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Civilian Radioactive Waste Management System
Management and Operating Contractor

REVIEW AND SELECTION OF UNSATURATED FLOW MODELS

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1. INTRODUCTION

Since the 1960's, ground-water flow models have been used for analysis of water resources problems. In the 1970's, emphasis began to shift to analysis of waste management problems. This shift in emphasis was largely brought about by site selection activities for geologic repositories for disposal of high-level radioactive wastes. Model development during the 1970's and well into the 1980's focused primarily on saturated ground-water flow because geologic repositories in salt, basalt, granite, shale, and tuff were envisioned to be below the water table. Selection of the unsaturated zone at Yucca Mountain, Nevada, for potential disposal of waste began to shift model development toward unsaturated flow models. This emphasis was greatly increased by the Nuclear Waste Policy Act Amendment in 1987 which named Yucca Mountain as the only site under investigation for potential disposal of high-level radioactive waste. Since the mid-1980's, pre-existing unsaturated flow models have been used, and many new unsaturated flow models have been developed. These models, which incorporate various flow submodels, have been developed on a somewhat independent basis by universities, national laboratories, and private companies. Interactions among developers, however, stimulated the development so that there is a considerable amount of similarity among the existing models. Also, during the development, as the significance of fractures was realized, models progressed from porous-media flow toward fractured flow through porous media.

Under the U.S. Department of Energy (DOE), the Civilian Radioactive Waste Management System Management and Operating Contractor (CRWMS M&O) has the responsibility to review, evaluate, and document existing computer models; to conduct performance assessments; and to develop performance assessment models, where necessary. In the area of scientific modeling, the M&O CRWMS has the following responsibilities:

- To provide overall management and integration of modeling activities
- To provide a framework for focusing modeling and model development
- To identify areas that require increased or decreased emphasis
- To ensure that the tools necessary to conduct performance assessment are available.

These responsibilities are being initiated through a three-step process. It consists of a thorough review of existing models, testing of models which best fit the established requirements, and making recommendations for future development that should be conducted. Future model enhancement will then focus on the models selected during this activity. Furthermore, in order to manage future model development, particularly in those areas requiring substantial enhancement, the three-step process will be updated and reported periodically in the future.

This document describes the CRWMS M&O approach to model review and evaluation (Chapter 2), and the requirements for unsaturated flow models which are the bases for selection from among the current models (Chapter 3). Chapter 4 identifies existing models and their characteristics. Through a detailed examination of characteristics, Chapter 5 presents the selection of models for testing. Chapter 6 discusses the testing and verification of selected models. Chapters 7 and 8 give conclusions and make recommendations, respectively. Chapter 9 records the major references for each of the models reviewed. Appendix A, a collection of technical reviews for each model, contains a more complete list of references. Finally, Appendix B characterizes the problems used for model testing.

2. APPROACH TO MODEL SELECTION

The approach used in this evaluation was to compile a list of existing models from those currently used in the DOE waste management programs and those used in the recent past. This list included appropriate models from the Basalt Waste Isolation Project, the Office of Nuclear Waste Isolation, and the Waste Isolation Pilot Plant, as well as those currently being used by the Yucca Mountain Site Characterization Project Office (YMPO). The models were then divided into categories such as subsystem models, subsurface natural processes, waste and repository induced processes, biosphere processes, and uncertainty/sensitivity analyses. Unsaturated flow models, the subject of this report, appeared in two categories: subsystem models and subsurface natural processes.

Because of the importance of unsaturated flow to waste isolation at Yucca Mountain, and because of the amount of model development being conducted in this area, unsaturated flow models were selected for a thorough evaluation. Waste isolation at Yucca Mountain is a function of fluid flow through fractured and porous media. The fluids, which are composed of liquid water, water vapor and air, flow through fractured and porous rocks which can be modeled by the concepts of porous media and fractured rock. For this reason, multiphase, single-phase liquid, single-phase gas, and discrete-fracture models were selected for evaluation. Table 1 presents a list of the unsaturated flow models that were evaluated.

The model evaluation was carried out by completing the following three steps:

- Technical Review
- Model Testing
- Programmatic Review.

The technical review of each model was based on documentation, publications, and discussions with the developers, where necessary. Appendix A presents the individual technical reviews, which serve as the basis of Chapters 4 through 6. These technical reviews form the basis for comparison of individual models with the requirements in Chapter 3 and for the selection of specific models for testing in Chapter 5.

Models selected for testing were installed on CRWMS M&O computers for component and site representative testing. Component tests consisted of comparison of simulated results with analytical solutions of simplified model equations. This comparison demonstrates that the coding of a specific mathematical model is correct (i.e., code verification). Site representative testing (Chapter 6) consisted of simulations which are more representative of the Yucca Mountain site to gain more familiarity with the models. Also, based on the review and testing of the models, recommendations for further enhancement of selected models are made in Chapter 8 of this report.

Because of the importance of model selection to performance assessment, and to the licensing of the repository, a program-wide review of the selection process, the results, and the recommendations for further development or enhancement was conducted. A draft of this document provided the basis for that review, and comments from the model developers aided greatly in making this evaluation more complete.

TABLE 1. Models Considered by the Technical Review

	DEVELOPING AGENCY	REFERENCE	SELECTED FOR TESTING
MULTI-PHASE			
FEHM	LANL	Zyvoloski et al. (1991)	X
MSTS	PNL	White and Nichols (1992) Nichols and White (1992)	X
NORIA	SNL	Bixler (1985)	
NUFT	LLNL	Nitao (1992)	X
TOUGH2	LBL	Pruess (1991)	X
V-TOUGH	LLNL, LBL	Nitao (1989)	
SINGLE-PHASE-LIQUID			
DCM3D	GRAM, SNL, NRC	Updegraff et al. (1991)	
FEMTRAN	SNL	Martinez (1985)	
FEMWATER/FEMWASTE	ORNL	Yeh (1987) Yeh and Ward (1981)	
LLUVIA-II	SNL	Eaton and Hopkins (1992)	X
NORIA-SP	SNL	Hopkins et al. (1991)	
SAGUARO	SNL	Eaton et al. (1983)	
TOSPAC	SPECTRA, SNL	Gauthier et al. (1992) Dudley et al. (1988)	X
TRACR3D	LANL	Birdsell and Travis (1991a)	X
VS2DT	USGS	Lappala et al. (1987)	X
SINGLE-PHASE-GAS			
TGIF	DISPOSAL SAFETY, SNL	Ross et al. (1992)	
DISCRETE-FRACTURE			
FRACMAN/MAFIC	GOLDER	Dershowitz et al. (1991), Miller (1990)	

3. MODEL-SELECTION REQUIREMENTS

The requirements for selection of flow models in the unsaturated zone are based on two regulatory requirements: one for calculating the pre-emplacement ground-water travel time (10 CFR 60), and one for calculating the release of radionuclides to the accessible environment over 10,000 years (40 CFR 191). The latter requires a detailed analysis of unsaturated flow under repository conditions which includes a significant input of thermal energy from the decaying waste. Also, the ground-water flow models will be used for analyses during site characterization, analyses of repository and waste package designs, and interpretation of the effects of natural events and processes which are expected to occur over the 10,000-year period. In addition to the regulations, the model requirements stem from the geologic characteristics of the Yucca Mountain site and from the theory of unsaturated flow itself.

The requirement of providing reasonable assurance that the pre-emplacement ground-water travel time from the disturbed zone of the repository to the accessible environment is greater than 1,000 years (10 CFR 60) combined with the geologic nature of Yucca Mountain produces the following model requirements:

- Water vapor and gas flowing through the mountain will affect the ground-water travel time. Changes in temperature and pressure due to topography and differences in rock-gas and atmospheric humidity levels cause gas to circulate within the mountain. This effect is degraded by the relatively high saturation levels of nonwelded tuff units and enhanced by the fractured nature of welded tuff units.

- Tuff layers having low hydraulic conductivity (nonwelded units) can cause perching of liquid water which produces a dominant lateral flow component. On this basis flow models must be capable of simulating both saturated and unsaturated water flow.

- Both requirements above lead to at least two-dimensional models (e.g., models which can solve ground-water flow problems in the space domain of a cross-section through the mountain). Here it is possible that heterogeneity in flow properties along the axis of Yucca Mountain may require a three-dimensional approach, or at least three-dimensional codes will need to be used to demonstrate the viability of the two-dimensional approach.

- The tuff units at Yucca Mountain contain both matrix and fracture porosities. Flow models must take both porosities into account.

- In underground openings in tuff and other rock types, dripping fractures have been observed within the unsaturated zone. These observations lead to the realization that disequilibrium conditions may exist between liquid in the fractures and liquid in the matrix.

Table 2 summarizes the requirements for the models needed to calculate ground-water travel time in the unsaturated zone. These requirements should be met or the models used should be shown to be conservative when compared to models that meet the requirements presented in Table 2.

Three factors suggest that the saturated zone at Yucca Mountain may be a significant consideration in the calculation of pre-emplacement ground-water travel time. These factors are summarized as follows: (1) 10 CFR 60 requires that the outer extremity of the disturbed zone be used as the starting point for the travel-time calculation. Depending upon how it is defined, the thermally disturbed zone, at higher thermal loads, may go below the water table; (2) it appears unlikely that any pre-emplacement, fracture-dominated flow channels connect the ground surface to the water table, and pass through the repository horizon. Nevertheless, establishing the non-existence of such flow channels may prove to be difficult and expensive; and (3) most likely, recent conceptualizations of the saturated zone will yield travel times that are substantially greater than 1,000 years. If this is true, it may be desirable to use only the saturated-zone travel time to demonstrate compliance with 10 CFR 60. However, because flow modeling in the saturated zone is better understood and accepted by the scientific community, and because performance assessment will require detailed modeling of flow in the unsaturated zone under repository conditions, the decision was made to limit this review to unsaturated flow models.

For the second regulatory requirement, the calculation of release of radionuclides to the accessible environment over 10,000 years, the input of thermal energy to Yucca Mountain must be considered. The input of thermal energy requires that the models include the capability of considering a heat pipe and an enhanced flow of gas through the mountain. In a heat pipe, water vaporizes near the heat source causing pressurization of the gas phase and flow of gas away from the heat source. The vapor is carried away from the heat source to cooler regions, where it condenses and deposits its heat. The water saturation profile, which increases with distance from the heat source, drives liquid water toward the heat source where it is vaporized. Near the Yucca Mountain repository, anisotropy in the fracture connectivity pattern will influence both the return flow of condensate and the outward flow of water vapor and latent heat.

In a heat pipe, heat transfer is primarily through convection. However, the model should be capable of handling convective, radiative, and conductive heat transfer. Outside the heat pipe, and perhaps near the waste as well, heat transfer is primarily by conduction. Near the waste, radiation may also contribute to the heat transfer. The conceptual design for thermal loading has not yet been developed, and the relative merits of a "hot" versus a "cold" repository are still being considered. Because of this, the capability to consider heat transfer caused by all three heat-transfer mechanisms must be maintained. Table 3 summarizes the requirements for calculation of unsaturated flow under repository conditions.

TABLE 2. Summary of Model Requirements for Ground-Water Travel-Time Calculations in the Unsaturated Zone

NUMBER	MODEL REQUIREMENT
1	Capability of considering mountain-scale water-vapor and gas flow under ambient conditions as affected by pressure and temperature changes due to topography
2	Capability of handling both saturated and unsaturated water flow
3	Capability of two- and three-dimensional flow
4	Capability of considering both disequilibrium and equilibrium conditions between fractures and matrix

TABLE 3. Summary of Model Requirements for Calculation of Unsaturated Flow Under Repository Conditions

NUMBER	MODEL REQUIREMENT
1	Capability of considering mountain-scale water-vapor and gas flow under ambient conditions as affected by pressure and temperature changes due to topography and barometric pressure changes
2	Capability of handling both saturated and unsaturated water flow
3	Capability of two- and three-dimensional flow
4	Capability of considering both disequilibrium and equilibrium conditions between fractures and matrix
5	Capability of considering mountain-scale water vapor and gas flow due to repository heat
6	Capability of considering a decaying heat source at temperatures that begin above boiling
7	Capability of considering the heat-pipe problem with heat transfer occurring by both convection and conduction

4. TECHNICAL REVIEW

4.1 MODEL IDENTIFICATION

The first step in the technical review process was to compile a list of those models which had either been used by or developed by the Yucca Mountain Site Characterization Project (YMP). For each such model, Table 1 gives model names, developing agencies, and major references. It also divides the flow models into four categories. Those designated as "multiphase, nonisothermal" consider flow processes for both liquid and gas phases. One two-phase model, TRACR3D, is not included in this category since it does not consider the nonisothermal processes of vaporization and condensation, which are crucially important for multiphase analyses of Yucca Mountain. However, TRACR3D has an excellent single-phase option, and Table 1 lists it as a single-phase liquid-flow model.

Models designated as "single-phase-liquid" use the Richards approximation to ground-water flow. This approximation assumes the gas phase to be infinitely mobile. One model, designated as "single-phase-gas," assumes 100 percent humidity levels in the rock gas. Disposal Safety's TGIF thus avoids a solution of the liquid phase and focuses on nonisothermal gas flow. Presently, a related pair of models have been designated as "discrete-fracture" models. Using borehole and outcrop data, FracMan develops statistical fracture properties and, from them, develops geometrical realizations of the fractured rock. FracMan is linked to a companion model MAFIC, but, because it can simulate only saturated flow, the companion model will be used only sparingly within the YMP. However, some of the algorithms which link it to FracMan may be directly transferable to a more general flow model.

4.2 MODEL CHARACTERIZATION

The second step in the technical review process was to identify model characteristics. This part of the technical review derived from documentation, publications, discussions with developers where necessary, and code listings, in some cases. Here, the primary goal was to identify internal algorithms, particularly those related to the code's performance and to its flow-process capabilities. Appendix A presents the model summaries developed during this review. To facilitate model comparisons, Table 4 characterizes multiphase models, and Table 5 characterizes single-phase liquid-flow models using the uniform set of characteristics described below.

4.2.1 Dimensions

Several geohydrologic factors indicate that multidimensional effects may be significant. These factors include gas flow through the mountain, lateral flow due to perched water, energy transfer through heat-pipe zones, and lateral flow between fractures and matrix, particularly in nonwelded units. As a concession to the computational difficulties, many Yucca Mountain calculations now assume one-dimensional flow. Such calculations may prove satisfactory, but they require extensive justification. To fully comply with Requirement 3 of Tables 2 and 3, the YMP will have to overcome the hardware and software limitations which now restrict problem dimensionality.

TABLE 4. General Characterization of Multiphase Models

	FEHM	MSTS	NORIA
DIMENSIONS	2, 3	1, 2, 3	2
FRACTURED-FLOW CONCEPTUALIZATION	Equivalent continuum Dual porosity Dual permeability	Equivalent continuum	Equivalent continuum
PHASES	2	1,2	2
HEAT	Yes	Yes	Yes
SPATIAL DISCRETIZATION	Finite element	Finite difference	Finite element
LINEARIZATION	Newton-Raphson	Newton-Raphson	Newton-Raphson
FLOW SOLVER	Conjugate gradient/gmres	Conjugate gradient/gmres[a] Direct	Direct
MISCIBLE COMPONENTS	Liquid? yes Gas? no	Liquid? yes Gas? no	No
CHAINING	Decay	Decay	None
GEOCHEMICAL REACTIONS	Linear sorption	Linear sorption	None
TRANSPORT SOLVER	Explicit Conjugate gradient/gmres	Conjugate gradient/gmres Direct	Direct

(a) Not yet available

TABLE 4. General Characterization of Multiphase Models (Continued)

	NUFT	PROFLOW	TOUGH2
DIMENSIONS	1, 2, 3	1,2,3	1,2,3
FRACTURED-FLOW CONCEPTUALIZATION	Equivalent continuum	Equivalent continuum Embedded planes	Equivalent continuum Multiple continuum
PHASES	1,2,...N[a]	3	2
HEAT	Yes	Yes	Yes
SPATIAL DISCRETIZATION	Integrated finite difference	Finite difference	Integrated finite difference
LINEARIZATION	Newton-Raphson	Picard	Newton-Raphson
FLOW SOLVER	Conjugate gradient/gmres Direct	Conjugate gradient/gmres Direct Successive overrelaxation Alternating directions	Conjugate gradient/gmres[b] Direct
MISCIBLE COMPONENTS	Liquid? Yes Gas? No	Liquid? Yes Gas? No	Liquid? Yes Gas? No
CHAINING	Decay	Decay Production	None
GEOCHEMICAL REACTIONS	Linear sorption	Linear sorption	None
TRANSPORT SOLVER	Conjugate gradient/gmres Direct	Conjugate gradient/gmres Direct Successive overrelaxation Alternating directions	Direct

(a) N is arbitrarily large
(b) Not yet available

TABLE 5. General Characterization of Single-Phase Models

	DCM3D	FEMTRAN	FEMWATER/FEMWASTE	LLUVIA-II	NORIA-SP
DIMENSIONS	1, 2, 3	2	2	2	2
FRACTURED-FLOW CONCEPTUALIZATION	Dual permeability	None	Equivalent continuum	Equivalent continuum	Equivalent continuum
PHASES	1	None	1	1	1
STEADY INITIAL CONDITIONS	No	None	Yes	Yes	No
HEAT	No	None	No	No	No
SPATIAL DISCRETIZATION	Finite difference	None	Finite element	Finite difference	Finite element
LINEARIZATION	Newton-Raphson	None	Picard	Newton-Raphson	Newton-Raphson
FLOW SOLVER	Method of lines	None	Successive overrelaxation Conjugate gradient/GMRES	Method of lines	Direct
FRACTURED-TRANSPORT CONCEPTUALIZATION	Dual permeability	Equivalent continuum	Equivalent continuum	Equivalent continuum	None
MISCIBLE COMPONENTS	Yes	Yes	Yes	No	No
CHAINING	Decay Production	Decay Production	Decay	None	None
GEOCHEMICAL REACTIONS	Linear sorption	Linear sorption	Linear sorption Ion exchange	None	None
TRANSPORT SOLVER	Method of lines	Direct	Successive overrelaxation Conjugate gradient/GMRES Direct	None	None

TABLE 5. General Characterization of Single-Phase Models (Continued)

	SAGUARO	TOSPAC	TRACR3D	VS2DT
DIMENSIONS	2	1	1, 2, 3	1, 2
FRACTURED-FLOW CONCEPTUALIZATION	Equivalent continuum	Equivalent continuum	Equivalent continuum Embedded planes	Equivalent continuum
PHASES	1	1	1,2	1
STEADY INITIAL CONDITIONS	Yes	Yes	No	No
HEAT	Yes	No	No	No
SPATIAL DISCRETIZATION	Finite element	Finite difference	Finite difference	Finite difference
LINEARIZATION	Picard	Newton-Raphson	Newton-Raphson	Hybrid
FLOW SOLVER	Direct	Direct	Conjugate gradient/GMRES	Strongly implicit
FRACTURED-TRANSPORT CONCEPTUALIZATION	Equivalent continuum	Dual permeability	Equivalent continuum	Equivalent continuum
MISCIBLE COMPONENTS	No	Yes	Yes	Yes
CHAINING	None	Decay Production	Decay Production	Decay
GEOCHEMICAL REACTIONS	None	Linear sorption	Linear sorption Nonlinear sorption Precipitation Nonequilibrium sorption	Linear sorption Nonlinear sorption Precipitation
TRANSPORT SOLVER	None	Direct	Explicit	Conjugate gradient/GMRES Strongly implicit

4.2.2 Fracture-flow Conceptualization

Unsaturated-flow models offer a variety of options for simulating fracture-flow conceptualizations:

- *Equivalent Continuum.* Assuming equilibrium, hydraulic property curves composite the effects of fractures and rock matrix. The approximation breaks down for rapid transients, a very tight rock matrix, and/or large fracture spacings.

- *Dual Permeability.* One continuum characterizes the fractures; the other, the rock matrix. This implementation permits fracture-to-matrix, fracture-to-fracture, and matrix-to-matrix fluid movements. Typically, it employs a pseudo-steady coupling of fracture and rock matrix. With current hardware and software, a fully transient coupling yields excessive computer execution times, so that only relatively small-scale simulations can be performed. The YMP must overcome this deficiency to satisfy Requirement 4 of Tables 2 and 3.

  To obtain a fully transient coupling, one defines a sufficiently large number of grid blocks within the rock matrix to accurately characterize the pressure gradients. Such an approach accurately characterizes the time behavior at times which are small compared with the time required to saturate the rock matrix. Alternatively, to obtain a pseudo-steady coupling, one uses a relatively small number of grid blocks within the rock matrix, generally separating neighboring fractures with only a single block thickness. The pseudo-steady approach becomes accurate only as the rock matrix nears saturation, when gradients are relatively small.

- *Dual Porosity.* As in the dual-permeability conceptualization, one continuum characterizes the fracture, and the other, the rock matrix. Unlike the dual-continuum approach, however, the dual-porosity approach assumes that the rock matrix acts predominantly as a storage mechanism, with large-scale flows occurring only within the fractures. Here, a fully transient coupling of fracture and matrix may be simulated efficiently.

- *Multiple Continuum.* This method is quite flexible. It will reduce to either dual-continuum or dual-porosity implementations with either pseudo-steady or fully-transient coupling of fractures and rock matrix. In addition, several porosity levels may be characterized (e.g., fractures, vugs, and rock matrix).

- *Embedded Planes.* Embedded fracture planes provide alternate flow pathways to the rock matrix. Fracture-matrix exchanges of fluid and contaminants are permitted only at grid-block interfaces. In analogy to an electric circuit, the fracture plane across a given grid block serves as a resistor in parallel to the rock matrix within that block.

4.2.3 Phases

In partially saturated rocks, two fluids, or phases, move simultaneously within the porous rock. Under pre-emplacement conditions, gas-phase pressure gradients are expected to be small, and a single-phase Richards-equation approximation should be adequate. Under repository conditions, repository heat will induce non-negligible gas-phase pressure gradients, thus requiring that two phases be considered.

4.2.4 Heat

Under repository conditions, repository heat will vaporize water, increase gas pressures, and thereby induce a heat-pipe-type transfer of energy. To consider this effect, the model must include heat transport, as well as liquid- and gas-phase flows.

4.2.5 Spatial Discretization

The efficiency of the matrix solver may depend sensitively upon the spatial-discretization method. The procedure used for assigning a number to each node yields an incidence matrix (a pattern of zeros and ones), and the incidence matrix influences solver design. The finite-element and integrated finite-difference methods yield a problem-dependent incidence matrix. In contrast, the finite-difference method yields a problem-independent incidence matrix, thereby facilitating the development of efficient direct solvers. For direct solvers, the relationship is relatively sensitive and, consequently, the finite-element and integrated finite-difference methods typically require substantially longer solution times when applied to two- and three-dimensional problems. However, because of their efficiency for large problems, iterative solvers are most appropriate for many Yucca Mountain analyses. For iterative solvers, the relationship between discretization method and solver appears to be much less sensitive, and, here finite-element and integrated finite-difference discretization methods yield computer execution times which are competitive with those arising from finite-difference discretization.

4.2.6 Linearization

Via their dependence on saturation levels, hydraulic-property functions cause multiphase systems to be highly nonlinear. This occurs even in the single-phase Richards approximation. Via their dependence on pressure, temperature, and composition, phase properties such as density, viscosity, and specific enthalpy also introduce non-linearities into multiphase systems. In the conservation equations characterizing flow and transport processes in porous media, this non-linearity appears in the coefficients of otherwise linear operators since the coefficients themselves become functions of the dependent variables. Assuming that the coefficients are relatively weak functions of the dependent variable, the Picard method evaluates these coefficients using dependent-variable values obtained from prior iterations. Starting from a residual expression of the conservation equations, the Newton-Raphson method expands this residual in a Taylor series. In contrast to the Picard method, this approach considers all first-order variations with respect to the dependent variables.

4.2.7 Flow Solver

For each nonlinear iterate, the solver evaluates the dependent variables. Both the numerical treatment of the time domain and the size of contemplated simulations dictate the type of solver to be used. Discretization of only the spatial derivatives of the transport terms yields a set of coupled ordinary equations, which may be solved by the method of lines. Discretization of the time derivatives of the accumulation terms as well, leads to either implicit or explicit types of solutions. For solution of the flow equation, stability considerations generally dictate the use of implicit solutions, and matrix-solution methods are required. For relatively small applications of one, perhaps two, dimensions, available computer memory and speed will allow the investigation to employ a direct matrix-solution method. Relatively large Yucca Mountain applications of two or three dimensions necessitate the use of iterative solution methods such as the successive-over-relaxation, alternating-direction implicit, conjugate-gradient/gmres, and strongly implicit methods.

4.2.8 Fracture-Transport Conceptualization

Most models use the same fracture conceptualization for both flow and transport. However, one model (TOSPAC) recognizes that the flow and transport mechanisms may require different conceptualizations for the fractured media.

