Ref

NUREG/CR-6114
PNL-8842
Vol. 1

Tech Docs

Application of an Infiltration Evaluation Methodology to a Hypothetical Low-Level Waste Disposal Facility

1456

Manuscript Completed: December 1993
Date Published: December 1993

Prepared by
P. D. Meyer

T. J. Nicholson, NRC Project Manager

Pacific Northwest Laboratory
Richland, WA 99352

Prepared for
Division of Regulatory Applications
Office of Nuclear Regulatory Research
U.S. Nuclear Regulatory Commission
Washington, DC 20555-0001
NRC FIN L2466

9609

Abstract

An analysis of infiltration and percolation at a hypothetical low-level waste (LLW) disposal facility was carried out. The analysis was intended to illustrate general issues of concern in assessing the performance of LLW disposal facilities. Among the processes considered in the analysis were precipitation, runoff, infiltration, evaporation, transpiration, and redistribution. The hypothetical facility was located in a humid environment characterized by frequent and often intense precipitation events. The facility consisted of a series of concrete vaults topped by a multilayer cover. Cover features included a sloping soil surface to promote runoff, plant growth to minimize erosion and promote transpiration, a sloping clay layer, and a sloping capillary barrier. The analysis within the root zone was carried out using a one-dimensional, transient simulation of water flow. Below the root zone, the analysis was primarily two-dimensional and steady-state.

Results of the simulations illustrated the limited value of daily precipitation data. For the humid site studied, hourly rainfall data provided significantly better estimates of the water balance. Results also demonstrated the importance of transpiration in removing water from the soil column, implying a need for accurate models of plant growth and water utilization. In addition, the amount of water predicted to percolate below the root zone was often less than the amount required to keep the clay barrier layer fully saturated, even in the relatively wet environment studied. This could be a concern if the clay were subject to shrinking under unsaturated conditions. The two-dimensional simulations showed that the sloping clay barrier diverted 75 percent of the water reaching it. The sloping capillary barrier, in contrast, diverted more than 99.99 percent of the water reaching it. Performance of the capillary barrier, however, was shown to vary significantly with the hydraulic properties of the two materials of which it is composed. Predicting performance simply by inspecting the water retention and hydraulic conductivity functions was difficult. An analytical expression was presented that can be used to estimate capillary barrier performance and to determine appropriate materials for construction.

Contents

Abstract iii

Foreword vii

Acknowledgments ix

1 Problem Description 1

1.1 Introduction 1
1.2 Site Description 1
1.3 Facility Design 2
1.4 Overview of Analysis 3

2 One-Dimensional Analysis 7

2.1 Summary of One-Dimensional Analysis 13

3 Two-Dimensional Analysis 15

3.1 Clay Barrier Simulation 15
3.2 Capillary Barrier Simulation 16

3.2.1 Analytical Capillary Barrier Solution 20

3.3 Summary of Two-Dimensional Analysis 21

4 Conclusions 23

4.1 Future Work 23

5 References 25

Appendix A: A Qualitative Discussion of Grid Discretization Error 27

Figures

1. Mean monthly precipitation and evaporation data representing the hypothetical facility site 1
2. Plan view of the hypothetical LLW disposal facility illustrating the arrangement of multiple vault/cover units 2
3. Cross section through one of the vault/cover units and details of the cover above the concrete vault 4
4. Conceptualization of infiltration/percolation at the hypothetical facility and division of the problem into a one-dimensional, transient analysis and a two-dimensional, steady-state analysis 5
5. Daily precipitation (Wagener, South Carolina) and pan evaporation (Blackville, South Carolina) for 1984 and 1985 7
6. Leaf area index and potential transpiration fraction for the hypothetical site 8
7. Root length density function for the hypothetical site 8
8. Transpiration sink factor for the hypothetical site 8
9. Volumetric water content and hydraulic conductivity as a function of tension for the one-dimensional model 10
10. Effect on rainfall rate of daily averaging. 10
11. Daily output from the one-dimensional simulation using hourly precipitation data 12

12. Model layout for the simulation of flow through the clay layer. 15

13. Cross-sectional output of the steady-state solution for flow through the clay layer: tension head, lateral flux, and vertical flux 17

14. Volumetric water content and hydraulic conductivity as a function of tension for the materials of the two-dimensional simulations 18

15. Tension profiles 4 m from left edge of concrete using high QC and low QC materials 18

16. Volumetric water content and hydraulic conductivity as a function of tension for the original, high QC and the modified, low QC materials 19

17. Effective capillary barrier length, L, as a function of the flux through the clay, q, as calculated by Equations 8 and 9 for the high QC materials 21

A-1. Layout of problem used to test discretization and slope approximation of the two-dimensional models 27

A-2. Pressure profiles for various grid configurations using the Two-Dimensional Princeton Unsaturated Code and MSTS 28

Tables

1. Parameters of hypothetical disposal facility materials 9

2. One-dimensional model results given in terms of percent of total 1984-85 precipitation 10

3. Comparison of UNSAT-H and HELP model results using 1984-85 Wagener precipitation data 11

4. Parameters for the modified (low QC) capillary barrier materials 19

5. Parameter values used in the analytical capillary barrier solution 21

Foreword

This technical report was prepared by Pacific Northwest Laboratory[1] under a research project with the Waste Management Branch in the Office of Nuclear Regulatory Research (FIN L2466). The report presents numerical simulation results and observations from the application of an infiltration evaluation methodology (previously documented in NUREG/CR-5523) to a hypothetical low-level waste (LLW) disposal facility. This work provides auxiliary infiltration analyses in support of NRC staff development and the testing of a performance assessment methodology for LLW facilities. This document also provides a technical discussion of issues arising from one- and two-dimensional infiltration analyses using a specific engineering design for given site conditions and processes.

NUREG/CR-6114 is not a substitute for NRC regulations, and compliance is not required. The approaches and/or methods described in this NUREG/CR are provided for information only. Publication of this report does not necessarily constitute NRC approval or agreement with the information contained herein.

[1] Pacific Northwest Laboratory is operated for the U.S. Department of Energy by Battelle Memorial Institute under Contract DE-AC06-76RLO 1830.

Acknowledgments

The author gratefully acknowledges the financial assistance of the Office of Nuclear Regulatory Research of the U.S. Nuclear Regulatory Commission (NRC). Tom Nicholson of the NRC is the Technical Monitor for the project, Application of Infiltration Evaluation Methodology to Low-Level Waste Performance Assessment Studies. His enthusiasm for the project has been appreciated. Mark Thaggard of the NRC has been most helpful in defining NRC needs with respect to low-level waste disposal performance assessment. Several staff members at Pacific Northwest Laboratory have contributed to this work. Glendon Gee has provided valuable direction to the project and has freely offered his wealth of experience. Mark Rockhold kindly tolerated an excessive number of questions and participated in numerous fruitful discussions. In addition, his review of this document is appreciated. Mike Fayer provided assistance with the UNSAT-H code. Will Nichols and Mark White provided guidance in using MSTS. Timely and thorough editorial assistance was provide by Kristin Manke. Finally, Richard Hills of New Mexico State University provided clear answers to many of my questions and, in addition, asked many insightful questions of his own that served to stimulate my analysis.

1 Problem Description

1.1 Introduction

One of the crucial issues in the performance assessment of shallow land burial facilities for low-level waste (LLW) disposal is the analysis of water movement within the unsaturated soils above and around the waste. Water moving through the soil cover and into the disposal facility itself is a potentially significant means by which contaminants can be released to the environment.

The primary objective of the infiltration analysis component of a LLW disposal facility performance assessment is to determine the amount of water coming into contact with the waste. The flux of water into the waste containment structure should be less than the natural recharge at the site while the site is operating as designed, and many years after construction when the facility may fail to operate as planned. The flow of water around and within a disposal facility will depend in large part on the local climate, hydrology, and geology and also on the specific facility design, construction, and operation. Predicting the occurrence and movement of water within the facility thus requires the availability of large amounts of data.

The purpose of this document is to illustrate general issues of concern in the analysis of infiltration and percolation for the assessment of LLW disposal facility performance. This analysis contributes to the infiltration evaluation methodology presented in Smyth et al. (1990). To facilitate the current analysis, a realistic but hypothetical LLW disposal facility design was used. The facility was located on a relatively well characterized site for which much of the required data was available. Only as much data as was required for the current analysis will be presented here.

Because an assessment of the disposal facility must be carried out before the facility is actually built, site performance is predicted using models of the facility and its environment. The analysis reported here used three numerical models of water flow in unsaturated porous media. A one-dimensional analysis using UNSAT-H (Fayer and Jones, 1990) was used to model the portion of the cover in and near the root zone. The lower portion of the cover was modeled using the Two-Dimensional Princeton Unsaturated Flow Code (Celia, 1991; Celia et al., 1990) and the Multiphase Subsurface Transport Simulator (White and Nichols, 1993; Nichols and White, 1993). The remainder of this section provides information on the climate and hydrology of the hypothetical site and details of the facility design. In addition, an overview of the method of analysis is given. Chapters 2 and 3 present results of the infiltration analysis.

1.2 Site Description

The hypothetical waste disposal facility is located in an environment typical of the southeast U.S. coastal plain region. Topography of the region is characterized by gently rolling hills, although the waste disposal facility itself is located in a relatively flat region. The climate is characterized by warm, humid summers and mild winters.

Climatic data were taken from a representative National Oceanic and Atmospheric Administration station. Mean annual precipitation is approximately 120 cm/year based on 29 years of data (1960-1989). Rainfall is slightly higher than average during the summer months and slightly lower during the fall as illustrated in Figure 1. Precipitation during the spring and summer months frequently occurs as local-

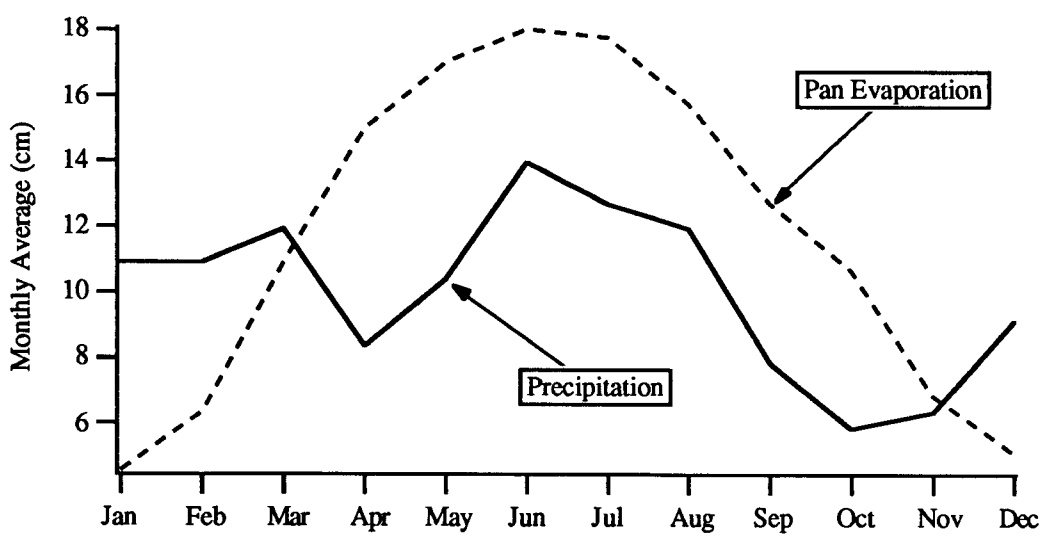


Figure 1. Mean monthly precipitation and evaporation data representing the hypothetical facility site

ized, intense thunderstorms. Winter precipitation tends to occur over a broader area.

The mean monthly measured pan evaporation, also shown in Figure 1, varies significantly with the seasons. Mean annual evaporation based on 26 years of data (1964-1989) is approximately 137 cm/year. Potential evapotranspiration (PET) was assumed to be equal to measured pan evaporation (i.e., a pan coefficient of 1.0 was used). Based on monthly averages, there is a precipitation excess during the winter months and thus an opportunity for significant deep percolation at this time.

Mean monthly maximum temperature ranges from approximately 60 to 90°F. Mean monthly minimum temperature ranges from approximately 35 to 70°F.

1.3 Facility Design

The hypothetical LLW disposal facility consists of an array of underground concrete vaults, each overlain by a multilayer cover. A plan view of the facility is shown in Figure 2. The surface of the covers are sloped to promote runoff. Plant growth on the surface limits erosion and promotes removal of water from the soil column through transpiration. A surface drainage system is located between the covers to effectively carry all runoff offsite.

