R   1   39    1
                  1.E5                    20.                    1.

ENDCY
```

Figure 6. TOUGH input deck for Sample Problem 2.

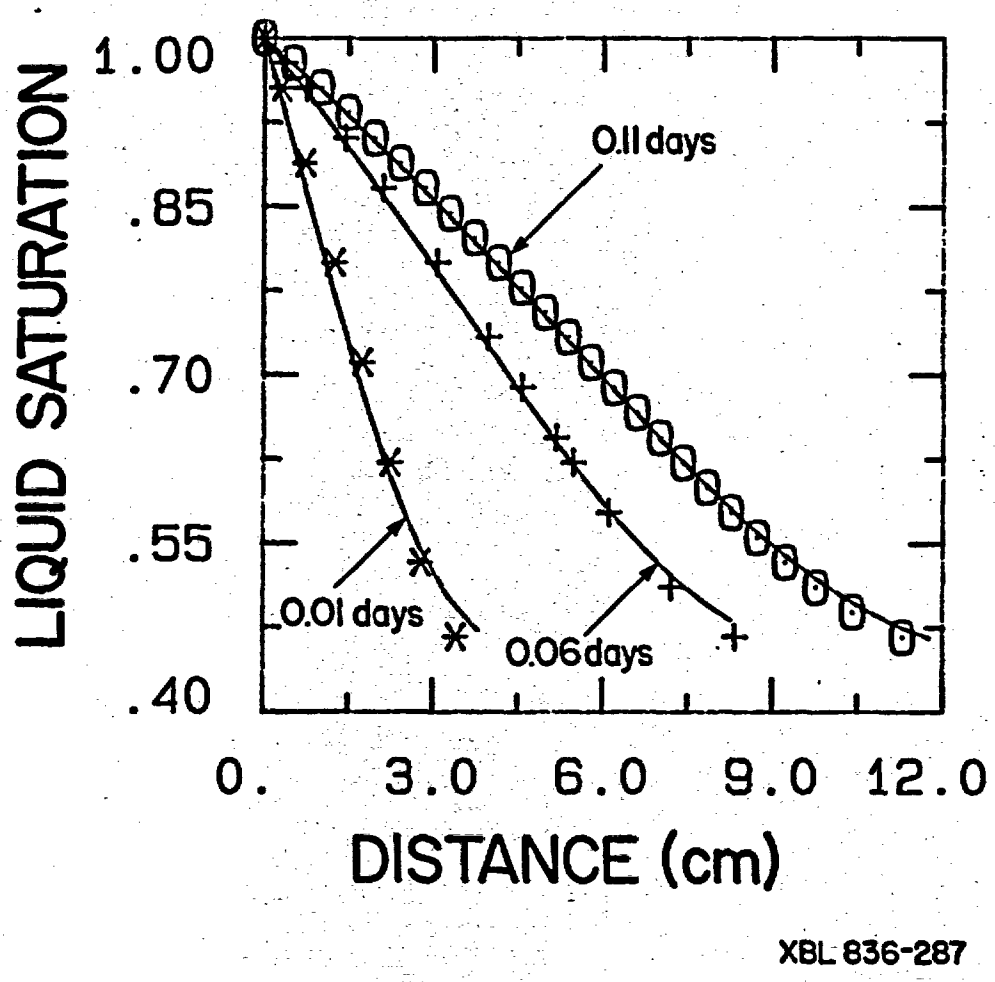


Figure 7. Liquid saturation profiles for Problem 2.

9.3 Problem No. 3 – 2-D Infiltration

Ross et al. (1982) proposed detailed specifications for a two-dimensional infiltration problem which includes gravity effects. The problem involves a rectangular section of soil 10 centimeters high and 15 centimeters long. The top 4 centimeters of the left boundary are held at a specified capillary pressure head $\psi = 6 - z$ (6 cm $\leq z \leq$ 10 cm). The right boundary is kept at constant (initial) capillary pressure head of -90 cm. All other boundaries are "no flow." The constant pressure head boundary conditions are realized in the TOUGH simulation by means of appropriate volume elements added at the periphery of the flow domain. Figure 8 gives a schematic of the problem, and explains the nomenclature used for the grid elements. The TOUGH input deck is shown in Figure 9, and Figures 10 and 11 present plots of computed results at a time of 0.508 days (8 time steps).

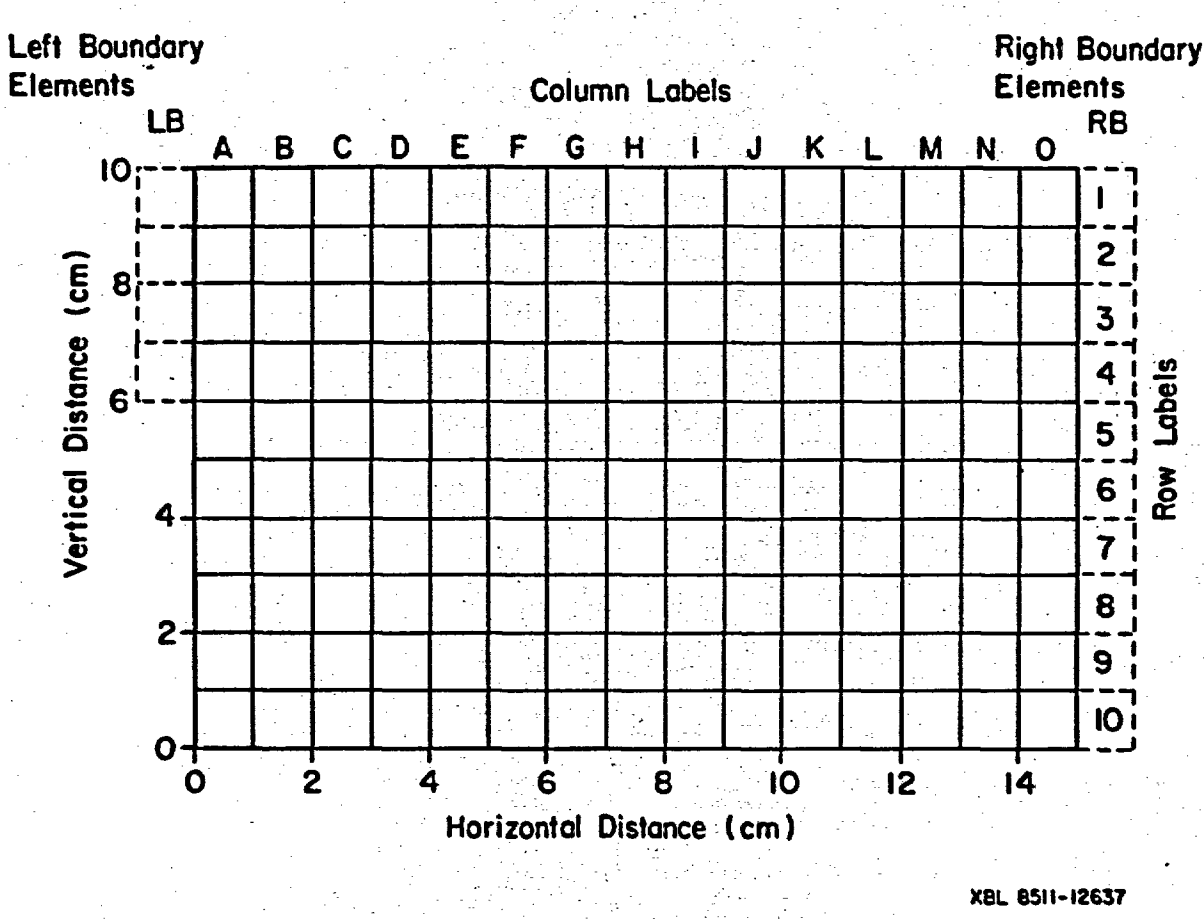


Figure 8. Flow geometry and discretization for Sample Problem 3.

