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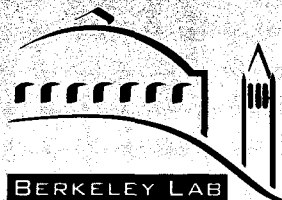et al.

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TOUGH2
SOFTWARE
QUALIFICATION

K. PRUESS
A. SIMMONS
Y.S. WU
G. MORIDIS

FEBRUARY 1996

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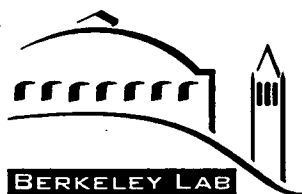
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1. INTRODUCTION

TOUGH2 is a numerical simulation code for multi-dimensional coupled fluid and heat flow of multiphase, multicomponent fluid mixtures in porous and fractured media. It belongs to the MULKOM ("MULti-KOMponent") family of codes (Pruess, 1983b, 1988) and is a more general version of the TOUGH simulator (Pruess, 1987). The MULKOM family of codes was originally developed with a focus on geothermal reservoir simulation. They are suited to modeling systems which contain different fluid mixtures, with applications to flow problems arising in the context of high-level nuclear waste isolation, oil and gas recovery and storage, and groundwater resource protection. TOUGH2 is essentially a subset of MULKOM, consisting of a selection of the better tested and documented MULKOM program modules.. The relationship of TOUGH and TOUGH2 to the MULKOM architecture is shown in Figure 1.
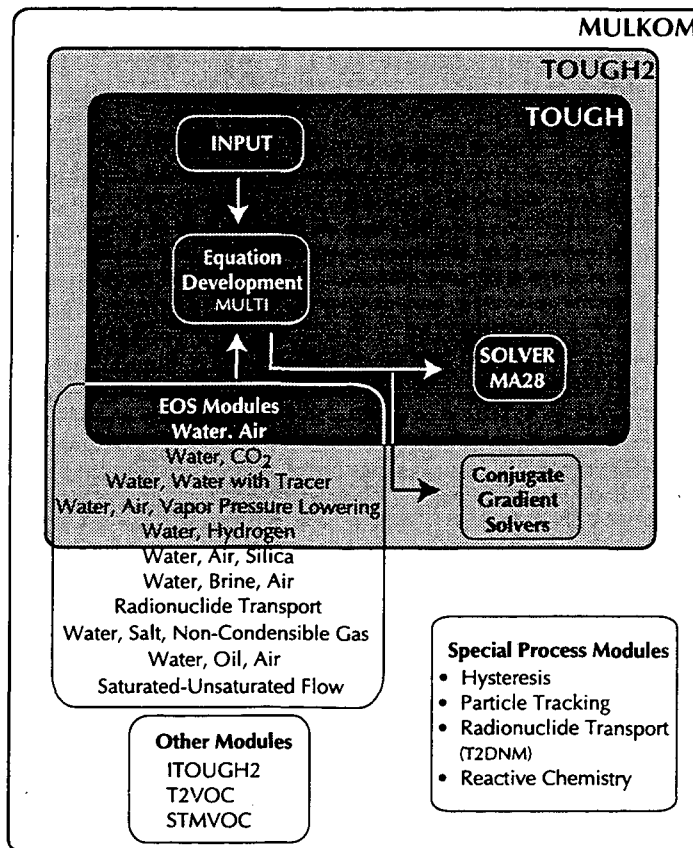
Figure 1. Relationship of TOUGH and TOUGH2 to the MULKOM architecture.

The purpose of this package of reports is to provide all software baseline documents necessary for the software qualification of TOUGH2. In accordance with Lawrence Berkeley National Laboratory (LBNL) Quality Implementing Procedure (QIP) SI.0, all components of the specified baseline documentation are provided. The software is not acquired, therefore no parts of the documentation are exempt from software verification and validation. This report contains the following sections: 1) Requirements Specification, 2) Design Description, 3) Software Validation Test Plan and Report, 4) Software User Documentation, and 5) Appendices. These sections comprise sequential parts of the

Software Life Cycle. They could have been written as a series of reports, but we chose to combine them into one report. The report components are not intended to stand alone but should be used in conjunction with the *TOUGH User's Guide* (Pruess, 1987) and with *TOUGH2 - A General Purpose Numerical Simulator for Multiphase Fluid and Heat Flow* (Pruess, 1991). The qualification package is complete with the attached Software Identification Form, executable source code, list of users, and bibliography of selected publications which utilized TOUGH or TOUGH2. No attempt was made to provide a conclusive bibliography; rather, the better known applications in geologic disposal of nuclear waste and geothermal reservoir processes are listed. Included in the package are several additional key publications that provide full details of the verification and validation test problems described herein and additional examples of TOUGH2 applications. They include the following: *Proceedings of the TOUGH Workshop* (Pruess, 1990); *TOUGH Simulations of Updegraff's Set of Fluid and Heat Flow Problems* (Moridis and Pruess, 1992); *Proceedings of the TOUGH Workshop '95* (Pruess, 1995); and *Flow and Transport Simulations Using T2CG1, a Package of Conjugate Gradient Solvers for the TOUGH2 Family of Codes* (Moridis and Pruess, 1995).

The version of TOUGH2 that is herein being qualified is the November 1994 Standard Version 1.11 housed at the Department of Energy's Energy Science and Technology Software Center (ESTSC) in Oak Ridge, Tennessee.

2. REQUIREMENTS SPECIFICATION

TOUGH2 is used for a multitude of applications, including oil and gas reservoir engineering, environmental problems involving contaminants, geothermal reservoir processes, and geologic disposal of nuclear waste. A list of requirements for representing conditions applicable to all of these settings would be long. Because Version 1.11 of TOUGH2 is being qualified for applications to the latter two modeling situations, a list of requirements was drawn up that is specific to representing the dominant fluid flow and heat transfer processes in geothermal reservoirs and in geologic disposal systems for nuclear waste. In order to simulate these processes, TOUGH2 must represent correctly the physical processes of multi-phase flow in saturated and unsaturated heterogeneous media. It therefore must provide an accurate description of constitutive physical laws and properties affecting each phase. It also must be capable of handling different geometries in one, two, and three dimensions. To handle the problems efficiently and smoothly, TOUGH2 must meet requirements for flexibility and timing. The multiple requirements for TOUGH2 with respect to geothermal and nuclear waste applications are listed below for ease of referral. The code underwent a long period of testing throughout development of the MULKOM code family and with a variety of settings and specifications, for the express purpose of determining whether the code accurately handles the processes of interest. Examples of some of the situations to which the code was applied are found in Appendix E, *Selected Bibliography*, and in application examples that follow. Furthermore, verification and validation tests have been performed that collectively address all of the listed requirements. These are described in Section 4, Software Validation Test Plan and Report.

2.1 Requirements

A. Flow processes driven by pressure, viscous, capillary, and gravity forces
   - single-phase fluid flow
   - single-phase gas flow
   - two-phase flow of liquid and gas
B. Constitutive relations
   - accurate description of thermophysical properties of water, vapor, and air
   - dissolution of air in water
   - vapor adsorption
   - vapor pressure lowering due to suction pressures
C. Phase change and interaction
   - appearance and disappearance of phases
   - interference between liquid and gas phases
   - enhancement of gas phase permeability from Knudsen (slip flow) effects
   - binary diffusion in gas phase
   - vapor-liquid phase change
D. Heat transport
   - heat conduction
   - heat convection
   - sensible and latent heat changes
   - conductive heat exchange with impermeable strata
   - coupled fluid and heat flow
E. Dimensionality
   - 1-D, 2-D, and 3-D flows

F. Geometry
        - Cartesian, cylindrical, irregular
G. Grid generation
H. Heterogeneities
        - heterogeneous formations
        - flow in porous and fractured media
I. Flexible specification of initial and boundary conditions, sources and sinks
J. Other
        - automatic time-stepping
        - restart capability
        - compatibility with TOUGH
        - user documentation
        - sample problems to illustrate code use and verify accuracy
        - internal version control
        - modularized structure for modifying or adding capabilities

2.2 Examples of Verification of Meeting Requirements

Hundreds of applications of the MULKOM family of codes over more than fifteen years have demonstrated that the codes, including TOUGH2, are applicable to complex problems in nuclear waste disposal, geothermal reservoir processes, environmental restoration, and that they obtain excellent results. Several successful simulations of field observations and laboratory experiments, as well as code verifications, were presented at the 1990 TOUGH Workshop (Pruess, 1990) and at the 1995 TOUGH Workshop (Pruess, 1995). Proceedings of both are included in this package. Many of the significant applications, particularly those in nuclear waste, are listed below in roughly chronological order.

An early comparative evaluation of geothermal reservoir simulation codes established important benchmarks for subsequent code developments (Stanford, 1980). MULKOM was extensively cross-checked against the SHAFT79 solutions developed for this DOE code comparison study. An analytical solution obtained by Lauwerier (1955) for non-isothermal flow in a homogeneous reservoir with conductive heat exchange to caprock and baserock was closely matched by a MULKOM simulation (Pruess and Bodvarsson, 1984).

Using the MINC (Multiple Interacting Continua) method, Pruess and Narasimhan (1985) demonstrated excellent agreement between MULKOM simulations and the Warren and Root (1963) double porosity solution for isothermal single-phase flow in a naturally fractured reservoir. Pruess et al. (1987) developed an analytical solution for the propagation of a boiling front during water injection into a depleted vapor zone in one-dimensional radial flow geometry. Numerical simulations with MULKOM closely matched the analytically predicted front location. Verma et al. (1985) numerically simulated a laboratory two-phase flow experiment for measuring steam-water relative permeability, obtaining good agreement with experimental data. Lam et al. (1988) successfully used MULKOM and the MINC method to model laboratory heat sweep experiments in a pressure vessel containing a configuration of regularly-shaped granite blocks.

McKibbin and Pruess (1989) presented analytical solutions for steady-state geothermal heat pipes with CO_2, which closely agreed with results of MULKOM simulations. Wu et al. (1990) developed a Buckley-Leverett type solution for immiscible displacement in composite porous media. Satisfactory agreement was obtained with

numerical simulations using MULKOM-GWF, a specialized version of MULKOM for three-phase flow of gas, water, and foam (Pruess and Wu, 1988). Doughty and Pruess (1990) investigated thermohydrologic conditions near heat-generating high-level nuclear waste packages. For the idealized problem of an infinite linear string of waste packages in a homogeneous porous medium with water as the single component, they obtained a semi-analytical similarity solution which was closely matched by numerical simulations with TOUGH.

Bodvarsson et al. (1990) reported three-dimensional well-by-well numerical simulations with MULKOM of the Olkaria, Kenya geothermal reservoir. Using actual flow rates and enthalpies from well data for the period from 1977 to 1983 to calibrate the reservoir model, they developed performance predictions that matched observed behavior of most wells from 1984 to 1987.

Falta and Pruess (1991) and Falta et al. (1992a, b) developed an enhanced version of TOUGH for three-phase component flow of water, air, and volatile organic compounds, known as STMVOC. They modeled steam injection experiments in one-dimensional laboratory cores performed by Hunt et al. (1988) and successfully predicted the migration of the steam condensation front, as well as profiles of temperature and pressure, and the removal of trichloroethylene from the column over time. Doughty and Pruess (1992) extended their earlier work on a similarity solution for fluid and heat flow near a linear heat source to a pore fluid consisting of water and air. The only simplifications made in their treatment involved flow geometry. The process complexities of highly non-linear, fully transient, two-phase, two-component fluid and heat flow with phase change were rigorously accounted for, making this the most difficult solvable two-phase fluid and heat flow problem presently available. Numerical simulations with TOUGH2 showed excellent agreement with the semi-analytical similarity solution.

Based on the observation that vapor pressures in vapor-dominated geothermal reservoirs under undisturbed conditions are close to saturated vapor pressure for measured temperatures (and thus contain water as both vapor and liquid phases), Pruess and O'Sullivan (1992) performed numerical simulations to investigate the nature and strength of fluid retention from capillary suction, vapor adsorption, and vapor pressure lowering. They ran the calculations with TOUGH2, which models vapor pressure lowering effects by means of the Kelvin equation.

2.2.1 Applications of TOUGH2 to Nuclear Waste Disposal

One motivation in developing the TOUGH2 code (Pruess, 1991) was from the need of performance assessment in the high-level nuclear waste disposal project. TOUGH2 has been used in many projects worldwide related to high-level nuclear waste projects from basic research to applications (Pruess, 1990 and 1995). The TOUGH/TOUGH2 code was used in the early research efforts in studies of unsaturated zone flow in Yucca Mountain (Rulon et al., 1986). In recent years, TOUGH2 has been used to develop the site-scale unsaturated zone model for moisture, gas and heat flow in Yucca Mountain (Wittwer et al., 1992, 1993, 1994, and 1995; and Bodvarsson et al., 1994). Furthermore, TOUGH2 has also been used to perform sensitivity studies of Yucca Mountain to understand effects of the ambient natural conditions on the mountain behavior (Wu et al., 1995; Ahlers et al., 1995a, 1995b). Associated with an inverse modeling tool (ITOUGH2, Finsterle, 1993), TOUGH2 has been used to analyze ventilation experiments at the Grimsel Rock Laboratory, Switzerland (Finsterle and Pruess, 1995) and to estimate the hydrogeological parameters, infiltration rate, water table, surface and lateral boundary conditions (Wu et al., 1995).

The general capability of TOUGH in handling fracture/matrix flow (Pruess, 1991) makes it useful in simulating groundwater infiltration and percolation within the welded unit at Yucca Mountain. It has been used for groundwater travel time calculations for the Yucca Mountain Site Characterization Project (Ho et al., 1994; and Arnold et al., 1995).

Niemi and Bodvarsson (1988) addressed the question of how hysteretic (history-dependent) capillary pressure-liquid saturation relations may affect flow and liquid saturation in a fractured rock system such as at Yucca Mountain. They used a hysteresis model to simulate a system consisting of discrete fractures and rock matrix under periodic infiltration pulses. They used material property values for densely welded tuffs at Yucca Mountain. Their model showed strongly hysteretic behavior in the uppermost layer of the matrix, which generated higher fracture flows and a more "smeared" matrix liquid saturation versus depth distribution for the hysteretic case.

TOUGH2 has also found wide applications in studies of thermohydrologic phenomena associated with thermal loading issues in high-level nuclear waste disposal (Witherspoon et al., 1996). TOUGH2 has been extensively used in thermal loading studies and performance assessment of high-level nuclear repositories (Pruess et al., 1990; Pruess and Tsang, 1993 and 1994; and Wu et al., 1995).

TOUGH2 has performed well on a series of fluid and heat flow problems that involved one, two, and three-dimensional flows, with varying degrees of non-linearity, coupling between fluid and heat flows, and complexity of boundary conditions. The verification process at this stage of the Software Life Cycle consisted of testing the MULKOM family of codes, including TOUGH2, over a period of years on the types of problems described above. These results, as well as verification and validation problems for the MULKOM/TOUGH codes, substantiate the accuracy of the process description employed in the code, and the mathematical and numerical approaches used. The latter two topics are discussed in the following section. Validation tests are discussed in Section 4.

3. DESIGN DESCRIPTION

This section describes the formal structure and architecture of TOUGH2. It details the functional requirements of the software and how they are implemented. It explains how TOUGH2 handles the physics of the processes modeled. It provides a description of numerical models and methods and the five fluid property (equation-of-state or EOS) modules. This section also describes the software structure, logic, and data structure and flow. It includes performance requirements and design constraints.

3.1 Background on MULKOM/TOUGH Family of Codes

TOUGH2's predecessor is the code MULKOM ("MULti-KOMponent"; Pruess, 1983b). MULKOM was built on the recognition that the governing equations for non-isothermal, multi-phase, multi-component flow are the same, regardless of the nature and number of fluid components present. MULKOM featured a modular architecture, in which a central module for flow and transport could be interfaced with several different fluid property modules to model systems with different fluid mixtures. The coding of MULKOM was never finalized but instead evolved into a collection of program modules for specialized applications. Nuclear waste-oriented applications spurred an effort to finalize and document a version of MULKOM for non-isothermal two-phase flows of water and air, which became TOUGH (Transport Of Unsaturated Groundwater and Heat) (Pruess, 1987). The methodological choices made in the development of MULKOM and their relationship to an earlier code, SHAFT79, were discussed by Pruess (1988).

TOUGH2 is a successor to TOUGH (Pruess, 1991). It is subroutine for subroutine very similar to TOUGH, but offers additional features such as internal mesh generation, an internal version control system, more convenient means of specifying boundary conditions, and an embedded fractured-media capability with the MINC method of "Multiple Interacting Continua". Unlike TOUGH, TOUGH2 provides the full multi-component, multi-phase flexibility previously available only in the undocumented MULKOM collection of modules. The name MULKOM is now used to refer to the particular modular architecture of the codes, while actual coding implementations are referred to as TOUGH and TOUGH2 (Moridis and Pruess, 1992).

The TOUGH2 family of codes includes: 1) TOUGH2 for two-phase multi-component fluid and heat flow with phase change; 2) T2DM, a TOUGH2 module for Fickian hydrodynamic dispersion (Oldenburg and Pruess, 1993); and 3) T2VOC (Falta et al., 1995) and M2NOTS (Adenekan, 1992; Adenekan et al., 1993) for three-phase multi-component fluid and heat flow (see Figure 1).

3.2 Structure and Architecture

TOUGH2 implements a flexible, general-purpose architecture (see Figure 2) for simulating fluid and heat flow in systems in which any number of components or species can be distributed among several coexisting phases. A key feature of the code architecture is an array structure that allows for flexible interfacing between the module that sets up and solves the fluid flow equations and the equation-of-state (EOS) modules, which represent fluid mixtures with different numbers of components and phases (see Table 1). Figure 3 provides a more detailed flow diagram of the code structure.
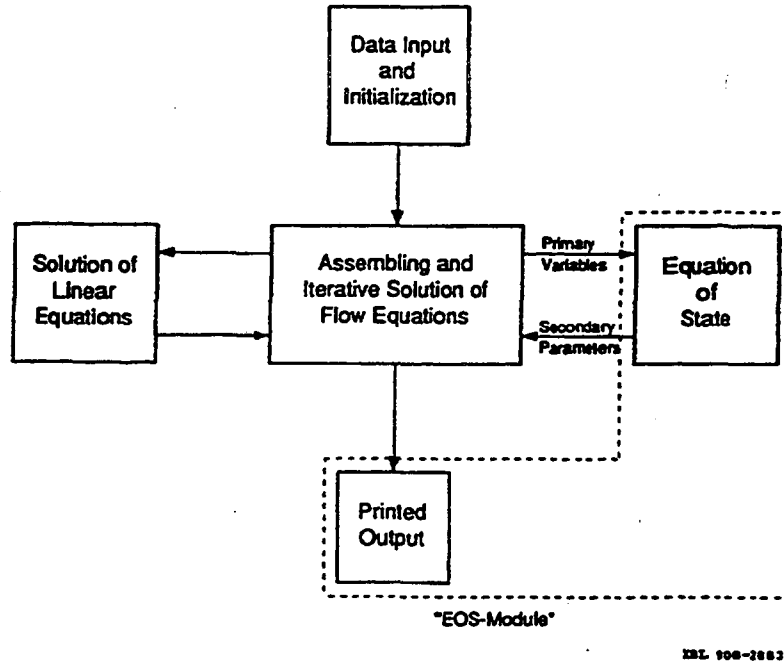
Figure 2. Modular architecture of MULKOM and TOUGH2.

Table 1. *TOUGH2 Fluid Property Modules*

MODULE	CAPABILITIES
EOS1	water, water with tracer*
EOS2	water, CO2
EOS3	water, air*[†]
EOS4	water, air, with vapor pressure lowering
EOS5	water, hydrogen*

*optional constant-temperature capability
[†]similar to the EOS-module of TOUGH

User features include flexible dimensioning of major arrays, capabilities for internal processing of flow geometry through automatic mesh generation (via MESHMAKER), and enhanced abilities for specifying initial and boundary conditions. TOUGH2 input formats are compatible with those of TOUGH, allowing TOUGH input files to be used with TOUGH2. However, some default parameter settings are different in TOUGH2, so that minor adjustments in TOUGH input files may be in order.

Much of what program units do is spelled out in internal comments and in printed output. TOUGH2 provides a tight version control system for meeting stringent demands on reliability and referenceability of code applications. Each program unit, when first called during a TOUGH2 simulation run, writes a one-line message specifying its name, version number and date, and purpose. All version messages are optionally printed to OUTPUT at the end of a simulation run. An example of an OUTPUT file for the end of a run is shown in Figure 4. This lists all of the program units used in the simulation, their version number and date, and what they do. Users who wish to modify the code can

therefore maintain an easily referenceable record of code changes and applications by updating version messages for each program unit they change for internal use. The coding complies with the ANSI X3.9-1978 (FORTRAN 77) standard.

Simplified Flow Chart of TOUGH2

TOUGH2
(main program)
-define parameters
-set up common blocks
-serve as main executive routine

IO
-open and assign disk files

INPUT
-read input data

MESHM:
RZ2D, WRZ2D,
PRZ2D
-mesh generation (optional)

RFILE
-initialize arrays for mesh, generation, and initial condition data

executive routine for time stepping

CYCIT

EOS
-initialize thermodynamic conditions

EOS satellite routines:
SAT, COWAT,
SUPST, VISW,
VISCO, COVIS,
VISS, RELP, PCAP

KON=2

Terminate?
NO
new time step

YES

STOP

ITER=0
KCYC=KCYC+1
KON=1
-set iteration and time step counter and convergence flag

KON?
KON=1
new iteration

ITER=ITER+1

(continued on next page)

Figure 3. Structure of TOUGH2.
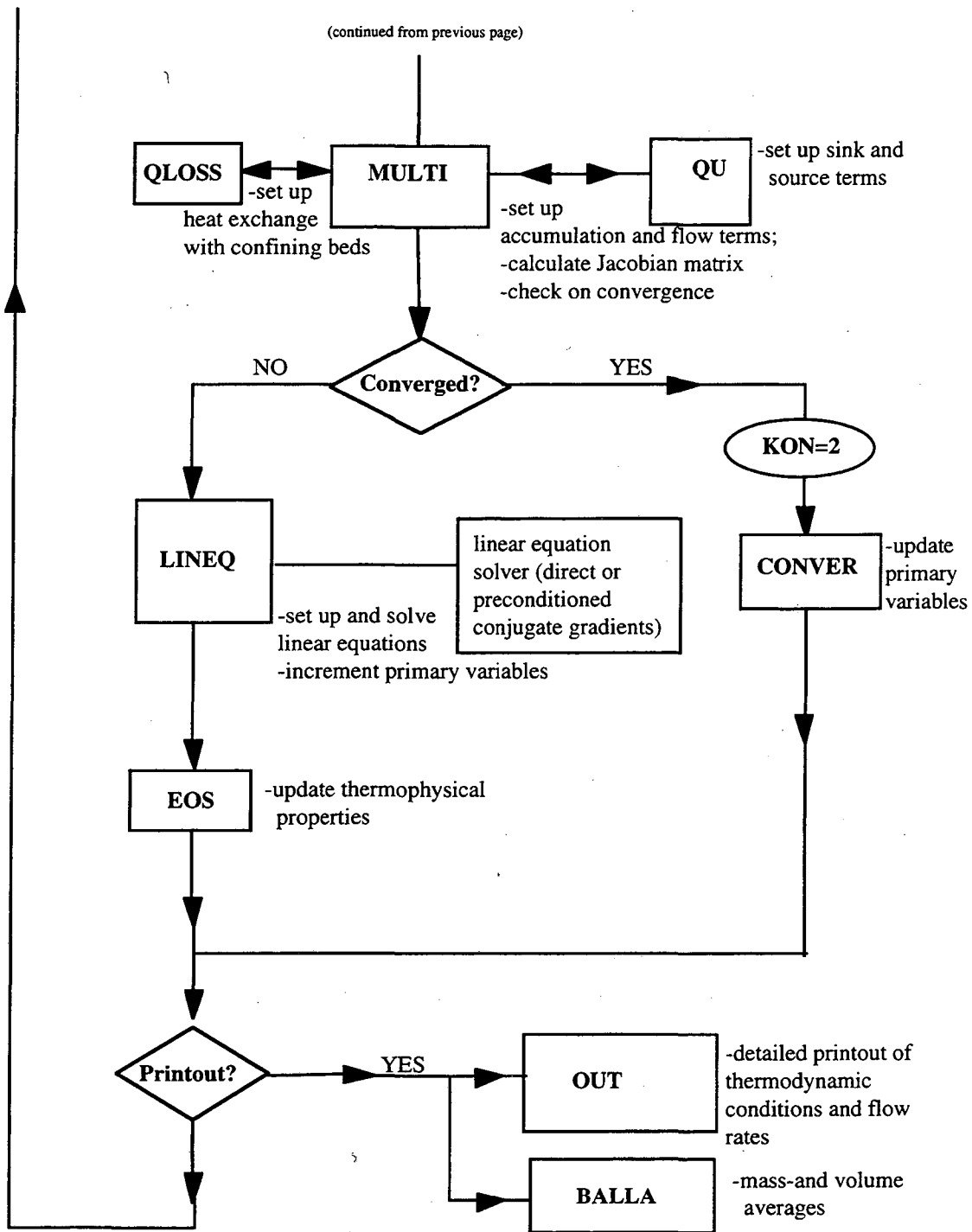
Figure 3 (cont.). Structure of TOUGH2.

```
!##############################################################################################
 #                                                                                            #
 #                              SUMMARY OF PROGRAM UNITS USED                                  #
 #                                                                                            #
 ##############################################################################################
```

UNIT	VERSION	DATE		COMMENTS
IO	1.0	15 APRIL	1991	OPEN FILES *VERS*, *MESH*, *INCON*, *GENER*, *SAVE*, *LINEQ*, AND *TABLE*
TOUGH2	1.0	29 MARCH	1991	MAIN PROGRAM
INPUT	1.0	11 APRIL	1991	READ ALL DATA PROVIDED THROUGH FILE *INPUT*
MESHM	1.0	24 MAY	1990	EXECUTIVE ROUTINE FOR INTERNAL MESH GENERATION
RZ2D	1.0	9 APRIL	1991	CALCULATE 2-D R-Z MESH FROM INPUT DATA
WRZ2D	1.0	26 MARCH	1991	WRITE DATA FOR 2-D R-Z MESH ON FILE *MESH*
PRZ2D	1.0	27 MARCH	1991	MAKE STRUCTURED PRINTOUT OF 2-D R-Z MESH
FLOP	1.0	11 APRIL	1991	CALCULATE NUMBER OF SIGNIFICANT DIGITS FOR FLOATING POINT ARITHMETIC
RFILE	1.0	23 APRIL	1991	INITIALIZE DATA FROM FILES *MESH* OR *MINC*, *GENER*, AND *INCON*
CYCIT	1.0	5 MARCH	1991	EXECUTIVE ROUTINE FOR MARCHING IN TIME
EOS	1.0	28 MARCH	1991	*EOS3* ... THERMOPHYSICAL PROPERTIES MODULE FOR WATER/AIR
SAT	1.0	22 JANUARY	1990	STEAM TABLE EQUATION: SATURATION PRESSURE AS FUNCTION OF TEMPERATURE
COWAT	1.0	22 JANUARY	1990	LIQUID WATER DENSITY AND INT. ENERGY AS FUNCTION OF TEMPERATURE AND PRESSURE
SUPST	1.0	29 JANUARY	1990	VAPOR DENSITY AND INTERNAL ENERGY AS FUNCTION OF TEMPERATURE AND PRESSURE
VISW	1.0	22 JANUARY	1990	VISCOSITY OF LIQUID WATER AS FUNCTION OF TEMPERATURE AND PRESSURE
VISCO	1.0	1 FEBRUARY	1990	CALCULATE VISCOSITY OF VAPOR-AIR MIXTURES
COVIS	1.0	1 FEBRUARY	1990	COEFFICIENT FOR GAS PHASE VISCOSITY CALCULATION
VISS	1.0	22 JANUARY	1990	VISCOSITY OF VAPOR AS FUNCTION OF TEMPERATURE AND PRESSURE
RELP	1.0	25 JANUARY	1990	LIQUID AND GAS PHASE RELATIVE PERMEABILITIES AS FUNCTIONS OF SATURATION
PCAP	1.0	4 MARCH	1991	CAPILLARY PRESSURE AS FUNCTION OF SATURATION
BALLA	1.0	5 MARCH	1991	PERFORM SUMMARY BALANCES FOR VOLUME, MASS, AND ENERGY
TSTEP	1.0	4 MARCH	1991	ADJUST TIME STEPS TO COINCIDE WITH USER-DEFINED TARGET TIMES
MULTI	1.0	30 MARCH	1991	ASSEMBLE ALL ACCUMULATION AND FLOW TERMS
QU	1.0	22 JANUARY	1990	ASSEMBLE ALL SOURCE AND SINK TERMS
LINEQ	1.0	22 JANUARY	1990	INTERFACE FOR THE LINEAR EQUATION SOLVER MA28
MC19A				HARWELL SUBROUTINE FOR SCALING MATRIX
CONVER	1.0	4 MARCH	1991	UPDATE PRIMARY VARIABLES AFTER CONVERGENCE IS ACHIEVED
PP	1.0	1 FEBRUARY	1990	CALCULATE VAPOR PRESSURE, DENSITY, INT. ENERGY AS F(P,T,X)
OUT	1.0	5 MARCH	1991	PRINT RESULTS FOR ELEMENTS, CONNECTIONS, AND SINKS/SOURCES
WRIFI	1.0	22 JANUARY	1990	AT THE COMPLETION OF A TOUGH2 RUN, WRITE PRIMARY VARIABLES ON FILE *SAVE*

Figure 4. Summary of program units and version history (from Pruess, 1991; Fig. 14)

3.3 Physical Processes and Approximations

Development of the TOUGH simulator was motivated by problems involving strongly heat-driven flow, for which conventional approaches to describing unsaturated flow are not applicable (Narasimhan, 1982). As temperatures approach or exceed the boiling point of water, vaporization takes 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 multiphase approach to fluid and heat flow, which fully accounts for the movement of gaseous and fluid phases, their transport of latent and sensible heat, and phase transitions between liquid and vapor. The gas phase in general will consist of a mixture of water vapor and air, and both components must be tracked separately.

