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Printed September 1996

Selection of a Numerical Unsaturated Flow Code for Tilted Capillary Barrier Performance Evaluation

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Prepared by
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Albuquerque, New Mexico 87185 and Livermore, California 94550
for the United States Department of Energy
under Contract DE-AC04-94AL85000

SF2900Q(8-81)

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Distribution
Category UC-2040

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ABSTRACT

Capillary barriers consisting of tilted fine-over-coarse layers have been suggested as landfill covers as a means to divert water infiltration away from sensitive underground regions under unsaturated flow conditions, especially for arid and semi-arid regions. Typically, the HELP code (Schroeder et al., 1994a,b) is used to evaluate landfill cover performance and design. Unfortunately, due to its simplified treatment of unsaturated flow and its essentially one-dimensional nature, HELP is not adequate to treat the complex multidimensional unsaturated flow processes occurring in a tilted capillary barrier. In order to develop the necessary mechanistic code for the performance evaluation of tilted capillary barriers, an efficient and comprehensive unsaturated flow code needs to be selected for further use and modification. The present study evaluates a number of candidate mechanistic unsaturated flow codes for application to tilted capillary barriers. Factors considered included unsaturated flow modeling, inclusion of evapotranspiration, nodalization flexibility, ease of modification, and numerical efficiency.

A number of unsaturated flow codes are available for use with different features and assumptions. The codes chosen for this evaluation are TOUGH2, FEHM, UNSAT2, SWMS_2D, and UNSAT-H. The UNSAT-H code was not selected for further evaluation because it is a one-dimensional code; a two- or three-dimensional capability is necessary for tilted capillary barriers. UNSAT2 was not evaluated because SWMS_2D is based on UNSAT2 and is a more recent code. The Oldenburg and Pruess (1993) tilted capillary barrier problem was selected for code comparison calculations.

All three codes chosen for this evaluation successfully simulated the capillary barrier problem chosen for the code comparison, although FEHM used a reduced grid. The numerical results are a strong function of the numerical weighting scheme. For the same weighting scheme, similar results were obtained from the various codes. Based on the CPU time of the various codes and the code capabilities, the TOUGH2 code has been selected as the appropriate code for tilted capillary barrier performance evaluation, possibly in conjunction with the infiltration, runoff, and evapotranspiration models of HELP.

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1.0 INTRODUCTION

Capillary barriers consisting of tilted fine-over-coarse layers have been suggested as landfill covers as a means to divert water infiltration away from sensitive underground regions under unsaturated flow conditions, especially for arid and semi-arid regions. The Hydrological Evaluation of Landfill Performance (HELP) model, which is sponsored by the Environmental Protection Agency (EPA), is generally used in the design of landfill covers. HELP is a quasi-two-dimensional model that predicts moisture movement into and through underground soil and waste layers including infiltration, evapotranspiration, unsaturated vertical drainage, lateral drainage, and leakage through liners. HELP has undergone considerable development over the past 15 years, with the latest version being HELP Version 3 (Schroeder et al., 1994a,b). The treatment of unsaturated flow in HELP is simplified in that capillary forces are ignored, the zone of evaporation is limited, and unsaturated flow is assumed to be one-dimensional. Therefore, HELP is not adequate to treat the complex multidimensional unsaturated flow processes occurring in a tilted capillary barrier, and a more mechanistic numerical code should be used.

Comparisons between HELP and various more mechanistic codes for horizontal landfill covers have been performed by a number of investigators. Thompson and Tyler (1984) compared the original HELP code and UNSAT1D (EPRI, 1981). Their results indicated that while HELP gives reasonable results for a one-dimensional landfill cover (horizontal layers) for humid conditions (Cincinnati, Ohio), HELP overpredicts the leakage rate through the landfill covers for semi-arid (Brownsville, Texas) and arid (Phoenix, Arizona) conditions, which are of primary importance for tilted capillary barriers. Fleenor and King (1995) compared HELP Version 3 with another mechanistic unsaturated flow model and reached similar conclusions for the above three locations. Nichols (1991) also concluded that HELP Version 2.0 predicts greater landfill cover leakage than UNSAT-H Version 2.0 (Fayer and Jones, 1990) for semi-arid conditions (Hanford, Washington).

In light of the above comparisons between HELP and more mechanistic codes for horizontal landfill covers, similar studies need to be performed for tilted capillary barriers, especially in arid and semi-arid environments. Large discrepancies are expected due to two factors: 1) the semi-arid and arid conditions expected for locations considering tilted capillary barriers, and 2) the lateral diversion capability (smaller leakage) of tilted capillary barriers compared to a horizontal landfill covers. Morris and Stormont (1996) recently considered the performance of tilted capillary barriers and conventional horizontal landfill covers. Noting the unsuitability of HELP to analyze tilted capillary barriers, they used the infiltration and evapotranspiration (ET) output from HELP as input to TRACR3D (Travis and Birdsell, 1991), a mechanistic unsaturated flow code. A similar scheme coupling HELP with a mechanistic unsaturated flow code may also be considered if the selected code does not currently include infiltration and evapotranspiration. In any event, coupling may be desirable because HELP is sponsored by EPA and is the current tool for designing horizontal landfill covers.

In order to develop the necessary mechanistic tool for this comparison, and for the performance evaluation of tilted capillary barriers, an efficient and comprehensive unsaturated flow code needs to be selected for further use and modification. The present study evaluates a number of candidate mechanistic unsaturated flow codes that can be used to more realistically describe the behavior of tilted capillary barriers in arid and semi-arid environments.

A number of unsaturated flow codes are available for use with different features and assumptions. For example, a number of codes assume that air is passive and only consider the flow of liquid (Richards equation), while others assume isothermal conditions. Some include evapotranspiration, while others ignore it. The purpose of the present investigation is to select an unsaturated flow code that has many of the features important to tilted capillary barrier performance and that can be easily modified to include the missing attributes and features. In light of previous comparisons between HELP and mechanistic unsaturated flow codes, and the unsuitability of HELP for tilted capillary barriers, the HELP code was not considered in the present code comparison.

2.0 CODE EVALUATION

2.1 Desirable Code Features

A summary of the desirable features of an unsaturated flow code for tilted capillary barrier use is given in Table 1. The five main criteria for selection include

1) unsaturated flow modeling,
2) evapotranspiration,
3) nodalization flexibility including flexible boundary conditions,
4) ease of modification, and
5) numerical efficiency.

Each feature is discussed in more detail below.