4.2.9 Miscible Components

For Yucca Mountain, radionuclides are the miscible components of interest. In contrast to immiscible components (phases), miscible components have no capillarity and may be dissolved in either liquid or gas phases, or both.

4.2.9 Chaining

Decay and production processes combine various nuclides into radioactive chains, or families. For the parent radionuclide, a single equation may be employed to characterize the combined effect of transport and decay. For daughter products, however, the radioactive production process must also be characterized. In this case, transport equations must be solved simultaneously to characterize the decay, production, and transport processes of each progenitor.

4.2.10 Geochemical Reactions

Four different algorithms are currently being used within the YMP to characterize geochemical reactions. They are:

- *Linear Sorption.* A constant ratio k_d of sorbed and dissolved concentrations is maintained.
- *Nonlinear Sorption.* The variable ratio k_d depends on the concentration level.
- *Non-equilibrium Sorption.* The variable ratio k_d depends on the time of exposure of rock to the dissolved concentration.

- *Saturation Limits.* Solubilities and catio-exchange capacities limit the amounts which may be dissolved and sorbed.

4.2.11 Transport Solver

The relative importance of advection to dispersion and diffusion (i.e., the Peclet number) determines the most desirable transport solver. If the effects of advection dominate (i.e., Peclet number greater than approximately two) then computer-performance considerations may dictate the use of an explicit solution. If the effects of dispersion and diffusion dominate (i.e., Peclet number less than approximately two) then stability considerations generally dictate the use of an implicit solution. For relatively small implicit solutions for one and two dimensions, available computer memory and speed will allow the investigator to employ a direct matrix-solution method. Relatively large Yucca Mountain applications of two or three dimensions necessitate the use of iterative solution methods such as the successive-over-relaxation, alternating-direction implicit, and conjugate gradient/gmres methods.

4.3 DISCUSSION

Tables 4 and 5 permit the reviewer to speculate on relative code performance. Linearization, for example, affects both computer time and robustness. In calculating single-phase flow, the Picard method used in PORFLOW, FEMWATER, and SAGUARO and the hybrid method used in VS2DT yield symmetric coefficient matrices, whereas the Newton-Raphson method used in all other codes yields an asymmetric coefficient matrix. For problems that are only moderately nonlinear, this reduces computer time by as much as a factor of four. However, for problems that are highly nonlinear, the Picard and hybrid methods converge poorly, and their computational advantage during each iteration is more than offset by the increased number of iterations required for convergence. Mixed results would be anticipated with models using the Newton-Raphson method yielding reduced computer times for highly nonlinear problems, and models using the Picard and hybrid techniques yielding reduced computer times for moderately nonlinear problems. The issue here is the viability of the Picard and hybrid methods for the levels of non-linearity to be encountered in Yucca Mountain analyses.

Some multiphase models (e.g., MSTS, NUFT, and TRACR3D) have a single-phase option. Some multiphase models (e.g., TOUGH2 and FEHM) do not have such an option. Because of design limitations, other models can perform only single-phase analyses. The use of two phases rather than one increases the order of the coefficient matrix by a factor of two. For a single iteration, this increases CPU time by a factor ranging from slightly less than 2^2 to 2^3, depending on the type of solver. Nevertheless, one cannot immediately conclude that, for a single-phase problem, the single-phase implementation will require the least CPU time. For multidimensional nonlinear problems, the added robustness of the two-phase approach can reduce the total number of iterations sufficiently to offset the CPU-time increase per iteration. Thus, as the dimensionality and level of non-linearity increase, one should expect the efficiency of two-phase simulations to approach and perhaps exceed that of single-phase simulations.

Tables 4 and 5 reveal that transport capabilities vary significantly. Some multiphase models (NORIA and TOUGH2) offer no transport capability at all. However, most multiphase models offer a minimal capability which includes radioactive decay, linear sorption, and an implicit solver. Only one (PORFLOW) offers radioactive production and decay. Models classified as single-phase liquid-flow models generally offer more transport options. Four models (DCM3D, FEMTRAN, TOSPAC, and TRACR3D) provide radioactive production and decay algorithms, and two models (TRACR3D and VS2DT) offer rather lengthy menus of geochemical-reaction options. One model (TRACR3D) offers both explicit and implicit solvers.

Tables 4 and 5 also indicate differing strategies for solution of the transport equation. Most models simultaneously simulate flow and transport using a single model. Some strategies, however, match a stand-alone flow model with a stand-alone transport model. FEMWASTE, for example, simulates transport using Darcy velocities generated by FEMWATER. Similarly, FEMTRAN simulates transport using Darcy velocities generated by FEMWATER, NORIA, NORIA-SP, or SAGUARO. For multidimensional analyses of Yucca Mountain, it may be inconvenient to store the relatively large files of Darcy velocities which are required by the transport analysis.

5. SELECTION OF MODELS FOR TESTING

The third step in the technical review process consisted of two activities, with the objective being to select models for testing. Section 5.1 compares model characteristics and model-selection requirements and describes general deficiencies. Section 5.2 then cross-compares model characteristics. With the understanding that final selection will follow testing, the objective here is to identify models which would be most suitable for further development in view of the general deficiencies that are identified in Section 5.1.

5.1 COMPARISON OF MODEL CHARACTERISTICS AND MODEL REQUIREMENTS

Assuming that discrete-fracture effects may be neglected, most analyses employ continuum conceptualizations. Tables 4 and 5 indicate that two models (PORFLOW and TRACR3D) offer the embedded-planes conceptualization for discrete-fracture analysis. However, this option has not been used in Yucca Mountain analyses, most likely due to its unrealistic treatment of fracture-matrix fluid exchanges. Tables 4 and 5 also indicate that many models offer equivalent-continuum, dual-porosity, and dual-permeability conceptualizations. One model (TOUGH2) offers a multiple-continuum conceptualization. In theory, the equivalent-continuum, dual-porosity, dual-permeability, and multiple-continuum conceptualizations may be employed in discrete-fracture implementations. However, except for small-scale implementations, that is not a practical reality. Thus, technologies for modeling discrete-fracture features of Yucca Mountain, such as an anisotropic fracture connectivity pattern, are not currently available within the project. The YMP will have to overcome this deficiency to completely satisfy Requirement 1 of Table 2 and Requirements 1, 5, and 7 of Table 3.

A fully transient characterization of non-equilibrium flow in fractured rocks can be characterized by a refined gridding near the fracture-matrix interface which is gradually graded into a coarse grid within the rock-matrix interior. In addition, a pseudo-analytic characterization of fracture-matrix coupling may prove sufficiently accurate and general that it too may be used to characterize non-equilibrium fracture flow. One-dimensional Yucca Mountain simulations can use the refined-gridding approach. Multidimensional simulations using this approach, while theoretically possible with the multiple-continuum implementation, are significantly limited by software inefficiency and excessive execution times. The equivalent-continuum conceptualization offered by most codes and the pseudo-steady, dual-permeability conceptualization offered by the a few flow models are unable to accurately characterize non-equilibrium flow in fractured rock. Thus, except at small spatial scales, Yucca Mountain models are unable to characterize the effects of non-equilibrium fracture-matrix flow. Requirement 4 of Tables 2 and 3 indicates that this capability is inadequate.

Private communications with code developers indicate that multiphase analyses are limited to a few thousand grid cells and that single-phase analyses based on a solution of Richards equation are generally limited to a few tens of thousands of grid cells. Here the efficiency of the flow solver is a primary consideration. A facility for performing transient, mountain-scale simulations of 100,000 grid cells or more, in computer processing times of 24 hours or less, would facilitate the resolution of many site-characterization and design issues. Such is not available at the present time. With such a facility, some realistic discrete-fracture and non-equilibrium fracture-flow calculations would be possible.

The discussion above points out three deficiencies which are generally present in all multiphase and single-phase liquid-flow models. Section 5.2 seeks to identify models which would provide the most suitable starting points for remedying these deficiencies.

5.2 CROSS-COMPARISON OF MODEL CHARACTERISTICS

Two ultimate objectives of the final selection process have influenced the selection of models for testing. These may be identified as follows:

- To provide code-to-code verification, both finite-difference and finite-element models should be selected.

- Both to provide code-to-code verification and to provide an efficient analysis capability for pre-emplacement problems, single-phase as well as multiphase flow models should be selected.

In addition, a desire to examine the efficiency of certain algorithms has also influenced the selection of models for testing.

5.2.1 Multiphase Models

FEHM. FEHM offers the most advanced finite-element capability within the YMP. As shown in Table 4, it has a three-dimensional capability, offers an iterative conjugate-gradient/gmres solver, and provides a selection of fractured flow and transport conceptualizations. As a finite-element model, it appears to offer a good host structure for developing a multiphase discrete-fracture capability. In addition, developing a single-phase, liquid-flow option for FEHM should be more cost effective than upgrading one of the existing single-phase, finite-element models. FEHM *was* selected for testing.

MSTS. MSTS is user friendly. It has an excellent graphics-based preprocessor. For complex multidimensional simulations of Yucca Mountain, data setup will be a time-consuming process, and such a capability will be useful. MSTS also implements boundary conditions in a flexible manner. It permits different types of conditions to be applied at the same boundary. This means, for example, that at the ground surface one could specify a Dirichlet condition with gas pressure equal to, say, atmospheric pressure, and one could also specify a Neumann condition with liquid flux equal to, say, the average annual recharge. This feature greatly facilitates code application and should be standardized on all multiphase codes used by the YMP. In order to examine these user-friendly features more carefully, MSTS *was* selected for testing.

Nevertheless, MSTS suffers from the fact that its internal algorithms closely resemble those of the older and more widely accepted TOUGH line of codes. Both MSTS and TOUGH2 use finite-difference, Newton-Raphson, and direct-solution algorithms. Furthermore, a conjugate-gradient/gmres solver is now being implemented in both.

NORIA. NORIA has one unique capability when compared to other multiphase flow codes, namely a non-equilibrium rate of vaporization. An appropriate choice for the value of an empirical constant of proportionality causes the vaporization rate to fall smoothly to zero with decreasing moisture content. However, non-equilibrium vaporization should not be an important effect at Yucca Mountain, given the large time scale of interest.

However, in choosing a multiphase finite-element model for the project, FEHM is the better choice. Table 4 indicates that NORIA is restricted to two dimensions, while FEHM offers a three-dimensional capability. NORIA offers only a direct solver. Though quite suitable for multiphase problems involving less than a few thousand elements, such a solver is inefficient for larger problems. FEHM's conjugate-gradient/gmres solver is more appropriate although it, too, will require upgrading for problems larger than a few tens of thousands of elements. Finally, NORIA offers only an equivalent-continuum conceptualization of fracture flow, while FEHM offers dual-permeability and dual-porosity conceptualizations, as well. For these reasons, NORIA *was not* selected for testing.

NUFT. NUFT represents a shell of executive and utility routines which support one of several flow and transport modules. It offers both direct and conjugate-gradient/orthomin solvers. With five different preconditioners, the latter represents a serious attack on the problem of software inefficiency. Liberal use of the "C" language is intended to make the maintenance of NUFT as easy as possible.

The general USNT module considers fully coupled flow and transport processes for N phases and N_c components where N and N_c are arbitrary. The more specialized US1P and US1C modules consider two-phase, Richards-equation flow with sequentially calculated transport of a single dilute species. In order to assess its computer efficiency relative to that of other Yucca Mountain codes, NUFT *was* selected for testing.

PORFLOW. PORFLOW has several positive characteristics. Its transport module offers a variety of features. Even so, its capability with respect to geochemical reactions is substantially less than that offered by VS2DT and by TRACR3D, as shown in Table 4. For both flow and transport modules, PORFLOW provides a large selection of solvers. However, PORFLOW omits one rather important option which TRACR3D includes, and, for relatively coarse-gridded transport problems resulting in relatively high Peclet numbers, the explicit option can be extremely important.

PORFLOW uses the Picard linearization method. Anticipating that the level of non-linearity in Yucca Mountain problems might rule out the use of this method, only one code employing the Picard method (VS2DT) was selected for testing. PORFLOW *was not* selected for testing.

TOUGH2. TOUGH2 derives from an old and well-established line of codes dating back to MULKOM. It is widely accepted, and its clean coding and clear organization have prompted improvements from scientists outside Lawrence Berkeley Laboratory (LBL). For example, starting from TOUGH, Lawrence Livermore National Laboratory

(LLNL) has optimized the coding for Cray computers, resulting in a version of the model called V-TOUGH. Others have added iterative solvers to improve computer efficiency. LBL itself is now including an iterative solver in their TOUGH2.

Like other models, TOUGH2 is capable of discrete-fracture and fracture-matrix disequilibrium simulations, but, because of efficiency considerations, this capability is restricted to relatively small problems. Nevertheless, as a finite-difference model, it offer an excellent host structure for further development. TOUGH2 *was* selected for testing.

V-TOUGH. In the future, LLNL plans to replace V-TOUGH with NUFT. In addition, one may note that LBL's TOUGH2 now incorporates some V-TOUGH features (e.g., vapor-pressure lowering) and that a forthcoming release of TOUGH2 employing a variant of the conjugate-gradient algorithm will supersede V-TOUGH's use of efficient direct solvers. Other superior V-TOUGH features include an upgraded time-stepping algorithm, an efficient steam-table evaluation procedure, and a detailed output-control algorithm. One may reasonably assume that future TOUGH2 development will also incorporate or supersede these features. Given then that both NUFT and TOUGH2 have been selected, V-TOUGH *was not* selected for testing.

5.2.2 Single-Phase Liquid-Flow Models

DCM3D. Like LLUVIA-II, DCM3D uses a method-of-lines solver. Because it is rarely used in hydrogeological investigations, this solver represents a natural choice. Consequently, one code using a method-of-lines solver (LLUVIA-II) was selected for model testing. DCM3D *was not* selected for testing.

FEMTRAN. Two different transport-solution strategies have been pursued in the development of models for the YMP. Many models simultaneously simulate flow and transport using a single model. Some strategies, however, match a stand-alone flow model with a stand-alone transport model. FEMTRAN results from the latter strategy. It simulates transport using Darcy velocities generated by FEMWATER, NORIA, NORIA-SP, or SAGUARO. Its ability to consider radionuclides upgrades the capability of FEMWASTE. However, none of its companion flow models were selected for testing. Furthermore, in comparison to TRACR3D and PORFLOW, its ability to simulate high-Peclet flow is limited, and, in comparison to TRACR3D and VS2DT, its options for characterizing geochemical reactions are limited. For these reasons, FEMTRAN *was not* selected for testing.

FEMWATER/FEMWASTE. Of the models considered by this review, only FEMWATER, NORIA-SP, and SAGUARO offer a single-phase, liquid-flow capability based on finite-element discretization. FEMWATER derives from a model published by Reeves and Duguid (1975) and FEMWASTE, from a model published by Duguid and Reeves (1976). The original Reeves-Duguid version of FEMWATER has three characteristics which make it inappropriate for Yucca Mountain analyses: Picard linearization, a direct solver, and two dimensions. Since 1975, FEMWATER development has removed one by adding two iterative solver options, but two limitations still remain. As noted in the discussion below, NORIA-SP development has also removed only one of the limitations found in the original Reeves-Duguid version of FEMWATER. FEMWATER/FEMWASTE *was not* selected for testing.

LLUVIA II. The uniqueness of the LLUVIA-II model derives from its use of an old and well-developed solver designed for "stiff" ordinary differential equations (ODEs). Differencing only the spatial-derivative terms in the flow equation yields a set of coupled ODEs in the time variable, which are solved by the ODE package (Shampine and Watts, 1980) which derives from the work of Hindmarsh (1981). This approach, known as the method of lines, is rarely used in hydrogeological investigations.

Some researchers contend that, for highly nonlinear unsaturated flow, this method provides a more efficient solution than more conventional methods. In addition, the benefit to be gained from parallelization is unknown. To further evaluate the method of lines, LLUVIA-II *was* selected for testing.

NORIA-SP. NORIA-SP is a single-phase, isothermal version of NORIA. In specializing NORIA, the object was to gain efficiency for single-phase implementations. In contrast to the TRACR3D development, which added a single-phase option, the NORIA-SP development elected to create a new version of the base model.

In comparison to other single-phase, finite-element models, NORIA-SP's use of Newton-Raphson linearization makes it relatively robust for highly nonlinear problems. However, for Yucca Mountain-scale problems, it is limited by its two dimensionality and by the poor efficiency of its direct solver. For these reasons, NORIA-SP *was not* selected for testing.

SAGUARO. As noted in Table 4, SAGUARO has a heat-transport capability. However, since the effects of vaporization and condensation are not included, it is not useful for Yucca Mountain analyses. Except for the heat-transport capability, SAGUARO's flow model is very close to that of the 1975 Reeves-Duguid version of FEMWATER. It therefore has three characteristics which make it inappropriate for Yucca Mountain analyses: Picard linearization, a direct solver, and two dimensions. For these reasons, SAGUARO *was not* selected for testing.

TOSPAC. TOSPAC was designed to be used as the flow module of the total system analyzer TSA. Nevertheless, it is of interest in the present review of detailed process models because of the emphasis of its design on efficiency. Although its steady-state model is used in the total-system studies, the efficiency of its transient solutions provides a benchmark for comparison with other models. TOSPAC *was* selected for testing.

TRACR3D. TRACR3D is a well-known and well-respected finite-difference model, which has been continually upgraded for more than a decade. Although it supports a two-phase capability, the lack of a thermal capability has led this review to consider only its single-phase flow capability for application to Yucca Mountain. In addition, TRACR3D offers one of the most advanced transport capabilities within the project.

As shown in Table 5, its facility for geochemical reactions is challenged only by VS2DT, and it is the only model to offer an explicit solution for high-Peclet transport. For these reasons, TRACR3D *was* selected for testing.

VS2DT. The uniqueness of the VS2DT model derives from two aspects of its implementation. First, its hybrid linearization is carefully designed to gain as much robustness as possible from the Newton-Raphson method while maintaining the symmetric coefficient matrix which is characteristic of the Picard method. (Theoretically, in obtaining a direct solution for a set of linear equations of order n, the solution time for a symmetric matrix is one fourth of that for an asymmetric matrix.) Second, rather than to use separate linearization and iterative solution loops like most codes do, VS2DT uses a single loop. This keeps the accuracy of the matrix solution in line with the accuracy of the linearization and further improves efficiency. Though it uses separate loops, TRACR3D accomplishes the same function by refining the tolerance of the matrix solution in accord with the accuracy of the linearization. Tests by both McCord (1991) and by Eaton (1992) showed VS2DT to be relatively fast in comparison to other single-phase liquid-flow models. However, these tests did not adequately test VS2DT's efficiency and robustness with hydraulic properties appropriate for Yucca Mountain. For these reasons, VS2DT *was* selected for testing.

5.3 MODEL SELECTION

As described above, a comparison with selection requirements and a cross-comparison of characteristics resulted in the selection of both multiphase and single-phase liquid-flow models for testing. The multiphase models are: FEHM, MSTS, NUFT, and TOUGH2. The single-phase liquid-flow models selected for testing are: LLUVIA-II, TOSPAC, TRACR3D, and VS2DT.

6. MODEL VERIFICATION AND TESTING

The codes selected for testing were first modified, if necessary, to run on a 486/33 personal computer with a Salford Fortran compiler. Documented test cases were then executed to show that the modifications had been done correctly and to become familiar with the codes. Once this phase (the verification phase) was completed, additional tests were performed to make code-to-code comparisons. To control these comparisons as carefully as possible and to understand differing results (Section 6.3), a test plan (Section 6.1) and a test strategy (Section 6.2) were developed.

6.1 TEST PLAN

Table 6 presents the plan developed to guide model testing. It identifies the models selected for testing and the problems to be executed by each. Footnoting indicates the extent to which this plan can been implemented at the present time. Appendix B discusses in detail the four problems, and the following paragraphs briefly characterize their relevance to the test plan.

6.1.1 Test Problems

The transient Jornada-Trench Problems consider the multidimensional, isothermal flow of unsaturated water in a dry heterogeneous soil. As shown in the table, they consist of Cases A_2, B_2, A_3, and B_3. Setting initial head values to -734 cm makes Cases A_2 and A_3 relatively easy to solve. Decreasing these values to -10,000 cm substantially increases the level of difficulty for Cases B_2 and B_3. At such dry moisture conditions, numerical oscillations to less-than-residual saturation levels introduce discontinuities in the moisture accumulation term. By considering such an effect, which occurs frequently in the analysis of dry soils, Cases B_2 and B_3 test the code's ability to minimize such oscillations. By introducing three-dimensionality, Cases A_3 and B_3 show the effect which an order-of-magnitude increase in the number of grid cells has on the efficiency of the code's solver.

Assuming steady initial conditions, the transient COVE2a Problem considers the one-dimensional, isothermal, unsaturated flow of water in a layered column of Yucca Mountain tuff. For this problem, the Paintbrush-tuff capillary-pressure and relative-permeability curves contain sharp variations. Rather than occurring at near-residual levels, such non-linearities occur at somewhat larger saturations. Had this problem assumed infiltrations greater than the levels of 0.1 and 0.2 mm/y used for steady and transient analyses, respectively, it would have more significantly engaged the rather severe non-linearities associated with fracture flow. However, the chosen problem definition is quite adequate to test the ability of a code's linearization algorithm to treat the type of non-linearity caused by continuous, yet rapidly varying, hydraulic properties.

In addition to non-linearities, the next two problems introduce complications related to the simulation of nonisothermal multiphase flow. The steady Pre-emplacement, Vapor-Diffusion Problem considers the one-dimensional, nonisothermal movement of water, vapor, and air in an undisturbed column of Yucca Mountain tuff. For a near-geothermal temperature gradient, it tests a code's ability to simulate the vastly different mobilities of gas and liquid phases and to simulate the counter-current flow fields of vapor and liquid which are present in

TABLE 6. Test Plan

CODE	PROBLEMS							
	Jornada Trench				COVE2a	Pre-Emplacement Vapor Diffusion		Repository Heat Pipe
	Case A_2	Case A_3	Case B_2	Case B_3		Case A	Case B	
FEHM	X		X	X(a)	X(a)	X(a)	X(a)	X(a)
LLUVIA-II	X		X					
MSTS (single phase)	X		X		X			
MSTS (two phase)	X		X					
NUFT	X(a)		X(a)	X(a)	X(a)	X(a)	X(a)	X(a)
TOSPAC					X			
TOUGH2	X		X	X(a)	X	X	X	X(a)
TRACR3D	X	X	X	X	X			
VS2DT	X		X		X			

(a) Here testing must await the implementation of recently released versions of FEHM, NUFT, and TOUGH2 (See Section 6.1 for a more complete explanation).

unsaturated rock. With a relative humidity of 50 percent prescribed at the top boundary, the problem also tests a code's algorithm for vapor-pressure lowering.

The transient Repository Heat-Pipe Problem considers the nonisothermal movement of water, vapor, and air, as influenced by the presence of repository heat. In contrast to the steady Pre-emplacement, Vapor-Diffusion Problem, the Repository Heat-Pipe Problem increases problem dimensionality from one to two dimensions, and it includes both saturated and unsaturated zones. Since the applied heat load causes repository temperatures to rise above boiling, this problem tests a code's ability to simulate the convective transport of latent heat. It also tests a code's ability to simulate, in a transient fashion, the cycle of vaporization and condensation which occurs.

6.1.2 Discussion

The test plan of Table 6 reflects code limitations. For example, an assumption of isothermal flow restricts TRACR3D to the Jornada-Trench and COVE2a Problems. An assumption of single-phase flow in the Richards approximation restricts LLUVIA-II and VS2DT to the same two problems. An additional assumption of one spatial dimension restricts TOSPAC to the COVE2a Problem only.

Except for rather minor considerations, the nonisothermal, multiphase codes FEHM, MSTS, NUFT, and TOUGH2 are capable of solving all four test problems. For these codes, the test plan reflects a strategy. As stated in Section 5.2, one objective of the final model selection process is to select both finite-difference and finite-element models. This means that FEHM, the only viable representative of the finite-element class, should be thoroughly tested to justify its selection. Broad acceptance by the scientific community conveys an advantage to the finite-difference model TOUGH2. It means that other finite-difference models need to evidence significant advantages over TOUGH2 in order to justify final selection. The technical review suggested that MSTS would not possess such advantages. To confirm this conclusion, MSTS was applied only to the Jornada-Trench and COVE2a Problems.

Implementation of the test plan of Table 6 is only partially complete. LANL's recent release of a new version of FEHM containing the vapor-diffusion algorithm did not permit execution of the Pre-Emplacement Vapor-Diffusion and Repository Heat-Pipe Problems prior to the scheduled release of this report. Similarly, LLNL's recent release of NUFT did not permit us to perform the indicated testing. In addition, time constraints did not permit us to report either the testing of FEHM with the Jornada-Trench Case B_3. Nevertheless, only in one case could additional testing affect the conclusions and recommendations of Chapters 7 and 8. A consideration of the relative merits of NUFT and TOUGH2 would necessitate a comparative testing of NUFT and a new version of TOUGH2 containing a conjugate-gradient/gmres solver.