```
1•SAM3• PROBLEM 4.2 OF ROSS ET AL. (1982)  ...  2-D INFILTRATION WITH GRAVITY
ROCKS
SOIL      2385.      .45          1.2E-14                    1.9          1030.
BOUND     2650.      .45          1.2E-14                    1.9          10000.

PARAM
   1  14 600   100000000000000  1
            43891.2        -1.          A  10     •9.80665                    1.
        1.E2        9.E2        2.E3        1.E4
     1.e-5             1.                                  1.E-7
                     1.E5                      .60 20.
RPCAP
     1                .333         -.1         1.
     1     9.79020E3  .333         1.
START
GENER

ELEME
LB   1    3    1BOUND     1.E50
A    1    9    1SOIL      1.E-4
B    1    9    1SOIL      1.E-4
C    1    9    1SOIL      1.E-4
D    1    9    1SOIL      1.E-4
E    1    9    1SOIL      1.E-4
F    1    9    1SOIL      1.E-4
G    1    9    1SOIL      1.E-4
H    1    9    1SOIL      1.E-4
I    1    9    1SOIL      1.E-4
J    1    9    1SOIL      1.E-4
K    1    9    1SOIL      1.E-4
L    1    9    1SOIL      1.E-4
M    1    9    1SOIL      1.E-4
N    1    9    1SOIL      1.E-4
O    1    9    1SOIL      1.E-4
RB   1    9    1BOUND     1.E50

CONNE
LB   1A   1    3    1    1    1    1.E-10   .0050      .01      0.
A    1B   1    9    1    1    1    .0050    .0050      .01      0.
B    1C   1    9    1    1    1    .0050     .005      .01        0.
C    1D   1    9    1    1    1    .0050     .005      .01        0.
D    1E   1    9    1    1    1    .0050     .005      .01        0.
E    1F   1    9    1    1    1    .0050     .005      .01        0.
F    1G   1    9    1    1    1    .0050     .005      .01        0.
G    1H   1    9    1    1    1    .0050     .005      .01        0.
H    1I   1    9    1    1    1    .0050     .005      .01        0.
I    1J   1    9    1    1    1    .0050     .005      .01        0.
J    1K   1    9    1    1    1    .0050     .005      .01        0.
K    1L   1    9    1    1    1    .0050     .005      .01        0.
L    1M   1    9    1    1    1    .0050     .005      .01        0.
M    1N   1    9    1    1    1    .0050     .005      .01        0.
N    1O   1    9    1    1    1    .0050     .005      .01        0.
O    1RB  1    9    1    1    1    .0050    1.E-10     .01        0.
A    1A   2    8    1    1    1    .0050    .0050      .01        1.
B    1B   2    8    1    1    1    .0050    .0050      .01        1.
C    1C   2    8    1    1    1    .0050    .0050      .01        1.
D    1D   2    8    1    1    1    .0050    .0050      .01        1.
E    1E   2    8    1    1    1    .0050    .0050      .01        1.
F    1F   2    8    1    1    1    .0050    .0050      .01        1.
G    1G   2    8    1    1    1    .0050    .0050      .01        1.
H    1H   2    8    1    1    1    .0050    .0050      .01        1.
I    1I   2    8    1    1    1    .0050    .0050      .01        1.
J    1J   2    8    1    1    1    .0050    .0050      .01        1.
K    1K   2    8    1    1    1    .0050    .0050      .01        1.
L    1L   2    8    1    1    1    .0050    .0050      .01        1.
M    1M   2    8    1    1    1    .0050    .0050      .01        1.
N    1N   2    8    1    1    1    .0050    .0050      .01        1.
O    1O   2    8    1    1    1    .0050    .0050      .01        1.

INCON
LB   1
                    1.E5              .02333                20.
LB   2
                    1.E5              .01667                20.
LB   3
                    1.E5               .010                 20.
LB   4
                    1.E5              .00333                20.
RB   1    9    1
                    1.E5               .600                 20.

ENDCY
```

Figure 9. TOUGH input deck for Problem 3.

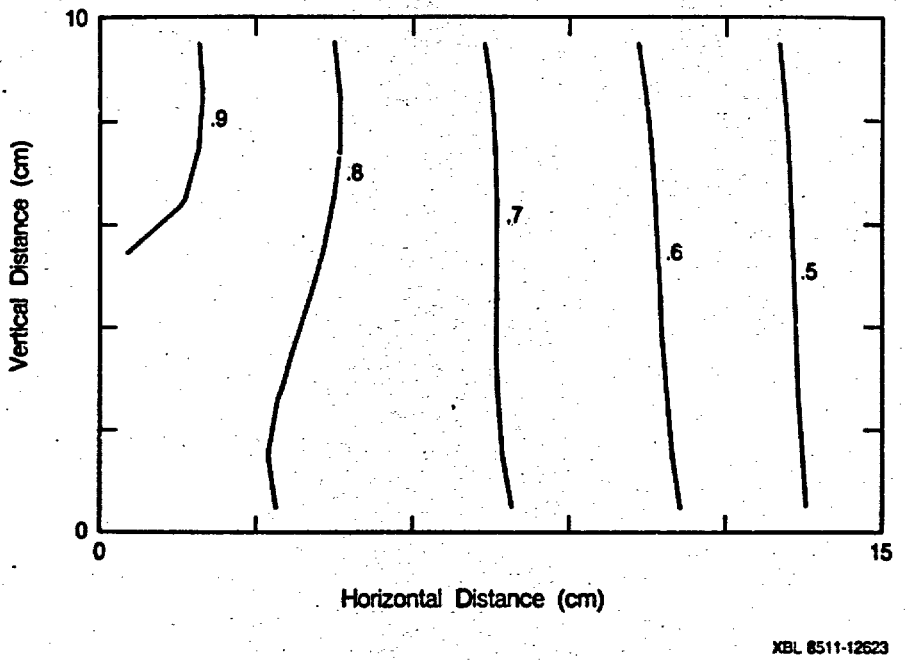


Figure 10. Liquid saturations after 0.508 days for Problem 3.

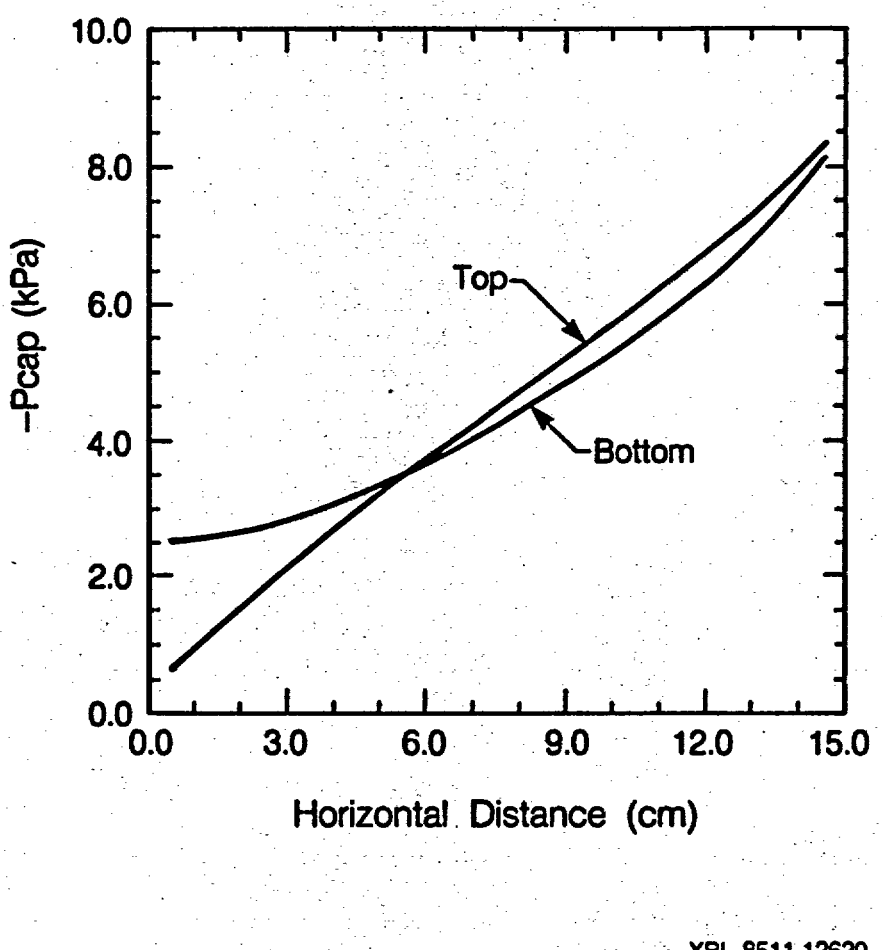


Figure 11. Capillary pressure profiles after 0.508 days for Problem 3.

9.4 Problem No. 4 – Flow to a Geothermal Well

Garg (1978) developed a semi-analytical theory for radial flow to a geothermal well, which accounts for phase transitions and propagating boiling fronts. He presented simulated results for production at a constant rate of 14 kg/s from a 100 m thick reservoir that is initially in single phase liquid conditions of T = 300 °C, P = 90 bars. In response to production pressures drop to the saturated vapor pressure, and a boiling front moves out into the reservoir. A slightly modified version of Garg's problem was later used in a code comparison study of geothermal reservoir simulators (Stanford Geothermal Program, 1980). Detailed problem specifications are given in the indicated references, or can be read off the TOUGH input deck as shown in Figure 12. The computational mesh consists of 10 grid blocks with ΔR= 1 m, and an additional 40 grid blocks with $\Delta R_{i+1}=\alpha \Delta R_i$ out to an outer radius of 2000 m. Simulated pressures in the wellbock (element AA1) are plotted versus time in Figure 13. The agreement with Garg's results is excellent.

