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BENCHMARK TESTING OF THERMOHYDROLOGIC COMPUTER CODES

Prepared for

Nuclear Regulatory Commission
Contract NRC-02-93-005

Prepared by

Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas

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ABSTRACT

Benchmark testing (i.e., code-to-code comparisons) of four general thermohydrologic codes was conducted to (i) compare and contrast their analysis capabilities, (ii) identify and understand any significant differences that may arise, and (iii) assess the robustness and computational efficiencies of the codes. The thermohydrologic codes tested were TOUGH2, FEHMN, CTOUGH, and MULTIFLO. The TOUGH2 and FEHMN codes are currently being used by U.S. Department of Energy (DOE) contractors, while the CTOUGH and MULTIFLO codes are used by the U.S. Nuclear Regulatory Commission (NRC) contractor. This report describes the codes tested, benchmark testing approach, results of computational testing, and comparisons of computational efficiencies.

The benchmark testing was performed in a systematic and structured manner using two sets of computational test cases. Each set of cases consisted of one- and two-dimensional simulations of isothermal and nonisothermal flow. The first set of test cases involved isothermal flow into relatively dry and heterogeneous systems. The second set required modeling coupled thermal and multiphase flow processes. Each set of test cases was progressively more difficult and involved simulating both porous and fractured-porous media systems. Calculational results produced by the thermohydrologic codes were compared on a graphical basis. In addition, computational statistics for each test case were summarized in tables.

In general, the benchmark testing showed that three of the four codes tested (TOUGH2, CTOUGH, and MULTIFLO) appear to possess sufficient capability to simulate the wide range of hydrologic and thermohydrologic conditions expected to be important in studies of the proposed high-level waste (HLW) repository at Yucca Mountain. In all the test cases considered, it was found that the numerical results produced by these three thermohydrologic codes agreed very well. The primary differences noted were in computational efficiency and, it was found that the MULTIFLO code was substantially faster than the other two codes. The fourth code, FEHMN, solved most of the test cases and the numerical results agreed adequately well with the results of the other codes. However, the FEHMN code experienced computational difficulties in two test cases; one case with high infiltration rates and another with flow in fractured-porous media. The latter problem appears to be related to a lack of a gridding capability to model discrete fractures.

CONTENTS

CONTENTS (Cont'd)

Section Page

FIGURES

TABLES

Table Page

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QUALITY OF DATA, ANALYSES, AND CODE DEVELOPMENT

DATA: No CNWRA-generated original data are contained in this report.

ANALYSES AND CODES: The TOUGH2, FEHMN, CTOUGH, and MULTIFLO computer codes were used in analyses contained in this report. These computer codes are not currently controlled under the CNWRA Software Configuration Procedure TOP-018. Codes, input and output files for all test cases will be archived as a QA record.

1 INTRODUCTION

1.1 BACKGROUND

Recent thermohydrologic modeling studies (Buscheck et al., 1995; Gansemer and Lamont, 1994) conducted for the proposed repository at the Yucca Mountain (YM) site led the U.S. Department of Energy (DOE) to consider a design that involves disposal of large spent fuel packages with thermal loading of 80 to 100 metric tons uranium (MTU) per acre. This thermal loading strategy is aimed at producing low relative humidity conditions (in the very near-field of the repository) for long time periods (i.e., thousands of years). This strategy could have the advantages of extending the containment time, delaying the period of controlled radionuclide release, and potentially reducing the sensitivity of total-system performance to hydrologic variability. Two potential disadvantages of the strategy, however, are the possible occurrence of channelized flow into the repository from perched water zones formed as a result of vapor condensation (Pruess and Tsang, 1994) and the induced thermal-hydrologic-mechanical-chemical couplings (Manteufel et al., 1994) make the assessment of isolation performance much more difficult.

Conceptually, such a thermal loading strategy could potentially enhance the compliance margin with the performance standard to be set by the U.S. Environmental Protection Agency and improve the overall robustness of the geologic repository. However, because of the complex nature of the coupled thermal and hydrologic processes, it is uncertain whether the advantages of this strategy will exceed potential disadvantages. Applications of thermohydrologic models will play an important role in the Nuclear Regulatory Commission (NRC) performance assessment studies (Nuclear Regulatory Commission, 1995) focused on the evaluation of the DOE strategy.

To date, the Center for Nuclear Waste Regulatory Analyses (CNWRA) has utilized the CTOUGH code, a modified version of the VTOUGH code (Nitao, 1989), in modeling thermohydrologic processes associated with the proposed repository. More recently, the CNWRA pursued development of a new thermohydrologic computer code referred to as MULTIFLO. This code is distinct in that in addition to modeling heat transfer and multiphase flow, it is capable of modeling chemical reactions and solute transport which may be important to thermo-hydro-chemical couplings. In this study, these two CNWRA codes were tested against the TOUGH2 (Pruess, 1991) and FEHMN (Zyvoloski et al., 1992) codes, currently being used by the DOE contractors.

Three major objectives of this benchmark testing study were to (i) compare and contrast the simulation capabilities of the NRC/CNWRA codes with those of the DOE, (ii) identify and understand any significant differences that may arise between DOE and NRC/CNWRA code applications, and (iii) assess the robustness and computational efficiencies of the codes. To this end, the four thermohydrologic codes were evaluated and compared in terms of capability to simulate diverse conditions and overall computational efficiency. In addition, working with the DOE thermohydrologic codes provided valuable insight that will be useful in conducting prelicensing reviews of the DOE performance assessment studies. Specifically, the experience gained from testing the DOE codes provided first hand knowledge of the conditions and situations where these sophisticated predictive tools typically encounter problems and/or are likely to produce unreliable results. This knowledge is expected to be directly applied in reviews of the performance analyses supporting the DOE site viability assessment.

1.2 BENCHMARK TESTING

The testing of the thermohydrologic codes was conducted according to the general approach outlined in Ross et al., (1982). However, no code verification (i.e., comparison with known solutions) tests were undertaken because most of the problems of interest here are highly nonlinear and cannot be solved analytically, even in their simplest form. Thus, the reliability of thermohydrologic codes could only be evaluated by benchmarking computational results with those produced by codes with similar capabilities (i.e., code-to-code comparisons). Close grouping of numerical results is considered a satisfactory result whereas a significant deviation from the group of numerical results is judged as unsatisfactory or questionable.

The benchmark test cases were designed to permit testing of specific code capabilities that are expected to be important in general applications to repository performance. For convenience, the test cases were grouped into either isothermal or nonisothermal flow. Both sets of test cases emphasized probing the robustness and computational efficiency of the four thermohydrologic codes. Robustness and computational efficiency are quantified in terms of capability of the codes to successfully simulate diverse conditions (i.e., complete the simulation and produce reasonable results) and computer execution speed (i.e., central processing unit time). In addition, benchmark testing was conducted to evaluate the major features and options of the computer codes.

1.3 DESCRIPTION OF COMPUTER CODES

The benchmark testing was performed using the TOUGH2, FEHMN, CTOUGH, and MULTIFLO computer codes. All four codes possess the capability to simulate one dimensional (1D), two dimensional (2D), or three dimensional (3D) systems. The TOUGH2 and FEHMN codes were selected because they were readily available and have been widely used in the DOE studies (Wittwer et al., 1995; TRW Environmental Safety Systems, Inc., 1995) of the proposed repository at the YM site. Other DOE codes such as NUFT, developed at Lawrence Livermore National Laboratory (LLNL), and MSTS, developed at Pacific Northwest Laboratory (Nichols and White, 1993), were considered for benchmark testing but not selected because they have not been widely used in the repository program. The CTOUGH code has been used by the CNWRA staff to conduct auxiliary analyses (Lichtner and Walton, 1994) for the NRC Iterative Performance Assessment activity. The MULTIFLO code, recently developed for the CNWRA, is currently being documented.

1.3.1 TOUGH2 Computer Code

The TOUGH2 code, like its predecessor TOUGH, was developed at the Lawrence Berkeley Laboratory (Pruess, 1987, 1991) for simulating the coupled transport of water, vapor, air, and heat in porous and fractured media. The acronym TOUGH refers to TranspOrt of Unsaturated Groundwater and Heat. The original version of the TOUGH code was developed as part of the DOE geothermal energy program. The TOUGH2 code, however, has been specifically tailored for use in studies of a high-level waste (HLW) repository in a partially saturated geologic media. This thermohydrologic code is perhaps the most widely used (Ho and Eaton, 1994; Buscheck and Nitao, 1993a, 1993b; Pruess et al., 1990a, 1990b; Tsang and Pruess, 1987) to investigate nonisothermal flow processes. Both the TOUGH and TOUGH2 codes have been extensively verified and benchmark tested (Updegraff, 1989; Moridis and Pruess, 1992).

A general mathematical model is implemented in the TOUGH2 code which is applicable to strongly heat-driven flow (i.e., liquid and gaseous phases). The flow model takes into account pressure, viscous, and gravity forces, as well as capillarity, binary diffusion, and phase transition effects. Air is assumed to behave as an ideal gas. The formulation of the heat transport model considers conduction (with thermal conductivity being a function of water saturation), convection, and binary diffusion. The code includes vapor pressure lowering effects, but Knudsen diffusion is neglected. Special equations of state modules are included for treating H_2O-CO_2, H_2O-air (with/without vapor pressure lowering), H_2O-H_2, and single-component nonisothermal H_2O systems.

An integral volume difference method is used to discretize the governing equations which permits the use of arbitrarily shaped grids. The computational algorithm treats all quantities fully implicitly and solves the system of equations simultaneously. A Newton-Raphson algorithm is used to accommodate the nonlinearities and the Jacobian terms are calculated numerically. The final system of matrix equations are solved using the MA28 direct solver (Duff, 1977) or iterative solvers with an incomplete lower upper (LU) factorization preconditioner. Some of the solver (i.e., accelerator) options include the following: (i) bi-conjugate gradient, (ii) Lanczos-type bi-conjugate gradient, and (iii) Generalized Minimum Residual (GMRES) method (Saad and Schultz, 1986).

1.3.2 FEHMN Computer Code

The FEHMN code, which is the YM version of FEHM, was developed at the Los Alamos National Laboratory (Zyvoloski et al., 1988; 1992). The acronym, FEHM, stands for Finite Element Heat and Mass transport code; the N is added to FEHM to designate a distinct version used in repository performance assessment. This code was designed to simulate thermal energy and coupled mass transfer for multiphase flow, as well as noncondensible gas flow in porous and permeable media. Another primary use of the FEHMN code is to simulate reactive transport (i.e., advection, dispersion, diffusion, sorption, and decay) of liquid and gaseous species with chemical reactions. However, the model formulation neglects changes in porosity and permeability arising from the chemical reactions (e.g., dissolution and precipitation).

The mathematical formulation of the governing equations is very general. FEHMN has options to allow subsets of the model to be exercised. For example, the code can be applied to these problems: (i) heat conduction, (ii) heat and mass transfer with pressure and temperature dependent properties, (iii) isothermal air-water transport (i.e., Richards' equation), (iv) heat and mass transfer with noncondensible gas, and/or (v) reactive transport of multiple solutes. In addition, the code has the capability of modeling physical systems in terms of either an equivalent porous medium or a double porosity/double permeability medium. Vapor pressure lowering effects are not considered.

A Galerkin finite element method was used to formulate the numerical approximations to the governing equations for multiphase flow. In addition, the FEHMN code has provisions to compute internode flows using a finite volume approach. The computational algorithm treats all quantities fully implicitly and solves the systems of equations simultaneously. A Newton-Raphson algorithm is used to accommodate the nonlinearities and the Jacobian terms are calculated analytically. The final system of matrix equations is solved using an iterative solver with incomplete LU preconditioners and a GMRES accelerator.

1.3.3 CTOUGH Computer Code

The CTOUGH code (CNWRA version of VTOUGH) is an enhanced version of the vectorized TOUGH or VTOUGH. The VTOUGH code was developed by LLNL (Nitao, 1989) to improve the computational efficiency for applications on a Cray supercomputer. In addition, LLNL refined the code by adding equivalent continuum formulation for dual porosity-fractured media, Knudsen diffusion, vapor pressure lowering effects, and improved computational algorithms (e.g., automatic time stepping and table look up for thermodynamic and hydraulic properties). The CNWRA further improved this code by including more efficient matrix solvers, and user interface features for generation of graphical output.

Because CTOUGH is basically an extension of the VTOUGH code, it possesses the equivalent mathematical theory, discretization approach, and computational algorithms. This code along with MULTIFLO will be used in NRC/CNWRA analyses of thermohydrologic processes.