6.2 TEST STRATEGY

The testing strategy consists of identifying essential code differences and understanding their effects. To facilitate this activity, Table 7 provides a detailed code characterization.

TABLE 7. Detailed Code Characterization[a]

CODE	TIME INTEGRATION			SPACE INTEGRATION			
	Time Step Controls	Technique	Options	Technique	Permeability Weighting		
					Absolute	Saturated	Relative
FEHM	Minimum and maximum step sizes Coupling to nonlinear iteration Recalculation/chopping controls	Finite difference	Backward Centered Variable	Finite element	Upstream None	NA	NA
LLUVIA-II	Step sizes adjusted via accuracy requirements	Method of lines	NA	Finite difference Point distributed[b]	Upstream Centered	NA	NA
MSTS	Acceleration factor Maximum step size Recalculation/chopping control	Finite difference	Backward	Finite difference	Harmonic Upstream Centered Geometric Linear	NA	NA
NUFT	Desired solution-vector changes Minimum and maximum step sizes Recalculation/chopping control	Finite difference	Backward	Finite difference Block centered	NA	Harmonic Upstream	Harmonic Upstream Centered
TOSPAC	Desired change in permeability or capillary pressure Block throughput time Maximum step-size change Recalculation/chopping control	Finite difference	Backward Centered Variable	Finite difference Block centered	Centered	NA	NA
TOUGH2	Maximum step size Coupling to nonlinear iteration Recalculation/chopping controls	Finite difference	Backward	Finite difference Block centered	NA	Harmonic Upstream	Harmonic Upstream Centered
TRACR3D	Minimum and maximum step sizes Coupling to nonlinear iteration Recalculation/chopping controls	Finite difference	Backward	Finite difference Block centered	NA	Harmonic	Upstream
VS2DT	Minimum and maximum step sizes Coupling to nonlinear iterations Recalculation/chopping control	Finite difference	Backward	Finite difference Block centered	NA	Harmonic	Geometric Upstream Centered Variable

(a) NA - not applicable
(b) Aziz and Setter (1979), p. 75

TABLE 7. Detailed Code Characterization (Continued) [a,b]

CODE	PHASES	NONLINEAR ITERATION		MATRIX SOLUTION	
		Linearization Technique	Convergence-Control Variables	Technique	Convergence-Control Variable
FEHM	2	Newton-Raphson with reduced degrees of freedom	Residual w.r.t. zero-th iterate	Conjugate gradient-GMRES	Residual w.r.t. zero-th iterate
LLUVIA-II	1	Newton-Raphson	Absolute change and relative change in capillary pressure	NA	NA
MSTS	1,2	Newton-Raphson	Residual w.r.t. mass or heat accumulation	Direct Conjugate gradient-GMRES[c]	NA Residual w.r.t. mass or heat accumulation
NUFT	1,2,...N[d]	Newton-Raphson	Change in solution vector	Direct Conjugate gradient/orthomin	Residual w.r.t. zero-th iterate
TOSPAC	1	Newton-Raphson	Relative change in capillary pressure	Direct	NA
TOUGH2	2	Newton-Raphson	Residual w.r.t. mass or heat accumulation and absolute value of residual	Direct Conjugate gradient-GMRES[c]	NA Residual w.r.t. mass or heat accumulation and absolute value of residual
TRACR3D	1,2	Newton-Raphson	Residual w.r.t. zero-th iterate	Conjugate gradient-GMRES	Residual w.r.t. zero-th iterate
VS2DT	1	Hybrid: Picard and Newton-Raphson	Change in total pressure	Strongly implicit	Change in total pressure

(a) NA - not applicable
(b) w.r.t. - with respect to
(c) Not yet available
(d) N is arbitrarily large

6.2.1 Time Integration

The column labeled "Options" lists the time-differencing methods offered by each code. Using the backward differencing option gave a high degree of similarity among the codes. However, one code, LLUVIA-II, uses a high-ordered time differencing scheme with a time-stepping algorithm based on accuracy requirements. LLUVIA's treatment of the time domain represents an essential code difference.

Other essential code differences are present. The column labeled "Time-Step Controls" identifies the types of parameters used by the automatic-time-stepping algorithms. Here, similar values were used for the minimum (initial) and maximum step sizes and for the magnification factor. Nevertheless, in relation to the single-phase codes, the two-phase codes can achieve specified error tolerances with larger values for the minimum and maximum step sizes and for the magnification factor. Most, but not all, codes control application of the magnification factor based on the ease of convergence, as measured by the number of iterations. One code, NUFT, also controls the magnitude of the magnification factor according to a desired change in the solution vector.

6.2.2 Space Integration

The column labeled "Space Integration - Permeability Weighting" lists the permeability-weighting methods which may be used by each code. Local similarity was achieved among the codes TOUGH2, TRACR3D, and VS2DT by using harmonic weighting of the saturated permeabilities and upstream weighting of the relative permeabilities. FEHM offers either no weighting at all or upstream weighting according to the prescription of Dalen (1979) for finite-element models. Here, upstream weighting was selected. For TOSPAC, only centered differencing was available. Although steps were taken to unify the analyses, differences persisted. Nevertheless, results suggest that these are nonessential differences. Only in one-dimensional applications does an essential code difference appear in the space-integration algorithms. Since the finite-element technique (FEHM) and the point-distributed finite-difference technique (LLUVIA-II) place nodes at cell boundaries, they cannot be specialized to one dimension.

6.2.3 Phases

Table 7 notes that all codes but FEHM and TOUGH2 can be executed in a single-phase mode. Thus, on the Jornada-Trench and COVE2a Problems, which can be executed with a single phase, the computer times required by FEHM and TOUGH2 might be expected to be significantly larger. One may understand this by considering the effect which a two-phase solution has on the solver, which is generally a dominant consumer of computer time. Using two phases where one would suffice means that the order of the coefficient matrix must be increased by a factor of two.

For a direct solver, computer time varies approximately as the cube of the order. Thus, for a single iteration, the two-phase solution would require a computer time which exceeds that of the single-phase solution by a factor of 2^3. For a conjugate-gradient type solver, the factor of 2^3 is replaced by a smaller, but still significant, factor. As noted above, however, the results below indicate that, for some problems, the improved stability of a two-phase solution reduces the total number of time steps and iterations sufficiently to offset the increased solution time of a conjugate-gradient solver. The number of phases must be identified as an essential code difference.

6.2.4 Nonlinear Iteration

Specification of an acceptable tolerance controls the number of iterations and, in some cases, the number of time-step reductions necessary to achieve nonlinear convergence. Computer execution times thus depend sensitively on the value specified for this parameter and on the performance variable to which it is applied. The column labeled "Convergence-Control Variable" identifies five different control variables and hence five different methods for applying convergence criteria.

To cope with such differences, the study arbitrarily adopted the absolute change in total head as the standard control variable. For the Jornada-Trench Case A_2, an absolute change of 1 cm of total head was specified for the final simulation time (30 days). For all but one of the codes (c.f., discussion of LLUVIA-II in Section 6.3) such a criterion appeared to establish a reasonable basis for code-to-code comparisons.

To achieve a uniform absolute change of 1 cm, the following procedure was implemented. By repeatedly running the problem, each time with a tighter tolerance, a reference run was defined. For the reference run, run-to-run changes, as determined by a post-processing step, indicated negligible variation. As necessary, additional runs were then performed to obtain a run suitable for code-to-code comparison. For the latter, the maximum change in total head, from the reference run, was required to be approximately equal to the adopted value (1 cm of total head). The tolerance settings derived for the Jornada-Trench Case A_2, were then used for all subsequent executions of the code. Code-to-code evaluations of the comparison runs should thus be reasonably free of any bias introduced through the use of differing nonlinear convergence methods. Except for LLUVIA-II, this study therefore classifies the differing nonlinear convergence-control variables as nonessential differences.

The column labeled "Linearization Technique" identifies two different algorithms. Except in one case, the codes selected for testing apply the Newton-Raphson linearization technique to both accumulation and transport terms. VS2DT applies the Newton-Raphson technique to its accumulation term and the Picard technique to its transport terms. This procedure retains the computer-time advantages of the latter for weakly nonlinear applications while incorporating some of the robustness of the former technique for more nonlinear applications. As indicated by the results below, this represents and essential code difference.

6.2.5 Matrix Solution

For solution of the test problems, four different matrix-solution techniques have been used: direct, conjugate gradient/gmres, conjugate gradient/orthomin, and strongly implicit. For problems containing a few thousand grid blocks (elements) or more, observable differences should appear with the iterative techniques having a significant computer-time advantage. For such problems, the computer time required by the iterative solvers grows in proportion to the order of the matrix raised to a power slightly less than two, while the computer time required by the direct technique grows in proportion to the order of the matrix raised to the power of three. Essential code differences are indicated.

6.3 TEST RESULTS

This section presents results, all of which were obtained using a 486/33 personal computer. In its interpretation of these results, it continues the discussion of essential code differences.

6.3.1 Jornada Trench

Testing here includes both multiphase (FEHM, MSTS, and TOUGH2) and single-phase (LLUVIA-II, MSTS, TRACR3D, and VS2DT) implementations. One code (MSTS) permits both multiphase and single-phase implementations. Another, the one-dimensional TOSPAC, is inappropriate for this problem. Here, the authors note with gratitude that, in order to facilitate the present effort, J. McCord (private communication, 1992), R.R. Eaton (private communications, 1992 and 1993), and S.O. Magnuson (private communication, 1992, and Magnuson *et al.*, 1990) provided their Jornada-Trench data sets for VS2DT, LLUVIA-II, and TRACR3D, respectively.

Figure 1 shows the calculated 30-day saturation profiles for Case A_2. All of the profiles agree nicely with each other. Figure 2 shows calculated 30-day saturation profiles for Case B_2. With only one exception, these profiles also agree nicely with each other. In comparison to the others, the VS2DT saturation front shows less lateral and vertical penetration. Apparently, the increased level of non-linearity in Case B_2 significantly impacts the robustness of VS2DT's linearization algorithm. Figures 3 and 4 give results for the three-dimensional Cases A_3 and B_3. For the code versions presently implemented by the CRWMS M&O, only TRACR3D and FEHM have the three-dimensional capability and the efficiency necessary to solve unsaturated-flow problems of approximately 25,000 nodes. Given that report deadlines did not permit us to include the testing of FEHM, these figures show only the 30-day saturation profiles determined with TRACR3D. Newly released versions of TOUGH2 and NUFT and a version of MSTS to be released in the near future have the efficiency necessary to solve problems of this size, thus permitting the results shown in Figures 3 and 4 to be expanded in the future.

Table 8 presents the computational parameters for the Jornada Trench problems. It indicates that, as long as the level of non-linearity is not too great, VS2DT is a very efficient code. After a second-place finish behind VS2DT for Case A_2, the two-phase code FEHM posted the smallest run time for Case B_2. Like FEHM, the single-phase implementation of TRACR3D uses a gmres implementation of a conjugate-gradient solver. For Cases A_2 and B_2, the TRACR3D CPU times ranked next to those of FEHM. Although TRACR3D evidenced a smaller CPU time per time step, FEHM required fewer time steps to achieve the same level of convergence.

Thus, for a problem of approximately 2,400 nodes, the enhanced stability of the two-phase approach can overcome the CPU-time penalty which the conjugate-gradient method attaches to the added solution of a transport equation for the air component. In order to include the beneficial effects of a second phase in TRACR3D (private communication, 1993), LANL recently released a new version of the code containing a fully coupled gas phase. When tested on Cases A_2 and B_2, this version of TRACR3D should give CPU times which more closely resemble those of FEHM.

Relatively large CPU times accompanied the Case-A_2 and Case-B_2 implementations of LLUVIA II, and the interpretation is quite interesting. For codes using matrix-solution techniques, CPU time generally increases monotonically with decreasing values of the tolerance parameter which controls nonlinear convergence. The procedure specified in Section 6.2 exploits this relationship in order to uniformly apply the same convergence criterion to all codes except LLUVIA II. For the method-of-lines solver used by LLUVIA II, the procedure was inappropriate. Here, CPU time decreased with decreasing values of the tolerance parameter until a minimum CPU time was achieved. Beyond this point, CPU time increased with decreasing values of the tolerance parameter.

In the error analysis for LLUVIA II, which was performed for Case A_2, the minimum CPU time corresponded to an accuracy level of approximately 4E-6 cm of total head with respect to the reference run. This represents a much higher level of accuracy than is generally required for hydrogeologic simulations. Attempts to degrade accuracy to the more reasonable level commensurate with that specified for the matrix-solution codes proved unsuccessful, yielding erratic results and excessive run times. Unlike the other codes listed in Table 8, the CPU times listed for LLUVIA II thus correspond to a minimum-CPU-time criterion, and not to a maximum total-head variation of 1 cm. The relatively large CPU times registered for LLUVIA II in Table 8 thus result from its demand for high accuracy. This demand, coupled with the relatively large CPU times resulting therefrom, will likely restrict the future use of LLUVIA II to utility applications.

For the two-phase solution of Case A_2, MSTS's CPU time per iteration exceeds that of TOUGH2 by over 80 percent. This indicates that TOUGH2's direct solver is more efficient than MSTS's direct solver. Nevertheless, the CPU times for TOUGH2 and MSTS are much larger than those of FEHM and TRACR3D. This indicates the desirability of the conjugate-gradient type solver used by the latter, even for problems as small as 2,400 nodes. To make this point more forcefully, it would be desirable to use one of the three-dimensional cases, which have approximately 25,000 nodes. However, the long run times which would be required by the direct solvers of TOUGH2 and MSTS precluded this activity, which will be possible only when new versions of these codes have been implemented on CRWMS M&O computers.

Expanding from two to three dimensions increases the number of nodes by a factor of ten. Table 8 shows that this increased the TRACR3D CPU time per iteration by a factor of approximately 20 for both Case A_3 and Case B_3. Assuming computer time to be proportional to N^{β}, where N is the number of nodes gives $\beta = 1.3$, approximately. For the gmres solution method used by TRACR3D, one would expect β to asymptotically approach a value closer to two. At 2,332 nodes, the two-dimensional problems are apparently too small to reveal the asymptotic behavior of this parameter.

6.3.2 COVE2a

Testing here includes both multiphase (FEHM and TOUGH2) and single-phase (MSTS, TOSPAC, TRACR3D, and VS2DT) implementations. Although MSTS permits both, only the single-phase implementation was employed on the COVE2a problem.

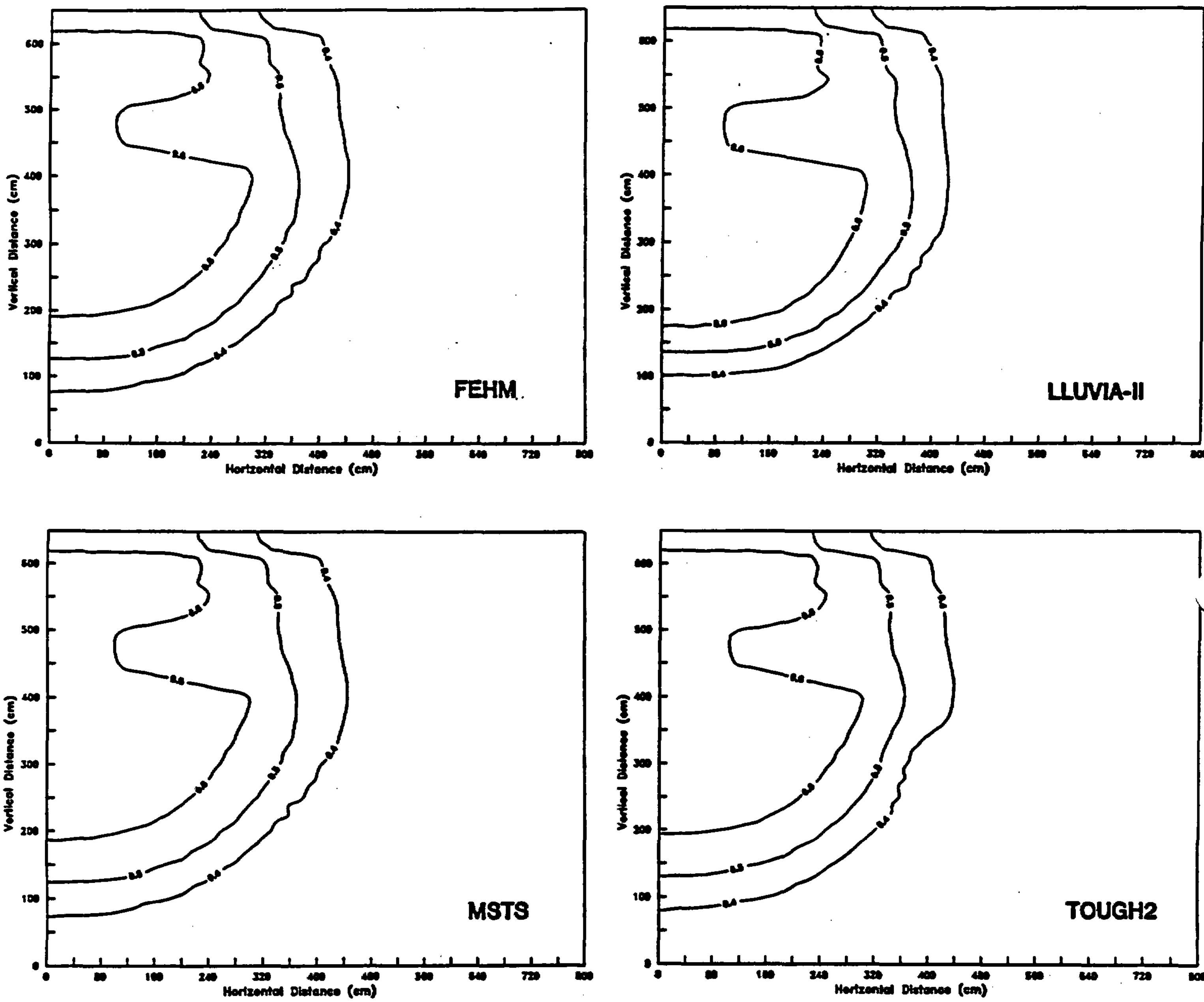
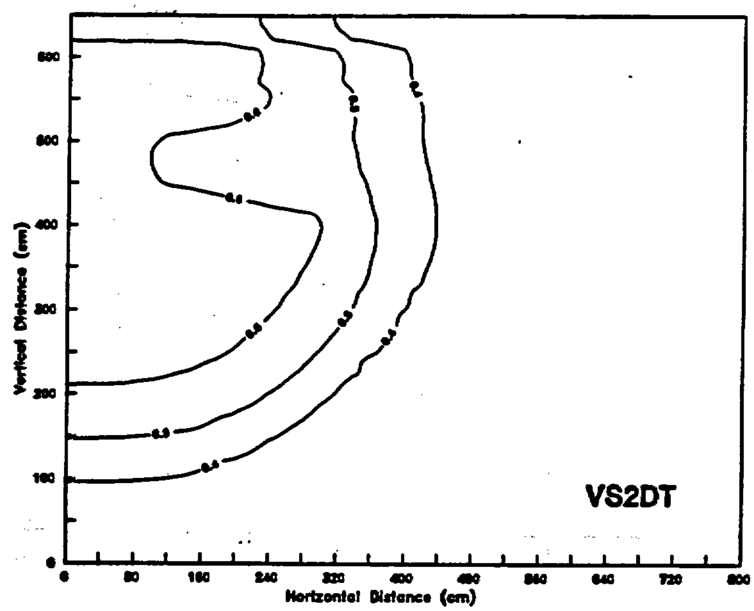


Figure 1. Calculated Saturation Profiles at 30 Days for the Jornada-Trench Problem, Case A_2.



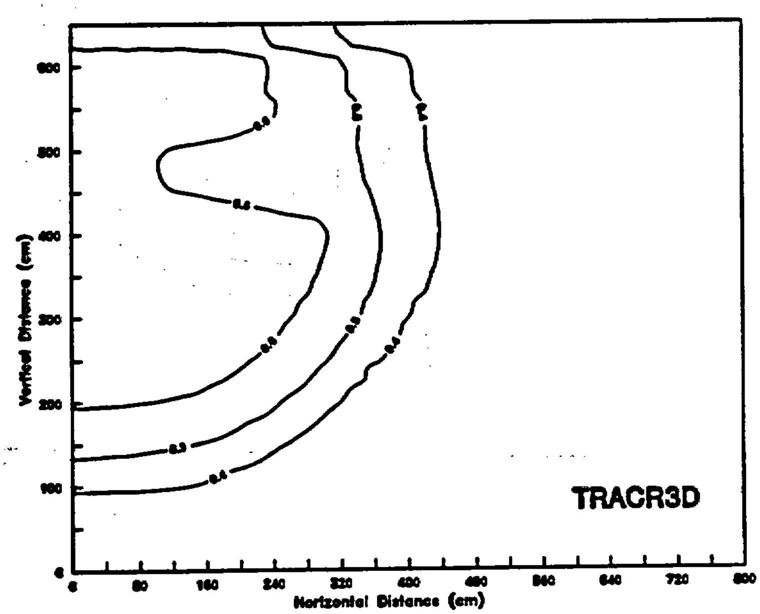


Figure 1. Calculated Saturation Profiles at 30 Days for the Jornada-Trench Problem, Case A_2 (Continued).

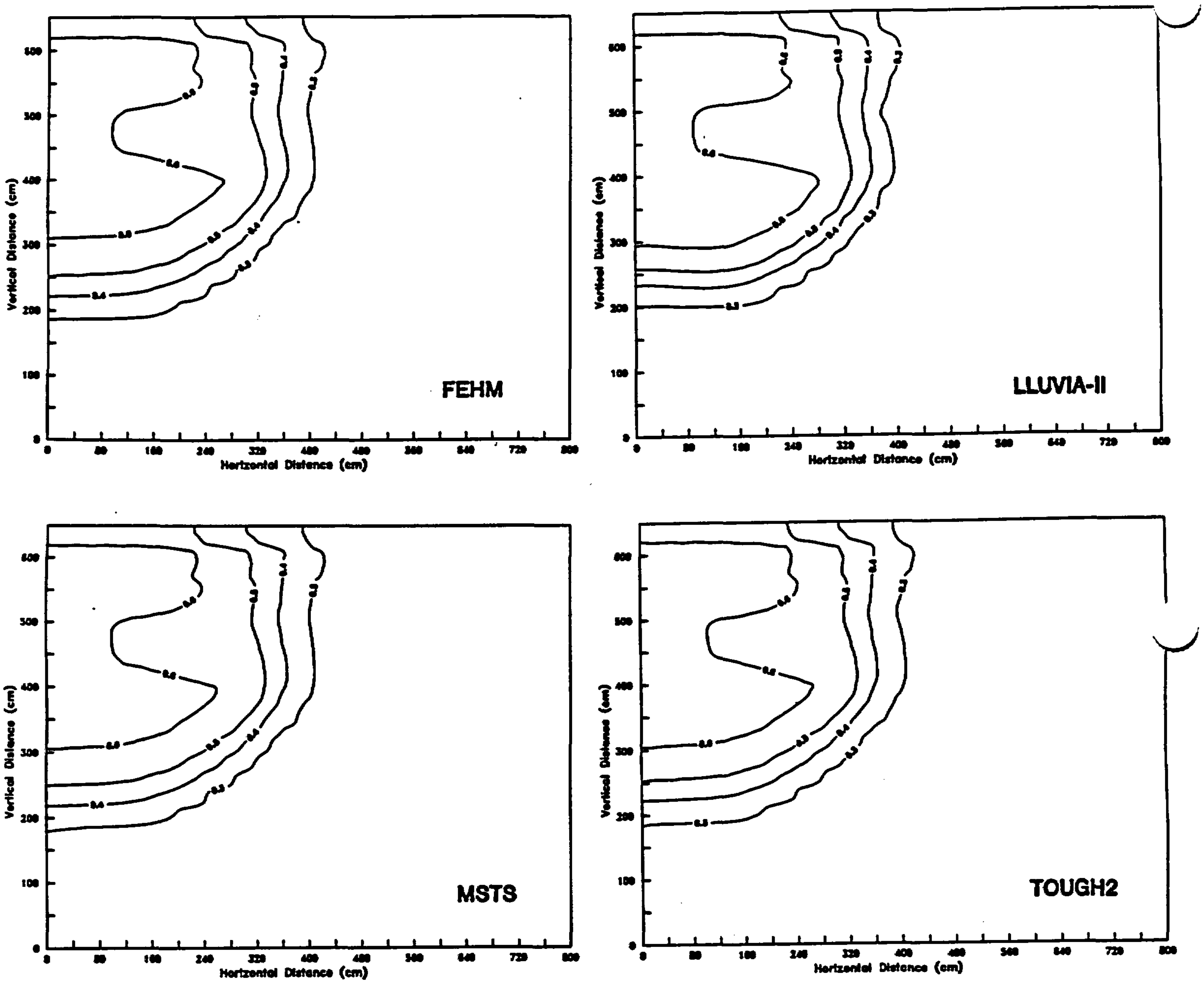


Figure 2. Calculated Saturation Profiles at 30 Days for the Jornada-Trench Problem, Case B_2.