```
*SAM4* GARG'S PROBLEM (CF. PAPER SPE-7479): FLOW TO A GEOTHERMAL WELL
ROCKS
LAY 1     2650.      .20           1.E-14                    4.20      1000.

START
PARAM
   1  50        50000300000000030
                   -1.                    AA  1
      2.

                 9.e6                  300.
RPCAP
    3      .30        .05
    1                 1.
ELEME ---     50     1    10   40   0.00000  2000.000
AA  1           LAY 1 3.142e+02
AA  2           LAY 1 9.425e+02
AA  3           LAY 1 1.571e+03
AA  4           LAY 1 2.199e+03
AA  5           LAY 1 2.827e+03
AA  6           LAY 1 3.456e+03
AA  7           LAY 1 4.084e+03
AA  8           LAY 1 4.712e+03
AA  9           LAY 1 5.341e+03
AA 10           LAY 1 5.969e+03
AA 11           LAY 1 7.634e+03
AA 12           LAY 1 9.797e+03
AA 13           LAY 1 1.261e+04
AA 14           LAY 1 1.627e+04
AA 15           LAY 1 2.106e+04
AA 16           LAY 1 2.731e+04
AA 17           LAY 1 3.549e+04
AA 18           LAY 1 4.620e+04
AA 19           LAY 1 6.025e+04
AA 20           LAY 1 7.869e+04
AA 21           LAY 1 1.029e+05
AA 22           LAY 1 1.347e+05
AA 23           LAY 1 1.766e+05
AA 24           LAY 1 2.316e+05
AA 25           LAY 1 3.041e+05
AA 26           LAY 1 3.996e+05
AA 27           LAY 1 5.253e+05
AA 28           LAY 1 6.909e+05
AA 29           LAY 1 9.092e+05
AA 30           LAY 1 1.197e+06
AA 31           LAY 1 1.576e+06
AA 32           LAY 1 2.077e+06
AA 33           LAY 1 2.737e+06
AA 34           LAY 1 3.607e+06
AA 35           LAY 1 4.756e+06
AA 36           LAY 1 6.271e+06
AA 37           LAY 1 8.271e+06
AA 38           LAY 1 1.091e+07
AA 39           LAY 1 1.439e+07
AA 40           LAY 1 1.899e+07
AA 41           LAY 1 2.505e+07
AA 42           LAY 1 3.306e+07
AA 43           LAY 1 4.363e+07
AA 44           LAY 1 5.758e+07
AA 45           LAY 1 7.600e+07
AA 46           LAY 1 1.003e+08
AA 47           LAY 1 1.324e+08
AA 48           LAY 1 1.748e+08
AA 49           LAY 1 2.307e+08
AA 50           LAY 1 3.045e+08
```

Figure 12. TOUGH input deck for Sample Problem 4.

```
CONNE
AA   1AA   2                    1 5.000e-01 5.000e-01 6.283e+02
AA   2AA   3                    1 5.000e-01 5.000e-01 1.257e+03
AA   3AA   4                    1 5.000e-01 5.000e-01 1.885e+03
AA   4AA   5                    1 5.000e-01 5.000e-01 2.513e+03
AA   5AA   6                    1 5.000e-01 5.000e-01 3.142e+03
AA   6AA   7                    1 5.000e-01 5.000e-01 3.770e+03
AA   7AA   8                    1 5.000e-01 5.000e-01 4.398e+03
AA   8AA   9                    1 5.000e-01 5.000e-01 5.027e+03
AA   9AA  10                    1 5.000e-01 5.000e-01 5.655e+03
AA  10AA  11                    1 5.000e-01 5.745e-01 6.283e+03
AA  11AA  12                    1 5.745e-01 6.602e-01 7.005e+03
AA  12AA  13                    1 6.602e-01 7.585e-01 7.835e+03
AA  13AA  14                    1 7.585e-01 8.716e-01 8.788e+03
AA  14AA  15                    1 8.716e-01 1.002e+00 9.883e+03
AA  15AA  16                    1 1.002e+00 1.151e+00 1.114e+04
AA  16AA  17                    1 1.151e+00 1.322e+00 1.259e+04
AA  17AA  18                    1 1.322e+00 1.519e+00 1.425e+04
AA  18AA  19                    1 1.519e+00 1.746e+00 1.616e+04
AA  19AA  20                    1 1.746e+00 2.006e+00 1.835e+04
AA  20AA  21                    1 2.006e+00 2.305e+00 2.087e+04
AA  21AA  22                    1 2.305e+00 2.649e+00 2.377e+04
AA  22AA  23                    1 2.649e+00 3.043e+00 2.710e+04
AA  23AA  24                    1 3.043e+00 3.497e+00 3.092e+04
AA  24AA  25                    1 3.497e+00 4.018e+00 3.532e+04
AA  25AA  26                    1 4.018e+00 4.617e+00 4.037e+04
AA  26AA  27                    1 4.617e+00 5.305e+00 4.617e+04
AA  27AA  28                    1 5.305e+00 6.096e+00 5.284e+04
AA  28AA  29                    1 6.096e+00 7.005e+00 6.050e+04
AA  29AA  30                    1 7.005e+00 8.049e+00 6.930e+04
AA  30AA  31                    1 8.049e+00 9.248e+00 7.941e+04
AA  31AA  32                    1 9.248e+00 1.063e+01 9.104e+04
AA  32AA  33                    1 1.063e+01 1.221e+01 1.044e+05
AA  33AA  34                    1 1.221e+01 1.403e+01 1.197e+05
AA  34AA  35                    1 1.403e+01 1.612e+01 1.374e+05
AA  35AA  36                    1 1.612e+01 1.852e+01 1.576e+05
AA  36AA  37                    1 1.852e+01 2.129e+01 1.809e+05
AA  37AA  38                    1 2.129e+01 2.446e+01 2.077e+05
AA  38AA  39                    1 2.446e+01 2.810e+01 2.384e+05
AA  39AA  40                    1 2.810e+01 3.229e+01 2.737e+05
AA  40AA  41                    1 3.229e+01 3.711e+01 3.143e+05
AA  41AA  42                    1 3.711e+01 4.264e+01 3.609e+05
AA  42AA  43                    1 4.264e+01 4.899e+01 4.145e+05
AA  43AA  44                    1 4.899e+01 5.629e+01 4.761e+05
AA  44AA  45                    1 5.629e+01 6.468e+01 5.468e+05
AA  45AA  46                    1 6.468e+01 7.433e+01 6.281e+05
AA  46AA  47                    1 7.433e+01 8.540e+01 7.215e+05
AA  47AA  48                    1 8.540e+01 9.813e+01 8.288e+05
AA  48AA  49                    1 9.813e+01 1.128e+02 9.521e+05
AA  49AA  50                    1 1.128e+02 1.296e+02 1.094e+06