Unsaturated Flow Modeling - In the modeling of unsaturated flow, the most comprehensive models use a full two-phase treatment to predict the movement of water and air in the soil; typical equations are summarized in the Appendix. In many situations, Richards equation is employed. Richards equation is a considerable simplification of the full two-phase treatment because the movement of air is not modeled and only water movement is considered. In this case, the air pressure is assumed to be constant, and only the water conservation equations are solved. This simplification often dramatically increases the numerical efficiency of the simulation without significantly influencing the results. Differences occur under high infiltration rates or ponding with a shallow water table when the underlying air cannot escape past the infiltrating water to the surface (Touma and Vauclin, 1986). The ideal combination is to have both options available in a given code so that either the full two-phase treatment or the Richards equation simplification can be selected. In addition, in the full two-phase treatment, inclusion of the energy equation is desirable to analyze diurnal and seasonal temperature variations. Drying of a capillary barrier with seasonal conditions may be important, especially in arid and semi-arid

Table 1
Desirable Computer Code Features for Tilted Capillary Barriers

Unsaturated Flow Modeling
- Richards equation as a minimum
- Full two-phase capability helpful to evaluate Richards equation
- Nonisothermal option helpful for drying and seasonal variations
- Hysteresis is helpful (wetting and drying cycles; fingering)

Evapotranspiration
- Surface Evaporation
- Plant-soil transpiration

Nodalization Flexibility
- Two-dimensional as a minimum
- Three-dimensional helpful
- Flexible Boundary Conditions

Ease of Modification
- Source code must be available and well written and documented

Numerical Efficiency
- Necessary for design calculations and sensitivity studies

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environments, in which case the full nonisothermal two-phase treatment is necessary. Hysteresis in the capillary pressure curve may also be significant in capillary barriers because the materials will undergo numerous wetting and drying cycles. In addition, the dominant failure mechanism of capillary barriers is most likely wetting-front instability, or gravity-driven fingering (Hill and Parlange, 1972; Glass et al., 1989a,b,c) as discussed by Oldenburg and Pruess (1993). According to Glass et al. (1989c) and Nieber (1996), hysteresis may control fingering processes, so the availability of a hysteresis model is desirable.

The unsaturated flow modeling capability of a code is the most important feature. Adding a full two-phase treatment to a simulator that uses the Richards equation simplification, or adding a nonisothermal option to an isothermal code, is a major modification and should only be considered if no code meets these requirements.

Solute transport has not been considered in the present list of desirable code features. Solute transport may be important in the evaluation of a landfill if the tilted capillary barrier fails and water flows through the protected underground region. However, adequate modeling of unsaturated flow and the diversion of water away from the protected region is considered to be much more important than a solute transport capability for the present study. If everything else were equal, a solute transport capability would be a plus. In addition, solute transport can often be evaluated as a post-processing step if the solute concentration is low. Therefore, solute transport was not a factor in the present evaluation.

Evapotranspiration - Evapotranspiration, which is the combination of evaporation due the surface conditions and transpiration of water by plants, should be included in any comprehensive treatment of capillary barrier performance. Evaporation, plant behavior, and the resulting water flow varies significantly with the seasons and from day to night and is dependent of the distribution and availability of water. This treatment is usually coupled to the unsaturated flow model as a sink/source of water and energy. Treatment of evapotranspiration is a plus, although modification of an existing code to include evapotranspiration models may be relatively straightforward once the computer code is selected.

Nodalization Flexibility including Boundary Conditions - The selected computer code must have sufficient nodalization flexibility to handle anticipated capillary barrier geometries including appropriate boundary conditions. A fully general three-dimensional treatment is obviously preferable, although two-dimensional geometries may be acceptable. Due to the tilted geometry and lateral diversion of capillary barriers being investigated in the present study, a one-dimensional code is not acceptable. In addition to the dimensionality of the code, the shape of the nodes must be flexible to allow for complicated geometries with possible non-orthogonal axes. Nodalization flexibility such as the dimensionality of the code and the geometries are such an inherent part of most codes that modification is impractical. Therefore, nodalization flexibility is the second most important feature after the unsaturated flow modeling capability. Boundary conditions must be capable of simulating diurnal and seasonal temperature and relative humidity variations as well as infiltration and runoff. As with evapotranspiration, modification of an existing code to simulate these conditions may be relatively straightforward.

Ease of Modification - The selected code must be able to be easily modified. The selected code may not have the full suite of desirable features, so modification will be necessary. The source code must be available so modifications can be performed locally, and the availability of the code developer is an obvious advantage. Ease of modification of the source code is a nebulous term that includes familiarization of the person with the code, the helpfulness and availability of the code developer, and the code layout. This attribute is very subjective and dependent on the personnel involved.

Numerical Efficiency - Finally, the code must be numerically efficient to allow the user to routinely investigate sensitivities and problem variations. Numerical efficiency of the codes can be quantitatively evaluated, although the results are dependent on the problem selected for evaluation. The problem selected for the present comparison is a two-dimensional tilted fine-over-coarse capillary barrier with a water table and uniform infiltration; evapotranspiration is not included. This problem primarily involves the unsaturated flow attribute of the tested codes.

The first phase of the code evaluation involves selection of candidate codes and an initial screening based on the mandatory features which, for the present case, is simply the dimensionality of the code. The second and final phase involves simulation of the capillary barrier problem and comparison of code predictions and numerical efficiency results.

2.2 Candidate Codes

The codes selected for comparison under this task are:

TOUGH2
FEHM
UNSAT2
SWMS_2D
UNSAT-H

There are a number of other unsaturated flow codes available such as TRACR3D (Travis and Birdsell, 1991), PORFLO-3 (Runchal and Sagar, 1989), VS2DT (Lapella et al., 1987), and FEMWATER (Yeh and Ward, 1979) among others; numerous code comparison exercises have also been performed (e.g., Baca and Magnuson, 1990; McCord and Goodrich, 1994), although none are directly applicable to tilted capillary barriers. The codes selected for the present code comparison were limited to those the authors were familiar with and those that have been extensively used in landfill cover and capillary barrier modeling efforts. Eventually, the selected code will be used and/or modified by the authors for tilted capillary barrier analysis and modeling, and familiarity with the code and/or direct applicability to the problem at hand is an advantage. Therefore, the selection of the final code is dependent on the authors' experience, and other codes may be just as appropriate for other users.

Brief descriptions of each candidate code are given below.

TOUGH2 - TOUGH2 has been developed at Lawrence Berkeley Laboratory by Pruess (1987, 1991). TOUGH2 uses a finite volume approach that can model arbitrarily shaped elements for unsaturated and saturated flow in three dimensions. A full two-phase treatment and a Richards equation approach (Pruess and Antunez, 1995) are available as well as isothermal and nonisothermal options. Conjugate gradient solvers have also recently been added to TOUGH2 to increase the speed of the code and to decrease the memory requirements, thereby allowing larger models to be employed (Moridis and Pruess, 1995). Hysteresis has been included in a version of TOUGH (Niemi et al., 1991a,b), which can probably be used in TOUGH2. Inverse modeling capabilities to estimate model parameters from data, which is useful in interpreting experimental data, are also available through the ITOUGH2 code (Finsterle and Pruess, 1995).

FEHM - FEHM has been developed over the past few years at Los Alamos National Laboratory by Zyvoloski et al. (1995a,b) and is a multidimensional, multiphase simulator for heat and mass transport in porous and fractured media using the finite element method. The code also has provisions to use the finite volume method.

