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Hydrologic Evaluation Methodology for Estimating Water Movement Through the Unsaturated Zone at Commercial Low-Level Radioactive Waste Disposal Sites

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Abstract

This report identifies key technical issues related to hydrologic assessment of water flow in the unsaturated zone at low-level radioactive waste (LLW) disposal facilities. In addition, a methodology for incorporating these issues in the performance assessment of proposed LLW disposal facilities is identified and evaluated. The issues discussed fall into four areas:

(1) Estimating the water balance at a site (i.e., infiltration, runoff, water storage, evapotranspiration, and recharge);
(2) Analyzing the hydrologic performance of engineered components of a facility;
(3) Evaluating the application of models to the prediction of facility performance; and
(4) Estimating the uncertainty in predicted facility performance.

An estimate of recharge at a LLW site is important since recharge is a principal factor in controlling the release of contaminants via the groundwater pathway. The most common methods for estimating recharge are discussed in Chapter 2. Many factors affect recharge; the natural recharge at an undisturbed site is not necessarily representative either of the recharge that will occur after the site has been disturbed or of the flow of water into a disposal facility at the site. Factors affecting recharge are discussed in Chapter 2.

At many sites engineered components are required for a LLW facility to meet performance requirements. Chapter 3 discusses the use of engineered barriers to control the flow of water in a LLW facility, with a particular emphasis on cover systems. Design options and the potential performance and degradation mechanisms of engineered components are also discussed.

Water flow in a LLW disposal facility must be evaluated before construction of the facility. In addition, hydrologic performance must be predicted over a very long time frame. For these reasons, the hydrologic evaluation relies on the use of predictive modeling. In Chapter 4, the evaluation of unsaturated water flow modeling is discussed. A checklist of items is presented to guide the evaluation. Several computer simulation codes that were used in the examples (Chapter 6) are discussed with respect to this checklist. The codes used include HELP, UNSAT-H, and VAM3DCG.

To provide a defensible estimate of water flow in a LLW disposal facility, the uncertainty associated with model predictions must be considered. Uncertainty arises because of the highly heterogeneous nature of most subsurface environments and the long time frame required in the analysis. Sources of uncertainty in hydrologic evaluation of the unsaturated zone and several approaches for analysis are discussed in Chapter 5. The methods of analysis discussed include a bounding approach, sensitivity analysis, and Monte Carlo simulation.

To illustrate the application of the discussion in Chapters 2 through 5, two examples are presented in Chapter 6. The first example is of a below ground vault located in a humid environment. The second example looks at a shallow land burial facility located in an arid environment. The examples utilize actual site-specific data and realistic facility designs. The two examples illustrate the issues unique to humid and arid sites as well as the issues common to all LLW sites. Strategies for addressing the analytical difficulties arising in any complex hydrologic evaluation of the unsaturated zone are demonstrated.

The report concludes with some final observations and recommendations.

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Executive Summary

This report identifies key technical issues related to hydrologic assessment of the unsaturated zone at low-level radioactive waste (LLW) sites. The issues discussed fall into four areas:

(1) Estimating the water balance at a site (i.e., infiltration, runoff, water storage, evapotranspiration, and recharge);

(2) Analyzing the hydrologic performance of engineered components of a facility;

(3) Evaluating the application of models to the prediction of facility performance; and

(4) Estimating the uncertainty in predicted facility performance.

There is a need for a summary of the information that is currently available for evaluating these hydrologic issues at LLW sites. We address these major issues and provide a review of the related current research in unsaturated zone hydrology. A methodology for incorporating these issues in the performance assessment of proposed LLW disposal facilities is identified and evaluated. This methodology is a revision and extension of the work reported in Smyth et al. (1990).