1.3.4 MULTIFLO Computer Code

The MULTIFLO code like the CTOUGH code is designed to model the coupled transport of liquid water, vapor, air, and heat in porous and fractured media. The acronym MULTIFLO refers to MULTIcomponent FLOw and transport. This generalized simulation code is designed to model both the thermohydrologic and reactive transport processes associated with a high-level nuclear waste repository. Development of this code was motivated by the recognition of possible important couplings between the hydrologic phenomena and pore-fluid chemistry (Lichtner, 1994). This recently developed code permits modeling of chemical species and reactions as well as changes in porosity and permeability due to dissolution and precipitation. Documentation for this code is expected to be published in late fiscal year 1996.

A general mathematical model for multiphase flow is incorporated in MULTIFLO that is comparable to that used in the TOUGH2 code. In addition, the code has options for solving subformulations such as single phase flow and pure conduction. The flow model takes into account the pressure, viscous, and gravity forces, as well as capillarity, binary diffusion, and phase transitions are incorporated. Air is assumed to behave as an ideal gas. The formulation of the heat transport model considers conduction (with thermal conductivity being a function of water saturation), convection, and binary diffusion. Also included are vapor pressure lowering effects.

An implicit finite difference method is used to discretize the governing equations and is formulated in a manner that permits Cartesian, cylindrical, or spherical coordinates in 3D. Thus, MULTIFLO is not applicable to simulation problems where unstructured grids are required. The computational algorithm treats all quantities fully implicitly and the system of matrix equations are solved simultaneously. A Newton-Raphson algorithm is used to accommodate the nonlinearities and the Jacobian terms are calculated analytically. The linearized matrix equations are solved using a direct elimination method with D-4 ordering (Price and Coats, 1973) or with an iterative method such as incomplete LU preconditioner with bi-conjugate gradient stabilized or GMRES accelerator, or nested factorization(Appleyard and Cheshire, 1983) preconditioner with ORTHOMIN accelerator (Vinsome, 1976). The thermodynamic properties of water are calculated using the International Formulation Committee functions. In addition, these functions may be used directly or through the use of internally generated tables for calculation of thermodynamic properties of liquid water and steam. The code is designed to accommodate maximum temperature and pressure values of 800 °C and 165 bars, respectively.

2 TESTING APPROACH

2.1 TEST OBJECTIVES

Thermohydrologic codes, such as those considered in this report, implement relatively sophisticated and complex mathematical models that rely heavily on a variety of numerical approximations and on the effectiveness of advanced computational methods. The primary objectives of the benchmark testing conducted in this study were:

- Compare and contrast the simulation capabilities of the NRC/CNWRA and DOE thermohydrologic codes.
- Identify and understand any significant differences that may arise between DOE and NRC/CNWRA code applications (which may be due to differences in computer implementation).
- Assess the robustness and computational efficiency of the codes.

Upon achieving these objectives, conclusions were reached regarding the likelihood that use of different codes could lead to distinct findings or interpretations about thermohydrologic processes and couplings.

2.2 TESTING PROTOCOL

In conducting the benchmark testing, a systematic and consistent approach was followed to ensure full and unbiased evaluations of the four thermohydrologic codes. Three general guidelines were used in testing: (i) ensure equivalent testing, (ii) use available code options that optimize computational performance, and (iii) provide progressively difficult test cases. Equivalent testing, as used here, means that test cases were posed to not put a particular code at a disadvantage. To ensure the best performance of all codes tested, available code options was exercised in an attempt to produce the fastest convergence and least CPU time. Test cases used in the benchmarking were developed to introduce increased complexity and therefore, greater computational difficulty in a progressive manner.

Equivalent testing was maintained by defining a set of test cases that could be readily accommodated by all four thermohydrologic codes. For example, all four codes possess the option to calculate interblock hydraulic properties using: (i) upstream weighting for mobility and enthalpy and (ii) harmonic averaging (Aziz and Settari, 1979) of intrinsic permeability. Thus, this option was exercised in all test cases. In addition, all four codes were set up to use the same or equivalent spatial discretizations. This ensured the computational effort and calculational accuracy would be equivalently specified for each code. Similarly, a uniform convergence criterion (associated with the Newton iterations) was also used in all test cases; specifically, the primary criterion used was that the infinity norm of the normalized Newton residual error vector be less than 10^{-5}.

In an effort to obtain the best computational performance, code options such as automatic time-stepping were used. In those codes providing different matrix solver options, the most efficient solver was utilized. Where major problems were encountered, the code developer was consulted to aid in the code application(s). All codes were run on the same computer, in this case a SUN SPARC20 workstation, using the standard compiler option (i.e., no compiler optimization). It is important to acknowledge, however, that the developers of the codes may be able to achieve better computational performance simply because they have much more experience applying the codes.

In developing the set of test cases, a range of physical settings and hydrologic conditions was considered that stressed the simulation capability of the codes in a progressive manner. The increasing level of difficulty was accomplished through the selection of problem geometry, initial and boundary conditions, and contrasts in hydraulic properties.

2.3 DESCRIPTION OF TEST CASES

Six test cases were developed for use in benchmark testing of the thermohydrologic codes. The first three test cases represented isothermal systems and the remaining three consisted of nonisothermal flow cases. Within each of these two groups of test cases, the formulation of the test cases was made progressively more difficult by varying: (i) problem geometry from 1D to 2D, (ii) system characteristics from homogeneous to heterogeneous porous media with discrete fractures, and (iii) severity of the boundary conditions and permeability contrasts. No 3D test cases were considered, primarily because of the high computational requirements of such test cases. The formulation of most of the test cases assumed that an equivalent porous continuum model was appropriate.

The following are brief descriptions of the six test cases used in the benchmark testing study. The test cases are grouped into isothermal flow (IF) and nonisothermal flow (NF) simulations.

IF-1 <u>One-Dimensional Flow in Layered Soil</u>. This case tested the capability of the codes to model flow into a layered soil column with contrasting hydraulic properties with dry initial conditions. Flow in the system is produced by infiltration at the soil surface. The simulation problem was made challenging by assuming relatively dry initial conditions (i.e., high initial suction head). This 1D problem was intended to test the capability of the codes to simulate isothermal flow in a porous medium with strongly nonlinear soil properties and large pressure head gradients.

IF-2 <u>Two-Dimensional Flow in Layered Soil</u>. To provide a test case of greater difficulty, the previous test case (IF-1) was extended to 2D and the hydraulic properties modified to produce greater contrasts. In addition, the inflow was treated as a point source and the magnitude of the source rate is increased by 20 times. This 2D test case was designed to test the code capabilities to simulate conditions where the flow system changes rapidly and the range of liquid saturation level is larger.

IF-3 <u>Two-Dimensional Flow in Fractured-Porous Media</u>. This isothermal flow problem progresses to a more complex and realistic test case. Flow into the 2D system was similar to the previous test case (IF-2) except that the system was conceptualized as a low permeability, homogeneous porous matrix with a system of discrete orthogonal fractures. Flow through this system was controlled by the matrix-fracture interactions (i.e., the matrix imbibes water while the fractures conduct water). The large permeability contrasts made this test case very challenging.

NF-1 <u>One-Dimensional Flow in a Soil Column with Heat Source</u>. In this test case, 1D flow into a large homogeneous soil column was considered. Constant temperature and pressure head were maintained at the top of the column. A point heat source was located at the bottom of the column which produced drying and induced upward flow of vapor and subsequent condensation. This test case exercised the multiphase flow components of the codes as well as the calculations of thermodynamic properties (i.e., pressure-volume-temperature relationships).

NF-2 Two-Dimensional Nonisothermal Flow in Layered Soil. A more detailed multiphase flow problem was considered here that involved both a point source of water and a line heat source. The physical system was a porous medium with high and low permeability layers. The hydrologic conditions resulted in regions of multiphase flow as well as formation of perched water zones. The objective of this test case was to more fully test the multiphase flow capabilities of the codes.

NF-3 Two-Dimensional Nonisothermal Flow in Fractured-Porous Media. The final test case was the most rigorous and challenging, as it considered the combined complexities of all previous isothermal and nonisothermal test cases. As in test case IF-3, the physical setting was a low permeability medium with a system of intersecting orthogonal fractures. Flow and heat sources were the same as those in test case NF-2.

3 BENCHMARK TEST CASES FOR ISOTHERMAL FLOW

3.1 ONE-DIMENSIONAL FLOW IN LAYERED SOIL

3.1.1 Problem Statement and Test Objectives

As an initial test case, the 1D problem originally studied by Hills et al. (1989) was selected that involved modeling flow into a field scale layered lysimeter. This test problem designated IF-1 was an excellent one because it consisted of flow into a relatively dry soil and exhibited relatively large pressure gradients. The upper boundary condition was a constant flux of q_l=2 cm/d at the soil surface. The bottom boundary was held at the initial pressure head. The initial pressure head profile is set to $h_i = -10^4$ cm. Five soil layers of alternating Bernino loamy fine sand and Glendale clay loam made up the 100-cm soil column. Each soil layer is 20 cm thick.

The objective of this test was to determine if the strong nonlinearity arising from the soil hydraulic properties and the dry initial conditions posed significant difficulty to the computer codes. This 1D test problem was previously solved for the single phase case (i.e., Richards' equation) using special computational techniques (Kirkland et al., 1992; Baca et al., 1996) that employed partitioned transforms. Consequently, it was expected that all the selected codes would, in fact, solve the isothermal flow problem but with contrasting rates of convergence and CPU times.

3.1.2 Input Specifications

The flow domain is sketched in Figure 3-1. For the finite difference codes, the 1D domain was discretized into a column of grid blocks with sizes of $\Delta x = \Delta y = 100$ cm, $\Delta z = 4$ cm. In the case of the finite element code, the mesh was comparable except the top and bottom elements were slightly larger. All four thermohydrologic codes were run for a total simulation period of 5 days. Soil hydraulic properties for the two distinct soil types were described by the van Genuchten (1980) formulas. These properties were taken directly from Hills et al. (1989) and are summarized in Table 3-1.

Table 3-1. Soil hydraulic properties for 1D flow problem

Layer	θ_s	θ_r	$\alpha (cm^{-1})$	n	$K_s (cm/d)$
Bernino Loamy Fine Sand	0.3658	0.0286	0.0280	2.2390	541.0
Glendale Clay Loam	0.4686	0.1060	0.0104	1.3954	13.1

TOUGH2, CTOUGH, and MULTIFLO codes required that the infiltration rate be treated as a mass source rather than as a flux boundary condition. Thus, the source strength was calculated by multiplying the flux rate by water density. This calculation produced a source rate of 2.31×10^{-4} kg/s, which was specified in the uppermost grid block. For the finite element code, FEHMN, the infiltration rate was treated as point sources specified at the two surface nodes. In contrast to the arithmetic averaging used by Hills et al. (1989), harmonic averaging was used in the calculation of the interblock intrinsic

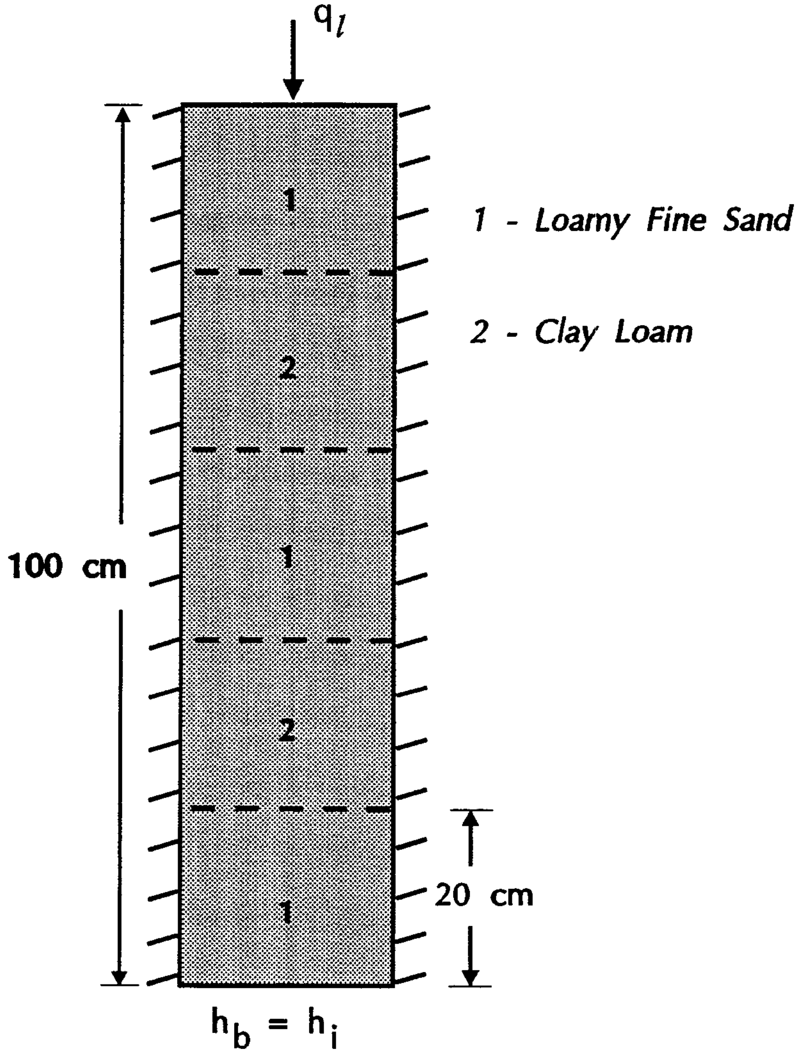


Figure 3-1. System sketch for 1D isothermal flow problem

permeabilities for the TOUGH2, CTOUGH, and MULTIFLO codes. The finite element code also utilized harmonic averaging in the calculation of element intrinsic permeabilities.