The TOUGH2 simulator takes account of the following physical processes with the governing equations provided in Appendix A. 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. Mass- and energy-balance equations are written in integral form for an arbitrary flow domain. In addition, TOUGH2 considers binary diffusion in the gas phase. It accounts for a simplified description of Knudsen diffusion by means of a Klinkenberg factor for permeability (Knudsen, 1909; Klinkenberg, 1941; Hadley, 1982). Capillary pressure, vapor adsorption, and vapor pressure lowering effects are taken into account for the liquid phase.

The transport equations are complemented with constitutive relationships, which express all parameters as functions of a set of thermodynamic variables. 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. The viscosity of air/vapor mixtures is computed from a formulation given by Hirschfelder et al. (1954), using steam table values for vapor viscosity. Air solubility in liquid water is represented by Henry's law. However, because air solubility in water is very small, the temperature dependence of Henry's constant is neglected. The value implemented in TOUGH2, $K_H=10^{10}Pa$, is accurate to within $\pm$ 10% in the temperature range from 40^0C to 100^0C (Loomis, 1928). Data for air solubility in water at higher temperatures has not been published and is not well known.

Heat transport occurs by means of conduction, with thermal conductivity dependent on water saturation; convection; and binary diffusion, which includes both sensible and latent heat. The description of thermodynamic conditions is based on assumed local equilibrium of all phases. (MULKOM has also been used to model non-equilibrium conditions, such as chemical reactions).

The governing equations used in TOUGH2 and their numerical implementation, are applicable to one-, two-, or three-dimensional anisotropic porous or fractured media. TOUGH2 does not perform deformation analysis of the host medium and its effects on the multiphase flow behavior, but it allows for porosity changes in response to changes in pore pressure (compressibility) and temperature (expansivity).

3.4 Mathematical and Numerical Methods

Continuum equations for mass- and energy-balance are discretized in space using the "integral finite difference" method (Edwards, 1972; Narasimhan and Witherspoon, 1976). (See Appendix B for a full derivation of methodology). Introducing appropriate volume averages, we have

$$\int_{V_n} Mdv = V_n M_n$$

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. 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. Five different weighting schemes for mobility averaging options are available for selection by the user.

The five weighting schemes include: (1) upstream weighting of both mobility and permeability; (2) upstream weighting of permeability and averaging of mobility between adjacent elements; (3) upstream weighting of mobility and harmonic weighting of permeability; (4) arithmetic averaging of mobility and harmonic weighting of permeability; and (5) harmonic weighting of the product of mobility and permeability. For each volume element (grid block N) there are a number of primary variables, the choice of which depends upon the phase composition needed to define the thermodynamic state of the flow system and therefore on the choice of EOS module. A coupled set of algebraic equations is obtained (see Pruess, 1987). The total number of mass- and energy-balance equations is equal to the product of the number of primary variables times the number of grid blocks. The equations 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 such as relative permeabilitites and capillary pressures. Because of these features of the equation system, TOUGH2 performs a simultaneous solution of the discretized mass- and energy-balance equations, taking all coupling terms into account. Non-linearities are handled by performing the Newton/Raphson iteration. The unknowns are the independent primary variables, which completely define the thermodynamic state of the flow system at time level t^{k+1}. Clarification is provided in the discussion of EOS modules, to follow.

Upon application of the Newton/Raphson iteration (see Pruess, 1987), a set of coupled linear equations is obtained. These can be solved with the direct solver MA28 (Duff, 1977) or with a preconditioned conjugate gradient solver, as discussed below. Iteration is continued until the residuals are reduced to a small fraction of the accumulation terms. See Appendix B for convergence criteria. Convergence is usually obtained in three to four iterations. If convergence cannot be achieved within a certain number of iterations, the time step size Δt is reduced and a new iteration process is started. All derivatives needed in the coefficient matrix are obtained by numerical differentiation. The resulting Jacobian matrix is solved to yield the changes in the primary variables in each element of the discretized domain from the previous iteration.

The entire geometric information of the space discretization is provided in the form of a list of grid block volumes, interface areas, nodal distances, and components of gravitational acceleration along nodal lines. The discretized equations are 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 can be expressed in terms of average conditions in grid blocks (see Pruess, 1987). A necessary condition for this is 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, the equations reduce to a conventional finite difference formulation (Peaceman, 1977).

In the original TOUGH2, the Jacobian was solved using MA28 (Duff, 1977) a direct solver using sparse matrix storage techniques. However, storage and execution time requirements of MA28 limited the use of TOUGH2 to a maximum of a few thousand equations. To address this limitation, Moridis and Pruess (1995) added T2CG1, a package of preconditioned conjugate gradient solvers to complement TOUGH2's direct solver and significantly increase the size of tractable problems. The conjugate gradient solvers decrease execution time and memory requirements substantially, and make possible the simulation of three-dimensional flow problems with tens of thousands of grid blocks on workstations and PCs.

3.5 Array Structure and Handling

The number of primary thermodynamic variables that is needed to specify completely the thermodynamic state of a flow system consisting of a number of NK components which are distributed according to local thermodynamic equilibrium among a number of NPH phases is NK+1. This is equal to the total number of balance equations per grid block, namely NK mass balance and one energy balance equation. The thermodynamic state of a discretized flow system containing NEL (number of elements) volume elements or grid blocks is then completely specified by a set of NEL*NK1 primary thermodynamic variables, to which correspond an equal number of mass and energy balance equations. For transient flow systems, these primary variables are time-dependent, and they represent the unknowns to be calculated in each time step. In TOUGH2 all of the NEL*NK1 variables are stored sequentially in a one-dimensional array X: first the NK1 variables for grid block #1, then the NK1 variables for grid block #2, and so on (see Figure 5). The starting location for primary variables for grid block N is NLOC +1, where NLOC = (N-1)*NK1. More detail on handling primary thermodynamic variables is found on pages 9-11 in Pruess (1991).

The choice of primary variables that define the thermodynamic state of the system when phase change is involved in fluid and heat flow processes is an important consideration. When a phase appears or disappears, the set of appropriate thermodynamic variables may change. This problem can be dealt with in two ways. One way is to use a set of "persistent" variables such as pressure and enthalpy, or density and internal energy, which remain independent even as phase conditions change, so that they can be used throughout the single and two-phase regions. The other possibility is to use the variables pressure and temperature only for single-phase conditions and to switch to variables such as pressure and saturation when a transition to two-phase conditions occurs. Experience has proven this variable-switching approach to be a robust method for treating multiphase systems and it has been implemented in the MULKOM, TOUGH, and TOUGH2 codes.

There are two additional arrays DX and DELX with structure identical to X. While X holds the primary variables corresponding to the last successful (converged) time step, DX holds the latest increments calculated during the Newton-Raphson iteration process. Thus the latest updated primary variables are the quantities X+DX. The array DELX holds small increments of the X themselves (typically on the order $10^{-7}*X$) which are used to calculate incremented parameters needed for the numerical calculation of the derivatives in the Jacobian matrix $J = -\partial R_n/\partial X_i$ (see Figure 6; x_i denotes the collection of all primary independent thermodynamic variables). At the conclusion of a converged time step, the primary variables X are updated, $X \rightarrow X+DX$.
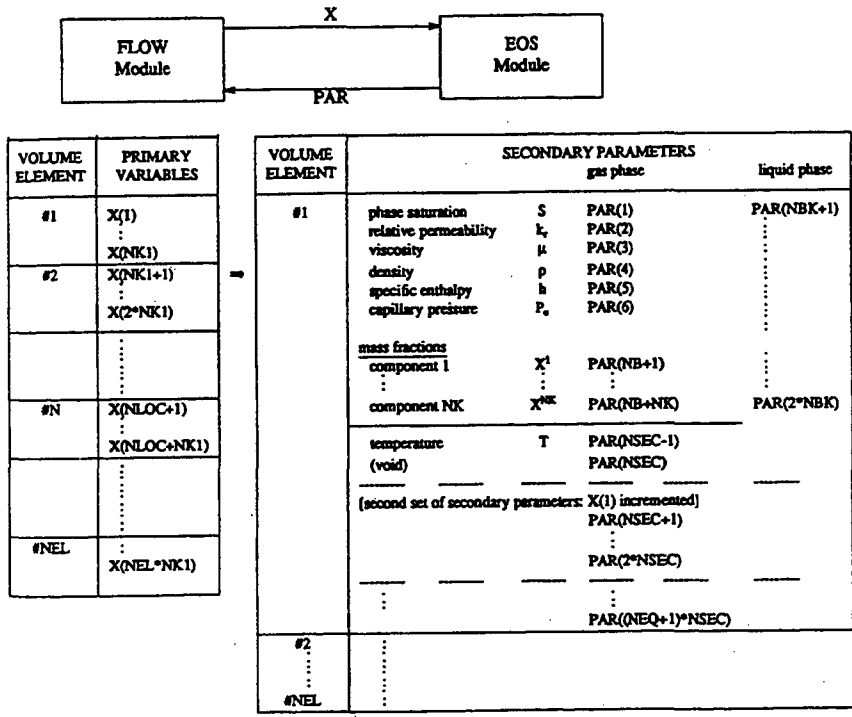
Figure 5. Structure of thermophysical property arrays in MULKOM and TOUGH2.

$$-\frac{\partial R_n^\kappa}{\partial x_i}\bigg|_p \qquad x_{i,p+1}-x_{i,p} \qquad = \qquad R_n^\kappa\bigg|_p$$

Figure 6. Linear equation structure.

As stated above, the number of mass- and energy-balance equations per grid block is the same as the number of NK1 primary thermodynamic variables. In many applications, however, the heat effects may be so small that temperature changes would be insignificant, and it would be sufficient to consider just the mass balance equations. The simplest way of forcing temperature changes to zero would be to assign the solid matrix an overwhelmingly large heat capacity, so that finite rates of heat exchange will cause negligible temperature change. This approach is possible with TOUGH2, but it has the disadvantage that the full number of balance equations must be solved, even though the energy balance reduces to the trivial statement $\partial T/\partial t = 0$. For certain EOS modules in which temperature is a primary variable, TOUGH2 offers a more elegant way of running problems without temperature changes which saves considerable computing time. In this method, TOUGH2 uses a parameter NEQ, distinct from NK, to number the balance equations per grid block, with the normal case being NEQ= NK+1. However, the user can choose to assign NEQ=NK in the INPUT file; then no energy equations are set up or solved, and the number of coupled equations per grid block is reduced from NK+1 to NK.

The EOS module calculates all thermophysical properties (secondary parameters) needed to assemble the mass- and energy-balance equations for the latest updated primary variables X+DX. These parameters are then stored sequentially in a large array "PAR" (see Figure 5). The number of secondary parameters other than component mass fractions is NB (usually NB=6); in addition there are NK mass fractions so that the total number of secondary parameters per fluid phase is NBK=NB+NK. The PAR array structure is shown in Figure 5 for the case of two fluid phases; however the coding permits any number of phases, as specified by the parameter NPH. The NPH*NBK phase-specific parameters are followed by temperature T and a void (unused) array member, so that the total number of secondary parameters is NSEC=NPH*NBK+2.

Note that the thermophysical properties are needed not only for calculating the residuals of the mass- and energy-balance equations, (Appendix B, Equation B.6) but also for calculating their derivatives in the Jacobian matrix (Eqs. B.7 and B.8) Thus, secondary parameters are required not only at the "state point" (latest X+DX), but also for the NEQ additional sets of primary variables in which one of the primary variables at a time is incremented by DELX. Therefore, the total number of secondary parameters per grid block is (NEQ+1)*NSEC. Secondary parameters for grid block #N start after location #NLOC2=(N-1)*(NEQ+1)*NSEC of the PAR array. More detail on thermophysical property array structure is found on pages 12-14 in Pruess (1991).

3.6 Linear Equation Setup

The data provided by the PAR-array are used in the flow module of TOUGH2 to assemble the linear equations (Eq. B.8) that are solved at each step of the Newton-Raphson iteration procedure. These equations are arranged and numbered sequentially, as shown in Figure 6, with the first NK equations per grid block representing component mass balances, while the last equation (#NK1) represents the energy balance. The row indices of the Jacobian matrix correspond to the sequence of primary variables in array X. If the option NEQ=NK is chosen, only NK mass balance equations will be set up per grid block. In this case only the first NK primary variables per grid block will contribute matrix columns, while variable #NK1, which must be temperature, remains passive and is not engaged or altered in the linear equation handling. However, all thermophysical parameters will be calculated at the temperature values specified in variable #NK1.

Note that the accumulation terms of the balance equations depend only on primary variables for one grid block, so that they will generate non-zero derivative terms only in an NEQ*NEQ submatrix that is located on the diagonal of the Jacobian J. The flow terms, being dependent on primary variables of two grid blocks, will generate two non-zero NEQ*NEQ submatrices of derivatives, which are located in the off-diagonal matrix locations corresponding to the two grid blocks.

In TOUGH2 all Jacobian matrix elements as well as the entries in the vector R of residuals are calculated in subroutine "MULTI". The calculation first assigns all matrix elements arising from the accumulation terms, of which there are NEQ*NEQ. These are stored sequentially in a one-dimensional array CO ("coefficients"); matrix elements for grid block N begin after location (N-1)*NEQ*NEQ in CO. The corresponding row and column indices are stored separately in arrays IRN and ICN, respectively. Calculation of the derivatives demands that each accumulation term is calculated NEQ+1 times; once for the state point (X+DX), and NEQ times for each of the NEQ primary variables incremented (X+DX+DELX). Additional contributions to diagonal terms in the Jacobian J may arise from sink and source terms, if present; these are assigned in subroutine QU called from MULTI. Subsequently all flux terms are evaluated. These depend in general on the 2*NEQ primary variables of the two connected grid blocks, so that a total of 2*NEQ+1 flux terms need to be evaluated for calculation of the state point as well as of all derivative terms.

After all matrix elements and members of the right-hand side vector of residuals have been preconditioned, the subroutine package MA28 (Duff, 1977) or the package of preconditioned conjugate gradient solvers (Moridis and Pruess, 1995) is called to solve the linear equations (Eq. B.8). The resulting increments in the primary variables are added to the array DX, and the process of linear equation setup and solution is repeated for the primary variables X+DX. This process continues until the residuals are reduced below a preset convergence tolerance. If convergence is not achieved within a specified maximum number of iterations (default 8), the time step is repeated with reduced time increment.

3.7 Dimensioning of Major Arrays

The major problem-size dependent arrays reside in COMMON blocks, which are dimensioned by means of a PARAMETER statement in the main TOUGH2 program. An informational statement on permissible problem size (number of grid blocks, etc.) is provided in the printed output of a TOUGH2 run. When problem specifications exceed array dimensions the execution stops with a diagnostic printout. The user must then increase PARAMETER assignments, recompile the main program, and relink. A list of major arrays used in TOUGH2 with their dimensions is given in Table 2.

Table 2. Summary of Major Common Blocks

REFERENCE TO	COMMON BLOCKS	LENGTH
Elements	E1-E6	NEL (=number of elements)
	VINWES, AHTRAN	
Primary variables	P1-P7	NEL*NK1[†]
Connections	C1-C11	NCON (=number of connections)
(interfaces)	COMPS, PORVEL	NCON*NPH
Linear equations	L1	$\geq$NZ=(NEL+2*NCON)*NEQ**2
	L2,L3	(2-4) *NZ
	L4	NEL*NEQ
	L5	NEL*5*NEQ
	L6	NEL*8*NEQ
	L7	NZ+5*NEQ*NEL+32
	L8	NEL*5*NEQ
	CGARA6	NZ+32*NEQ*NEL+1000
Secondary parameters	SECPAR	NEL*(NEQ+1) *NSEC

[†]NKI≡NK+1

3.8 Equation-of-State Modules

The thermophysical properties of fluid mixtures needed in assembling the governing mass- and energy-balance equations are provided by equation-of-state (EOS) modules. The MULKOM (and hence TOUGH2) formulation in the general sense accommodates any number of fluid components and phases that may be present, but the number of phases and components modeled is determined by the EOS module that is selected.

Besides providing values for all secondary (thermophysical) parameters as functions of the primary variables, the EOS module must fulfill three additional functions:

1) the phase conditions pertaining to a given set of primary variables must be recognized (element-for-element),
2) the appearance and disappearance of phases must be diagnosed as primary variables change during the Newton-Raphson iteration process, and
3) primary variables must be switched in response to a change of phase.

The primary variables/secondary parameters concept as implemented in MULKOM and TOUGH2 eliminates any direct connection between the choice of primary variables and the secondary parameters that are used to set up the flow equations. This provides maximum flexibility in the choice of primary variables because only secondary parameters are used in the flow equations. Only one exception to this separation exists; pressure of a reference phase is by convention always the first variable and it is used directly in the flow equations. The choice of all other primary variables is open. Note that only one EOS module at a time should be linked with other TOUGH2 modules.

3.8.1 EOS1 (Water, Water with Tracer): This is the most basic EOS module. It provides a description of pure water in its liquid, vapor, and two-phase states, and has a capability of representing two waters of identical physical properties which contain different trace elements. The default parameter settings for a single water component are (NK, NEQ, NPH, NB) = (1, 2, 2, 6). The option NEQ = 1 is available for running problems that involve only liquid water, or only superheated steam, under constant

pressure conditions. The primary variables are (P, T) for single-phase points, and (P_g, S_g) for two-phase points. For the convenience of the user, it is possible to initialize two-phase points as (T, S_g); a numerical value of the first primary variable less than 374.15 will automatically be taken to mean temperature (in °C) instead of gas pressure, and will cause variables to be internally converted from (T, S_g) to $(P_{sat}(T), S_g)$ prior to execution.

The two-waters capability can be invoked by specifying (NK, NEQ, NPH, NB) = (2, 3, 2, 6) in data block "MULTI" (see below). With this option, two water mass balances will be set up, allowing separate tracking of the two components. The primary variables in this case are (P, T, X) for single-phase points, and (P_g, S_g, X) for two-phase points, where X is the mass fraction of Water 2 present. All thermophysical properties (density, specific enthalpy, viscosity) are assumed independent of the component mixture; i.e., independent of the mass fraction X. This approximation is applicable for problems in which the identity of different waters is distinguished by the presence of different trace constituents, which occur in concentrations low enough to have no effect on the thermophysical properties.

All water properties (density, specific enthalpy, viscosity, saturated vapor pressure) are calculated from the steam table equations as given by the International Formulation Committee (1967). See Figure 7 and Table 3 for ranges. The formulation includes subregion 1 (subcooled water below T = 350°C, subregion 2 (superheated steam) and subregion 6 (saturation line up to T = 350°C). Within these regions, density and internal energy are represented within experimental accuracy. Viscosity of liquid water and steam are represented to within 2.5% by correlations given in the same reference. (Refer to the original publication for details).
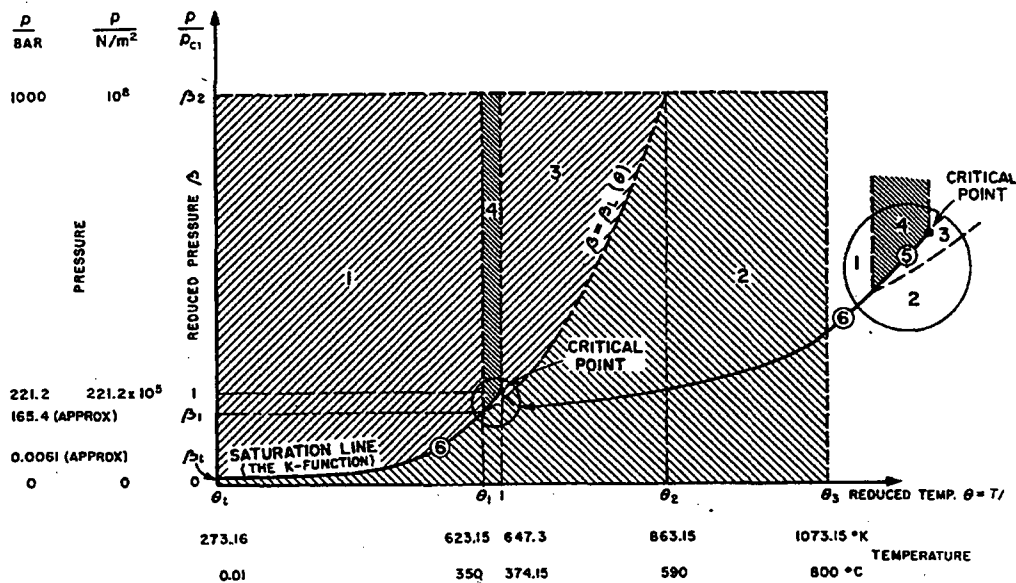
Figure 7. *Illustration of Subregions on the Pressure-Temperature Diagram (from International Formulation Committee, 1967).*

Table 3. Ranges of Thermophysical Parameters for Phase Regions in Figure 7.

Subregion	Temp (°C)	Sat. Vapor Pressure
1	0.01-350	0.0061-1000
2	350-374.15	165.4-221.2
3	0.01-374.15	0-165.4

The phase diagnostic procedures are as follows. When initializing a problem, each grid block has two primary variables (X1, X2). Whether X2 means gas saturation (two-phase) or temperature (single phase) is decided from the numerical value: for X2 > 1.5, X2 is taken to be temperature in °C, otherwise it is gas saturation. (Although physically saturation is restricted to the range $0 < S < 1$, it is necessary to allow saturations to exceed 1 during the Newton-Raphson iteration). If X2 is temperature, single phase conditions exist; specifically, for P (=X1) > $P_{sat}(T)$ there is single phase liquid; otherwise there is single phase steam. After initialization, the phase condition is identified simply based on the value for S_g, as stored in the array PAR. $S_g = 0$: single phase liquid; $S_g = 1$: single phase vapor; $0 < S_g < 1$: two-phase.

Phase change is recognized as follows. For single phase points the temperature (second primary variable) is monitored, and the corresponding saturation pressure is compared with P. For a vapor (liquid) point to remain vapor (liquid), it is required that P < $P_{sat}(P>P_{sat})$; if this condition is violated, a transition to two-phase conditions takes place. The primary variables are then switched to (P_g, S_g) and these are initialized as $P_g = P_{sat}(T)$, $S_g = 0.999999$ if the point was in the vapor region, and $S_g = 0.000001$ if it was in the liquid region. For two-phase points S_g is monitored; it is required that $0 < S_g < 1$ for a point to remain two-phase. If $S_g < 0$ this indicates disappearance of the gas phase; the primary variables are then switched to (P, T) and the point is initialized as single phase liquid, with T taken from the last Newton/Raphson iteration, and P = 1.000001 * $P_{sat}(T)$. For $S_g > 1$ the liquid phase disappears; again the primary variables are switched to (P, T) and the point is initialized as single phase vapor, with T taken from the last Newton/Raphson iteration, and P = 0.999999 * $P_{sat}(T)$. In these transitions temperature is preserved, rather than pressure, from the last iteration. A summary of EOS1 specifications and parameters is given in Table 4 below.

Table 4. Summary of EOS 1

COMPONENTS	#1: water
	#2: "water 2" (optional)

PARAMETER CHOICES	
(NK, NEQ, NPH, NB)=	(1,2,2,6) one water component, non-isothermal (default)
	(1,1,2,6) only liquid, or only vapor, isothermal
	(2,3,2,6) two waters, non-isothermal*

PRIMARY VARIABLES

single phase conditions
   (P, T, [X])-(pressure, temperature, [mass fraction of water 2]†)

two-phase conditions
   (P$_g$,S$_g$,[X])-(gas phase pressure, gas saturation, [mass fraction of water 2]†)

---

*two waters cannot be run in isothermal mode, because in this case temperature is not the last primary variable
†optional, for NK=2 only

   3.8.2 EOS2 (Water, CO$_2$): This fluid property module was developed by O'Sullivan et al. (1985) for describing fluids in gas-rich geothermal reservoirs, which often contain CO$_2$ mass fractions from a few percent to occasionally 80% or more (Atkinson et al., 1980). It accounts for non-ideal behavior of gaseous CO$_2$, and dissolution of CO$_2$ in the aqueous phase according to Henry's law with heat-of-solution effects. The thermophysical property correlations are based on the model of Sutton and McNabb (1977); a formulation from Pritchett et al. (1981) is used for the viscosity of vapor-CO$_2$ mixtures. Specifications and parameters of EOS2 are summarized in Table 5.

Table 5. Summary of EOS2

COMPONENTS	#1: water
	#2: CO$_2$

PARAMETER CHOICES	
(NK, NEQ, NPH, NB)=	(2,3,2,6) no other options are available

PRIMARY VARIABLES
single phase conditions
   (P, T, PCO$_2$)-(pressure, temperature, CO$_2$ partial pressure)
two-phase conditions
   (P$_g$,S$_g$,PCO$_2$)-(gas phase pressure, gas saturation, CO$_2$ partial pressure)

   3.8.3 EOS3 (Water, Air): This module is an adaptation of the EOS module of TOUGH for the TOUGH2 program, and implements the same thermophysical properties model (see Pruess, 1987). All water properties are represented by the steam table equations (International Formulation Committee, 1967). Air is approximated as an ideal gas, and additivity is assumed for air and vapor partial pressures in the gas phase, P$_g$ = P$_a$ + P$_v$. The viscosity of air-vapor mixtures is computed from a formulation given by Hirschfelder et al. (1954). The solubility of air in liquid water is represented by Henry's

law; i.e., dissolved air mole fraction $x_l^{(air)}$ is proportional to air partial pressure in the gas phase.

EOS3 differs from the EOS module of TOUGH in the choice of primary thermodynamic variables. In TOUGH the variables are (P, T, X) for single phase conditions and (P$_g$, S$_g$, T) for two-phase conditions. The choice made in EOS3 is (P, X, T) for single phase and (P$_g$, S$_g$ +10, T) for two-phase. The rationale for the choice of S$_g$ +10 as a primary variable is as follows. As an option, we wish to be able to run isothermal two-phase flow problems with the specification NEQ = NK, so that the then superfluous heat balance equation needs not be engaged. This requires that temperature (T) be the third primary variable. The logical choice of primary variables would then appear to be (P, X, T) for single phase and (P$_g$, S$_g$, T) for two-phase conditions. However, both X and S$_g$ vary over the range (0, 1) so that this would not allow a distinction of single phase from two-phase conditions solely from the range of primary variables. By taking the second primary variable for two-phase conditions to be X2 = S$_g$ +10, the range of that variable is shifted to (10, 11) and a distinction between single and two-phase conditions can be made. Primary variables can optionally be initialized identical to TOUGH specifications by setting MOP(19) = 1. A summary of EOS3 specifications is given in Table 6.

Table 6. Summary of EOS3

COMPONENTS	#1: water
	#2: air
PARAMETER CHOICES	
(NK, NEQ, NPH, NB)=	(2,3,2,6) water and air, nonisothermal (default)
	(2,2,2,6) water and air, isothermal
PRIMARY VARIABLES*	
single phase conditions	
(P, X, T)-(pressure, air mass fraction, temperature)	
two-phase conditions	
(P$_g$,S$_g$+10,T)-(gas phase pressure, gas saturation plus 10, temperature)	

*By setting MOP (19)=1, initialization can be made with TOUGH-style variables (P, T, X) for single phase, (P$_g$,S$_g$, T) for two-phase.

3.8.4 EOS4 (Water, Air, with Vapor Pressure Lowering Capability):

This EOS differs from EOS3 in that provision is made for vapor pressure lowering effects. Vapor pressure is expressed by Kelvin's equation (Eq. A.9); it is a function not only of temperature, but depends also on capillary pressure, which is a function of saturation. The primary variables are (P, T, P$_a$) for single-phase conditions and (P$_g$, S$_g$, P$_a$) for two-phase conditions. Temperature is not among the primary variables for two-phase conditions but is determined from the relationship P$_g$ - P$_a$ = P$_v$, with P$_v$ = P$_v$ (T, S$_l$) as given in (Eq. A.9).