UNSAT2 - UNSAT2 was developed by Neuman and colleagues (Davis and Neuman, 1983) and is a two-dimensional finite element code for unsaturated and saturated flow including evapotranspiration. Flow geometries are restricted to a horizontal plane, axisymmetric flow, or a vertical plane with irregular boundaries. A Richards equation simplification is used as only the liquid-phase flow equation is solved. Isothermal conditions are assumed. SWMS_2D is a more recent code based on UNSAT2.

SWMS_2D - SWMS_2D is based on the UNSAT2 code as distributed by the U.S. Department of Agriculture (Simunek et al., 1994). Similar to UNSAT2, it is a two-dimensional finite element code for unsaturated and saturated flow including evapotranspiration using a Richards equation approximation and assuming isothermal flow. In addition, SWMS_2D solves the advection-dispersion equation for solute transport.

UNSAT-H - UNSAT-H Version 2.0 was developed by Pacific Northwest Laboratory (Fayer and Jones, 1990) and is not related to UNSAT2. UNSAT-H is a one-dimensional code for unsaturated flow including evapotranspiration and heat. A Richards equation approach is used to simplify the unsaturated flow modeling.

2.3 Initial Code Screening

The first phase of the code evaluation involves an initial screening of the selected codes based on the mandatory features which, for the present case, is simply the dimensionality of the code. The UNSAT-H code, which was written to evaluate the hydrologic performance of protective barriers (Fayer and Jones, 1992), did not meet the mandatory requirements of the present study since it is a one-dimensional code. In addition, the UNSAT2 code (unrelated to UNSAT-H) was also screened out in this first phase since SWMS_2D is a more recent version. Therefore, the codes TOUGH2, FEHM, and SWMS_2D are considered for further evaluation by comparison to the test problem.

2.4 Code Comparison Problem

The second phase of the evaluation process involves application of the codes to a tilted capillary barrier. The problem chosen for this comparison is a two-dimensional tilted fine-over-coarse capillary barrier with a water table and uniform infiltration along the top boundary; no evapotranspiration is included (Oldenburg and Pruess, 1993). A sketch of the capillary barrier is given in Figure 1; properties and problem parameters are summarized in Table 2. A fine layer 50 m thick overlies a coarse layer 10 m thick; the layers are tilted at a 5° angle with respect to the horizontal. Infiltration occurs at the top of the fine layer at a constant rate of 0.60 m/year. A water table is present at a depth of 59 m along the left boundary. The steady-state leakage, or breakthrough, across the fine-coarse boundary is desired for comparison with the Ross (1990) solution.

Unfortunately, the results given by Oldenburg and Pruess (1993) and by Ross (1990) are only for steady-state conditions, while the situation for real capillary barriers involves transient infiltration events and diurnal and seasonal variations in temperature and evapotranspiration. While the problem has its shortcomings, and selection of an evaluation problem by the author of TOUGH2 (Pruess) may seem unfair or biased, their problem is the only known published

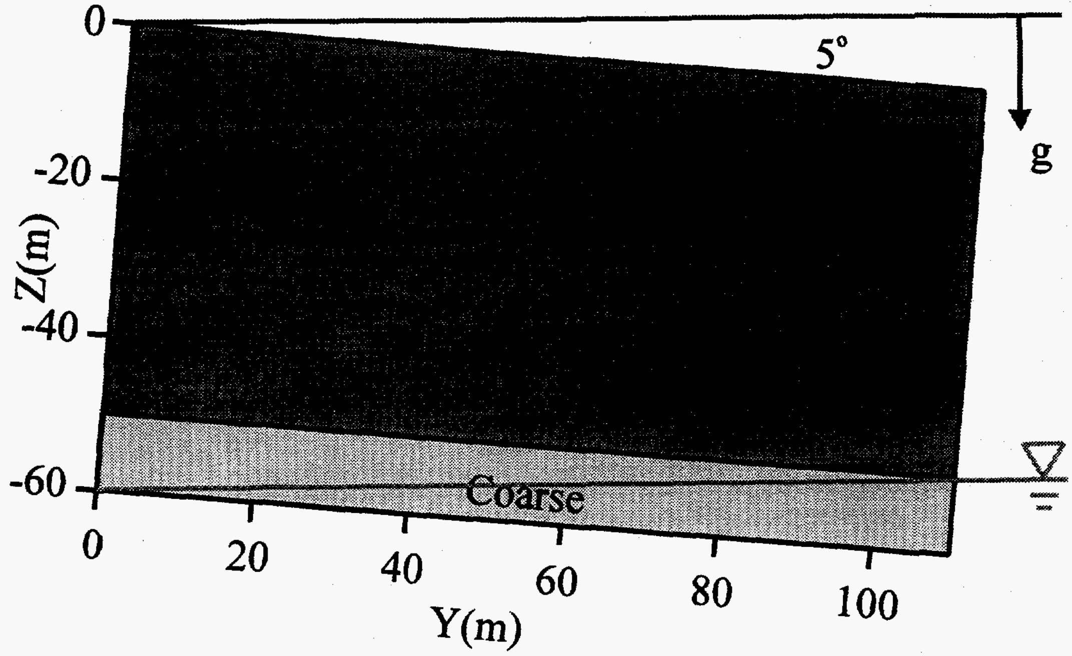


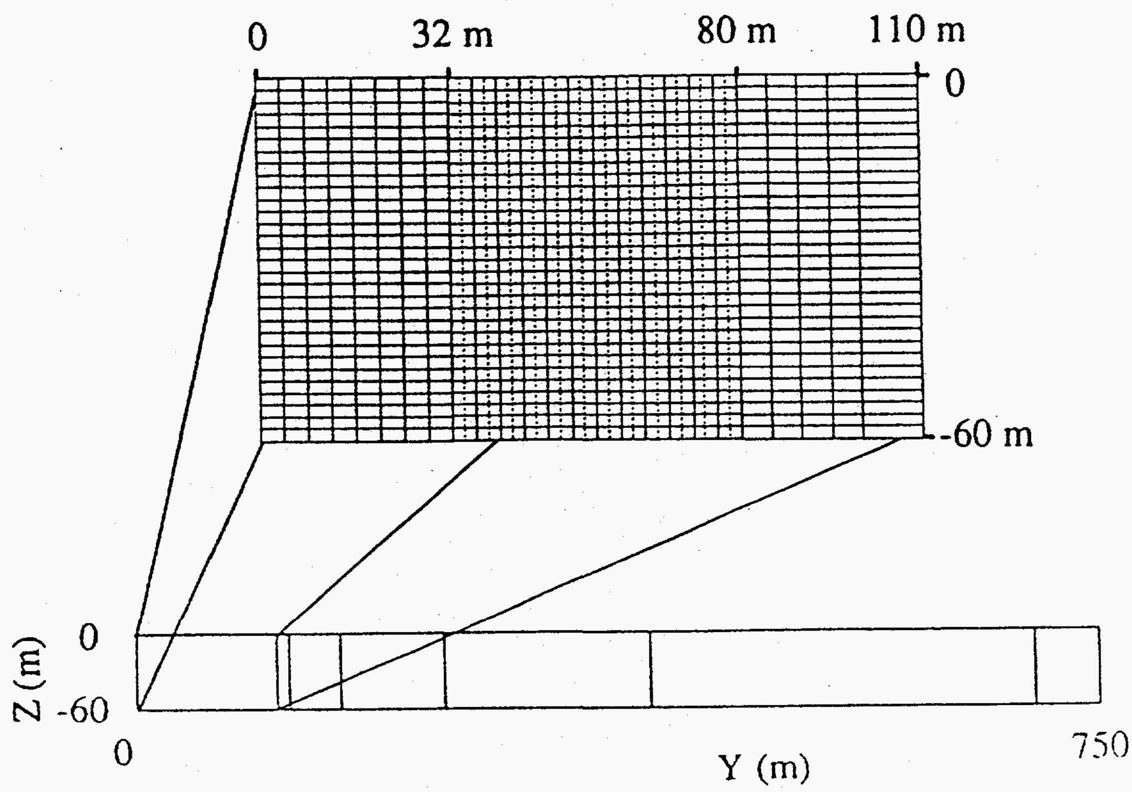
Figure 1
Comparison Problem Schematic
(after Oldenburg and Pruess, 1993)