3.1.3 Evaluation of Results

All four thermohydrologic codes applied to this 1D isothermal test problem produced successful results. As can be noted from the water saturation profiles in Figure 3-2, the numerical results for all four codes agree very well. In applying the thermohydrologic codes, no significant computational difficulties were encountered with either nonlinear soil properties, contrasting hydraulic properties, or dry initial conditions. Although not presented here, other test runs were made for this 1D test problem in which the source rate was increased to values close to the saturated hydraulic conductivity of the upper layer. It was found that the FEHMN code required finer time stepping to accommodate the larger source rates. The finer time stepping resulted in the larger CPU time.

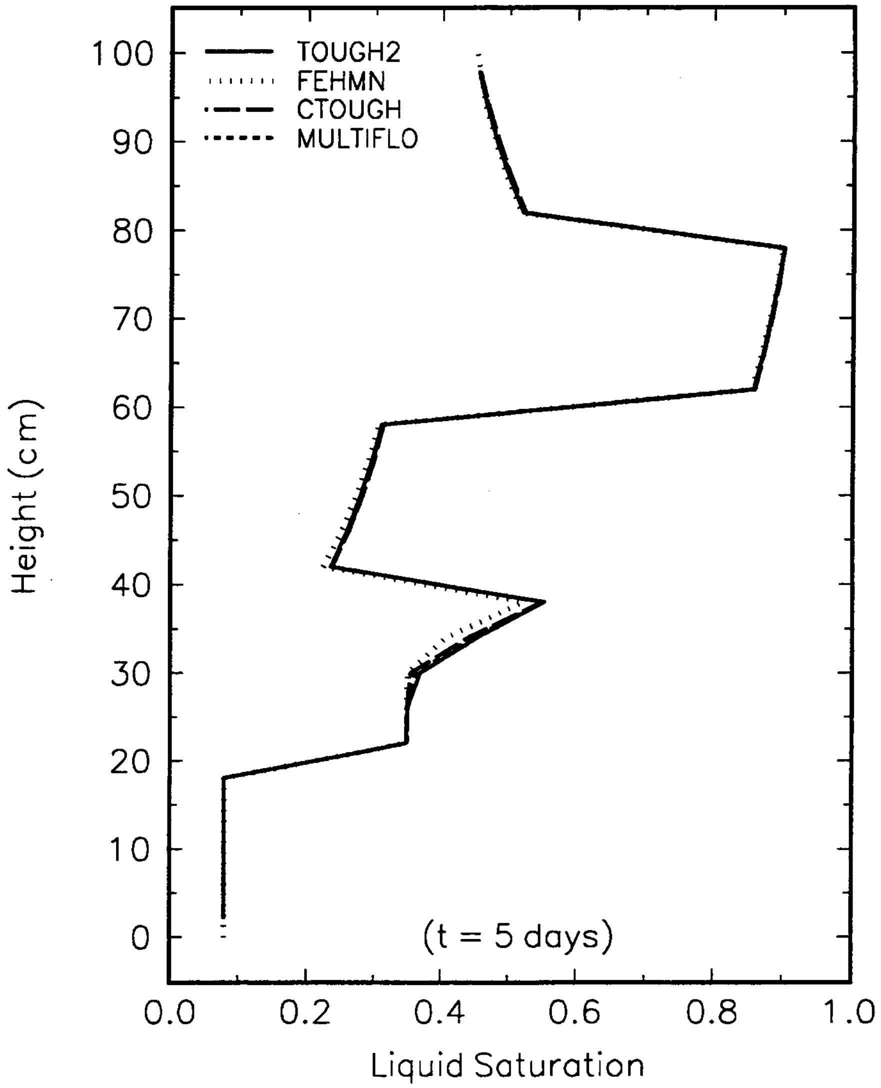


Figure 3-2. Comparison of liquid saturation profiles for 1D test problem

The main conclusion drawn from this particular test problem was that all four thermohydrologic codes can effectively simulate infiltration into heterogeneous soils with relatively dry initial conditions and strongly nonlinear hydraulic properties. The MULTIFLO code required the smallest CPU time and the FEHMN the largest. On a per step basis, the FEHMN code is relatively efficient, however, it required much smaller time steps The computational statistics for each of the thermohydrologic codes are summarized in Table 3-2.

Table 3-2. Computational statistics for 1D isothermal flow problem

Parameter	TOUGH2	FEHMN	CTOUGH	MULTIFLO
Total Run Time (CPU s)	6.93	64.98	16.12	1.33
Total Time Steps	39	571	271	40
Total Newton Iterations	105	1096	333	117
Total Step Cuts	0	N/A	0	0
Average CPU/Step	0.1777	0.11380	0.0595	0.0333
Average Iterations/Step	2.7	1.9	1.2	2.9
Average CPU/Element/Step	7.11E-3	4.55E-3	2.38E-3	1.33E-3
Average CPU/Element	.277	2.599	.648	.0532
Minimum Time Step (s)	1E2	N/A	2.74E-3	86.4
Maximum Time Step (s)	3.24E5	N/A	3.01E3	2.27E4
Ratio of Total Run Time to Minimum Run Time	5.21	48.86	12.12	1

3.2 TWO-DIMENSIONAL FLOW IN LAYERED SOIL

3.2.1 Problem Statement and Test Objectives

This second isothermal test case (IF-2) considered 2D flow in a relatively dry, multilayered vadose zone. The domain of this hypothetical system was a rectangular region 2,500 cm high and 700 cm wide. Flow into the system is introduced by an internal source located in the upper left corner of the domain. The top and vertical boundaries of the system were set as no flow boundaries. The bottom boundary was set to a fixed pressure equal to the initial pressure head of $h_i = -10^4$ cm. As in the previous test case, the system consisted of alternating soil layers with contrasting hydraulic properties. The hydraulic conductivities of the soil layers were anisotropic and the vertical conductivity was larger than the horizontal conductivity.

One of the objectives of this test problem was to determine how well the thermohydrologic codes simulated transient flow in a heterogeneous medium where the infiltration occurred only over a small portion of the soil surface. This specification was similar to a condition of focused recharge. Under this boundary condition, the fluid flow exhibited distinct 2D behavior as it moved horizontally along interfaces and vertically through individual soil layers. Another objective of this problem was to test the codes in a wetter fluid regime. Thus, to create higher saturation levels, a high infiltration rate was assumed. This high infiltration rate produced large pressure head gradients and enhanced the dynamics of flow, both of which made the problem more computationally challenging.

3.2.2 Input Specifications

The geometry for this flow domain and the location of the internal source are shown in Figure 3-3. The computational grid used to represent the domain consisted of 7 grid blocks in the x-direction, 1 in the y-direction, and 25 in the z-direction. The grid system was uniform with block sizes of $\Delta x = \Delta y = \Delta z = 100$ cm. The duration of the simulation period was 30 days and automatic time stepping was used. The internal source was set to a value of 4.62×10^{-3} kg/s, a factor of 20 greater than the previous test case. This value was selected after the TOUGH2 and FEHMN codes failed to complete the simulation for a larger source rate (e.g., 100 times greater).

Each layer of this soil system is 500 cm thick. The hydraulic properties for the two layers are variations of those properties used in the previous 1D test problem. To add different facets to this 2D test case, the porosities for the two layers were chosen to be smaller, like the residual moisture contents. In addition, the hydraulic conductivity in the horizontal direction K_x was assigned a value of one-tenth K_z. The soil properties used in this 2D test problem are summarized in Table 3-3.

Table 3-3. Soil hydraulic properties for 2D isothermal flow problem

Layer	θ_s	θ_r	$\alpha (cm^{-1})$	n	$K_z (cm/d)$
High K Layer	0.05	0.010	0.0280	2.2390	5410.0
Low K Layer	0.10	0.025	0.0104	1.3954	131.0

3.2.3 Evaluation of Results

This isothermal test case provided a vehicle for evaluating the capabilities of the thermohydrologic codes to simulate transient two-phase (i.e., air-water) flow in 2D. For the selected source rate, all four codes successfully simulated the moisture build-up below the mass source, localized perching at the first layer interface, and redistribution in the multilayered medium. Saturation profiles computed from the numerical results are shown in Figure 3-4. These plots clearly show that all four codes produced comparable results. Slight differences are evident for the FEHMN code results due to the slightly different computational grid required to maintain an equivalent number of nodes.

The computational results for this particular test problem supported the conclusion that all four thermohydrologic codes can effectively simulate variably saturated flow into layered media with relatively dry initial conditions. The anisotropic properties did not appear to pose any problem for the codes. As in the previous test problem, the MULTIFLO code required the least CPU time and the CTOUGH the largest. Computational statistics for each of the thermohydrologic codes are summarized in Table 3-4.

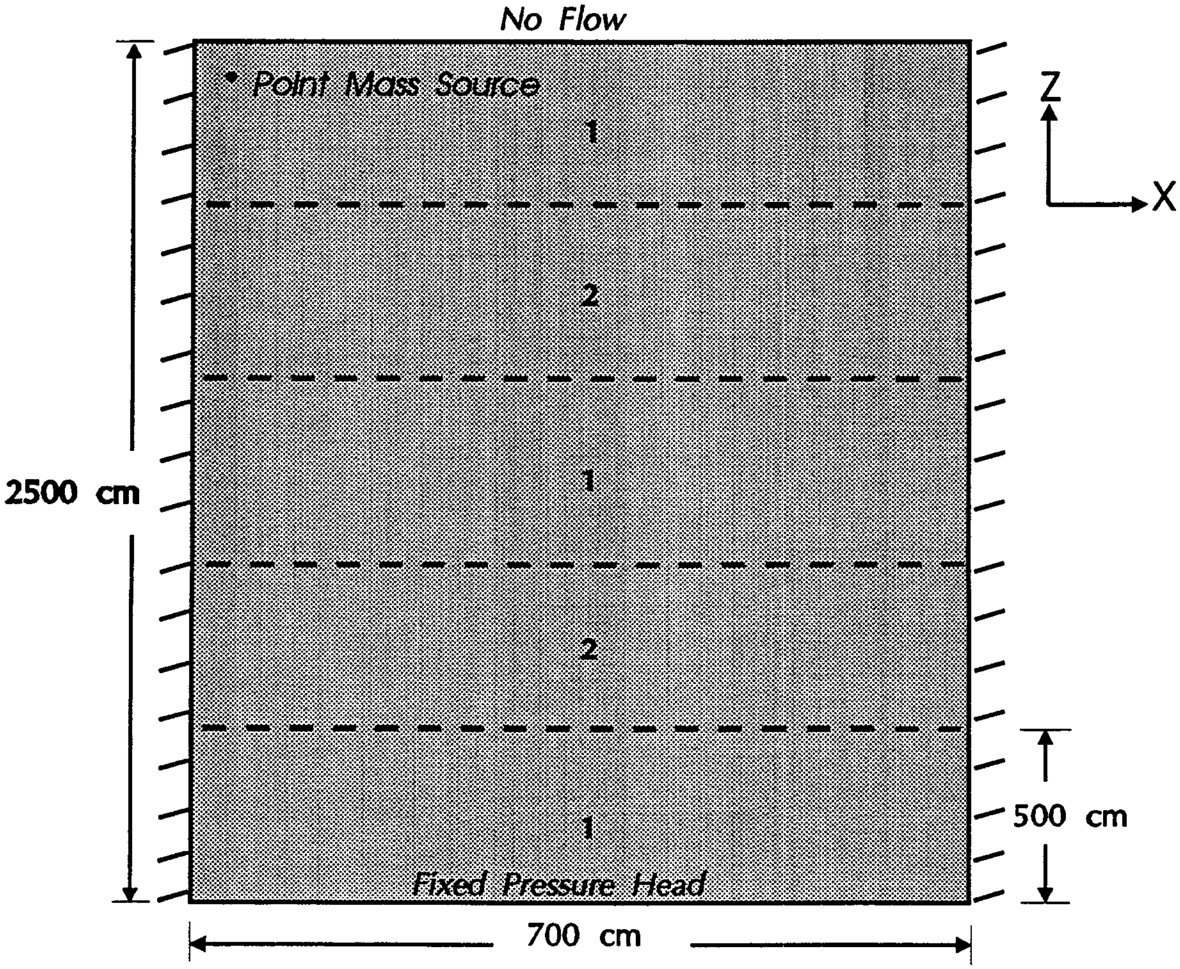


Figure 3-3. System sketch for 2D isothermal flow problem

3.3 TWO-DIMENSIONAL FLOW IN FRACTURED-POROUS MEDIUM

3.3.1 Problem Statement and Test Objectives

The final isothermal test problem was designed to be much more challenging than the previous test problems and required modeling flow in a fractured porous medium. The physical system is a 2D homogeneous porous medium with very low permeability and a network of orthogonal fractures. The domain of this hypothetical system is a rectangular region 1001.0 cm high and 700.8 cm wide. The domain is traversed by 10 horizontal and 8 vertical fractures. The fracture spacing and aperture are