GENER
AA   1PRO 1                          MASS       -14.

INCON

ENDCY
```

Figure 12. TOUGH input deck for Sample Problem 4 (continued).

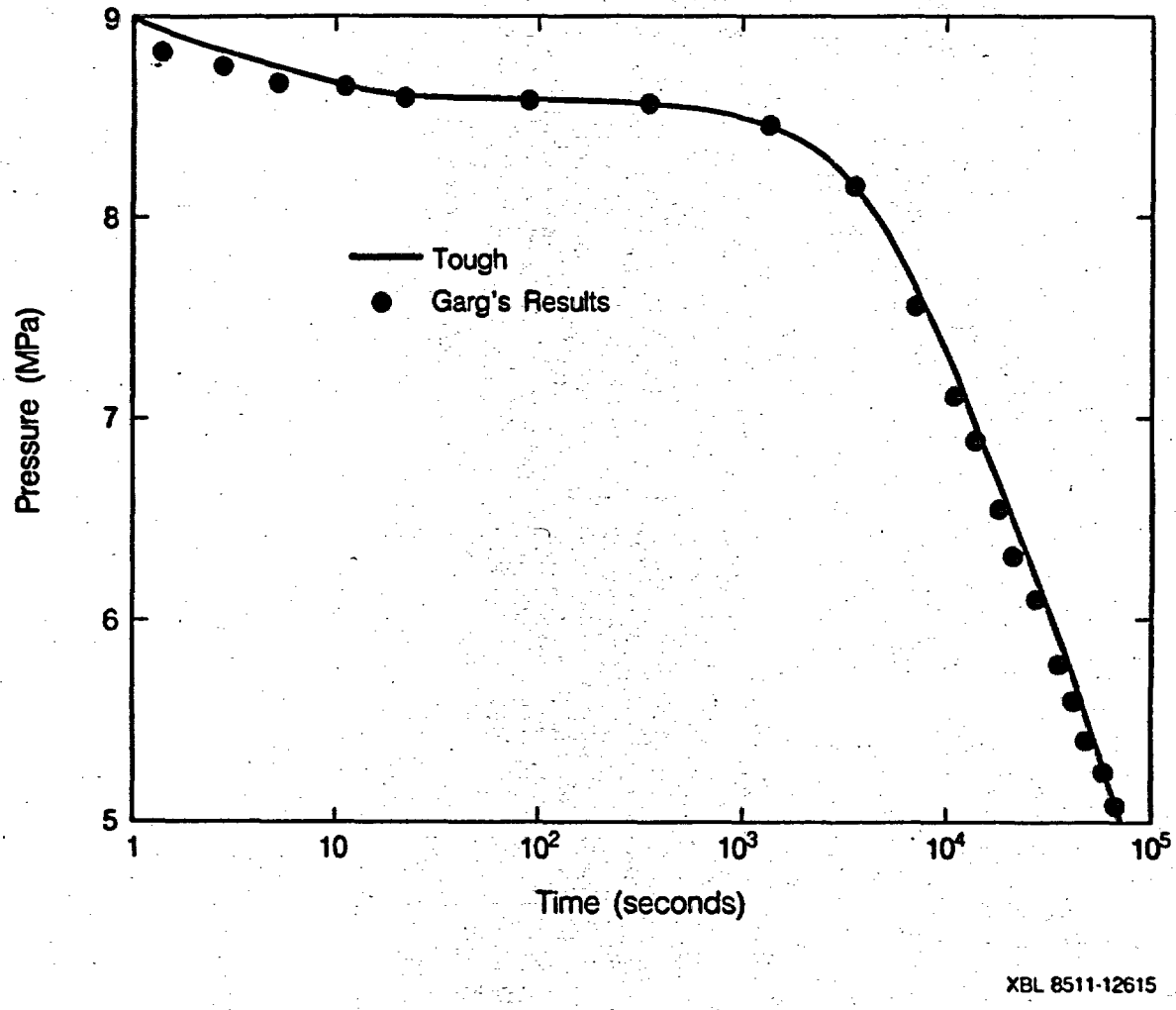


Figure 13. Wellblock Pressures for Problem 4.

9.5 Problem No. 5 – Waste Package in a Partially Saturated Medium

A study of thermohydrological conditions near high-level nuclear waste packages emplaced in a partially saturated fractured medium was recently made by Pruess, Tsang, and Wang (1985). These authors used an experimental version of the TOUGH code which takes effects of vapor pressure lowering into account. The present problem is similar to the one studied by Pruess et al., except that vapor pressure lowering effects are ignored.

Figure 14 shows the highly idealized geometry of the flow system. We consider an infinite linear string of waste packages, which is intersected by a set of plane, parallel fractures at a spacing of 0.22 m. The formation parameters used in this study are listed in Table 8. Most of these parameters were taken from a compilation of Hayden et al. (1983). We wish to emphasize that these parameters were chosen here to define a test case with large fracture and small matrix permeability; they do not necessarily represent conditions expected for a hypothetical nuclear waste repository at Yucca Mountain.

Because of the symmetry of the problem it is only necessary to model a 0.11 m thick section (see Figure 14). The parameters of the two-dimensional computational grid are given in Table 9, and part of the TOUGH input deck (excluding the data blocks ELEME and CONNE) is shown in Figure 15. For convenience we have multiplied all volumes and interface areas in blocks ELEME and CONNE by a factor 4.5/0.11, so that our calculation is normalized to one waste package (assumed to be 4.5 m long). The time-dependent heat generation data were obtained from Hayden et al. (1983). The initial conditions reflect assumed suction equilibrium between matrix and fractures; these conditions were obtained by running a two-element matrix-fracture problem with $S_{l,matrix}$=80% to equilibrium. Gravity effects were ignored.