Other sets of primary variables, in particular temperature, could be used in two-phase conditions. However, test calculations indicated that the choice (P$_g$, S$_g$, P$_a$) usually led to better convergence behavior than the choice (P$_g$, S$_g$, T). With the variables (P$_g$, S$_g$, T), the amount of air present in a grid block becomes controlled by the difference between total gas pressure, P$_g$, and effective vapor pressure, P$_v$ = P$_{sat}$(T) • f$_{VPL}$(T,S$_l$), which can be subject to severe numerical cancellation. From the applications viewpoint, however, initialization of the flow problem with the set (P$_g$, S$_g$, T) may be more convenient. EOS4 allows one to initialize two-phase points as (P$_g$, S$_g$, T); this capability can be selected by

specifying MOP(19) = 1 in the INPUT file. The default option for MOP(19) = 0 is (P_g, S_g, P_a). The choice MOP(19) = 2 allows EOS4 to be initialized with EOS3 variables of (P, X, T) for single phase, $(P_g, S_g + 10, T)$ for two-phase. In this way, continuation runs with EOS4 can be made from EOS3-generated conditions.

When using MOP(19) ≠ 0 options, data block or file INCON must terminate on a blank record (' '). If '+++' is encountered in INCON, it is assumed that primary variables are provided in agreement with internal usage; MOP(19) is then reset to zero and a message to this effect is printed.

The ability to handle vapor pressure lowering effects makes it possible for a liquid phase to be present under conditions where vapor partial pressure and gas phase total pressure are less than the saturation pressure. In EOS4 the pressure at which liquid phase density, enthalpy, and viscosity are evaluated is taken as $P_l = \max (P_g, P_{sat})$. A difficulty here is that temperature is not among the variables in two-phase conditions, so that P_{sat} is only implicitly known; moreover, vapor pressure lowering effects are functionally dependent on liquid phase density, which is also a function of temperature. This leads to a potentially unstable situation with regard to the choice of liquid phase pressure under conditions where $P_g = P_{sat}$, which is common in boiling regions. To avoid this problem liquid water density in the Kelvin equation is evaluated for vapor pressure lowering (Eq. A.9) at $P_l = P_{sat}$, which is a good approximation due to the small compressibility of water. In all accumulation and flow terms, the density of liquid water is evaluated at $P_l = \max (P_g, P_{sat})$. Vapor pressure lowering can be optionally suppressed by setting MOP(20) = 1. A summary of EOS4 specifications is given in Table 7.

Table 7. Summary of EOS4

COMPONENTS	#1: water
	#2: air
PARAMETER CHOICES	
(NK, NEQ, NPH, NB)=	(2,3,2,6) water and air, nonisothermal
	(no other choices available)
MOP (20)=1: optionally suppress vapor pressure lowering effects	
PRIMARY VARIABLES*[†]	

single phase conditions
    (P, T, P_a)-(pressure, temperature, air partial pressure)
two-phase conditions
    (P_g,S_g, P_a)-gas phase pressure, gas saturation, air partial pressure)

---

*By setting MOP (19)=1, initialization of two-phase conditions can be made with (P_g, S_g, T).
[†]By setting MOP (19)=2, initialization can be made with EOS3-style variables of (P, X, T) for single phase, (P_g, S_g + 10, T) for two-phase.

3.8.5 EOS5 (Water, Hydrogen): This property module was developed to study the behavior of groundwater systems in which hydrogen release is taking place. It is related to EOS3, the main difference being that the air component is replaced by hydrogen, with different thermophysical properties (see Table 8). The assignment and handling of primary thermodynamic variables in EOS5 is identical to EOS3 (see Table 6). The main differences in the assignment of secondary parameters are as follows. Density of hydrogen gas is computed from the ideal gas law. Viscosity and water solubility of hydrogen are

interpolated from the data given in Table 8. For temperatures in excess of 25°C, the solubility at 25°C is used. The parameter specifications of EOS5 are identical to those of EOS3 as given in Table 6, with "air" replaced by "hydrogen".

***Table 8.** Thermophysical Properties of Hydrogen*

Density at P=1 bar	Experimental*	Ideal Gas Law[†]
T=280K	.086546 kg/m³	.08660 kg/m³
T=300K	.080776 kg/m³	.08082 kg/m³
Viscosity*		
	T=0°C	T=100°C
P=1 bar	8.40x10⁻⁶Pa·s	10.33x10⁻⁶Pa·s
P=100 bar	8.57x10⁻⁶Pa·s	10.44x10⁻⁶Pa·s
Solubility in water at P=1 bar[§]		
T=0°C	1.92x10⁻⁶gH₂/gH₂O	
T=25°C	1.54x10⁻⁶gH₂/gH₂O	

*from Vargaftik (1975), p. 39.
[†]universal gas constant R=8314.56J/mol/°C; molecular weight of hydrogen 2.0160.
[§]after Dean (1985).
Solubility at different pressures is computed from Henry's law.

3.9   Specification of Flow Geometry

Handling of flow geometry in TOUGH2 is compatible with TOUGH input formats and data handling. As in other "integral finite difference" codes (Edwards, 1972; Narasimhan and Witherspoon, 1976), flow geometry is handled by means of a list of volume elements (grid blocks) and a list of flow connections between them. This formulation can handle regular and irregular flow geometries in one, two, and three dimensions. Single- and multiple-porosity systems (porous and fractured media) can be specified, and higher order methods, such as seven- and nine-point differencing, can be implemented by means of appropriate specification of geometric data (Pruess and Bodvarsson, 1983).

Volume elements in TOUGH2 are identified by five-character names, such as 'ELE10'. Flow connections are specified as ordered pairs of elements, such as "(ELE10,ELE11)". A variety of options and facilities is available for entering and processing the corresponding geometric data (see Figure 8). As in TOUGH, element volumes and domain identification can be provided by means of a data block "ELEME" in the INPUT file, while a data block "CONNE" can be used to supply connection data, including interface area, nodal distances from the interface, and orientation of the nodal line relative to the vertical. These data are internally written to a disk file MESH, which in turn initializes the geometry data arrays used during the flow simulation. The data formats on the file MESH are identical with the format specifications for data blocks ELEME and CONNE.
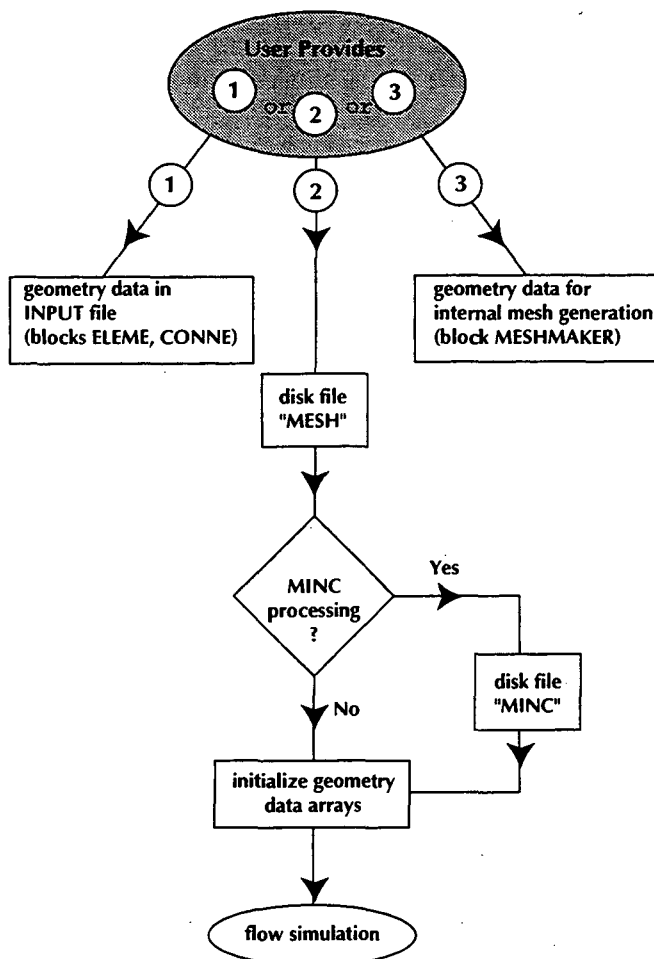
Figure 8. User options for supplying geometric data.

TOUGH2 offers additional avenues for defining flow system geometry. By means of the keyword 'MESHMAKER' in the INPUT file, a special program module can be invoked to perform a number of mesh generation and processing operations. The MESHMAKER module itself has a modular structure; present sub-modules include "RZ2D" for generating two-dimensional radially symmetric (R-Z) meshes, and "XYZ" for one-, two-, and three-dimensional Cartesian grids. Multiple-porosity processing for simulation of flow in naturally fractured reservoirs can be invoked by means of the keyword 'MINC', (Pruess and Narasimhan, 1982, 1985; Pruess, 1983a; see Appendix C). The MINC process operates on the data of the "primary" (porous medium) mesh as provided on disk file "MESH", and generates a "secondary" mesh containing fracture and matrix elements with identical data formats on file "MINC". (The file MESH used in this process can be either directly supplied by the user, or it can have been internally generated either from data in INPUT blocks ELEME and CONNE, or from RZ2D or XYZ mesh-making; see Figure 8). The internal mesh generation process will also write nodal point coordinates on file MESH for graphical display. These data are written in 3E10.4 format into columns 51-80 of each grid block entry in data block ELEME. At present, no internal use is made of nodal point coordinates in TOUGH2.

In TOUGH2 elements are referenced by names consisting of a string of five characters, '12345'. These are arbitrary, except that the last two characters (#4 and 5) must

be numbers. Specific naming conventions have been adopted in the internal mesh generation process. For RZ2D, the last two characters directly number the radial grid blocks, from 1 through 99. Character #3 is blank for the first 99 radial blocks, and then runs through the sequence 1, 2, ...9, A, B, ..., Z for a maximum of 3599 radial blocks. The second character counts up to 35 grid layers as 1, 2, ..., 9, A, B, ..., Z. The first character is 'A' for the first 35 layers, and is incremented to B, C, ..., A, 1, 2, ..., 9 for subsequent groups of 35 layers.

For rectilinear meshes generated by XYZ, characters 4 and 5 together number the grid blocks in X-direction, while character #3 = 1, 2, ..., 9, A, B, ..., Z numbers Y-direction grid blocks, and character #2, running through the same sequence as #3, numbers grid blocks in Z direction. Overflows with more than 99 X-blocks, or more than 35 Y- or Z-blocks advance character #1 through the sequence A, B, C, ..., Z. Both RZ2D and XYZ assign all grid blocks to domain #1 (first entry in block "ROCKS"); a user desiring changes in domain assignments must do so by hand, either through editing of the MESH file, or by appropriate source code changes in subroutines WRZ2D and GXYZ. TOUGH2 runs that involve RZ2D or XYZ mesh generation will produce a special printout, showing element names arranged in their actual geometric pattern.

The naming conventions for the MINC process are somewhat different from those originally adopted in the GMINC program (Pruess, 1983a) and are as follows. For a primary grid block with name '12345', the corresponding fracture subelement in the secondary mesh is named '2345' (character #1 replaced with a "blank"). The successive matrix continua are labeled by running character #1 through 2, ..., 9, A, B, ..., Z. The domain assignment is incremented by 1 for the fracture grid blocks, and by 2 for the matrix grid blocks. Thus, domain assignments in data block "ROCKS" should be provided in the following order: the first entry is the single (effective) porous medium (POMED), then follows the effective fracture continuum (FRACT), and then the rock matrix (MATRX). An example is given in Sample Problem 3 in Appendix G that follows.

Mesh generation and/or MINC processing can be performed as part of a simulation run. Alternatively, by closing the INPUT file with the keyword 'ENDFI' (instead of 'ENDCY'), it is possible to skip the flow simulation and only execute the MESHMAKER module to generate a MESH or MINC file. These files can then be used, with additional user-modifications by hand if desired, in a subsequent flow simulation. MESHMAKER input formats are described in the Software User Documentation Report under "Preparation of Input Data", and examples of practical applications are given in the sample problems in Appendix G. Execution of MESHMAKER produces printed output which is self-explanatory.

3.10 Initial Conditions and Restarting

As in the TOUGH code, initial thermodynamic conditions for the volume elements in the flow domain can be assigned to identical default values for all elements, or they can be prescribed for each element individually by means of a data block "INCON". A file "INCON" written to the same specifications as data block "INCON" should also be used for initialization.

A simulation problem can be run in several segments. At the end of a simulation run TOUGH2 writes the primary thermodynamic variables of all elements on a disk file "SAVE" with format specifications identical to "INCON". For a subsequent continuation run, file SAVE can be merged into the INPUT file as data block INCON or it can be

renamed as file INCON. In the latter case, no data block INCON should be present in the INPUT file, as this would cause the INCON file to be overwritten.

TOUGH2 also offers the facility of assigning initial conditions uniformly throughout selected zones of the simulation grid. This is invoked by means of a data block INDOM, which provides information on the thermodynamic conditions in user-defined domains. The format specifications for block INDOM are similar to those used in INCON. Thermodynamic conditions given in block INDOM take precedence over default assignments for the entire flow domain; specifications for individual grid blocks in INCON supersede all other assignments.

The normal way of defining initial conditions is by directly providing the primary thermodynamic variables. Note that these variables are generally different for different EOS modules. The thermodynamic state variables that are used internally in TOUGH2 as primary dependent variables may not always be the most convenient variables for a user to initialize a flow problem. The parameter MOP(19) offers a variety of choices, which permit initialization with variables different from the internally used primary variables. These choices are different for different EOS modules, and they are documented in the printout produced by each EOS.

At the end of a simulation run, file SAVE will always be written with the internal primary variables of the EOS module used. When modifying an INPUT file for a continuation run, MOP(19) might therefore have to be changed to its default value MOP(19)=0 for proper initialization. To minimize the possibility of user error, an automatic switch has been implemented in TOUGH2, as follows. The file SAVE as internally written by TOUGH2 terminates on a record with '+++' in the first three columns, followed by one record with restart information. When the data block INCON or file INCON terminates on '+++' rather than a blank line, it is assumed that this INCON was internally generated in a previous TOUGH2 run and that it is therefore written with the internally used set of primary variables. Accordingly, when '+++' is encountered in INCON the switch MOP(19) is reset to zero, and a message to that effect is printed.

3.11 Boundary Conditions

Boundary conditions are generally specified by means of appropriately chosen volume elements, flow connections, and sinks and sources. Boundary conditions can be of two basic types. Dirichlet conditions prescribe thermodynamic conditions, such as pressure or temperature on the boundary, while Neumann conditions prescribe fluxes of mass or heat crossing boundary surfaces. A special case of Neumann boundary conditions is "no flux", which in the integral finite difference framework is handled by not specifying any flow conditions across the boundary. More general flux conditions are 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 specified by introducing appropriate boundary elements and connections. A connection consists of an interface area, and a pair of adjacent nodes at some distance 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.

TOUGH2 implements Dirichlet conditions with the simple device of "active" and "inactive" elements. By convention, elements encountered in data block ELEME (or files MESH or MINC) are taken to be "active" until the first element entry with a zero or negative volume is encountered. The first element with volume less than or equal to zero, and all subsequent elements, are taken to be inactive. For the inactive elements no mass or energy balance equations are set up, and their primary thermodynamic variables are not included in the list of unknowns. Otherwise, inactive elements can appear in flow connections and initial condition specifications like all other elements. This feature can be used to specify Dirichlet boundary conditions by gathering all elements beyond the desired flow domain boundary at the end of the ELEME block and inserting a dummy volume element of zero volume in front of them. Thermodynamic conditions for the inactive elements are maintained as initially prescribed during a simulation run.

The specification of inactive elements can also be used in the MESHMAKER module to steer the MINC-process of subgridding volume elements. By convention, inactive elements will remain unpartitioned, i.e., they will be treated as a single porous medium. Users should beware that the MINC process may lead to ambiguous element names when the inactive element device is used to keep a portion of the primary mesh as unprocessed porous medium.

3.12 Software and Hardware Considerations (Efficiency, Portability, etc.)

TOUGH2 is portable to platforms that have an ANSI (FORTRAN 77) compiler. It can run on a PC, a Macintosh, a UNIX workstation (Sun, etc.), or a mainframe. It is easily maintained because of the flexibility of its modularization and through its internal version control, which allows the user to note version updates and to document personalized changes to the program. Numerous tests have shown that it produces consistent results on various platforms. TOUGH2's efficiency has been demonstrated clearly in Moridis and Pruess (1995). The authors chose sixteen test problems of variable complexity and size and compared the efficiency of the direct solver method using MA28 to methods using three different conjugate gradient solvers. For each solver they tabulated the grid size, number of equations, number of time steps, simulation time, number of Newtonian iterations, and CPU time. The conjugate gradient solvers were invariably faster, often by orders of magnitude, than the MA28 direct solver in all 16 problems. MA28 could not solve most of the large and medium size problems; it was limited in size to less than 2000 grid blocks for 2-D problems, and less than 400 for 3-D problems. Performance of the solvers was specific to the problem, compiler, and machine. The conjugate gradient solvers had well-defined memory requirements, which were lower than requirements for the MA28. These low memory requirements and the speed of the routine made possible the solution of 20,000 equation problems needed for these exercises on personal computers. TOUGH2, in fact, can handle problems with as many as 100,000 equations using the conjugate gradient solver approach. Theoretically, there is no upper bound to the number of equations it is capable of solving. Occasionally a specific solver failed for a particular problem, but in all test problems, one or more solvers produced a fast, efficient and accurate solution.

3.13 Performance Requirements and Design Constraints

Version 1.11 of TOUGH2 uses no pre- or post-processors and requires no interfaces with external hardware or software. TOUGH2 has no prescribed requirements for performance beyond its ability to model accurately the processes listed in the Requirements Specification, Section 2. Its flexible modularization and choice of solvers remove constraints on the size, dimensions, and complexity of design of a problem that can be handled by the code. Therefore, this section applies primarily to caveats in problem specification and choice of solver.

As with any code, proper set-up of the problem is necessary to obtaining reliable results. Key to successful application of TOUGH2 is a careful consideration of the physical processes that are involved in a given flow problem. In particular, space discretization, time-stepping, and interface-weighting procedures need to be selected carefully so that accurate results may be obtained. Without attention to these issues, application of TOUGH2 may result in both inefficient performance and inaccurate results.

In selecting the conjugate gradient solvers over the direct solver, the user trades the robustness and slow performance of a direct solver for the speed and reduced memory requirements of an iterative solver. However, because they are case-, problem-, and machine-specific, iterative solvers may be less reliable if they are not carefully applied. Because of the case-specificity of the solvers, the user must watch carefully both the convergence and the evolution of residuals over the time increments of the simulation. In cases of unsatisfactory convergence, the user should examine the conjugate gradient performance statistics in the file LINEQ generated by TOUGH2 runs, paying close attention to the parameters IERR and ERR (see Moridis and Pruess, 1995 for more details).

Because a wide variety of options is available in a complex code such as TOUGH2, the user must give careful consideration to peculiar features of a given problem when setting it up if a reasonably accurate and efficient solution is to be obtained. TOUGH2 is intended to be a "general-purpose" simulator. For example, there is no single weighting scheme for general transient two-phase flows in composite media that simultaneously preserves optimal accuracy for single-phase or steady two-phase flows. Another problem arises in the weighting scheme for interface densities. For certain flow problems spatial interpolation of densities may provide more accurate answers than a weighting scheme. Issues of interface weighting and associated discretization errors are especially important when non-uniform or irregular grids are used. Additional complications related to interface weighting arise in flow problems that involve hydrodynamic instabilities. Discussion of examples of the nuances and pitfalls of modeling multiphase flows is provided in Pruess (1991). In general, in the design and implementation of numerical schemes for multi-phase flows, a trade-off occurs between accuracy and efficiency on the one hand, and flexibility and robustness on the other. For a particular problem, small modifications in the source code may produce substantial gains in accuracy and efficiency.

When making changes in the code, it is essential to preserve a continuous dependence of all secondary parameters on the primary thermodynamic variables. True numerical discontinuities, such as a non-zero capillary air entry pressure, are inadmissible. They may lead to an unstable situation in which the residuals in the governing equations (Eq. B.6) become discontinuous functions of the primary variables, so that it may be impossible to reduce them to small values. A finite transition region for continuous variation of parameters must be provided.

3.14 Future Developments

As stated previously, the Version 1.11 of TOUGH2 that is being qualified here includes the better tested MULKOM program modules. LBNL has developed additional modules, however, and these are expected to become part of future releases of TOUGH2. They include EOS modules for multiphase fluid mixtures containing hydrocarbon and non-Newtonian fluids, capabilities for modeling rock-fluid interactions with dissolution and precipitation processes and associated porosity and permeability change, coupled radionuclide transport in porous fractured media, modules for production and injection well operations and scheduling, preprocessor programs for higher-order differencing schemes to minimize space discretization errors, and specialized routines for the study of multiphase flow processes in fractured media, including hysteresis effects.

3.15 Verification of Design Description

Verification that TOUGH2 meets the design description and structure depicted in Figure 3 was conducted during testing and debugging of the code. Sample runs were set up to test the ability of the EOS modules to handle primary variables in the manner described above. Once the runs were completed, sample problems were constructed to demonstrate the code. These are found in Appendix G.

4. SOFTWARE VALIDATION TEST PLAN AND REPORT

4.1 Validation Test Plan

The Validation Test Plan for TOUGH2 is quite straight-forward. It calls for implementing the code in the variety of applications specified by requirements, testing and debugging the code for errors, and subsequently verifying and validating the code. The terms "verification" and "validation" are used differently in quality assurance software terminology than in scientific research. In quality assurance terms, "software verification" means checking to ensure that a following stage (e.g. implementation) fulfills the requirements of a preceding stage (e.g. design), where the Software Life Cycle is built on a "waterfall approach" in which requirements are established, followed by code design, then code implementation, and finally validation. Validation means that the operational code satisfies all the requirements specified for it in the requirements stage (Mangold, 1993). The verification process has been described in the two preceding sections, in which the requirements are specified and the code design is explained. Verification testing and debugging took place as each module of the code was created. Some of the verification tests performed to ensure that the code is able to model the processes specified by the requirements are given as sample problems in Appendix G.

4.1.1 Acceptance Criteria: A number of additional verification problems were run to compare the results obtained by TOUGH2 against known analytical solutions to such formalized problems as the Theis solution, for example. The acceptance criterion for establishing that the TOUGH2 results showed sufficient agreement to the analytical solution was demonstration that the obtained results for TOUGH2 and the analytical solution differed by five percent or less (95% or better agreement). The five percent choice is somewhat arbitrary; depending upon the nature of the problem, it may be possible (and is always desirable) to achieve much closer agreement. The validation problems are summarized in Table 9. A short summary of each, along with a graphical comparison of TOUGH2 and the analytical solution, is found in the paragraphs following. For some applications, comparison could not be made to an analytical solution but could be made to experimental results in the laboratory or field. In the world of scientific conceptual models, this type of comparison is called "model validation". Comparisons of TOUGH2 solutions with experimental results are also included in Table 9 and described in the following section along with a graphical comparison. Acceptance criteria are difficult to quantify for comparisons against experimental or field data because the closeness of fit will depend partly on the goodness of original data, experimental artifacts, and heterogeneity in the natural system. Where possible, we try to obtain an agreement of 90% or better. The reader is referred to references listed in Column 6 of Table 9 for further details of the problem set up and specifications.

In the terminology of software engineering, "validation" tests are those that ensure that the software meets the requirements specified for it. The "verification" tests also fulfill the definition of "validation", because in order to obtain good results when compared to analytical solutions, the software must be able to model the processes of interest in the problem. However, additional validation problems were run for this qualification effort to cover specified requirements of TOUGH2 that are not part of the problem descriptions for tests listed in Table 9. A summary of the validation test problems and results is provided below. Full descriptions of these validation tests will be found in a future report.

Throughout the development of the MULKOM/TOUGH codes an effort was made to maintain continuity in numerical performance, i.e., different code variations were

exercised on several earlier benchmark problems to guard against errors in coding. Therefore, verification or validation exercises performed with any member of the MULKOM/TOUGH family are significant in establishing credibility for all other members as well.

Table 9. Summary of Validation Problems

#	PROBLEM TITLE	DIMENSIONS	FEATURES	ISSUES	REFERENCES
1	infiltration	1-D, linear horizontal	isothermal	code verification against known semi-analytical solution (Philip, 1955; Ross et al., 1982)	#2 in Pruess (1987); also #1 in Moridis and Pruess (1992)
2	flow to a geothermal well	1-D, radial	water and steam only, no air; sensible and latent heat effects; coupled fluid and heat flow	phase transitions; propagating boiling front; code verification against known semi-analytical and numerical solutions (Garg, 1978, 1980)	#4 in Pruess, (1987), also #4 in Moridis and Pruess (1992)
3	transient heat pipe	1-D, linear	coupled fluid and heat flow with air; liquid-gas counter-flow with very strong binary diffusion; sensible and latent heat effects	code verification against similarity solution (Doughty and Pruess, 1991, 1992)	Pruess (1991); Doughty and Pruess (1992)
4	coupled heat and mass transport	1-D, linear	non-isothermal convection, diffusion	code verification (Avdonin, 1964, Ross, 1982)	# 2 in Moridis and Pruess (1992)
5	heat transport	1-D, radial	single phase non-isothermal, convection, diffusion, sensible and latent heat effects	code verification (Avdonin, 1964, Ross, 1982)	#3 in Moridis and Pruess (1992)
					#2 in Moridis and Pruess (1995)
6	Theis problem (flow toward a well)	1-D, radial	single-phase, isothermal, viscous forces	validation against analytical solution (Theis, 1935)	#1 in Moridis and Pruess (1995)
7	Coupled fluid and heat flow in fracture	1-D, radial	heat conduction, MINC, fracture-matrix flow, single-phase, non-isothermal	verification	Pruess and Wu (1993)
8	infiltration	2-D, cartesian	isothermal, two-phase heterogeneous medium, seepage face mixed boundary condition, interference between liquid and gas, gravity effects	validation against experimental data (Vauclin et al., 1979)	#6 in Moridis and Pruess (1995)

Table 9 (cont). Summary of Validation Problems

#	PROBLEM TITLE	DIMENSIONS	FEATURES	ISSUES	REFERENCES
9	convection cell	2-D, cylindrical	single phase, non-isothermal, heterogeneous soil, no mass flow boundary, flow channeling, sensible and latent heat effects	validation against lab experiment (Reda, 1984)	#7 in Moridis and Pruess (1992) 3 in Moridis and Pruess (1995)
10	two-phase flow	2-D, cylindrical	simultaneous heat and mass flow, phase change, time-variant pressure boundary, interference between liquid and gas phase	validation against lab experiment (Kruger and Ramey, 1974; Faust and Mercer, 1979)	#8 in Moridis and Pruess, 1992
11	Warren-Root Solution	1-D, radial	transient flow, double-porosity medium	code verification against analytical solution (Warren and Root, 1963)	this paper
12	Lauwerier heat transfer solution	2-D, cartesian	conductive and convective heat transfer in porous media	code verification against analytical solution (Lauwerier, 1955)	this paper
13	handling of thermophysical properties	NA	water, water vapor, air	TOUGH2 calculated properties compared to steam tables (CRC, 1993)	this paper
14	vapor pressure lowering	NA	coupling between capillary and vapor adsorption effects, and vapor pressure	comparison with predictions from Kelvin's equation	this paper
15a	heterogeneous	1-D	single-phase slightly compressible liquid	code verification against analytical solution of Moridis (1995)	this paper
15b	flow to single well with anisotropic formation	2-D	single-phase, slightly compressible fluid, infinite anisotropic aquifer	code verification against analytical solution (Papadapoulos, 1965)	this paper
16	single-phase transient flow with irregular gird	2-D, cartesian	transient flow in horizontal, isotropic, isothermal aquifer	verification of irregular grid capability using Theis solution	this paper

Table 9 (cont). Summary of Validation Problems

#	PROBLEM TITLE	DIMENSIONS	FEATURES	ISSUES	REFERENCES
17a	heat conduction	1-D, linear	semi-infinite rock column, step change in T; ignores flow effects	code verification against analytical solution of Carslaw and Jaeger (1959)	this paper
17b	binary vapor diffusion	1-D	vapor and air diffusion in gas phase, semi-infinite rock column; ignores vapor adsorption	code verification against analytical solution of Carlsaw and Jaeger (1959)	this paper
17c	gas flow with Klinkenberg effects	1-D	steady single-phase gas flow across linear rock column, isothermal	code verification of gas permeability enhancement at low pressures (Klinkenberg, 1941)	this paper
18	horizontal well with compressible liquid	3-D	anisotropic reservoir	code verification against analytical solution of Goode and Thambynayagam (1987)	this paper
19	single-phase gas flow	1-D, radial	flow to single vertical well at center of bounded cylindrical formation	code verification against analytical solution of Kabir and Hasen (1986)	this paper
20	water absorption into porous matrix	1-D, radial	fracture-matrix interaction in two-phase flow	code verification against semi-analytical solution	Zimmerman et al, (1990)

4.2 Validation Tests (Keyed to Table 9)

1. Infiltration - 1-D, Linear (Pruess, 1987; Moridis and Pruess, 1992)
This is a one-dimensional problem that considers 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 infiltration boundary in the problem is represented by means of a very large element (LB0), with a nodal distance set to a small non-zero value, to avoid relative permeability at the boundary to be taken from the downstream element designated as F1. The solution obtained by Philip (1955) treats the gas phase as a passive spectator at constant pressure. This approximation is enforced by surrounding the soil tube with a ring of very large volume, which is assigned a pressure of P = 1 bar. Different interface weighting procedures were used, labeled 0, M1, and M2 in Figure 9. The simulated
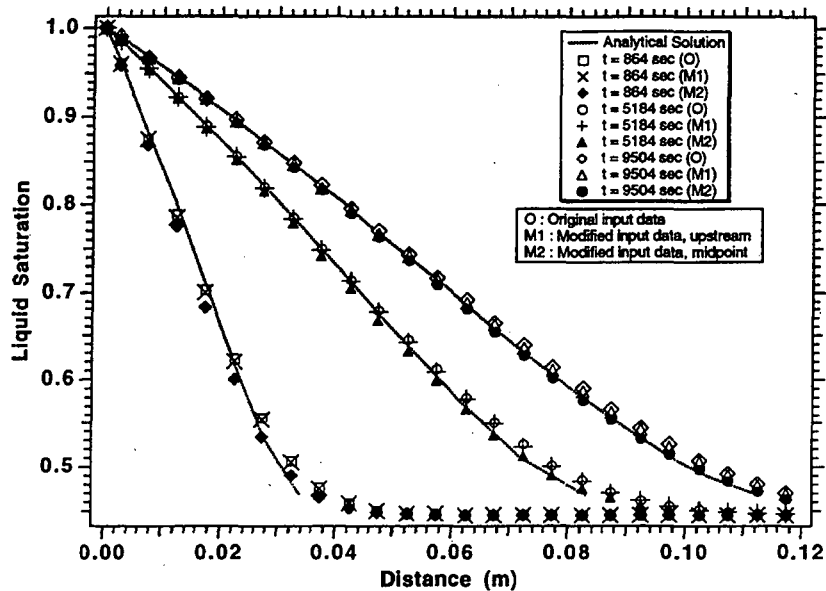
Figure 9. Liquid saturation profiles for verification problem 1 (from Moridis and Pruess, 1995).

results are seen to agree well with the semi-analytical solution given by Ross et al. (1982) and meet the acceptance criterion of 95% or better agreement.