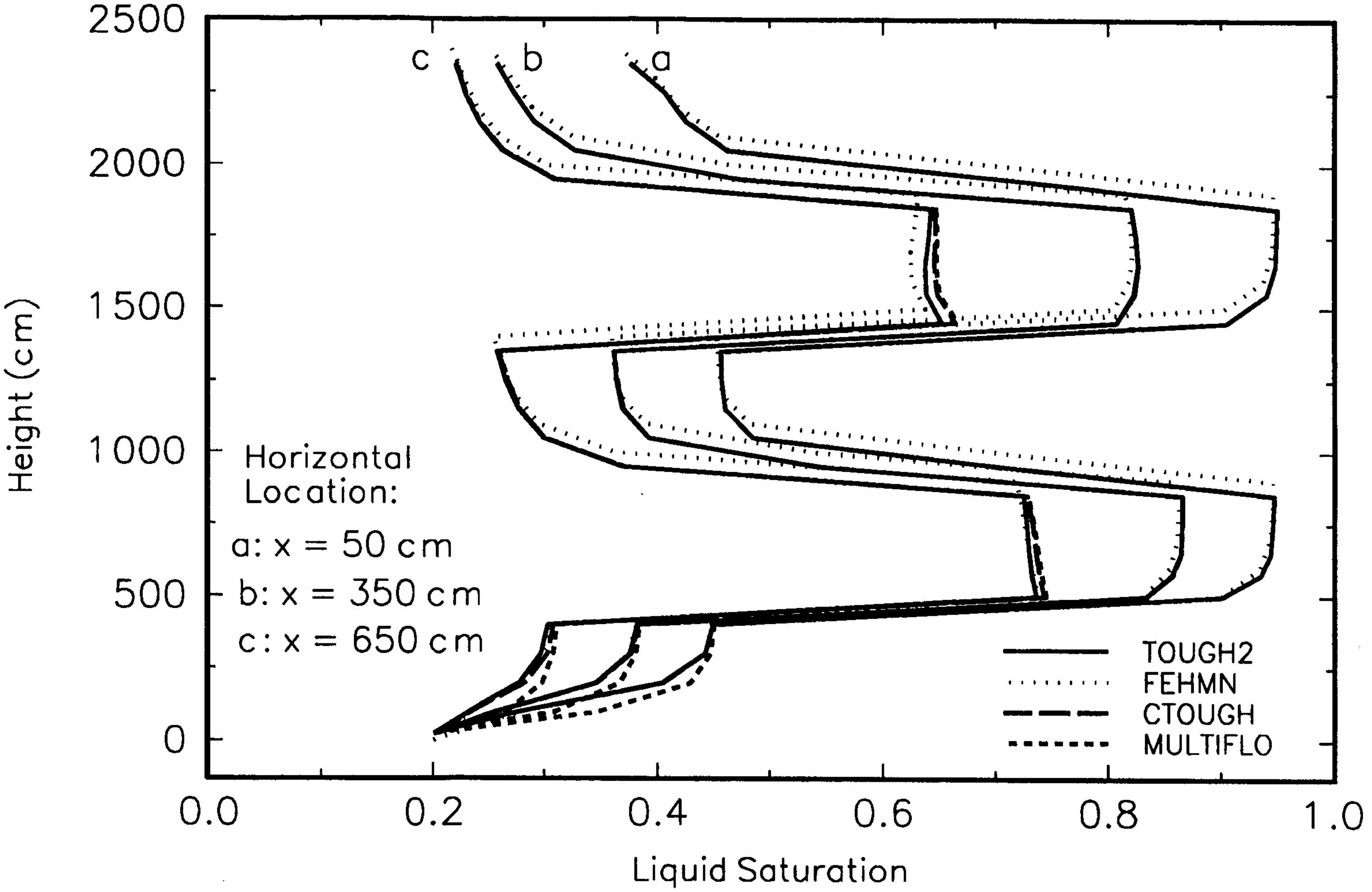


Figure 3-4. Comparison of liquid saturation profiles for 2D isothermal test problem

Table 3-4. Computational statistics for 2D isothermal flow problem

Parameter	TOUGH2	FEHMN	CTOUGH	MULTIFLO
Total Run Time (CPU s)	168.60	272.12	288.4	124.82
Total Steps	59	409	142	157
Total Newton Iterations	212	964	432	477
Total Step Cuts	0	N/A	0	1
Average CPU/Step	2.86	0.665	2.03	0.795
Average Iterations/Step	3.59	2.35	3.04	3.04
Average CPU/Element/Step	0.016	3.8E-3	0.012	4.54E-3
Average CPU/Element	.96	1.55	1.65	.713
Minimum Time Step (s)	1E2	N/A	1.04E2	1.51E2
Maximum Time Step (s)	4.14E5	N/A	.85E5	9.85E4
Ratio of Total Run Time to Minimum Run Time	1.35	2.10	2.31	1

uniform with values of 100 cm and 0.01 cm, respectively. As in the previous problem, flow was introduced to the system by a mass source located in the upper left corner of the domain. The top and vertical boundaries of the system were set as no flow boundaries. The bottom boundary was set to a fixed pressure equal to the initial pressure head of $h_i = -10^3$. The hydraulic properties for porous matrix and fractures were highly contrasting producing large pressure gradients across the system.

The main objective of this test problem was to determine how well the thermohydrologic codes modeled flow in a medium in which the matrix blocks principally provide water storage while the discrete fractures transmit water and hydraulically interconnect the source to rest of the domain. Under the boundary conditions, the fluid flow exhibited distinct 2D behavior as it moved vertically and horizontally through the individual fractures. Another objective of this problem was to test the robustness of the codes to handle large permeability contrasts representative of a realistic system.

3.3.2 Input Specifications

The system geometry and the location of the internal source are illustrated in Figure 3-5. The computational grid used to represent the domain consisted of 15 grid blocks in the x-direction, 1 in the y-direction, and 20 in the z-direction. The grid system for the porous matrix was uniform with block sizes of $\Delta x = \Delta y = \Delta z = 100$ cm. Each fracture was represented with a thin block equal to the fracture aperture. The duration of the simulation period was 30 days and automatic time stepping was used. The internal source was the same as the preceding test case which was set to a value of 4.62×10^{-3} kg/s.

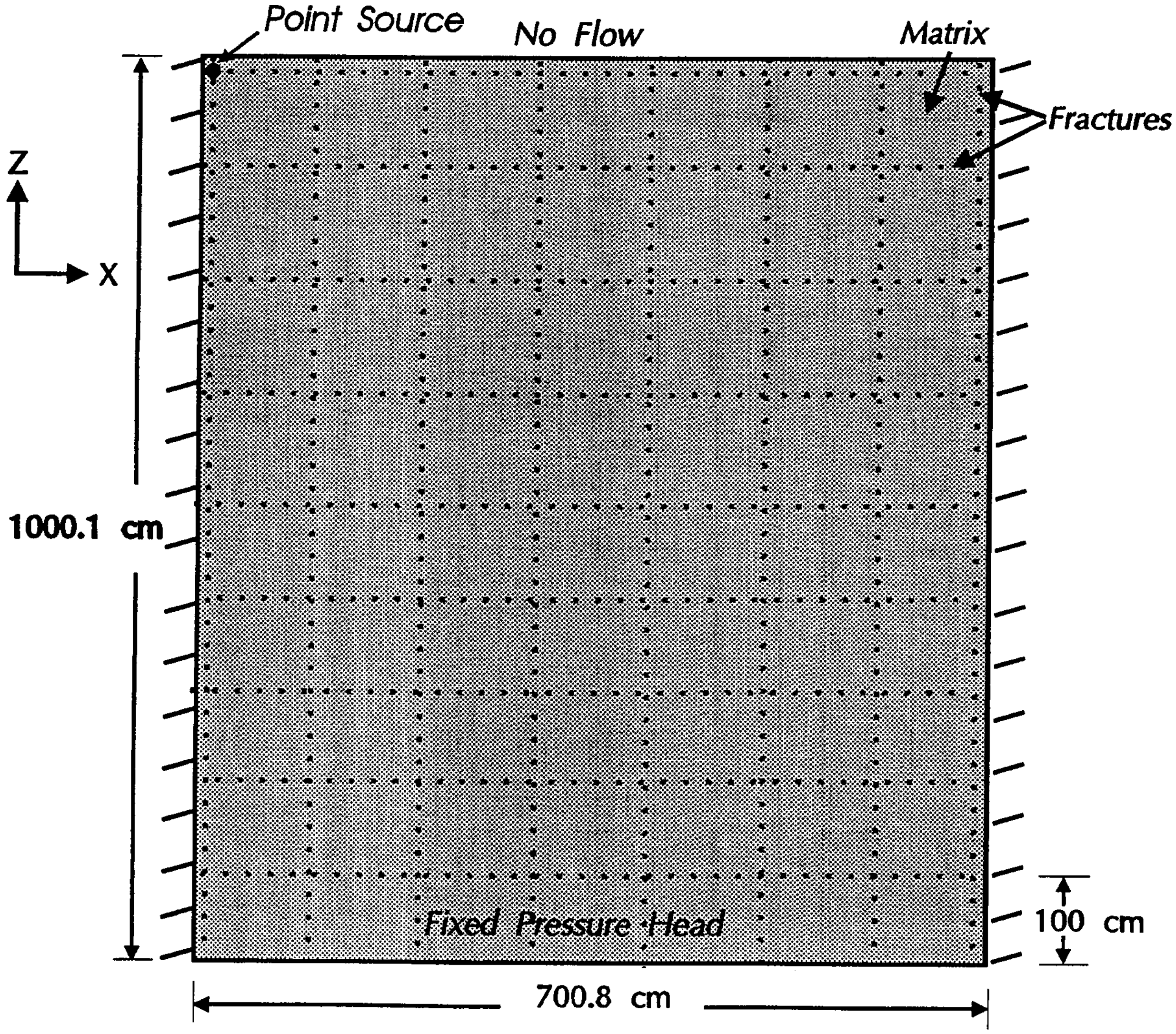


Figure 3-5. System sketch for 2D fracture flow problem

Each matrix block in the flow domain was bounded by fractures and, therefore, isolated from the other matrix blocks. This geometry, along with the low matrix permeability, constrained the system to behave like a dual porosity medium. The hydraulic conductivity assigned to the fractures was set to large arbitrary value. The permeability contrast between the fractures and matrix is in excess of 7 orders of magnitudes. In addition, the van Genuchten parameters assigned to the fractures were selected to ensure that water drains rapidly through the fractures; this was accomplished by choosing a large van Genuchten n and large α (i.e., low air entry pressure) values. The combination of contrasting permeabilities and van Genuchten parameters (between matrix and fractures) make this test case exceptionally challenging but not atypical of practical applications. The hydraulic properties used in this 2D test problem are summarized in Table 3-5. It is noted, however, that the van Genuchten parameters were selected after an initial attempt to use a linear capillary pressure relation for the fractures resulted in the TOUGH2 code failing to complete the simulation.