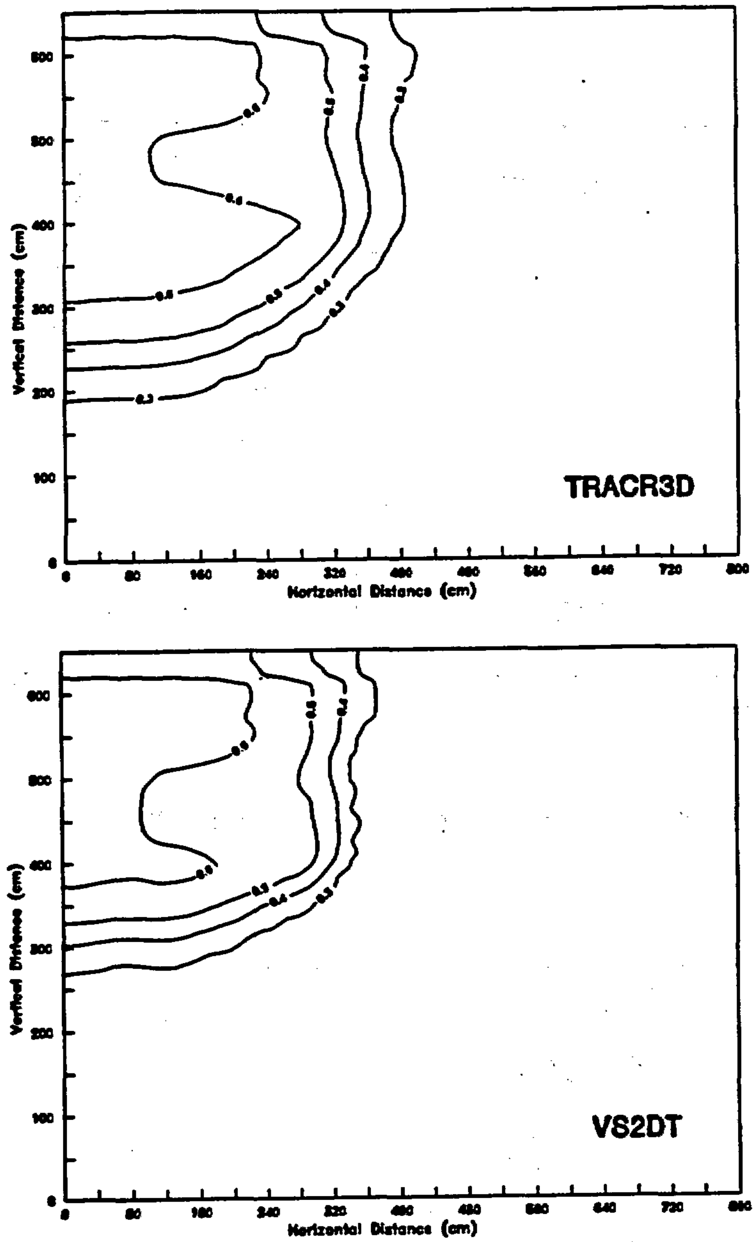


Figure 2. Calculated Saturation Profiles at 30 Days for the Jornada-Trench Problem, Case B_2 (Continued).

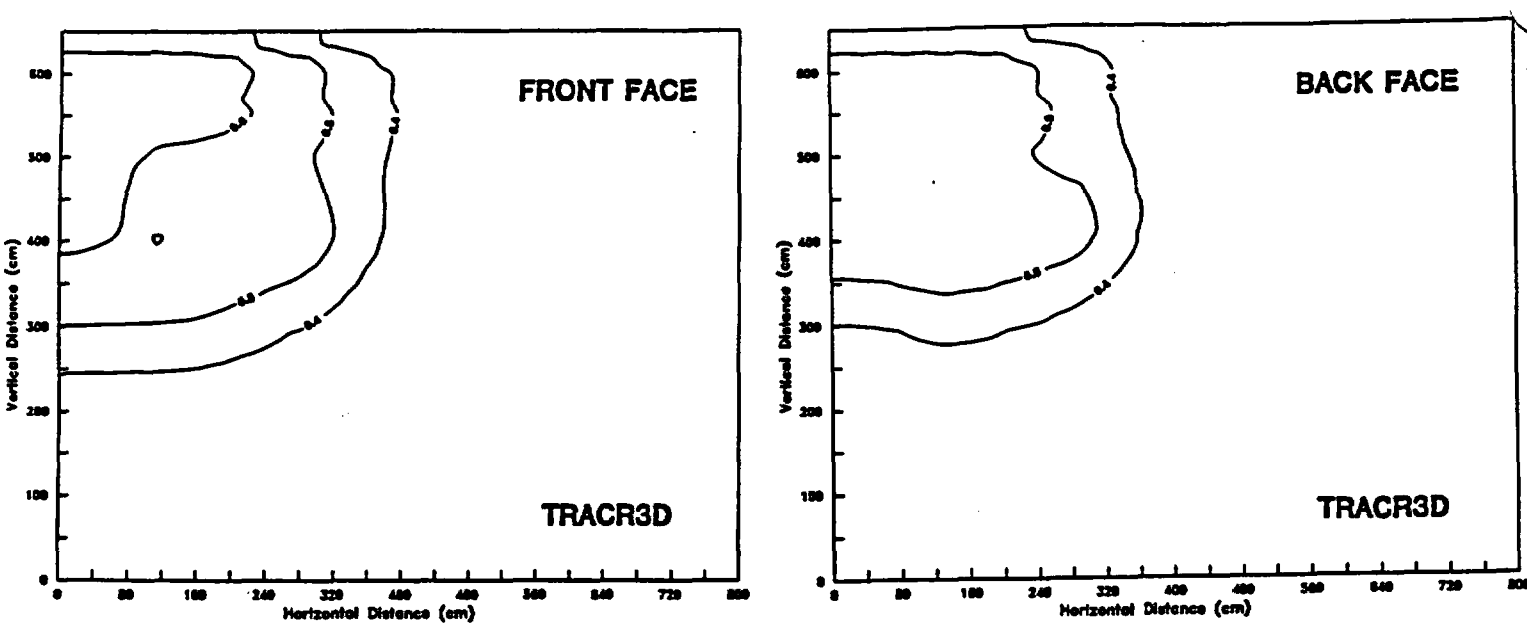


Figure 3. Calculated Saturation Profiles at 30 Days for the Jornada-Trench Problem, Case A_3.

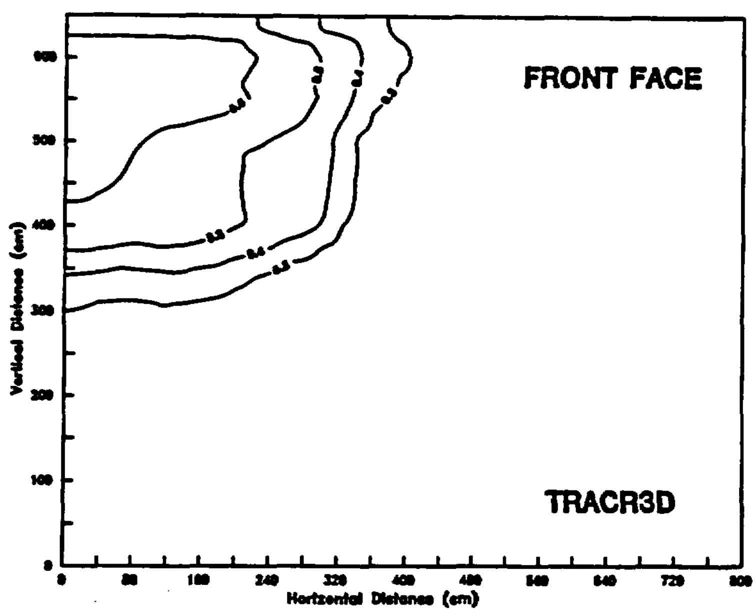


Figure 4. Calculated Saturation Profiles at 30 Days for the Jornada-Trench Problem, Case B_3.

TABLE 8. Computational Parameters for the Jornada-Trench Problems

CASE	CODE	NUMBER OF PHASES[a,b]	CPU TIME (sec)	NUMBER OF TIME STEPS	NUMBER OF ITERATIONS
A_2	LLUVIA-II	1	16,200	-	-
	MSTS	1	10,860	133	308
	TRACR3D	1	1,811	131	819
	VS2DT	1	840	131	1,016
	FEHM	2	1,157	37	82
	MSTS	2	45,180	45	176
	TOUGH2	2	18,422	37	130
B_2	LLUVIA-II	1	24,372	-	-
	MSTS	1	27,288	162	731
	TRACR3D	1	3,231	190	1,511
	VS2DT	1	7,320	1,521	9,138
	FEHM	2	1,444	37	117
	TOUGH2	2	40,743	37	182
A_3	TRACR3D	1	27,900	131	646
B_3	TRACR3D	1		163	1,172

(a) Time-stepping parameters depended on the number of phases according to the following:

NUMBER OF PHASES	INITIAL TIMESTEP (sec)	MAGNIFICATION FACTOR	MAXIMUM TIME STEP (day)
1	600	1.3	0.247
2	600	2.0	1.0

(b) LLUVIA-II automatically controlled time steps to achieve prescribed accuracy requirements.

Figure 5 gives steady-state capillary pressure profiles for an infiltration rate of 0.1 mm/yr. Figure 6 gives corresponding saturation profiles. With only one exception, these profiles agree well both with each other and with those given in the COVE2a benchmarking reports (Birdsell and Travis, 1991b, and Gauthier *et al.*, 1991). In comparison to those of other codes, the VS2DT capillary-pressure (Figure 5) and saturation profiles (Figure 6) evidence insufficient wetting of the Paintbrush nonwelded unit. Just as for the Jornada-Trench Case B_2, excessive CPU times indicate poor convergence.

Through numerical experimentation, it was found that the poor convergence could be attributed primarily to hydraulic properties of the Paintbrush tuff. Here, the van Genuchten λ parameter is largely responsible for the shape of the hydraulic-property curves, and larger values of this parameter increase the level of non-linearity. Figure 7 shows the conductivity curve specified by Appendix B, corresponding to the value $\lambda = 0.8545$. It also shows a curve corresponding to a value $\lambda = 0.5000$, for which improved convergence was obtained. Even so, the VS2DT computer time was excessive in comparison to other codes, indicating that the problem of poor convergence had not been completely removed by the reduced value of λ. In obtaining the steady-state solution with $\lambda = 0.5000$ for the Paintbrush tuff, VS2DT required 1,020 seconds, and TRACR3D required 110 seconds. Figure 8 gives transient capillary pressure profiles, and Figure 9 gives corresponding saturation profiles. With initial conditions prescribed by the steady-state profiles of Figures 5 and 6, the transient analyses assume an infiltration rate of 0.2 mm/yr. These profiles agree well both with each other and with those given in the COVE2a benchmarking reports (Birdsell and Travis, 1991b, and Gauthier *et al.*, 1991).

In its presentation of computational parameters, Table 9 shows the effects of two phases (TOUGH2 and FEHM) and two dimensions (FEHM) in slowing computer processing. Whereas the CPU times of TRACR3D and MSTS differed substantially for the Jornada-Trench analyses (Table 8), they differed insignificantly here. For a one-dimensional problem, this indicates an insensitivity of CPU time to solver differences. Thus, the principal advantage of the TOSPAC transient algorithm lies not in its efficiency, but in its user friendliness as a one-dimensional utility code.

6.3.3 Pre-Emplacement Vapor Diffusion

The test plan (Table 6) calls for testing FEHM, TOUGH2, and NUFT. Because of time constraints on the study, only TOUGH2 analyses have been completed.

Using Kelvin's law to characterize the effect of vapor-pressure lowering, this problem assumes that capillary pressures maintain the surface soil gas at a 50 percent humidity level. This causes water vapor to diffuse to the surface from the near 100 percent levels at depth, resulting in a general drying of the system. Figure 10 presents liquid saturations. Calculated for a time period of one million years, it represents a steady-state solution to a two-phase, hydrothermal problem. Figure 5 (COVE2a problem) presents liquid saturations corresponding to a steady infiltration rate of 0.1 mm/yr. A comparison of Figures 5 and 10 indicates the extent to which this evaporation process affects moisture levels.

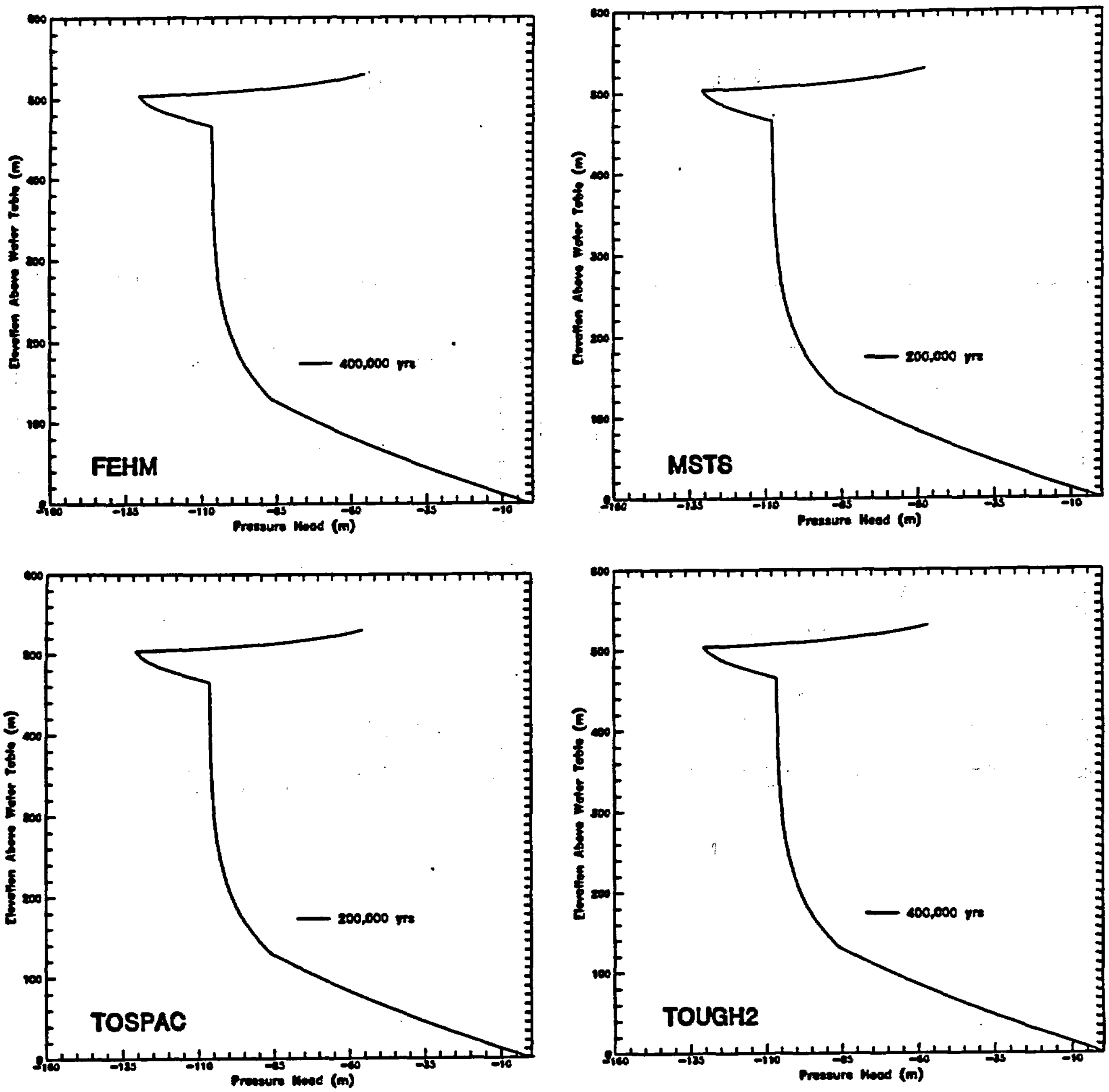


Figure 5. Calculated Capillary-Pressure Profiles at Steady State for the COVE2a Problem.

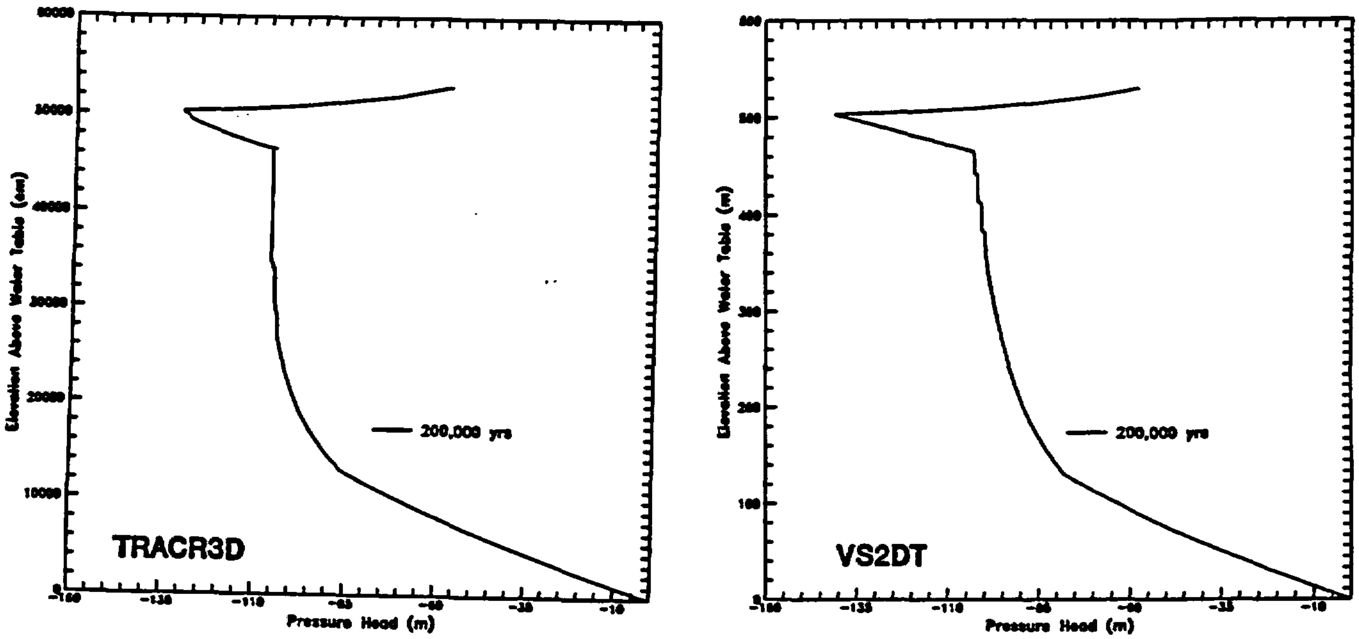


Figure 5. Calculated Capillary-Pressure Profiles at Steady State for the COVE2a Problem (Continued).

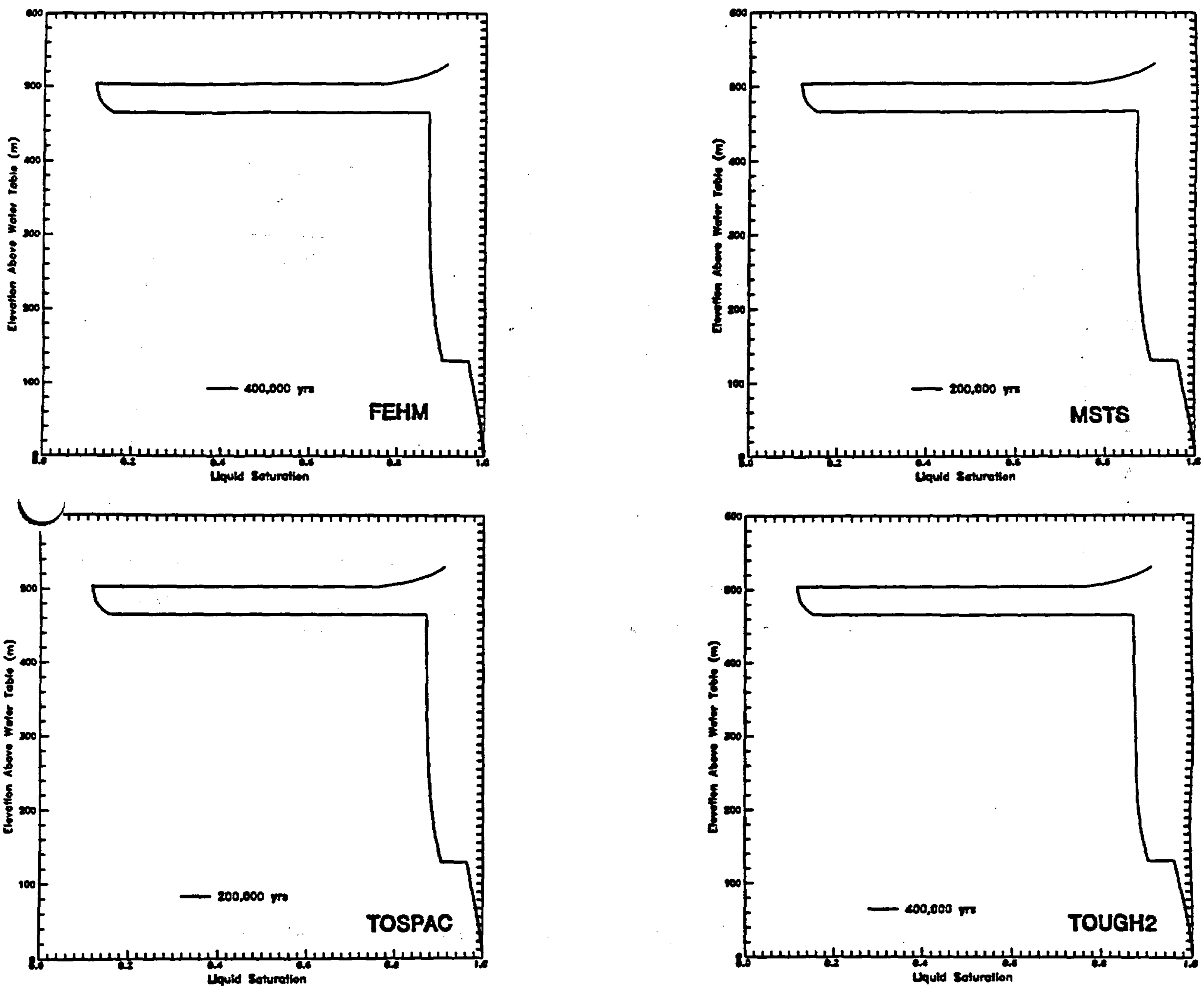


Figure 6. Calculated Saturation Profiles at Steady State for the COVE2a Problem.

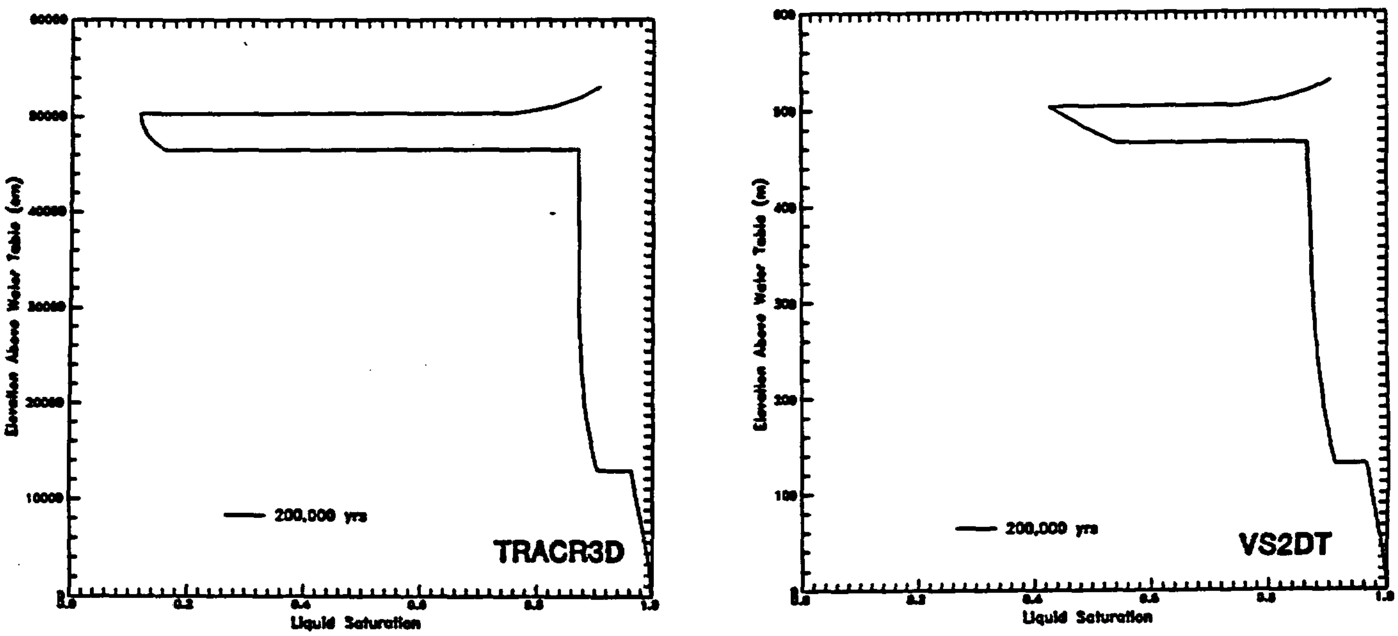


Figure 6. Calculated Saturation Profiles at Steady State for the COVE2a Problem (Continued).