A cross section through a portion of one of the vault/cover units along with further detail of the cover construction is shown in Figure 3. The figure illustrates several features of the design, in addition to the sloping surface, that restrict water from contacting the waste. The top-soil layer is sufficiently thick to permit plant growth. The sand layer immediately beneath the top-soil functions as a filter to prevent small particles from entering the gravel layer. The gravel is intended to prevent significant root and animal penetration. A sloping clay layer overlain by permeable material provides a low-permeability barrier to flow and promotes subsurface lateral drainage of water that percolates below the root zone. The clay layer is located beneath the region subject to freezing. Immediately beneath the clay is a layer of fine material overlying a much coarser material. These two layers function as a capillary barrier, scavenging water pass-

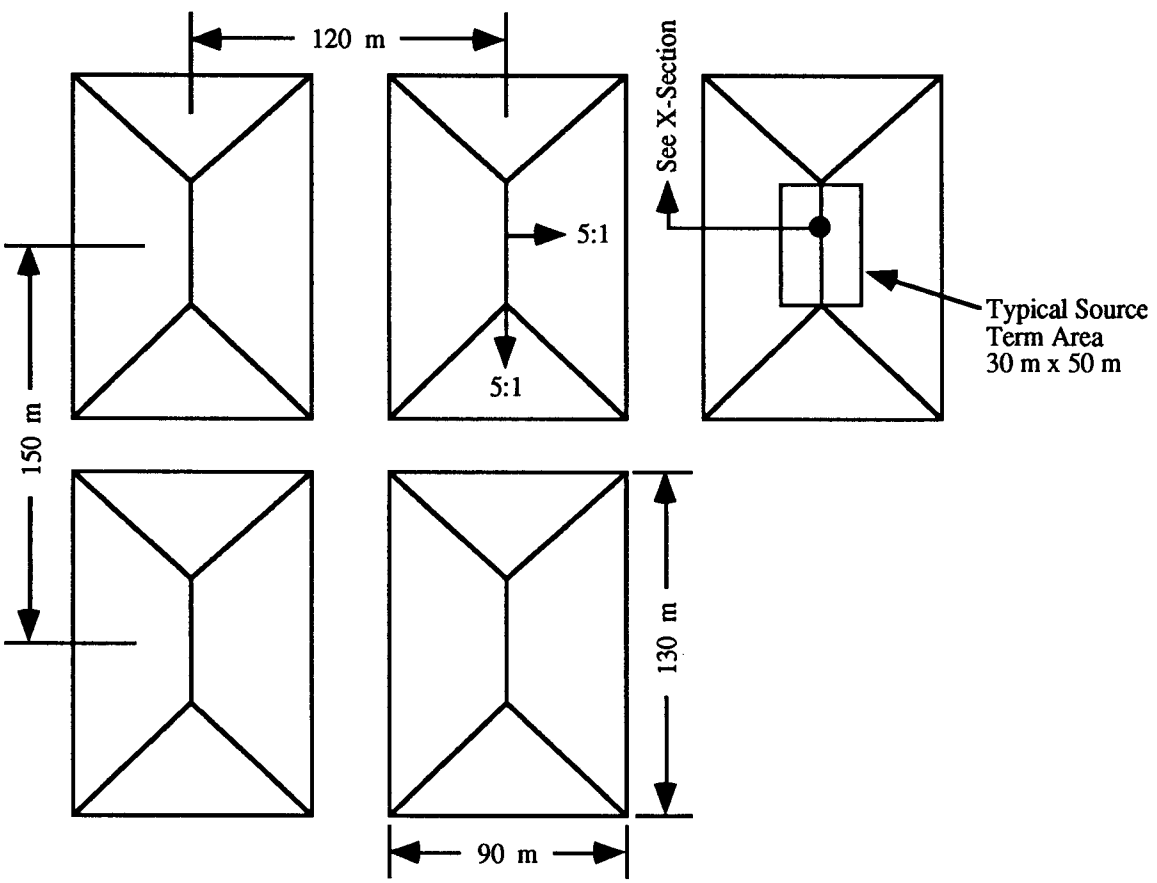


Figure 2. Plan view of the hypothetical LLW disposal facility illustrating the arrangement of multiple vault/cover units

ing through the clay and diverting it around the waste. The final barrier to water flow is the concrete vault itself, which has a low permeability and a sloping top surface to divert water. In addition, the concrete is covered by low permeability bentonite panels

1.4 Overview of Analysis

The approach adopted for the analysis of infiltration and percolation at the hypothetical facility was to divide the problem into relatively independent pieces that could be separately analyzed. The problem was divided according to the time scale of the relevant transient processes. At the surface and within the root zone, transient processes such as rainfall and the variation of evapotranspiration (ET) throughout the day are significant and take place over the course of hours or days. The analysis of this region must account for this transience. Below the root zone, and particularly below the clay layer, the important transient processes are deep penetration of roots, degradation of the clay and concrete barriers, and fouling of the capillary barrier. Because these processes take place over years or tens of years, a steady-state analysis may be applicable for this region.

Figure 4 illustrates some of the relevant processes involved in the movement of water from the surface of the disposal facility to the concrete vault. In general, the time scale of the processes increases from top to bottom. The dashed boxes represent the division in the analysis. The upper box contains processes that were examined using a transient, one-dimensional analysis. Processes contained in the lower box were part of a two-dimensional, primarily steady-state analysis. The following two chapters discuss the one-dimensional and two-dimensional analyses. The particular models used in each analysis are presented as well as results from the application of the models.

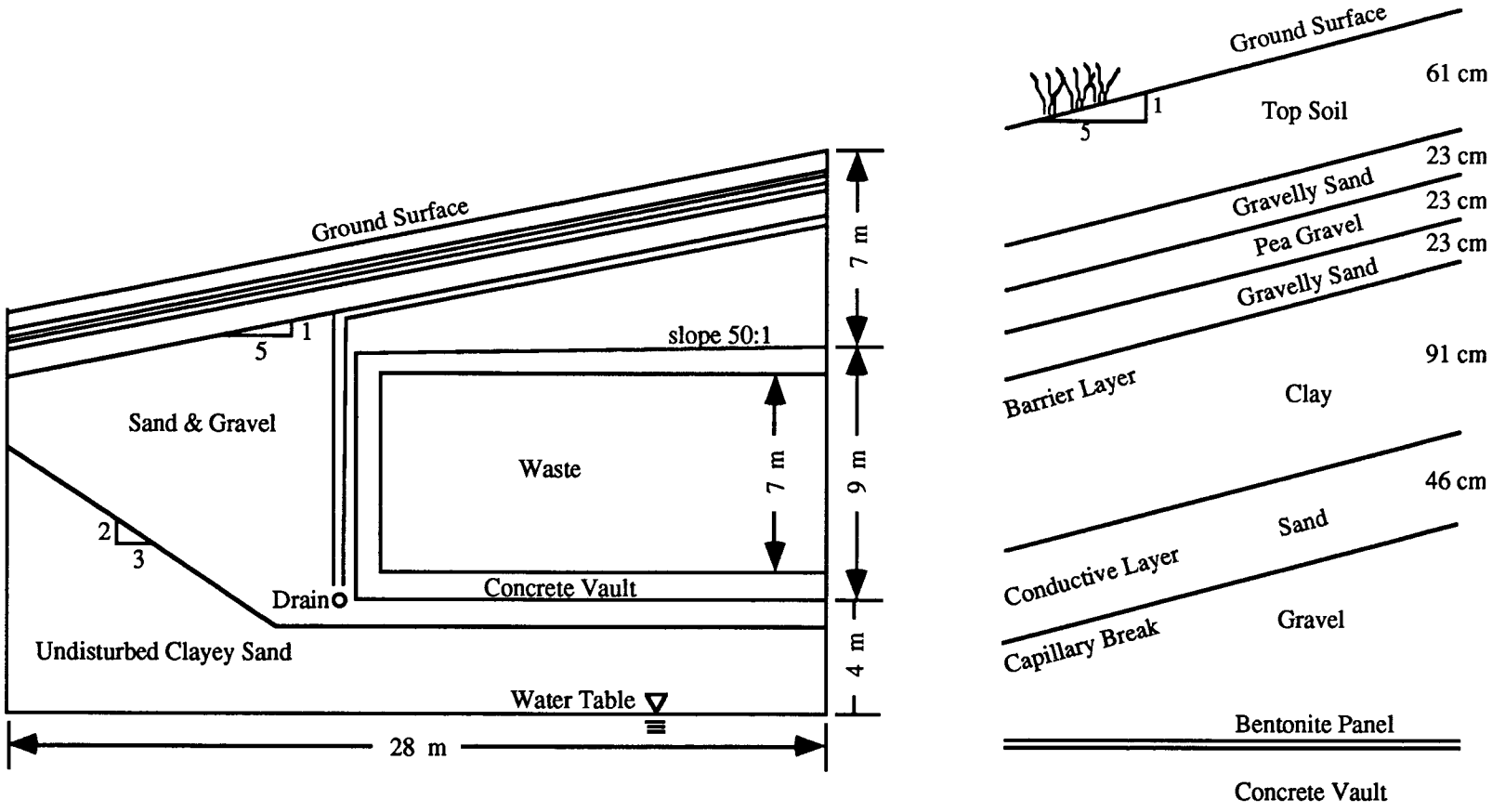


Figure 3. Cross section through one of the vault/cover units (left) and details of the cover above the concrete vault (right)

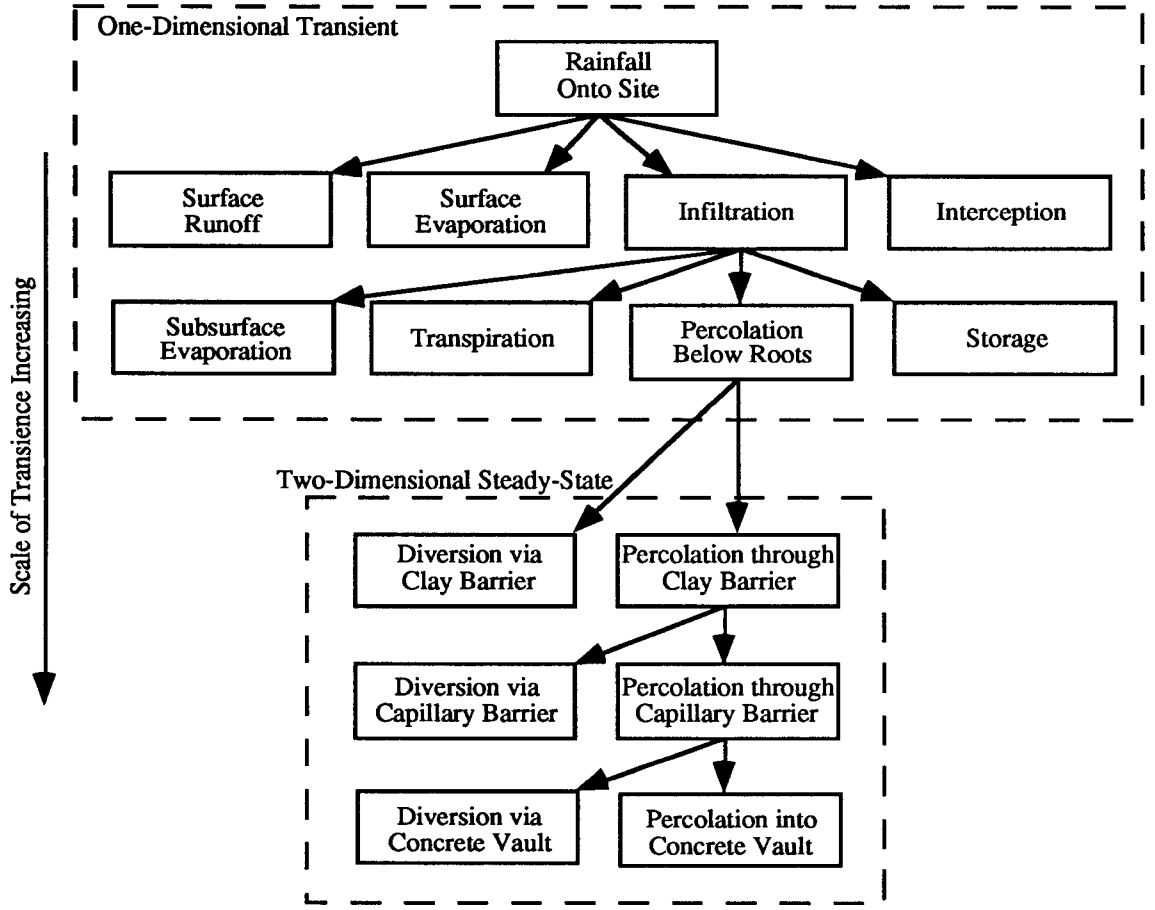


Figure 4. Conceptualization of infiltration/percolation at the hypothetical facility and division of the problem into a one-dimensional, transient analysis and a two-dimensional, steady-state analysis

2 One-Dimensional Analysis

The illustrations of the site design (Figures 2 and 3) clearly show that two- (and perhaps three-) dimensional flow of water will take place throughout the facility. The success of the facility depends on this. It is nevertheless possible to learn much of importance about the performance of the facility design using a simpler one-dimensional analysis. Although surface runoff will clearly have a large horizontal component, water that infiltrates will primarily flow in a vertical direction until reaching the clay layer. Thus, the first step in the analysis was the development of a one-dimensional model of the top four layers of the cover. This model was used to address several important issues: determination of the key processes influencing the near-surface water balance, estimation of the surface and subsurface drainage requirements, and estimation of the amount of water available for percolation into the clay layer.

The one-dimensional code selected for use was UNSAT-H (Fayer and Jones, 1990). The physical processes modeled by this code include precipitation, evaporation from the soil surface, infiltration, transpiration, redistribution, and drainage. During rainfall, however, UNSAT-H does not allow evaporation or transpiration. Precipitation and evaporation inputs are allowed to vary over time. Evaporation can be calculated from either daily weather data or PET values input by the user. For the hypothetical site, PET values derived from measured pan evaporation were used. As previously mentioned, the pan coefficient used was 1.0; thus, PET was equivalent to pan evaporation. Representative hourly precipitation measurements were obtained from the National Climatic Data Center for Wagener, South Carolina. Daily precipitation data for the same years at Blackville, South Carolina, were also used (hourly data was not available). The years of 1984 and 1985 were selected for the initial analysis because the total precipitation for each year (116 and 125 cm, respectively, for Wagener; 123 and 112 cm, respectively, for Blackville) was close to the average (120 cm). Interception was assumed to be negligible. Daily pan evaporation measured at Blackville was also used. Total yearly pan evaporation for the two years was 151 and 144 cm. Daily values of rainfall and evaporation are plotted in Figure 5.