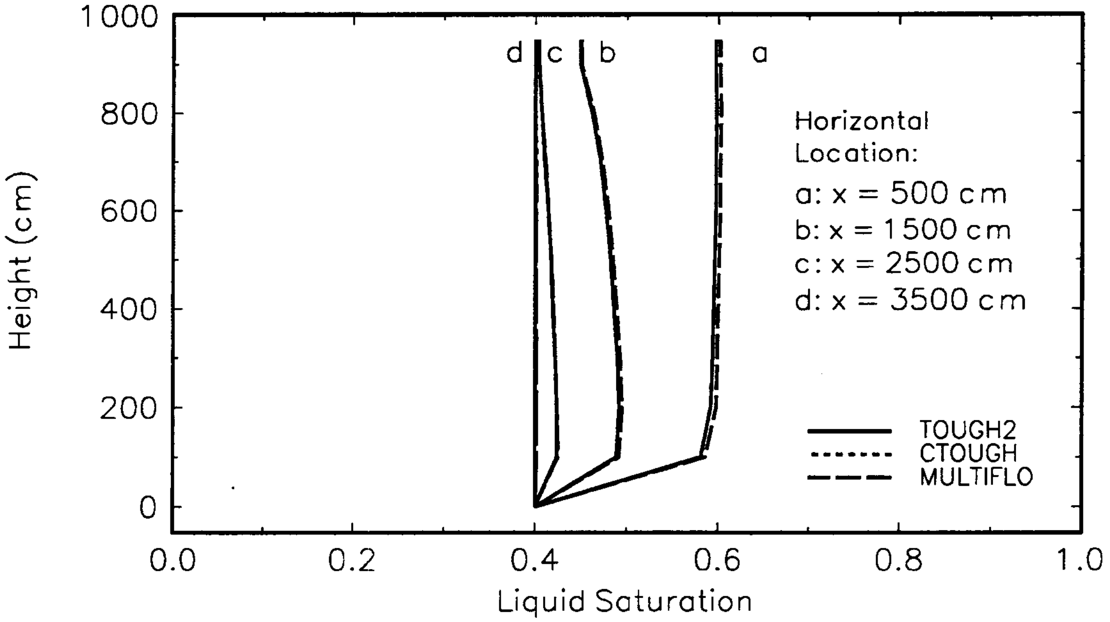
Table 3-5. Soil hydraulic properties for 2D isothermal flow in fractured media

Layer	θ_s	θ_r	$\alpha (cm^{-1})$	n	$K_s (cm/d)$
Matrix	0.30	0.1050	0.01019	1.395	8.478E-4
Fractures	0.45	0.0045	0.09790	4.000	7.056E4

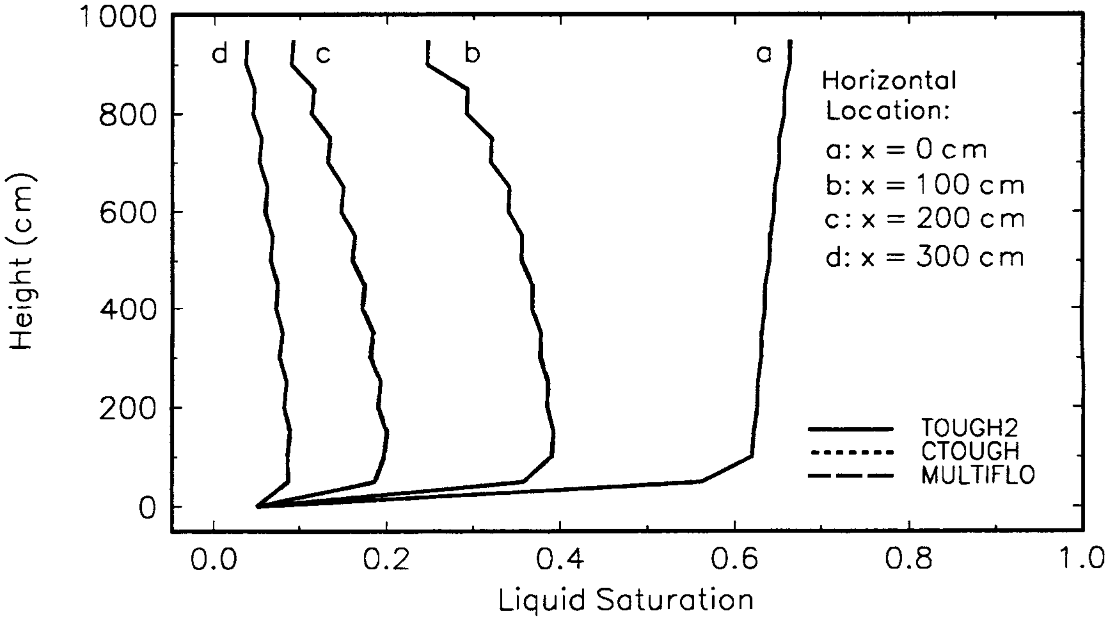
3.3.3 Evaluation of Results

This 2D isothermal test problem was intended to provide a basis for evaluating the capabilities of the four thermohydrologic codes to model flow in a system with characteristics relevant to the proposed repository site. In setting up the computational grids for this test case, it was found that the capability of TOUGH2, CTOUGH, and MULTIFLO easily accommodated the matrix-fracture geometry while the FEHMN code gridding required many more nodes (because the elements use vertex based nodes). This inconsistency in computational grid violated the basic guideline of test equivalence (see Section 2.2). Moreover, even for short simulation times, the FEHMN code with a fine grid required excessive CPU time. The high permeability contrasts may also have contributed to the computational difficulty. As a result, the FEHMN code was excluded from this test case. It is believed that the FEHMN code could overcome the gridding limitation by the addition of line elements (Baca et al., 1984) or plate elements (Lopez and Smith, 1995) to the code.

Liquid saturation profiles plotted from the numerical results of the three codes are shown in Figure 3-6. The first series of curves in Figure 3-6(a) show the vertical saturation profiles for the vertical fractures while those in Figure 3-6(b) are for the matrix blocks only. Omitted from Figure 3-6(b) are the saturations in the horizontal fractures which exhibit similar values for adjacent vertical fractures. These plots clearly show that the results agree exceptionally well. The computational results for this particular test problem supported the conclusion that the TOUGH2, CTOUGH, and MULTIFLO codes can effectively simulate variably saturated flow into media with large contrasts in permeability as well as in geometry. Neither the high mass source nor the contrasting retention properties of the fracture and matrix posed any problem for the codes. The MULTIFLO and CTOUGH codes needed the least CPU time while the TOUGH2 code required the largest. Computational statistics for each of the thermohydrologic codes are summarized in Table 3-6.



(a) Matrix



(b) Fracture

Figure 3-6. Comparison of saturation profiles for 2D isothermal flow in fractured media

Table 3-6. **Computational statistics for 2D isothermal flow in fractured media**

Parameter	TOUGH2	FEHMN	CTOUGH	MULTIFLO
Total Run Time (CPU s)	2701.12	—	643.25	157.60
Total Steps	341	—	188	134
Total Newton Iterations	1801	—	345	352
Total Step Cuts	107	—	0	0
Average CPU/Step	7.92	—	3.42	1.176
Average Iterations/Step	5.28	—	1.835	2.63
Average CPU/Element/Step	.026	—	.011	3.92E-3
Average CPU/Element	9.00	—	2.14	.525
Minimum Time Step (s)	1E-7	—	1.8E-5	8.64E-6
Maximum Time Step (s)	1.5E4	—	6.19E5	4.32E5
Ratio of Total Run Time to Minimum Run Time	17.14	—	4.08	1

4 BENCHMARK TEST CASES FOR NONISOTHERMAL FLOW

4.1 ONE-DIMENSIONAL FLOW IN A SOIL COLUMN WITH HEAT SOURCE

4.1.1 Problem Statement and Test Objectives

In this 1D nonisothermal test case (designated NF-1), the thermohydrologic codes were applied to the problem of modeling coupled heat transfer and fluid flow with phase transitions. The homogeneous soil column was 34,000 cm high with uniform initial conditions: (i) temperature of 55 °C, (ii) liquid saturation of 0.40, and (iii) gas phase pressure of 1 bar (10^5 Pa). The upper boundary conditions are held fixed at these values while the bottom boundary was specified as no flow and no heat flux. The hydraulic and thermal properties of the porous matrix were chosen to produce a range of multiphase conditions. Heat was introduced into the soil column by a point source at the lowermost grid block. This resulted in conduction of thermal energy from the source which, in turn, created the high fluid temperatures and pressures. A drying front developed near the heat source and induced upward vapor flow with subsequent condensation.

The objective of this test case was to assess the ability of the thermohydrologic codes to describe the (i) interaction between gravity, capillarity, and viscous forces; (ii) phase changes; and (iii) rapidly changing thermodynamic conditions. The range of thermohydrologic conditions produced in this test case fully exercised the computational algorithms for coupled heat and flow as well as the calculation of thermodynamics properties. This test case was deceptively simple and, in actuality, more than an adequate challenge to probe code strengths and weaknesses.

4.1.2 Input Specifications

The geometry of the idealized soil column and associated boundary conditions are shown in Figure 4-1. For the finite difference codes, this domain was discretized into a grid of 35 blocks with uniform block sizes of $\Delta x = \Delta y = 1{,}000$ cm and $\Delta z = 1{,}000$ cm except at the top and bottom of the grid where $\Delta z = 500$ cm. For the finite element code, the grid was composed of 34 elements of $\Delta x = \Delta y = \Delta z = 1{,}000$ cm. The lateral boundaries of the column of grid blocks were set to no flow and no heat flux conditions. The soil column was assigned a heat source of 10^3 J/s, bulk density of 2300 kg/m^3, specific heat of 840 J/kg-K, and thermal conductivity of 10.0 W/m-K. Thermal conductivity was arbitrarily set to a large value to enhance heat conduction. Soil hydraulic properties assigned to the soil column are summarized in the following Table 4-1. The total simulation period for this test case was 15 days.

Table 4-1. Soil hydraulic properties for 1D nonisothermal flow problem

Layer	θ_s	θ_r	$\alpha (Pa^{-1})$	n	$k_m x 10^{-10} (cm^2)$
Porous Matrix	0.200	0.02	5.555E-5	2.000	9.87

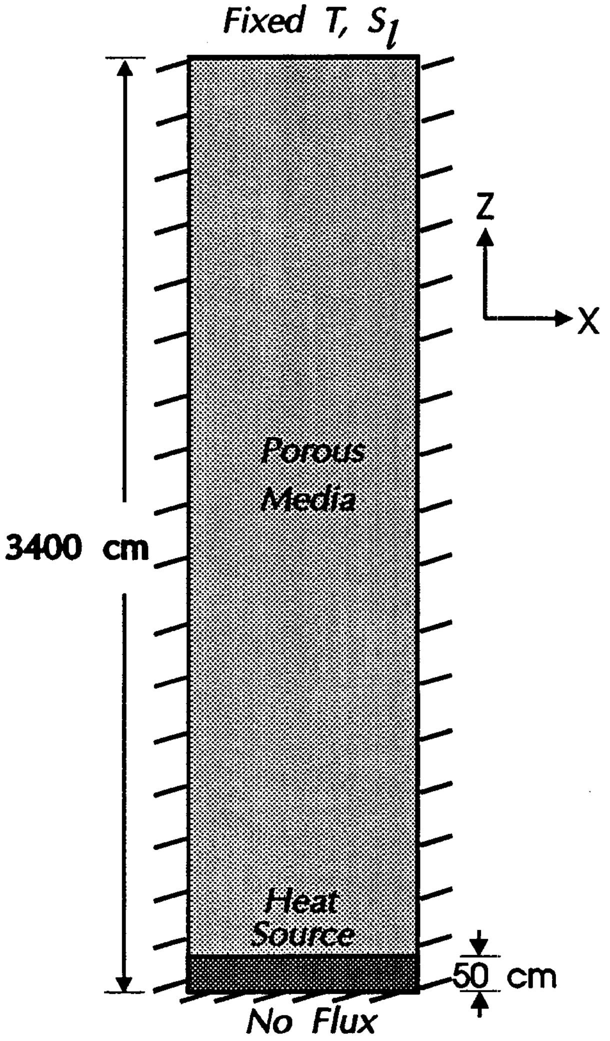
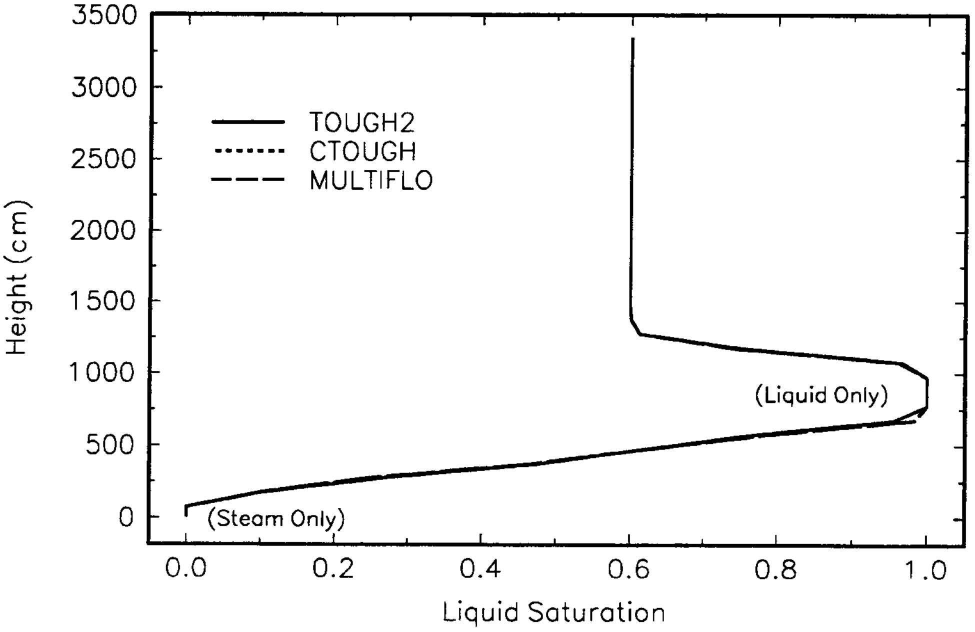