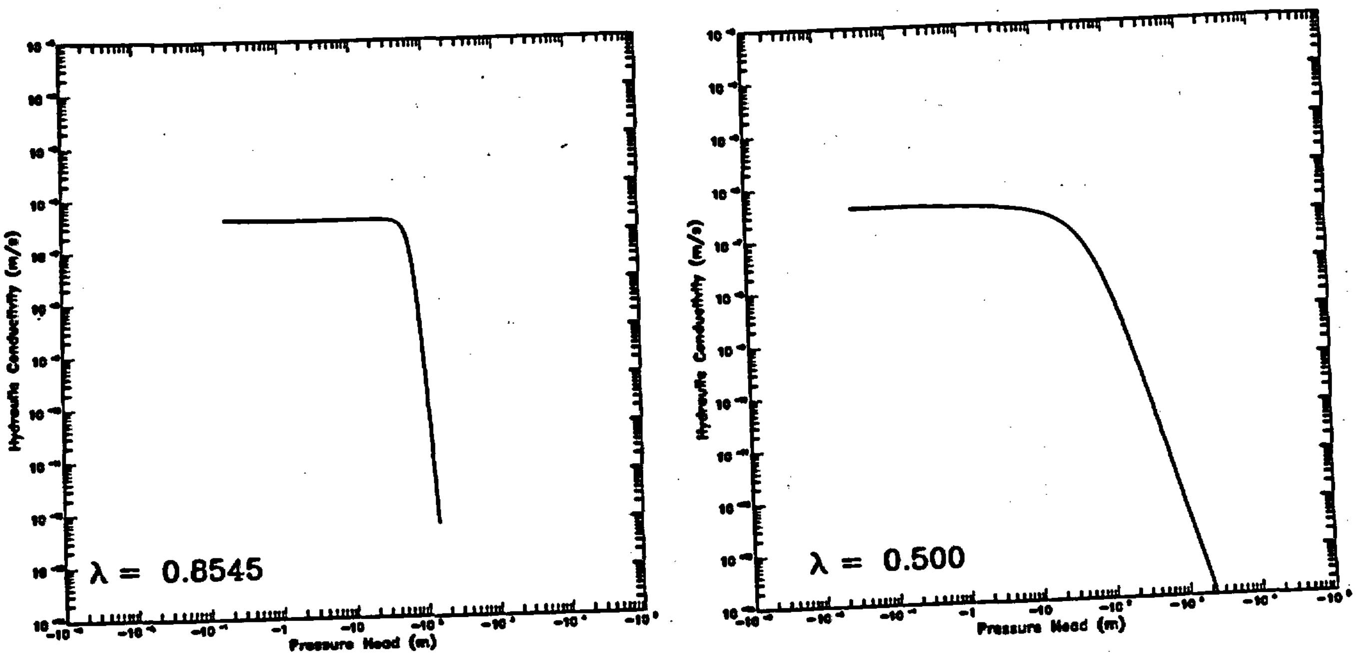


Figure 7. Conductivity Curves for the Paintbrush Unit.

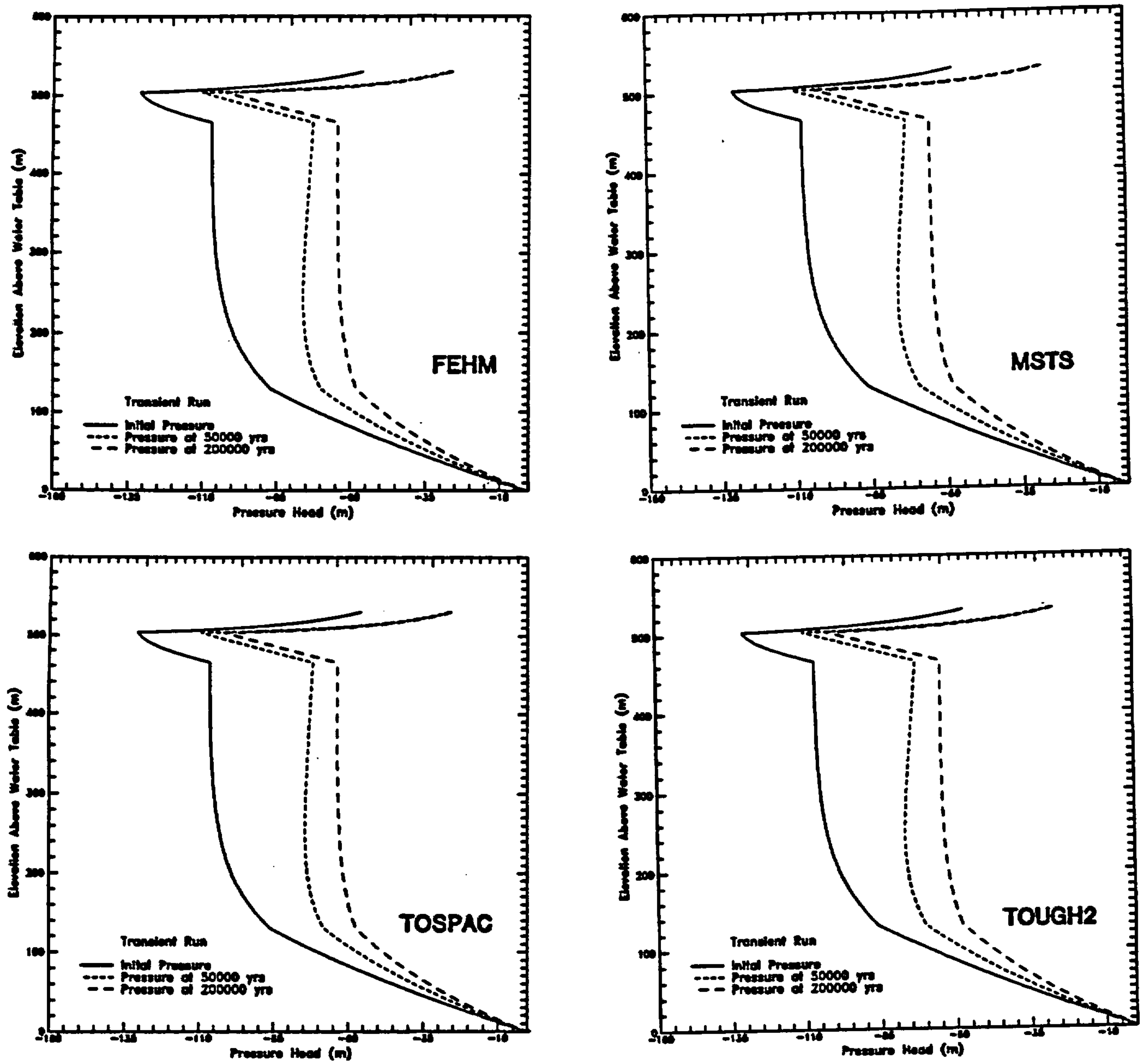


Figure 8. Calculated Capillary-Pressure Profiles for the COVE2a Problem.

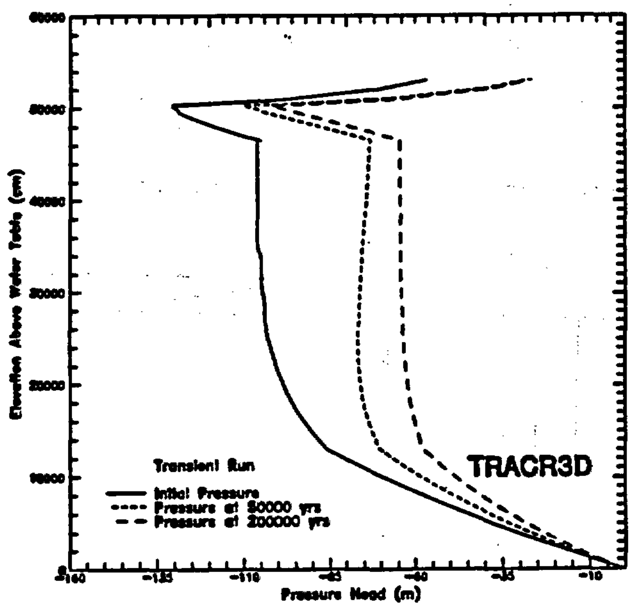


Figure 8. Calculated Capillary-Pressure Profiles for the COVE2a Problem (Continued).

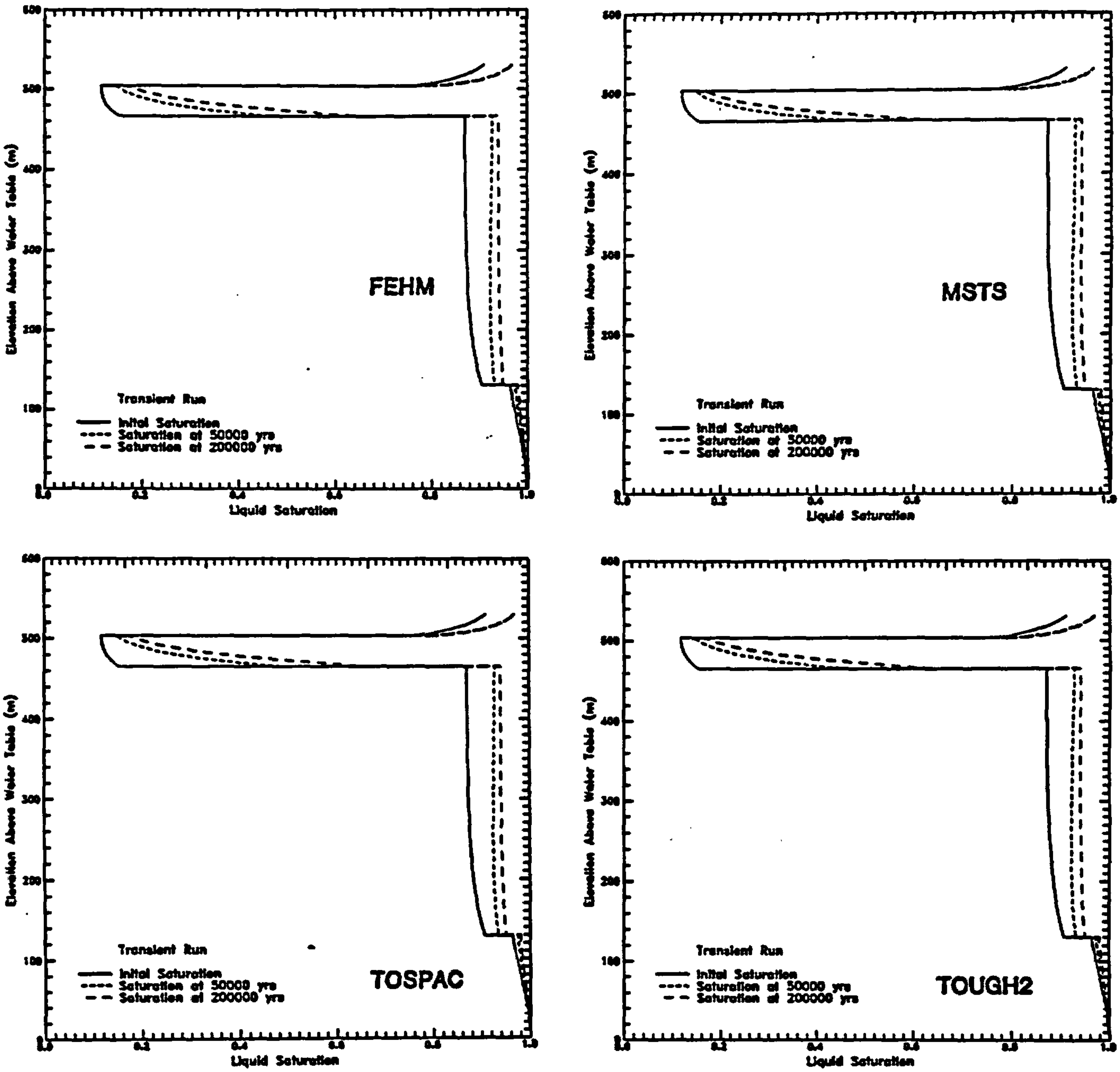


Figure 9. Calculated Saturation Profiles for the COVE2a Problem.

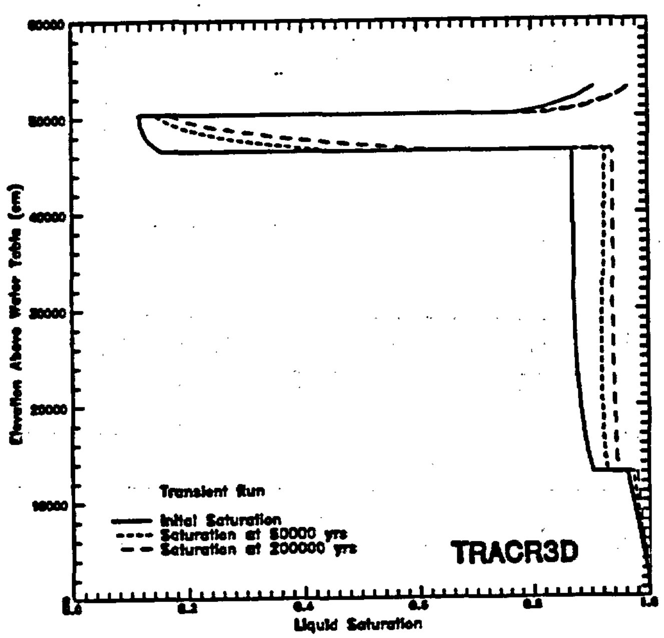


Figure 9. Calculated Saturation Profiles for the COVE2a Problem (Continued).

TABLE 9. Computational Parameters for the COVE2a Problem

CODE	NUMBER OF PHASES[a]	CPU TIME (sec)	NUMBER OF TIME STEPS	NUMBER ITERATIONS
MSTS	1	120	48	86
TOSPAC	1	95	-	135
TRACR3D	1	108	65	231
FEHM[b]	2	204	31	72
TOUGH2	2	342	42	167

(a) Time-stepping parameters depended on the number of phases according to the following table:

NUMBER OF PHASES	INITIAL TIME STEP (yr)	MAGNIFICATION FACTOR	MAXIMUM TIME STEP (yr)
1	3.0	1.3	10,000
2	3.0	2.0	10,000

(b) Two-dimensional calculation

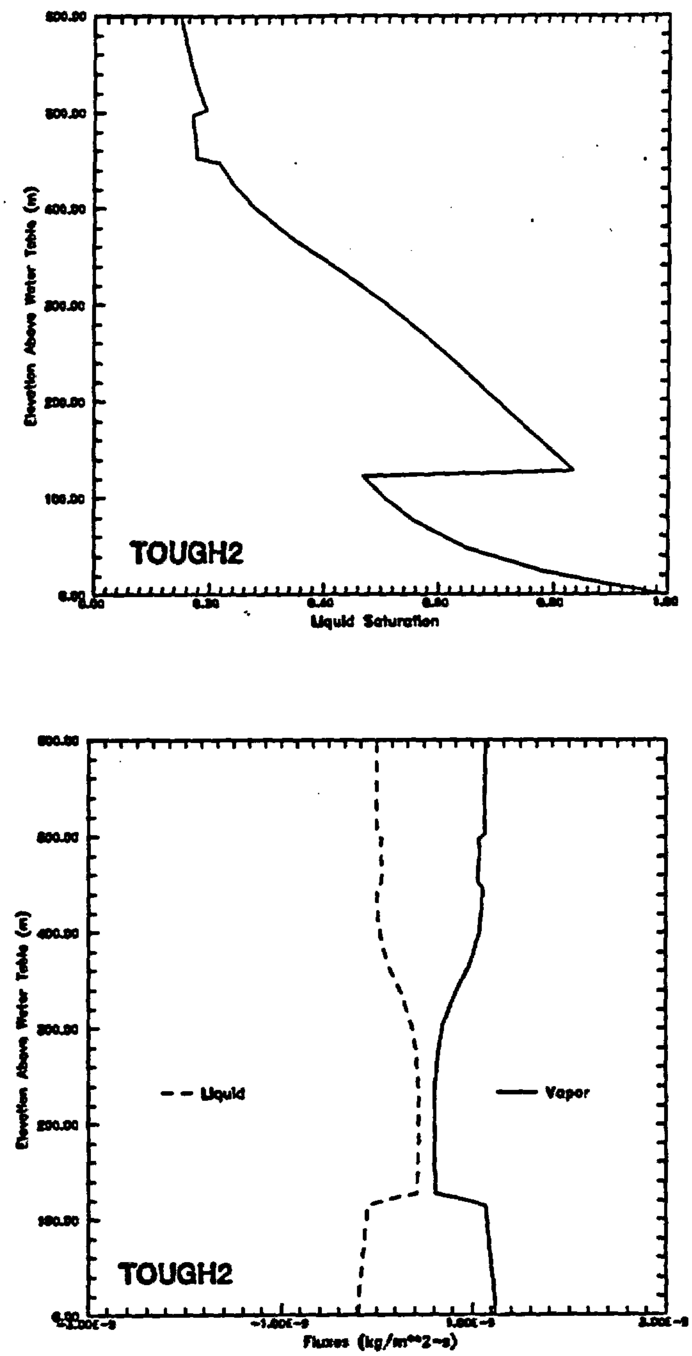


Figure 10. Calculated Saturation and Flux Profiles at Steady State for the Pre-Emplacement Vapor-Diffusion Problem.

Figure 10 shows the extent to which liquid and vapor flows mirror each other. When combined, they yield a net upward flow of 0.03 mm/yr. The TOUGH2 CPU time measured 47.3 seconds on a 486/33 personal computer.

6.3.4 The Repository Heat Pipe

The test plan (Table 6) calls for testing FEHM, TOUGH2, and NUFT. Because of time constraints on the study, this testing has not been completed.

7. CONCLUSIONS

This study has led to two different sets of conclusions. One set, identified as "General Conclusions" considers a general comparison of model capabilities with model requirements. It identifies deficiencies which now exist. A second set of conclusions, identified as "Model-Specific Conclusions" considers specific codes. It identifies noteworthy characteristics of the various implementations.

7.1 GENERAL CONCLUSIONS

Tables 2 and 3 list the model requirements. In addition to the regulations of 10 CFR 60 and 40 CFR 191, these model requirements derive from the geologic nature of Yucca Mountain and from the theory of unsaturated flow. A comparison of model capabilities with the model requirements of Tables 2 and 3 yields the following conclusions:

- Several models address the physical and numerical requirements of Tables 2 and 3 sufficiently well that they may be used as host structures for future development. Future development can thus focus manpower and financial resources on upgrading selected existing codes.

- Several models can simulate Yucca Mountain problems of moderate size using the approximation of a fracture-matrix continuum with isotropic fracture connectivity. However, Requirement 1 of Table 2 and Requirements 1, 5, and 7 of Table 3 will necessitate a consideration of the fracture-matrix discontinuum with anisotropic connectivity. Models in current use by the YMP cannot adequately characterize this effect.

- Only in one-dimensional implementations can currently available models characterize the effect of non-equilibrium fracture-matrix flow. Requirements 3 and 4 of Tables 2 and 3 indicate that this capability is inadequate.

- The efficiency demands for simulating a fracture-matrix discontinuum and non-equilibrium fracture-matrix flow are significant. Substantial improvements in both hardware and software are needed in order to meet these requirements.

- Single-phase, liquid-flow models based on the Richards equation are appropriate for site-characterization and test-design analyses relating to the system prior to waste emplacement. However, the inability of such models to characterize the effect of temperature on the movement of water in liquid and gaseous phases makes such models inappropriate for performance assessment of the post-emplacement system (Requirement 1 of Table 2 and Requirements 5, 6, and 7 of Table 3).

7.2 CODE-SPECIFIC CONCLUSIONS

This study has considered two different groups of models. One group comprises the various codes used within the project to characterize unsaturated liquid flow and transport. Here the conclusions derive both from a cross-comparison of model capabilities and code testing. The other group comprises the two relatively unique models, FracMan and TGIF.

7.2.1 Model Capabilities

A cross-comparison of model capabilities (Sections 4.3, 5.1, and 5.2) led to the following conclusions:

- The TOUGH2 model offers a very capable multiphase, nonisothermal flow model using a finite-difference implementation. However, NUFT has similar capabilities, and further examination of this recently released code may show it to be an attractive alternative to TOUGH2.

- FEHM offers the most capable multiphase, nonisothermal flow model using a finite-element implementation.

- TRACR3D provides the most capable transport model. TRACR3D also provides the most capable single-phase flow model using a finite-difference implementation.

- MSTS has an excellent input preprocessor, and a flexible implementation of boundary conditions facilitates its application. The clarity of its coding is excellent. Otherwise, however, it does not add significantly to the capabilities present in TOUGH2.

- TOSPAC's user interface may be the best in the project and, like MSTS, the clarity of its coding is excellent. In addition to its usefulness as the flow and transport module of the total system analyzer TSA, TOSPAC makes an excellent utility code.

7.2.2 Code Testing

The above conclusions, together with a desire to test several relatively unique algorithms, led to a selection of codes for testing. Using the problems defined in Appendix B, four multiphase, nonisothermal flow models (FEHM, MSTS, NUFT, and TOUGH2) and four single-phase liquid-flow models (LLUVIA-II, TOSPAC, TRACR3D, and VS2DT) were tested. The results (Section 6.3) may be summarized in the following manner:

- Except in special cases, the Picard and hybrid methods appear to be inappropriate for the non-linearities caused by Yucca Mountain moisture conditions and hydrogeologic properties.

- Because of enhanced robustness, the CPU times of two-phase simulations can be quite competitive with the CPU times of single-phase, Richards-equation simulations.

- For transient simulation of the one-dimensional COVE2a problem, the single-phase results were quite similar both in terms of the saturation profiles obtained and the CPU times required. Although TOSPAC's user friendliness make it highly desirable as a utility code, its one-dimensional coding appears to offer only marginal efficiency improvement over that obtainable through one-dimensional implementations of the three-dimensional codes TRACR3D and MSTS.

- For optimal efficiency, the method-of-lines solver used by LLUVIA-II requires a high level of accuracy. Here, the simulation error is several orders of magnitude smaller than is necessary for practical applications, and the CPU time is relatively large. The latter characteristic appears to rule out all but specialized applications of the method of lines to Yucca Mountain problems.

7.2.3 FracMan

Sections A.6 and A.14 (Appendix A) report the reviews of two models which have relatively unique capabilities. FracMan develops statistical fracture properties and, from them, develops geometrical realizations of fractured rock. TGIF simulates the mountain-scale movement of water vapor and gas. The review of FracMan may be summarized in the following manner:

- Requirement 1 of Table 2 and Requirements 1, 5, and 7 of Table 3 necessitate a consideration of the fracture-matrix discontinuum and its anisotropic connectivity.
- In its focus on the geometrical characteristics of fractured rock, FracMan provides one of two capabilities needed to satisfy these requirements.
- The second capability, namely the abilities to simulate the multiphase and unsaturated single-phase flow does not presently exist within the YMP.

7.2.4 TGIF

The review of TGIF may be summarized in the following manner:

- Requirement 1 of Table 2 and Requirements 1 and 5 of Table 3 call for a consideration of mountain-scale movements of water vapor and gas.
- Multiphase flow models can simulate the movements of water vapor and gas, but an excessive demand for computer resources rules out mountain-scale analyses. Thus, at the present time, TGIF alone is capable of performing such simulations.
- However, TGIF cannot adequately consider either the effect of the repository heat pipe on the mountain-scale movements of water vapor and gas or the effect of the latter on repository temperature.
- Furthermore, in common with other flow models used by the project, TGIF cannot account for the fracture-matrix discontinuum and its anisotropic connectivity.

8. RECOMMENDATIONS

8.1 GENERAL RECOMMENDATIONS

Where the general recommendations below require additional development, selected codes should be the basis for that development.

- Several models address the physical and numerical requirements of Tables 2 and 3 sufficiently well that they may be used as host structures for future development. Thus, the development of new stand-alone models should be sharply curtailed, thereby permitting future development to focus on upgrading selected existing codes.

- To satisfy the requirements of 10 CFR 60 and 40 CFR 191 relating to the prevalence of fractured rock at Yucca Mountain, future model development should consider a simulation capability for discrete-fracture effects, including an anisotropic connectivity.