We ran the problem out to 51.4 days (66 time steps). Calculated results are shown in Figures 16 and 17. For comparison we have also plotted results obtained from a one-dimensional radial flow calculation in which fracture effects were ignored.

Our results are similar to those reported by Pruess et al. (1985) for a case with vapor pressure lowering. A detailed discussion of physical phenomena observed in the simulation is given in the paper by Pruess et al., and will not be repeated here.

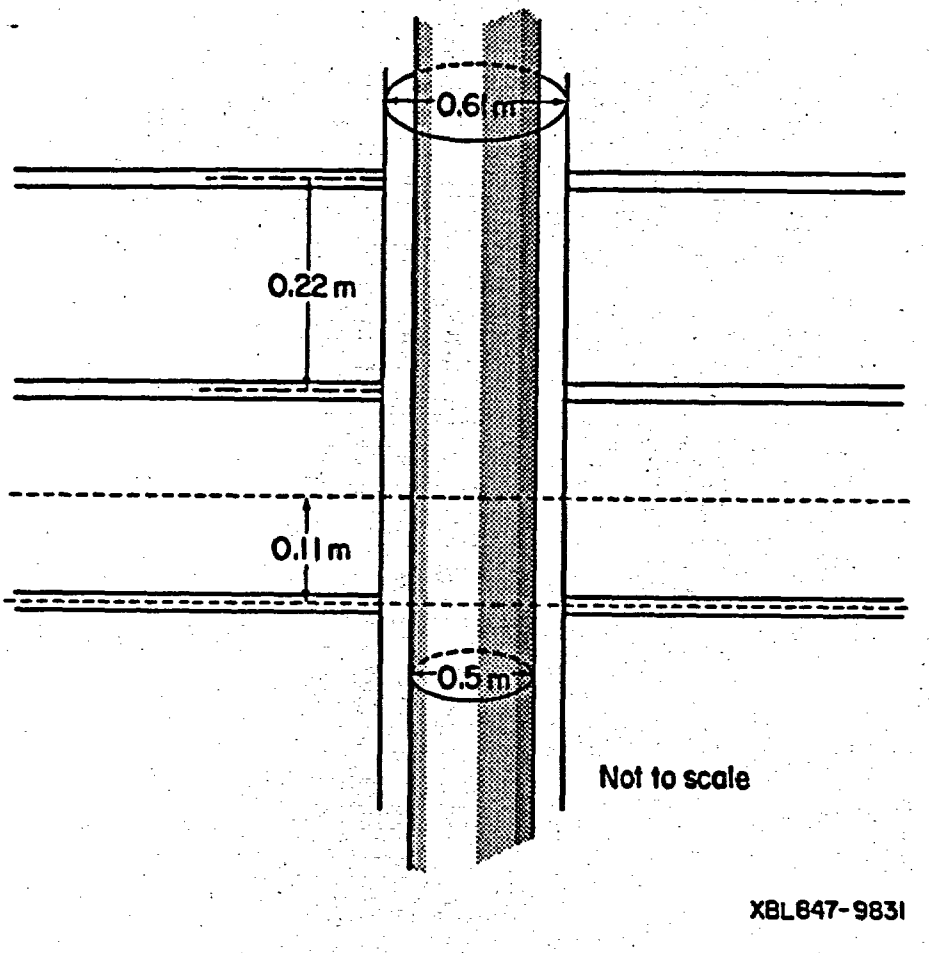


Figure 14. Idealized geometry for Sample Problem 5.

Table 8
Formation Parameters for Sample Problem 5

Matrix	
rock grain density	$\rho_R = 2550$ kg/m^3
rock specific heat	$C_R = 768.8$ J/kg°C
rock heat conductivity	$K = 1.6$ W/m°C
porosity	$\phi_m = 10.3\%$
permeability	$k_m = 32.6 \times 10^{-18}$ m^2
suction pressure	$P_{suc}(S_l) = -1.393\,(S_{EF}^{-1/\lambda}-1)^{1-\lambda}$ MPa
relative permeability to liquid (van Genuchten, 1980)	$k_{rl}(S_l) = \sqrt{S_{EF}}\,[1-(1-S_{EF}^{1/\lambda})^{\lambda}]^2$ where $S_{EF} = (S_l - S_{lr})/(1 - S_{lr})$, $S_{lr} = 9.6 \times 10^{-4}$, $\lambda = 0.45$
relative permeability to gas	$k_{rg}(S_l) = 1 - k_{rl}$
Fractures (one set)	
aperture	$\delta = 2$ mm
porosity	$\phi_f = 20\%$
spacing	$D = .22$ m
average continuum permeability	$\bar{k}_f = 10^{-13}$ m^2
permeability per fracture*	$k_f \approx \bar{k}_f \cdot D/\delta = 11 \times 10^{-12}$ m^2
equivalent continuum porosity	$\phi_f \approx \phi_f\,\delta/D = 0.182\%$
suction pressure	$P_{suc}(S_l) = -500\,(.0099 - S_l)/.0099$ MPa
relative permeability to liquid	$k_{rl}(S_l) = (S_l - 0.01)/0.99$
relative permeability to gas	$k_{rg}(S_l) = 1 - S_l$
Initial Conditions	
temperature	$T = 26$°C