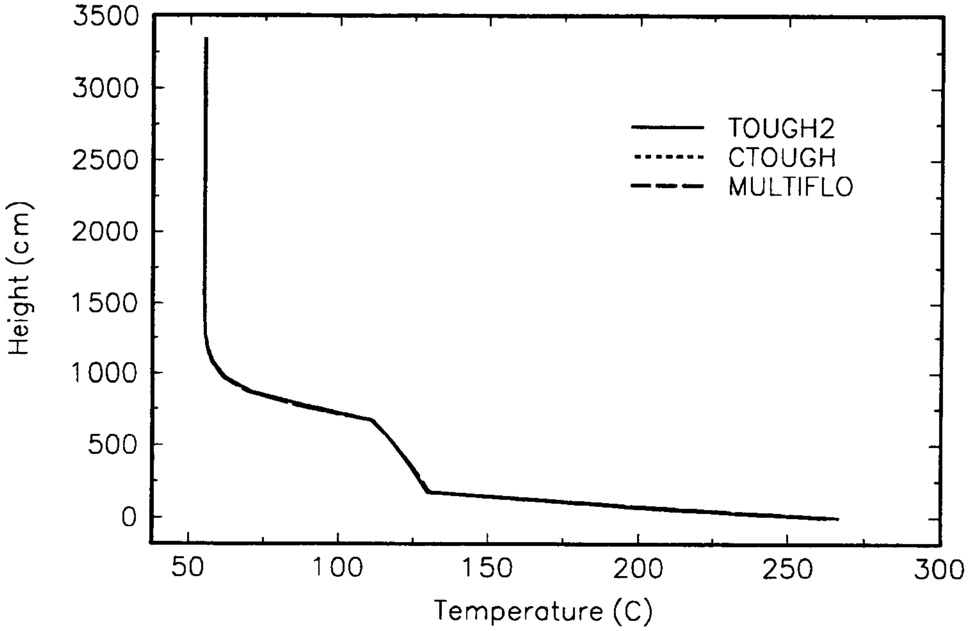
Figure 4-1. System sketch for 1D nonisothermal flow problem

4.1.3 Evaluation of Results

Numerical results for this test case, which are illustrated in Figure 4-2, suggested a complex interaction of driving forces in the vicinity of the heat source. The liquid saturation and temperature profiles shown in this figure indicate that water influx from the top boundary was essentially driven by gravity with little contribution by capillary imbibition. In the lower portion of the soil column, rapid phase transitions occurred with flow conditions changing from two-phase, to all liquid, back to two-phase, and finally to all steam. A condensation region formed above the heat source where temperatures were cooler [see Figure 4-2(a)].



(a) Saturation Profile



(b) Temperature Profile

Figure 4-2. Liquid saturation and temperature profiles for 1D test problem

From the code comparisons in Figure 4-2, it is evident that the results produced by TOUGH2, CTOUGH, and MULTIFLO code agree well, in fact, the curves overlay almost perfectly. Not shown in the figure are the results for the FEHMN code. In running the FEHMN code, it executed properly for a simulation period of about 5 days. At this point the code encountered numerical difficulties and the execution time became prohibitive. This occurred as a result of the repetitive reductions of the time step. Assistance of the FEHMN code developer was sought but the problem was not resolved. It is believed the problem may be associated with the high source rate.

The main conclusion drawn from this particular test problem was that three of the four thermohydrologic codes can very effectively simulate coupled heat and flow in the multiphase regime. Specifically, it appears that the codes properly describe conduction heat transfer and multiphase flow patterns consistent in terms of temperature rise at the heat source, creation of boiling conditions, occurrence of phase change, and upward vapor flow. The MULTIFLO code required the smallest CPU time. The computational statistics for each of the thermohydrologic codes are summarized in Table 4-2.

Table 4-2. Computational statistics for 1D nonisothermal flow problem

Parameter	TOUGH2	FEHMN	CTOUGH	MULTIFLO
Total Run Time (CPU s)	1407.98	incomplete run	887.73	5.68
Total Steps	2046	—	3309	180
Total Newton Iterations	10960	—	15234	526
Total Step Cuts	964	—	1345	1
Average CPU/Step	.3349	—	.3191	.0314
Average Iterations/Step	2.54	—	5.69	2.67
Average CPU/Element/Step	9.30E-3	—	8.86E-3	8.734E-4
Average CPU/Element	3.66E-3	—	1.56E-3	3.27E-4
Minimum Time Step (s)	15.2	—	17.97	8.64
Maximum Time Step (s)	.461E4	—	1.21E4	6.10E3
Ratio of Total Run Time to Minimum Run Time	247.88	—	156.29	1

4.2 TWO-DIMENSIONAL MULTIPHASE FLOW IN LAYERED SOIL

4.2.1 Problem Statement and Test Objectives

This next test case, NF-2, considered nonisothermal flow in a 2D multilayered porous medium. The system geometry is the same as the previous 2D isothermal flow problem (see Section 3.2.2) and consists of a rectangular region 2,500 cm high and 700 cm wide. Flow into the system was introduced by an internal water source located in the upper left corner of the domain. Heat sources were introduced in 3 grid blocks located near the middle of the domain. The initial temperature and pressure head were uniformly set to 20 °C and 1 bar, respectively. The top boundary of the system was set to fixed pressure head and temperature, corresponding to the initial values. The lateral and bottom boundaries were no flow and no heat flux. The soil column was assumed to be composed of alternating soil layers with contrasting hydraulic properties. The permeabilities of the soil layers were anisotropic with the vertical permeability set to 10 times larger than the horizontal permeability.

The main objective of this 2D test problem was to determine how well the thermohydrologic codes simulated multiphase flow in a heterogeneous medium where the infiltration occurred only over a small portion of the soil surface. Under these boundary conditions, the fluid flow exhibited distinct 2D behavior as it moved horizontally along interfaces and vertically through the individual soil layers. Another objective of this problem was to test the codes in a wetter fluid regime. Thus, to create higher saturation levels a high infiltration rate was assumed. This high infiltration rate produced large pressure head gradients and enhanced the dynamics of flow, both of which made the problem more computationally challenging.

4.2.2 Input Specifications

The system geometry (see Figure 4-3) and grid used in this test case are similar to those used in the previous 2D isothermal flow problem (see Section 3.2.2). The primary difference is the placement of heat sources in 3 grid blocks near the middle of the column. The computational grid consisted of 7 grid blocks in the x-direction, 1 in the y-direction, and 25 in the z-direction. Location of the internal heat sources were (i,j,k)=(3,1,13), (i,j,k)=(4,1,13), and (i,j,k)=(5,1,13). The vertical and horizontal grid block sizes were uniform with $\Delta x = \Delta y = \Delta z = 100$ cm, except at the boundaries where $\Delta x = \Delta z = 50$ cm. The soil column was assigned a heat source of 2,000 J/s, bulk density of 2,300 kg/m^3, specific heat of 1,000 J/kg-C, and thermal conductivity of 5 W/m-C. The duration of the simulation period was 30 days.

Each layer of this idealized porous medium is 500 cm thick. The hydraulic properties for the two soils are variations of those properties used in the previous isothermal 1D test problem. To add different facets to this nonisothermal flow test case, the porosities for the two soils were chosen to be smaller, as were the residual moisture contents. In addition, the permeability in the horizontal direction was assigned a value of one-tenth that in the vertical. Hydraulic properties used in this 2D test problem are summarized in Table 4-3.

4.2.3 Evaluation of Results

This test case provided a basis for evaluating the capabilities of the thermohydrologic codes to simulate transient multiphase flow in 2D. In contrast to the previous test case, all four codes successfully simulated heat transfer, multiphase flow, and moisture redistribution. Liquid saturation and temperature profiles generated from the code output are shown in Figure 4-4. The profiles for various locations show that the TOUGH2, FEHMN, CTOUGH, and MULTIFLO agree very well. The saturation and temperature profiles for TOUGH2, CTOUGH, and MULTIFLO are exceptionally close, while slight differences are evident for the FEHMN code. These differences are due to the slightly different computational grid required to maintain an equivalent number of nodes.

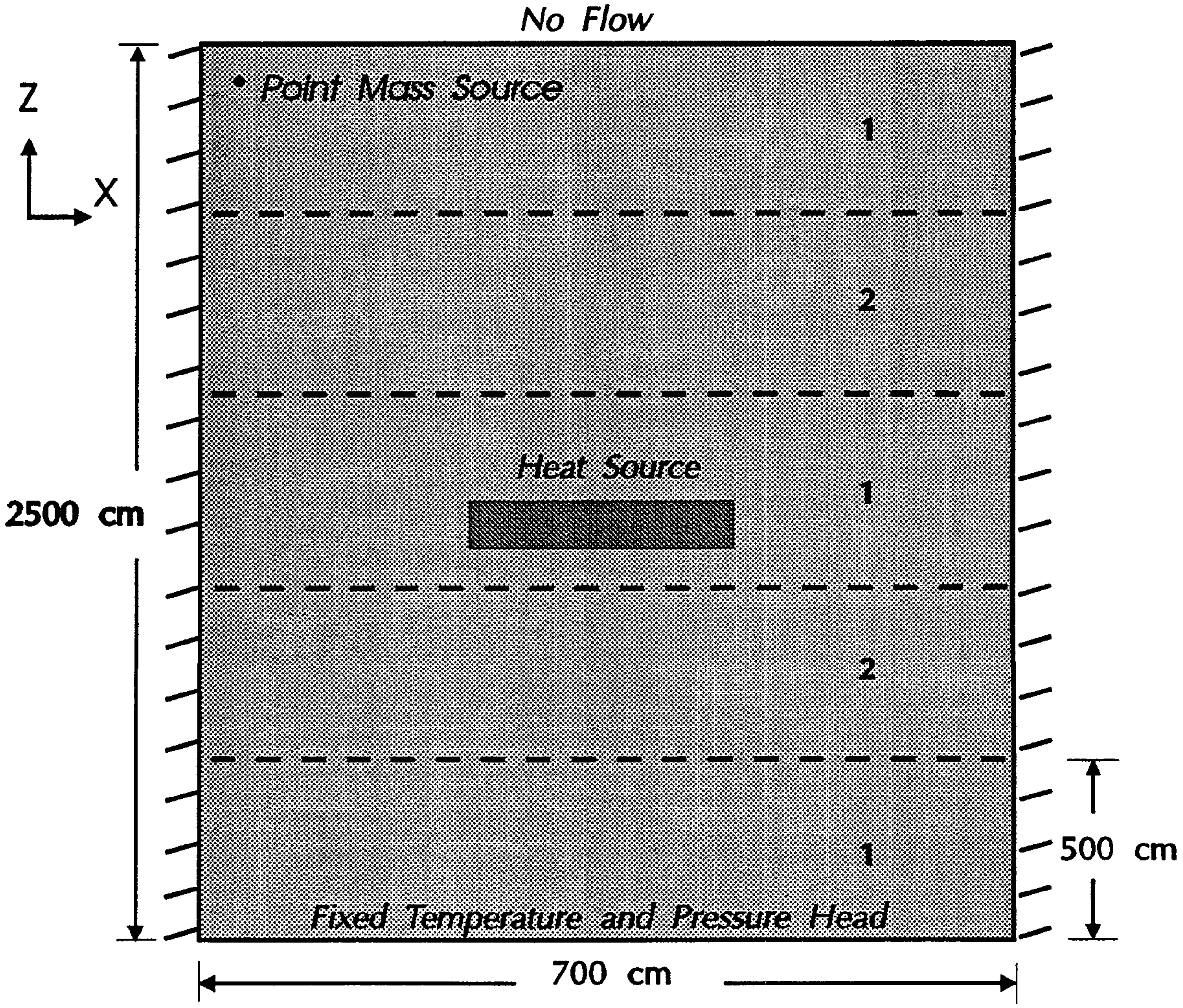
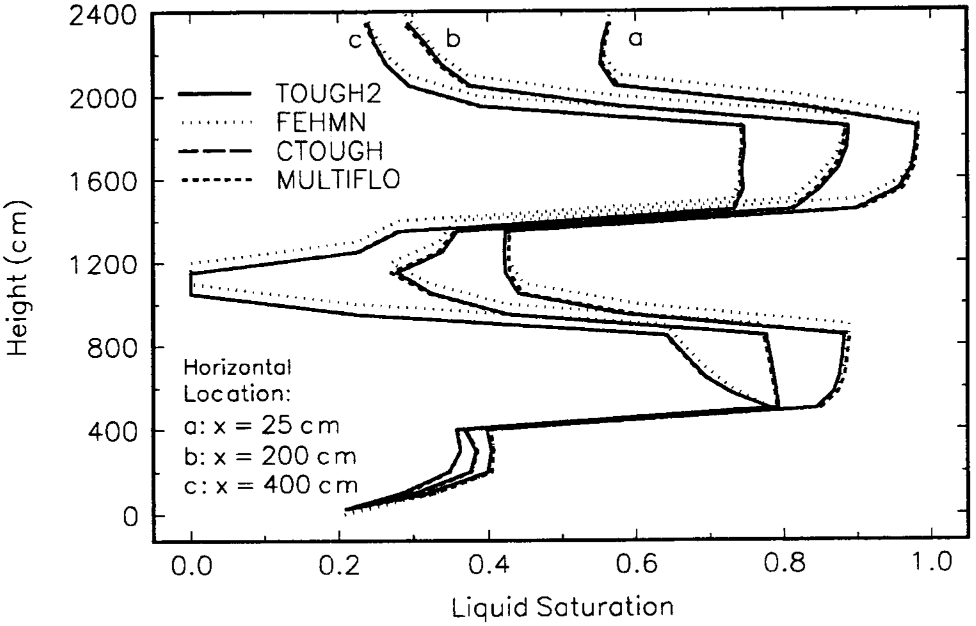