Estimating water flow within the unsaturated zone at a LLW site is important because it is this water that plays a principle role in controlling the release of contaminants via the groundwater pathway. An estimate of the natural (undisturbed site) recharge is used in the regional groundwater flow component of LLW site performance assessment. An estimate of the flow of water into a waste disposal facility, a term we call seepage, is required for the source term component of performance assessment. We emphasize the difference between these two terms – the natural recharge at an undisturbed site may not be a conservative estimate either of recharge at the same site after it has been disturbed, or of seepage into an engineered facility at the site. This is because site surface conditions (e.g., soil and plant characteristics), which are always modified from their natural state, strongly control the flow of water into a waste disposal facility.

Estimation of Recharge

The most common methods for estimating recharge, at undisturbed or disturbed sites, are discussed in Chapter 2 and include water budget analysis, lysimetry, zero-flux plane, unit hydraulic gradient, and tracers. The water budget method can provide reliable estimates of recharge at humid sites, but is problematic for arid sites, primarily because recharge is usually calculated as the difference between precipitation and evapotranspiration. At arid sites, one can be very nearly equal to the other; such a calculation has an inherently large error (often several orders of magnitude).

Lysimetry is the only method available for directly measuring recharge. One of the strengths of lysimetry is that it provides a control volume in which a number of water balance components can be measured directly, thus providing the necessary data to calibrate numerical models, which can then be used to forecast recharge. Lysimeters have several disadvantages. They are usually fixed in space and are therefore limited in their ability to quantify the effects of spatial variability. The natural stratification or layering of soils is usually not preserved in a lysimeter. For determining recharge at a LLW site, however, this may not be a disadvantage since the natural layering may not be representative of the final engineered disposal facility. The primary disadvantage of lysimetry is that the length of the data record is often relatively short, so that meaningful long-term averages may be difficult to obtain.

Applying the zero-flux plane and the unit gradient methods to recharge estimation is often impractical. These methods can typically provide reliable estimates only when the water profile is fairly constant in time and the soil profile is homogeneous.

Tracers, most commonly chloride, chlorine-36 (^{36}Cl), and tritium (^{3}H), are a reliable means to estimate natural, undisturbed-site recharge. Tracers provide an estimate of recharge averaged over the period of time in which the tracer resides in the soil. For ^{36}Cl and ^{3}H, this period of time is less than 40 years, which makes it difficult to estimate recharge at low flux rates using these tracers. The use of ^{36}Cl and ^{3}H is also limited because their movement in the root zone is significantly affected by plant uptake, macropore flow, and other near-surface processes. Studies have shown that when recharge rates are below 20 mm/yr., estimates of recharge with ^{36}Cl are not reliable. Chloride provides a recharge estimate that represents a historical average over a long period of time and appears to be the most reliable tracer for arid and semi-arid locations, especially for low recharge rates.

Engineered Barriers

At many sites, engineered barriers are required for the facility to meet performance requirements. For a hydrologic evaluation of LLW disposal facilities, engineered barriers are those components that provide structural stability or limit the movement of water into the waste and the movement of contaminant from the disposal facility into the environment. The role of engineered cover systems and waste containment structures in controlling the flow of water in a LLW facility is discussed in Chapter 3. Emphasis is on cover systems because they are the primary means of reducing seepage into a facility.

Cover system components are categorized as surface layer, protective layer, drainage layer, and barrier layer. The functions of the surface layer are to manage runoff, minimize erosion, and maximize evapotranspiration. The protective layer, often placed directly beneath the surface layer, protects underlying layers from degradation through repeated freeze/thaw cycles, repeated excessive wetting/drying, and plant, animal, or human intrusion. A drainage layer is typically placed beneath the protective layer and above the barrier layer to collect water that has infiltrated and to divert this water laterally so that it has no opportunity to contact the waste. The barrier layer is often the most critical component of the cover system; its low permeability is usually the primary means of limiting seepage to the extremely small value necessary for a facility to meet the performance requirements.

Options in materials and design for each of the cover system components are discussed. The types of barrier layers discussed are compacted soil (clay), geomembrane, geosynthetic clay liner, asphalt mixture, and capillary barriers. Composite barriers made up of more than one of these types are also examined. The potential performance and probable failure mechanisms are discussed for each of the barrier types, including composites. Field, laboratory, and analytical evidence for the behavior of barrier layers is presented.