Runoff is calculated in UNSAT-H as the amount of precipitation applied at a rate in excess of the maximum infiltration rate. The maximum infiltration rate is determined by the maximum pressure head, a parameter input by the user. For the hypothetical facility, the maximum pressure head of the

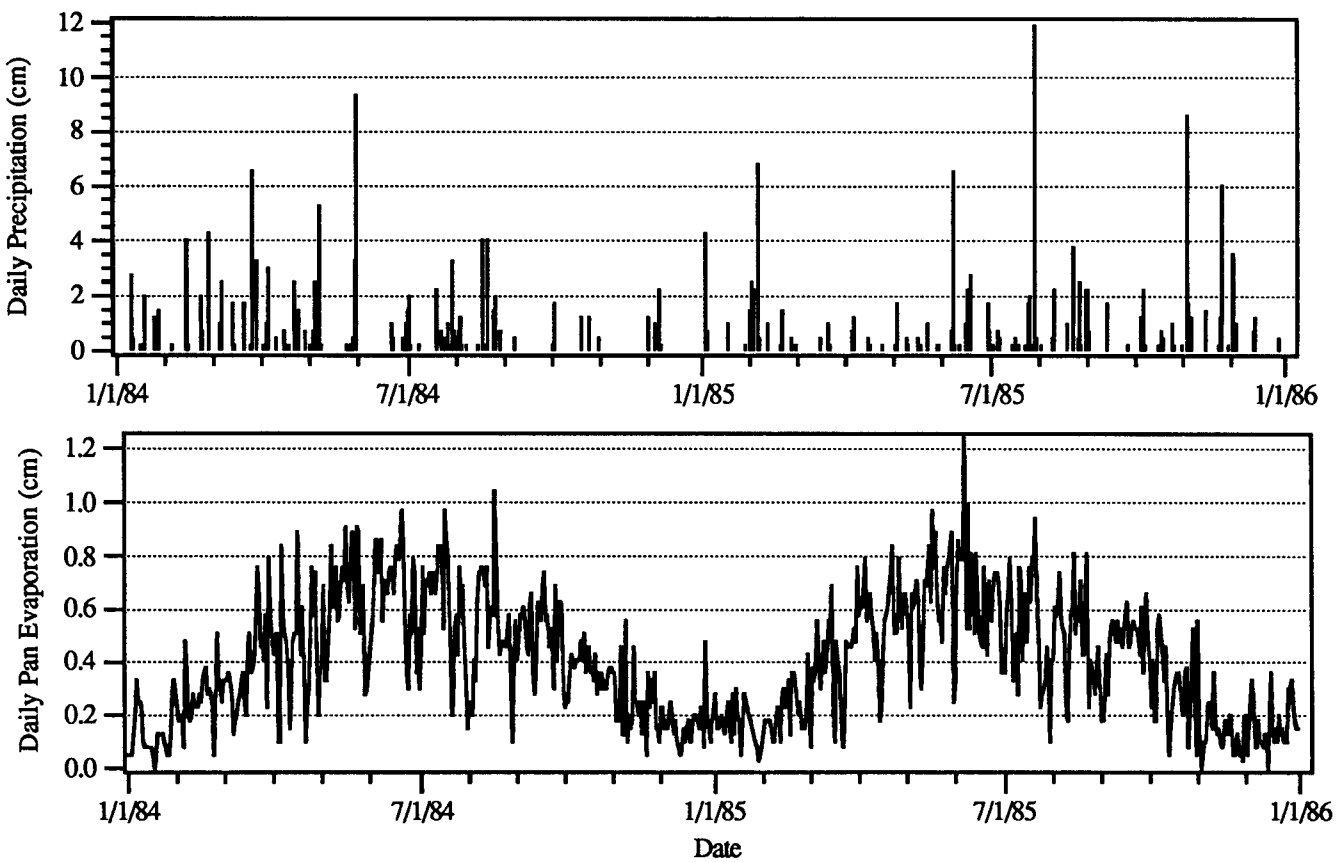


Figure 5. Daily precipitation (Wagener, South Carolina) and pan evaporation (Blackville, South Carolina) for 1984 and 1985

top soil was taken to be zero. Therefore, positive pressure at the soil surface during a precipitation event resulted in a portion of the precipitation being partitioned into a runoff component. Infiltration is defined here as the vertical movement of water into the soil surface.The method used by UNSAT-H results in a maximum amount of runoff. Under actual conditions, plant growth may limit runoff and enhance infiltration and, potentially, drainage. If this is the case, UNSAT-H may underpredict the amount of drainage.

Transpiration, or water uptake by plants, is represented in UNSAT-H as a sink at nodes within the root zone. The potential (maximum) transpiration (PT) is calculated as a fraction of PET and is a function of the leaf area index (LAI). The LAI used to model the hypothetical site varied over the year such that PT constituted 97 percent of PET during June, 94 percent of PET during July and August, and 100 percent of PET during the rest of the year (see Figure 6).

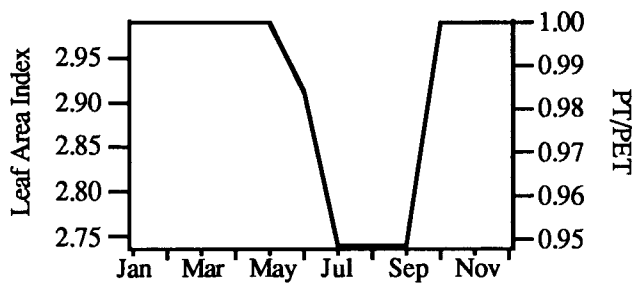


Figure 6. Leaf area index and potential transpiration fraction for the hypothetical site

UNSAT-H distributes PT over the root zone according to the root density, which declines exponentially with depth. The maximum depth of root penetration for the hypothetical site was 50 cm, limiting root growth to the top-soil layer. Figure 7 shows the root length density function used.

Actual transpiration at each node will be less than PT, depending on the node's tension *(h)*. (Tension is the negative of the pressure head, ψ). At a tension below $h=H_n$, plants cease to transpire because of anaerobic conditions. When the tension is high, plants have difficulty drawing water from the soil. The point at which transpiration begins to be reduced is denoted as H_d. The tension above which plants wilt and all transpiration ceases is denoted as H_w. Representative values for H_n, H_d, and H_w were chosen as 30 cm; 10,000 cm; and 14,000 cm; respectively. Figure 8 illustrates the transpiration fraction as a function of the moisture content.

The UNSAT-H code solves the pressure-based form of Richards equation for unsaturated flow (Richards, 1931), which can be written as

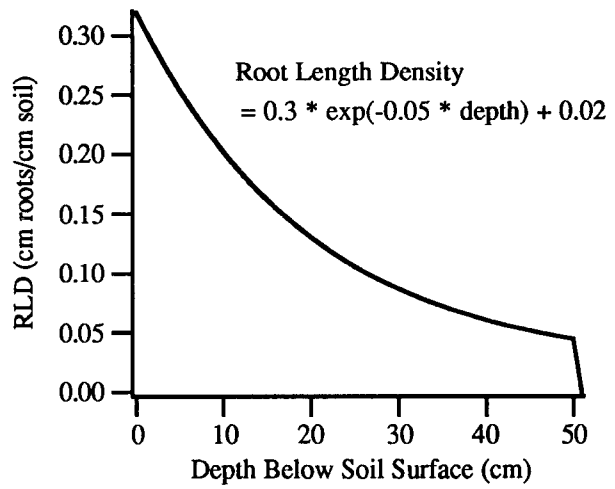


Figure 7. Root length density function for the hypothetical site

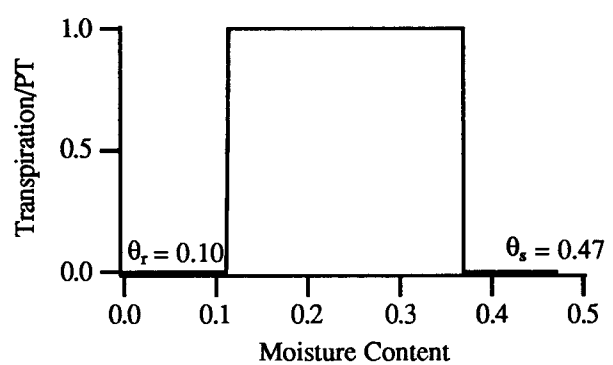


Figure 8. Transpiration sink factor for the hypothetical site

$$C(\psi)\frac{\partial\psi}{\partial t} = \nabla\bullet K(\psi)\nabla\psi - \frac{\partial K}{\partial z} \qquad (1)$$

where ψ is pressure head, $C(\psi)=d\theta/d\psi$ is the specific moisture capacity, and $K(\psi)$ is the unsaturated hydraulic conductivity. The constitutive equations used to relate the unsaturated hydraulic conductivity and the moisture content to the pressure head were the van Genuchten functions (van Genuchten, 1978):

$$\theta(\psi) = \theta_r + (\theta_s - \theta_r)\,[1 + (\alpha\psi)^n]^{-m} \qquad (2)$$

where α, m, and n are curve fitting parameters with $m=1-1/n$ and θ_r and θ_s are the residual and saturated moisture content, respectively. The conductivity function was that derived by van Genuchten (1980) based on the Mualem model (Mualem, 1976)

Table 1. Parameters of hypothetical disposal facility materials

Material Name (refer to Figure 3)	Water Content		van Genuchten Parameters		Saturated Hydraulic Conductivity (cm/s)
	Residual	Saturated	α (cm^{-1})	n	
Top Soil	0.10	0.47	0.0440	1.523	1.00e-04
Upper Gravelly Sand	0.02	0.32	0.1008	2.922	1.00e-02
Pea Gravel	0.03	0.26	4.6950	2.572	1.00e+00
Lower Gravelly Sand	0.02	0.34	0.1008	2.922	1.00e-02
Clay	0.0001	0.36	0.0016	1.203	1.00e-07
Sand (Conductive Layer)	0.045	0.37	0.0683	2.080	3.00e-02
Gravel (Capillary Break)	0.014	0.51	3.5366	2.661	1.85e+00
Concrete	0.08	0.40	0.0063	1.080	1.00e-08
Undisturbed Clayey Sand	0.21	0.30	0.0035	3.000	1.40e-07

$$K(\psi) = K_s \frac{\{1 - (\alpha\psi)^{n-1}[1 + (\alpha\psi)^n]^{-m}\}^2}{[1 + (\alpha\psi)^n]^{0.5m}} \quad (3)$$

where K_s is the saturated hydraulic conductivity. Hysteresis was not simulated. The parameter values required for this model can be found in Table 1. Volumetric water content and hydraulic conductivity are plotted as a function of tension in Figure 9, respectively, for the top four layers (the upper and lower sand are nearly identical).

Nodal spacing of the one-dimensional model varied with depth; spacing was reduced at the surface and at the interfaces between layers. The total number of nodes used was 104 over the 1.2 m depth simulated. The geometric average was used for internodal conductivities. During rainfall, a specified flux was applied at the upper boundary equal to the precipitation rate. If at any time the pressure head exceeded 0.0 cm, the surface node was held at a constant pressure of 0.0 cm until the pressure fell below this value. Similarly, a flux equal to the potential evaporation was applied at the surface node between rainfall events. If the pressure fell below the minimum allowable value of -15.3 m, the surface node was held constant at this value. The bottom boundary was specified to have unit hydraulic head gradient.

Three simulations were carried out using daily rainfall data from Blackville, daily rainfall from Wagener, and hourly rainfall data from Wagener. All three simulations used daily PET data from Blackville. The error generated by using Blackville PET data with Wagener precipitation data was expected to be small because of the proximity of the two measurement stations. No attempt was made to determine the correlation between Blackville and Wagener rainfall data. Such a correlation analysis would be necessary in an actual site application. All three simulations extended over a 2-year period using 1984 and 1985 precipitation data. For the simulations in which daily precipitation values were used, the total daily rainfall amount was evenly applied over a 24-hour period. For the simulation in which hourly precipitation data was used, each hour's rainfall was applied over that hour only.

Averaging the precipitation over 24 hours has a pronounced effect on the rainfall rate. Figure 10 illustrates the effect for a 2-week period of the Wagener data. Using daily precipitation values significantly reduces the rate of precipitation and can consequently be expected to reduce the amount of runoff, and increase the amount of infiltration.

Table 2 shows the results of the simulations in terms of the partitioning of total cumulative precipitation over the 2-year period. Note that interception losses are assumed to be negligible and that all evaporative losses occur from the soil surface after infiltration.When daily average precipitation is used, very little of the rainfall ends up as surface runoff. Nearly all of the precipitation infiltrates and a large proportion (about 30 percent) ends up draining out the bottom of the soil column. In contrast, using hourly rainfall data

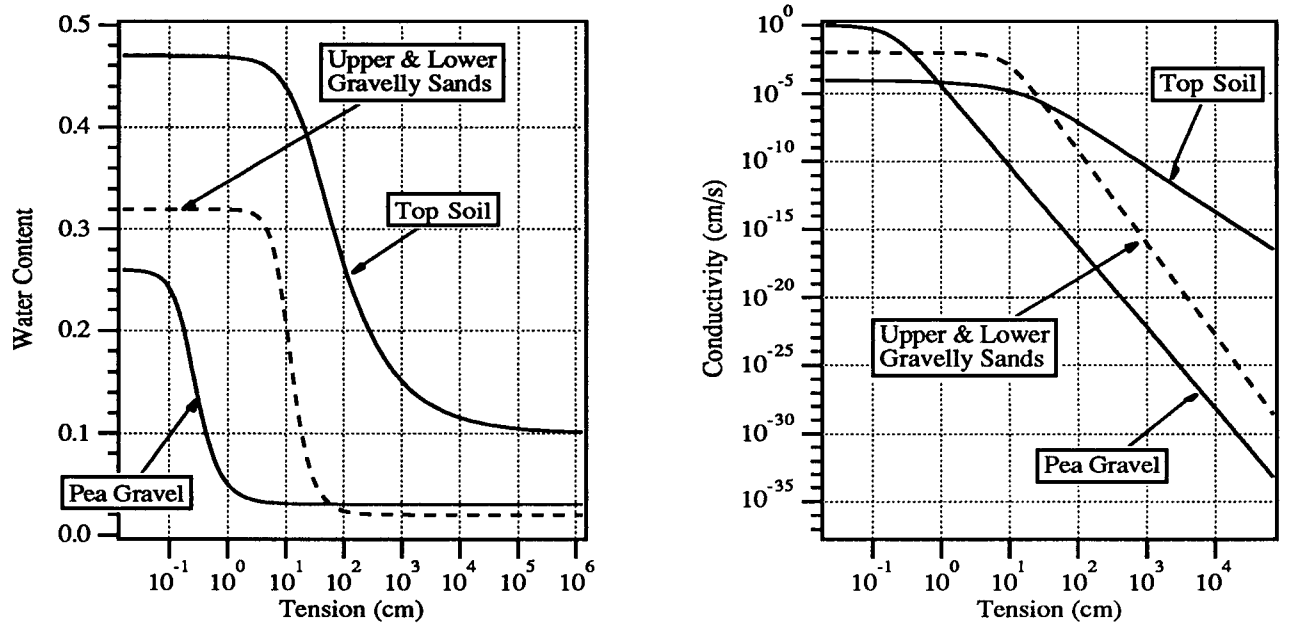


Figure 9. Volumetric water content (left) and hydraulic conductivity (right) as a function of tension for the one-dimensional model

results in the allocation to surface runoff of over one-third of the precipitation. Drainage is correspondingly reduced to a few percent of precipitation. In all cases nearly two-thirds of the precipitation is allocated to ET. The net change in storage over the 2-year simulation is small, as would be expected over the long term. This results from applying initial tensions of 50 cm to the top soil, 20 cm to the upper sand, 2 cm to the gravel, and 15 cm to the lower sand. Because these results clearly indicate that inaccuracies are introduced by the use of daily precipitation data at this site, the remainder of this section will discuss the hourly precipitation results only.