Figure 4-3. System sketch for 2D nonisothermal flow problem

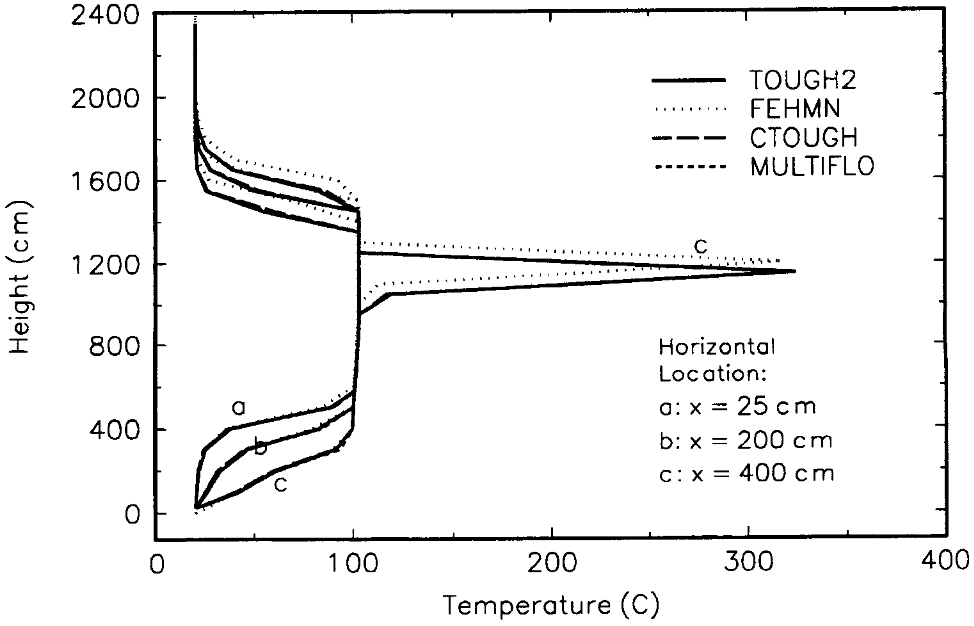
Table 4-3. Soil hydraulic properties for 2D nonisothermal flow problem

Layer	θ_s	θ_r	$\alpha (cm^{-1})$	n	$K_z (cm/d)$
High K Layer	0.05	0.010	0.0280	2.2390	5410.0
Low K Layer	0.10	0.025	0.0104	1.3954	131.0

The graphical results in Figure 4-4 suggested that the four codes capture the physics of nonisothermal flow for this test case. Overall, these results supported the conclusion that all four thermohydrologic codes effectively simulate multiphase flow in a layered porous medium. Neither the



(a) Saturation Profile



(b) Temperature Profile

Figure 4-4. Comparison of liquid saturation and temperature profiles for 2D nonisothermal test problem mass source rate or the anisotropic properties appeared to have posed any problem for the four codes. As in the previous test cases, the MULTIFLO code required the least CPU time and the FEHMN code the largest. Computational statistics for each of the thermohydrologic codes are summarized in Table 4-4.

Table 4-4. Computational statistics for 2D nonisothermal flow problem

Parameter	TOUGH2	FEHMN	CTOUGH	MULTIFLO
Total Run Time (CPU s)	1054.47	2289.22	1353.4	307.27
Total Steps	125	1312	628	371
Total Newton Iterations	664	3976	2058	1405
Total Step Cuts	15	N/A	12	10
Average CPU/step	8.44	1.74	2.16	.828
Average Iteration/Step	5.31	3.03	3.27	3.79
Average CPU/Element/Step	.0482	9.94E-3	.012	4.73E-3
Average CPU/Element	6.03	13.08	7.73	1.76
Minimum Time Step (s)	1E2	N/A	1.03E2	43.2
Maximum Time Step (s)	7.62E4	N/A	2.16E4	2.57E4
Ratio of Total Run Time to Minimum Run Time	3.42	13.08	4.4	1

4.3 TWO-DIMENSIONAL MULTIPHASE FLOW IN FRACTURED-POROUS MEDIUM

4.3.1 Problem Statement and Test Objectives

The final isothermal test problem (NF-3) was designed to be much more challenging than the previous test problems and required modeling flow in fractured-permeable medium. The physical system was a 2D homogeneous porous medium with very low permeability and a system of orthogonal fractures. The domain of this hypothetical system is a rectangular region 1,001.0 cm high and 700.8 cm wide. The domain is traversed by 10 horizontal and 8 vertical fractures. The fracture spacing and aperture are uniform with values of 100 cm and 0.1 cm, respectively. As in the previous problem, flow was introduced to the system by a mass source located in the upper left corner of the domain. The top and vertical boundaries of the system were no flow boundaries. The bottom boundary was set to a fixed temperature, capillary pressure, and gas saturation equal to the initial values of 30 °C, 1 bar, and 0.4, respectively.

The main objective of this test problem was to determine how well the thermohydrologic codes modeled multiphase flow in a fractured-porous medium. The fluid flow exhibited distinct thermal and flow behavior along the fractures and interacts with the porous matrix. Another objective of this problem was to test the robustness of the codes to handle very large permeability contrasts which are quite common in detailed simulations of actual geologic systems.

4.3.2 Input Specifications

The system geometry and the location of the internal source are shown in the diagram presented in Figure 4-5. The computational grid used to represent the domain consisted of 7 grid blocks in the x-direction, 1 in the y-direction, and 10 in the z-direction. The computational grid for this test case was largely uniform with block sizes of $\Delta x = \Delta y = \Delta z = 100$ cm; grid blocks half this size were used at boundaries of the domain. Each fracture was represented with a thin block equal to the fracture aperture. The duration of the simulation period was 30 days. The internal source was the same as the previous test case and was set to 4.62×10^{-3} kg/s.

Matrix blocks in the flow domain are bounded by vertical and horizontal fractures. As a result, each block is isolated from the other matrix blocks. This geometry, along with the low matrix permeability, constrained the flow and thermal behavior of the system. The permeability contrast between the fractures and matrix is in excess of 7 orders of magnitudes. In addition, the van Genuchten parameters assigned to the fractures were selected to ensure that water drains rapidly through the fractures. The combination of contrasting permeabilities and van Genuchten parameters make this test case exceptionally challenging. The specific matrix and fracture properties used in this 2D test problem are summarized in Table 4-5.

Table 4-5. Soil hydraulic properties for 2D isothermal flow in fractured media

Medium	θ_s	θ_r	$\alpha (cm^{-1})$	n	$K_s (cm/d)$
Matrix	0.30	0.1050	0.01019	1.395	8.478E-4
Fractures	0.45	0.0045	0.09790	4.000	7.056E4

4.3.3 Evaluation of Results

This final test problem involved the most complex of thermal and hydraulic characteristics. As such, it represented a calculational acid test for the thermohydrologic codes. Only the three finite difference codes were applied to this test case because the finite element code required a much finer grid (see Section 3.3.3). For the purposes of making direct comparisons, the liquid saturation and temperature profiles were separately plotted for fractures and porous matrix. The locations of these profiles were selected to bound and traverse the heat source. The graphical comparisons for liquid saturations are presented in Figure 4-6(a) and (b). Similarly, the temperature profiles are shown in Figure 4-6(c) and (d).

As can be seen from these plots, the three codes (TOUGH2, CTOUGH, and MULTIFLO) produced results that agree very well. The three saturation profiles for the vertical fractures, overlay almost perfectly like those for the porous matrix. Similarly, both sets of temperature profiles show close agreement except at the peak temperatures [see Figure 4-6(c)]. Quite interestingly, the CTOUGH agreed better with the MULTIFLO results than with TOUGH2 results. This is a surprising result because both the CTOUGH and TOUGH2 codes are extensions of the original TOUGH code (Pruess, 1987).

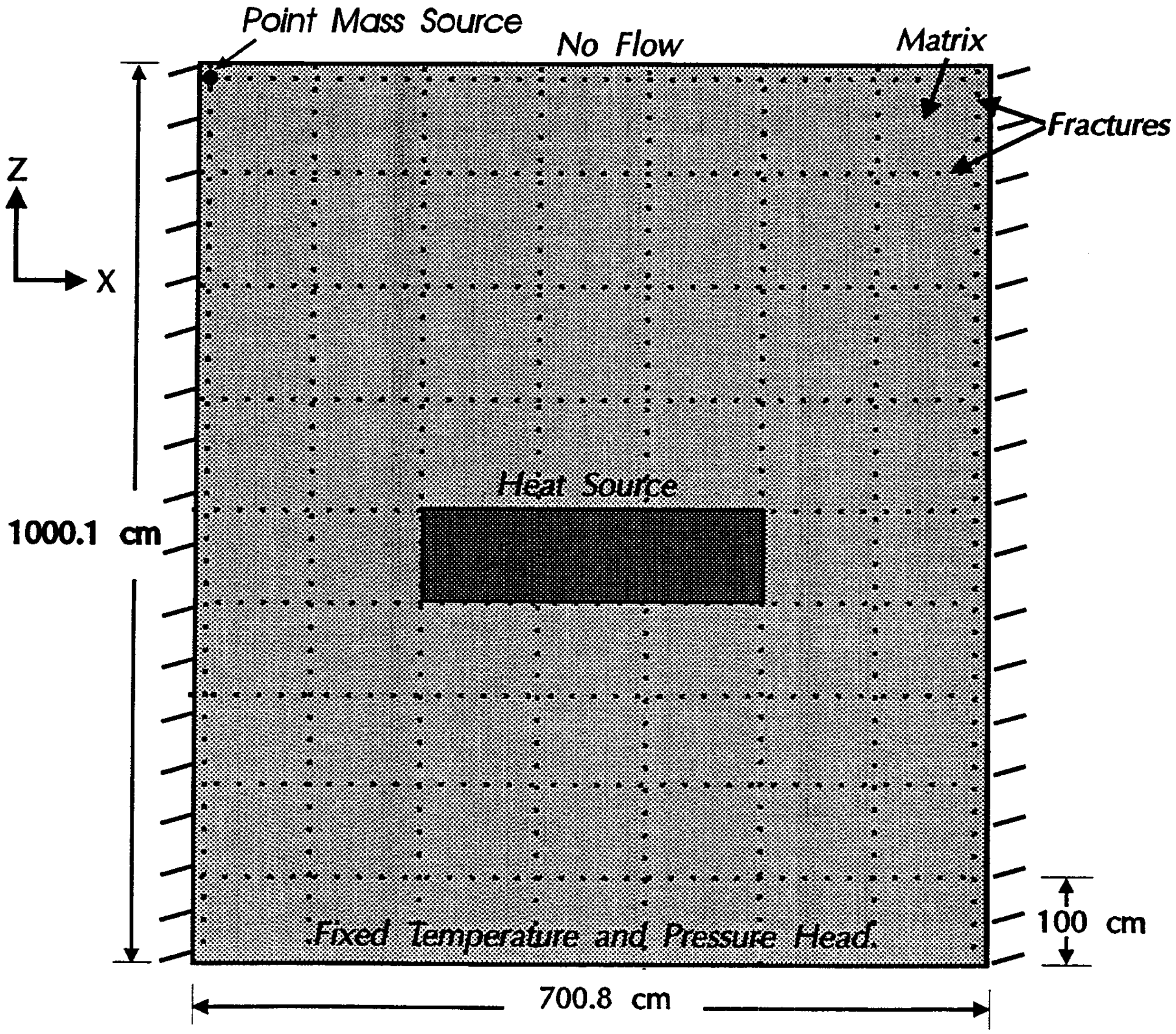
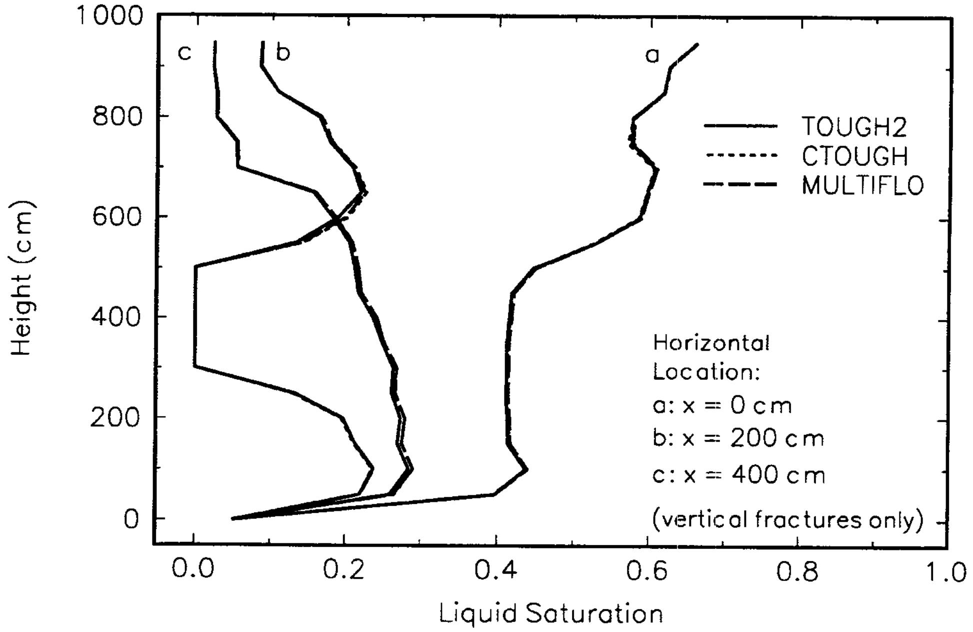