- To satisfy the requirements of 10 CFR 60 and 40 CFR 191 relating to the prevalence of fractured rock at Yucca Mountain, future model development should consider a multidimensional simulation capability for non-equilibrium fracture-matrix flow.

- The demands for improvement in computational efficiency are substantial. These demands stem both from the requirements of 10 CFR 60 and 40 CFR 191, as expressed above, and from the needs of site-characterization and design calculations. Strong focus and project-wide coordination is needed. Strategies for future development should consider software improvements, including those appropriate for massive parallelization. A suitable goal would be the solution of a multiphase, nonisothermal Yucca Mountain problem of 100,000 grid cells in a CPU time of less than 24 hours.

- Since future model-development problems will be difficult and funds are limited, the number of stand-alone codes to be carried forward should be minimized.

8.2 CODE-SPECIFIC RECOMMENDATIONS

This section presents recommendations for future model development. These recommendations assume that both finite-difference and finite-element codes are needed with one of them, the primary code, performing most of the calculations and the other, the secondary code, providing cross-verification. The recommendations also assume that, in addition to a multiphase capability, a single-phase flow capability is also needed, at least for the present. They are:

- To avoid unnecessary duplication of effort, future development should focus on certain selected codes. They may be regarded as host structures for future development. The selected codes are: FEHM, TGIF, TOUGH2, TRACR3D, and FracMan, with one possible exception. Further analysis of the NUFT code may show it to be an attractive alternative to TOUGH2.

- As a primary multiphase, continuum model, use TOUGH2.

- As a primary multiphase, discrete-fracture flow model, link FracMan and FEHM.

- As a primary single-phase liquid-flow model, use TRACR3D.

- If a secondary single-phase liquid-flow model is desired, put a single-phase switch in FEHM.

- As a single-phase, discrete-fracture, gas-flow model, link FracMan and TGIF. Then expand TGIF to characterize the coupled effects of a repository heat pipe and mountain-scale gas flow. This expansion should be aimed at maintaining TGIF's mountain-scale advantage over the multiphase models.

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APPENDIX A

MODEL REVIEWS

A.1 DCM3D

1. Name of the Model

DCM3D

2. General Program Information

2.1 *Program size.* DCM3D has approximately 10,000 lines of source code.

2.2 *Programming language.* ANSI standard FORTRAN

2.3 *Computer system on which it operates.* The user's manual reports the use of a Cray XMP-24. Updegraff, the author, reports (private communication, 1991) that the program also operates on a VAX 8700 and an IBM PC.

2.4 *Compiler(s) used.* DCM3D uses standard compilers for each of these computers.

2.5 *Location of code and availability.* Inquiries on code availability should be directed to C.D. Updegraff at GRAM, Inc., 1709 Moon Street Northeast, Albuquerque, New Mexico 87112.

2.6 *Brief description of model/code history.* The U.S. Nuclear Regulatory Commission (NRC) is developing a performance assessment methodology for analyzing the long-term disposal of high-level radioactive waste (HLW). The program's development was prompted by the NRC's need to provide independent regulation and evaluation of the U.S. Department of Energy's (DOE) HLW disposal activities. As part of the program, NRC contracted Sandia National Laboratories (SNL) to assist in the development of a computer code to model isothermal ground-water flow in an unsaturated, fractured, porous medium. The result of this work is DCM3D, a code developed by Updegraff et al. (1991).

3. Status of Model

3.1 *Development (Is the model now undergoing significant development or modification? or continuing maintenance?).* To our knowledge, no new developments on DCM3D are currently underway.

3.2 *Documentation.* DCM3D: A Double-Continuum, Three-Dimensional, Ground-Water Flow Code for Unsaturated, Fractured, Porous Media (Updegraff et al., 1991)

3.3 *Status of verification and validation.* The DCM3D user's manual (Updegraff et al., 1991) includes four illustrative problems. Only one (Problem 2) is new. Two are recommended as benchmarks by an NRC-funded study (Ross et al., 1982) and have been executed by other codes. Updegraff (1989) and Moridis and Pruess (1992) report results for one of these (Problem 1) using NORIA (Bixler, 1985), TOUGH

(Pruess, 1987), and PETROS (Hadley, 1985). For the other (Problem 3), an unpublished NRC benchmarking report gives results using several codes, including SWIFT II (Reeves et al., 1986). Problem 4 derives from the experimental work of Vauclin (1978). These problems are discussed separately below:

Problem 1 - One-Dimensional Infiltration. An infiltration front enters a semi-infinite horizontal tube filled with a homogeneous soil. Air is not accounted for and is a passive spectator. This problem, one of the benchmarks adopted by Ross et al. (1982), compares the DCM3D solution with the semi-analytical results of Philip (1955). To characterize infiltration for 9,504 s, 40 grid blocks were used. The Cray XMP-24 analysis required 90 time steps and 0.30 s of CPU time, and the VAX 8700 analysis required 162 time steps and 3.0 s.

Problem 2 - One-Dimensional Flow Through a Saturated Fractured Medium. A constant flux of water enters one end of a horizontal column containing a fractured medium. As it flows through the fractures, water enters the rock matrix at a rate determined by the transfer coefficient. Water also moves horizontally within the rock matrix, but at a much slower rate than within the fractures. Updegraff et al. (1991) solved this problem both analytically and numerically. Using only 10 grid blocks, the Cray XMP-24 analysis required 293 time steps and 0.31 s of CPU time, and the VAX 8700 analysis required 221 time steps and 2.7 s.

Problem 3 - Production from a Saturated Fractured Medium. As in the Theis problem, water is pumped from a well at a constant rate. Initially, the fractures provide most of the water, and the rate of production is relatively large. Later, following a period of transition, the rock matrix provides most of the water, and the rate of production is relatively small. This problem, one of the benchmarks adopted by Ross et al. (1982), compares the DCM3D solution with the analytical results of Streltsova-Adams (1978). Apparently, DCM3D does not have an option for cylindrical coordinates. For this, a radially symmetric problem, a two-dimensional 40-by-40 Cartesian grid was used. The Cray XMP-24 analysis required 412 time steps and 155 s of CPU time, and the VAX 8700 analysis required 227 time steps and 917 s.

Problem 4 - Two-Dimensional Infiltration. In this problem, a 2-m-high by 3-m-long vertical slab of soil is recharged at a rate of 4.11E-5 m/s over a 0.5-m long region at the top left corner of the slab. The slab is bound on the bottom and one side by impermeable boundaries. A trench bounds the other side of the slab, the top portion of which comprises a seepage face. The lower portion of the trench contains water, which is maintained at a constant depth of 0.65 m. This problem compares the numerical results of DCM3D with the experimental results of Vauclin et al. (1979). A 100-by-18 grid was chosen and, with exception to the seepage face, it faithfully implemented the boundary conditions specified by Vauchlin et al. (1979). Since DCM3D does not have a seepage-face option, a no-flow condition was prescribed along the top portion of the trench. Updegraff et al. (1991) note some differences between numerical and experimental results, perhaps arising from this boundary-condition or, as the authors suggest, from heterogeneities distributed throughout the slab and especially at a depth of 0.5 m. The Cray XMP-24 analysis required 579 time steps and 245 s of CPU time, and the VAX 8700 analysis required 552 time steps and 2,330 s.

Given a common data base and hydrogeologic characterization of the Yucca Mountain site, participants in the PACE-90 study determined the movement of radionuclides to the accessible environment. This exercise verified the ability of different researchers to independently conceptualize a complex site in a physically consistent manner. Although code implementations varied among the five participants, the study may be considered as a code-verification effort in a broad sense because of similarity of the results. To simulate flow, participants chose DCM3D and five other flow codes. The problem is briefly described as follows:

PACE-90 analysis. DCM3D simulated partially saturated flow in a one-dimensional column extending from the water table to the bottom of the repository and located near drill hole G-4. The conceptualization used fifteen materials with varying hydrologic characteristics and thicknesses. Flow was simulated in both the matrix and fractures. A total of 122 grid blocks discretized the column. At the upper boundary, a net infiltration rate of 0.01 mm/yr recharged the system, and, at the lower boundary, a pressure of zero fixed the water-table elevation for matrix and fractures. The flow field calculated by DCM3D was then transferred to NEFTRAN (Longsine et al., 1987) for the radionuclide-transport simulation.

3.4 *Status of Quality Assurance (QA)*. DCM3D is under an NRC sponsored QA program.

4. Type of Model (Phenomena/Processes Modeled)

DCM3D, a multi-dimensional (one-, two-, or three-dimensional) numerical model, simulates unsaturated flow in a fractured, porous medium. It utilizes a dual-permeability approach with the continuum of one permeability characterizing the rock matrix and the other characterizing the fractures. A transfer term provides coupling between the two continua. Richards' relation provides the equation of motion for both fractures and matrix. Assumed to have a constant pressure throughout, the air component does not require a governing equation. Air, however, is not entirely a "passive spectator" since its presence leads to both capillary-pressure and relative-permeability effects.

5. Governing Equations

The model solves two coupled Richards equations in three dimensions for two continua. It assumes that fractures are sufficiently well connected and uniformly distributed that their effect upon the flow system can be adequately accounted for by means of REV averages. The fractures constitute one continuum; the porous matrix, the other. A transfer term, proportional to the pressure difference, couples the flow within the two continua. For this coupling strategy, known as a pseudo-steady-state approximation, the coefficient of proportionality is assumed to be proportional to the relative permeability of the porous matrix. Typically, DCM3D uses the functional forms developed by van Genuchten (1980) and Maulem (1976) to characterize the dependence of relative permeability and capillary pressure upon saturation. However, the model's function sub-programs may be rewritten to handle different functional forms. Water and rock are assumed to be only weakly compressible. The model accounts for changes in density and pore volume in the accumulation (temporal derivative) terms, but not in the transport (spatial derivative) terms.

6. Method of Solution

DCM3D applies the finite-difference technique only to the spatial domain, retaining the time variable as a continuous variable. The flow equations thus transform to a coupled set of ordinary differential equations (ODEs). This approach constitutes a significant departure from the approaches used by TOUGH, TRACR3D, MSTS, and NORIA. By employing a differencing procedure also within the time domain, the latter codes become dependent upon a linear-equation solver. In contrast, DCM3D becomes dependent upon ODE methods for stiff systems. Stiffness arises through the variability of specific-storage coefficients and relative permeabilities. DCM3D uses ODEPACK. Developed by Hindmarsh (1983), ODEPACK was applied by Brown and Hindmarsh (1987) to stiff ODE systems similar to those anticipated for DCM3D.

7. Type of Input Parameters

Data input for DCM3D consists of two types: non-hydrologic parameters necessary to run the code and hydrologic data. The following data are grouped and presented in the order in which they are read by the code.

Non-Hydrologic Data:

- Title
- Subtitle
- Analyst
- Name of file to which plot data are to be written
- Options telling code to run and type of media being solved
- Density, dynamic viscosity, and compressibility of water
- Gravitational acceleration, including its x-, y-, and z-direction components
- Relative and absolute convergence criteria for LSODES
- Newton-Raphson convergence criteria
- Maximum number of time steps permitted
- Maximum number of time steps permitted between write times

- Start time for the simulation
- Initial time-step size
- Minimum time-step size permitted between write times .
- Maximum time-step size permitted between write times
- Maximum CPU time permitted
- Number of grid blocks in the x-, y-, and z-directions
- Information on grid-block spacing in the x-, y-, and z-directions
- Number of write times
- Time at which output is sent to an output file, plot file, or save file
- Control flag indicating whether to calculate moisture content, saturations, or Darcy velocities at particular write times.

Hydrologic/Material Data:

- Number of materials
- Name of material (rock) type
- Minimum and maximum index range for a particular material in i, j, and k directions
- Bulk compressibility of porous media
- Porosity of porous material
- Intrinsic permeability of porous material in the x-, y-, and z-directions
- Moisture content of porous material under fully saturated and residual moisture conditions
- van Genuchten capillary-pressure parameters for the power denominator and for the entire expression
- Parameter in the denominator of the van Genuchten equation
- Bulk compressibility of fractured material
- Porosity of fractured material

- Intrinsic permeability of fractured material in x-, y-, and z-directions

- Transfer factor between porous and fractured materials

- Moisture content of fracture material under fully saturated and residual moisture conditions

- Initial conditions

- Number of non-zero flux and pressure boundary conditions tables

- Number of data pairs or triplets in the boundary-condition table

- Type of porous medium and fracture boundary conditions

- Distribution of the boundary conditions between porous and fractured media

- Boundary condition ranges, minimum and maximum index in the x-, y-, and z-directions

- Time at which boundary conditions are to be applied

- Value of the boundary conditions for porous medium and fractures

- Number of source term tables in modeled region

- Number of data pairs or triplets in the table of source term data

- Distribution of source term between porous medium and fractures

- Source term range (i.e., minimum and maximum index in the x-, y-, and z-directions)

- Time at which source term is applied and value of the source term for the porous medium and fractures.

Restart Data:

- Restart information
- Name files, specify options
- Time step data
- Write times
- X-, y-, and z-direction boundary condition data
- Source term data.

8. Type of Output and User Options

Primary output from DCM3D includes porous media and fracture velocity fields, pressures, and moisture contents (or saturations). From these data, ground-water travel times can be obtained. The user has the option of specifying the times at which the above information is written to either a plot file, an output file, or a save file.

9. Model Interactions (emphasize needed processors)

9.1 *Does the model interface with any other models?* Yes, see below.

9.2 *Source code and type of information needed.* Not applicable.

9.3 *Receiving code and type of information provided.* DCM3D provides velocity fields, pressures, and moisture contents which may be transferred to a transport code. If flow occurs predominantly within the porous media, then the NRC-funded code NEFTRAN (Longsine et al., 1987) may be used. Currently, NRC is funding the development of a radionuclide transport code to simulate transport in a fractured porous media.

9.4 *Any pre- or postprocessing needed?* Postprocessing of the output data is needed since DCM3D has no graphics capability *per se*. DCM3D stores output data in a plot file. A FORTRAN computer code, READPL, reads this file, reformats the data, and creates the desired graphics. Assuming that the user will need to modify it, the user's guide (Updegraff et al., 1991) lists READPL.

10. Model Application

10.1 *Usage within the Civilian Radioactive Waste Management System (CRWMS) program.* Within the CRWMS program, DCM3D can be used for code-verification studies. However, it is unclear to what extent a NRC-developed code should be used in licensing calculations by the DOE. DCM3D has the ability to characterize flow and to determine travel times to the accessible environment.

10.2 *Usage outside the program.* At this point, DCM3D has been used only for analyses related to Yucca Mountain.

11. Codes With Similar or Same Capabilities

11.1 *Within the program.* The Yucca Mountain Site Characterization Project (YMP) has funded the development of several models which are comparable to DCM3D. These codes include TOUGH2 at LBL, V-TOUGH (Nitao, 1989) at LLNL, NORIA (Bixler, 1985) and LLUVIA-II (Eaton and Hopkins, 1992) at SNL, TRACR3D (Birdsell and Travis, 1991) and FEHM (Zyvoloski et al., 1992) at LANL (Los Alamos National Laboratory), and PORFLO-3 and MSTS at PNL (Pacific Northwest Laboratory). In terms of the processes considered, many of the latter codes are more general. Except for LLUVIA-II and PORFLO-3, which are also based on Richard's equation, all of the latter include a gas phase. Some of the latter also consider heat transport, and, appropriately, they include a condensing vapor component within the gas phase. Like DCM3D, TOUGH has the ability to perform dual-permeability calculations. Otherwise, DCM3D would be unique in this respect. Its major claim to uniqueness, however, is its method of solution. Only DCM3D and LLUVIA-II use a technique for coupled ordinary differential equations (ODEs) specially designed for stiff systems.

11.2 *Outside the program.* In addition to DCM3D, the NRC funded the documentation of TOUGH (Pruess, 1987). Further, a number of codes have been developed within the petroleum industry. In terms of the number of processes considered, the "black-oil" and compositional models (Peaceman, 1977) provide a capability which is superior to that of DCM3D. Developed for use in the area of reservoir engineering, these codes are proprietary, and that constitutes a major impediment to their use in licensing. They include ECLIPSE (Exploration Consultants, Ltd.), VIP (J.S. Nolen and Associates, Inc.), THERM (SSI-Intercomp, Inc.), and TETRAD (DYAD 88 Software, Inc.). All of these codes consider multiple phases and components. In addition, THERM and TETRAD simulate nonisothermal processes.

12. Major Assumptions and Limitations

DCM3D assumes the following:

- Applicability of the concept of a dual continuum
- Richards' extension of Darcy's law to partially saturated media
- Spatial changes in water density are much smaller than temporal changes and are therefore neglected
- Water is slightly compressible
- Both fracture and porous medium are slightly elastic

DCM3D does not consider the following:

- Fully transient coupling between fracture and porous matrix continua
- Radionuclide transport processes, e.g., decay-production, dispersion, or sorption
- Heat induced processes
- Vaporization and condensation
- Gas-phase diffusive or convective transport.

13. Remarks/General Observations/Discussion

DCM3D conceptualizes the fractured porous media of Yucca Mountain as a dual-permeability model. In using a transfer function, the model assumes a pseudo-steady-state coupling of fracture and porous-media continua. This represents a generalization of the equivalent-porous medium assumption of Klavetter and Peters (1986), but falls short of fully transient coupling such as that used by SWIFT II (Reeves et al., 1986).

The adequacy of a pseudo-steady-state coupling depends on the response of Yucca Mountain to storm events. It also relates to fracture separations and fracture skins. In his analysis of interference tests, Moench (1984) concludes that both fully transient and pseudo-steady-state approaches are appropriate within the saturated zone at the Nevada Test Site. DCM3D does not consider either heat or gas-phase transport processes. Depending on results of future characterization studies, such processes may be important in determining radionuclide release to the accessible environment.

Potentially, the method of lines can be useful for licensing studies. Apparently this approach is quite competitive with standardly used techniques. For Problems 1 and 4 above, DCM3D is faster than TOUGH by factors of three to four, and, for Problem 1, DCM3D is faster than NORIA (Bixler, 1985) by several orders of magnitude. Standard techniques are basically sequential. It is possible that the method of lines lends itself more readily to parallelization. The M&O team should examine this issue in greater depth.

14. Comparison to Other Models

See Chapters 4, 5, and 6 of the main text.

15. Summary and Recommendations

- The NRC developed DCM3D for use in their Yucca-Mountain project.

- DCM3D is a detailed process code which is useful for site characterization, site suitability, and detailed design review. For some applications, it may be limited by excessive computer time.

- DCM3D permits either equilibrium or disequilibrium between fracture and matrix. However, it is appropriate only for a pseudo-steady state and may be physically incorrect for a highly transient storm event.

- Like other process codes, DCM3D is too detailed for probabilistic analysis of the total system and is limited by excessive computer time.

- DCM3D does not consider gas-flow, heat-transport, or radionuclide transport processes. Although the last deficiency is remedied by using a compatible receiving code such as NEFTRAN (Longsine et al., 1987), the first two will require substantial code modification.

- DCM3D uses the method of lines. LLUVIA-II also uses the method of lines. The M&O should evaluate this technique.

- Rather than DCM3D, however, it is recommended that the M&O obtain a reference copy of LLUVIA-II. As a more simple implementation, the latter should offer a better vehicle for testing the method of lines. It is thus recommended that DCM3D not be considered for either component or site-representative testing. However, depending on the nature of future interactions with NRC, it may be appropriate to reconsider the latter recommendation.

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A.2 FEHM

1. Name of the Model

FEHM

2. General Program Information

2.1 *Program size.* Approximately 10,000 lines of source code

2.2 *Programming language.* FORTRAN 77

2.3 *Computer system on which it operates.* FEHM (Zyvolosky et al., 1992) runs on Cray, Sun, VAX, and IBM PC. The Sun version is under quality-assurance (QA) control. An in-house processor performs the relatively minor changes necessary to adapt the source code to each computer.

2.4 *Compiler(s) used.* Standard compilers are used for each machine.

2.5 *Location of code and availability.* Only the QA Group EES-13 at LANL (Los Alamos National Laboratory) can release the quality-controlled FEHMN version. Uncontrolled versions of FEHM may be obtained from the author, G. Zyvoloski at LANL.

2.6 *Brief description of model/code history.* Using finite-element discretization, the original version of FEHM (Zyvoloski et al., 1988), was designed for geothermal applications. It simulated the nonisothermal, two-phase flow of a single component (water) in three dimensions. With the addition of a non-condensing gas component (air) to its flow module, FEHM (Zyvoloski et al., 1992) now simulates two-phase, non-isothermal flow problems which are of interest to the Yucca-Mountain Project. in two and three dimensions. It also simulates the transport of reactive tracers.

3. Status of Model

3.1 *Development (Is the model now undergoing significant development or modification? or continuing maintenance?).* As permitted by funding, LANL is adding facilities for radionuclide chains and for stress calculations.

3.2 *Documentation.* Zyvoloski et al. (1992) provide a model description and a user's manual. This document, which is thorough and easily followed, meets U.S. Nuclear Regulatory Commission (NRC) requirements as specified in NUREG-0856. A separate document (Zyvoloski and Dash, 1992) addresses the issues of verification and validation.

3.3 *Status of verification and validation.* At the present time, the verification of FEHM is limited to the two example problems contained in (Zyvoloski et al., 1992). However, LANL has completed a draft verification document (Zyvoloski and Dash, 1992). When released, it will include nine problems designed to activate the major processes simulated by the code. These problems focus on heat transport, single and multiphase flow, coupled flow and heat transport, and tracer transport.

Of the example problems presented by Zyvoloski et al. (1992), the results of two have been compared with those of other codes. Both assume the presence of a production well in a geothermal reservoir. Water vapor represents the dominant component of the gas phase, with the non-condensible gas component having only a negligible effect on reservoir behavior. One of the problems is the Toronyi example (Toronyi and Farouq Ali, 1977). This problem has been used in the code-verification effort reported by Molloy (1980), which included Thomas and Pierson (1978). For a simulation time corresponding, approximately, to removal of 19 percent of the original water mass, the results of FEHM compare reasonably well with those of Thomas and Pierson (1978).

The other geothermal problem is Problem 5, Case A of the DOE Code-Comparison Project. A moving two-phase region characterizes this problem, with the produced fluid replaced by cold-water recharge at the outer boundaries. Zyvoloski et al. (1992) compare the results of FEHM with those of six researchers (Molloy, 1980). For the temperature of the produced fluid and the downhole pressure of both the production well and an observation well, the results of FEHM show good agreement with those of the other codes.

3.4 *Status of Quality Assurance (QA).* LANL has placed its FEHMN version under QA control.

4. Type of Model (Phenomena/Processes Modeled)

FEHM (Zyvoloski et al., 1992) is a multi-dimensional (one-, two-, or three-dimensional) numerical model designed to simultaneously simulate nonisothermal liquid and gas flow and multi-component tracer transport. Features present in the code include:

- Fluid flow in both liquid and gas phases under pressure, viscous, and gravity forces according to Darcy's equation
- Capillarity between liquid and gas phases
- Dual-porosity treatment of fracture-matrix coupling
- Dual-permeability treatment of fracture-matrix coupling
- Transport of sorbing tracers by advection, dispersion, and diffusion in both liquid and gas phases.

5. Governing Equations

For partially saturated nonisothermal flow, the model solves three governing equations in as many as three dimensions. One equation effects mass conservation for the water component in both liquid and gas phases, while a second effects mass conservation for a non-condensible gas component in both phases. A third equation yields energy conservation within liquid and gas phases and within the rock. Additional equations establish mass conservation for an arbitrary number of tracer components in both phases. Limited only by computer time and space requirements, the maximum number of tracer components is currently set at ten.

6. Method of Solution

FEHM (Zyvoloski et al., 1992) uses finite-element spatial discretization for both flow and transport. Rather than Gauss quadrature, one may elect to use Lobatto integrations over the volume of each element. In contrast to Gauss quadrature, Lobatto integration does not introduce corner connections, thereby reducing the density of the coefficient matrix and decreasing execution time. For a rectangular grid, Lobatto gives a node-connection pattern which is identical to that of a finite-difference algorithm. The resulting equations employ fully implicit finite-difference discretization in the temporal domain, obtaining thereby a coupled set of nonlinear difference equations.

A Newton-Raphson technique linearizes the solution of these equations. Application of the Newton-Raphson method yields a set of linear equations with a non-symmetrix coefficient matrix (the Jacobian matrix). FEHM solves the linearized equations for liquid pressure, temperature, and gas saturation using the minimum-residual technique gmres (Saad and Schultz, 1986), a variant of the conjugate-gradient approach which is suitable for non-symmetric matrices. As a preconditioner, the incompletely factorized Jacobian matrix is applied to the full Jacobian matrix. This minimizes core-storage requirements, and, depending on the size of the problem, it may also minimize the CPU time.

For simulation of fractured systems, FEHM provides dual-porosity and dual-permeability algorithms. Though somewhat limited in its design, the transient fracture-matrix coupling provided by its dual-porosity algorithm provides a substantial upgrade to the conventional pseudo-steady approach.