pressure	$P = 10^5$ Pa ($\equiv 1$ bar)
liquid saturation in matrix	$S_{l,m} = 80\%$ (suction
liquid saturation in fractures	$S_{l,f} = .0098783674683$ equilibrium)

*Note that we do not imply a parallel-plate model for the fractures; k_f is less than the parallel plate permeability $(\phi_f\,\delta)^2/12 = 1.33 \times 10^{-8}$ m^2.

Table 9
Grid Specifications for Problem 5

The grid extends from the wall of the canister (r = 0.25 m) out to r = 300 m, at which distance boundary conditions of T = 26°C, P = 1 bar, S_l = 0.80 are maintained. Discretization in r - direction is made with a series of concentric cylinders with the following radii.

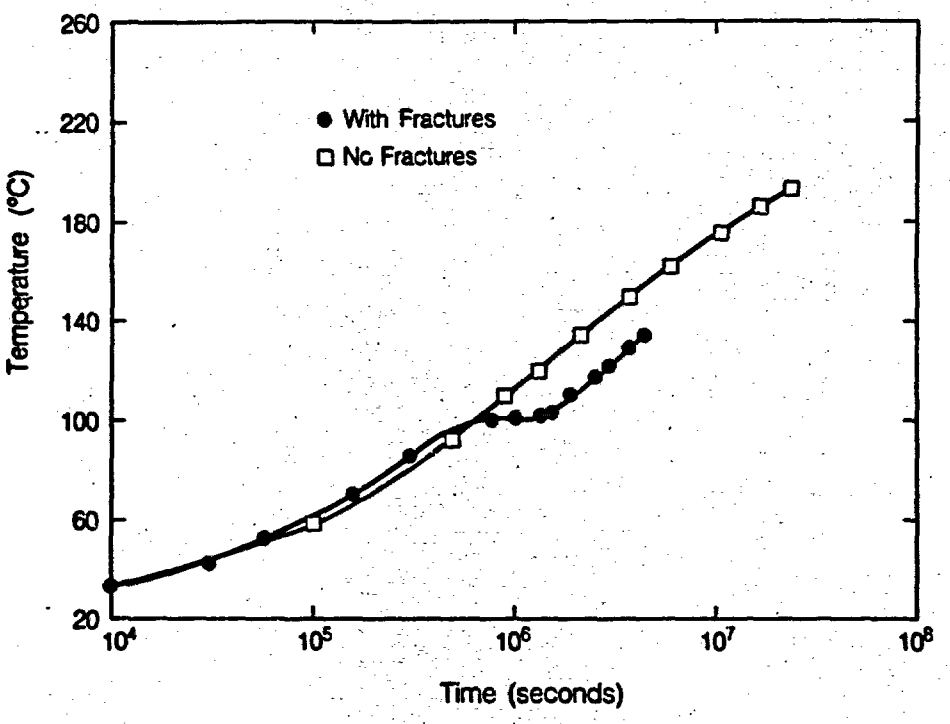
grid element	radius (m)	grid element	radius (m)	grid element	radius (m)
1	.2700	17	3.096	31	38.49
2	.3050	18	3.563	32	45.24
3	.3660	19	4.465	33	53.12
4	.4359	20	5.517	34	62.33
5	.5159	21	6.747	35	73.07
6	.6075	22	8.182	36	85.62
7	.7124	23	9.857	37	100.3
8	.8326	24	11.81	38	117.4
9	.9702	25	14.10	39	137.3
10	1.128	26	16.76	40	160.6
11	1.308	27	19.88	41	187.8
12	1.515	28	23.51	42	219.6
13	1.751	29	27.75	43	256.7
14	2.023	30	32.71	44	300.0
15	2.334				
16	2.689				

In z-direction we discretize into four layers, the first of which represents (half of) the fracture:

layer	thickness (m)
A	1×10^{-3}
B	4×10^{-3}
C	1.5×10^{-2}
D	9.0×10^{-2}

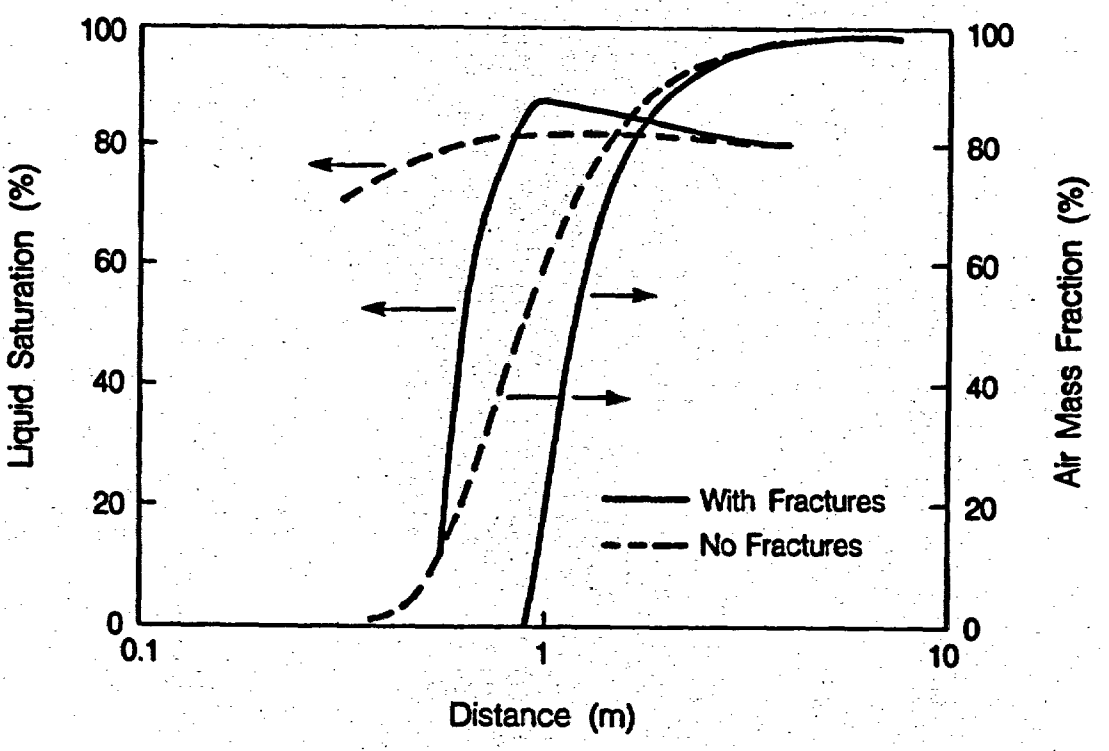
```
*SAM5* Waste Package in Partially Saturated Fractured Porous Medium -- 2-D
ROCKS
FRACT    2     2550.       .20   11.E-12   11.E-12   11.E-12      1.80      768.8
                          1.60       .25
    1          1.E-2         0.        1.        1.
    1           5.E8    0.0E-4      .0099
WTUFF    1     2550.      .103 3.2631E-173.2631E-173.2631E-17      1.80      768.8
                          1.60       .25
BOUND    1     2550.      .103 3.2631E-173.2631E-173.2631E-17      1.80       1.E4
                          1.60       .25