Table 2
Comparison Problem Parameters

	Upper Layer (Fine)	Lower Layer (Coarse)
Thickness	50 m	10 m
Length	750 m	750 m
Permeability	10^{-13} m^2	2 x 10^{-13} m^2
Porosity	0.30	0.40
Relative Permeability	$k_{r,w} = e^{\alpha\psi}$; $\alpha = 0.1$ m^{-1}	$k_{r,w} = e^{\alpha^*\psi}$; $\alpha^* = 4.$ m^{-1}
Capillary Pressure	$P_c = -10^6\ (1.-S_l)$	$P_c = -10^6\ (1.-S_l)$

Boundary Conditions

Left Side	No flow.
Right Side	No flow.
Top	Uniform infiltration rate (0.60 m/year).
Bottom	Horizontal water table at a depth of 59 m at left boundary.



<u>Figure 2</u>
Comparison Problem Discretization
(from Oldenburg and Pruess, 1993)

capillary barrier application that is simple enough to be performed by different codes quickly yet complex enough to test the physics and numerics of the codes for tilted capillary barrier problems.

The discretization employed by Oldenburg and Pruess (1993) is shown in Figure 2. Thirty rows 2 m deep were used with varying column dimensions. The initial column width was 4 m out to 80 m downdip that increased thereafter. A higher resolution grid was examined between 32 and 80 m downdip using 2 m wide columns. The results from the original grid and the higher resolution grid are essentially the same.

The two-phase characteristic curves employed in the analysis include a linear capillary pressure and the quasi-linear wetting-phase relative permeability, or

$$k_{r,w} = e^{\alpha\psi} \tag{1}$$

where α is the sorptive number and ψ is the moisture potential ($\psi = P_c / \rho g$). Because none of the codes had the quasi-linear wetting-phase relative permeability, each code had to be modified, thus providing a measure of how easily each code could be modified.

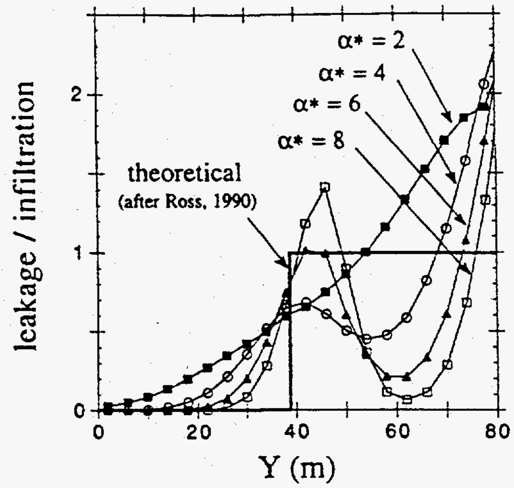
The results from the capillary barrier simulations are compactly presented as a ratio of the leakage past the fine-coarse boundary divided by the infiltration rate. A value of zero shows complete diversion of the infiltrating water, while a value of 1.0 means no diversion. The ratio should increase with distance downdip until breakthrough occurs, which is defined as a ratio of 1.0. Values higher than 1.0 are expected further downstream as initially diverted water flows into the coarse layer.

Oldenburg and Pruess (1993) investigated two different numerical weighting schemes. The two numerical weighting schemes for the permeability-mobility product ($k\, k_{r,i} / \mu_i$) (see the Appendix) indicate some of the complexities associated with unsaturated flow modeling. Harmonic weighting, which considers the upstream and downstream parameters, is appropriate for steady-state one-dimensional flow without phase change or phase propagation based on flux conservation and should honor the property contrast across layers. However, for transient conditions, upstream weighting must be used because flux conservation is not directly applicable. Upstream weighting, which only uses the upstream parameters, does not preserve the contrast between the layers but it is numerically much more robust. The use of harmonic weighting for transient unsaturated flow can lead to large errors (Aziz and Settari, 1979; Tsang and Pruess, 1990), and unphysical results can be obtained. Therefore, upstream weighting is usually employed in unsaturated flow simulations.

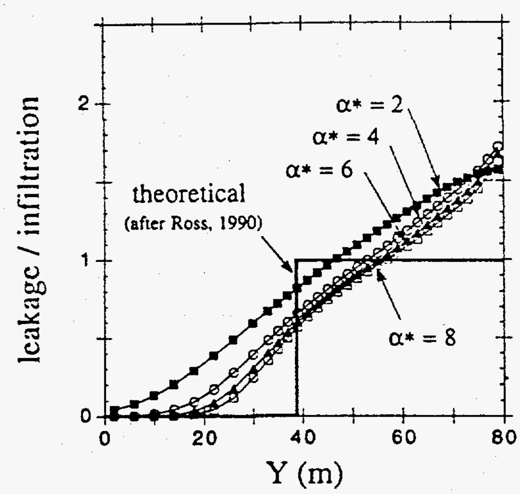
The calculated leakage/infiltration ratio from Oldenburg and Pruess (1993) for these two weighting schemes is shown in Figure 3 as a function of distance downdip and the sorptive number for the coarse layer, α^*; note that the sorptive number for the fine layer, α, is constant in their simulations. For the present code comparison, only the results for a coarse layer sorptive number of 4.0 m^{-1} will be considered. The results for the two weighting schemes are significantly different. The ratio for harmonic weighting shows an initial breakthrough at about 40 m. The ratio decreases slightly after this location since some of the water has flowed into the coarse layer. The ratio then increases again; note that the water table and fine-coarse contact intersect at 103 m downdip. In contrast, for upstream weighting, the ratio increases monotonically with distance.