2. Flow to a Geothermal Well (Pruess, 1987; Moridis and Pruess, 1992)
This problem deals with radial 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. The computational mesh consists of 10 grid blocks with $\Delta R = 1$ 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 wellblock (element AA1) are plotted versus time in Figure 10. Comparison of TOUGH with Garg's results is excellent and meets the acceptance criterion of 95% or better agreement.
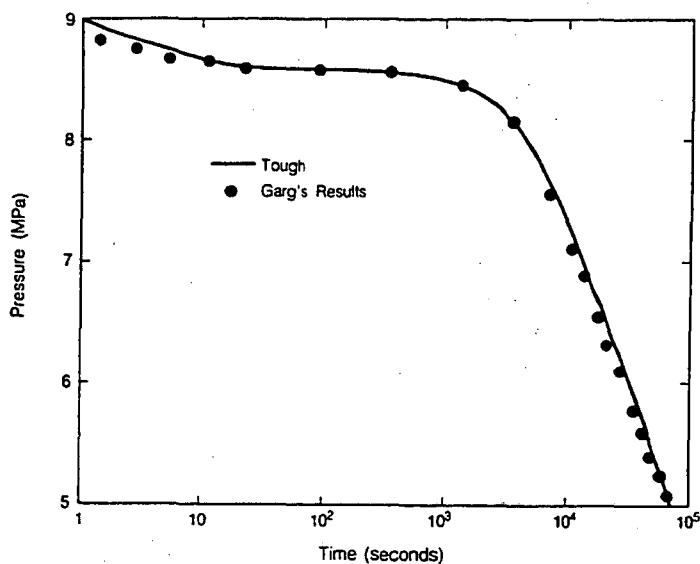
Figure 10. Wellblock pressures for verification problem 2 (from Pruess, 1987).

3. Heat Pipe (Pruess, 1991; Doughty and Pruess, 1992)

Validation Problem 3 simulates a heat pipe with cylindrical geometry. It considers a case in which a heat pipe (a heat transfer system which operates via a liquid-vapor counterflow process) is artificially induced by nuclear heat-generating waste packages in a partially saturated medium. The TOUGH2 input file uses the EOS3 fluid properties module. The problem places a constant strength, linear heat source in an infinite homogeneous medium with uniform initial conditions. The MESHMAKER module is used to generate a one-dimensional radial grid extending to a large radius, which for practical purposes can be considered infinite. Boundary conditions are constant. Most of the formation parameters are identical to data used in previous modeling studies at Yucca Mountain (Pruess et al., 1990). Because fracture effects are not included in the simulation, heat pipe effects would be very weak at the low rock matrix permeabilities (on the order of one microdarcy) encountered at Yucca Mountain. To obtain a more pronounced heat pipe effect, absolute permeability was arbitrarily increased to 20 millidarcy and capillary pressures were reduced by a factor of 100 compared to that at Yucca Mountain. To examine space discretization effects, runs were made with a coarse, medium, and fine mesh using MESHMAKER. As shown in Figure 11, excellent agreement is obtained by comparing the fine mesh results with those of an exact similarity solution (Doughty and Pruess, 1991, 1992). Under constant initial conditions the governing partial differential equations in radial distance r and time t reduce to ordinary differential equations through the introduction of a similarity variable $\eta = r/t^{1/2}$. The resulting equations are coupled and nonlinear, necessitating a numerical integration (Doughty and Pruess, 1991, 1992).

The input file for problem 3 can also be executed with the EOS4 fluid property module, which includes vapor pressure lowering effects. This can serve as a benchmarking reference for the EOS4 module. The results are quite similar to those obtained with EOS3 when the problem is set up with a constant rate of heat generation, except that because of very strong vapor pressure lowering effects, dryout near the heater is slowed. Comparison of this problem with the similarity solution affords the most comprehensive code verification available, because all of the non-linearities of two-phase
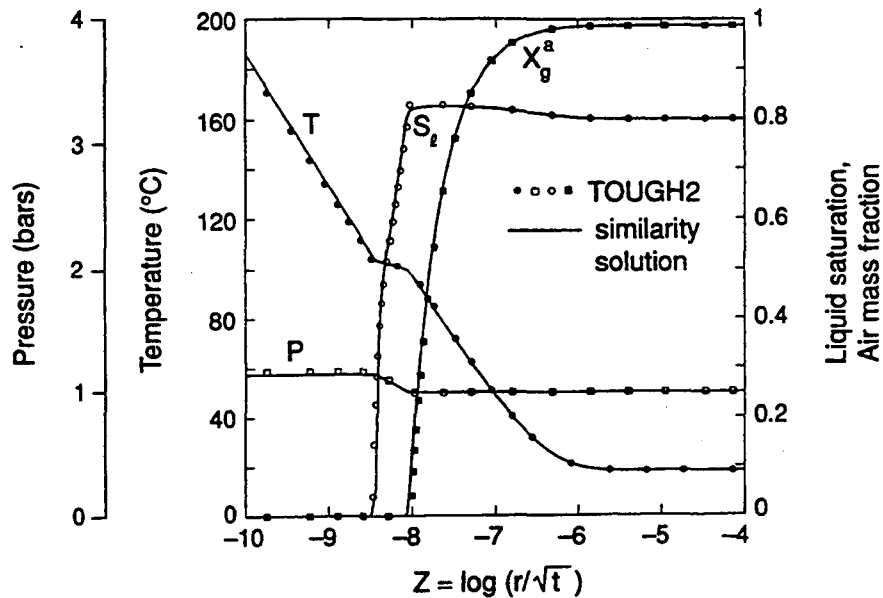
Figure 11. *Comparison of TOUGH2 with similarity solution for problem 3 (from Pruess, 1991).*

flow behavior and of fluid and heat flow coupling are rigorously described by the similarity solution.

4. <u>Coupled Heat and Mass Transport - Avdonin Problem</u> (Moridis and Pruess, 1992)
The analytical solution to this problem of one-dimensional heat and mass transport was developed by Avdonin (1964). Ross et al. (1982) described the problem and presented a solution. Cold water is injected into a semi-infinite, high-temperature aquifer at a specified constant mass flow rate. The overburden and underburden are impermeable to mass and heat flow, acting as no-flow and adiabatic boundaries and reducing the equation governing heat transport to that of convection-diffusion. Updegraff (1989) modeled this problem in his comparison study of three simulation codes that model strongly coupled mass and heat flow in unsaturated porous media (TOUGH, NORIA, and PETROS). Moridis and Pruess (1992) discuss their simulation of Updegraff's set of fluid and heat flow problems and the difference between their results using TOUGH and those of Updegraff.

The space discretization used by Updegraff (1989) consisted of 500 equally spaced gridblocks and two boundary gridblocks. The space and time discretization were based on criteria established by Reeves et al. (1986). A very large volume was assigned to the boundary grid blocks, thus ensuring constant boundary pressures and temperatures during the simulation. An initial pressure distribution varying from the left-hand to the right-hand boundary was distributed across the grid blocks. The prescribed pressure differential on the boundaries created an influx which resulted in an equivalent system. For this flux to equal the desired injection rate, Updegraff specified an appropriate permeability.

It turned out that Updegraff used erroneous water property values. The differences between his values and those in the steam tables had a significant impact on the solution. Therefore, Moridis and Pruess (1992) computed the analytical solution using values from the steam tables. They also corrected Updegraff's error in relative permeability. Moridis and Pruess (1992) created three modified data sets. The first used an upstream weighting

of mobilities, permeabilities, and thermal properties. The second data set used a midpoint weighting scheme. The second and third data sets differed in boundary conditions and in the treatment of sources and sinks. The use of direct injection into the first grid block in these two data sets reduced the size of the input data file by 90%. Strictly speaking, constant rate injection into a flow system initially at uniform pressure will result in a transient change of flow rates away from the injection point, rather than giving steady-state mass flow throughout. However, because of the large permeability and the small compressibility of liquid water, the pressure diffusivity at these conditions is very large, so that the region with practically steady flow expands rapidly and runs well ahead of the thermal front.

The corrected analytical and the TOUGH solutions obtained with the modified input files are shown in Figure 12. The runs required 1300 time steps to reach the maximum simulation time of t_{max} = 130,000 sec because of the time-step constraint of $\Delta t \leq$ 100 sec. Moridis and Pruess (1992) concluded that with upstream weighting TOUGH properly predicts the midpoint of the front, but there is a certain amount of numerical dispersion which results in a broadening of the front. On the other hand, it is a more robust numerical weighting scheme, being more stable in difficult situations with long time steps. The midpoint weighting scheme is more accurate and in excellent agreement with the analytical solution. This test meets the acceptance criteria of 95% or better agreement.
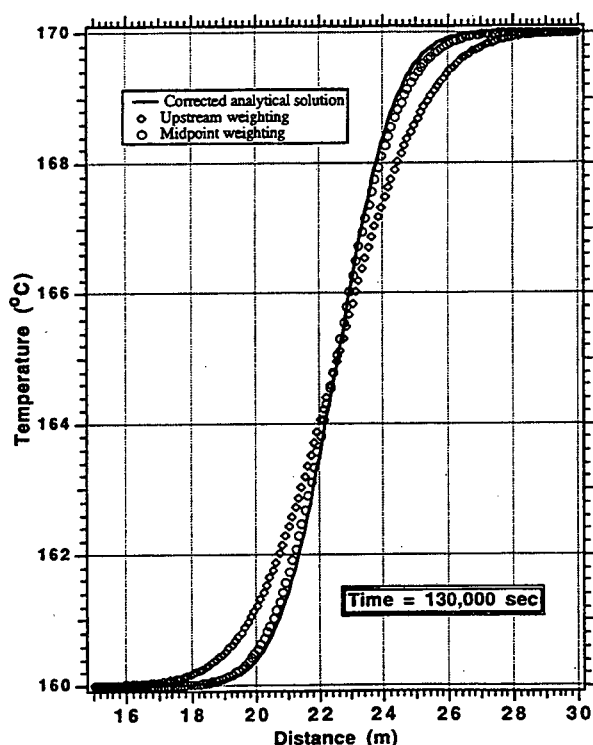
Figure 12. Comparison of the analytical solution to the TOUGH solutions in validation problem 4 (from Moridis and Pruess, 1992).

5. Radial Heat Transport (Moridis and Pruess, 1992; Moridis and Pruess, 1995)
The radial heat transport in this problem was originally solved analytically by Avdonin (1964) and was later described by Ross et al. (1982). Cold water is injected into a semi-

infinite, high-temperature aquifer. This problem is very similar to the one-dimensional heat transport problem described in validation problem 4, except that it uses radial rather than Cartesian coordinates. The overburden and underburden are impermeable to mass and heat flow, acting as no-flow and adiabatic boundaries and reducing the equation governing heat transport to that of convection-diffusion.

The radius of the aquifer is sufficient to approximate semi-infinite behavior (1000 m), at which a constant temperature (equal to the initial temperature of 170^0C) is imposed. TOUGH2 predictions of the temperature distribution in Figure 13 at $t = t_{max} = 10^9 \, sec$ after initiation of the cold water injection are shown for comparison to the analytical solution.

This simulation was performed using the EOS1 fluid property module with NK = 1 and NEQ = 2. The number of gridblocks used was 127, resulting in a total of N = 254 equations. The grid was generated with the MESHMAKER submodule. A very large volume ($10^{38} \, m^3$) was assigned to the single boundary grid block in the radial direction (127th), thus ensuring constant boundary pressures and temperatures during the duration of the simulation. With flow rate directly specified through a mass source, the problem becomes insensitive to the precise value of permeability.

Figure 13 shows excellent agreement between the analytical and the TOUGH2 solutions at $t = 10^9 \, sec$. This is well within the acceptance criterion of 95% or better agreement. This problem has a "similarity solution" in terms of the variable r^2/t (O'Sullivan, 1981; Doughty and Pruess, 1990, 1992). The TOUGH2 results are consistent with the r^2/t invariance that exists in the problem so that at $t = 10^9 \, sec$. the TOUGH2 solution virtually coincides with the analytical solution.
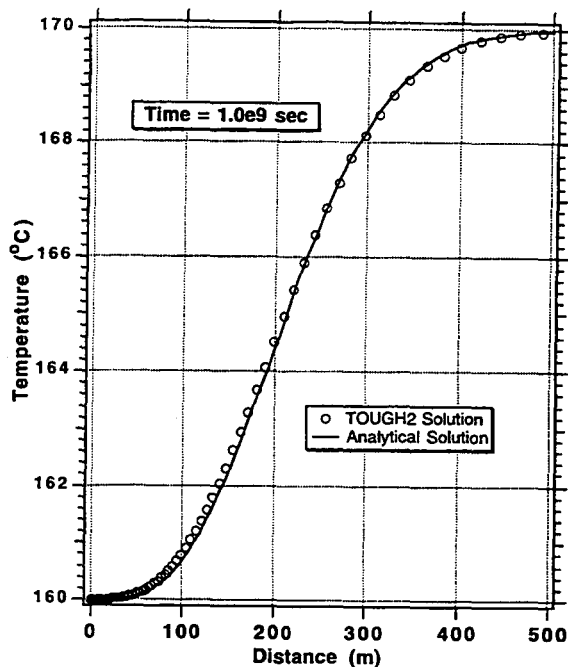
Figure 13. Comparison of the analytical and TOUGH2 solutions to the radial heat transport problem in validation problem 5 (from Moridis and Pruess, 1992).

6. Theis solution (Moridis and Pruess, 1995)

This problem represents the classical Theis (1935) problem of one-dimensional radial flow toward a well of radius $r_w \to 0$ in a homogeneous circular aquifer with infinite-acting boundaries. Input parameter values are given in Moridis and Pruess (1995). The EOS1 fluid property module with NK = 1 and NEQ = 1 was used for the TOUGH2 simulation. The outer boundary extends to 10^6 m, which is sufficient for the aquifer to act as infinite. A total of N = 104 equations are solved, as the domain is subdivided into 104 grid blocks. Figure 14 shows the analytical solution and the TOUGH2 solution obtained for an aquifer temperature of 20^0C. The two solutions are virtually identical. Therefore, the acceptance criterion for validation is met. Note that in this and similar problems of single-phase flow in confined aquifers (where the compressibility is small and the only variable changing is pressure) the convergence criterion for the relative error in the Newtonian iterations must be set to a sufficiently small number. More specifically, the parameter RE1 in Record PARAM.3 of the PARAM data block must be reset from its default value of 10^{-5} to a number several orders of magnitude smaller. The maximum RE1 value should not be larger than 10^{-8}.
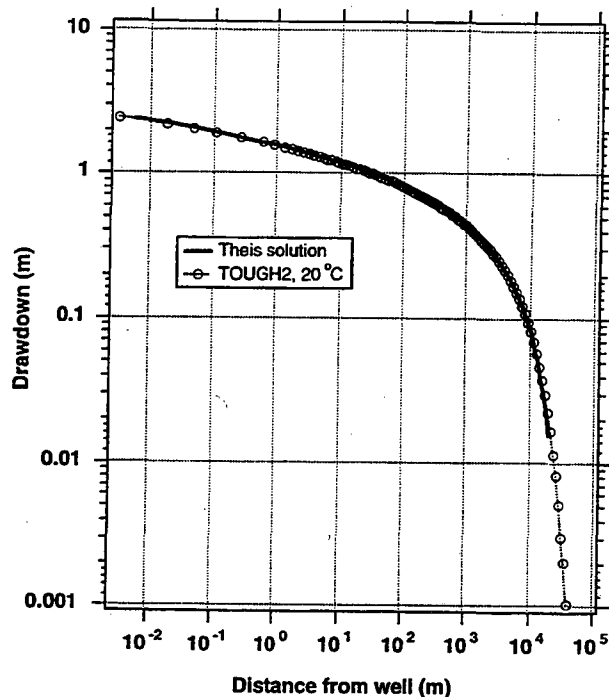
Figure 14. Comparison of the analytical and the TOUGH2 solutions to the THEIS problem at $t = t_{max} = 10$ *days (from Moridis and Pruess, 1995).*

7. Coupled fluid and heat flow in fracture (Pruess and Wu, 1993)

Pruess and Wu (1993) developed a new method for modeling fluid and heat flow in fractured reservoirs which is an extension of a technique developed by Vinsome and Westerveld (1980) for calculating heat exchange between permeable layers and impermeable semi-infinite confining beds during thermally enhanced oil recovery. Pruess and Wu's method combined a finite-difference description of global flow in the fractures with an analytical representation of interporosity flow by means of trial functions for fluid pressures and temperatures in the matrix blocks. The trial functions contain adjustable

parameters which are calculated for each time step in a fully coupled way based on matrix block shapes and dimensions. They incorporated the method into MULKOM and verified it by comparison with exact analytical solutions for fluid and heat exchange with individual matrix blocks. Applications were made to geothermal well test and production-injection problems with interporosity fluid and heat flow. A shown in Figure 15, the MULKOM simulation using multiple-interacting-continua (MINC) and numerical solution show excellent agreement.
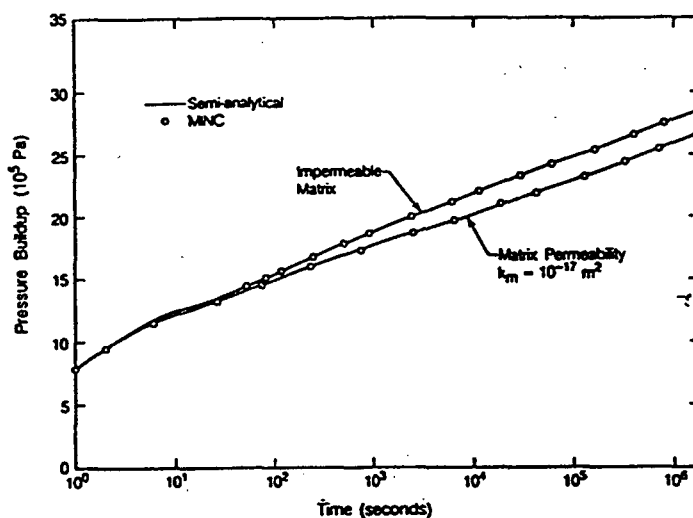
Figure 15. *Comparison of MULKOM to semi-analytical solution for pressure buildups for non-isothermal injection into a fractured reservoir for validation problem 7 (from Pruess and Wu, 1993).*

Test problems 8 through 10 are verification problems for the purposes of software engineering, but are validation problems in the sense of scientific model validation. Instead of comparisons to analytical solutions, the TOUGH2 simulated results are compared to results obtained from field or laboratory experiments to ascertain the "validity" of the conceptualization of the model presented in the TOUGH2 problem.

8. Infiltration - Vauclin Problem (Moridis and Pruess, 1992; 1995)

Test problem 8 describes a two-dimensional infiltration laboratory experiment conducted by Vauclin et al. (1979), who provided measurement data and a numerical solution (therefore this is both a verification and a "validation" problem). Water infiltrates at a rate of 4.111×10^{-5} m/sec over a length of 0.5 m of a vertical slab of soil. Due to symmetry only half of the problem needs to be modeled. The bottom boundary and the left boundary (line of symmetry) are considered impermeable to flow. Below z = 0.65 m the right boundary is a constant pressure boundary with a water saturation of 1 at the bottom; above z = 0.65 m it is a seepage surface, i.e. a mixed type of boundary condition which sets the water flux equal to zero when the medium is unsaturated and has a head equal to the hydraulic head when the medium is saturated.

For this simulation the domain was subdivided into 378 grid blocks. The MESHMAKER facility in TOUGH2 was used to generate the grid. A very large volume (10^{29} m^3) was assigned to the right-hand boundary grid blocks, thus ensuring constant boundary pressures, saturations, and temperatures throughout the simulation. The

simulation was performed with the EOS3 fluid property module, using NK = NEQ = 2 (isothermal conditions) in block MULTI to solve just two equations per grid block. This results in a total of N = 756 equations. A more complete discussion of the data input is provided by Moridis and Pruess (1992).

An upstream weighting scheme for mobilities (MOP (11) = 2) was used in this simulation. A no-flow top boundary was used because previous simulations had indicated that the mass transfer through this block was insignificant. Water was injected directly into four specific grid blocks by specifying appropriate sources.

Initial pressures and saturations were hand-calculated and assigned using the hydrostatic pressure distribution below the water table and the capillary pressure vs. water content relationship in Vauclin et al. (1979). Coding the capillary pressure function into TOUGH2 is a small effort; the FORTRAN code for the Vauclin et al. (1979) capillary pressure function is provided in Moridis and Pruess (1995).

Figure 16 shows the TOUGH2 predictions and the experimental observations at the desired locations and times. The agreement between experimental data and numerical simulation results is good, but measurable local deviations are observed. Therefore, not all areas of the curve meet an acceptance of 90% or better agreement to experimental data. The reason for the deviations is due to the heterogeneity of the soil slab; this is discussed extensively in Moridis and Pruess (1992).
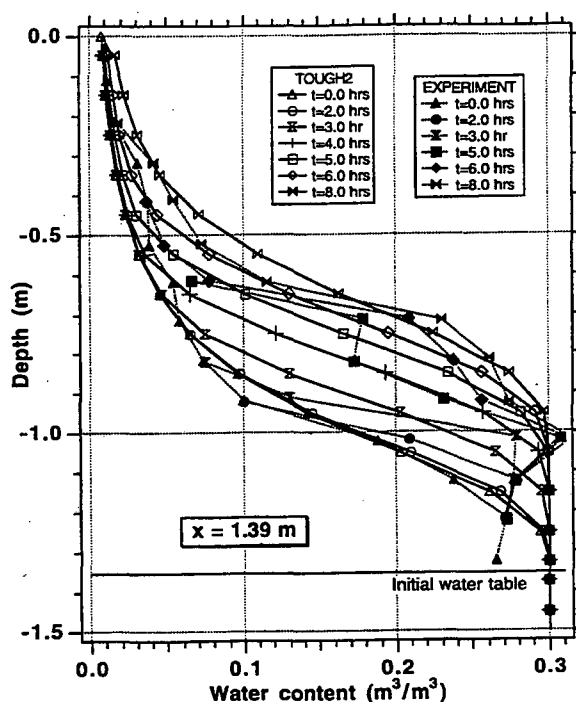

Figure 16. TOUGH2 predictions and experimental infiltration measurements at x = 1.39 m in test 8 (from Moridis and Pruess, 1995).

## 9. Convection Cell (Moridis and Pruess, 1992; 1995)

This problem involves a laboratory convection cell experiment described, performed, and modeled by Reda (1984). A porous medium consisting of glass beads with an average diameter of 0.65 mm fills the annular region between two vertical concentric cylinders. Application of heat generates a thermal buoyancy force, giving rise to the development of convection cells. This problem was used to test the ability of TOUGH2 to simulate transient two-dimensional simultaneous heat and mass flow, and was discussed in detail by Moridis and Pruess (1992).

To evaluate TOUGH2, numerical predictions were compared to measurements of the thermal response of the surface of the inner cyliner at the elevations z = 0.4192, 0.6288, 0.7336, and 0.7860 m (i.e. $z/\Delta r$ = 2, 3, 3.5, and 3.75.). These comparisons were made over a period of $t = t_{max} = 10^5$ sec for a power level of 278.3 W/m. The strong variation of temperature in the immediate vicinity of the heater, combined with the need to include permeability enhancement effects in the simulations, required a grid with sufficiently fine discretization near the heater. The MESHMAKER facility of TOUGH2 was used to generate the grid. Finer spatial discretization was used near the heater with successively larger blocks at increasing distance from the heater.

Two simulations were run. The first did not consider permeability enhancement. The second simulation used nine different sub-domains of porous media. Initial pressure and temperature conditions were set. No separate step of gravity equilibration was needed because the process occurs very fast. The EOS1 fluid property module was used for this simulation with NK = 1 and NEQ = 2. The 416 grid blocks resulted in a total of N = 832 equations.

Simulation results were compared with the measurements made by Reda (1984) at various distances from the heater over time. Figures 17 a and b compare the experimental measurements and numerical predictions. Numerical results with and without permeability enhancement are shown. A very good agreement between experiment and prediction is observed for the period of transient convection, as well as for the eventual steady state. Most parts of the curves show 90% or better agreement and therefore meet the acceptance criterion for comparison to experimental data. Figure 17 a shows an extreme sensitivity of temperature to radial distance from the heater in the immediate vicinity of the inner radius. A less dramatic dependence of temperature on radial distance r above the heater is shown in Figure 17 b.

Results of the simulation show that permeability enhancement has a significant impact on the temperature distribution. Temperatures predicted without permeability enhancement are consistently higher above and below the heater. The temperature differential is small initially, but keeps increasing during the transient period and stabilizes as steady-state is approached. Furthermore, the temperature differential appears earlier and is more pronounced at the top of the heater. This indicates that without flow channeling initiation of convection is slower, and a weaker convection process occurs at later times when steady-state is approached. Neglecting channeling effects does not produce more accurate results despite its apparent better agreement with measurements near the steady-state because of very steep temperature gradients near the heater. A more detailed discussion is found in Moridis and Pruess (1992; 1995).
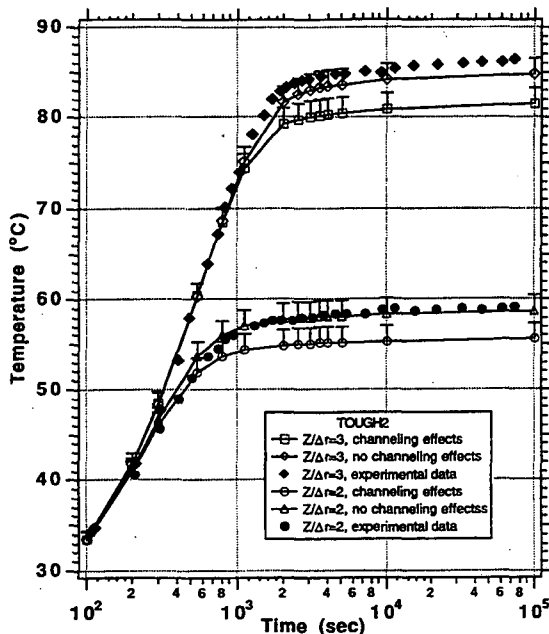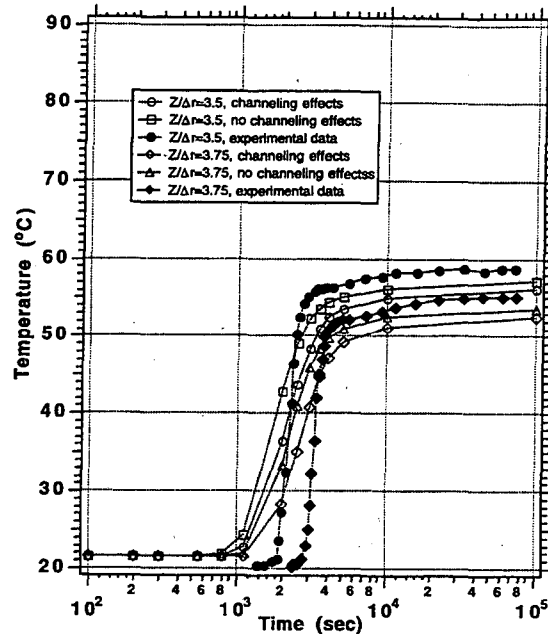
Figure 17.

a. Comparison of TOUGH2 predictions with experimental data at the top and bottom ($z/\Delta r$ = 3 and 2 respectively) of the heating element in test problem 9.

b. Comparison of TOUGH2 predictions with experimental data at $z/\Delta r$ = 3.5 and $z/\Delta r$ = 3.75 (from Moridis and Pruess, 1995).