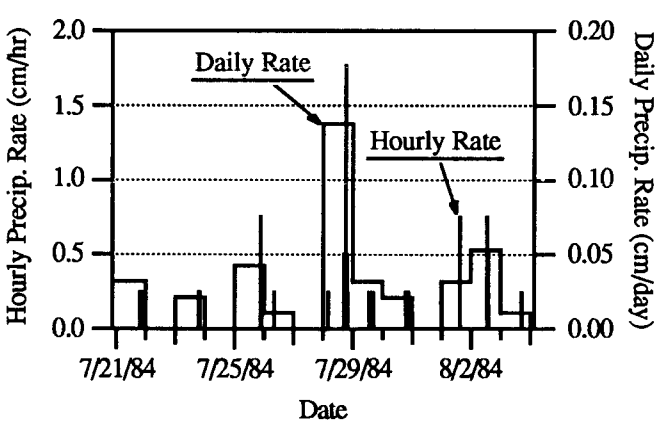


Figure 10. Effect on rainfall rate of daily averaging

Table 2. One-dimensional model results given in terms of percent of total 1984-85 precipitation

	Blackville Precipitation (Daily Only) (%)	Wagener Precipitation (%)	
		Daily	Hourly
Runoff	2.9	7.0	36.7
Infiltration	97.1	93.0	63.3
Evapotranspiration	62.2	63.8	60.5
Drainage	35.0	29.5	4.0
Storage	0.0	-0.2	-1.3

Figure 11 shows daily results for the simulation using hourly precipitation data from Wagener. The top plot shows daily storage (left axis) and drainage at the bottom of the column (right axis). Note that the majority of drainage during the 2-year period occurs during the early months of the simulation. Twenty percent of the drainage occurs on the first 2 days, in fact. This is a result of the wet initial conditions. To investigate the effect on the overall results, the initial conditions were altered by simulating water flow through the column during 1983 using hourly data from Wagener and average PET data.The final pressures from this simulation were used as the initial conditions for 1984.

This resulted in drier initial conditions, but little change in the results of Table 2 (third column). Drainage was reduced from 4.0 to 3.1 percent of precipitation. The change in storage was reduced from -1.3 to -0.5 percent. Runoff, infiltration, and ET were unchanged.

Figure 11 shows that storage and drainage remained high throughout the spring of 1984 until plant transpiration began to dominate the water balance. Storage recovered somewhat during the second winter, but there was insufficient rain to produce significant drainage during this period. The latter half of 1985 was fairly wet and storage had recovered somewhat by the end of the simulation. Drainage, however, continued to decrease. Figure 11 also illustrates the importance of runoff. The largest daily rainfall of the 2 years occurred at the end of July 1985. Of the 12 cm that fell, only 2 cm infiltrated. This large rainfall had a marginal effect on storage and no effect on drainage.

Evapotranspiration represents the single largest sink of water. Figure 11 illustrates the relatively slight contribution to ET of the evaporation component. Of the total predicted ET, approximately 90 percent occurred as transpiration. This is a consequence of the plant model used, as previously discussed.

The amount of ET predicted by UNSAT-H represents just 50 percent of the PET. Transpiration is limited by two factors. First, during rain events, no transpiration (or evaporation) occurs. Table 2 suggests, however, that the total amount of ET at the hypothetical facility is insensitive to the average rate of rainfall. The second factor limiting transpiration is the reduction that takes place when soil water pressure becomes very high or very low. This is controlled by the plant parameters H_w, H_d, and H_n. A comparison of Figure 11 and the PET plot of Figure 5 shows that a lack of water in the soil column limited transpiration during all but the first few months of the simulation. Obtaining accurate values for the plant parameters may thus be crucial to accurately predict ET and drainage.

The integrity of the clay barrier is a critical factor in the success of the cover. The clay directly prevents water movement because of its low permeability, but it also limits the amount of water reaching the capillary barrier. If the clay barrier fails, the likelihood of the capillary barrier failing is increased. There are two primary mechanisms by which the clay layer may fail to restrict the flow of water. If there is insufficient water to keep the clay layer nearly saturated, it is possible that the clay may shrink, resulting in cracking and the opening of macropores in the clay. In this event, water may percolate through the clay layer at a rate much higher than the saturated hydraulic conductivity of the clay matrix. The amount of drainage predicted when using hourly precipitation data is approximately 1.5×10^{-7} cm/s (4 percent of 241 cm over 2 years). This is slightly larger than the saturated hydraulic conductivity of the clay, $K_s = 1.0\times10^{-7}$ cm/s. The majority of the drainage occurs during just a few months, however, and during the remainder of the simulation the flux of water arriving at the clay layer is 10 to 100 times less than K_s of the clay.

Evidence that desiccation of a clay barrier can occur on a significant scale and in a short period of time was recently presented by Melchior et al. (1993). Their large-scale field test examined several cover designs including one similar to the hypothetical design used here. Melchior et al. found that a 60 cm compacted soil liner (17 percent clay, 26 percent silt, 52 percent sand, and 5 percent gravel; lab measured $K_s = 1.0\times10^{-8}$ cm/s) overlain by 25 cm of coarse sand and 75 cm of grass-vegetated top-soil began to pass significant quantities of water after only 20 months of operation. Preferential flow paths had been opened through desiccation during a dry summer. This occurred despite careful construction procedures and minimization of shrinkage potential through appropriate choice of materials (clay composition was 50 percent illite, 30 percent smectite, and 20 percent kaolinite and chlorite). In the fifth year of operation, sufficient quantities of water passed through the compacted soil layer to cause failure of an underlying capillary barrier. At the same location and over the same period of time, desiccation did not occur in a cover design utilizing a flexible membrane liner (welded high-density polyethylene) immediately above the compacted soil layer (Melchior et al., 1993).

In the long term, the integrity of the clay layer may also be compromised by the penetration of roots and animals. A gravel layer is probably insufficient protection against this type of degradation, especially with respect to root penetration.

As a point of reference, the one-dimensional simulation results were compared to results generated using the HELP model (Schroeder et al., 1992). The parameters of the HELP model were set such that the two simulations were approximately equivalent. Because HELP is largely an empirical model and UNSAT-H is largely a mechanistic model, the two simulations could not be made strictly equivalent. Daily precipitation data from Wagener was used. The four layers above the clay were modeled: depth, porosity, saturated hydraulic conductivity, and initial water content in each layer were identical to the UNSAT-H simulations. The moisture retention functions (Figure 9) were evaluated at tensions of 33 cm and 1500 cm to determine field capacity and wilting point, respectively, for each layer. The evaporative depth was 50 cm, the leaf area index was 2.99, the vegetative cover was excellent grass, and the SCS runoff curve number was 80.

Summary results for the 2-year HELP simulation are presented in Table 3. The HELP model predicts about the same amount of runoff as UNSAT-H (using daily rainfall data), but predicts substantially more ET, and consequently less drainage.The difference in ET values may be accounted for by the plant models used. UNSAT-H takes less water from

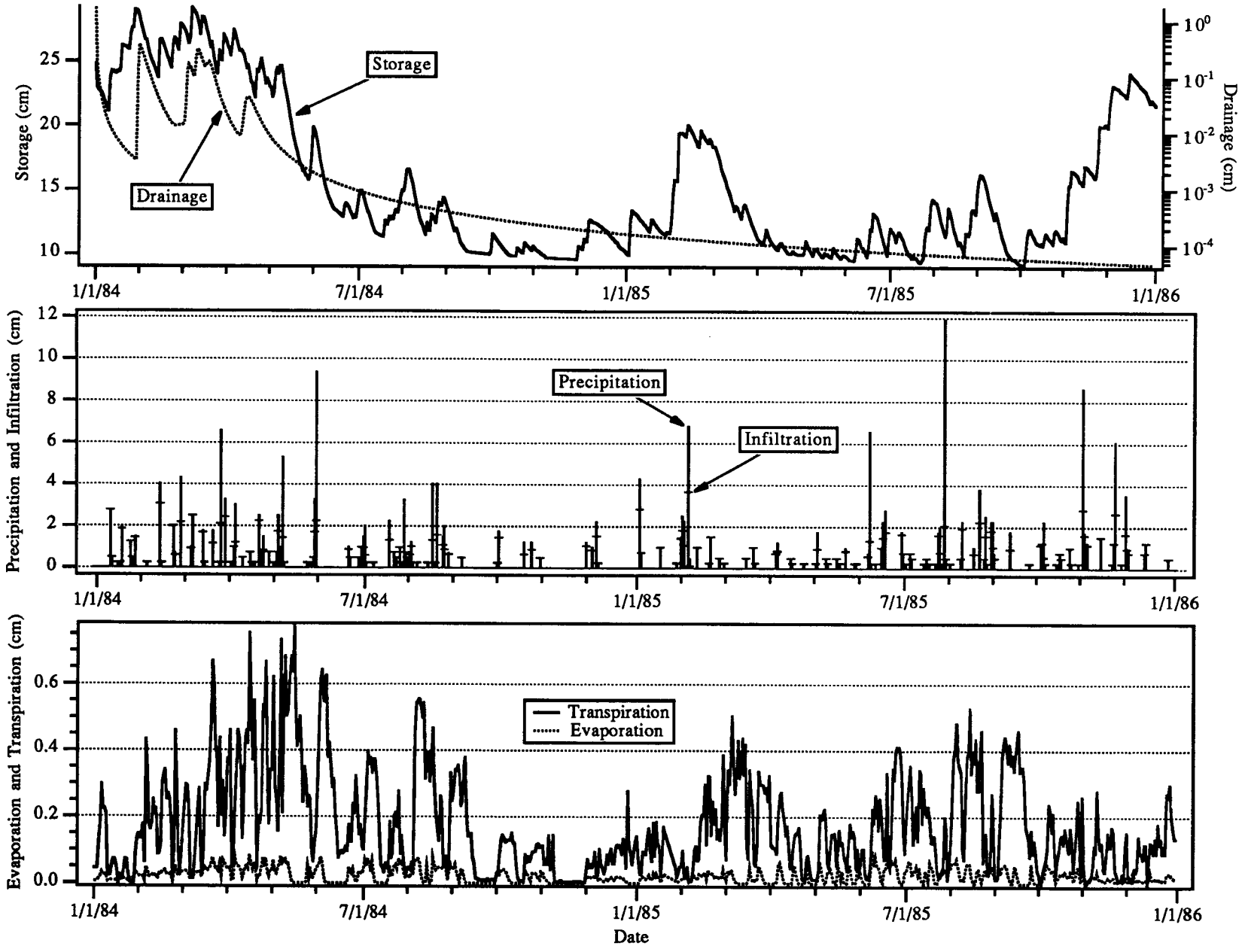


Figure 11. Daily output from the one-dimensional simulation using hourly precipitation data

depth because of the exponential decay in root density (Figure 7). HELP does not account for changes in tranpiration with depth. The hourly results from UNSAT-H are also given in Table 3 for reference. Differences in the HELP results and the UNSAT-H hourly results can be attributed to the use of daily rainfall data by HELP and to the plant models used, as described above.

Table 3. Comparison of UNSAT-H and HELP model results using 1984-85 Wagener precipitation data

	UNSAT-H Daily (%)	HELP Daily (%)	UNSAT-H Hourly (%)
Runoff	7.0	8.9	36.7
Evapotranspiration	63.8	80.7	60.5
Drainage	29.5	8.9	4.0

2.1 Summary of One-Dimensional Analysis

The results of the one-dimensional simulations illustrate, above all, the limited value of daily precipitation data in predicting the manner in which rainfall will be partitioned between runoff and drainage. For a humid site subject to short duration, intense rainfall events, hourly data are required.If hourly data are not available, assumptions about the actual distribution of rainfall must be made to produce results that are both more realistic and more conservative. The simulation results also demonstrate the importance of transpiration in removing water from the soil column and thus controlling percolation. Accurate models of plant growth and water utilization are therefore of prime importance. Finally, the results showed that during much of the year the amount of water reaching the clay layer may be less than that required to keep it saturated, even in a relatively wet environment. If the success of the facility cover depends on maintaining a nearly saturated clay barrier, then a flexible membrane liner above the clay, or some alternative barrier method, may be required. Simulating water flow through a flexible membrane liner poses some difficulties and it may be difficult to predict the behavior of such a cover system.

The one-dimensional analysis discussed above assumes that all plant and soil properties are homogeneous in space and constant in time. In reality, neither of these conditions is likely to be true. Variations in properties over space and time can have a significant impact on the flow of water through the cover. In addition, the 2-year simulation is too short to adequately sample the year-to-year variability in climate. Both short- and long-term predictions of the amount of water percolating to the clay layer are thus uncertain. Incorporation of this uncertainty in the analysis remains a topic for future study.

3 Two-Dimensional Analysis

The one-dimensional simulation of the top four layers of the cover incorporated the transient processes of most importance at the site: precipitation and evapotranspiration (ET). These transient processes produce a transient drainage at the base of the column. The drainage exhibits much less variability, however, than either precipitation or transpiration (see Figure 11). The analysis presented in this section assumes that the fluctuations in drainage have little effect on the flow of water within and below the clay layer. With this assumption, the focus of the analysis becomes the determination of the steady-state pressure field.

The design of the disposal facility requires that a multidimensional analysis be carried out to obtain accurate estimates of the pressure. The sloping clay layer and the sloping capillary barrier produce significant lateral flow. The analysis described in this section is primarily steady-state and two-dimensional, and involves the simulation of a cross section through one of the vaults.

The analysis of this chapter includes neither the bentonite panel located above the concrete nor a low permeability geomembrane potentially located above the clay layer. These two components were not included in the analysis because of the difficulty in incorporating them into conventional models of unsaturated flow. In addition, the long-term integrity of these materials is very uncertain.

3.1 Clay Barrier Simulation

The results of the one-dimensional simulation suggest that, unless the integrity of the clay barrier is compromised, assuming a flux through the clay equal to its saturated hydraulic conductivity will be conservative. That is, the amount of water available for percolation into the clay layer will be no more, and may often be less, than K_s of the clay. Because the clay layer is sloped to promote lateral drainage, however, the flux of water through the clay may vary spatially. At the peak of the facility cover, the flux will be smaller than near the edges of the facility. In order to investigate the nature of flow through the clay layer, a simple two-dimensional, three-layer model was developed.

The simulation was carried out using MSTS, a public-domain, two-phase, two-component, flow and transport simulator for variably saturated porous media (White and Nichols, 1993; Nichols and White, 1993). MSTS uses an integrated finite difference solution method and a Newton-Raphson linearization. In two dimensions and using a Cartesian coordinate system, MSTS discretizes the domain into rectangular control volumes. Irregular boundaries can be accommodated by specifying inactive nodes, which are excluded from the computations.

The model consisted of a layer of clay sandwiched between two layers of gravelly sand, as shown in Figure 12. The hydraulic properties of the materials were previously given in Table 1. (The lower gravelly sand was used.) Parts of the domain were specified as inactive. Some of the boundary conditions were thus specified on interior cell faces. The lower boundary was located a sufficient distance from the clay layer such that it did not influence the solution at the base of the clay. A sand channel was left open at the lower end of the clay layer to allow the passage of water draining down the clay.