7. Type of Input Parameters

Preprocessor GENMSH and a number of input macros provide the input for FEHM (Zyvoloski et al., 1992). In order to simplify geometric considerations, GENMSH and FEHM divide the solution space into a number of blocks. Blocks are then subdivided into elements, the smallest computational units. Although element types may vary from block to block, each block contains elements of the same type. Volumetric weight factors, specified for each direction, control element volumes, which may vary within a block. For two-dimensional problems, GENMSH and FEHM permit either quadrilaterals with four nodes or triangles with three nodes. For three-dimensional problems, GENMSH and FEHM permit either quadrilateral polyhedrons of eight nodes or triangular prisms of six nodes. GENMSH writes FEHM input files for the COOD and ZONE macros.

The following discussion characterizes each of the FEHM input macros:

CAP. Capillary pressure data. Assignment of capillary pressure curve to specified nodes or to a spatial block. Optional.

COOR. Node coordinate data. GENMSH output may be used. Required.

COND. Thermal conductivity data. Assignment of values to specified nodes or to a spatial block. GENMSH output may be used. Required.

CONT. Contour plot data. Optional.

CTRL. Program control parameters. Control nonlinear and linear-solution iterations, time stepping, and implicitness of solution. Optional.

DUAL. Input for dual-porosity solution. Includes only geometric data for rock matrix. Optional.

ELEM. Element node data. GENMSH does generates this data. Required.

EOS. Equation-of-state data. Includes parameters for vapor-pressure, density, and viscosity submodels and reference enthalpy data. Optional.

FLOW. Source-strength data for heat and water component. Optional.

HFLX. Heat-flux data. Optional.

INIT. Initial-value data. Specification of initial data may also require PRES macor. Optional.

ITER. Iteration parameters. Additional nonlinear and linear-solution controls (see CTRL). Optional.

NGAS. Non-condensible gas (air) data. Includes data for partial-pressure submodel and gas sources (sinks). Optional.

NODE. Node numbers for output and time histories. Required.

PERM. Absolute-permeability data. Required.

PPOR. Data for variable porosity and permeability submodels. Optional.

PRES. Initial data for nonuniform pressure and enthalpy distributions.

RLP. Relative permeability data. Assignment of relative-permeability curves to specified nodes or spatial block. Optional.

ROCK. Absolute rock-density, specific-heat, and porosity data. Required.

SOL. Solution specifications. Identifies flow and heat-transport equations to be solved. Specifies Labatto or Gauss quadrature for element integrations. Required.

STEA. Steady-state solution generated as initial condition. Optional.

STOP. Signals end of input. Required.

TEXT. Text input. Optional.

TIME. Time-stepping data (also see CTRL) for both simulation and output. Required.

TRAC. Tracer data. Includes initial data, implicitness, and linear-solution controls. Optional.

ZONE. Geometric definition of grid. GENMSH output may be used here. Optional.

8. Type of Output and User Options

In addition to hard copy, FEHM (Zyvoloski et al., 1992) provides graphical output. The documentation for FEHM describes two graphics routines. Technically both use the DISSPLA graphics package. However, since only primitive line-drawing commands are utilized, they are easily convertible to other systems. For each of the nodes specified through input macro CTRL, postprocessor FEHPLTR plots time histories of temperature, pressure, enthalpy, flow rate, concentration, and capillary pressure. For each of the output distributions specified through input macro CONT, postprocessor FECPLTR constructs contour plots.

9. Model Interactions (emphasize needed processors)

9.1 *Does the model interface with any other models?* See Section 9.4 below.

9.2 *Source code and type of information needed.* Not applicable.

9.3 *Receiving code and type of information provided.* Not applicable.

9.4 *Any pre- or postprocessing needed?* FEHM (Zyvoloski et al., 1992) uses preprocessor GENMSH and graphical postprocessors FEHPLTR and FECPLTR, as discussed above.

10. Model Application

10.1 *Usage within the Civilian Radioactive Waste Management Systems (CRWMS) program.* If an equivalent continuum is assumed, FEHM (Zyvoloski et al., 1992) can be used to characterize the coupled nonisothermal flow and transport processes within the partially saturated zone. Potentially, FEHM could also be used to characterize the transport of gases although it is somewhat limited by its exclusion of decay processes.

For highly transient episodes, such as storm events, where the equivalent-continuum approximation is inappropriate, FEHM's dual-porosity algorithm is too restricted. For such periods, FEHM offers only a direct gridding approach, the poor efficiency of which makes it practical only for relatively small systems containing few fractures. Given that this deficiency is quite common, one may still note that, for the Yucca-Mountain unsaturated zone, FEHM is just as applicable to highly transient episodes as other detailed process models within the Yucca-Mountain Project.

FEHM may also be used for simulating saturated flow processes. This capability has been used to design tracer tests for the C-well project.

10.2 *Usage outside the program.* Originally, FEHM (Zyvoloski et al., 1992) was developed for use as a geothermal simulator. It may still be used in that capacity. It might also have application for near-surface disposal of low-level radioactive and hazardous wastes.

11. Codes With Similar or Same Capabilities

11.1 *Within the program.* The Yucca-Mountain Project has funded the development of several codes with multiphase flow capabilities similar to those of FEHM. These codes include TOUGH2 (Pruess, 1991) at LBL (Lawrence Berkeley Laboratory), V-TOUGH (Nitao, 1989) at LLNL (Lawrence Livermore National Laboratory), NORIA (Bixler, 1985) at SNL (Sandia National Laboratory), MSTS at PNL (Pacific Northwest Laboratory), and TRACR3D (Birdsell and Travis, 1991) at LANL. Like FEHM (Zyvoloski et al., 1992), three of these codes (TOUGH2, V-TOUGH, and MSTS) also consider nonisothermal processes.

The codes differ in terms of conceptualization options, i.e., dimensionality (two or three dimensions) and fracture characterization (equivalent continuum, dual porosity, dual permeability, or discrete fractures). They also differ in terms of numerical solution, i.e., spatial-discretization (finite difference or finite element) and linear-equations solver (direct solution, successive over-relaxation, method of lines, or gmres).

The Yucca-Mountain Project has funded the development of several codes with transport capabilities, some of which are superior to those of FEHM. With radionuclide chaining and a detailed chemical reaction model, TRACR3D at LANL provides a notable example of the latter. Other transport codes include stand-alone transport codes like FEMTRAN (Martinez, 1985) and LLUVIA-S at SNL. They also include total-system codes with imbedded transport routines, like SUMO (Eslinger et al., 1990) at PNL and TOSPAC (Dudley, et al., 1988) at SNL. In terms of conceptualization options and numerical solution, the codes differ in the same respects as the flow codes, with two important exceptions. In contrast to multiphase flow, the effects of non-linearity tend to be much less severe for transport, with transport and chemical-process parameters evidencing either independence or only a weak dependence on concentration.

If it were not for the second item, advection, this weak non-linearity would make the numerical simulation of transport much more efficient than the numerical simulation of flow. However, advection can be a much more dominant process for transport than for multiphase flow, and this tends to degrade computer efficiency.

11.2 *Outside the program.* In their Yucca-Mountain project, the NRC has funded the documentation of TOUGH (Pruess, 1987) and the development of DCM3D (Updegraff et al., 1991). The former has a general capability for treating multiphase flow while the capability of the latter is limited to that of a dual-permeability implementation of the Richards equation.

Further, a number of codes have been developed within the petroleum industry. In terms of the multiphase-flow processes considered, both black-oil and compositional models (Peaceman, 1977) provide a capability superior to FEHM (Zyvoloski et al., 1992). Developed for use in the area of reservoir engineering, these codes are proprietary, and that constitutes a major impediment to their use in licensing. Compositional models include THERM (SSI-Intercomp, Inc.) and TETRAD (DYAD 88 Software, Inc.). These codes consider more than two phases and two components, and they are nonisothermal.

Other federally funded projects have developed transport codes to characterize the movement of radionuclide chains. SWIFT II (Reeves et al., 1986), a saturated flow and transport code provides one example. The NRC developed this code for their salt-repository project.

12. Major Assumptions and Limitations

- A steady-state option is not available. For large problems, running through a transient sequence to achieve steady state represents a costly and needless expenditure of computer time. Since most transient characterization runs assume steady-state initial conditions, this is a significant consideration. Further development may be required.

- The dual-permeability treatment of FEHM (Zyvoloski et al., 1992) does not consider the transient fracture-matrix flow occurring during and after a rain-storm event.

- The dual-porosity treatment of FEHM permits only two nodes in a direction perpendicular to the fracture. This is not sufficient for characterizing the transient fracture-matrix flow and transport processes occurring during and after a rain-storm event. Transient matrix flow is particularly significant for nonwelded units, where it, most likely, removes most of the infiltration water from the fractures before it reaches the repository.

- An ideal gas is assumed. Uncertainties due to non-ideal behavior should be acceptable.

- The liquid is assumed to be compressible under saturated conditions, but incompressible under unsaturated conditions. This is an acceptable assumption requiring no additional development.

- FEHM assumes tracer concentrations to be small and thus includes only ordinary diffusion dependent on the concentration gradient. This is a standard assumption requiring no additional development. Bird et al. (1966, pp. 563 ff.) provide a general discussion of multicomponent diffusion.

- FEHM does not consider radionuclide decay and production processes.

- The dispersion tensor is assumed to be dependent on fluid velocity only. Although the literature has questioned this assumption, no acceptable alternative has yet been offered. Thus, no additional development is required at this time.

13. Remarks/General Observations/Discussion

In terms of the basic physics of its flow code, FEHM (Zyvoloski et al., 1992) is similar to TOUGH2 (Pruess, 1991) although the latter is more widely accepted. Since it permits an arbitrary number of nodes within the matrix, the TOUGH2 (Pruess, 1991) treatment of matrix flow by its MINC facility is more general than that of FEHM, which permits only two nodes within the matrix. However, in terms of its numerical efficiency, TOUGH2 would profit by implementing a static-condensation solution procedure like that of FEHM, suitably generalized to more than two nodes within the matrix. SWIFT II (Reeves et al., 1986) employs a generalized version of the static condensation procedure. In addition, TOUGH2 efficiency will benefit from the currently ongoing effort to install a gmres solver like that used by FEHM.

Although the models have similar transport capabilities, TRACR3D is superior to FEHM. TRACR3D offers radioactive decay and production processes, while FEHM offers only decaying tracers. TRACR3D also offers a more extensive menu of possible reactions between dissolved constituents and mineral substrates. In addition, TRACR3D offers a facility for high Peclet-number transport which is not currently included in FEHM.

Another significant point about FEHM consists in noting that it is a finite-element code using a gmres solver. The rather arbitrary node-to-node connection pattern (connection molecule) of a finite-element model severely restricts the choice of direct solvers to a banded or frontal solution technique. Consequently, finite-element codes employing only a direct solver generally are significantly less efficient than a comparable finite-difference code, which requires a standard connection molecule. However, the use of a gmres solver should even the gap between finite-element and finite-difference codes for the large problems to be encountered at Yucca Mountain. Such a possibility is significant for geometrically complex systems.

14. Comparison to Other Models

See Chapters 4, 5, and 6 of the main text.

15. Summary and Recommendations

- FEHM is a two-phase, detailed-process code. Its flow code is appropriate for non-stochastic applications, which may be either isothermal or nonisothermal.

- FEHM is the only three-dimensional, finite-element code in the Yucca-Mountain Project. Although the integrated finite-difference approach of TOUGH, also provides a general geometric capability, a finite-element model is the more common choice for geometric flexibility. Furthermore, if an alternative solution approach is necessary, then FEHM is a likely candidate.

- FEHM is one of the two operational codes within the project which currently use a gmres solver. TRACR3D, another LANL code, shares this distinction. For preconditioning, both use incomplete factorization. Gmres solvers, perhaps with alternative preconditioning options, and massive parallelization, may help alleviate the excessive demand for computer resources which now severely limits the application of detail-process codes.

- In consideration of the above, it is recommended that FEHM be included in the component-testing task.

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A.3 FEMTRAN

1. Name of the Model

FEMTRAN

2. General Program Information

2.1 *Program size.* FEMTRAN (Martinez, 1985) contains approximately 3,000 source statements.

2.2 *Programming language.* FORTRAN 77

2.3 *Computer system on which it operates.* VAX and Cray.

2.4 *Compiler(s) used.* Standard compilers.

2.5 *Location of code and availability.* A copy of FEMTRAN resides in a permanent-file library at Sandia National Laboratories (SNL).

2.6 *Brief description of model/code history.* Duguid and Reeves (1976) developed the original version of FEMTRAN under DOE (U.S. Department of Energy) funding. At that time the code was used, in conjunction with the flow code reported by Reeves and Duguid (1975), to analyze partially saturated flow and transport problems for the low-level waste-burial grounds at Oak Ridge, TN. Yeh and Ward (1980) revised the original flow code in order to obtain a continuous velocity field. They named the flow code "FEMWATER" and the transport code "FEMWASTE". Martinez (1985), using DOE funding from the Yucca-Mountain Project, upgraded FEMWASTE. He added a capability for solving radionuclide chains and named the new version "FEMTRAN".

3. Status of Model

3.1 *Development (Is the model now undergoing significant development or modification? or continuing maintenance?).* No.

3.2 *Documentation.* Martinez (1985) provides a readable discussion of governing equations and data input. The model has changed insignificantly since 1985.

3.3 *Status of verification and validation.* At the present time, the verification of FEMTRAN consists of three different items.

Sample Problems. In addition to illustrating the application of FEMTRAN, their intended use, the three sample problems of Martinez (1985) also serve as code verifications. Each of these problems considers the transport of a three-member chain. Problem 1, a one-dimensional implementation, assumes equal retention factors, an assumption which simplifies the corresponding analytic solution. The result of the FEMTRAN calculation compares quite favorably with analytic results in spite of a rather poor mass balance near the radionuclide source. This circumstance may be understood by recognizing that bilinear basis functions do <u>not</u> conserve mass, a fact that may be proved theoretically. Nevertheless, the minimization of residuals, inherent in the Galerkin weighted-residuals method, generally yields accurate results at nodal points.

Problems 2 and 3 are taken from the INTRACOIN Level-1 Study (SKI, 1984). These problems are quite similar, with dimensionality being the primary difference. Problem 2 is one dimensional, and Problem 3 is two dimensional. Both assume unequal retention factors. Although many similar codes have executed these two problems, Martinez (1985) compared FEMTRAN results for Problem 2 only with the results of RANCH (Haderman and Patry, 1981). Again, the results compare nicely in spite of a poor mass balance near the radionuclide source. Martinez (1985) compares the results of Problem 3 only with the results of Problem 2 to show the effect of transverse dispersion.

Cove-1 Benchmark Calculations. COVE-1 exercises focused on a two-dimensional isothermal water-drainage and contaminant-transport problem for variably saturated porous media (Hayden, 1985 and Eaton and Martinez, 1986). Six flow-transport code combinations participated, including FEMTRAN, which was coupled with the single-phase flow code SAGUARO (Eaton et al., 1983).

In COVE 1N, material properties and boundary conditions were consistent with those of Pickens et al. (1979), who assume a system consisting of a medium-grained sand. In COVE 1YMa and 1YMb, material properties were representative of a nonwelded tuff, and boundary conditions were varied. All three problems used the same geometric configuration. In order to add transport to the problem definition of Pickens et al. (1979), a non-decaying contaminant was assumed to be initially distributed within the upper 0.1 m.

Using the flow field generated by SAGUARO, FEMTRAN successfully completed the three COVE-1 problems and provided transport results which were similar to those of other participants. The discussion of Hayden (1985, pp. 4-15 ff.), is quite interesting. It focuses on discrepancies between the results of FEMTRAN and the results of LANL's finite-difference code TRACR3D (Birdsell and Travis, 1991). Hayden (1985) attributes the discrepancies to two factors. Except for the portion of the boundary adjacent to a tile drain, the right-hand boundary of the system is specified by a no-flow condition. The bilinear basis functions used by SAGUARO and by FEMTRAN cannot reproduce this condition exactly, and this results in a small, but spurious, flow of contaminants from the system. In addition, the FEMTRAN analysis uses approximately one-third as many time steps as the TRACR3D analysis. Since both analyses use backward-in-time differencing, it is assumed that enhanced levels of numerical dispersion also caused the FEMTRAN results to deviate from those of TRACR3D.

PACE-90 Radionuclide Transport Problem. Given a common data base and a common hydrogeologic characterization of the Yucca-Mountain Site, participants in the PACE-90 study determined the movement of radionuclides to the accessible environment assuming an undisturbed, isothermal flow field. This exercise verified the ability of different researchers to independently conceptualize a complex site in a physically consistent manner. Nevertheless, computed results largely agreed, thus providing verification of code executions. To simulate flow, participants chose FEMTRAN and NORIA and five other codes, or code combinations.

The FEMTRAN-NORIA analysis considers a two-dimensional cross-section lying between drill holes G-4 and UE-25a. With a total of 1,260 quadrilateral elements, the NORIA analysis divides this cross-section into nine hydrogeologic units extending from the water table to the top of the Tpt-TM section of the Topapah Spring unit. With the bottom boundary held at a pore pressure of zero to characterize the water table, the two sides are assumed to be no-flow boundaries. For the top boundary, a net infiltration of 0.01 mm/y is prescribed.

Using Darcy velocities and an average moisture-content value taken from NORIA results and a source strength generated by the AREST code (Apted, 1989), the FEMTRAN analysis focuses on a small section of the total cross-section considered by the NORIA analysis. Containing both wells, it extends vertically downward from the repository horizon and measures 100 m in thickness. It is divided into 552 elements. The FEMTRAN analysis indicates that the peak concentration travels only 20 m below the repository and that the farthest extremity of the plume travels less than 50 m in 100,000 years. As a check, FEMTRAN is also used in a one-dimensional vertical analysis. As expected, one- and two-dimensional results agree nicely except near the sides of the repository.

3.4 *Status of Quality Assurance.* FEMTRAN is *not* under QA control.

4. Type of Model (Phenomena/Processes Modeled)

FEMTRAN is a two-dimensional, finite-element model for simulating radionuclide transport in a saturated or unsaturated porous medium. Processes considered include the following:

- Advection
- Dispersion and diffusion
- Linear sorption
- Radioactive decay and production.

5. Governing Equations

FEMTRAN solves the coupled mass-conservation equations for a chain of radionuclides. Only two spatial dimensions are permitted, and branching is not allowed.

6. Method of Solution

To spatially discretize the transport equations, FEMTRAN uses the Galerkin finite-element method with bilinear basis functions. The Galerkin approach requires that weighting and basis functions be identical. Unlike SAGUARO (Eaton et al., 1983) and NORIA (Bixler, 1985), which allow subparametric mappings from global to local coordinate systems, FEMTRAN permits only isoparametric mappings. Like the basis function, the mapping function is also bilinear. The code employs the upstream-weighting formulation of Huyakorn and Nilkuha (1979).

To temporally discretize the transport equations, FEMTRAN input allows the analyst to specify a weighting factor ω, denoting differing degrees of implicitness in the solution algorithm. A value $\omega=½$ corresponds to centered (Crank-Nicholson) differencing, while a value $\omega=1$ corresponds to backward differencing. FEMTRAN input also allows the analyst to select mass lumping. Rather than to prescribe off-diagonal accumulation terms, a mass-lumping procedure adds them to the diagonal term.

7. Type of Input Parameters

Data input required for the execution of FEMTRAN may be divided into the 15 data sets listed below:

Data Set 1: Problem Identification. Contains problem number and problem title.

Data Set 2: Control Parameters. Contains control parameters for defining the problem including mesh input control, boundary control, time increments, and number of materials.

Data Set 3: Conversion Factors. Provides for conversion of the hydrodynamic solution when computed by SAGUARO (Eaton et al., 1983). Optional.

Data Set 4: Time Integration Parameters. Contains parameters for controlling the time step sequence. Includes specification of leach times under transient boundary conditions.

Data Set 5: Printed Output Control. Specifies the time planes at which printed output is desired.

Data Set 6: Auxiliary Storage and Flow Field Control. Allows for control of the amount of flow field print output and the timeplanes for which species concentration solutions are stored.

Data Set 7: Material Properties. Data set specifies material properties for the number of materials present. Data includes bulk density, dispersivities, porosity, etc.

Data Set 8: Species and Material Dependent Properties. Contains data on properties which depend both on species and material type. Includes such properties as decay constants and distribution coefficients.

Data Set 9: Nodal Point Coordinates. Optional.

Data Set 10: Element Connectivities. Optional.

Data Set 11: Material Corrections. Used if material changes are made. Optional.

Data Set 12: Initial Conditions. Initial conditions are specified for all members of the decay chain being analyzed.

Data Set 13: Dirichlet Boundary Conditions. Optional.

Data Set 14: Neumann Boundary Conditions. Default boundary condition, need not be specified explicitly.

Data Set 15: Cauchy Boundary Condition. Optional.

Input requirements needed for mesh specifications and hydrodynamic variables may either be provided by the user or obtained from other sources. FEMTRAN contains the same mesh generation subroutine found in FEMWATER (Yeh and Ward, 1980) to facilitate mesh specification. Mesh data can also be provided from a disk file after construction by the mesh generator codes QMESH or DECODE (Martinez and Bixler, 1984). Hydrodynamic variables may be specified through a user-supplied subroutine, or they may be computed using one of the following codes: FEMWATER (Yeh and Ward, 1980), MARIAH (Gartling and Hickox, 1982), or SAGUARO (Eaton et al., 1983).

8. Type of Output and User Options

In addition to an echo of input data, FEMTRAN allows the user to choose the time planes at which computed data are desired. Output at the specified times may include mass-balance data, concentrations, and material fluxes. Additionally, the user may control the amount and type of flow-field output obtained. Flow-field output may include mass balances, Darcy velocities, moisture contents, and the hydraulic heads.

9. Model Interactions (emphasize needed processors)

9.1 *Does the model interface with any other models?* Yes, see below.

9.2 *Source code and type of information needed.* FEMTRAN assumes a prior calculation of the flow field. The COVE-1 exercises demonstrate the coupling procedure. Here SAGUARO (Eaton et al., 1983) computed transient Darcy-velocity and moisture-content fields, which were transferred to FEMTRAN. Other flow codes such as NORIA (Bixler, 1985), MARIAH (Gartling and Hickox, 1982), and FEMWATER (Yeh and Ward, 1980) may be used as well, providing that a reformatting facility is provided. DECODE (Martinez and Bixler, 1984) and MERLIN (Gartling, 1981) provide examples of such a facility.

9.3 *Receiving code and type of information provided.* Not applicable.

9.4 *Any pre- or postprocessing needed?* Plotting packages provide time histories of radionuclide transport. For the PACE-90 calculations, the output was reformatted for the BLOT graphics package.

10. Model Application

10.1 *Usage within the CRWMS program.* FEMTRAN provides a stand-alone transport capability for those, principally SNL, flow codes (MARIAH, SAGUARO, and NORIA) which do not have a built-in transport capability. It may be used for both near- and far-field applications.

10.2 *Usage outside the program.* Potentially, FEMTRAN could be used in a variety of waste-management areas, including hazardous waste and low-level nuclear waste. However, the availability of many other codes with similar or enhanced capabilities may limit its use.

11. Codes With Similar or Same Capabilities

11.1 *Within the program.* The Yucca Mountain Project has funded the development of several transport capabilities. In some cases, these capabilities are implemented within modules of a general flow and transport simulator. TRACR3D (Birdsell and Travis, 1991) and FEHM (Zyvoloski et al., 1992) at LANL (Los Alamos National Laboratory), MSTS, SUM0, and PORFLO-3 (Sagar and Runchal, 1989) at PNL (Pacific Northwest Laboratory), TOSPAC (Dudley et al., 1988) and SPARTAN (Sinnock and Lin, 1989) at SNL, VS2DT (Lappala et al., 1987 and Healy, 1990) at USGS (U.S. Geological Survey) have transport modules. In other cases, a transport capability is implemented in a separate stand-alone code. SNL's LLUVIA-S, a version of the Dykhuizen (1987) fractured media transport simulator, and FEMTRAN are stand-alone transport simulators.

11.2 *Outside the program.* The Nuclear Regulatory Commission has funded the development of DCM3D (Updegraff et al., 1991) with its Yucca-Mountain project. Other government funded efforts have yielded codes with capabilities similar to those of FEMTRAN. SWIFT (Reeves et al., 1984) and NEFTRAN (Longsine et al., 1987) provide examples of such efforts.

12. Major Assumptions and Limitations

- A dual-continuum option is not available. Without substantial modification, fracture-matrix disequilibrium cannot be accounted for in field-scale simulations.

- A high-order differencing option is not available for the advection term. Without substantial code modification, code applications will require a highly refined spatial mesh.

- An iterative solution option is not available. This limits rather severely the size of the problem the code can consider.

- A stand-alone flow calculation is required. The amount of data transfer and the required synchronization of time steps makes this a cumbersome procedure.