10. Two-phase flow (Moridis and Pruess, 1992)

This problem modeled flashing (vaporizing) flow from a synthetic sandstone core. The experiment was performed and modeled by Kruger and Ramey (1974). Faust and Mercer (1979) later independently modeled the experiment. This problem tests TOUGH2's ability to simulate simultaneous heat and mass flow, as well as vaporization of water (phase change). The saturated core cylinder is placed in an oven and heated to 198.9°C. The left boundary is insulated to prevent mass and energy flux, while the right end of the core is a "time-variable-pressure" boundary with a pressure decline described by Updegraff (1989). Prior to emplacement in the oven, the saturated core is brought to an initial pressure and heated so as to affect a linear temperature variation between the left and right end. The relative permeability curves in the experiment were described by Corey's equations (Kruger and Ramey, 1974). Numerical predictions were compared to the measured temperature distribution along the length of the core cylinder at a time of t = 300 sec.

Moridis and Pruess (1992) performed numerical simulations using TOUGH and compared them to the results obtained by Updegraff (1989). The boundary conditions of Updegraff's approach did not approximate the ones described in the Kruger and Ramey (1974) experiment. Updegraff asserted that TOUGH could not handle the type of boundary conditions called for by the experiment, but in fact it can handle them easily, these being the constant temperature boundary at the outside edge of the core, zero temperature gradient boundary, and the transient pressure boundary. Moridis and Pruess (1992) modified Updegraff's approach and data inputs by creating two new data sets, but kept his space discretization. To simulate the constant temperature boundary, they added a second set of grid blocks, which formed a ring surrounding the cylindrical core and

assigned a very large volume to each of the grid blocks of this domain. The addition of the ring boundary created essentially a two-dimensional problem.

Moridis and Pruess (1992) introduced a very general transient-pressure boundary condition by treating air as an ideal gas and submitting it to suitable time-dependent rates of air injection and withdrawal. They created two data sets, one with the ring boundary and one without, and made TOUGH runs using both files. By treating the boundary conditions in the manner described in full detail in Moridis and Pruess (1992), they were able to eliminate all of the problems encountered by Updegraff. Figure 18 shows numerical results compared to experimental data of Kruger and Ramey (1974). The agreement is satisfactory in meeting the acceptance criterion for comparison to experimental data; observed discrepancies may reflect that experimentally achieved boundary conditions at the core outlet may be more complex than presumed in the idealized one-dimensional model.
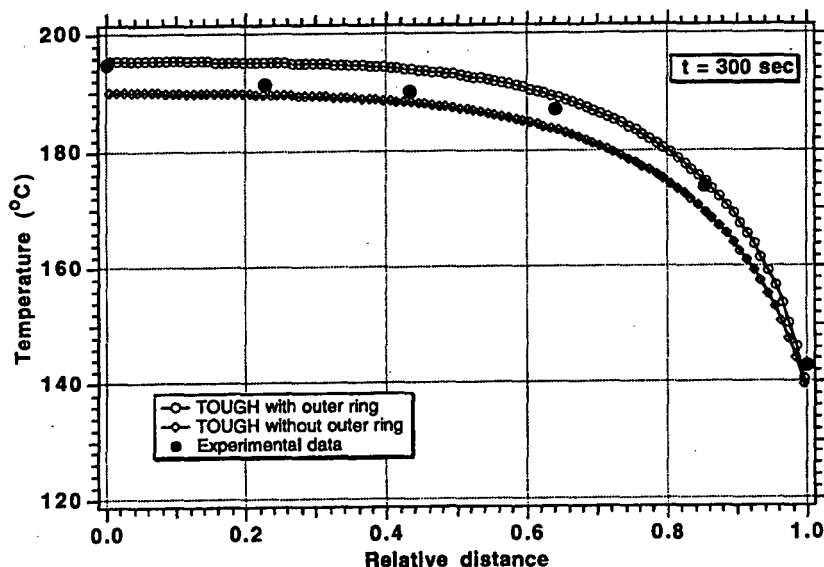
Figure 18. Comparison of TOUGH data and experimental data for problem 10 (from Moridis and Pruess, 1992).

11. Warren-Root double-porosity solution (this paper):
This problem is designed to examine the capability and accuracy of TOUGH2 in simulating transient flow in a double-porosity medium. The problem concerns transient behavior of water injection into liquid in a horizontal, uniformly fractured, infinite and isothermal formation. Warren and Root (1963) presented an analytical solution for this problem using a double-porosity approach.

A one-dimensional radial grid was generated for the TOUGH2 simulation. The infinite radial fractured/matrix domain is represented by 50 elements with an outer radius of 1,000 m and thickness of 10 m. The three-dimensional fracture network and cubic matrix system are used in the TOUGH2 discretization. The matrix blocks are represented by 1 x 1 x 1 m cubes. The fracture permeability and aperture are correlated by the cubic law.

The fracture/matrix properties and fluid parameters used are: fracture porosity ϕ_f = 0.0006; matrix porosity ϕ_m = 0.3; fracture permeability k_f = 1.0 x $10^{-12}m^2$; matrix

permeability $k_f = 1.0 \times 10^{-16} m^2$; temperature $T = 25^0C$; rock compressibility $C_r = 0$; fluid compressibility $C_f = 4.48 \times 10^{-10}$ Pa^{-1}; and fluid viscosity $\mu = .898 \times 10^{-3}$ Pa•s. The double-porosity parameters as defined by Warren and Root (1963) are: $\alpha = 60$; $\omega = 2.0 \times 10^{-3}$; $\lambda = 6 \times 10^{-5}$. The injection rate at the well is 0.01 m^3/s, wellbore radius is 0.1 m, and the outer boundaries are treated as a constant pressure condition in the TOUGH2 simulation instead of an infinite system. The early time solution will not be affected by the boundary.

A comparison of the TOUGH2 simulation and the Warren-Root solution is shown in Figure 18 for the well pressure response. Figure 19 indicates that the TOUGH2 simulated result is in excellent agreement with the analytical solution for this problem, and meets the acceptance criteria of 95% or better agreement, indicating typical double-porosity behavior of two-parallel semi-log straight lines on a pressure plot.
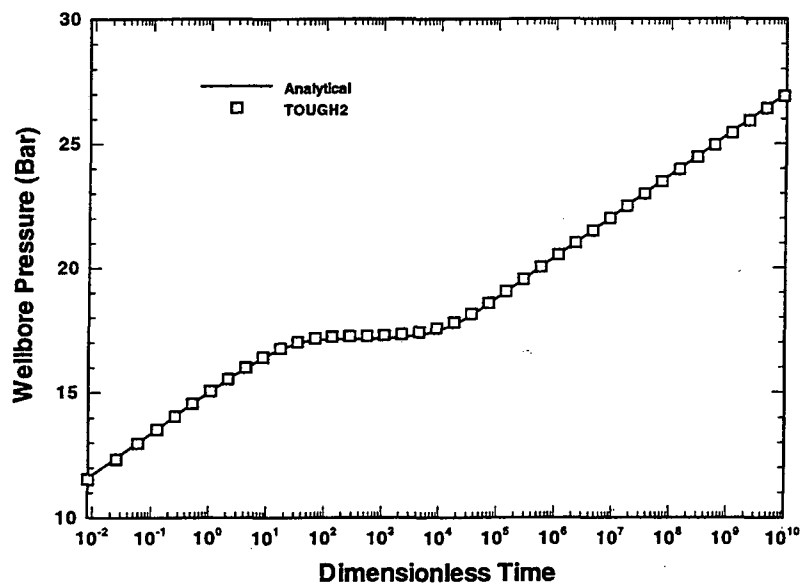
Figure 19. Comparison of TOUGH2 to Warren-Root double-porosity solution.

12. Lauwerier heat transfer solution (this paper):

This problem is designed to examine the capability and accuracy of the TOUGH2 code in simulating two-dimensional conductive and convective heat transfer in porous media. The problem concerns hot water injection into a linear water layer with a constant injection rate, displacing the in-situ "cold" water, in which thermal conduction is ignored. At the same time, heat transfer occurs perpendicularly into impermeable layers, in which only the heat conduction in the direction perpendicular to the linear water layer is considered. Lauwerier (1955) derived an analytical solution for this two-dimensional heat transfer problem, against which results of a TOUGH2 simulation were compared.

A two-dimensional rectilinear grid of 4,400 elements was generated using the TOUGH2 MESHMAKER for a grid of 10 × 60 m. In order to reduce the effects of spatial discretization on the numerical solution, a very fine grid was used; the 10 m length, parallel to the linear water layer, was divided into 200 uniformly spaced gridblocks. Along the direction perpendicular to the water layer, the 60 m width was divided into 22 rows non-uniformly, with the finest spacing next to the water layer. Also the mesh connections

in the direction parallel to the water layer were deleted in the input file for consistency with the analytical treatment which includes transverse heat conduction only.

The formation properties and fluid parameters used are: water layer porosity ϕ_1 = 1.0; impermeable layer porosity ϕ_2 = 0.3; water layer permeability k_1 = .89 × 10^{-13} m^2; half width of water layer b = 0.05 m; rock compressibility Cr = 0; fluid compressibility C_f = 4.48×10^{-10} Pa $^{-1}$; fluid viscosity μ = .89× 10^{-3} Pa•s; water specific heat c_w = 4.17965 J/kg•°C; rock specific heat c_r = 1,000 J/kg•°C; water density ρ_w = 1,000 kg/m^3; and rock grain density ρ_r = 1,600 kg/m^3. The boundary and initial conditions are: pore velocity in water layer from injection V_w = 5.0035 m/s; injection temperature T_0 = 26 ° C; and initial temperature T_i = 25 ° C. The outlet end conditions for both water layer and impermeable layer were treated as constant temperature boundaries.

A comparison of temperature profiles along the water layer from the TOUGH2 simulation and the analytical solution is shown in Figure 20 for three different times. Figure 20 indicates that the TOUGH2 simulated results are in excellent agreement with the analytical solution for this problem and meet the acceptance criteria for having 5% or less discrepancy, except at the thermal front where some slight numerical dispersion effects exist.

Figure 20. Temperature profiles for the analytical solution and the TOUGH2 simulation for the Lauwerier heat transfer solution in Problem 12.

13. Correct handling of thermophysical properties (this paper):
This is a trivial problem designed to confirm the validity of the thermophysical properties of the reservoir fluids in TOUGH2 simulations. The fluids considered in TOUGH2 include
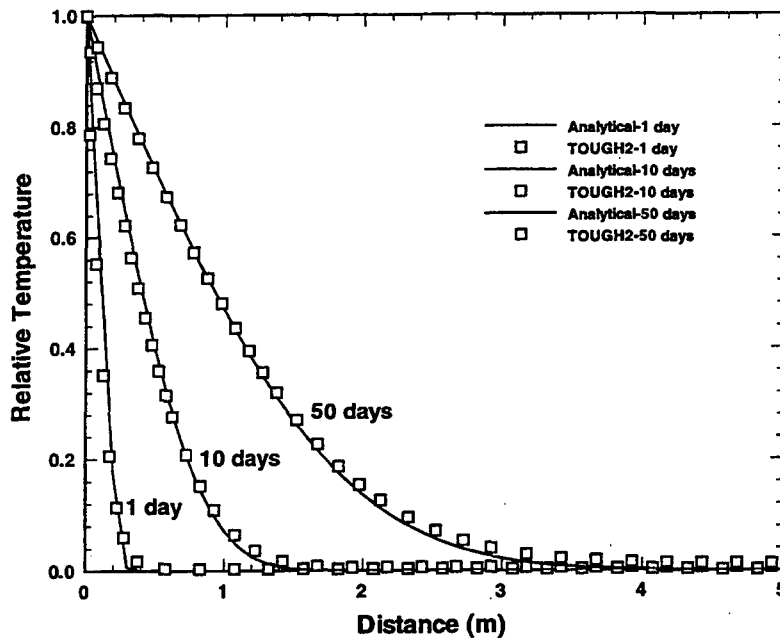
(a) water, (b) water vapor, (c), air, (d) CO_2, and H_2. In this verification exercise only the first three are considered.

TOUGH2 was run with a small number of gridblocks and with no communication between them, thus affecting invariable conditions. The fluid properties at the different conditions were then printed out, and were tabulated. In Table 10 the TOUGH2-calculated properties are compared to values obtained from CRC (1993) for a variety of pressure and temperature conditions. The two sets of property values practically coincide, thus confirming the correctness of thermophysical properties calculated in TOUGH2 and meeting the acceptance criteria for being within 5% of actual values. In this case one would want the TOUGH2 and actual values to match more closely than by 95%, and in fact, they fall within less than 1% discrepancy.

Table 10. Comparison of TOUGH2 to thermophysical property data from steam tables in validation problem 13.

Substance	P (Pa)	(°C)	TOUGH2 RESULTS		TABLES	
			ρ_g, ρ_L (kg/m^3)	H_g, H_L (J/kg)	ρ_g, ρ_L (kg/m^3)	H_g, H_L (J/kg)
Air	1.013×10^5	20	1.2036 (ρ_g)	9.8825×10^4 (H_g)	1.2036 (ρ_g)	9.8824×10^4 (H_g)
	3.0×10^5	10	3.6903 (ρ_g)	8.8624×10^4 (Hg)	3.6903 (ρ_g)	8.8624×10^4 (H_g)
	6.0×10^5	50	6.4671 (ρ_g)	1.2943×10^5 (H_g)	6.4671 (ρ_g)	1.2944×10^5(H_g)
Water/Vapor	1.013×10^5	5	1000.00 (ρ_L)	2.1107×10^4 (H_L)	1000 (ρ_L)	2.1107×10^4 (H_L)
	1.013×10^5	20	998.32 (ρ_L)	8.3955×10^4 (H_L)	998.32 (ρ_L)	8.3955×10^4 (H_L)
	1.013×10^5	90	965.13 (ρ_L)	3.7696×10^5 (H_L)	965.13 (ρ_L)	3.7696×10^5 (H_L)
	1.013×10^5	100	0.59758 (ρ_g)	2.676×10^6 (H_L)	0.59758 (ρ_L)	2.676×10^6 (H_L)
	1.013×10^5	150	0.52323 (ρ_g)	2.7762×10^6 (H_g)	0.52323 (ρ_L)	2.7762×10^6 (H_L)
	3.0×10^5	10	999.89 (ρ_L)	4.2267×10^4 (H_L)	999.89 (ρ_L)	4.2267×10^4 (H_L)
	5.065×10^5	10	999.99 (ρ_L)	4.2488×10^6 (H_L)	999.99 (ρ_L)	4.2488×10^4 (H_L)
	5.065×10^5	30	995.93 (ρ_L)	1.2612×10^5(H_L)	995.93 (ρ_L)	1.2612×10^5 (H_L)
	5.065×10^5	150	916.79 (ρ_L)	6.3217×10^5 (H_L)	916.79 (ρ_L)	6.3217×10^5 (H_L)
	4.6709×10^5	149.3	2.5032 (ρ_g)	2.7445×10^6 (H_g)	2.5032 (ρ_L)	2.7445×10^6 (H_L)
			917.43 (ρ_L)	6.2911×10^5 (H_L)	917.43 (ρ_L)	6.2912×10^5 (H_L)

Table 10 (cont.). Comparison of TOUGH2 to thermophysical property data from steam tables in validation problem 13.

		TOUGH2 RESULTS		TABLES	
1.013×10^6	100	958.56 (ρ_L)	4.1975×10^5 (H_L)	958.56 (ρ_L)	4.1975×10^5 (H_L)
1.013×10^6	150	917.9 (ρ_L)	6.3248×10^5 (H_L)	917.9 (ρ_L)	6.3248×10^5 (H_L)
5.065×10^6	150	919.44 (ρ_L)	6.35×10^5 (H_L)	919.44 (ρ_L)	6.3501×10^5 (H_L)
11.437	29.84	8.1787×10^{-5} (ρ_g)	2.5572×10^6 (H_g)	8.18×10^{-5}	2.557×10^6

14. Vapor Pressure Lowering (this paper):

This problem examined the implementation of vapor pressure lowering as a function of decreased matrix saturation (increased capillary suction). An analytical relationship for this problem, known as the Kelvin equation, was presented by Edlefsen and Anderson (1943).

A one-dimensional grid composed of eight gridblocks was generated for this simulation. Each gridblock was assigned a different liquid saturation, while all other properties remained constant from block to block. The saturations tested varied from 0.5 to 0.001 (fully saturated = 1.0). Temperature was kept constant for all times at 26.85 ^{0}C (300K), and all the properties of water were evaluated at this temperature. Other relevant properties, which were used to calculate both the analytical solution and the numerical (TOUGH2) solution were: vapor pressure of free water = 0.03531 bar, atmospheric pressure = 1.01325 bar, molecular (formula) weight of water = 18.016 kg/kmole, and the density of water = 997.0 kg/m^3. Capillary suction was evaluated using a standard van Genuchten (1980) model, and values for the van Genuchten parameters were chosen arbitrarily to be representative of a tuff matrix. The parameters chosen were α = 0.001 and m = 0.412.

Agreement between the TOUGH2 calculations and the analytically calculated values is excellent, as shown in Table 11. None of the numerically calculated values differed from the analytical solution by greater than one-one hundred thousandths (0.00001) of a bar. In no case did the relative error exceed three-hundredths (0.03) of one percent. Therefore, the validation acceptance criterion was easily met for this test case.

Table 11. Comparison of vapor pressure lowering between TOUGH2 and Analytical solution (Edlefsen and Anderson, 1943).

Saturation	Pv (TOUGH2)	Pv (Analytical)	Delta (bar)	% error
0.5	0.03532	0.03531	0.00001	0.03
0.1	0.03531	0.03530	0.00001	0.03
0.05	0.03530	0.03529	0.00001	0.03
0.01	0.03514	0.03513	0.00001	0.03
0.005	0.03483	0.03482	0.00001	0.03
0.003	0.03431	0.03430	0.00001	0.03
0.002	0.03354	0.03354	0.00000	0.00
0.001	0.03075	0.03074	0.00001	0.03

15a. Flow in a Heterogeneous Formation with Multiple Wells (this paper):

Single-phase, Slightly Compressible Liquid, 1-Dimensional, Heterogeneous
This problem describes flow in a horizontal heterogeneous system with multiple wells and finite boundaries. The analytical solution to this problem was developed by Moridis (1995) using the Transformational Decomposition method, which first defines the conditions at the boundaries of the heterogeneous subdomains and then describes the pressure distribution using analytical sub-solutions within each subdomain.

The problem has five subdomains. The various rocks in the subdomains are assumed incompressible. The reservoir geometry, dimensions, and properties (porosity ϕ and permeability k), as well as the well rates and the well locations, are presented in Table 12. The initial pressure is $p_0 = 5000$ psi and the water compressibility is considered constant at $c_W = 3.134 \times 10^{-6}$ psi^{-1} (2.200×10^{-3} Pa^{-1}). For the TOUGH2 simulation, the domain was discretized into a total of 178 gridblocks.

Figure 20 shows the pressure drawdown at t = 200 days obtained from the analytical method and the TOUGH2 simulation. It is obvious that the two solutions literally coincide and therefore that the acceptance criterion for the validation are met.

Table 12. *Reservoir Properties, Geometry, and Discretization in Test Problem 15a*

Dimensions in (x,y,z): 5000 x 300 x 50 (ft)

Discretization: $M_x = 178$ Dx's of variable size, $M_y = M_z = 1$

Sub-domain	k (md)	ϕ	Subdomain length (ft)	# of Wells	Well Rates (bbl/D)	Well position (local x, ft)
1	50	0.2	800	2	-30, 20	100, 560
2	20	0.18	1200	3	-20 (all)	300, 770, 910
3	8	0.12	1400	1	-25	490
4	6	0.08	800	1	-25	650
5	2	0.07	800	0	-	-
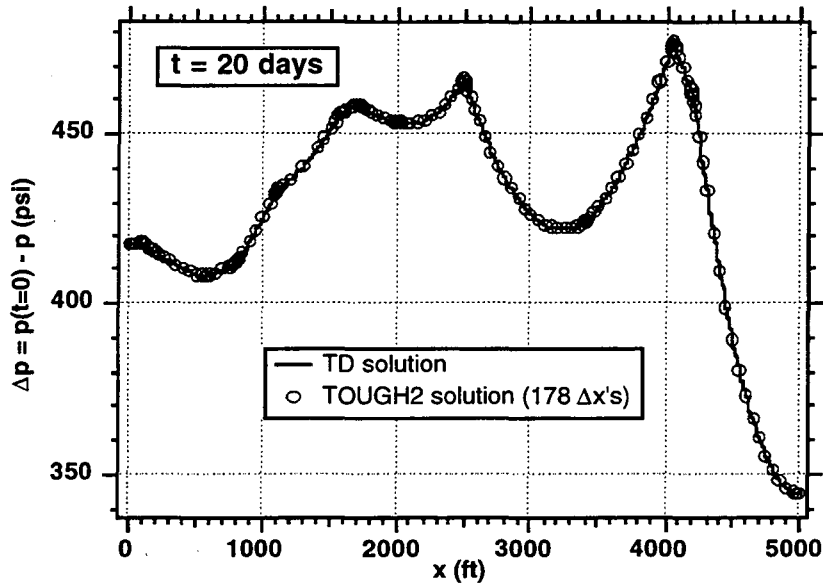
Figure 21. *Comparison of the analytical and the TOUGH2 solutions to the problem of 1-D flow through a heterogeneous formation with multiple wells for problem 15a.*

15b. Flow to a Single Well at the Center of an Infinite Reservoir (this paper):
Single-phase, Slightly Compressible Liquid, 2-Dimensional, Anisotropic

In this problem we compare the TOUGH2 and the analytical solutions of flow of water to a vertical well located in the center ($x = 0$, $y = 0$) of an aquifer which is infinite in areal extent, homogeneous, anisotropic, and of uniform thickness. The two-dimensional analytical solution to this problem was developed by Papadopulos (1965) using integral transforms in an approach very similar to the Theis (1935) solution, which assumes a fully penetrating well and constant water and formation properties.

The analytical and the TOUGH2 solutions at $t = 20$ days were computed using the following reservoir and fluid properties: $T_x = 1000$ m^2/day, $T_y = 100$ m^2/day (directional transmissivities), $\phi = 0.3$ (formation porosity), $S = 1.0 \times 10^{-4}$ (storage coefficient), $h_z = 50$ m (formation thickness), $q = 1000$ m^3/day. For the TOUGH2 simulation, the domain was discretized into a total of 3,600 gridblocks (60×60 in x,y). Due to symmetry, only one quarter of the domain was considered (from 0 to infinity in both x and y).

Figure 22 shows the pressure drawdown along the x axis at $y = 0$ m, as well as along the x=y axis. The agreement between the analytical and the TOUGH2 solutions is excellent and falls well within the acceptance criterion of having less than 5% discrepancy.
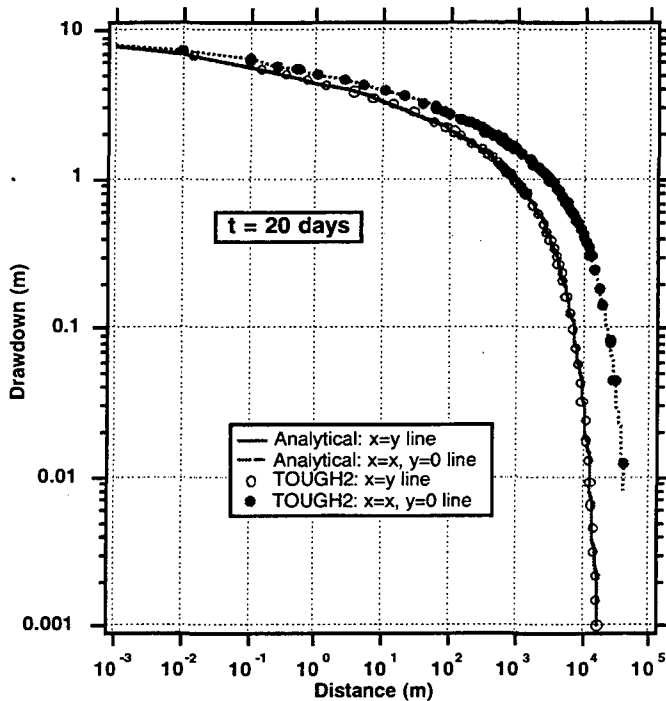
Figure 22. *Comparison of the analytical and the TOUGH2 solutions to the problem of 2-D flow to a single well in an anisotropic aquifer for problem 15b.*

16. Single-phase transient flow simulation using an irregular grid (this paper):

This problem is designed to examine the capability and accuracy of the TOUGH2 code in simulating transient flow using an irregular grid. The problem concerns transient flow of a slightly compressible liquid in a horizontal, uniform, infinite, and isothermal aquifer, for which the analytical solution of Theis (1935) is available. The system is initially at static conditions and is fully saturated with water. Water is injected through a fully penetrating well with constant volumetric rate from t = 0.

The two-dimensional grid of the TOUGH2 simulation is shown in Figure 23. Because of the symmetry of the problem, only a quarter of the flow geometry is discretized and simulated. The infinite radial flow domain is represented by a rectangular domain of 2,000 x 2,000 m with thickness of 10 m. The irregular integral finite difference grid, as shown in Figure 22, was generated based on randomly selected block centers, with a total of 1,000 elements. Three locations of A (x=9.67m, y=8.33m), B (x=26.90m, y=73.02m), and C(x=305.12m, y=118.12m) are chosen at which pressures from the analytical and numerical solutions were compared.
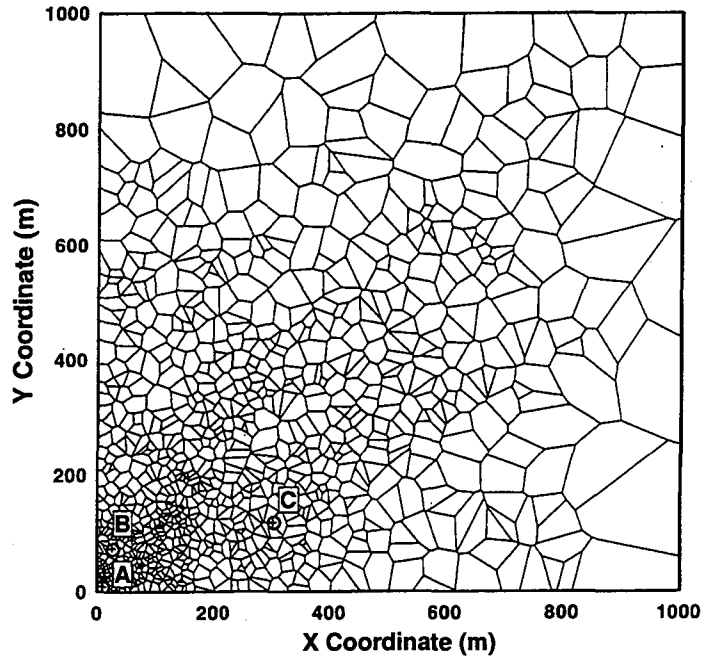
Figure 23. Irregular grid constructed for problem 16.

The rock and fluid parameters used are: porosity $\phi = 0.2$; permeability $k = 1.0 \times 10^{-12}$m^2; temperature $T = 25^0$C; rock compressibility $C_r = 0$; fluid compressibility $C_f = 4.48 \times 10^{-10}$ Pa^{-1}; and fluid viscosity $\mu = .898 \times 10^{-3}$ Pa•s. The injection rate at the well is 0.001 m^3/s, and the outer boundaries in the TOUGH2 simulation are treated as a first-type, constant pressure condition. Therefore, the early time numerical solution can be compared with the analytical solution before the finite boundary effects take place.

Comparison of the TOUGH2 simulation and the Theis solution is shown in Figure 24, for the three observations points, indicating overall excellent agreement between the two solutions for all the three locations and demonstrating that the comparison meets the acceptance criteria of having 5% or less discrepancy. It should be mentioned that a well is represented as a line source in the Theis solution; however, the well is approximated in the TOUGH2 simulation by a finite soil column with a top area of 17.8 m^2. This explains why a small difference exists between the two solutions at location A, which is close to the well.
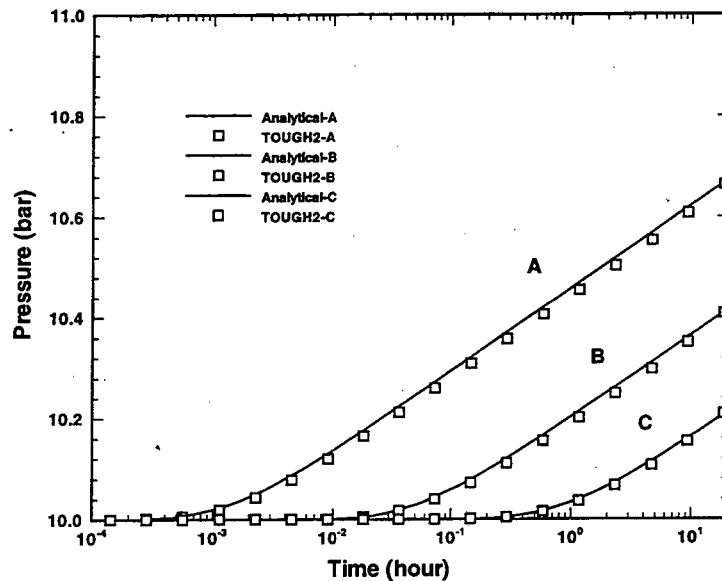
Figure 24. Comparison of TOUGH2 simulation with Theis solution for an irregular grid, as described in problem 16.