The uniform discretization used in the simulation was 15.2 cm in width and 6.1 cm in depth (67 by 77 nodes). Geometric averaging was used to calculate internodal conductivities in this and all subsequent MSTS simulations. The steady-state flux applied at the top was 1.53×10^{-7} cm/s, which is a rate equivalent to the average drainage flux over the 2-year simulation period predicted by the one-dimensional model using hourly rainfall data (Table 2). The bottom boundary was held at a pressure head of zero. For a discussion of the errors resulting from the chosen grid dis-

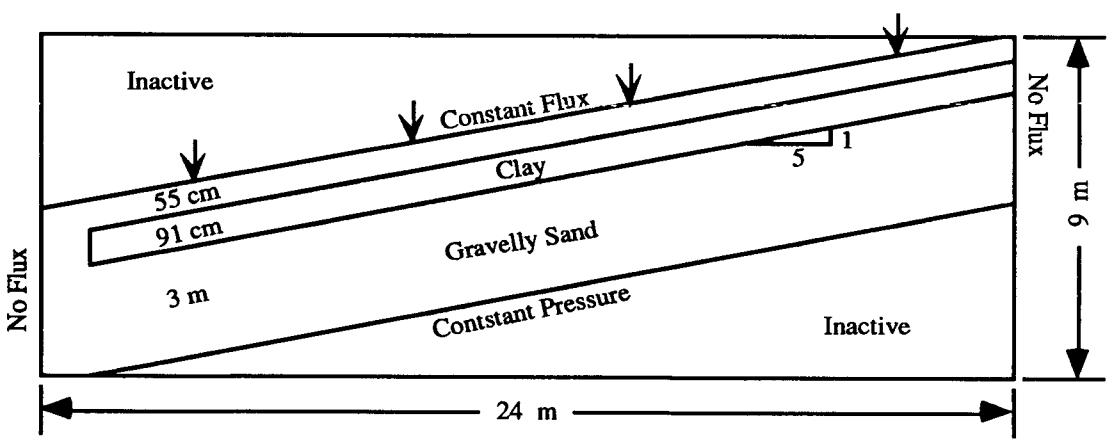


Figure 12. Model layout for the simulation of flow through the clay layer. Arrows at top of active domain indicate locations of cross-sectional output

cretization and the use of a rectangular grid to approximate a sloping boundary, see Appendix A.

Selected cross sections through the top sand layer and the clay layer of the steady-state solution obtained with MSTS are shown in Figure 13. Soil tension decreases from the top of the active domain, reaching a minimum value just above the top of the clay layer. This is the point of maximum saturation. The tension then increases with depth until reaching a constant value just below the bottom of the clay. Variation in tension with distance from the left boundary is apparent, but relatively small (less than 5 cm).

In contrast to the tension, the fluxes vary with distance from the left boundary by approximately an order of magnitude at the top of the clay layer. In addition, the fluxes are discontinuous at this point. Lateral flow takes place primarily immediately above the clay layer. Flow is downslope (in the negative x-direction, although it is plotted as positive in Figure 13) at this point. Within and below the clay the lateral component of flow is much smaller and takes place in the positive x-direction because of the increasing saturation in the downslope direction. The vertical flow takes place exclusively in the downward direction and is nearly constant within and below the clay layer. The flux through the clay, 4.0×10^{-8} cm/s, is approximately 25 percent of the upper boundary flux and is only 40 percent of the saturated hydraulic conductivity of the clay (1.0×10^{-7} cm/s). Note that the vertical flux through the clay varies only marginally with distance from the left boundary.

3.2 Capillary Barrier Simulation

This section describes a two-dimensional model of the waste disposal facility that uses the bottom of the clay layer as the upper boundary with a constant flux set to K_s of the clay. This model is conservative in the sense that it will predict a larger than expected flux through the capillary barrier and into the concrete vault.

The Two-Dimensional Princeton Unsaturated Code (Celia, 1991) was used in the capillary barrier model. The Princeton code solves the mixed formulation of the Richards equation

$$\frac{\partial\theta}{\partial t} = \nabla\bullet\, K(\psi)\,\nabla\,\psi + \frac{\partial K}{\partial z} \qquad (4)$$

using a modified Picard linearization (Celia et al., 1990). The numerical solution method is finite elements using both triangular and rectangular elements with linear and bilinear basis functions, respectively. Thus, the code can exactly represent the geometry of sloping layers such as those found in the hypothetical facility.

The Princeton code was written for instructional and research uses and therefore does not have all the features and options of many of the commercial codes. One of the necessary improvements that was made to the code was the addition of an iterative solver. The NSPCG package (Oppe et al., 1988) was integrated into the code. NSPCG contains a wide variety of iterative solvers; the conjugate gradient method with a modified incomplete LU preconditioner was selected for solving the unsaturated flow problem. Additional changes were made to improve the output generated by the code.

The layout of the model is identical to the two-dimensional cross section shown in the left side of Figure 3, minus the top five layers. As stated, the upper boundary was set at a constant flux equal to the saturated hydraulic conductivity of the clay layer. The lower boundary was set to a constant pressure head of zero. The side boundaries were specified as zero flux. The boundary on the right arises from symmetry conditions while that on the left was assumed to be far enough from the concrete vault to minimize its effect on the region of concern.The model contained 99 nodes in the horizontal direction and 75 nodes in the vertical direction. Spatial discretization was variable. The finite element formulation of the Princeton code uses the arithmetic average for internodal conductivities.

As with the previous simulations, the van Genuchten model was used for the water retention and hydraulic conductivity relationships. Parameters for this model were given in Table 1. The waste was assumed to have characteristics identical to the concrete. The pressure saturation and pressure-conductivity relationships for the materials of the two-dimensional model are shown in Figure 14. The functions for clay are included for completeness.

The Princeton code was used to run a transient simulation of the hypothetical facility. The initial pressure head at each node was set equal to the elevation of that node above the water table. Using this initial condition, all water redistribution was caused by the influx at the top boundary.

Figure 15(A) is a plot of tension profiles near the top of the model domain. The profiles were taken at a location approximately 4 m from the left edge of the concrete vault. Each profile is labeled with a corresponding simulation time. The results suggest that the capillary barrier is successfully diverting nearly all of the water being input at the top of the model. After 1050 days, there has been no change in the tension 30 cm below the capillary break interface.

A close examination of Figure 15(A) indicates, however, that the system has not reached steady state after 1000 days. It therefore cannot be said with certainty that the capillary barrier will ultimately prevent percolating water from reaching the concrete vault. As Figure 15(A) shows, the tension head at the capillary break interface reaches the critical value of 1 cm after about 1000 days. This is the tension at which the hydraulic conductivity of the capillary break is nearly equal to that of the conductive layer (see Figure 14).

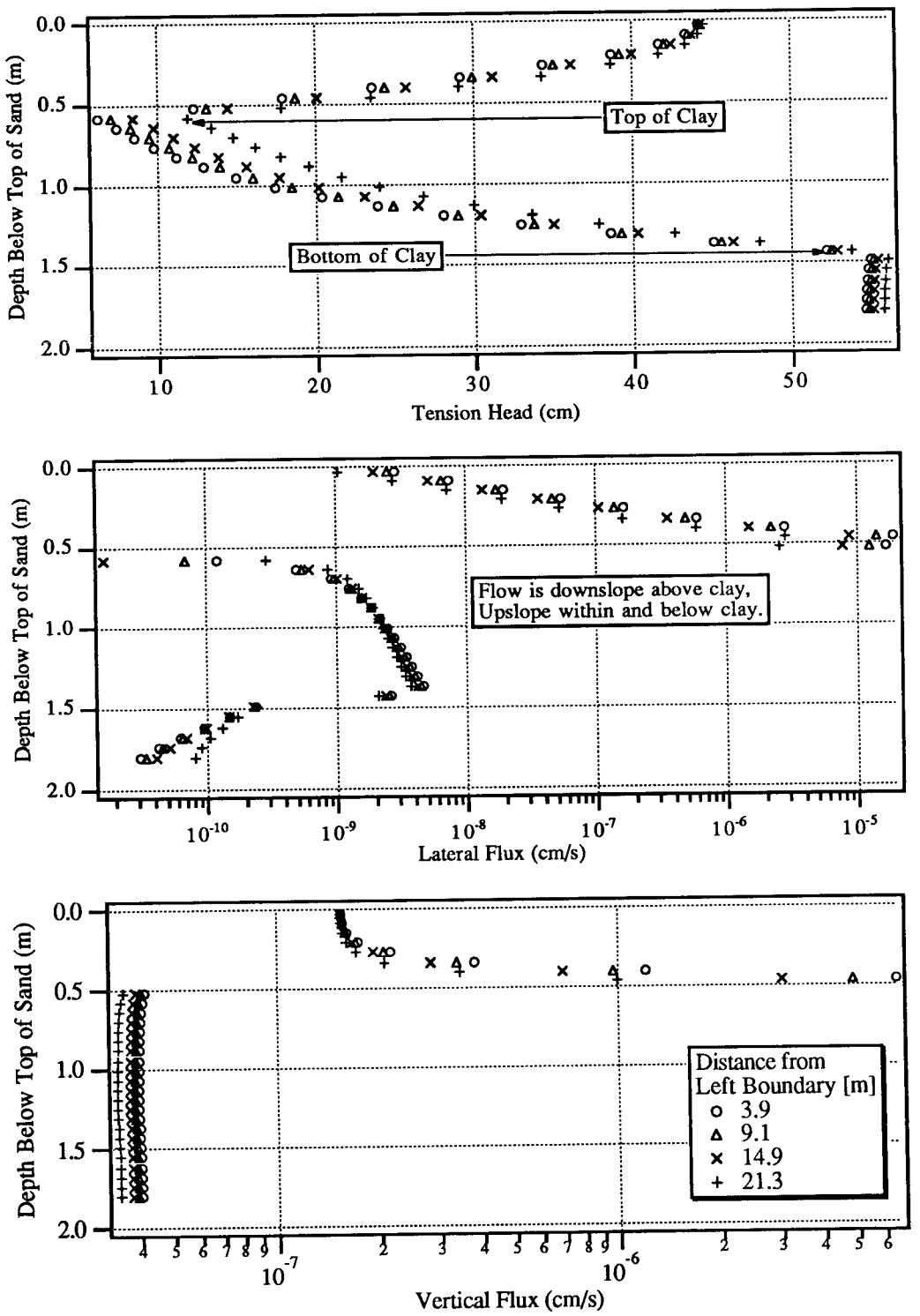


Figure 13. Cross-sectional output of the steady-state solution for flow through the clay layer: tension head (top), lateral flux (middle), and vertical flux (bottom). Refer to Figure 12 for locations of cross-sections. Note that lateral flux above the clay layer is plotted as positive, but occurs in the negative x-direction (downslope).

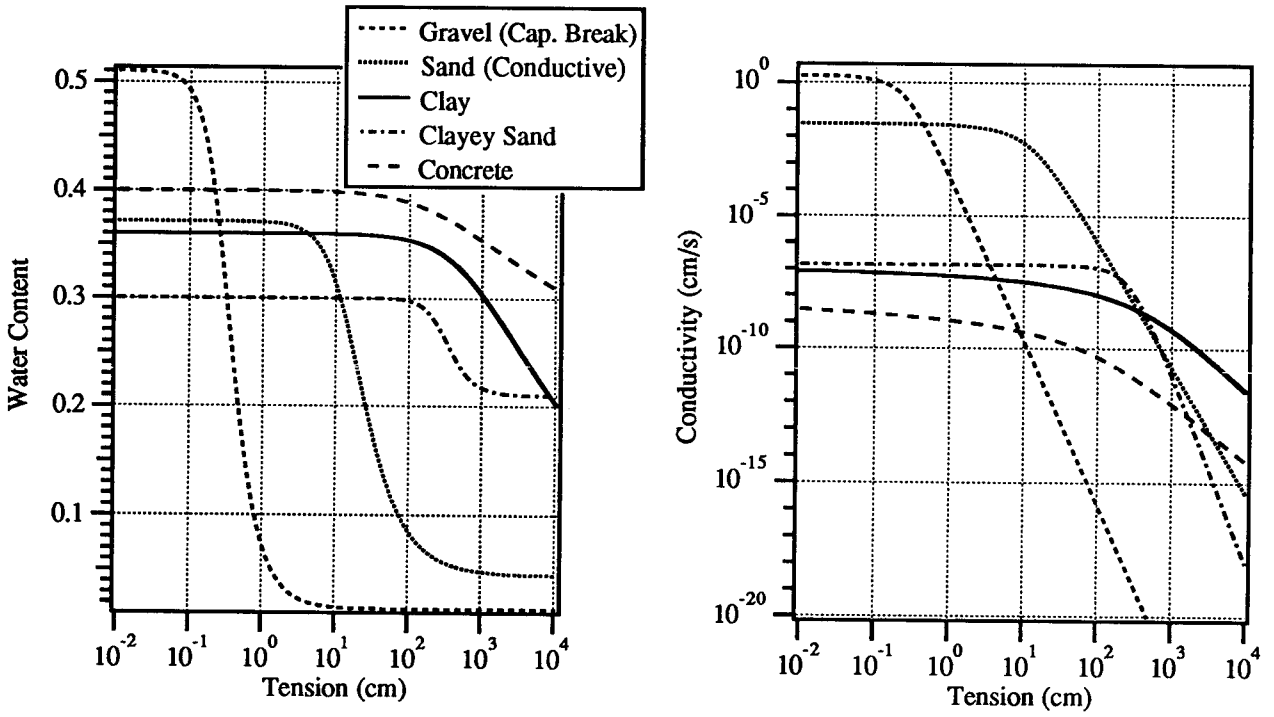


Figure 14. Volumetric water content (left) and hydraulic conductivity (right) as a function of tension for the materials of the two-dimensional simulations

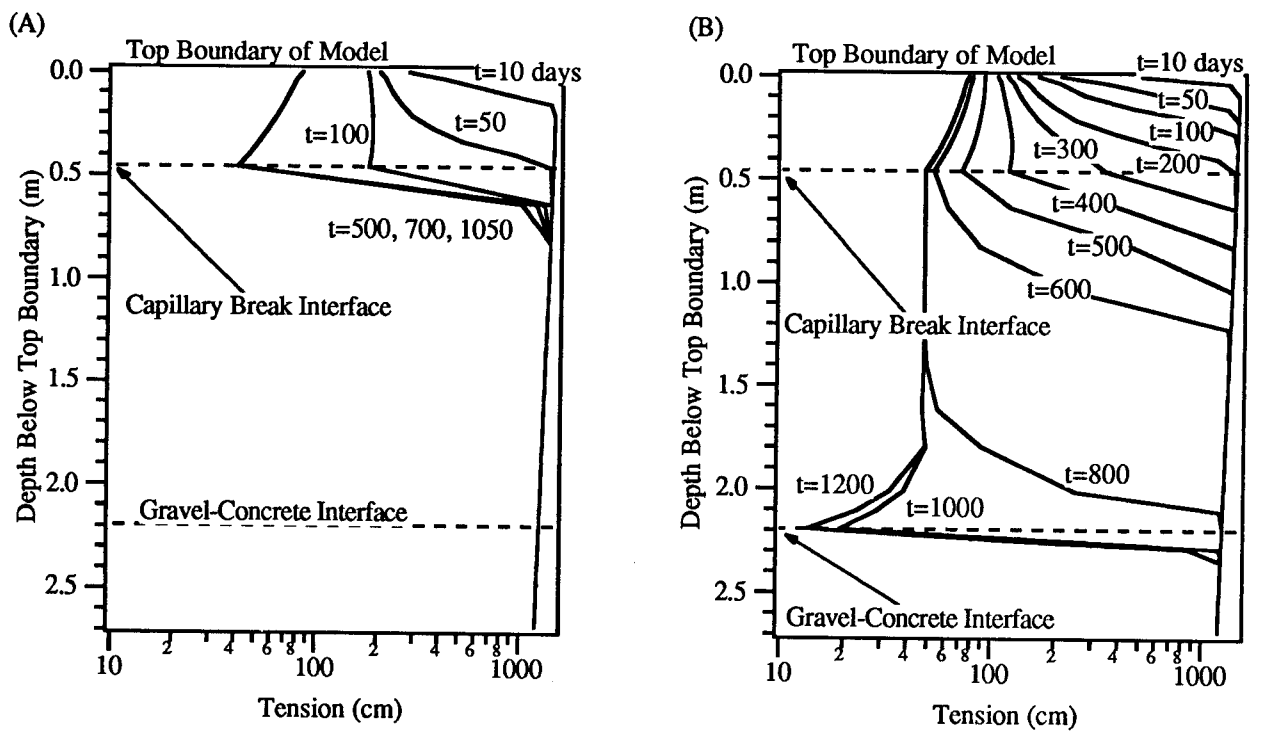


Figure 15. Tension profiles 4 m from left edge of concrete using high QC (A) and low QC (B) materials. Time of each profile is indicated.