- Only liquid-phase transport components may be considered. Vapor flow is not allowed.

- Only two spatial dimensions are considered. This will be sufficient for many applications. However, some applications will undoubtedly require three dimensions.

13. Remarks/General Observations/Discussion

Relative to the ORNL versions which preceded it, FEMTRAN contains a few organizational changes. For example, a facility for obtaining a continuous flow field was first implemented in the flow code by Yeh and Ward (1980). Martinez (1985) made this facility available as an option for the transport code. He also generalized the mass-balance calculations. The major modification in FEMTRAN appears to be that of chain decay and production. (The ORNL versions do not consider radioactive production.) Unfortunately, however, many of the limitations present in the earlier versions still appear in FEMTRAN.

To date, all FEMTRAN applications to Yucca Mountain have assumed an undisturbed repository, a steady-state isothermal flow field, and negligible fracture flow. If the isothermal condition is removed with transients limited to the relatively long-term behavior inherent in the heat source, then liquid-flow vectors will, most likely, point inward. In this case, there may be little or no transport from the repository for 10,000 years. If a transport code is necessary for analyzing the nonisothermal problem for a steady-state recharge, FEMTRAN should be appropriate. If transients due to large storm events are permitted, then fracture flow will likely occur, and FEMTRAN will <u>not</u> be appropriate. If, further, the effects of climate change, volcanism, or seismic events are considered, then FEMTRAN's limitation to relatively small systems dominated by porous-media flow will prove disabling for many, perhaps most, applications.

14. Comparison to Other Models

See Chapters 4, 5, and 6 of the main text.

15. Summary and Recommendations

Section 12 lists the limitations of FEMTRAN, and Section 13 suggests the areas in which they may affect future licensing calculations. Since other codes within the project have overcome many of these limitations, it is recommended that FEMTRAN <u>not</u> be considered further.

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A.4 FEMWASTE

1. Name of the Model

FEMWASTE

2. General Program Information

2.1 *Program size.* FEMWASTE (Yeh and Ward, 1981) contains approximately 2,000 source statements.

2.2 *Programming language.* FORTRAN 77

2.3 *Computer system on which it operates.* Duguid and Reeves (1976) ran the model on IBM-360 computers at ORNL (Oak Ridge National Laboratory). Since that time, it has been used on other machines, as well, including VAX, CDC, and personal computers.

2.4 *Compiler(s) used.* Standard compilers.

2.5 *Location of code and availability.* The model may be obtained from the Environmental Sciences Division at ORNL.

2.6 *Brief description of model/code history.* A variety of modeling problems in the early 1970s led to the development of the original model. These problems related to the Oak Ridge burial grounds for radioactive wastes, to the International Biological Program, and to several projects funded by the EPA (U.S. Environmental Protection Agency). Since that time, the model has been enhanced using funding both from the NRC (U.S. Nuclear Regulatory Commission) and the DOE (U.S. Department of Energy).

3. Status of Model

3.1 *Development (Is the model now undergoing significant development or modification? or continuing maintenance?).* Since 1981, the model has been enhanced in several ways. Point Gauss-Seidel and conjugate-gradient solvers have been added, and a high-order treatment of the convection term has been implemented. A mass-balance algorithm has been written. In addition, algorithms for nonlinear sorption and ion-exchange have been added, and the model has been expanded to three dimensions.

3.2 *Documentation.* Yeh and Ward (1981) update the original documentation of Reeves and Duguid (1976). These two documents provide a comprehensive and readable description of the model, including both theory and data input.

3.3 *Status of verification and validation.*

Lapidus and Amundson's (1952) Equilibrium Case (Duguid and Reeves, 1976): Water moves at a constant velocity through a one-dimensional ion-exchange column. With an initial concentration of zero, the boundary concentration is fixed at a constant value. For the same values of retardation, interstitial velocity, and dispersion, the numerical results of Duguid and Reeves agree nicely with the analytic results of Lapidus and Amundson.

Seepage Pond [Duguid and Reeves (1976), Yeh and Ward (1980), Yeh and Ward (1981) and Yeh (1987)]: Water from a seepage pond moves through a highly permeable sand to a sloping seepage face and a stream. Infiltration due to rainfall is small in comparison to seepage from the pond and is neglected. Assuming a concentration of unity in the pond, the problem calls for concentration contours at 20 years. To approximate the dependence of sorption on the exposed surface area, Reeves and Duguid assume that sorption is proportional to water content. Yeh and Ward assume that sorption is independent of water content. Results are quite similar to those of Reeves and Duguid, except near the seepage face. There, the change in the sorption model plus the improved calculations of Darcy-velocity and mass flux give concentration contours which are more physically reasonable than those of Duguid and Reeves. All calculations use a grid consisting of 595 nodes and 528 elements.

3.4 *Status of Quality Assurance (QA).* The EPA (U.S. Environmental Protection Agency) has brought FEMWASTE under QA control.

4. Type of Model (Phenomena/Processes Modeled)

FEMWASTE simulates radionuclide transport in either a two-dimensional (x-y) plane or a two-dimensional vertical (x-z) cross-section. As indicated by its name, the code uses the finite-element method. a variably saturated porous medium. Processes considered include the following:

- Advection
- Dispersion and diffusion
- Sorption and ion exchange
- Radioactive decay.

5. Governing Equations

FEMWASTE solves the advective-dispersion equation for a decaying radionuclide.

6. Method of Solution

Yeh and Ward (1981) made two major changes to the code of Duguid and Reeves (1976). After solving for the concentration at a given time step, Duguid and Reeves differentiate this variable to obtain mass-flux components. This procedure can lead to non-conservation of mass at element interfaces. To avoid the problem, Yeh and Ward apply the Galerkin approach and then use an implicit solution procedure like that used to obtain concentration values. The procedure is identical to that used to obtain Darcy velocities. Generally, the computer time will increase by a factor less than three for a two-dimensional problem (Yeh, 1981). This is of little consequence, however, since the solution of the flow equation is, by far, the time-limiting factor.

Following the work of Huyakorn and Nilkuha (1979), Yeh and Ward introduce an upstream-weighting option into the code. For advection-dominated transport, this option allows the analyst to stabilize the solution algorithm with numerical dispersion. However, the analyst must exercise caution since the solution so obtained may be physically unrealistic.

Yeh and Ward also made three relatively minor changes to the code of Duguid and Reeves. The latter authors take the distribution coefficient k_d to be linearly dependent on moisture content. An unsaturated soil, it is assumed, will incompletely expose its sorbing surfaces. This is consistent with the sorption mechanism identified by a soil chromatograph (Reeves, Francis, and Duguid, 1977). Citing several references, Yeh and Ward argue that, in general, k_d depends on moisture content in a complicated manner but that, to first order, one should assume k_d is independent of water content. They change the code accordingly. Consistent with changes introduced in FEMWATER, Yeh and Ward also introduce mass lumping and mid-difference weighting into the time-integration algorithm.

7. Type of Input Parameters

Generally speaking, integer and real parameters appear on separate records with formats of 16I5 and 8F10.0, respectively. Control and temporal gridding parameters come first, followed by material properties. Then, depending on the option selected by the analyst, spatial gridding information may be either input or read from a file prepared by a prior execution of FEMWATER. If the former option is chosen, then some rudimentary facilities for automatic mesh generation are available. Typically, mesh generation is a non-trivial exercise for a finite-element model.

Mesh dependent quantities follow. Initial conditions are prescribed. Then, as the final items of the data set, come the specification of sources and sinks and the specification of possibly three different types of boundary conditions. Dirichlet conditions (constant concentrations) may be prescribed at either interior or exterior nodes. Neumann conditions (constant fluxes) may be prescribed on exterior element sides. Cauchy conditions (convective transfer through boundary) may also be prescribed on exterior element sides.

8. Type of Output and User Options

FEMWASTE output includes an echo of all input data, initial conditions, and boundary conditions. Concentration, mass-flux, and Darcy-velocity tables are output at times specified by the input. This output includes time increment, time-step number, and elapsed simulation time. In addition to hard copy, plot files may be prepared during execution.

9. **Model Interactions (emphasize needed processors)**

9.1 *Does the model interface with any other models?* Yes, see below.

9.2 *Source code and type of information needed.* FEMWASTE assumes a prior calculation of the flow field. FEMWATER writes Darcy velocities on a file, which, FEMWASTE reads during the course of the mass-transport calculation.

9.3 *Receiving code and type of information provided.* Not applicable.

9.4 *Any pre- or postprocessing needed?* A plotting package provides time histories and contour plots.

10. **Model Application**

10.1 *Usage within the Civilian Radioactive Waste Management System (CRWMS) program.* FEMWASTE provides a stand-alone transport capability for FEMWATER. It may be used for both near- and far-field applications.

10.2 *Usage outside the program.* FEMWASTE has been used in a variety of waste-management areas, including hazardous waste and low-level nuclear waste. However, the availability of many other codes with similar or enhanced capabilities limit its usefulness.

11. **Codes With Similar or Same Capabilities**

11.1 *Within the program.* The Yucca Mountain Project has funded the development of several transport capabilities. In many cases, these capabilities are implemented within modules of a general flow and transport simulator. TRACR3D (Birdsell and Travis, 1991) and FEHM (Zyvoloski et al., 1992) at LANL (Los Alamos National Laboratory), MSTS and SUMO at PNL (Pacific Northwest Laboratory), TOSPAC (Dudley et al., 1988) and SPARTAN (Sinnock and Lin, 1989) at SNL, VS2DT (Lappala et al., 1987 and Healy, 1990) at USGS (U.S. Geological Survey) and PORFLOW (Runchal and Sagar, 1991) have transport modules. In other cases, a transport capability is implemented in a separate stand-alone code. SNL's LLUVIA-S, a version of the Dykhuizen (1987) fractured media transport simulator, and FEMTRAN are stand-alone transport simulators.

11.2 *Outside the program.* The NRC has funded the development of DCM3D (Updegraff et al., 1991) with its Yucca-Mountain project. Other government funded efforts have yielded codes with capabilities similar to or exceeding those of FEMWASTE. SWIFT (Reeves et al., 1986) provides an example of such an effort.

12. **Major Assumptions and Limitations**

- A dual-continuum option is not available. Without substantial modification, fracture-matrix disequilibrium cannot be accounted for in field-scale simulations.

- Radioactive chaining is not considered.
- A stand-alone flow calculation is required. The amount of data transfer and the required synchronization of time steps makes this a cumbersome procedure.
- Only liquid-phase transport components may be considered. Vapor flow is not allowed.
- Only two spatial dimensions are considered. This will be sufficient for many applications. However, some applications will undoubtedly require three dimensions.

13. Remarks/General Observations/Discussion

Although the precursor to FEMWASTE (Duguid and Reeves, 1976) was one of the first of its kind, FEMWASTE's general performance capabilities are now duplicated by many other codes, as indicated in Section 11. Most have built-in transport modules, which are more convenient to use than stand-alone transport modules like FEMWASTE, and some have capabilities which are more advanced than those of FEMWASTE.

Nevertheless, the current evolution of FEMWASTE, now called HYDROGEOCHEM, should be followed by the M&O. The expanded capabilities for convection-dominated transport and for sorption and ion exchange may rival those offered by TRACR3D (Birdsell and Travis, 1991), which are the most advanced such capabilities in the Yucca-Mountain project.

14. Comparison to Other Models

(See Chapters 4, 5 and 6 of the main text.)

15. Summary and Recommendations

Section 12 lists the limitations of FEMWASTE. Since several transport modules of other codes within the project overcome many of these limitations, it is recommended that FEMWASTE <u>not</u> be considered further.

16. References

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A.5 FEMWATER

1. Name of the Model

FEMWATER

2. General Program Information

2.1 *Program size.* FEMWATER (Yeh, 1987) contains approximately 4,500 source statements.

2.2 *Programming language.* FORTRAN 77

2.3 *Computer system on which it operates.* Reeves and Duguid (1975) developed and ran the original version of FEMWATER on IBM-360 computers at ORNL (Oak Ridge National Laboratory). Since that time, the code has been used on other machines, as well, including VAX, CDC, and personal computers.

2.4 *Compiler(s) used.* Standard compilers.

2.5 *Location of code and availability.* The code may be obtained from the Environmental Sciences Division at ORNL.

2.6 *Brief description of model/code history.* A variety of modeling problems in the early 1970s led to the development of the original model by Reeves and Duguid (1975). These problems related to the Oak Ridge burial grounds for radioactive wastes, to the International Biological Program, and to several projects funded by the EPA (U.S. Environmental Protection Agency). Since that time, the model has been enhanced using funding from a variety of sources, including the NRC (U.S. Nuclear Regulatory Commission) and DOE (U.S. Department of Energy). Two documents (Yeh and Ward, 1980) and Yeh (1987) discuss the more recent versions of the model.

3. Status of Model

3.1 *Development (Is the model now undergoing significant development or modification? or continuing maintenance?).* Since 1987, the model has been expanded to three dimensions, and another iterative-solver option has been added. The latter is based on the preconditioned conjugate-gradient method.

3.2 *Documentation.* Yeh and Ward (1980) and Yeh (1987) update the original documentation of Reeves and Duguid (1975). These three documents provide a comprehensive and readable description of the model, including both theory and data input.

3.3 *Status of verification and validation.* Several different documents report problems which have been solved with FEMWATER. These problems illustrate the use of the code. Furthermore, since many of them have been run with other codes, these problems also verify FEMWATER.

Coweeta Inclined Soil Column (Reeves and Duguid, 1975): Investigators of The Coweeta Hydrologic Laboratory in North Carolina have made extensive use of inclined physical soil models. This problem focuses on one of their studies. An inclined concrete trough is filled, for the most part, with Halewood sandy loam. Under the outflow level, the soil is graded to sand, gravel , and rock to simulate stream bank conditions. After soaking the upper surface for several days, the structure was covered with plastic to prevent evaporation. A physically reasonable estimate of the unsaturated hydraulic-conductivity curve yielded simulated outflow rates which, for the simulated 10-day period, matched the measured values to a reasonable degree of approximation. The spatial mesh for this two-dimensional problem consisted of 612 elements and 690 nodes.

Freeze's Idealized Flow System [Reeves and Duguid (1975) and Yeh and Ward (1980)]: Freeze (1971a, 1971b, 1972a, and 1972b) applied his finite-difference code to a number of partially saturated flow systems. Parenthetically, it is interesting to note the closing comments of his (1971b) article. There, he identifies computer performance as the major limitation of a physics-based approach. Ironically, computer performance remains a major limitation in determining performance at the Yucca-Mountain site, in spite of the software and hardware advances of the last twenty years.

The flow system of interest assumes recharge through an upland plateau, seepage along a sloping surface, and discharge downdip to a stream. Steady-state heads, as calculated by Reeves and Duguid and by Yeh and Ward, show good agreement with those determined by Freeze. However, the discharge rates calculated by Reeves and Duguid differ from those calculated by Freeze. This may be due to the error inherent in the velocity calculation of Reeves and Duguid, and, hence, it would have been interesting to see the discharge rates determined by the velocity algorithm of Yeh and Ward. Unfortunately, these authors do not report their results. The spatial mesh for this two-dimensional problem consisted of 571 nodes.

Seepage Pond [Duguid and Reeves (1976), Yeh and Ward (1980), Yeh and Ward (1981) and Yeh (1987)]: Water from a seepage pond moves through a highly permeable sand to a sloping seepage face and a stream. Infiltration due to rainfall is small in comparison to seepage from the pond and is neglected. Duguid and Reeves, Yeh and Ward (1980), Yeh and Ward (1981) and Yeh calculate steady-state pressure and velocity fields. Results differ negligibly. Each uses a grid consisting of 595 nodes and 528 elements.

Huyakorn's (1986) One-Dimensional Column (Yeh, 1987): During a 10-day period, water, at a rate of 5 cm/day, infiltrates into a 200-cm vertical column containing a highly permeable soil (saturated conductivity, 10 cm/day). At the end of the tenth day, infiltration ends and evaporation begins, at a rate of 0.5 cm/day. This problem, which is simulated for a twenty-day period, tests the algorithm used to chop the time step. To calculate head as a function of depth and time, the analysis uses a grid consisting of 40 elements and 82 nodes.

Two-Dimensional Drainage Problem (Yeh, 1987): Two parallel drains, separated by a distance of 20 m, extend downward to the top of an impermeable aquifuge, a depth of 10 m. Infiltrating water, which enters the top surface at a flux of 0.006 m/day, discharges through the drains, the levels of which are maintained at a height of 2 m above the top of the aquifuge. Above the water level, the walls of the drains are assumed to be impermeable. The analysis determines the steady-state head distribution using 121 nodes and 100 elements.

3.4 *Status of Quality Assurance (QA).* The EPA has brought FEMWATER under QA control.

4. Type of Model (Phenomena/Processes Modeled)

Using a single-phase approximation to the two-phase equations, FEMWATER simulates variably saturated flow in a two-dimensional geometry, which may be a horizontal Cartesian (x-y) plane, a vertical Cartesian (x-z) cross-section, or a vertical radial (r-z) cross-section. As indicated by its name, the model uses the finite-element method.

5. Governing Equations.

FEMWATER uses the Richards equation.

6. Method of Solution

Yeh and Ward (1980) made one major change to the code of Reeves and Duguid (1975). After solving for head at a given time step, Reeves and Duguid differentiate this variable. This procedure can lead to discontinuous velocity components at element interfaces. Generally, the effect worsens with increasing permeability contrast between neighboring elements. To avoid this problem, Yeh and Ward apply the Galerkin approach and then use an implicit solution procedure like that used to obtain heads. If the availability of core storage permits, then the coefficient matrix of the velocity equation may be factored and stored. Then, the additional computer time required to obtain the velocities will be negligible. Otherwise, the computer time will increase by a factor less than three for a two-dimensional problem (Yeh, 1981).

Yeh (1987) made three major changes. First, to the direct method used by the original code, he added a Gauss-Seidel point-iteration method. Second, he improved the implementation of triangular elements. The original model permits the user to coalesce two nodes of a quadrilateral to obtain a triangular element. Yeh directly implements the basis functions for a triangular element, thereby decreasing the number of nodes and replacing a numerical element quadrature with an analytic integration. For a gridding containing mostly triangular elements, this represents a significant improvement in efficiency. Third, Yeh added a radial-geometry option.

Yeh and Ward (1980) made several relatively minor changes to the code of Reeves and Duguid (1975). To the variable-weighting scheme of the original model, they added mid-difference and mass-lumping options. Instead of allowing nonlinear parameters such as conductivity and water capacity to vary across an element, Yeh and Ward use the element average. Here they introduce numerical dispersion in an apparent effort to stabilize the algorithm.

Yeh (1987) also added several relatively minor changes. Although it requires relatively few coding changes, the mass-balance facility is quite useful. It provides a check on the numerical scheme and the consistency of the computer code. Treating conductivity tensors whose axes deviate from the coordinate axes improves the ability of the code to simulate anisotropic and heterogeneous media. A facility for time-step chopping enables the code to automatically reset the time step, thereby alleviating the need for troublesome external manipulations. The addition of Cauchy and time-dependent boundary conditions further broadens the model's range of application.

7. Type of Input Parameters

Generally speaking, integer and real parameters appear on separate records with formats of 16I5 and 8F10.3, respectively. Control and temporal gridding parameters come first, followed by material properties. Spatial gridding information comes next, including some rudimentary facilities for automatic mesh generation. Typically, mesh generation is a non-trivial exercise for a finite-element model.

Mesh dependent quantities follow. Initial or, if steady-state initial conditions are to be calculated, pre-initial conditions are prescribed. Then come source and boundary conditions. This input can be quite substantial since four different boundary conditions (Dirichlet, Neumann, Cauchy, and variable) are permitted and since each source and boundary condition may be specified by a table of time-dependent values.

In addition, SPROP may be regarded as input. Rather than to offer specific options for relative conductivity and moisture characteristic, the authors of FEMWATER expect the code user either to input these curves in tabular form or to write a SPROP routine which will generate them from analytical formulas. Section 5.2 of Yeh (1987) provides the necessary instructions for writing this routine.

8. Type of Output and User Options

FEMWATER output includes an echo of all input data, initial conditions, and boundary conditions. Pressure heads, total heads, moisture contents, and mass balances are output at the times specified by the input. Output also includes the time-step number, elapsed simulation time, and convergence characteristics, including the number of iterations. In addition to hard copy, plot files, and FEMWASTE files of moisture contents and Darcy velocities may be prepared during execution.

9. **Model Interactions (emphasize needed processors)**

9.1 *Does the model interface with any other models?* Yes, see below.

9.2 *Source code and type of information needed.* Not applicable.

9.3 *Receiving code and type of information provided.* FEMWATER writes Darcy velocities and water contents on a file, which FEMWASTE reads during the course of the mass-transport calculation.

9.4 *Any pre- or postprocessing needed?* Separate preprocessors and postprocessors plot the grid and provide time histories and contour plots.

10. **Model Application**

10.1 *Usage within the Civilian Radioactive Waste Management System (CRWMS) program.* Possibly the best use of FEMWATER within the CRWMS program would be the design of laboratory and field experiments. Under appropriate approximations, FEMWATER could also be used as a performance-assessment model. However, because of its assumption of isothermal flow, its role would be limited to analysis of the undisturbed case.

10.2 *Usage outside the program.* FEMWATER has been used in a variety of waste management areas, including hazardous waste and low-level nuclear waste. However, the availability of many other codes with similar capabilities limits its usefulness.

11. **Codes With Similar or Same Capabilities**

11.1 *Within the program.* The Yucca Mountain Project has funded the development of other flow and transport codes with capabilities which are either similar to or greater than those of FEMWATER. To characterize variably saturated flow, LLUVIA-2, NORIA-SP, and TOSPAC (Dudley et al., 1988) from SNL (Sandia National Laboratories) and SUMO (Eslinger et al., 1990) from PNL (Pacific Northwest Laboratory), TRUST (Reisenauer et al., 1982 and Narasimhan, 1975) from both PNL and LBL (Lawrence Berkeley Laboratory), and VS2DT (Lappala et al., 1987 and Healy, 1990) solve the single-phase Richards equation, as does FEMWATER. TOUGH2 (Pruess, 1991) at LBL (Lawrence Berkeley Laboratory), TRACR3D (Birdsell and Travis, 1991) and FEHM (Zyvoloski et al., 1992) at LANL (Los Alamos National Laboratory), MSTS at PNL, PORFLOW (Runchal and Sagar, 1991), and NORIA (Bixler, 1985) at SNL solve general multiphase equations, which include the Richards equation as a special case.

11.2 *Outside the program.* With its Yucca-Mountain project, the Nuclear Regulatory Commission has funded the documentation of TOUGH (Pruess, 1987), a multiphase solver, and DCM3D (Updegraff et al., 1991), a single-phase solver. Other government funded efforts yielded UNSAT2 (Davis and Neuman, 1983) and VAM2D (Huyakorn et al., 1989).

12. Major Assumptions and Limitations

- Thermal effects are not considered. Such effects may be quite significant at Yucca Mountain.
- Vapor flow is not considered.
- The Picard sequential updating procedure is used to linearize the nonlinear flow equation. For simulating dry environments, a Newton-Raphson procedure is required.
- A dual-continuum option is not available. Without substantial modification, fracture-matrix disequilibrium cannot be accounted for in field-scale simulations.
- Upstream conductivity weighting is not permitted.
- Only two spatial dimensions are considered. This will be sufficient for many applications. However, some applications will undoubtedly require three dimensions.

13. Remarks/General Observations/Discussion

For a relatively wet environment, such as that encountered at Oak Ridge, non-linearities can generally be handled with the Picard method. For relatively dry environments, like that of Yucca Mountain, non-linearities can be more severe. For an equivalent-continuum conceptualization, this is particularly apparent during a change from fracture to matrix-dominated flow. There, a Newton-Raphson option is desirable. After testing the Newton-Raphson algorithm on a suite of problems, Reeves and Duguid (1975) concluded that the algorithm increased both computer time and code complexity for the class of problems they were considering. They elected <u>not</u> to include this algorithm in the public-release version of the code. For the rock properties present at Yucca Mountain, their conclusion is not valid, and the more powerful Newton-Raphson method is required.

As indicated in Section 12, and as amplified above, FEMWATER has major limitations when considered in the context of the Yucca-Mountain project. Nevertheless, its current evolution is not without merit. In fact, Yeh's currently unpublished work with the multi-grid technique should be watched carefully since the implementation of such a technique may ease the computer-performance limitation which currently afflicts physics-based models in the Yucca-Mountain project.

14. Comparison to Other Models

See Chapters 4, 5, and 6 of the main text.

15. Summary and Recommendations

The relevance of a Richards-equation code is an issue at the Yucca-Mountain site. Nevertheless, the M&O needs to be prepared to perform simulations with such a code. However, the performance capability of FEMWATER is duplicated by many other codes, some of which employ algorithms which are more appropriate for the Yucca-Mountain site. It is therefore recommended that FEMWATER not be considered for component testing.

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