17a. One-dimensional heat conduction (this paper):

This problem is designed to examine the accuracy of the TOUGH2 code in simulating conductive heat transfer in porous media. The problem concerns heat conduction into a semi-infinite linear rock column. Initially, the system is at uniform temperature, and a step change in temperature is imposed on the boundary from t=0. Then heat starts to conduct into the column. When effects of water flow on the heat transfer can be ignored, the heat transfer problem becomes one of heat conduction in solids, for which many analytical solutions are available. For the test problem of interest, an analytical solution from Carslaw and Jaeger (1959) is used.

In the TOUGH2 simulation, a one-dimensional linear grid of 1,000 elements was generated using the TOUGH2 MESHMAKER for a ten meter domain of unit cross area. In order to eliminate the effects of fluid flow, rock porosity and permeability were set to zero. The formation properties and thermal parameters used are: permeability $k = 0.0$ m^2; rock compressibility $C_r = 0$; rock specific heat $c_r = 1,000$ J/kg $°C$; thermal conductivity $K=2.0$ W/m$°C$; and rock grain density $\rho_r = 1,600$ kg/m^3. The boundary and initial conditions are: boundary temperature $T_0 = 50 ° C$; and initial temperature $T_i = 25 ° C$. The outlet end condition for the rock column was treated as a constant temperature boundary, the same as the initial condition.

A comparison of the temperature profiles along the rock column from the TOUGH2 simulation and the analytical solution is shown in Figure 25 for three different times, 1, 10, and 50 days. Figure 25 indicates that the TOUGH2 simulated temperature results are in excellent agreement with the analytical solution for this problem and meet the acceptance criteria of having 5% or less discrepancy from the analytical solution. In fact, it is difficult to detect any discrepancy between the two.
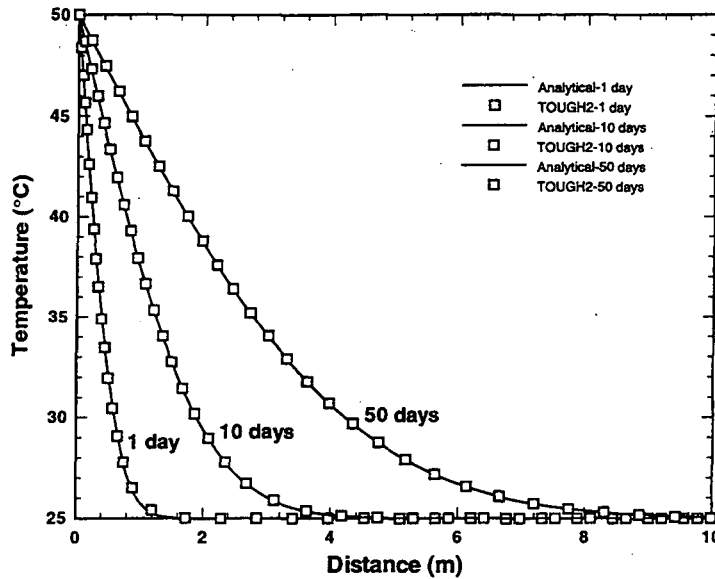
Figure 25. *Comparison of analytical solution and TOUGH2 results for heat conduction problem in problem 17a.*

17b. One-dimensional binary vapor diffusion (this paper):

This problem is designed to examine the accuracy of the TOUGH2 code in simulating vapor and air diffusion in the gas phase. The problem concerns air component diffusion into a semi-infinite linear rock column. The system initially contains single-phase gas at isothermal conditions of 25°C. The gas phase consists of air and water vapor only, and initially the mass fraction of vapor is 0.990 throughout. The adsorption of air or vapor on the rock solids is ignored. At t = 0, the air mass fraction on the boundary is increased to 1. Then the air component starts to diffuse into the column by binary diffusion. For this test problem, the governing partial differential equation, boundary and initial conditions are identical to a heat conduction problem (pure diffusion). Therefore, an analytical solution of heat conduction from Carslaw and Jaeger (1959) is used in this comparison study.

In the TOUGH2 simulation, a one-dimensional linear grid of 1,000 elements was generated using the TOUGH2 MESHMAKER for a 10 m domain of unit cross area. The EOS3 fluid property module was used. In order to eliminate effects of advective gas flow, the water saturation and the rock permeability were set to zero. The formation properties and diffusion parameters used are: permeability $k = 0.0$; rock compressibility $Cr = 0$; formation temperature $T = 25$ °C; porosity $\phi = 1$; tortuosity $\tau = 1$; effective diffusivity $\phi S_g \tau D = 4.0975 \times 10^{-4} m^2/s$ and binary diffusion coefficient, $D = 1.1707 \times 10^{-5} m^2/s$. The boundary and initial conditions are: boundary air mass fraction $Xair = 1.0$; and initial air mass fraction $Xair = 0.99$. The outlet end condition for the rock column was treated as a constant mass fraction boundary, the same as the initial condition.

A comparison of the air mass fraction profiles along the rock column from the TOUGH2 simulation and the analytical solution is shown in Figure 26 for three different times, 1, 5, and 10 days. Figure 26 indicates that the TOUGH2 simulated results are in excellent agreement with the analytical solution for this problem and meet the acceptance criteria of having 5% or less discrepancy from the analytical solution.
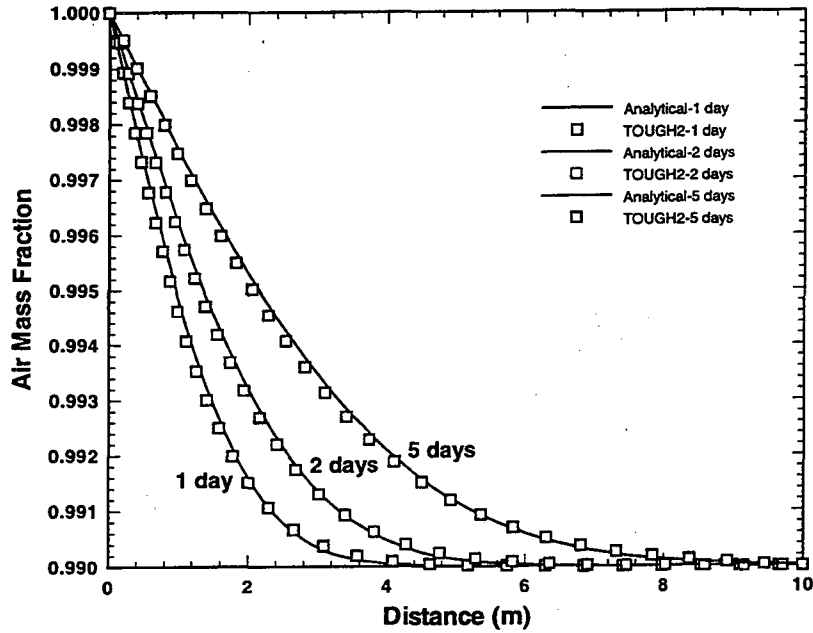
Figure 26. Comparison air mass fraction profiles showing TOUGH2 results and analytical solution for problem 17b.

17c. One-dimensional gas flow with Klinkenberg effects (this paper):

This problem is designed to examine the capability and accuracy of the TOUGH2 code in simulating porous medium gas flow with the Klinkenberg effect (1941). The problem concerns a steady gas flow problem across a linear rock column. The system contains single-phase gas at isothermal conditions, and a constant gas mass injection rate is imposed on the inlet of the rock column. The outlet end of the rock column is kept at a constant pressure. Klinkenberg (1941) gave the following relation:

$$\kappa_g = \kappa_\infty \left(1 + \frac{b}{P}\right) \tag{1}$$

where κ_g is the gas-phase permeability; and κ_∞ is the gas permeability at infinite pressure; b is the Klinkenberg coefficient (Pa); and P is the gas-phase pressure.

Under the steady state flow condition stated above, an analytical solution can be derived for the gas pressure distribution along the rock column,

$$P(x) = -b + \left[b^2 + P_b^2 + 2b\,P_b + 2q_m\mu(L-x)/\beta\,\kappa_\infty\right]^{1/2} \tag{2}$$

where P_b is the outlet boundary pressure; q_m is the gas mass injection rate per unit area; μ is the gas viscosity; L is the length of the rock column; and $\beta = M_g/RT$ is the gas compressibility factor.

In the TOUGH2 simulation, a one-dimensional linear grid of 1,000 elements was generated using the TOUGH2 MESHMAKER for a 10 m domain of unit cross sectional area. In order to eliminate the effects of liquid, the water saturation was set to zero. The formation and Klinkenberg parameters were selected from a laboratory study of welded tuff at Yucca Mountain (Reda, 1987). The parameters used are: porosity $\phi = 0.3$; permeability $k = 5\times10^{-19}$ m²; Klinkenberg coefficient $b = 7.6\times10^{5}$ Pa; rock compressibility $Cr = 0$; formation temperature $T = 25\,°C$; and compressibility factor $\beta = 1.1885\times10^{-5}$ kg/Pa•m³. The boundary conditions are: air mass injection rate $q_m = 1\times10^{-6}$ kg/s; and outlet boundary pressure $P_b = 1$ bar.

A comparison of the pressure profile along the rock column from the TOUGH2 simulation and the analytical solution is shown in Figure 27. Figure 27 indicates that the TOUGH2 simulated pressure distribution is in excellent agreement with the analytical solution for this problem and meets the acceptance criterion of having less than 5% discrepancy.
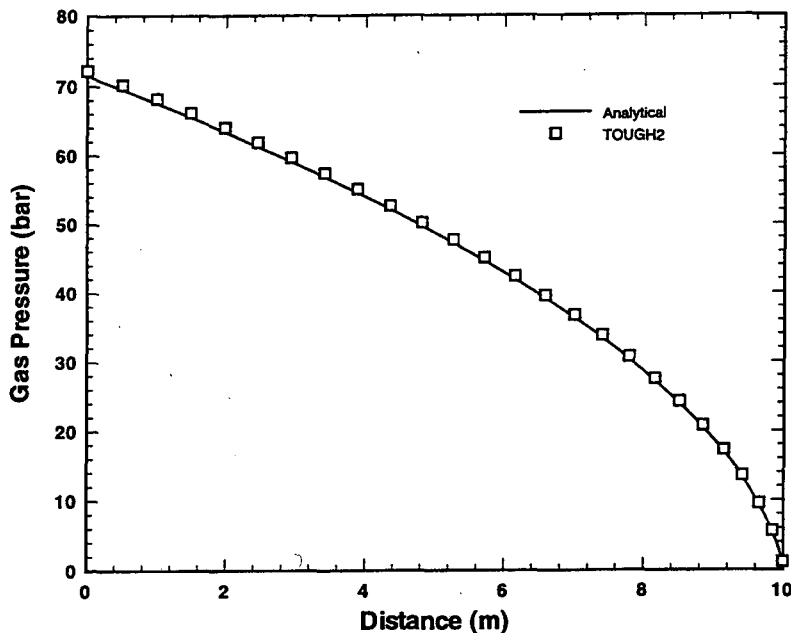
Figure 27. Comparison of the pressure profile along the rock column from the TOUGH2 simulation and the analytical solution for problem 17c.

18. 3-D Flow to a Horizontal Well (this paper):

Single-phase, Slightly Compressible Liquid, 3-Dimensional, Anisotropic
This problem involves verification of TOUGH2 against the analytical solution for flow of a single-phase fluid to an infinite-permeability horizontal well located in a semi-infinite homogeneous and anisotropic reservoir of uniform thickness and width. The three-dimensional analytical solution to this problem was developed by Goode and Thambynayagam (1987) using successive integral transforms. The solution involves a slightly compressible liquid with constant compressibility, assumes constant liquid and formation compressibilities, and neglects gravitational effects.

Figure 28 shows a schematic of the horizontal well model and identifies a number of important parameters. In the problem used for the comparison between the analytical and the TOUGH2 solutions the following reservoir and fluid properties were used: $k_x = 100$ md, $k_y = 50$ md, $k_z = 10$ md (formation permeabilities), $\phi = 0.1$ (formation porosity), $c_t = 3.134 \times 10^{-6}$ psi^{-1} ($= 2.200 \times 10^{-3}$ Pa^{-1}, total system compressibility), $h_z = 220$ ft (formation thickness), $h_x = 2200$ ft (formation width), $L_{zb} = 110.5$ ft, $L_{za} = 109.5$ ft, $L_{xd} = 800$ ft, $L_w = 500$ ft, $q = 2000$ STB/D (3.68×10^5 m^3/S, well flow rate), $m = 1.0$ cp (viscosity) and $B_o = 1.0025$ (formation volume factor, corresponding to a fluid density of water (998.3 kg/m^3). The initial reservoir pressure is $p_0 = 5000$ psi.

For the TOUGH2 simulation, the domain was discretized into a total of 9,996 gridblocks ($17 \times 28 \times 21$ in x,y,z) of non-uniform size. A very high permeability (5.0×10^7 md) was assigned to the k_x permeability of the wellbore to simulate the infinite permeability assumption in the analytical solution. The well flow rate was distributed uniformly over the length of the well.

Figure 29 shows the pressure drawdown at the well (x = 1100 ft, y = 0 ft, z = 110 ft) over time. An excellent agreement between the analytical and the TOUGH2 solutions is observed, well within the acceptance criterion of less than 5% discrepancy, thus confirming the validity of the TOUGH2 solution for this type of problem.
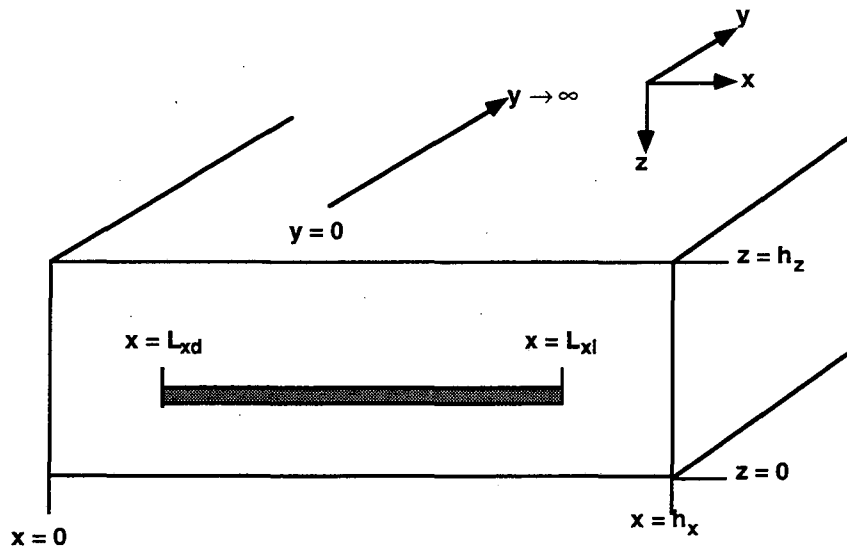
Figure 28. Schematic of the horizontal well system.
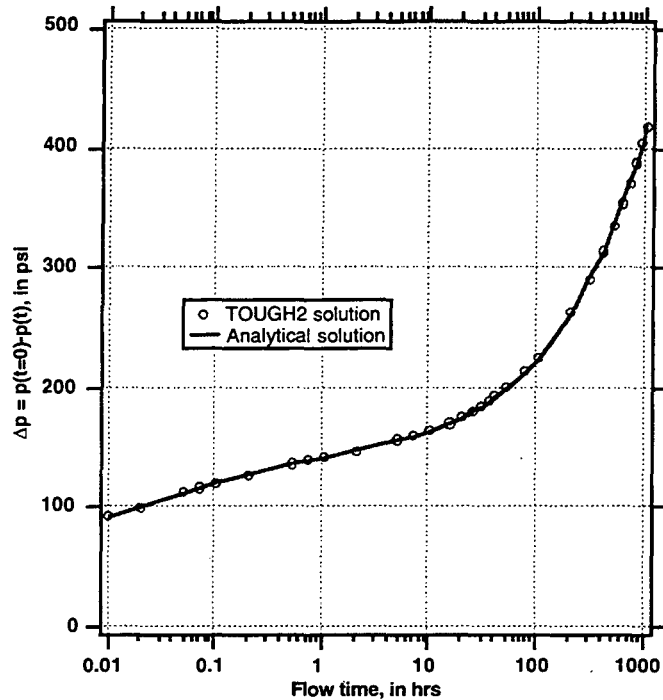
Figure 29. Comparison of the analytical and the TOUGH2 solutions (pressure drawdown at the well) to the problem of 3-D flow to a horizontal well in an anisotropic aquifer for problem 18.

Analytical solutions are generally not available for three-dimensional problems because their full complexity cannot be verified. However, the problem described above with a 3-D horizontal well validates TOUGH2's ability to model three-dimensional problems accurately. It is also worth noting the three-dimensional simulations described by Moridis and Pruess (1995) because they obtained good results using data from nuclear waste and geothermal settings. Their Test 10 featured single- and two-phase flow under non-isothermal conditions in a three-dimensional geothermal reservoir model, as described by Antunez et al. (1994). Moridis and Pruess (1995) employed an irregular grid in Test 11 to a three-dimensional model of the Cerro Prieto geothermal field featuring non-isothermal multi-phase flow with phase changes and fracture-matrix interactions. A similar test was their Test 13 which depicted channelized two-phase flow in fractured media in three dimensions at Yucca Mountain, as described by Pruess and Tsang (1994).

19. 1-D Radial Flow of a Compressible Gas (this paper):

Single-phase, Compressible Gas, 1-Dimensional, Homogeneous

This problem involves radial flow of a gas (compressible fluid) to a single vertical well located at the center of a bounded cylindrical formation. The analytical solution to this problem was developed by Kabir and Hasan (1986) using perturbation techniques.

In the problem the reservoir is finite but infinite-acting due to its very large radius. The following reservoir properties were used: $k_r = 2.367 \times 10^{-12}$ m^2 (formation permeability), $\phi = 0.35$ (formation porosity), and $h_z = 50$ m (formation thickness). In both TOUGH2 and the analytical solution the gas properties were taken to be those of air, which was considered an ideal gas. The initial reservoir pressure was $p_0 = 6 \times 10^5$ Pa, and the

initial temperature was $T_0 = 50\ ^\circ\text{C}$. Gas was removed from the system at a rate of 1.15573 kg/sec. For the TOUGH2 simulation, the domain was discretized into a total of 114 gridblocks of non-uniform size.

Figure 30 shows the distribution of the pressure drawdown along the r-axis at a time t = 6.89 days from the beginning of gas removal. Under the assumption of ideal gas properties, there is an excellent agreement between the analytical and the TOUGH2 solutions, well within the acceptance criterion of having less than 5% discrepancy.
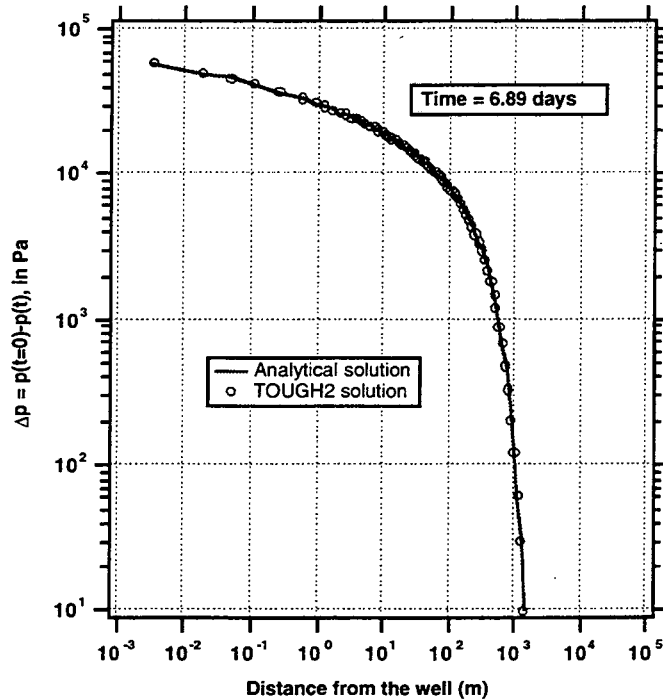
Figure 30. Analytical and TOUGH2 predictions of the pressure drawdown distribution in the gas reservoir for problem 19.

20. Water absorption into porous matrix

This is a problem designed to examine the capability and accuracy of the TOUGH code in simulating transient interaction between fractures and matrix in two phase flow conditions. Zimmerman et al. (1990) developed an approximate analytical solution for calculating water absorption into porous spherical, cylindrical and slablike matrix blocks whose characteristic curves are of van Genuchten-Mualem type. Here, the analytical solution is used to check the numerical results from the TOUGH code.

A slab shape of blocks was chosen in this study, and a one-dimensional radial grid was generated for the TOUGH simulation. the half thickness of the slab is 0.20 m, and is subdivided into 20 grid blocks of equal volume. The block is initially at uniform saturation of 0.6765. Then, the outer boundary is saturated with water at zero water potential from t=0, so that water begins imbibing into the block.

The fracture/matrix properties used are those that have been estimated for the Topopah Spring member of the Paintbrush Tuff of Yucca Mountain: matrix porosity

ϕ_m=0.14; matrix permeability $k_m = 3.9 \times 10^{-18}$ m^2; and van Genuchten parameters, n=3.04; m=0.671; S_s=0.984; S_r=0.318; and α=1.147$\times 10^{-5}$; water viscosity μ=0.001 Pa.s.

A comparison of the TOUGH simulation and the analytical solution is shown in Figure 31 for the relative water influx versus dimensionless time. Figure 31 indicates that the TOUGH2 simulated result is in reasonable agreement with the analytical solution for this problem, in terms of estimation of water imbibition flux into the slab block.
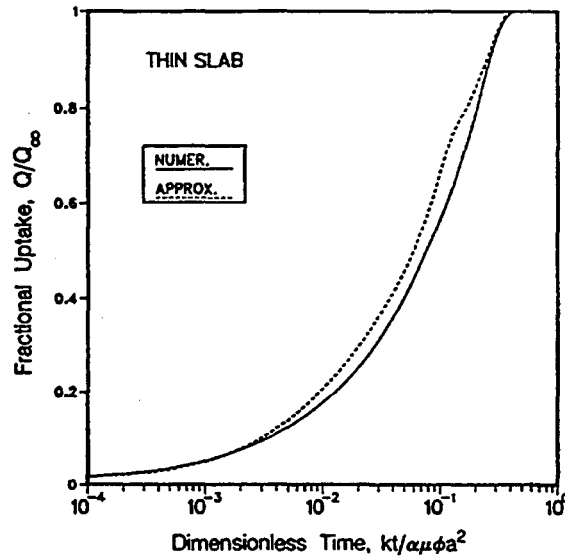
Figure 31. *Normalized cumulative liquid flux for TOUGH and semi-analytical solution in slab absorption problem of test problem 20.*

4.3 Summary

Verification of design of TOUGH2 was met exclusively through numerical tests and did not require the employment of additional procedures or confirmatory methods. Software validation of TOUGH2 was accomplished by testing in the 20 test cases described above. As a demonstration that the specified requirements for TOUGH2 have been met, Table 13 provides a cross-check of the requirements against the validation problems described above that satisfy those requirements. As shown in Table 13, the validation tests that were run for qualification purposes collectively satisfy the Requirements Specification and all meet the acceptance criteria.

As additional examples of TOUGH2 applications that fit the software engineering definition of "validation" because they demonstrate that the code can model the processes it purports to model, the TOUGH2 Selected Bibliography (Appendix E) lists papers that applied TOUGH2 to solve problems involving the processes listed under Requirements Specification (e.g., heat pipe, infiltration, convection cell).

Table 13. *Requirements Validation Cross-Check*

Requirement	Test Case	Acceptance Criteria	Reference
A. flow processes			
gravity effects capillary forces viscous forces	8, 9 3, 8 6, 8, 11, 15a, 15b, 18, 19	met	Pruess (1987) Moridis and Pruess (1992,1995)
single-phase gas flow	1, 6, 9, 11, 15a, 15b, 16, 18, 19	met	Pruess (1987) Pruess and Wu (1993) this paper , Moridis and Pruess (1992, 1995)
two-phase flow of liquid and gas	3, 8, 10	met	Moridis and Pruess (1992, 1995)
B. Constitutive Relations			
accurate description of thermophy: properties	13	met	this paper
dissolution of air in water	13	met	this paper Pruess (1987) Moridis and Pruess (1992)
vapor adsorption	14	met	this paper Pruess (1987) Moridis and Pruess (1992)
vapor pressure lowering due to suction pressure	14	met	this paper; Pruess (1987)
C. Phase Change /interaction			
phase (dis)appearance	2, 10	met	Moridis and Pruess (1992)
phase interference (liquid and gas)	3, 8, 10	met	Moridis and Pruess (1992, 1995)
permeability enhancement from slip flow effects (Knudsen)	17c	met	this paper
binary diffusion in gas phase	3, 17b	met	this paper Pruess (1987) Moridis and Pruess (1992)
vapor-liquid phase change	2, 3, 10	met	Pruess (1987) Moridis and Pruess (1992)

Table 13 (cont.). Requirements Validation Cross-Check

Requirement	Test Case	Acceptance Criteria	Reference
D. Heat Transport			
conduction	7, 12, 17a	met	this paper
convection	4, 5, 9	met	Moridis and Pruess (1992, 1995)
sensible and latent heat changes	2, 3, 5, 9, 10	met	Pruess (1987) Moridis and Pruess (1992, 1995)
conductive heat exchange with impermeable strata	7, 12	met	Pruess and Wu (1993), this paper
coupled fluid and heat flow	2, 3, 4, 7, 10, 12	met	Pruess and Wu (1993) Moridis and Pruess (1992) Pruess (1987)
E. Dimensionality			
1-D	1, 3, 4, 6, 7, 11, 15a, 17a, 17c, 19	met	this paper; Pruess (1987) Pruess and Wu (1993) Moridis and Pruess (1995)
2-D	8, 9, 10, 12, 15b, 16	met	Moridis and Pruess (1992) this paper Moridis and Pruess (1995)
3-D	18	met	this paper
F. Geometry			
Linear	1, 3, 4, 17a, 17b,17c	met	this paper, Moridis and Pruess (1992) Pruess (1987)
Cartesian	8, 12	met	this paper
cylindrical	9, 10	met	Moridis and Pruess (1995) Moridis and Pruess (1992)
radial	2, 6, 7, 11, 19	met	this paper, Pruess and Wu (1993), Pruess (1987) Moridis and Pruess (1995)
irregular	16	met	this paper
G. Grid Generation	8, 12, 17a, 17b, 17c	met	this paper
H. Heterogeneities			
heterogeneous formations flow in porous media	8, 15a, 15b, 18 4, 6, 15a, 15b, 18, 20	met met	this paper Moridis and Pruess (1992, 1995)

Table 13 (cont.). Requirements Validation Cross-Check

Requirement	Test Case	Acceptance Criteria	Reference
flow in fractured media	7, 8, 11	met	this paper Pruess and Wu (1993) Moridis and Pruess (1995)
I. flexible handling of boundary conditions, etc.	8, 10	met	Moridis and Pruess (1992)
J. Other			
automatic time-stepping	all cases	met by its existence	this paper; Pruess (1991)
restart capability	NA	met by its existence	this paper; Pruess (1991)
compatible with TOUGH	1, 2, 3	demonstration that TOUGH and TOUGH2 obtain same results	this paper; Pruess (1987) Moridis and Pruess (1992)
user documentation	all cases	met by its existence	this paper; Pruess (1991)
illustrative sample problems-code demonstration and accuracy	sample problems 1-4 Sect. 5.5 this paper	met by their existence	this paper; Pruess (1991)
internal version control	all cases	met by its existence; see Fig. 4 in this paper	this paper; Pruess (1991)

5. SOFTWARE USER DOCUMENTATION

5.1 Installation Procedures

The distribution media for TOUGH2 varies. For installation options on a work station or mainframe, information should be obtained from the ESTSC distribution center at Oak Ridge[†]. For a PC, the program is installed by inserting the diskette into drive B and typing "install". Instructions for operating TOUGH2 will appear in the "README" file, which is included as Appendix F to this document.

5.2 Hardware and Software Operating Environments

As stated previously, TOUGH2 can be operated in any type of environment: on a mainframe computer, at a workstation, and on a PC or a Macintosh.

5.3 Input and Output

This section describes input and output files, file formats, options, default parameters data files, commands, and execution. TOUGH2 does not specify acceptable ranges of inputs and outputs; these are determined exclusively by whether the results make reasonable sense and require knowledge on the user's part of operative processes. Likewise, any errors that result will come about primarily due to the user's choice of options, parameter values, and problem setup. The MULKOM family of codes, including TOUGH2, has been tested and debugged for over a decade with scores of applications. Only one coding error is known to exist. This occurs in the naming convention for very large grids in the meshmaking RZ2D submodule. The error will be corrected in an updated version of TOUGH2. For code nomenclature see Appendix D.