A steady-state analysis is required to determine the ultimate fluxes in the system.

The simulations using the Princeton code were not carried out to steady state because of the computational expense. A simpler, steady-state model of the capillary barrier was solved using MSTS, however. This model was similar to the clay barrier model of Figure 12 with the exception that the materials of the capillary barrier, sand and gravel, replaced the gravelly sand and clay, respectively. Results of this simulation indicated the potential effectiveness of the capillary barrier. The steady-state, vertical flux of water through the gravel layer was less than 0.01 percent of the input flux.

It is difficult to predict the performance of the capillary break system simply by comparing the tension-conductivity relationships of the conductive layer and the capillary break. To illustrate the difficulty, the original materials comprising the conductive layer and the capillary break were modified in the full two-dimensional model (as before, similar to Figure 3). The conductive layer was modified from a coarse sand to a silty sand. The capillary break layer was modified from a gravel to a gravelly sand. These changes reflect a possible problem in construction: the mixing of coarse sand with silty material, for example. The original materials will be designated the high quality control (QC) case and the modified materials the low QC case. The main effect of the modification was to reduce the air entry pressure of the capillary break material. The parameters of the van Genuchten/Mualem model for the modified, low QC materials are given in Table 4. As with the original materials, the Princeton code was used to simulate the modified problem.

Table 4. Parameters for the modified (low QC) capillary barrier materials

	High QC Materials (Table 1)		Low QC Materials	
	Sand	Gravel	Silty Sand	Gravelly Sand
θ_r	0.045	0.014	0.098	0.02
θ_s	0.371	0.51	0.35	0.34
α (cm^{-1})	0.0683	3.5366	0.0440	0.1008
n	2.08	2.661	1.523	2.922
K_s (cm/s)	3.0e-2	1.85	1.0e-4	1.0e-2

The modified parameters are referred to as low QC because the contrast in their properties is less extreme than the original materials. This is illustrated by comparing the water retention and hydraulic conductive functions for the two cases, as shown in Figure 16. With the high QC materials,

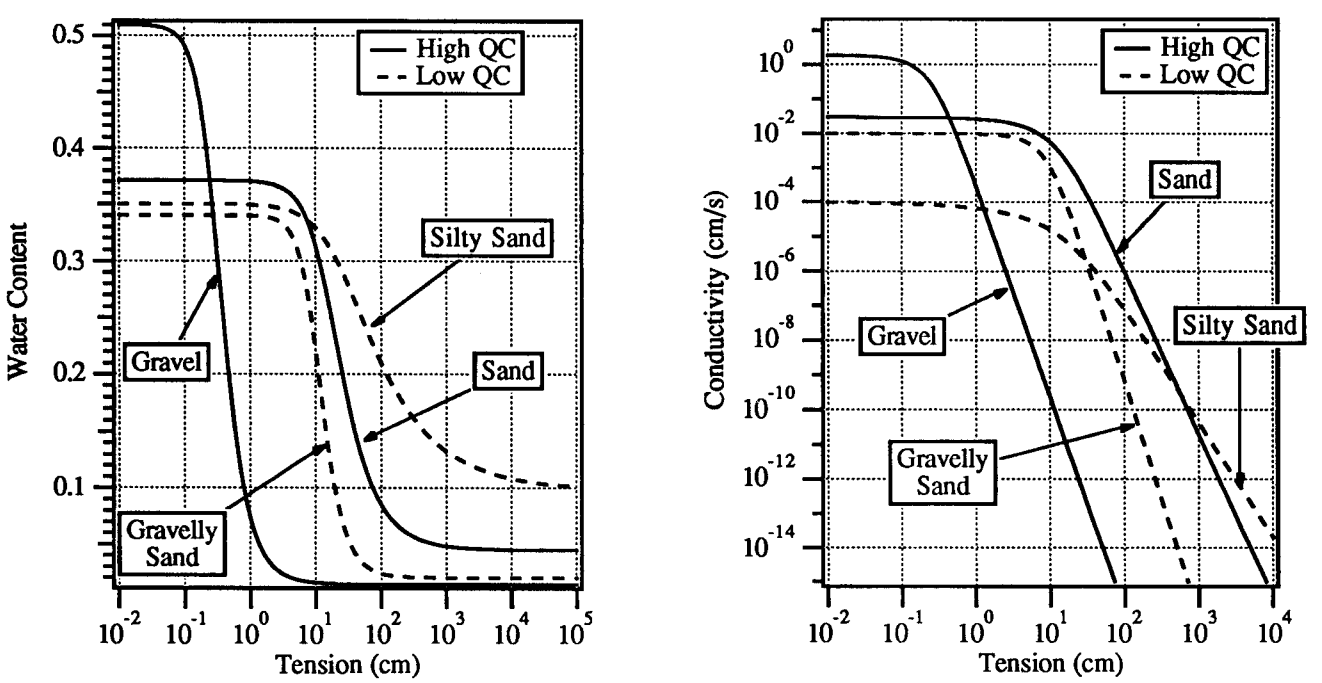


Figure 16. Volumetric water content and hydraulic conductivity as a function of tension for the original, high QC and the modified, low QC materials

the conductivity of the conductive layer remains greater than that of the capillary break for tensions greater than 1 cm. This cross-over point is at about 40 cm for the low QC materials. At the initial tension of 14 m, the hydraulic conductivity of the silty sand is approximately 10^6 times larger than the conductivity of the gravelly sand. With an input flux on the top boundary of only 1.0×10^{-7} cm/s, these materials might still be expected to perform as a capillary break.

The effect of using the low QC materials can be seen in Figure 15(B), which shows tension profiles at the same location as Figure 15(A). The results of this simulation show that the capillary barrier, using the modified materials, provides little or no resistance to the passage of the front. Between 200 and 400 days the front passes across the capillary break interface. At about 1000 days, water begins to percolate into the concrete vault.

The modeling results using the low QC materials suggest that an inspection of the pressure-saturation and pressure-conductivity curves may be insufficient to determine the performance of a capillary break system. Relatively small changes in the characteristic curves may produce drastically different results. This is particularly important because the characteristic curves will likely be derived from lab experiments on a small number of samples and thus may be somewhat uncertain. This uncertainty will carry over into the results predicted by a model.

3.2.1 Analytical Capillary Barrier Solution

The performance of the capillary barrier is critical to the success of the disposal facility but is difficult to predict because it depends on several factors. Flow of water through the capillary barrier is a function of the hydraulic properties of both the fine and the coarse materials, the slope of the interface, and the flow of water through the clay layer. A numerical analysis of barrier performance can be time consuming given the presence of a sloping interface, which requires a two-dimensional analysis.

To facilitate the design analysis and the determination of appropriate capillary barrier materials, an analytical solution (Ross, 1990, 1991) for flow through a capillary barrier can be used. Ross derived an expression for the steady-state, effective length of a capillary barrier, where this length is defined by the point at which the flux across the sloping interface is equal to the infiltration rate. For the hypothetical facility design, the infiltration rate is given by the flow through the clay layer. Ross' solution assumes that the capillary barrier is located far above the water table and that the thickness of the conductive layer does not restrict the flow of water.

The solution for the effective capillary barrier length, L, is given in Ross (1990) as

$$L = -\frac{K_s S}{q}\int K_r dh \qquad (5)$$

where $K_r = K/K_s$ is the relative permeability of the conductive material, S is the slope of the interface, and q is the infiltration rate. All other parameters were previously defined. Ross (1991) presents the solution of Equation 5 when the relative permeability is given by Philip's quasilinear relationship (Philip, 1969). The van Genuchten permeability function used in this analysis cannot always be well-represented by the quasilinear relationship. As an alternative, Equation 5 was solved using the relative permeability expression introduced by Brooks and Corey (1964).

$$K_r = \left(\frac{h}{h_a}\right)^{-\lambda'} \qquad h \geq h_a \qquad (6)$$

$$K_r = 1 \qquad h < h_a \qquad (7)$$

The parameters h_a is the air entry tension; λ' is a fitting parameter related to the pore size distribution. The solution of Equation 5 using the Brooks-Corey relative permeability relationship is

$$L = \frac{K_s S}{q}\left[\frac{h_a\left(\frac{h_w^*}{h_a}\right)^{\lambda'} - h_w^*\left(\frac{q}{K_s}\right)^{\frac{1}{\lambda'}-1}}{(1-\lambda')\left(\frac{h_w^*}{h_a}\right)^{\lambda'}\left(\frac{q}{K_s}\right)^{\frac{1}{\lambda'}-1}}\right] \qquad (8)$$

when $h_a \leq h_w^*$, and

$$L = \frac{K_s S}{q}\,\frac{h_a\left(1-\left(\frac{q}{K_s}\right)^{\frac{1}{\lambda'}-1}\right)}{(1-\lambda')\left(\frac{q}{K_s}\right)^{\frac{1}{\lambda'}-1}} + h_a - h_w^* \qquad (9)$$

when $h_a > h_w^*$. The parameters h_a and h_w^* in these expressions are the air entry pressure of the conductive material and the water entry pressure of the capillary break material, respectively. These parameters can be estimated from an inspection of the water retention functions. λ' is the Brooks-Corey fitting parameter for the conductive material. K_s is the saturated conductivity of the conductive material. The van Genuchten parameters α and n are related to h_a and λ'. Van Genuchten (1980) suggests the following approximate relationships.

$$h_a \sim \alpha^{-1} \qquad (10)$$

$$\lambda' = \frac{5n-1}{2} \tag{11}$$

Equations 8 and 9 were used to estimate the effective length of the capillary barrier when using both the high QC and the low QC materials (see Figure 16 and Table 4). The effective barrier length was estimated to be over 4000 m for the high QC materials and less than 1 m for the low QC materials. These results were obtained using parameter values given in Table 5 and are consistent with the simulation results presented earlier.

Table 5. Parameter values used in the analytical capillary barrier solution

	High QC Materials	Low QC Materials
q (cm/s)	1.0×10^{-7}	1.0×10^{-7}
K_s (cm/s)	3.0×10^{-2}	1.0×10^{-4}
S	0.2	0.2
h_a (cm)	7.0	14.0
h_w^* (cm)	1.5	68.0
λ'	4.7	3.3

An analytical solution such as that given by Equations 8 and 9 is particularly useful in examining the impact of uncertainty in parameter values. The infiltration rate, q, is one parameter that is expected to increase over time. The effect on L of a change in q can be easily determined and is plotted in Figure 17 for the high QC materials. The required effective capillary barrier length for the hypothetical facility is approximately 20 m, which is exceeded by the high QC materials as long as the flux through the clay is less than about 2×10^{-5} cm/s.

3.3 Summary of Two-Dimensional Analysis

The two-dimensional analysis has examined several issues related to the performance of the hypothetical LLW disposal facility. A model of steady-state flow through the sloping clay layer showed that approximately 75 percent of the water arriving at the clay was diverted to lateral drainage. The flux of water transmitted through the clay was 40 percent of its saturated hydraulic conductivity. Volumetric water content of the clay remained very close to its saturated value. This simulation was carried out using a constant input flux to the top of the clay that was 50 percent larger than the clay's saturated conductivity. The one-dimensional simulations described in the previous chapter indicated that the flux input to the clay will be variable and often much less than the value used in the two-dimensional steady-state simulation. The impact of this variability on the water content of the clay (and potential desiccation) remains an item of future study. The application of a closed-form stochastic approach (Dagan and Bresler, 1983; Bresler and Dagan, 1983) as presented in Smyth et al. (1990) may also be appropriate in this case.

The simulations of flow through the capillary barrier demonstrated the sensitivity of barrier performance to the water retention characteristics of the two materials comprising the capillary barrier. This makes it difficult to predict the performance based on an inspection of the relationships between tension and water content or hydraulic conductivity. An analytical solution was presented that can be used to determine proper materials to use in the construction of a capillary barrier and to predict the barrier's performance.