Figure 4-5. System sketch for 2D nonisothermal flow in fractured-porous media

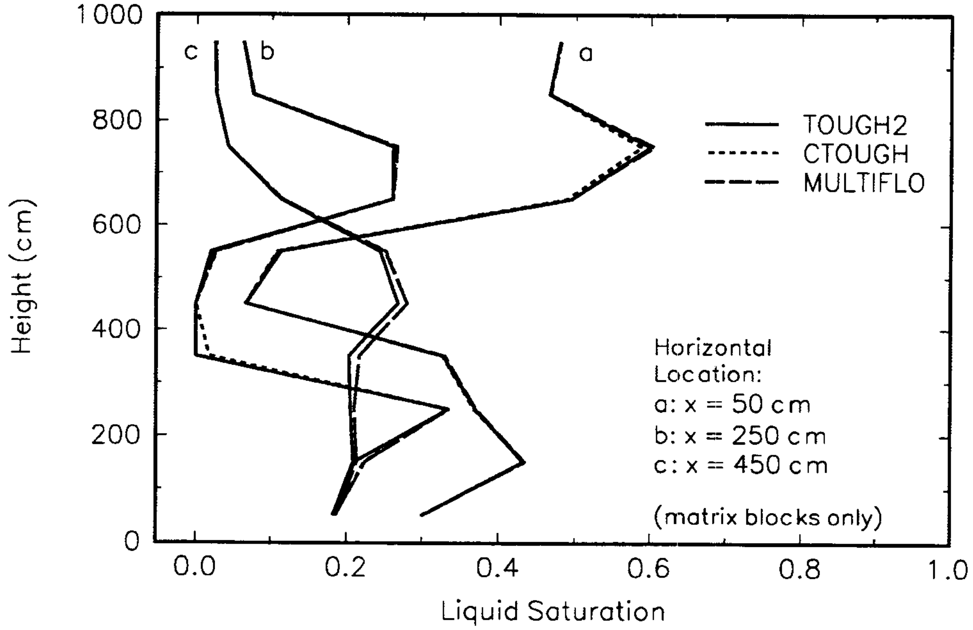
The computational results for this particular test problem supported the conclusion that the TOUGH2, CTOUGH, and MULTIFLO codes possess comparable capabilities to simulate multiphase flow in fractured-porous media. Among the four codes, the main differences in code capabilities are in the computational performance (see Table 4-4). As in previous test cases, the MULTIFLO code required the least CPU time and TOUGH2 the largest.

Table 4-6. Computational statistics for 2D isothermal flow in fractured media

Parameter	TOUGH2	FEHMN	CTOUGH	MULTIFLO
Total Run Time (CPU s)	7418.30	N/A	2833.52	721.07
Total Steps	744	N/A	539	386
Total Newton Iterations	2706	N/A	1576	1377
Total Step cuts	12	N/A	4	2
Total Elements	300	N/A	300	300
Average CPU/step	9.97	N/A	5.26	1.87
Average Iteration per Step	3.64	N/A	2.92	3.57
Average CPU/Element/Step	.0332	N/A	.0175	6.233E-3
Average CPU/Element	24.73	N/A	9.45	2.404
Minimum Time Step (s)	.1E-8	N/A	1.8E-5	.86E-5
Maximum Time Step (s)	.43E4	N/A	3.23E4	.43E5
Ratio of Total Run Time to Minimum Run Time	10.29	N/A	3.93	1

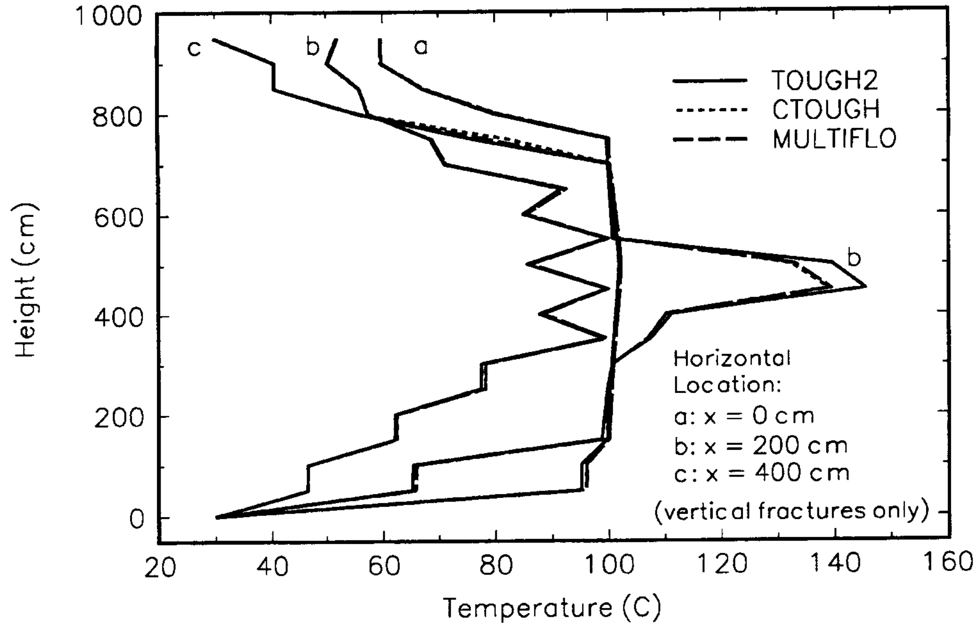


(a) Fracture

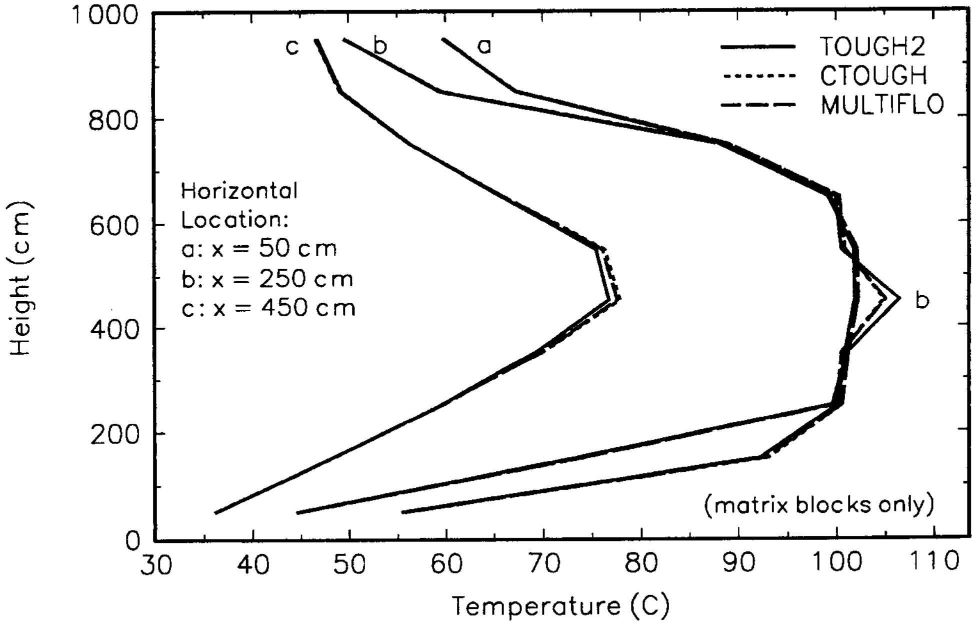


(b) Matrix

Figure 4-6. Comparison of saturation and temperature profiles for 2D nonisothermal flow in fractured media



(c) Fracture



(d) Matrix

Figure 4-6. Comparison of saturation and temperature profiles for 2D nonisothermal flow in fractured media

5 SUMMARY OF FINDINGS AND CONCLUSIONS

Computational testing of the TOUGH2, FEHMN, CTOUGH, and MULTIFLO codes was conducted with three main objectives: (i) compare and contrast the analysis capability of the four thermohydrologic codes, (ii) identify and understand any significant differences that may arise between DOE and NRC/CNWRA code applications (as a result of computer implementation), and (iii) assess the robustness and computational efficiency of the codes. These objectives were accomplished through code benchmark testing (i.e., code-to-code comparisons). Graphical comparisons of pressure, temperature, and liquid saturation calculations were performed. The benchmark testing of the four thermohydrologic codes used a protocol that tested each code in an equivalent way, permitted each code to achieve the best performance, and tested the major capabilities of the codes in a progressive manner.

5.1 GENERAL FINDINGS

From the computational results of the six benchmark test cases, it was generally found that the TOUGH2, CTOUGH, and MULTIFLO codes produced numerical results that agreed most closely. Results produced by the FEHMN code that deviated from this group primarily are due to the discretization approach. Specifically, the FEHMN used vertex centered nodes in contrast to the other three codes which used cell centered nodes. The observed differences can be explained and resolved through grid refinement. Thus, the conclusion of this study is that the DOE and NRC are not likely to arrive at different interpretations of important thermohydrologic processes and couplings, as a result of using different computer codes, so long as process assumptions and parameter values are uniform.

It was found, however, that the DOE FEHMN code appears to have some computational limitations. These limitations are associated with using infiltration rates (or mass source rates) and modeling discrete fractures. The first limitation is significant in that the code was unable to model flow for cases with moderate to high infiltration rates (see Sections 3.1.3 and 3.2.2). Thus, the current version of the code may not be capable of analyzing pluvial climate scenarios. This particular limitation was manifested in the FEHMN code by the necessity of very small time steps. Similar problems with the FEHMN code were recently noted by a DOE contractor using the FEHMN code to model drift-scale thermohydrologic phenomena (for the proposed repository). The contractor report (TRW Environmental Systems, Inc., 1995) stated that "numerical difficulties prevented the use of an infiltration rate greater than 0.3 mm/yr." The second limitation is significant in that the code cannot feasibly model heat transfer and/or fluid flow in porous media with systems of discrete fractures, because of prohibitive CPU requirements. In addition, it is believed that the high permeability contrast between fracture and matrix was also a factor causing numerical difficulties in the fracture flow cases (see Sections 3.3.3 and 4.3.3). FEHMN also encountered difficulties in simulating 1D nonisothermal flow in a homogeneous porous medium with fixed boundary conditions (see Section 4.1.3). This particular simulation was terminated because of excessive CPU requirements.

5.2 COMPUTATIONAL ASPECTS

For each test case, various computational parameters were tabulated to provide an indication of the efficiency of the computer codes. In all cases, the MULTIFLO code was found to perform better, in terms of CPU time, than the other three thermohydrologic codes. This superior performance appeared to be due to three factors: (i) efficiency of Newton iteration (based on analytic calculation of Jacobian terms), (ii) speed of the iterative solvers, and (iii) effectiveness of the automatic time-stepping algorithm.

The computational speed of the CTOUGH code was in most cases faster than the TOUGH2 code. These three codes exhibited a high degree of robustness in solving the full set of benchmark test cases. Although the FEHMN code did not have the same success as the other codes, the limitations identified in this study can be overcome with nominal code enhancements.

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