5.3.1 Preparation of Input Data: TOUGH2 input is provided through a file INPUT, organized into data blocks which are labeled by five-character keywords. With a few exceptions, the order of data blocks is arbitrary. TOUGH2 input formats are compatible with those of TOUGH. Figure 32 gives a listing of TOUGH input formats and indicates a number of optional additional parameters that in TOUGH2 are provided through the same data blocks. TOUGH2 also has a number of new, optional data blocks. These are listed in Table 14, and the corresponding input formats are shown in Figure 33.

[†] Energy Scicence Technology Software Center
P.O. Box 1020, Oak Ridge, Tennessee 37831, U.S.A.
Phone: (423) 576-2606, Fax: (423) 576-2865

Figure 32. TOUGH input formats with TOUGH2 extensions
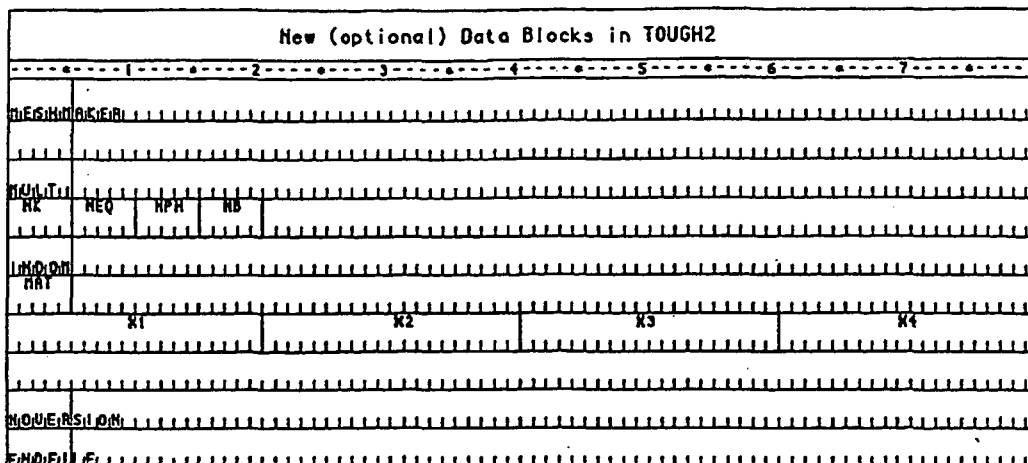
Figure 33. Input formats for new TOUGH2 data blocks

Table 14. New data blocks in TOUGH2 (optional)

Keyword	Function
MESHM	invokes internal mesh generation and processing facilities
MULTI.	allows to select number of fluid components and balance equations per grid block; applicable only with certain EOS modules that offer different options
INDOM	permits domain-specific initialization of thermodynamic conditions
NOVER	if present, optionally suppresses a printout of versions and dates of the program units executed in a TOUGH2 run
ENDFI	alternative to "ENDCY" for closing a TOUGH2 input file; will cause flow simulation to be skipped; useful if only mesh generation is desired

The following discussion first summarizes the new parameters and options of TOUGH2 in the TOUGH data blocks. It then discusses the input formats and choices available through the new data blocks. For a discussion of input variables that are identical to the ones used in TOUGH, one should refer to the *TOUGH User's Guide* (Pruess, 1987).

5.3.2 Enhancements in TOUGH Blocks: Comments or text can be inserted between data blocks anywhere in a TOUGH2 input file. Such records will generate a one-line printed output that says "Have read unknown block label '(first five characters)' - ignore this and continue reading input data", but will otherwise be ignored. (In TOUGH, execution simply stopped when an unknown block label was encountered).

Several of the MOP parameters (first record in block 'PARAM') that control optional printout and some calculational choices, have different options and settings than in TOUGH. Each TOUGH2 run will produce a one-page informative printout of available selections and options chosen. Additional parameters provided through TOUGH data blocks are as follows (see Figure 32). The second (optional) record in block 'ROCKS' has

a parameter GK which is the Klinkenberg parameter b in the gas phase permeability relationship $k = k_0(1+b/P)$. In partially saturated media, vapor diffusion can be considerably enhanced in comparison to the expression given in Eq. A.7, due to phase change effects (condensation/evaporation) at the pore level. Such enhanced diffusion can be modeled by specifying a suitable value, typically or order 1, for the parameter $B= \phi S_g \tau$. This is to be entered as parameter BE in the first record in block PARAM. In block ELEM, AHTX is the contact area of a grid block with the top or bottom boundary of the flow system. This can be used with certain EOS modules for a heat exchange calculation with semi-infinite half spaces that represent the confining beds of a flow system (as in Sample Problem 3, Appendix G). The X, Y, Z data in element records are nodal point coordinates. These are not used at all in TOUGH2, but can be optionally provided in the ELEME block to facilitate plotting.

When working with different EOS modules, there is a need to be able to specify injection of different fluid components (or heat). Table 15 lists the TYPE specifications that can be used in data block GENER in the input file.

Table 15. *Specifications for Generation Types*

Component Index	Code Words (variable "Type" in block GENER)	Component EOS1	EOS2	EOS3	EOS4	EOS5
#1	COM1, MASS, WATE	water1	water	water	water	water
#2	COM2, AIR, WATR	water2	CO_2	air	air	H_2
#3*	COM3	-	-	-	-	-
#4*	COM4	-	-	-	-	-
#NK1[†]	HEAT	heat	heat	heat	heat	heat

*not used in EOS1 through EOS5
[†]NK1=NK+1

Thus, a user working with the "two waters" option of EOS module EOS1 would specify TYPE=COM1 (or MASS, or WATE) to inject "water 1", while specification of TYPE=COM2 (or AIR, or WATR) would allow injection of "water 2".

5.3.3 Input Formats for MESHMAKER: At present there are three sub-modules available in MESHMAKER (see Figure 34): keywords 'RZ2D' or 'RZ2DL' invoke generation of one- or two-dimensional radially symmetric R-Z meshes; 'XYZ' initiates generation of a one, two, or three-dimensional Cartesian X-Y-Z mesh; and 'MINC' calls a modified version of the 'GMINC' program (Pruess, 1983a) to sub-partition a "primary" porous medium mesh into a secondary mesh for fractured media, using the method of "multiple interacting continua" (Pruess and Narasimhan, 1982, 1985). The meshes generated under keyword 'RZ2D' or 'XYZ' options, or assignment of 'ELEME' and 'CONNE' blocks in the INPUT file must precede the MESHMAKER/MINC data. See Pruess (1991) for preparation of input data for the three MESHMAKER sub-modules. Complicated geometric settings may require application of external mesh generators.

MESHMAKER - Two-dimensional R-Z Grids

MESHMAKER

RZ2D

RRAD
NRAD

RC(1)   RC(2)   RC(3)   RC(NRAD)

EQUID
NEQU   DR

LOGAR
NLOG   RLOG   DR

LAYER
NLAY

H(1)   H(2)   H(3)   H(NLAY)

MESHMAKER-Rectilinear Grids

MESHMAKER

XYZ
DEG

NX1   DEL
DX(1)   DX(2)   DX(3)   DX(NX1)

NX2   DEL
DX(NX1+1)   DX(NX1+2)   DX(NX1+NX2)

NY   DEL
DY(1)   DY(2)   DY(3)   DY(NY)

NZ   DEL
DZ(1)   DZ(2)   DZ(3)   DZ(NZ)

MESHMAKER - MINC Processing for Fractured Media

MESHMAKER

MINC
TYPE   DUAL
PART
J NVOL WHERE   PAR(1)   PAR(2)   PAR(3)   PAR(4)   PAR(5)   PAR(6)   PAR(7)
VOL(1)   VOL(2)   VOL(3)   VOL(NVOL)

Figure 34. Input formats for MESHMAKER module.

5.4 User Features

Much of the data handling in TOUGH2 is accomplished through disk files which are written in a format of 80 characters per record, so that code users can edit and modify them with any normal text editor. Table 16 summarizes the disk files other than (default) INPUT and OUTPUT used in TOUGH2. Most of these are also used in TOUGH, and files with the same names in both codes have identical formats. The use and function of these files is described in the following sections and in the Appendix G Sample Problems (Pruess, 1991). Further information is available in the *TOUGH User's Guide* (Pruess, 1987).

Table 16. TOUGH2 Disk Files

File	Use
MESH	written in subroutine INPUT from ELEME and CONNE data, or in module MESHMAKER from mesh specification data
	read in REFILE to initialize all geometry data arrays used to define the discretized flow problem
GENER	written in subroutine INPUT from GENER data
	read in RFILE to define nature, strength, and time-dependence of sinks and sources
INCON	written in subroutine INPUT from INCON data
	read in RFILE to provide a complete specification of thermodynamic conditions
SAVE	written in subroutine WRIFI to record thermodynamic conditions at the end of a TOUGH2 simulation run
	compatible with formats of file or data block INCON for initializing a continuation run
MINC	written in module MESHMAKER with MESH-compatible specifications, to provide all geometry data for a fractured-porous medium mesh (double porosity, dual permeability, etc.)
	read (optionally) in subroutine RFILE to initialize geometry data for a fractured-porous system
LINEQ	written in linear equation solver "MA28", to provide informative messages on linear equation solution
TABLE	(optional; available only with certain EOS modules) written in subroutine QLOSS to record data on heat exchange with impermeable confining layers, or heat and fluid exchange with embedded matrix blocks in a fractured-porous medium
	read in QLOSS in a continuation run
VERS	written in all TOUGH2 program units with informational message on version number, date, and function
	read in main program "TOUGH2" and printed to default OUTPUT at the conclusion of a TOUGH2 simulation run; printing of version information is suppressed when keywork 'NOVER' is present in INPUT file

5.5 Summary

Verification of this phase of the Software Life Cycle which relates to installation, user documentation, and provision of code demonstration cases was completed by providing with this package the report *TOUGH2 - A General Purpose Numerical Simulator for Multiphase Fluid and Heat Flow* (Pruess, 1991) and the sample problems described in Appendix G which demonstrate how the user sets up certain types of problems and manipulates various aspects of the code.

5.6 Version History

TOUGH2 was released in May 1991 and transferred to the National Energy Software Center, which performed some tests on it before the Center was disbanded. The code was then transferred to DOE's Energy Science and Technology Software Center (ESTSC). TOUGH2 remained unchanged until November 1994 when the T2CG1 package of conjugate gradient solvers was added. The November 1994 Version 1.11 of TOUGH2 is the version described in this software qualification package. An adaptation of this version for PC's was transferred to ESTSC in January 1995. It includes only very minor modifications, and is not considered a separate, distinct version of the code. Additional TOUGH2 modules are in use, e.g. a module with hydrodynamic dispersion. These will be released in due course, following extensive testing, documentation, and some packaging. When they are ready for release, a new version of TOUGH2 will be sent to ESTSC.

ACKNOWLEDGMENTS

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APPENDIX A. MASS AND ENERGY BALANCES

The basic mass- and energy-balance equations solved by MULKOM, TOUGH and TOUGH2 can all be written in the following general form:

$$\frac{d}{dt} \int_{V_n} M^{(\kappa)} dV = \int_{\Gamma_n} F^{(\kappa)} \bullet n \, d\Gamma + \int_{V_n} q^{(\kappa)} dV \tag{A.1}$$

The integration here is over an arbitrary subdomain Vn of the flow system under study, which is bounded by the closed surface Γ_n. The quantity M appearing in the accumulation term denotes mass or energy per unit volume, with $\kappa = 1, \ldots,$ NK labeling the mass components, and $\kappa = NK + 1$ for the heat "component."

The general form of the mass accumulation term is

$$M^{(\kappa)} = \phi \sum_{\beta=1}^{NPH} S_\beta \rho_\beta X_\beta^{(\kappa)} \tag{A.2}$$

The total mass of component κ is obtained by summing over all fluid phases $\beta = 1, \ldots,$ NPH. S_β is the saturation (volume fraction) of phase β, ρ_β is density of phase β, and $X_\beta^{(\kappa)}$ is the mass fraction of component κ present in phase β. Similarly, the heat accumulation term in a multi-phase system is

$$M^{(NK+1)} = \phi \sum_{\beta=1}^{NPH} S_\beta \rho_\beta u_\beta + (1-\phi) \rho_R C_R T \quad , \tag{A.3}$$

where u_β denotes internal energy of fluid phase β.

The mass flux term is a sum over phases

$$F^{(\kappa)} = \sum_{\beta=1}^{NPH} X_\beta^{(\kappa)} F_\beta \tag{A.4}$$

for $\kappa = 1, \ldots,$ NK. Individual phase fluxes are given by a multi-phase version of Darcy's law:

$$F_\beta = -\kappa \frac{\kappa_r \beta}{\mu_\beta} \rho_\beta \left(\nabla P_\beta - \rho_\beta g \right) \tag{A.5}$$

Here k is absolute permeability, $k_{r\beta}$ is relative permeability of phase β, μ_β is viscosity, and

$$P_\beta = P + P_{c,\beta} \tag{A.6}$$

is the pressure in phase β, which is the sum of the pressure P of a reference phase, and the capillary pressure of phase β relative to the reference phase. g denotes the vector of gravitational acceleration. Gas phase permeability can be specified to depend on pressure, according to the Klinkenberg relationship $k = k_0(1 + b/P)$, where k_0 is absolute

permeability at high pressure (Klinkenberg, 1941). In addition to Darcy flow, TOUGH2 also includes binary diffusion in the gas phase for fluids with two gaseous (or volatile) components κ, κ'

$$\mathbf{f}^{(\kappa)}_{\beta=gas} = -\phi\, S_g\, \tau D_{\kappa\kappa'}\rho_g\, \nabla\, X_g^{(\kappa)} \tag{A.7}$$

$D_{\kappa,\kappa'}$ is the coefficient of binary diffusion which depends on the nature of the gaseous components and on pressure and temperature. τ is a tortuosity factor. When binary diffusion is present the flux-term (A.7) simply gets added to that of (A.4).

Heat flux contains conductive and convective components (no dispersion)

$$\mathbf{F}^{(NK+1)} = -K\nabla T + \sum_{\beta} h_\beta \mathbf{F}_\beta \tag{A.8}$$

where K is thermal conductivity of the medium, and $h_\beta = u_\beta + P/\rho_\beta$ is the specific enthalpy of phase β.

MULKOM and TOUGH2 can model vapor pressure lowering due to capillary and phase adsorption effects. This is represented by Kelvin's equation (Edlefsen and Anderson, 1943):

$$P_v(T,S_l) = f_{VPL}(T,S_l) \cdot P_{sat}(T) \tag{A.9a}$$

where

$$f_{VPL} = \exp\left\{\frac{m_l \cdot P_c(S_l)}{\rho_l R(T+273.15)}\right\} \tag{A.9b}$$

is the vapor pressure lowering factor. P_{sat} is saturated vapor pressure of bulk liquid, P_c is the difference between liquid and gas phase pressures, m_l is the molecular weight of the liquid, and R is the universal gas constant.

APPENDIX B. SPACE AND TIME DISCRETIZATION[†]

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

$$\int_{V_n} M \, dV = V_n \, M_n \tag{B.1}$$

where 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}:

$$\int_{\Gamma_n} F^\kappa \bullet n \, d\Gamma = \sum_m A_{nm} \, F_{nm} \tag{B.2}$$

Here F_{nm} is the average value of the (inward) normal component of **F** over the surface segment A_{nm} between volume elements V_n and V_m. The discretization approach used in the integral finite difference method and the definition of the geometric parameters are illustrated in Fig. 35.
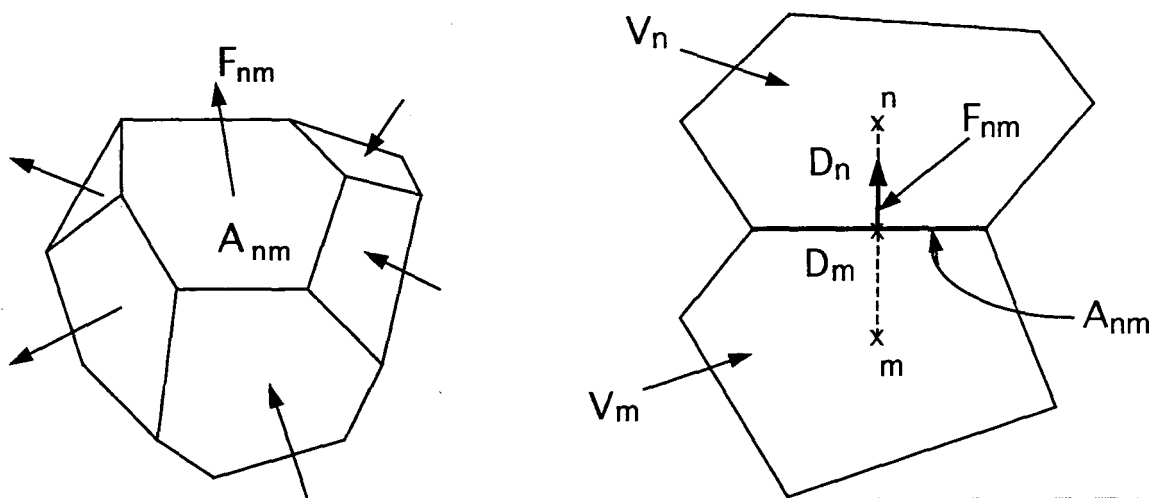
Figure 35. *Space discretization and geometry data in the integral finite difference method.*

The discretized flux is expressed in terms of averages over parameters for elements V_n and V_m. For the basic Darcy flux term, Eq. (A.5), we have

$$F_{\beta,nm} = -k_{nm} \left[\frac{k_{r\beta}\, \rho_\beta}{\mu_\beta} \right]_{nm} \left[\frac{P_{\beta,n} - P_{\beta,m}}{D_{nm}} - \rho_{\beta,nm}\, g_{nm} \right] \quad (B.3)$$

where the subscripts (nm) denote a suitable averaging at the interface between grid blocks n and m (interpolation, harmonic weighting, upstream weighting). D_{nm} is the distance between the nodal points n and m, and g_{nm} is the component of gravitational acceleration in the direction from m to n.

The discretized form of the binary diffusive flux in the gas phase is

$$J_{g,nm}^{\kappa} = -\left(\phi\, S_g\, \tau_g\right)_{nm} \left(D_g^\kappa\right)_{nm} \rho_{g,nm} \frac{X_{g,n}^\kappa - X_{g,m}^\kappa}{D_{nm}} \quad (B.4).$$

For the group (ϕ S τ) geometric weighting is used at the interface, while D and ρ are averaged between grid blocks n and m.

Substituting Eqs. (B.1) and (B.2) into the governing Eq. (A.1), a set of first-order ordinary differential equations in time is obtained.

$$\frac{dM_n^\kappa}{dt} = \frac{1}{V_n} \sum_m A_{nm}\, F_{nm}^\kappa + q_n^\kappa \quad (B.5)$$

Time is discretized as a first order finite difference, and the flux and sink and source terms on the right hand side of Eq. (B.5) are evaluated at the new time level, $t^{k+1} = t^k + \Delta t$, to obtain the numerical stability needed for an efficient calculation of multiphase flow. This treatment of flux terms is known as "fully implicit," because the fluxes are expressed in terms of the unknown thermodynamic parameters at time level t^{k+1}, so that these unknowns are only implicitly defined in the resulting equations; see e.g. Peaceman (1977). The time discretization results in the following set of coupled non-linear, algebraic equations

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

$$= 0 \quad (B.6)$$

where we have introduced residuals $R_n^{\kappa,k+1}$. For each volume element (grid block) V_n there are NEQ equations ($\kappa = 1, 2, \ldots$ NEQ; usually, NEQ = NK + 1), so that for a flow system with NEL grid blocks (B.6) represents a total of NEL • NEQ coupled non-linear equations. The unknowns are the NEL • NEQ independent primary variables $\{x_i; i = 1, \ldots,$ NEL • NEQ$\}$ which completely define the state of the flow system at time level t^{k+1}. These equations are solved by Newton/Raphson iteration, which is implemented as follows. We introduce an iteration index p and expand the residuals $R_n^{\kappa,k+1}$ in Eq. (B.6) at iteration step p + 1 in a Taylor series in terms of those at index p.

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

$$+ \dots = 0 \tag{B.7}$$

Retaining only terms up to first order, we obtain a set of NEL • NEQ linear equations for the increments $(x_{i,p+1} - x_{i,p})$:

$$- \sum_i \frac{\partial R_n^{\kappa,k+1}}{\partial x_i}\bigg|_p (x_{i,p+1} - x_{i,p}) = R_n^{\kappa,k+1}(x_{i,p}) \tag{B.8}$$

All terms $\partial R_n/\partial x_i$ in the Jacobian matrix are evaluated by numerical differentiation. Eq. (B.8) is solved by sparse direct matrix methods (Duff, 1977) or iteratively by means of preconditioned conjugate gradients (Moridis and Pruess, 1995). Iteration is continued until the residuals $R_n^{\kappa,k+1}$ are reduced below a preset convergence tolerance. The selection and switching of primary variables in a TOUGH2 solution depend on the phase conditions. The variable switching procedure affects the updating for secondary dependent variables but does not affect the equation setup because the equations are still mass and energy conservation equations for each block.

$$\left| \frac{R_{n,p+1}^{\kappa,k+1}}{M_{n,p+1}^{\kappa,k+1}} \right| \le \varepsilon_1 \tag{B.9}$$

The default (relative) convergence criterion is $\varepsilon_1 = 10^{-5}$. When the accumulation terms are smaller than ε_2 (default $\varepsilon_2 = 1$), an absolute convergence criterion is imposed, $|R_n^{\kappa,k+1}| \le \varepsilon_1 \cdot \varepsilon_2$. Convergence is usually attained in 3 - 4 iterations. If convergence cannot be achieved within a certain number of iterations (default 8), the time step size Δt is reduced and a new iteration process is started.

It is appropriate to add some comments about our space discretization technique. The entire geometric information of the space discretization in Eq. (B.6) 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 (B.3, B.4) can be expressed in terms of average conditions in grid blocks. A general requirement 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), Eq. (B.6) is identical to a conventional finite difference formulation (e.g. Peaceman, 1977).

APPENDIX C. DESCRIPTION OF FLOW IN FRACTURED MEDIA[#]

Figure 36 illustrates the classical double-porosity concept for modeling flow in fractured-porous media as developed by Warren and Root (1963). Matrix blocks of low permeability are embedded in a network of inter-connected fractures. Global flow in the reservoir occurs only through the fracture system, which is described as an effective porous continuum. Rock matrix and fractures may exchange fluid (or heat) locally by means of "interporosity flow," which is driven by the difference in pressures (or temperatures) between matrix and fractures. Warren and Root approximated the interporosity flow as being "quasi-steady," with rate of matrix-fracture interflow proportional to the difference in (local) average pressures.
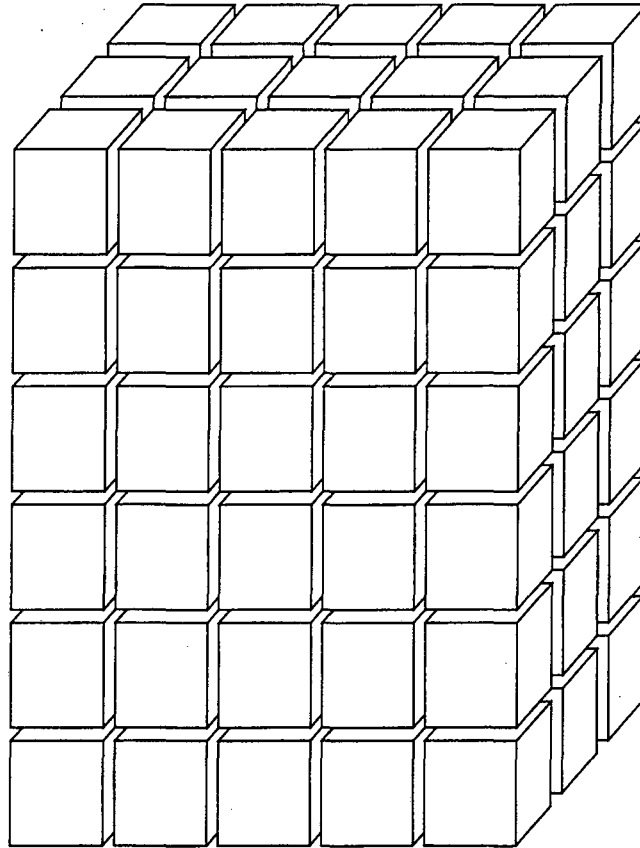
Figure 36. Idealized "double porosity" model of a fractured porous medium.

The quasisteady approximation is applicable to isothermal single phase flow of fluids with small compressibility, where pressure diffusivities are large, so that pressure changes in the fractures penetrate quickly all the way into the matrix blocks. However, for multiphase flows, or coupled fluid and heat flows, the transient periods for interporosity flow can be very long (tens of years). In order to accurately describe such flows it is necessary to resolve the driving pressure, temperature and mass fraction gradients at the matrix/fracture interface. In the method of "multiple interacting continua" (MINC; Pruess and Narasimhan, 1982, 1985), resolution of these gradients is achieved by appropriate subgridding of the matrix blocks, as shown in Fig. 37. The MINC concept is based on the

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[#] Adapted from TOUGH2 report, Pruess (1991).

notion that changes in fluid pressures, temperatures, phase compositions, etc. due to the presence of sinks and sources (production and injection wells) will propagate rapidly through the fracture system, while invading the tight matrix blocks only slowly. Therefore, changes in matrix conditions will (locally) be controlled by the distance from the fractures. Fluid and heat flow from the fractures into the matrix blocks, or from the matrix blocks into the fractures, can then be modeled by means of one-dimensional strings of nested grid blocks, as shown in Fig. 37.
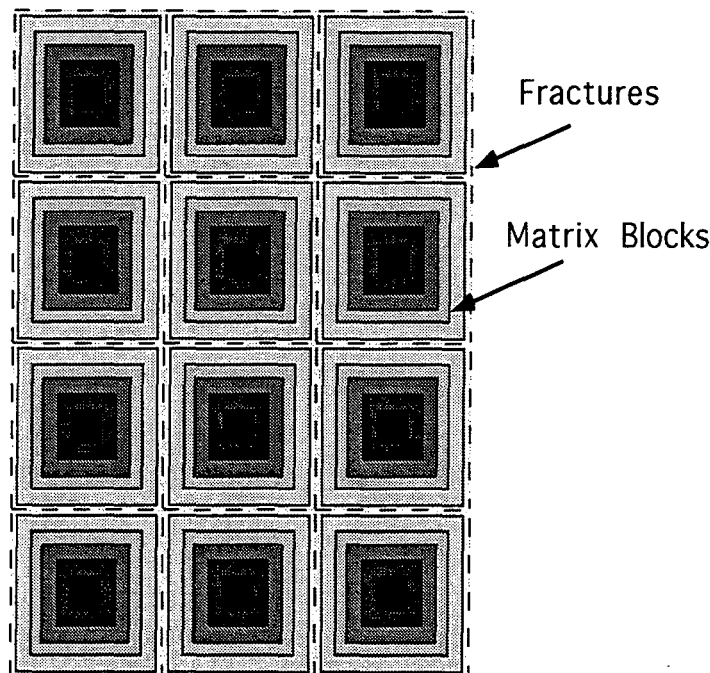
Figure 37. Subgridding in the method of "multiple interacting continua" (MINC).

In general it is not necessary to explicitly consider subgrids in all of the matrix blocks separately. Within a certain reservoir subdomain (corresponding to a finite difference grid block), all fractures will be lumped into continuum # 1, all matrix material within a certain distance from the fractures will be lumped into continuum # 2, matrix material at larger distance becomes continuum # 3, and so on. Quantitatively, the subgridding is specified by means of a set of volume fractions VOL(j), j = 1, ..., J, into which the "primary" porous medium grid blocks are partitioned. The MINC-process in the MESHMAKER module of T2VOC operates on the element and connection data of a porous medium mesh to calculate, for given data on volume fractions, the volumes, interface areas, and nodal distances for a "secondary" fractured medium mesh. The information on fracturing (spacing, number of sets, shape of matrix blocks) required for this is provided by a "proximity function" PROX(x) which expresses, for a given reservoir domain V_o, the total fraction of matrix material within a distance x from the fractures. If only two continua are specified (one for fractures, one for matrix), the MINC approach reduces to the conventional double-porosity method. Full details are given in a separate report (Pruess, 1983a).