The hypothetical facility design analyzed in this document has potential failure mechanisms that have not been discussed. Because most of the water passing through the clay barrier flows to a drain located at the bottom of the conductive channel, the proper functioning of this drain is essential to the success of the facility. If the drain should fail during the life of the facility, saturations would rise in the conductive channel. The capillary barrier along the side of the concrete vault may fail in this case allowing water to move laterally into the vault. In addition, the analysis carried out here has assumed that the interface between the two materi-

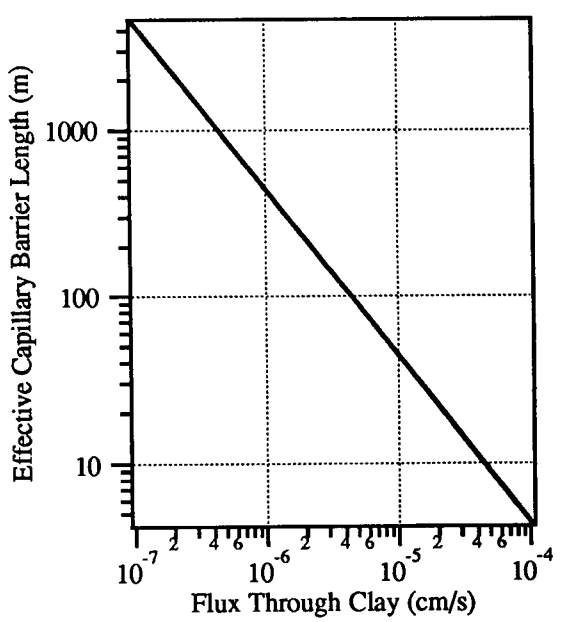


Figure 17. Effective capillary barrier length, L, as a function of the flux through the clay, q, as calculated by Equations 8 and 9 for the high QC materials

als of the capillary barrier is well-defined and constant over time. To accomplish this in the actual system will require careful control of the construction process and also additional components such as a filter to prevent fine material from washing down into the coarser barrier material. The presence of material heterogeneities and construction imperfections will result in a higher flow of water through the capillary barrier. These and related issues should be considered in the assessment of cover performance.

It is likely that the hydraulic properties of the disposal facility materials will change over the lifetime of the facility. As previously discussed, the clay barrier may become more porous because of desiccation and the penetration of roots; the performance of the capillary break system may degrade because of movement of fines from the conductive layer into the capillary barrier layer. In addition, the concrete may degrade, increasing its permeability to water. If changes in material properties over the lifetime of the facility can be determined, a model incorporating these changes can be developed.

4 Conclusions

An analysis of infiltration into and percolation through a hypothetical LLW disposal facility has been presented. The facility consisted of a series of concrete vaults topped by a multilayer cover. A single vault/cover unit was examined. The cover contained several design features intended to minimize the flow of water into the concrete vault, including a sloping soil surface to promote runoff, plant growth to minimize erosion and promote transpiration, a sloping clay layer, and a sloping capillary barrier. The latter two features act as low permeability barriers to flow and promote subsurface lateral drainage. The hypothetical facility was located in a humid environment characterized by frequent and often intense precipitation events. Hourly and daily rainfall data from two sites in South Carolina were used in the analysis.

The analysis consisted of a series of simulations of water flow through the cover to determine the performance of the facility design. Major observations and conclusions resulting from the analysis are summarized here.

- Many of the processes influencing the flow of water through the facility vary over time, although the scale of the variation differs for each process. Precipitation, for instance, may vary significantly over a period of a few minutes while the degradation of concrete may take place over decades. If possible, the analysis should be simplified by partitioning the problem into transient and steady-state portions. In the present work, a transient analysis was primarily considered only in the region within and above the root zone.

- The facility design considered here contains several features that divert the flow of water around the waste, thereby creating significant lateral subsurface flow. Accurate prediction of the flux of water into the waste requires consideration of this lateral flow. The transient analysis of flow within and above the root zone was one dimensional, however, and therefore neglected lateral flow in this region. Below the root zone, the analysis was restricted to two dimensions. Certain design features (such as the multiple concrete vaults of the hypothetical facility) may call for a three-dimensional analysis.

- For the humid site examined here, the variability in precipitation was on a time scale much shorter than 1 day. This variability required that hourly precipitation data be used to obtain accurate predictions of the water balance. Using daily-averaged rainfall data resulted in underestimation of the amount of surface runoff and overestimation of drainage below the root zone.

- Comparison between the largely empirical HELP model and a mechanistic model of unsaturated flow (UNSAT-H) illustrated large differences in the predicted water balance. Much of the difference may be caused by the restriction of HELP to the use of daily average precipitation data.

- Evapotranspiration represented the single largest sink of water, accounting for approximately 60 percent of the precipitation. Obtaining reliable estimates for parameters describing water utilization by plants may thus be necessary to accurately predict the flux of water passing below the root zone.

- The flux of water predicted to reach the clay barrier varied over the course of a 2-year simulation and was often much less than that required to keep the clay layer fully saturated. This has consequences for facility performance because desiccation of the clay may increase its permeability. Complete failure of the clay barrier, and potentially the capillary barrier also, may result.

- Two-dimensional simulations estimated that the sloping clay barrier, when intact, will divert 75 percent of the water reaching it. In addition, the flux through the clay may be less than its saturated hydraulic conductivity even when the input flux is greater than K_s of the clay.

- Performance of the capillary barrier will vary significantly with the hydraulic properties of the two materials of which it is composed. The capillary barrier is potentially able to divert more than 99 percent of the water passing through the clay layer.

- Predicting barrier performance simply by inspecting the water retention and hydraulic conductivity functions is difficult. An analytical expression for the effective length of a capillary barrier was presented. This expression is easy to evaluate and can be used to estimate barrier performance and to determine appropriate materials for construction.

4.1 Future Work

During the discussion of the results of the infiltration/percolation analysis, several issues have been raised that require further analysis to resolve. Foremost among these is the analysis of uncertainty. Many of the parameters needed to carry out the simulations can be only approximately determined. In addition, material properties will be spatially variable and may vary significantly over time as well. The resulting uncertainty is not accounted for in the output of deterministic simulations such as those presented in this document.

Unfortunately, the analysis of uncertainty typically requires either a greatly expanded computational effort, or a gross simplification of the problem. Future efforts will focus on

incorporating existing tools such as the stochastic method of Dagan and Bresler (1983) and the analytical capillary barrier solution of Ross (1990) into the design and performance assessment analyses.

Although the analysis presented here has been limited to two dimensions, the actual flow of water through the facility will be three dimensional. It is possible that the three-dimensional characteristics of the design influence the performance of the facility in ways that cannot be determined with a two-dimensional analysis. This possibility will be investigated with VAM3DCG, a fully three-dimensional model (Huyakorn and Panday, 1993).

During the next 2 years, four specific tasks will be undertaken to develop an improved Infiltration Evaluation Methodology (IEM). These four tasks will focus on activities that are intended to meet U.S. Nuclear Regulatory Commission licensing needs in the evaluation of water infiltration for performance assessments at LLW sites.

Task 1. Infiltration uncertainties. The aim of this task is to develop methods of estimating hydrologic impacts on engineered structures and to improve and integrate the analysis of climatic, vegetative, and soil processes. This task will develop an improved analysis of parameter uncertainty for near-surface water balance calculations. We will expand the present IEM by identifying acceptable procedures for estimating evapotranspiration and surface runoff, and accounting for snowmelt and extreme rainfall events. Key parameters will be accounted for in a systematic manner and additional testing of the impact of climatological data (use of hourly versus daily values) will be investigated for dry (arid, western) site conditions.

Task 2. Capillary barrier analysis. The capillary barrier has been shown to play a dominant role in the performance of multilayer cover systems. This task will expand on the present work by more rigorously examining the physics of the capillary barrier and by evaluating the effect on flow through the barrier with stochastic variation in barrier hydraulic properties. Performance of capillary barriers with variable hydraulic properties and infiltration rates will be tested numerically. The performance of sloping capillary barriers under these conditions will be documented.

Task 3. Water flow code comparisons. This task will compare selected codes, using two- and three-dimensional configurations, for analyses of water balance at LLW sites. The purpose of this task is to develop insight into those situations requiring a three-dimensional analysis. VAM3DCG will be evaluated in both two and three dimensions. In addition, other codes such as MSTS and the Two-Dimensional Princeton Code will be tested and compared with VAM3DCG. Performance criteria will be established to evaluate the selected codes based on accuracy, efficiency, and ease of use.

Task 4. Infiltration data – model test comparisons. Infiltration, redistribution, and drainage (recharge) data at two field sites, Las Cruces, New Mexico, and Richland, Washington (Hanford Site), will be used to test the performance of selected models. Detailed characterization data sets as well as sparse data sets will be used. Monte Carlo simulations using improved numerical methods for solving flow and transport problems will be tested against the available data sets. Field data will be used to evaluate the limitations of simplified, one-dimensional screening models with respect to more comprehensive two- and three-dimensional models.

5 References

Bresler, E. and G. Dagan. "Unsaturated flow in spatially variable fields, 2, Application of water flow models to various fields." *Water Resources Research*, 19(2), 421-428, 1983.

Brooks, R. H. and A. T. Corey. *Hydraulic Properties of Porous Media*. Hydrology Paper No. 3, Civil Engineering Dept., Colorado State Univ., Fort Collins, CO, 1964.

Celia, M. A. "The Two-Dimensional Princeton Unsaturated Code." Distributed at the Princeton University Short Course: Fundamentals of Unsaturated Zone Modeling, 24-28 June 1991.

Celia, M. A., E. T. Bouloutas, and R. Zarba. "A general mass-conservative numerical solution for the unsaturated flow equation." *Water Resources Research*, 26(7), 1483-1496, 1990.

Dagan, G. and E. Bresler. "Unsaturated flow in spatially variable fields, 1, derivation of models of infiltration and redistribution." *Water Resources Research*, 19(2), 413-420, 1983.

Fayer, M. J. and T. L. Jones. PNL-6779, "UNSAT-H Version 2.0: Unsaturated Soil Water and Heat Flow Model." Pacific Northwest Laboratory, Richland, WA, 1990.

Huyakorn, P. S. and S. Panday. *VAM3DCG - Variably Saturated Analysis Model in Three-Dimensions with Preconditioned Conjugate Gradient Matrix Solvers, Documentation and User's Guide, Version 1.1*. HydroGeoLogic, Inc., Herndon, VA, 1993.

Melchior, S., K. Berger, B. Vielhaber, and G. Miehlich. "Water Balance and Efficiency of Different Landfill Cover Systems." Geoconfine 93, Arnould, Barrès, and Côme (eds.), Balkema, Rotterdam, ISBN 90 5410 330 2, 1993.

Mualem, Y. "A new model for predicting the hydraulic conductivity of unsaturated porous media." *Water Resources Research*, 12(3), 513-522, 1976.

Nichols, W. E. and M. D. White. PNL-8637, "MSTS: Multiphase Subsurface Transport Simulator User's Guide and Reference." Pacific Northwest Laboratory, Richland, WA, 1993.

Oppe, T. C., W. D. Joubert, and D. R. Kincaid. *NSPCG User's Guide, Version 1.0, A Package for Solving Large Sparse Linear Systems by Various Iterative Methods*. CNA-216, Center for Numerical Analysis, The University of Texas at Austin, Austin, TX, 1988.

Philip, J. R. "Theory of infiltration." *Advances in Hydroscience*, 5, 215-296, 1969.

Richards, L. A. "Capillary conduction of liquids in porous mediums." *Physics*, 1:318-333, 1931.

Ross, B. "The diversion capacity of capillary barriers." *Water Resources Research*, 26(10), 2625-2629, 1990.

Ross, B. "Reply." *Water Resources Research*, 27(8), 2155-2156, 1991.

Schroeder, P. R., B. M. McEnroe, R. L. Peyton, and J. W. Sjostrom. "Hydrologic Evaluation of Landfill Performance (HELP) Model, Vol. IV: Documentation for Version 2." U.S. Army Corps of Engineers Internal Working Document EL-92-1 (Approved for Public Release), 1992.

Smyth, J. D., E. Bresler, G. W. Gee, and C.T. Kincaid. NUREG/CR-5523, "Development of an Infiltration Evaluation Methodology for Low-Level Waste Shallow Land Burial Sites." U.S. Nuclear Regulatory Commission, Washington, D.C., 1990.

van Genuchten, M. Th. "A closed-form equation for predicting the hydraulic conductivity of unsaturated soils." Soil Science Society of America Journal, 44, 892-898, 1980.

White, M. D. and W. E. Nichols. PNL-8636, "MSTS: Multiphase Subsurface Transport Simulator Theory Manual." Pacific Northwest Laboratory, Richland, WA, 1993.

Appendix A: A Qualitative Discussion of Grid Discretization Error

A small test problem was used to investigate the effect of grid discretization and the use of a rectangular discretization to approximate a sloping interface. The test problem modeled flow at the interface between sand and an underlying, sloping clay layer, as shown in Figure A-1. The soil properties were identical to those used in the hypothetical facility. The constant flux input at the top of the domain was 1.5×10^{-7} cm/s, identical to that used in the large-scale simulations. A unit gradient condition was specified at the bottom boundary while zero flux conditions were specified on the lateral boundaries.

To test the effect of approximating the interface with rectangular elements, the domain was discretized using rectangular elements only, of size 7.5 by 3.0 cm. The Two-Dimensional Princeton Unsaturated Code was used to solve for the steady-state pressure field. The elements along the interface were then subdivided into two triangular elements, exactly representing the sloping interface. The Princeton code was also used to solve this problem. The left side of Figure A-2 shows the results. Tension is given as a function of depth, 135 cm from the left edge of the domain. For this problem, the use of rectangular elements to represent a sloping interface appears to be satisfactory. Increasing the size of the elements to 11.25 by 4.5 cm and solving the problem with exclusively rectangular elements also gives a good solution (see Figure A-2, left).

In contrast to the Princeton code, the MSTS code requires that all computational elements be rectangular (rectangular parallelepipeds in three dimensions). MSTS was used with computational elements of several sizes to test the effect of the grid discretization. The steady-state tension profiles are shown in the right side of Figure A-2. Tensions in the sand vary little with the grid size. The coarser discretizations result in progressively lower tensions being predicted in the clay. These results provide an indication of the errors that can be expected from the simulations. In the majority of the MSTS solutions discussed in this document, a coarse grid of 15×6 cm was used. The error accompanying the use of such a coarse grid was accepted in the interest of obtaining solutions to the full-scale problem with reasonable computational effort.

Small differences between the solutions obtained with the Princeton code and with MSTS are apparent in Figure A-2 upon close inspection. These differences are caused by the dependence of water viscosity and density on temperature in MSTS. The default temperature used by MSTS is 20°C.

Although MSTS allows the refinement of the grid in regions of particular interest, this feature of the code was not utilized. Refining the grid only where large pressure gradients are expected improves the efficiency of the solution. The full-scale simulations with the Princeton code used such a customized grid. Producing such a grid requires a significant amount of time using either the Princeton code or MSTS. In addition, refined grids are difficult to modify with either code. The difficulty in building and modifying grids tailored to the particular problem being modeled is an important limitation.