START
PARAM
   2  75 600  7510003000000002 40          2.13e-5
              4.44e6        -1.          AA  3
      1.e3      9.e3       2.e4
     1.E-4     1.E00                                      1.E-7
                1.E5                    .20 26.
RPCAP
    7         0.45000    9.6E-4        1.
    7         0.45000    9.6E-4 7.178E-07       5.E8         1.
TIMES
    1
    4.44e6

GENER
AA  1CAN                      101     HEAT
 0.                .3155760E+08  .6311520E+08  .9467280E+08
  .1262304E+09  .1577880E+09  .1893456E+09  .2209032E+09
  .2524608E+09  .2840184E+09  .3155760E+09  .3471336E+09
  .3786912E+09  .4102488E+09  .4418064E+09  .4733640E+09
  .5049216E+09  .5364792E+09  .5680368E+09  .5995944E+09
  .6311520E+09  .6627096E+09  .6942672E+09  .7258248E+09
  .7573824E+09  .7889400E+09  .8204976E+09  .8520552E+09
  .8836128E+09  .9151704E+09  .9467280E+09  .9782856E+09
  .1009843E+10  .1041401E+10  .1072958E+10  .1104516E+10
  .1136074E+10  .1167631E+10  .1199189E+10  .1230746E+10
  .1262304E+10  .1293862E+10  .1325419E+10  .1356977E+10
  .1388534E+10  .1420092E+10  .1451650E+10  .1483207E+10
  .1514765E+10  .1546322E+10  .1577880E+10  .1609438E+10
  .1640995E+10  .1672553E+10  .1704110E+10  .1735668E+10
  .1767226E+10  .1798783E+10  .1830341E+10  .1861898E+10
  .1893456E+10  .1925014E+10  .1956571E+10  .1988129E+10
  .2019686E+10  .2051244E+10  .2082802E+10  .2114359E+10
  .2145917E+10  .2177474E+10  .2209032E+10  .2240590E+10
  .2272147E+10  .2303705E+10  .2335262E+10  .2366820E+10
  .2398378E+10  .2429935E+10  .2461493E+10  .2493050E+10
  .2524608E+10  .2556166E+10  .2587723E+10  .2619281E+10
  .2650838E+10  .2682396E+10  .2713954E+10  .2745511E+10
  .2777069E+10  .2808626E+10  .2840184E+10  .2871742E+10
  .2903299E+10  .2934857E+10  .2966414E+10  .2997972E+10
  .3029530E+10  .3061087E+10  .3092645E+10  .3124202E+10
  .3155760E+10
  .3051000E+04  .2943166E+04  .2881139E+04  .2820725E+04
  .2761883E+04  .2704571E+04  .2648748E+04  .2594375E+04
  .2541413E+04  .2489825E+04  .2439575E+04  .2390627E+04
  .2342947E+04  .2296501E+04  .2251257E+04  .2207182E+04
  .2164246E+04  .2122418E+04  .2081670E+04  .2041972E+04
  .2003298E+04  .1965619E+04  .1928909E+04  .1893143E+04
  .1858296E+04  .1824344E+04  .1791262E+04  .1759028E+04
  .1727620E+04  .1697015E+04  .1667192E+04  .1638131E+04
  .1609811E+04  .1582213E+04  .1555318E+04  .1529107E+04
  .1503563E+04  .1478666E+04  .1454401E+04  .1430751E+04
  .1407699E+04  .1385229E+04  .1363327E+04  .1341977E+04
  .1321164E+04  .1300875E+04  .1281096E+04  .1261813E+04
  .1243012E+04  .1224682E+04  .1206810E+04  .1189384E+04
  .1172392E+04  .1155822E+04  .1139664E+04  .1123906E+04
  .1108538E+04  .1093550E+04  .1078932E+04  .1064673E+04
  .1050765E+04  .1037199E+04  .1023964E+04  .1011053E+04
  .9984572E+03  .9861678E+03  .9741770E+03  .9624769E+03
  .9510599E+03  .9399185E+03  .9290455E+03  .9184337E+03
  .9080764E+03  .8979669E+03  .8880985E+03  .8784651E+03
  .8690604E+03  .8598783E+03  .8509132E+03  .8421591E+03
  .8336107E+03  .8252625E+03  .8171093E+03  .8091460E+03
  .8013675E+03  .7937690E+03  .7863458E+03  .7790933E+03
  .7720071E+03  .7650828E+03  .7583161E+03  .7517029E+03
  .7452392E+03  .7389212E+03  .7327449E+03  .7267067E+03
  .7208030E+03  .7150302E+03  .7093850E+03  .7038641E+03
  .6984641E+03

INCON
AA  3    41    1
                1.E5      0.9901216325317                  26.

ENDCY
```

Figure 15. TOUGH input deck for Problem 5.



XBL 8511-12616

Figure 16. Temperatures at a distance R = 0.3355 m from canister centerline (Problem 5).



XBL 8511-12617

Figure 17. Profiles of liquid saturation and gas phase composition after 51.4 days (Problem 5).

9.6 Problem No. 6 – Heat Pipe

Heat pipes are devices which achieve large heat fluxes for small applied temperature gradients by means of two-phase countercurrent flow in a porous medium (Eastman, 1968). Liquid is vaporized at the hot end, and the vapor is driven by a pressure gradient towards the cold end, where it condenses, releasing latent heat. The condensate then returns to the hot end by means of capillary suction.

The heat pipe problem presented here includes non-condensible gas (air) and binary diffusion of air and vapor in the gas phase. The problem therefore engages all mass- and energy-balance equations, and flux terms, which are present in TOUGH. Selection of this problem was motivated by the recent publication of a semi-analytical solution for the steady state of a heat pipe with non-condensible gas (Udell and Fitch, 1985), which could be used to verify the accuracy of the TOUGH simulator for a complex problem.

The TOUGH input deck (see Figure 18) models a one-dimensional horizontal porous column of 2.25 m length and 1 m cross-sectional area, which is discretized into 90 volume elements of 2.5 cm length each. A boundary condition of zero capillary pressure is maintained at one end of the column while a heat flux of 100 W/m^2 is injected at the other end. Detailed problem specifications were given by Udell and Fitch (1985), and can be read off the TOUGH input deck. Note, however, that in order to obtain a semi-analytical solution, Udell and Fitch made a number of simplifying assumptions, which are not made in the TOUGH simulator. The most important simplification was to neglect the temperature dependence of fluid properties. Because of this difference we do not expect a perfect agreement between the TOUGH simulation and the semi-analytical solution.

The simulation reaches a steady state after 876.6 days (80 time steps). Figure 19 shows that the TOUGH results agree well with the semi-analytical solution of Udell and Fitch (1985). As a further check we modified TOUGH to implement the same simplifying assumptions as were made by Udell and Fitch. This resulted in an excellent agreement with their solution.

```
*SAM6* HEAT PIPE WITH NON-CONDENSIBLE GAS AFTER UDELL AND FITCH.
ROCKS
SAMPL    2     2600.       0.4    1.E-12    1.E-12    1.E-12 1.13     700.
                    0.582     0.5
    6     0.150
    6     632455.53 0.150
LBND     2     2600.       0.4    1.E-12    1.E-12    1.E-12 1.13     700.    E4
                    0.582     0.5
    1     0.1       0.8       0.2       0.9
    1     0.        0.1       0.9

START
PARAM
 8 2 100      200000001000000004000000000 2.6   E-5 1.   E-10
0.                  1.000                SAM 1     9.817     5.

101330.             0.5                  70.
ELEME
LBD00          LBND 1.     E30
SAM00   89    1SAMPL 0.025

CONNE
LBD00SAM00                      1 1.   E-10 .0125    1.        0.
SAM00SAM01   88    1    1      1 .0125    .0125     1.        0.

GENER
SAM89Q   1                           HEAT 100.