The MINC-method as implemented in the MESHMAKER module can also describe global matrix-matrix flow. Figure 38 shows the most general approach, often referred to as "dual permeability," in which global flow occurs in both fracture and matrix continua. It is also possible to permit matrix-matrix flow only in the vertical direction. For any given

fractured reservoir flow problem, selection of the most appropriate gridding scheme must be based on a careful consideration of the physical and geometric conditions of flow. The MINC approach is not applicable to systems in which fracturing is so sparse that the fractures cannot be approximated as a continuum.
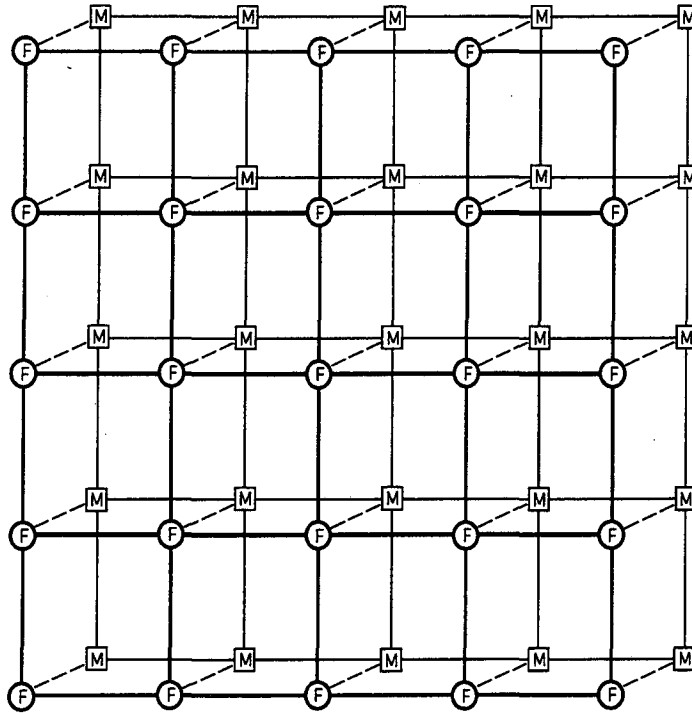
Figure 38. Flow connections in the "dual permeability" model. Global flow occurs between both fracture (F) and matrix (M) grid blocks. In addition there is F-M interporosity flow.

APPENDIX D. NOMENCLATURE

A	area, m^2
b	Klinkenberg parameter, Pa
B	effective vapor diffusion strength parameter, replaces the group $\phi S_g \tau$ in Eq. (A.7), dimensionless
C	specific heat, J/kg·°C
d	penetration depth for heat conduction, m
D	diffusion coefficient, m^2/s
D	distance, m
DELX	small increments of primary variables for computing numerical derivatives
DX	increments of primary variables during Newton-Raphson iteration
f	diffusive flux, $kg/m^2 \cdot s$
f_{VPL}	vapor pressure lowering factor, dimensionless (Eq. A.9)
F	mass or heat flux, $kg/m^2 \cdot s$ or W/m^2
g	gravity acceleration, m/s^2
h	specific enthalpy, J/kg
i	index of primary thermodynamic variable
J	Jacobian matrix
k	intrinsic permeability, $m^2 (10^{-12} m^2 \approx 1\ darcy)$
k_r	relative permeability, dimensionless
K	thermal conductivity, W/m·°C
K_H	Henry's constant, Pa
m	index of volume element (grid block)
m_{air}	molecular weight of air
m_{H_2O}	molecular weight of water
m_l	molecular weight of liquid
M	accumulation term in mass or energy balance equation, kg/m^3 or J/m^3
n	index of volume element (grid block)
N	index of volume element (grid block)
NB	number of secondary parameters other than mass fractions in PAR array (usually NB = 6)
NBK	NB + NK
NEL	number of volume elements (grid blocks) in flow domain
NEQ	number of balance equations per volume element; NEQ = NK1 or NEQ = NK
NK	number of mass components present
NK1	NK + 1
NLOC	storage location after which primary variables start for grid block N; NLOC = (N – 1)*NK1
NLOC2	storage location after which secondary parameters start for grid block N;NLOC2 = (N – 1*(NEQ + 1)*NSEC
NPH	number of phases
NSEC	number of secondary parameters per volume element; NSEC = NPK*NBK + 2
p	index in Newton-Raphson iteration
P	pressure, Pa
$P_{a.e.}$	air entry pressure, Pa
P_c	capillary pressure, Pa

P_{sat}	saturated vapor pressure, Pa
q	volumetric sink or source rate, $kg/m^3 \cdot s$ or W/m^3
r	radius, m
R	residuals in mass or energy balance equations, kg/m^3 or J/m^3
R	universal gas constant, $8314 \cdot 56$ J/°C·mole
S	saturation (void fraction occupied by a fluid phase), dimensionless
t	time, s
T	temperature, °C
u	specific internal energy, J/kg
V	volume, m^3
x	distance, m
x,X	primary thermodynamic variable
$x_\beta^{(\kappa)}$	mol fraction of component κ in phase β
$X_\beta^{(\kappa)}$	mass fraction of component κ in phase β
$z = \log[r/(t)^{1/2}]$	similarity variable for cylindrical flow geometry

Greek

β	phase index (β = liquid, gas)
θ	thermal diffusivity, m^2/s
κ	component index
ρ	density, kg/m^3
Γ	area, m^2
ϕ	porosity, dimensionless
τ	tortuosity factor, dimensionless
μ	viscosity, Pa·s

Subscripts

a	air
β	phase
c	capillary
f	fracture
g	gas
i	initial
l	liquid
r	relative
R	rock
v	vapor

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APPENDIX F. README FILE

TOUGH2 Version 1.11 January 1994
with preconditioned conjugate gradient module T2CGl
(PC Version December 1994)

RE@.ME RFM.ME READ.ME READ.ME
Update 12/94

This flyer contains brief instructions for installing and running TOUGH2 under DOS or WINDOWS operating systems on an IBM PC or compatible. The TOUGH2-PC code can be executed on 386 machines or better. With present dimensioning (PARAMETER statements in main program) for up to 800 grid blocks and 2400 connections, memory requirements are approximately 4 Mb of RAM when one of the conjugate gradient solvers is being used. When using the direct solver MA28 the same 4 MB of RAM will allow the execution of models with a maximum of 500 grid blocks and 1500 connections.

The TOUGH2 code requires 64-bit arithmetic, while the 386, 486 and 585 (Pentium) machines have 32-bit wordlength. Accordingly, in the TOUGH2-PC version all floating point variables have been declared "real*811 (double precision), and all floating point constants have been converted from Ew.d to Dw.d format. The only other changes in TOUGH2-PC relative to the mainframe version are:

(1) Subroutines SECOND, ELDAYS, and ADDAYS have been appended to module t2cgi for obtaining CPU times.

(2) FORMAT statements with more than 127 'XI field spaces have been modified according to 129X --> 12OX,9X, to avoid a problem with the LAHEY compiler, Version 5.XX.

No modifications in function names are needed, because TOUGH2 uses generic FORTRAN77 function names throughout.

TOUGH2-PC is distributed on a 3.511 high-density diskette, formatted under the MS-DOS operating system for IBM PC's or compatibles. THOUGH2PC is set to be compiled and linked using a LAHEY Fortran compiler version 5.00 or better. other compilers that can access extended memory (memory beyond 1 Mb) may be used instead with minor changes to the CPU timing subroutines. A quick fix to the CPU timing routine is explained in detail in the 'Additional notes' section in this flyer.

The distribution diskette includes the following 17 files:

(1) read.me - the file you're reading

(2) t2cgl.for - contains the main program of TOUGH2, with PARAMETER statements for flexible dimensioning of all major arrays, and initialization of disk files; also includes a revised version of subroutine LINEQ that calls a suite of preconditioned conjugate gradient routines; t2cgl.for replaces the program module t2m.for of the previous version of TOUGH2 (Version 1.0, April 1991);

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(3) meshm.for - module with internal mesh generation capabilities

(4) eosl.for - equation of-st@t6@;fo@,;water-or,@two-waters

(5) eos2.for - equation of state for water/CO2 mixtures

(6) eos3.for - equationof state for water/air (similar to TOUGH)

(7) eos4.for - equation of state for water/air with vapor pressure lowering capability

(8) eos5.for - equation of state for water/hydrogen; otherwise similar to eos3.for

(9) t2f.for - the core module of TOUGH2; it reads input data, initializes arrays and parameters, sets up the Newton-Raphson iteration, and performs time stepping; it also contains the water property routines (steam table equations) and the relative permeability and capillary pressure function which are Used in the equation-of-state modules

(10) ma28.for linear equation solver from the Harwell subroutine librar written by I.S. Duff. (MA28 is subject to proprietary restrictions, and use outside of TOUGH2 requires proper license. Contact: The Harwell Subroutine Library Liaison officer, Mr. S. Marlow, Building 8.9, Harwell Laboratory, Didcot, Oxon OXII ORA, United Kingdom.)

(11) makefile file that contains the required commands and instructions to compile, link and create an executable file using the LAHEY Fortran compiler Ver. 5.XX. Can be modified to customize installation of TOUGH2, or to compile and link the code with other equation of state (EOS) modules.

(12) install.bat file to install and create the required directories to start using the program according to the suggested structure in the "makefile" file

(13) delet.bat utility file to erase TOUGH2 generated output files between runs. This file should be used with caution and customized to the specific needs of a run.

In addition, there are four input files for sample problems.

(14) sami - input file for sample problem 1 (code demonstration and comparison with TOUGH)

(15) rhp - input file for sample problem 2 (heat pipe in cylindrical geometry)

(16) rvf - input file for sample problem 3 (heat sweep in a vertical fracture)

(17) rfp - input file for sample problem 4 (five-spot geothermal production/injection)

Files (2) - (10) contain the TOUGH2 source code. The only change in comparison to version 1.0, April 1991, is the replacement of file t2m.for with t2cgi.for, the preconditioned conjugate gradient module. When compiling and linking TOUGH2, t2cgl.for should come first, then meshm.for, then the desired EOS-module, then t2f.for, and finally ma28.for. Note that only one of the EOS modules must be linked at a time.

On an IBM PC, or compatible 386 machine or better with a DOS-based operating system, using LAREY compiler Ver. 5.00 or later, small simulations may be run from

DOS. The number of elements in a simulation model will depend on the amount of extended memory (XMS) available in the machine. For big simulation jobs using the LAHEY compiler Ver. S.XX, it is necessary that all extended memory (memory beyond 1 Mb) must be made available to the LAHEY compiler prior to compilation and linking. To perform this operation all Terminate and Stay Resident Programs (TSR) must be removed. it is recommended to use stripped-down versions of the CONFIG.SYS and AUTOEXEC.BAT files specific for running TOUGH2. MS-DOS Version 6.0 or later allow the use of multiple CONFIG.SYS and AUTOEXEC.BAT files, see the MS-DOS and FORTRAN compiler manuals for details. Running TOUGH2 under WINDOWS using the LAHEY Fortran compiler, has the advantage of accessing virtual memory (temporary space on a hard drive). This allows large simulation jobs to run on machines with limited amount of RAM. The trade-off is a slower execution due to data swapping between physical RAM and virtual memory. On machines with 16 MB of RAM and more, it is possible to run TOUGH2 under WINDOWS in the background and use other WINDOWS application in the foreground.

To install and run TOUGH2 using the LAHEY Fortran compiler Ver. 5.XX proceed as follows. (This procedure assumes that the compiler is properly installed)

(1) Insert the distribution diskette in drive B:, type INSTALL and press <enter>. The install file will create a TOUGH2 directory, and copy TOUGH2-PC into this directory. It will also create a DEVELOP subdirectory into which it will copy the input files for the sample problems.

(2) Customize the "makefile" file as desired.

(3) Within the TOUGH2 directory, type the following command:

        make

        The code will then be compiled and linked and, if the "makefile" file provided on the distribution diskette was not modified, an executable Ilt2eosl.exell incorporating the EOS1 fluid property module will be written to the TOUGH2\DEVELOP directory.

        To check on proper code installation, within the TOUGH2\DEVELOP directory execute sample problem No.4, five-spot geothermal production and injection, with the following command.

        t2eosl <rfp >rfp.out

        The first part of the command uploads the Ilt2eosl.exell file and runs it using the 'Irfpll file as the input deck. The output is redirected to the 'Irfp.out" file. The ll>rfp.out" part of the command is optional; if it is not present, all output will be displayed on the screen.

Additional notes.

        An effort was made to have the TOUGH2 source code comply with the ANSI X3.9-1978 (FORTRAN 77) standard, and on most machine and compiler combinations, the code should compile and run without modifications. TOUGH2 makes several calls to an external routine "SECOND" for obtaining elapsed CPU times, such as

        CALL SECOND(TZERO).

The PC version of TOUGH2 includes the subroutines SECOND, ADDAYS and ELDAYS that work together to provide the elapsed CPU times, and are compatible with the LAHEY Fortran compiler. Different compilers have different conventions for obtaining CPU time, and appropriate adjustments must be made. In some cases no facility for assigning CPU time may be available; the user may then relinquish the CPU timing by replacing the subroutine SECOND at the end of file t2m.for with a dummy routine, as follows.

```
SUBROUTINE SECOND(T)
REAL*8 T
CHARACTER ELTIME*11, FECHA*8
COMON /ELTIM/ELTIME, FECRA
T=0.DO
ELTIME='00:00:00.00'
FECHA ='01/01/01'
RETURN
END
```

This dummy subroutine will avoid an "unsatisfied external,, error; all execution times and dates will be reported as 0.0 and 01, respectively, in the printout.

The file t2cgl.for includes the following routines:

(i)   revised versions of the program units normally supplied in t2m.for,

(ii)   a version of subroutine LINEQ that is appropriately modified for interfacing with the conjugate gradient solvers, and

(iii) a set of preconditioned conjugate gradient routines.

The presence of a modified version of subroutine LINEQ in t2cgl.for will create a situation of "duplicate names" during the linking process, as a subroutine LINEQ is also present in standard TOUGH2 (file t2f.for). On most computers the linker will simply use the first program unit with a given name, and will ignore subsequent program units with the same name. On some computers the presence of duplicate names during linking will create a fatal error. The simplest way to avoid this is to change the names of the unwanted program units. Specifically, the name conflict can be avoided by renaming LINEQ in t2f.for to LINEX, say, prior to compilation and linking. In the PC version of TOUGH2 LINEQ was removed from t2f.for.

The only user-definable input parameter associated with the conjugate gradient module is MOP(21) in block PARAM, which selects different solvers as follows.

MOP(21) =   0:   default; is set internally to MOP(21) = 3.
            1:
            2:   direct solution with MA28 (as in TOUGH2, Version 1.0). routine
                 DSLUBC: biconjugate gradient solver with incomplete LU-
                 factorization.
            3:   routine DSLUCS: Lanczos-type biconjugate gradient solver with
                 incomplete LU-factorization.
            4:   routine DSLUGM: generalized minimum residual solver with

~incomplete LU-@tactori-z-a-tion.@:.-

Apart from the choice of the linear equation solver, there are no userdefinable parameters, and the conjugate gradient package would be run with unmodified TOUGH2 input files.

The computational work for iterative solvers increases much less with problem size and matrix bandwidth than is the case for direct solvers. Therefore, iterative solution is the method of choice for virtually all 3-D problems, and for I-D and 2-D problems with more than a few thousand simultaneous equations. Present dimensioning of the PC version of t2cgi.for is for up to 800 grid blocks and up to 3 ecluations per grid block. Maximum problem size can be easily changed in PARAMETER statements in the main program. If the number of grid blocks exceeds 4 digits (9999), FORMAT statement # IS05 in subroutine RPILE in *t2f.for* must be changed from 2014 to 16IS.

Iterative solvers such as conjugate gradients do not, generally speaking, have the same robustness as direct solution techniques, and the performance of the different algorithms is problem-dependent. The default solver option invokes the LancZOB-type biconjugate gradient solver which often is the most computationally efficient. Our simulations of a broad variety of flow problems indicate that each of the 3 conjugate gradient solvers included in the T2CGI package is optimal for certain cases, while failing for others (Moridis et al., 1994). Therefore, for any given flow problem, users are encouraged to experiment and try the different solvers offered.

As mentioned before, T2CGI requires no user-definable parameters other than the choice of linear equation solver. Occasionally users may wish to modify the default settings for iteration and convergence parameters. These parameters are defined upon the first call (ICALL = 1) in subroutine LINEQ in module T2CGI, as illustrated in the following code fragment.

```
        IF(ICALL.EQ.1) THEN
        WRITE(11,899)
899 FORMAT(6X,ILINEQ    0.91 CG 31 JANUARY    19941,6X,
        XIINTERFACE FOR LINEAR EQUATION SOLVERS'/
        X47X,ICAN CALL MA28 OR A PACKAGE OF CONTUGATE GRADIENT',
        XI SOLVERS')
c
        MATSLV=MOP(21)
        IF(MATSLV.EQ.O.OR.MATSLV.GT.4) MATSLV=3
        NMAXIT=MAX(20,NEL*NEQ/10)
        ICLOSR=2
        IF(MATSLV.EQ.4) ICLOSR=O
        CLOSUR=I.D-6
        ISYM=O
        IL7NIT=O
        NVECTR=30
        SEED=1.D-25
        ENDIF
```

For very difficult problems, it may be necessary to tighten the convergence criterion CLOSUR beyond the default of I.D-6, and to increase the maximum number of iterations beyond the value specified in NMAXIT (NEL*NEQ is the order of the matrix of the linear equation system). Information on convergence behavior for each Newtonian iteration is

written onto a disk file ILINEQI.

Files (14) - (17) contain input files for the sample problems presented in the TOUGH2 report. Users should run several of the sample p@o@iems@ to check on proper code installation. Due to machine-dep@ndent roundoff, TOUGH2 may produce slightly different results on different computers. For same-size time steps, all primary variables (pressure P, temperature T, saturation 9, etc.) and their changes (DX1, DX2 ....) should agree to typically four digits or better. However, on different computers the iteration sequence for a time step may be slightly different, and occasionally a different number of iterations may be required for convergence. If automatic time stepping is used, a different number of iterations for convergence may subsequently cause different-size time steps to be taken; naturally this will then produce somewhat larger discrepancies in results because of different time truncation errors.

Of all the numbers processed by TOUGH2, the most sensitive are the residuals, i.e., the differences between left hand sides (accumulation terms) and right hand sides (flow terms) of the governing equations. During the Newton/Raphson iteration process these residuals are reduced to smaller and smaller values, until they drop below specified convergence tolerances. As convergence is approached, the residuals are subject to increasingly severe numerical cancellation, arising from subtracting two numbers with diminishing difference. Maximum residuals are (optionally printed during the iteration process as "MAX. RES.", and are also printed in the header of a full time step printout (as "MAX. RES." or "RERMII). These numbers can serve as a convenient check when evaluating reproducibility of code applications. Small numerical differences due to roundoff etc will first show up in different values for "MAX. RES.", long before giving any visible changes in primary variables or their increments.

TOUGH2 is documented in:

> K. Pruess, TOUGH2 - A General-Purpose Numerical Simulator for
> Multiphase Fluid and Heat Flow, Lawrence Berkeley Laboratory Report
> LBL - 29400, May 1991.

The TOUGH2 report is not a self-contained free standing document. For instructions on preparing input data, users also need the following report:

> K. Pruess, TOUGH User's Guide, Lawrence Berkeley Laboratory Report
> LBL - 20700, June 1987 (also available as Nuclear Regulatory
> Commission Report NUREG/CR-4645).

Information on the conjugate gradient algorithms and applications to large 2-D and 3-D flow problems are presented in:

> Moridis, G., K. Pruess, E. Antunez, and C. Oldenburg. T2CGI, A Package of
> Preconditioned Conjugate Gradient Solvers for the TOUGH2 Family of Codes,
> Lawrence Berkeley Laboratory Report LBL-35518, Lawrence Berkeley
> Laboratory, Berkeley, CA, 1994.

> Antunez, A., G. Moridis and K. Pruess. Large-Scale Geothermal Reservoir
> Simulation on PCs, Lawrence Berkeley Laboratory Report LEL-35192, presented
> at 19th Workshop on Geothermal Reservoir Engineering,
> Stanford University, Stanford, CA, January 1994.

The DSLUBC and DSLUCS routines used in the conjugate gradient package were written by Anne Greenbaum (Courant Institute) and Mark K. Seager (Lawrence Livermore National Laboratory). DSLUGM was written by Peter Brown, Alan Hindmarsh, and Mark K. Seager (all of LLNL). These routines were adapted and improved for incorporation into the TOUGH2 code by George Moridis (Lawrence Berkeley Laboratory). Interfacing with TOUGH2 was done by George Moridis and Karsten Pruess. Emilio Antunez (LBL) performed the adaptation to PC.

Distribution of the TOUGH2 code is handled by:

Energy Science and Technology Software Center
P.O. Box 1020
Oak Ridge, Tennessee 37831
U.S.A.

phone (615) 576-2606
fax   (615) 576-2865
email: estsc @ adonis.osti.gov
The address of the code developer is:
Karsten Pruess
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Lawrence Berkeley Laboratory
Berkeley, CA 94720
U.S.A.
fax: (510) 486-5686
email: k_pruess @ lbl.gov

APPENDIX G. SAMPLE PROBLEMS

Pruess (1991) provides sample problems that are useful for checking the proper installation of TOUGH2 and cross-referencing it to TOUGH and for handling common applications of the code. The problems are summarized briefly here; however, the user is urged to consult Pruess (1991) for printouts of the input files, schematics of problem set-up, and data plots.

G.1 Sample Problem 1

Problem 1 is identical to sample problem 1 from the *TOUGH User's Guide* (Pruess, 1987) and is a good check on proper installation of TOUGH2. It consists of a number of one- and two-element subproblems which are independent of one another, but which are run simultaneously and therefore must go through the same sequence of time steps. The subproblems perform flow and/or injection and withdrawal of water, air, and heat, with highly non-linear phase and component (dis)appearances that require subtle numerical procedures. The input file for the EOS3 fluid properties module is almost completely identical to that of TOUGH sample problem 1, except that a few MOP-parameters are set differently because of different defaults in TOUGH2. Table 17 lists the elements and features of the subproblems in problem 1. As shown in Pruess (1991, Figure 9), the results are virtually identical to those generated by TOUGH. Minor differences occur in the maximum residuals during the iteration process. After time step 2, TOUGH2 takes different time steps because of different default settings. Sample input and output are shown in Figures 39 and 40 respectively.

Table 17. Summary of Sample Problem #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 form 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

```
*SAM1* CODE DEMONSTRATION: PHASE TRANSITIONS, COMPONENT (DIS-)APPEARANCES
       THIS INPUT FILE IS SLIGHTLY DIFFERENT FROM THAT FOR SAMPLE PROBLEM 1
       OF TOUGH. THESE COMMENTS ARE INSERTED TO NOTE THE DIFFERENCES. KEYWORDS
       ARE FOLLOWED BY A COLUMN COUNTER TO FACILITATE PROPER ALIGNMENT OF DATA.
       A FEW MOP-OPTIONS ARE SET DIFFERENTLY (SEE SECTION 7.1 IN TOUGH2 GUIDE).
ROCKS----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
TRANS          2650.         .50   1.E-14                           2.10     1000.
SHOME     2    2850.         .50   1.E-14                           2.10     1000.
                             1.8          .1
       3         .40         .10
       1        1.E5         .2    1.

START----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
PARAM----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
    2   4        11000301000000200711
                       -1.                F   1
         1.E2     5.E3

              45.E5                  .5                   250.
RPCAP----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
       3       .30         .05
       1                  1.
TIMES----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
       1     3              2.E3
          1.E3
ELEME----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
F   1    9    1TRANS       10.
SHO 1    9    1SHOME       10.
SHO11    1    1SHOME       1.E4

CONNE----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
F   1F   2                   1     5.         5.         1.
F   3F   4                   1     5.         5.         1.
F   5F   6                   1     5.         5.         1.

INCON----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
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                 200.                  0.
SHO11
              50.E5                 240.
SHO12
              40.E5                 100.

GENER----1----*----2----*----3----*----4----*----5----*----6----*----7----*----8
F   7AIR                            AIR     5.E-3    9.802E4
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
SHO11WEL00                       2  DELV    1.E-12                 1.E2
SHO12WEL00                          DELV    2.E-12       1.E6      1.E2

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

Figure 39. Input file for sample problem 1 - code demonstration.

Figure 40. Selected output for sample problem 1.

G.2 Sample Problem 2

Sample Problem 2 simulates thermal interference along a preferential flow path by modeling nonisothermal injection into and production from a single vertical fracture. The fracture is bounded by semi-infinite half-spaces of impermeable rock, which provide a conductive heat supply. A special feature of the problem is that the semi-analytical method of Vinsome and Westerveld (1980) is used to describe heat conduction in the confining layers, reducing the dimensionality of the problem from 3-D to 2-D. Water remains in single-phase liquid conditions throughout so that capillary pressures and relative permeability are not needed.

The problem uses the EOS1 fluid property module and is run in three separate segments. The first run produces mesh generation only. Steps required for mesh generation using MESHMAKER are explained in Pruess (1991). The second step calculates a hydrostatic pressure equilibrium in the fracture under isothermal conditions. This calculation uses the MESH file obtained in step one, and requires the following modifications in the input file. The time step counter MCYC is reduced to 4, the generation items are removed, convergence tolerance is decreased to achieve a tighter control on gravity equilibrium, the 'ENDCY' statement is removed, and the semi-analytical heat exchange calculation is disengaged by setting MOP(15)=0. The third step is the

production/injection run using an input file along with the MESH file as used in the gravity equilibration. A plot of the transient temperature changes at the producing element is given in Figure 42.
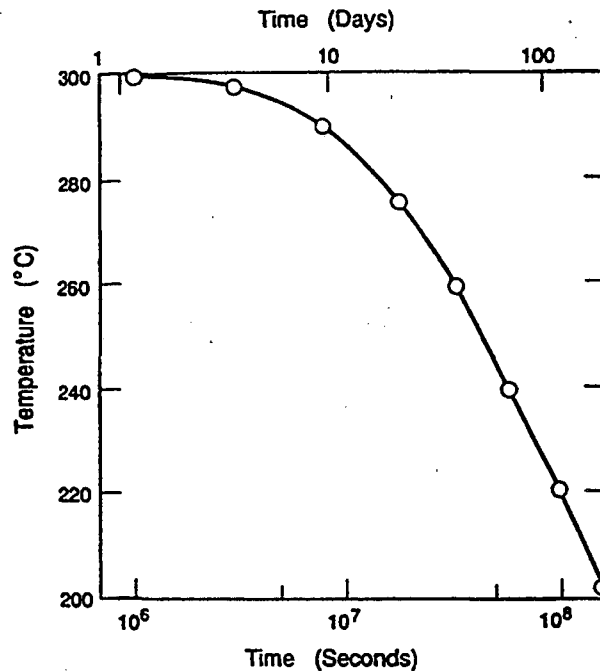

Figure 41. *Produced fluid temperature versus time for vertical fracture problem in sample problem 2.*

G.3 Sample Problem 3

Sample Problem 3 is the five-spot problem of geothermal production/injection. It considers a large well field with wells arranged in a "five-spot" configuration. Because of symmetry, only 1/8 of the problem needs to be modeled. The computational grid was generated by means of a separate preprocessor program that has not yet been integrated into the TOUGH2 package. The problem specifications correspond to conditions that may typically be found in deeper zones of hot and fairly tight fractured two-phase reservoirs (Pruess and Narasimhan, 1985). The input file for use with the EOS1 fluid property module models the system as a fractured medium with embedded impermeable matrix blocks in the shape of cubes. The matrix blocks are assigned a small porosity so that they will contain a small amount of water. This prevents the water mass balance equation from degenerating to 0. The MESHMAKER module is used to perform MINC-partitioning of the primary grid. Alternatively, the MINC process can be disabled and the problem run as an effective porous medium. Figure 38 shows temperature profiles along a line of injection to production well for a porous medium and two different fracture spacings.

By small adjustments to input files in Problems 2 and 3, a number of problem variations can be run, e.g. injection into vapor-dominated systems for Problem 2, and heat exchange with confining beds for Problem 3.
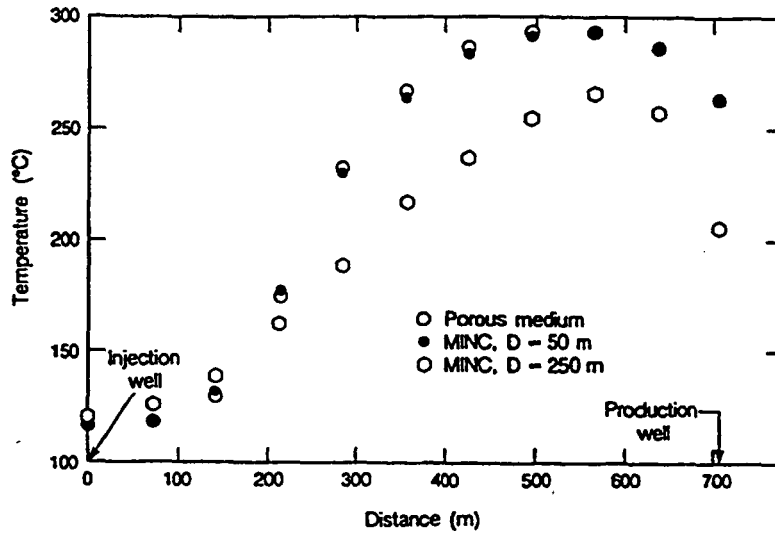
Figure 42. *Temperature profiles for problem 3 along a line of injection to production well after 36.5 years. MINC results for a 50 m fracture spacing are virtually identical to porous medium results while MINC results for a 250 m fracture spacing show lower temperatures.*