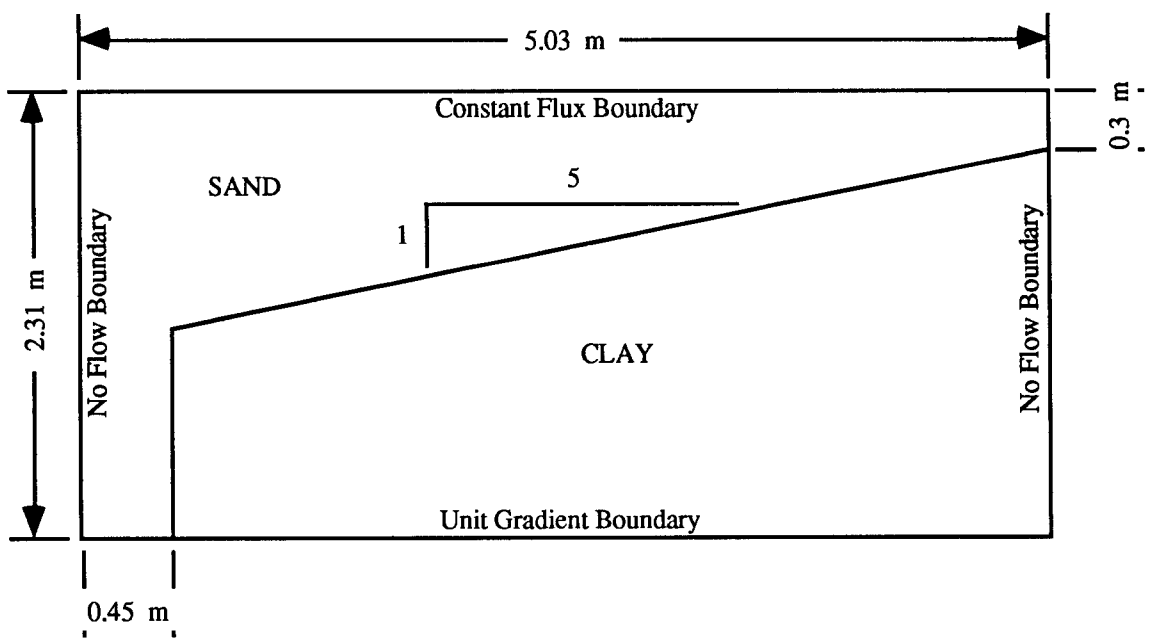


Figure A-1. Layout of problem used to test discretization and slope approximation of the two-dimensional models

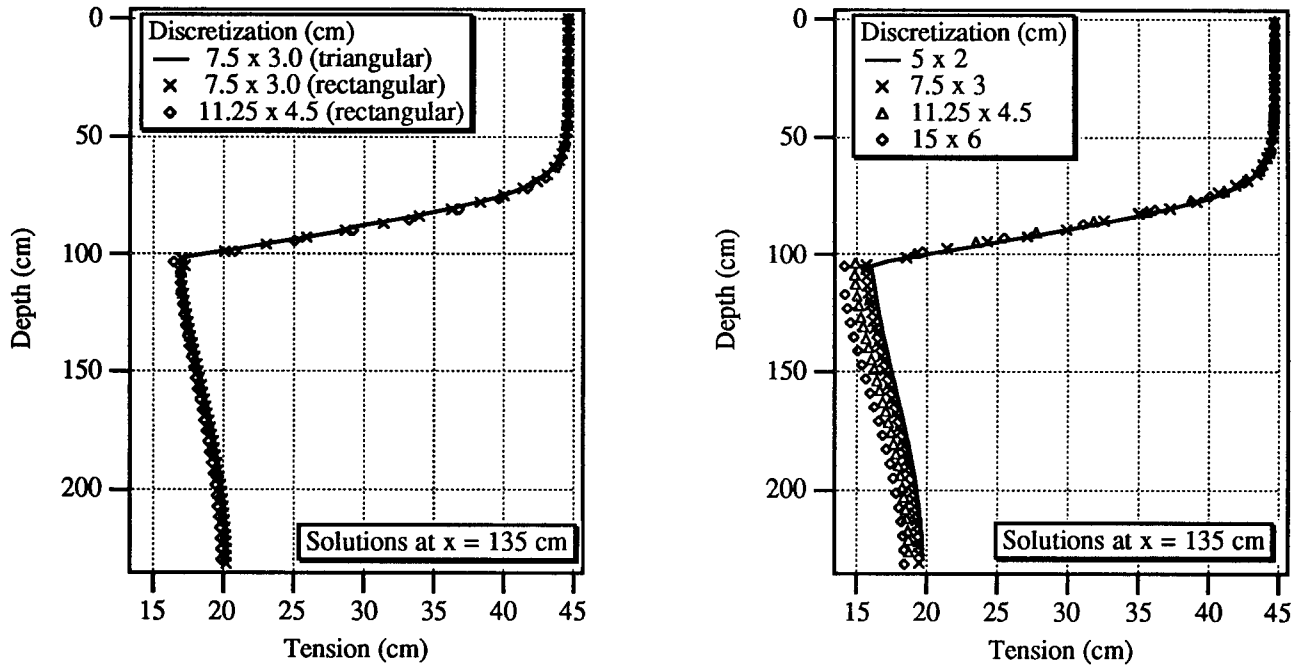


Figure A-2. Pressure profiles for various grid configurations using the Two-Dimensional Princeton Unsaturated Code (left) and MSTS (right)

Distribution

No. of Copies

OFFSITE

5 T. J. Nicholson
U.S. Nuclear Regulatory Commission
Office of Nuclear Regulatory Research
Mail Stop NL-005
Washington, DC 20555

U.S. Nuclear Regulatory Commission
Director, Division of Regulatory Applications
Office of Nuclear Regulatory Research
Mail Stop NL/S-260
Washington, DC 20555

U.S. Nuclear Regulatory Commission
Chief, Waste Management Branch
Division of Regulatory Applications
Office of Nuclear Regulatory Research
Mail Stop NL/S-260
Washington, DC 20555

U.S. Nuclear Regulatory Commission
Director, Division of Low Level Waste
Management and Decommissioning
Office of Nuclear Material Safety & Safeguards
Mail Stop 44-3
Washington, DC 20555

U.S. Nuclear Regulatory Commission
Document Control Center
Division of Low Level Waste Management
Office of Nuclear Material Safety & Safeguards
Mail Stop 44-3
Washington, DC 20555

5 R. Cady
U.S. Nuclear Regulatory Commission
Office of Nuclear Regulatory Research
Mail Stop NL/S-260
Washington, DC 20555

S. Amter
Disposal Safety Incorporated
1660 L Street NW, Suite 314
Washington, DC 20036

No. of Copies

G. S. Campbell
Agronomy Department
Washington State University
Pullman, WA 99164

M. A. Celia
Dept. of Civil Engineering and Operations
Research
Princeton University
Princeton, NJ 08544

P. Davis
Sandia National Laboratory
Division 6416
P.O. Box 5800
Albuquerque, NM 87185

Dr. T. Hakonson
Los Alamos National Laboratory
Mail Stop K495
Los Alamos, NM 87547

R. G. Hills
Department of Mechanical Engineering
Box 30001, Department 3450
New Mexico State University
Las Cruces, NM 88003

T. L. Jones
Department of Crop and Soil Sciences
Box 3Q
Las Cruces, NM 88003

W. A. Jury
Department of Soils
University of California
Riverside, CA 92502

K. Keller
Geology Department
Washington State University
Pullman, WA 99164

J. Kool
HydroGeoLogic, Inc.
1165 Herndon Parkway
Suite 900
Herndon, VA 22070

No. of
Copies

M. W. Kozak
Sandia National Laboratory
Division 6416
P.O. Box 5800
Albuquerque, NM 87185

T. J. McCartin
U.S. Nuclear Regulatory Commission
Office of Nuclear Regulatory Research
Mail Stop NL/S-260
Washington, DC 20555

J. McCord
Sandia National Laboratory
Division 6416
P.O. Box 5800
Albuquerque, NM 87185

D. B. McLaughlin
Ralph M. Parsons Laboratory, 48-209
Department of Civil Engineering
Massachusetts Institute of Technology
Cambridge, MA 02139

J. W. Mercer
GeoTrans, Inc.
46050 Manekin Plaza
Suite 100
Sterling, VA 22170

H. J. Morel-Seytoux
57 Selby Lane
Atherton, CA 94027-3926

S. P. Neuman
Department of Hydrology and Water Resources
University of Arizona
Tucson, AZ 85721

V. Rogers
Rogers & Associates Engineering Corp.
P.O. Box 330
Salt Lake City, UT 84107

F. Ross
U.S. Nuclear Regulatory Commission
11555 Rockville Pike
Rockville, MD 20852

No. of
Copies

B. Sagar
Center for Nuclear Waste Regulatory Analysis
6220 Culebra Road
P.O. Drawer 28500
San Antonio, TX 78284

R. K. Shulz
University of California-Berkeley
108 Hilgard Hall
Berkeley, CA 84720

J. B. Sisson
EG&G
P.O. Box 1625, MS 2107
Idaho Falls, ID 83415

E. P. Springer
Environmental Science Group
HSE 12
Health, Safety and Environment Division
Los Alamos National Laboratory
Los Alamos, NM 87545

M. Thaggard
U.S. Nuclear Regulatory Commission
11555 Rockville Pike
Rockville, MD 20852

S. W. Tyler
Desert Research Institute
P.O. Box 60220
Reno, NV 89506

W. J. Waugh
UNC GeoTech
P.O. Box 14000
Grand Junction, CO 81502

E. P. Weeks
U.S. Geological Survey
Federal Center Mail Stop 413
Denver, CO 80225

P. J. Wierenga
Dept. of Soil and Water Science
429 Shantz Bldg.
University of Arizona
Tucson, AZ 85721

No. of
Copies

M. H. Young
Dept. of Soil and Water Science
429 Shantz Bldg.
University of Arizona
Tucson, AZ 85721

ONSITE

42 Pacific Northwest Laboratory

M. P. Bergeron
M. D. Campbell
J. W. Cary
C. R. Cole
M. J. Fayer
M. D. Freshley
G. W. Gee
M. J. Graham
C. T. Kincaid
R. R. Kirkham
R. J. Lenhard
P. D. Meyer (15)
W. E. Nichols
J. C. Ritter
M. L. Rockhold
R. J. Serne
C. S. Simmons
R. L. Skaggs
J. L. Smoot
G. P. Streile
J. E. Szecsody
Publication Coordination
Technical Report Files (5)

Routing

R. M. Ecker
P. M. Irving
C. S. Sloane
P. C. Hays (last)

NRC FORM 335 (2-89) NRCM 1102, 3201, 3202

U.S. NUCLEAR REGULATORY COMMISSION

BIBLIOGRAPHIC DATA SHEET

(See instructions on the reverse)

1. REPORT NUMBER (Assigned by NRC, Add Vol., Supp., Rev., and Addendum Numbers, if any.)

NUREG/CR-6114
PNL-8842
Vol. 1

2. TITLE AND SUBTITLE

Application of an Infiltration Evaluation Methodology to a Hypothetical Low-Level Waste Disposal Facility

3. DATE REPORT PUBLISHED

MONTH	YEAR
December	1993

4. FIN OR GRANT NUMBER

L2466

5. AUTHOR(S)

P.D. Meyer

6. TYPE OF REPORT

Technical

7. PERIOD COVERED *(Inclusive Dates)*

8. PERFORMING ORGANIZATION – NAME AND ADDRESS *(If NRC, provide Division, Office or Region, U.S. Nuclear Regulatory Commission, and mailing address; if contractor, provide name and mailing address.)*

Pacific Northwest Laboratory
Richland, WA 99352

9. SPONSORING ORGANIZATION – NAME AND ADDRESS *(If NRC, type "Same as above"; if contractor, provide NRC Division, Office or Region, U.S. Nuclear Regulatory Commission, and mailing address.)*

Division of Regulatory Applications
Office of Nuclear Regulatory Research
U.S. Nuclear Regulatory Commission
Washington, D.C. 20555-0001

10. SUPPLEMENTARY NOTES

11. ABSTRACT *(200 words or less)*

An analysis of infiltration and percolation at a hypothetical low-level waste (LLW) disposal facility was carried out. The analysis was intended to illustrate general issues of concern in assessing the performance of LLW disposal facilities. Among the processes considered in the analysis were precipitation, runoff, infiltration, evaporation, transpiration, and redistribution. The hypothetical facility was located in a humid environment characterized by frequent and often intense precipitation events. The facility consisted of a series of concrete vaults topped by a multilayer cover. Cover features included a sloping soil surface to promote runoff, plant growth to minimize erosion and promote transpiration, a sloping clay layer, and a sloping capillary barrier. The analysis within the root zone was carried out using a one-dimensional, transient simulation of water flow. Below the root zone, the analysis was primarily two-dimensional and steady-state.

Results of the simulations illustrated the limited value of daily precipitation data. For the humid site studied, hourly rainfall data provided significantly better estimates of the water balance. Results also demonstrated the importance of transpiration in removing water from the soil column, implying a need for accurate models of plant growth and water utilization. In addition, the amount of water predicted to percolate below the root zone was often less than the amount required to keep the clay barrier layer fully saturated, even in the relatively wet environment studied. This could be a concern if the clay were subject to shrinking under unsaturated conditions. The two-dimensional simulations showed that the sloping clay barrier diverted 75 percent of the water reaching it. The sloping capillary barrier, in contrast, diverted more than 99.99 percent of the water reaching it. Performance of the capillary barrier, however, was shown to vary significantly with the hydraulic properties of the two materials of which it is composed. Predicting performance simply by inspecting the water retention and hydraulic conductivity functions was difficult. An analytical expression was presented that can be used to estimate capillary barrier performance and to determine appropriate materials for construction.

12. KEY WORDS/DESCRIPTORS *(List words or phrases that will assist researchers in locating the report.)*

Low-Level Waste Disposal
Infiltration
Percolation
Unsaturated Flow
Numerical Modeling
Performance Assessment

13. AVAILABILITY STATEMENT

Unlimited

14. SECURITY CLASSIFICATION

(This Page)

Unclassified

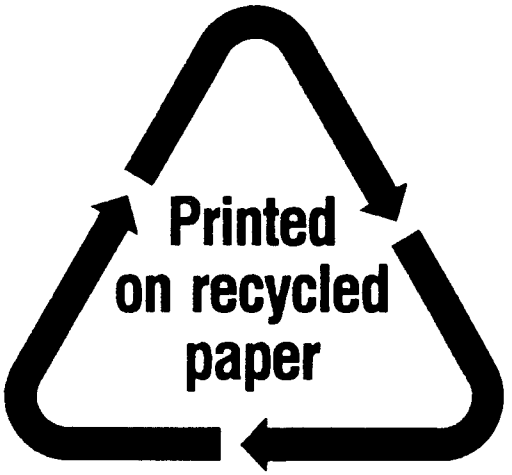
(This Report)

Unclassified

15. NUMBER OF PAGES

16. PRICE

NRC FORM 335 (2-89)



Federal Recycling Program