ENDCY
```

Figure 18. TOUGH input deck for Sample Problem 6.

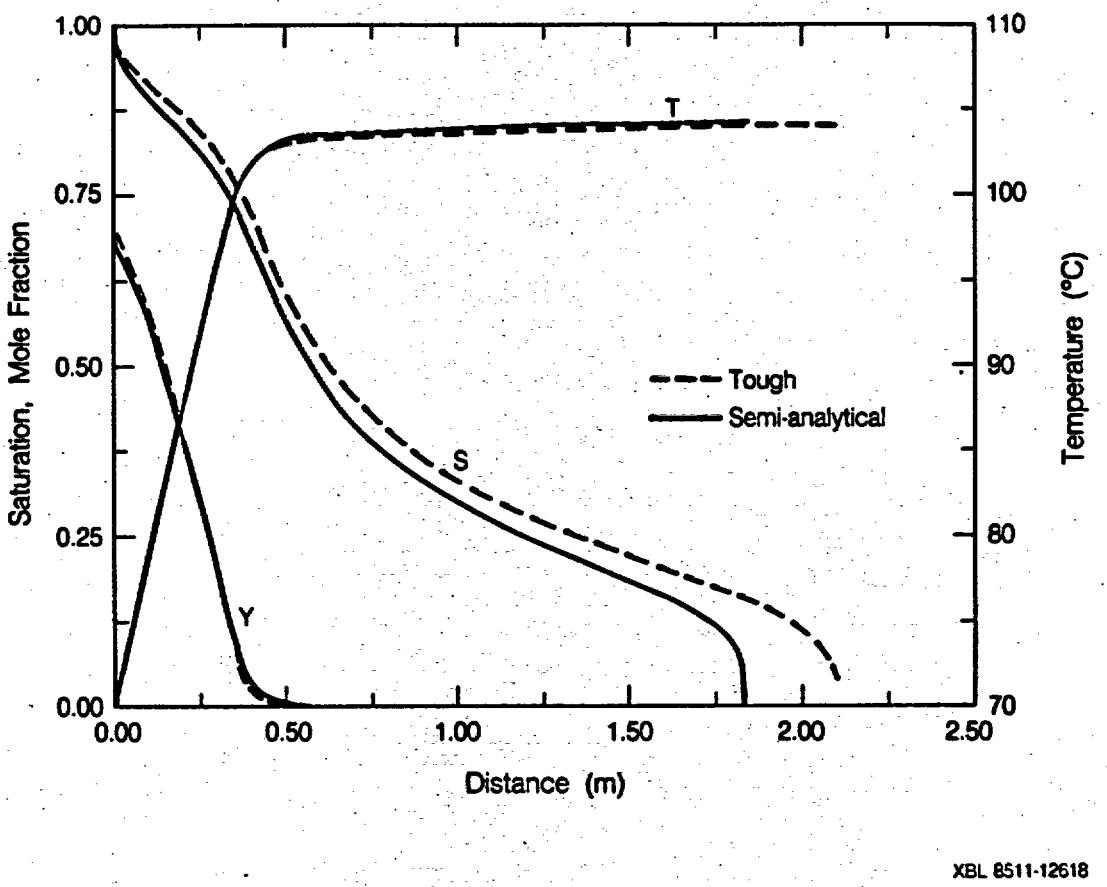


Figure 19. Simulated Steady State Conditions in Problem 6, Compared with Approximate Semi-Analytical Solution (T - temperature; S - scaled liquid saturation, $S = (S_l - S_{lr})/(1-S_{lr})$; Y - air mole fraction in gas phase).

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Appendix A: Relative Permeability Functions

IRP = 1 **linear functions**

k_{rl} increases linearly from 0 to 1 in the range
$RP(1) \leq S_l \leq RP(3)$;
k_{rg} increases linearly from 0 to 1 in the range
$RP(2) \leq S_g \leq RP(4)$
Restrictions: $RP(3) > RP(1)$; $RP(4) > RP(2)$.

IRP = 2

$$k_{rl} = S_l ** RP(1)$$
$$k_{rg} = 1.$$

IRP = 3 **Corey's curves**

$$S^* = (S_l - S_{lr})/(1 - S_{lr} - S_{sr})$$
$$k_{rl} = (S^*)^4$$
$$k_{rg} = (1-S^*)^2 (1 - [S^*]^2)$$

where $S_{lr} = RP(1)$; $S_{sr} = RP(2)$
Restriction: $RP(1) + RP(2) < 1$

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

$$S^* = (S_l - S_{lr})/(1 - S_{lr} - S_{sr})$$
$$k_{rl} = [S^*]^4$$
$$k_{rg} = 1 - k_{rl}$$

where $S_{lr} = RP(1)$; $S_{sr} = RP(2)$.
Restriction: $RP(1) + RP(2) < 1$

IRP = 5 **"All perfectly mobile"**

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

IRP = 6 **functions of Fatt and Klikoff (1959)**

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

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

where $S_{lr} = RP(1)$.
Restriction: $RP(1) < 1$.

IRP = 7 **Sandia - functions (Hayden et al., 1983; van Genuchten, 1980)**

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

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

where $\lambda = RP(1)$, $S_{lr} = RP(2)$, $S_{ls} = RP(3)$

IRP = 8 **function of Verma et al. (1985)**

$$S^* = (S_l - S_{lr})/(S_{ls} - S_{lr})$$
$$k_{rl} = (S^*)^3$$
$$k_{rg} = A + BS^* + C[S^*]^2$$

Parameters as measured by Verma et al. for steam-water flow in an unconsolidated sand:

$S_{lr} = RP(1) = .2$
$S_{ls} = RP(2) = .895$
$A = RP(3) = 1.259$
$B = RP(4) = -1.7615$
$C = RP(5) = .5089$

If the user wishes to employ other relative permeability relationships, these need to be programmed into subroutine RELP. The routine has the following structure:

```
      SUBROUTINE RELP (  )

      GOTO (10,11,12,---), IRP

   10 CONTINUE
      .
      .
      .
(IRP = 1)
      REPL = ...
      REPG = ...
      RETURN
   11 CONTINUE
      .
      .
      .
(IRP = 2)
      REPL = ...
      REPG = ...
      RETURN
      .
      .
      .
      END
```

To code an additional relative permeability function, the user needs to insert a code segment analogous to those shown above, beginning with a statement number which would also appear in the GOTO statement. The RP( ) parameters as read in input can be utilized as parameters in the assignment of liquid and gas relative permeability (REPL and REPG, respectively).

Appendix B: Capillary Pressure Functions

ICP = 1 **linear function**

$$P_{cap} = \begin{cases} -CP(1) \text{ for } S_l \leq CP(2) \\ 0 \text{ for } S_l \geq CP(3) \\ -CP(1) \cdot \dfrac{CP(3) - S_l}{CP(3) - CP(2)} \text{ for } CP(2) < S_l < CP(3) \end{cases}$$

Restriction: $CP(3) > CP(2)$.

ICP = 2 **function of Pickens et al. (1979)**

$$P_{cap} = -P_o \left\{ \ln \left[\frac{A}{B} \left(1 + \sqrt{1 - B^2/A^2}\right) \right] \right\}^{1/x}$$

with $A = (1 + S_l/S_{lo})(S_{lo} - S_{lr})/(S_{lo} + S_{lr})$

$B = 1 - S_l/S_{lo}$

where $P_o = CP(1)$, $S_{lr} = CP(2)$,

$S_{lo} = CP(3)$, $x = CP(4)$.

Restrictions: $0 < CP(2) < 1 \leq CP(3)$;

$CP(4) \neq 0$.

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

$$P_{cap} = \begin{cases} -P_e - P_o \left(\dfrac{1 - S_l}{S_l - S_{lr}} \right)^{1/\eta} \text{ for } S_l < 1 \\ 0 \text{ for } S_l = 1 \end{cases}$$

where $P_o = CP(1)$, $S_{lr} = CP(2)$, $\eta = CP(3)$, $P_e = CP(4)$.

Restrictions: $CP(2) \geq 0$;

$CP(3) \neq 0$.

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

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

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

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

Restriction: $CP(1) \geq 0$.

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

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

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

$$P_{cap} = -P_o \cdot \sigma\,(T) \cdot f$$

where $P_o = CP(1)$, $S_{lr} = CP(2)$,

σ = surface tension of water (supplied internally in TOUGH).

Restriction: $0 \leq CP(2) < 1$

ICP = 7 **Sandia function** (Hayden et al., 1983; van Genuchten, 1980)

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

$$P_{cap} = \begin{cases} 0 \text{ (if } S_l \geq S_{ls}) \\ -P_o \{[S^*]^{-1/\lambda} - 1\}^{1-\lambda} \\ -P_{max} \quad (\text{if } P_o \{[S^*]^{-1/\lambda} - 1\}^{1-\lambda} \geq P_{max}) \end{cases}$$

where $\lambda = CP(1)$, $S_{lr} = CP(2)$, $P_o = 1./CP(3)$,

$P_{max} = CP(4)$, $S_{ls} = CP(5)$

Additional capillary pressure functions can be programmed in subroutine PCAP in a fashion completely analagous to that for relative permeabilities (see Appendix A).

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This document contains a technical description of the TOUGH computer program, which was developed at Lawrence Berkeley Laboratory for simulating the coupled transport of water, vapor, air and heat in porous and fractured media. The physical processes taken into account in TOUGH are discussed, and the governing equations actually solved by the simulator are stated in full detail. A brief overview is given of the mathematical and numerical methods, and the code architecture. The report provides detailed instructions for preparing input decks. Code applications are illustrated by means of six sample problems.

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