In addition to comparison of results between various codes, the results can also be compared to the capillary barrier lateral diversion formula of Ross (1990). Steenhuis et al., (1991) and Stormont (1995) present additional diversion length expressions. For the conditions of the problem summarized in Table 2 ($\alpha = 0.1$ m^{-1}; $\alpha^* = 4.0$ m^{-1}), the predicted capillary diversion length is 39.3 m; this value is shown along with the results.

Concerns about the relatively poor quantitative agreement between the TOUGH2 simulations and Ross' formula have been raised. Oldenburg and Pruess (1993) attribute the differences to a



(a) Harmonic Weighting Results



(b) Upstream Weighting Results

<u>Figure 3</u>
Comparison Problem Leakage/Infiltration Ratio Results
(from Oldenburg and Pruess, 1993)

number of factors. The numerical simulations show a gradual increase in the leakage across the fine-coarse interface, which is expected. In contrast, Ross (1993) assumed that breakthrough would occur all at once and that the leakage which increase as a step function. In addition, Oldenburg and Pruess (1993) suggest that the numerical simulations reflect wetting-front instability, or gravity-driven fingering, which is the most likely failure mechanism of capillary barriers as discussed earlier in section 2.1. This behavior is not considered in the analytical solution given by Ross (1990). Another concern has been raised about the proximity of the water table. In the Oldenburg and Pruess (1993) simulations, the water table is only a few meters below the fine-coarse interface when breakthrough occurs. Ross' derivation assumed that the water table was infinitely far away from the fine-coarse interface. The water table proximity question has recently been addressed by Webb (1996). He found that as the water table gets further away from the interface, the agreement between the numerical simulations and Ross' solution improves significantly. However, these results were not available at the time that the present simulations were performed. Therefore, the present report used the original Oldenburg and Pruess (1993) results for comparison.

In order to more efficiently perform the code modifications and the code runs, personnel familiar with each code were selected. For the TOUGH2 code, Stephen Webb performed the modifications and runs, while Clifford Ho and Mehdi Eliassi worked on FEHM and SWMS_2D, respectively. The results from each code are presented below. The runs were performed on an HP 735/125 Workstation.

2.5 Comparison Problem Results

2.5.1 TOUGH2

The TOUGH2 simulations of the capillary barrier problem of Oldenburg and Pruess (1993) are discussed in this section. The model used the mesh shown previously in Figure 2, which extends 750 m along the tilted horizontal axis. Due to the numerical options in the TOUGH2 code, and the sensitivities shown by Oldenburg and Pruess, four cases were considered. Two numerical weighting schemes, upstream and harmonic, and two unsaturated flow modeling options, the full two-phase treatment and the Richards equation simplification were used and the results compared. The isothermal option was also employed.

Differences in the two numerical weighting schemes have been studied by Oldenburg and Pruess (1993) as mentioned earlier. The use of the full two-phase treatment and the simplified Richards equation approach allows for a comparison of the results, both from a prediction viewpoint and from a numerical efficiency perspective. While Richards equation may not be appropriate in every situation as discussed earlier, it may be adequate for scoping studies and other situations.

The problem was run in two parts. Initial conditions were established by running a false transient to steady-state. The properties in both layers were made essentially the same for the steady-state runs so the entire domain time constants would be equal. Performing the steady-state run posed some problems with the full two-phase treatment, as the solution and the time steps oscillated. The problem with obtaining steady-state conditions was also noted by Oldenburg (Oldenburg, private communication, 1994). He got around the problem by running reduced problem domains to steady-state and then adding on more columns. For example, the first column was analyzed separately for steady-state conditions, and then an additional 1 or 2 columns were added to the problem with the first column as boundary conditions. This approach, although cumbersome, was also used in the present study. This oscillatory behavior was not seen in the Richards equation option as steady-state conditions were readily obtained. Therefore, a possible way to initialize a full two-phase problem would be to run the steady-state with Richards equation option and use these conditions for the full two-phase treatment. This difficulty with initializing TOUGH2 with the full two-phase treatment is not considered serious since steady-state conditions are readily calculated with Richards equation.

The infiltration transient was performed by using the calculated initial conditions and applying the infiltration along the top surface. The simulation was run until the time step approached 10^{13} seconds. The leakage across the fine-coarse boundary was then compared to the infiltration rate to determine the leakage/infiltration ratio.

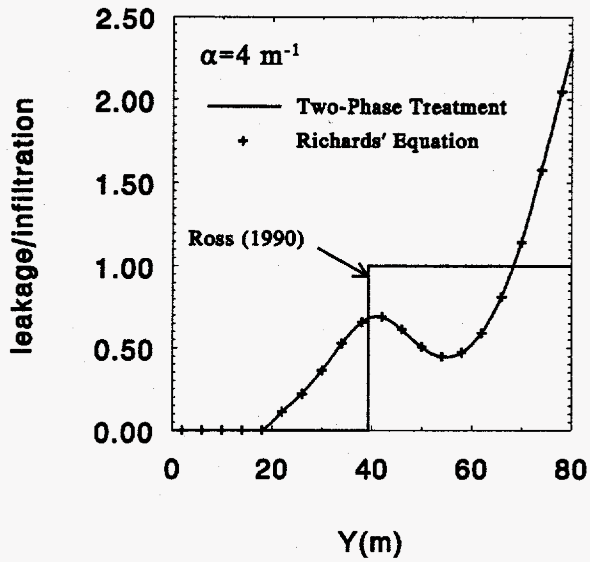
The leakage/infiltration results for these four combinations are shown in Figure 4. Differences between the full two-phase treatment and Richards equation are small for the present problem, being less than 1% for both weighting schemes. The results are essentially the same as given by Oldenburg and Pruess (1993) including the significant influence of the numerical weighting scheme employed as discussed earlier. The numerical efficiency results are presented and discussed later.

Modification of TOUGH2 to include the quasi-linear relative permeability relationship was straightforward. A separate routine calculates relative permeabilities, and an option for the quasi-linear model was simple to add.

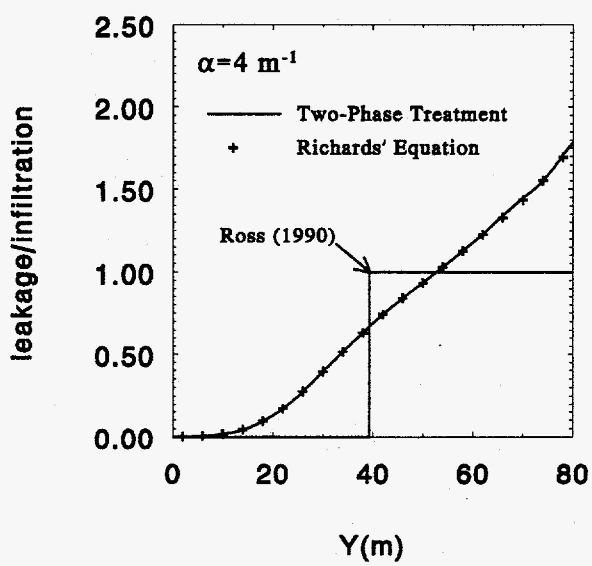
2.5.2 FEHM[1]

The capillary barrier configuration of Oldenburg and Pruess has also been analyzed using the FEHM (Finite Element Heat and Mass) code (Zyvoloski et al., 1995a,b). The mesh for the FEHM model was created by mapping the TOUGH2 mesh used by Oldenburg and Pruess into FEHM. Because FEHM uses a finite element formulation, the coordinates of the nodes comprising the elements had to be specified. The nodal coordinates for FEHM were specified as the centroids of the TOUGH2 volume elements. Conceptually, the only difference between the two grids is that the centroids of the TOUGH2 elements are now the nodes of the FEHM elements. In FEHM, material properties are specified at the nodes rather than at the elements themselves. Therefore, placement of the nodes of the FEHM elements at the centroids of the

[1]- written by Clifford Ho and Stephen Webb



(a) Harmonic Weighting Results



(b) Upstream Weighting Results

<u>Figure 4</u>
TOUGH2 Leakage/Infiltration Ratio Results

TOUGH2 elements yields consistency between the two codes when upstream weighting is used for flow between the interface of the coarse and fine layers.

A note should be made regarding the orientation of these grids. Rotation of the initially orthogonal grid creates dipping lateral boundaries as well. Because the upper boundary is specified using a uniform infiltration, anomalous low downward fluxes are expected to occur along the upstream lateral boundary, especially at lower elevations. Ideally, the lateral boundaries for this problem should be vertical. The decision by Oldenburg and Pruess (1993) to use the rotated orientation probably resulted from the convenience of simply rotating the gravity vector while maintaining an orthogonal grid (which was aligned with the strata) in TOUGH2. For consistency, this orientation was implemented in FEHM as well, although different configurations are possible (and probably preferred) as shown in Figure 5.

Unfortunately, the rotated grid in FEHM that corresponded to the Oldenburg and Pruess model yielded "negative finite element coefficients", perhaps indicating that the mesh was not consistent with a Delaunay formulation (Zyvoloski et al., 1995b). This problem resulted in spurious solutions from FEHM. As a result, the domain was reduced from its original 34 columns of nodes to only the first 27 columns of nodes, yielding a domain that was 138 m wide in the downdip direction. Although this smaller domain also yielded "negative finite element coefficients", the finite volume option was added that resulted in solutions for this domain. This smaller domain, consisting of 27 columns and 30 rows, was used in the FEHM results presented in this section.

A Richards equation option was employed with reference conditions of 20°C and 0.1 MPa, and full upstream weighting of the permeability-mobility product was specified; a harmonic weighting option equivalent to that used in TOUGH2 is not available. The material properties and boundary conditions specified by Oldenburg and Pruess (1993) were implemented in the FEHM model. Difficulties were encountered in running FEHM on the HP Workstation. Therefore, the simulation was performed on a Sun Workstation and the CPU time was translated to an HP Workstation time value by ratioing CPU times for the equivalent TOUGH2 run.

This system was first simulated for 1×10^{10} days without infiltration to establish hydrostatic conditions, which were used as initial conditions for the subsequent simulation with infiltration. After another 1×10^{10} days of simulated time with infiltration, the leakage/infiltration ratio was calculated along the interface between the fine and coarse layers. Figure 6 shows the results of this FEHM simulation, which are quite similar to the results from TOUGH2. The leakage increases fairly uniformly from the upstream end towards the downstream end. The leakage/infiltration ratio is slightly higher at 80 m for FEHM than for TOUGH2 but it is in general agreement.

The quasi-linear model used for the liquid relative permeability was easily implemented in FEHM, although the first derivative of the function also had to be included in the modification. This requirement could present additional problems if a more complex function were needed.

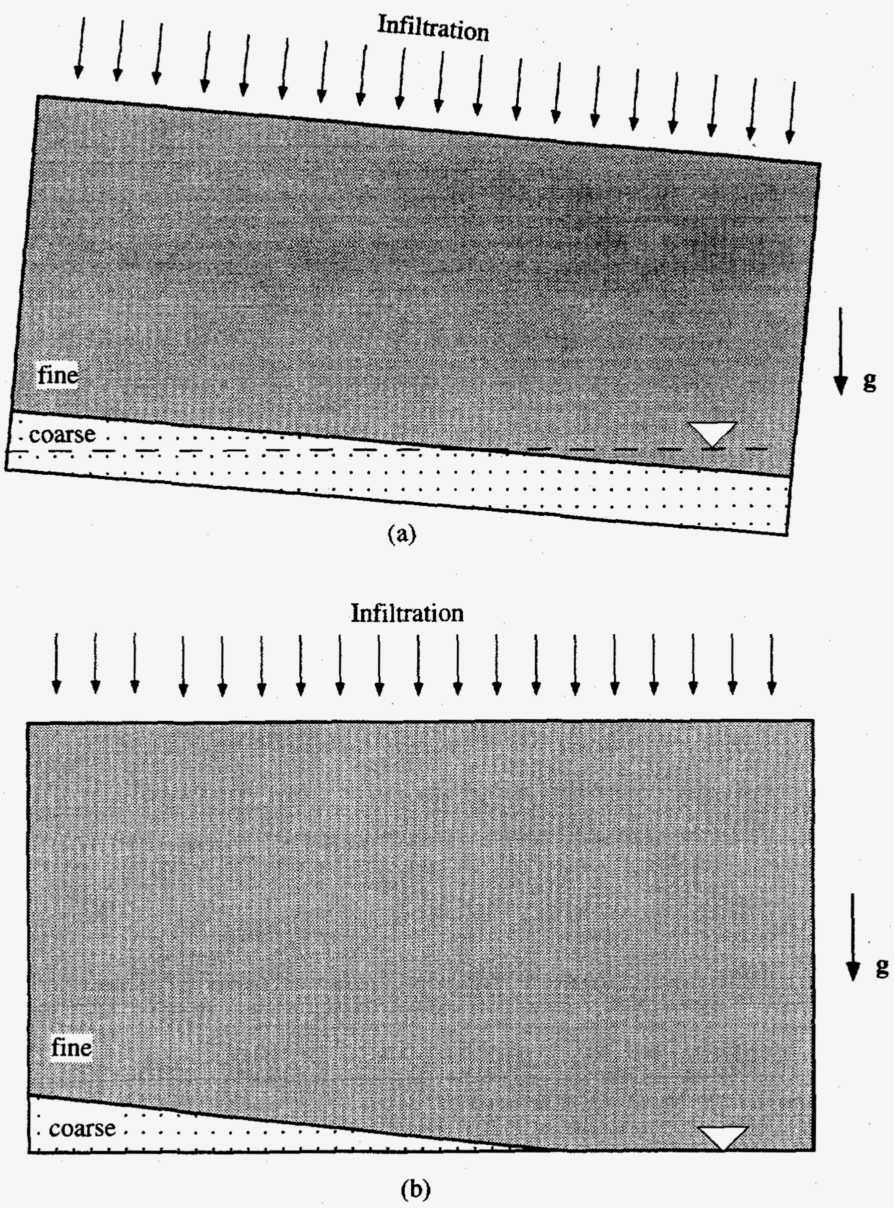


Figure 5
Different Possible Orientations for the Capillary Barrier Problem
(a) Oldenburg and Pruess
(b) Possible Preferred Orientation

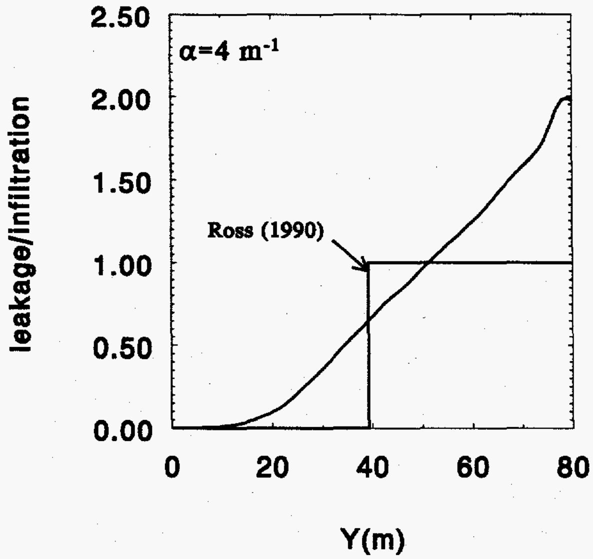


Figure 6
FEHM Leakage/Infiltration Ratio Results for Upstream Weighting

2.5.3 SWMS_2D[1]

The finite element code SWMS_2D (Simunek et al. 1994) was used to simulate the Oldenburg and Pruess capillary barrier problem using Richards equation. Two different meshes were used in the investigation. The first mesh mapped the finite elements directly onto the TOUGH2 finite volumes, or elements, so the nodes were at TOUGH2 element boundaries; this mesh is referred to as TOUGH2 boundaries. The second mesh specified the finite element nodes at the TOUGH2 element centers similar to the FEHM mesh and is referred to as TOUGH2 element centers. The full domain used in the TOUGH2 simulations was used in SWMS_2D.

Recognizing that the saturation is a linear function of the pressure potential, the initial conditions were input directly to the code. The boundary conditions for the problem were easily enforced. The material properties specified by Oldenburg and Pruess were used. A liquid residual moisture content of 0.001 was also specified. Oldenburg and Pruess (1993) showed that different results can be obtained depending upon the mobility weighting. SWMS_2D does not employ either harmonic or upstream weighting for flow calculations. Rather, SWMS_2D uses a simple (arithmetic) averaging technique for the unsaturated hydraulic conductivity.

Because steady-state conditions are of primary interest in the present comparison, the infiltration problem was simulated with time steps that were allowed to increase to as high as

[1]- written by Mehdi Eliassi and Stephen Webb

10^{13} seconds; this criterion was also used by Oldenburg and Pruess (1993). Figure 7 depicts the leakage/infiltration ratio results obtained using SWMS_2D for the two mesh systems employed; the figure also includes Ross's results. The results are different than either the harmonic or upstream weighting results given by TOUGH2 or FEHM and depend on the mesh employed. The sensitivity to the mesh is probably due to the change in location of the interface. In the TOUGH2 boundaries grid, the material interface corresponds to a finite element boundary, which is probably more appropriate for the arithmetic average weighting technique used in SWMS_2D. The TOUGH2 element centers mesh is probably more appropriate for upstream weighting.

In order to compare the SWMS_2D results to the other model results, another TOUGH2 simulation was performed with a weighting technique similar to the one used by SWMS_2D. The averaging technique used in the TOUGH2 run averages the mobilities of adjacent elements and harmonically weights the permeabilities. Because the permeabilities only vary by a factor of 2 from the fine to the coarse layer in the selected problem, there is very little difference between harmonic weighting and an average value of the permeability. The TOUGH2 results are shown in Figure 8. The results are similar to the SWMS_2D runs, indicating reasonable agreement between the codes.

SWMS_2D was fairly easy to modify to incorporate the quasi-linear relative permeability function due to the modular nature of the code. The manual is well documented and all important variables and their various functions are explained.

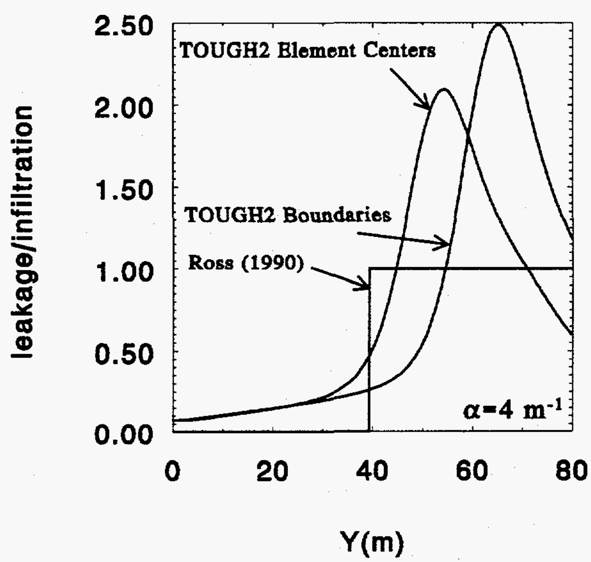


Figure 7
SWMS_2D Leakage/Infiltration Ratio Results

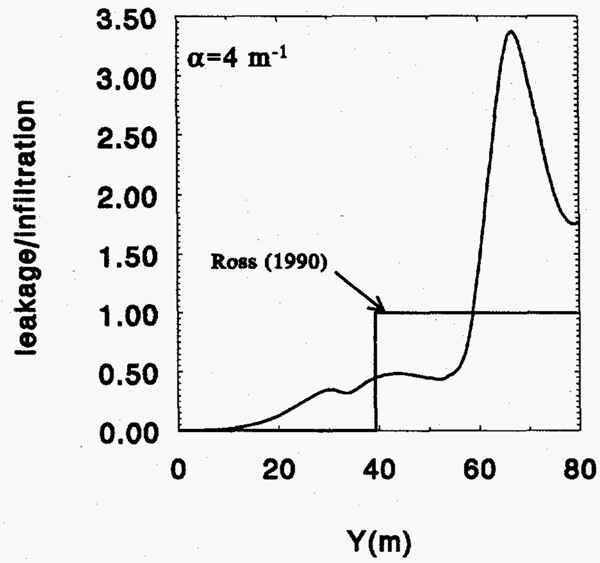


Figure 8
TOUGH2 Leakage/Infiltration Ratio Results for Arithmetic Average Weighting

2.5.4 CPU Time Comparison

Table 3 summarizes the numerical efficiency results; all CPU times are for an HP 735/125 Workstation. For TOUGH2, the computer times vary by about 2 orders of magnitude. Using Richards equation is about an order of magnitude faster than the full two-phase treatment, and the use of upstream weighting is another order of magnitude more efficient than harmonic weighting. The improved efficiency of upstream weighting is due to the fact that it only considers the upstream conditions, while harmonic weighting depends on upstream and downstream variables. As discussed earlier, upstream weighting is often necessary for transient unsaturated flow modeling, especially for propagating phase fronts such as the wetting front in capillary barriers; harmonic weighting can result in gross errors under these conditions.

The elapsed time for the FEHM simulation is considerably longer than the analogous TOUGH2 simulations (>60 minutes vs. 1.3 minutes), but this may be a result of the grid orientation, which is not ideally suited for FEHM. The SWMS_2D CPU times depended on the grid. For the same grid and weighting scheme as TOUGH2 (TOUGH2 Boundaries), SWMS_2D takes about 7 times as long as TOUGH2. For the alternate grid based on the centers of the TOUGH2 element centers, the CPU time is about 4 times as long as TOUGH2. Based on these results, TOUGH2 is clearly the most numerically efficient code for the capillary barrier problem used in this comparison.

Table 3
CPU Time Results
(HP 735/125 Workstation)

TOUGH2	
Full Two-Phase Treatment	
Harmonic Weighting	160 minutes
Upstream Weighting	16 minutes
Richards Equation	
Harmonic Weighting	21 minutes
Upstream Weighting	1.3 minutes
Arithmetic Average Weighting	1.2 minutes
FEHM - reduced domain	
Richards Equation	
Upstream Weighting	>60 minutes
SWMS_2D	
Richards Equation	
Arithmetic Average Weighting	
TOUGH2 Boundaries	8.6 minutes
TOUGH2 Element Centers	4.6 minutes

3.0 DISCUSSION AND CONCLUSIONS

All the codes simulated the capillary barrier problem chosen for the code comparison, although FEHM simulations used a reduced grid. The numerical results are a strong function of the numerical weighting scheme. For the same weighting scheme, similar results were obtained from the various codes. Upstream weighting is the preferred approach even though the layer contrast is not preserved. Harmonic weighting can result in large errors or unphysical results for transient simulations.

The results from the present code evaluation are summarized in Table 4; HELP is also included in the table since it is the model generally used at present for landfill cover analysis and design. The desirable code features for tilted capillary barriers have been summarized in Table 1 and were discussed earlier in Section 2.1 Based on this study, the TOUGH2 code has been selected as the appropriate code for further tilted capillary barrier design work. Not only does TOUGH2 have various unsaturated flow, weighting, and isothermal and nonisothermal options, but the geometry is flexible and the code is numerically efficient. The only obvious drawbacks to TOUGH2 are the lack of an evapotranspiration model and the limited boundary conditions including infiltration and runoff. As discussed earlier, infiltration, runoff, and evapotranspiration could be included by linking TOUGH2 and HELP similar to the procedure used by Morris and Stormont (1996), while generalization of the boundary conditions should be straightforward. In

Table 4 - Summary of Code Evaluation

	Unsaturated Flow Modeling	ET[1]	Nodalization Flexibility	Ease of Modification	Numerical Efficiency
TOUGH2	Full two-phase Richards equation Nonisothermal Isothermal option Hysteresis version Inverse capability with ITOUGH2	No	General 3-D Non-orthogonal Limited boundary conditions	Fairly easy	Fast
FEHM	Richards equation Nonisothermal	No	2-D	Fairly easy	Slow
UNSAT2[2]	Richards equation Isothermal	Yes	2-D		
SWMS_2D	Richards equation Isothermal	Yes	2-D	Fairly easy	Moderate
UNSAT-H[3]	Richards equation Nonisothermal	Yes	1-D Only		
HELP[4]	Simplified - no capillary forces	Yes	Quasi 2-D 1-D unsat. flow		Very Fast

[1]- evapotranspiration.
[2]- not evaluated due to similarity to SWMS_2D.
[3]- not evaluated due to 1-D restriction.
[4]- current landfill cover design code.

addition, hysteresis, which is important in the dominant failure mechanism of capillary barriers, or fingering, can be added to TOUGH2 based on the work of Niemi (1991a,b).

The present code comparison only evaluated steady-state behavior because those are the only results presented by Oldenburg and Pruess (1993) and Ross (1990). While comparison to steady-state results is important, the ultimate application will be to unsteady-state tilted capillary barrier performance where transient conditions dominate. Comparison of TOUGH2 predictions to tilted capillary barrier data by Webb and Stormont (1995) did not show good agreement. However, the differences in those comparison have been attributed to experimental difficulties such as instrument problems and inhomogeneous layers (R.E. Finley and E.E. Ryder, SNL, private communication 7/96), and the lack of evapotranspiration in the TOUGH2 model could be a factor. In contrast, TOUGH2 predictions of the two-dimensional infiltration data of Vauclin et al. (1979) show very good overall agreement (Moridis and Pruess, 1992). Therefore, TOUGH2 should be able to predict the transient unsaturated capillary barrier conditions.

In addition to the capabilities of TOUGH2, inverse modeling is available through the ITOUGH2 code (Finsterle and Pruess, 1995). This capability may be invaluable in the interpretation of experimental data.

4.0 ACKNOWLEDGMENTS

I want to acknowledge the contributions of Clifford Ho and Mehdi Eliassi of the Geohydrology Department for their help in running the problems on FEHM and SWMS_2D, respectively.

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6.0 NOMENCLATURE

g	gravity
k	permeability
k_r	relative permeability
P	pressure
V	Darcy velocity
x	linear dimension
z	vertical dimension

Greek

α	sorptive number for fine layer
α^*	sorptive number for coarse layer
ρ	fluid density
μ	viscosity
ψ	moisture potential

Subscripts

c	capillary
nw	nonwetting phase
w	wetting phase

Appendix
Two-Phase Flow Equations

The Darcy velocity of each fluid is commonly assumed to be given by a two-phase extension of Darcy's Law, or (de Marsily, 1986)

$$V_j = - k \frac{k_{r,j}}{\mu_j} \left(\nabla P_j + \rho_j g \nabla z \right) \qquad \textbf{(A-1)}$$

The equations for one-dimensional flow for each phase for horizontal flow (no gravity) reduce to

$$V_w = - k \frac{k_{r,w}}{\mu_w} \frac{dP_w}{dx} \qquad \textbf{(A-2)}$$

and

$$V_{nw} = - k \frac{k_{r,nw}}{\mu_{nw}} \frac{dP_{nw}}{dx} \ . \qquad \textbf{(A-3)}$$

The difference in the phasic pressures is determined by the capillary pressure curve which is usually expressed as a function of the local saturation. For the case of a wetting and a nonwetting fluid, the capillary pressure is defined as

$$P_c = P_{nw} - P_w \ . \qquad \textbf{(A-4)}$$

Relative permeability is also typically represented as a function of saturation.

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