Evaluating Models

Water flow in a LLW disposal facility must be evaluated before construction of the facility. In addition, hydrologic performance must be predicted over a very long time frame. For these reasons, hydrologic evaluation relies on the use of predictive modeling. In Chapter 4 the evaluation of unsaturated water flow modeling is discussed.

To understand the modeling process and how to evaluate its use, we view the development of a model for evaluating hydrologic processes at a LLW facility as a three-step process: development of a conceptual model; predictive simulation using a mathematical model that represents the key aspects (processes) of the conceptual model; and interpretation of results from the simulations in terms of the conceptual model.

All three steps are crucial in the development of a capable model and its successful application. The use of a computer code does not replace the human tasks of defining an acceptable conceptualization of the real physical system or interpreting the results in light of the limiting assumptions made in the conceptualization. Justification for code selection must therefore be based on a realistic conceptualization.

Site characterization and modeling efforts should be intimately connected. A data collection program that is not guided by the needs of the model(s) may collect unnecessary data and neglect to obtain critical information, thereby wasting time and resources. Even during construction and after closure, an ongoing data collection program should include among its purposes collection of data necessary to verify the initial hydrologic assessment by updating parameters to “as built” values.

A checklist of items to guide the evaluation of model use is presented in Table 4.1. Each criterion in the checklist is discussed in more detail throughout Chapter 4. When combined with the use of professional judgement, the checklist can reduce the introduction of modeling errors. Several codes that are used in the examples of Chapter 6 are also discussed with respect to the checklist. The codes used in the examples include HELP, UNSAT-H, and VAM3DCG.

Uncertainty Analysis

Many processes and phenomena involved in the flow of water through a LLW disposal facility are characterized by randomness and are consequently unpredictable to some degree. To provide a defensible estimate for predictions of water flow in a LLW disposal facility, the uncertainty associated with model predictions must be considered.

The sources of uncertainty are many. Among climatic processes and parameters that exhibit significant spatial and temporal variability, precipitation is particularly important because of its direct effect on all water balance components. Air temperature, wind velocity, and solar radiation primarily affect evapotranspiration. In addition, because the size of a LLW facility is small relative to the spatial variability of these climatic processes, the temporal variability is of greatest concern.

The inherent variability of natural geologic formations and soils can be quite large. Studies of soils data indicate that saturated hydraulic conductivity has the greatest variability of these parameters, as measured by the coefficient of variation. The water retention parameter related to the air entry pressure (van Genuchten’s α) also exhibits significant variability. The porosity and the water retention parameter related to the pore size distribution (van Genuchten’s n) have the least amount of variability.

Consideration of the temporal variability of vegetation is important in an uncertainty analysis simply because a plant community on a LLW disposal facility will change over time, either through natural succession or through catastrophic events such as fires and large storms.

The long-term performance of engineered barriers is uncertain due to a number of causes, most importantly construction defects and long-term aging and degradation, including subsidence. Engineering judgement and sensitivity analysis can be used to estimate the relative importance of each of these processes. For those processes judged to be of greatest importance, their potential variability (spatial or temporal) can be characterized using literature-derived values and pilot studies.

The methods of uncertainty analysis discussed for evaluating water movement at a LLW disposal facility are Monte Carlo simulation, the bounding approach, and sensitivity analysis. The method of uncertainty analysis that is appropriate is usually determined by the complexity of the problem and the available data. In many cases, more than one method can be applied simultaneously. Expert (engineering) judgement is also an uncertainty evaluation method. We acknowledge the use of expert judgement as essential to a credible and defensible performance assessment, and suggest that it should always be used in conjunction with one or more of the approaches described in Chapter 5.

Application Examples

To illustrate the application of the discussions in Chapters 2 through 5, two examples are presented in Chapter 6. The first example is of a below ground vault located in a humid environment. The second example looks at a shallow land burial facility located in an arid environment. The examples utilize actual site-specific data and realistic facility designs. The two examples illustrate the issues unique to humid and arid sites as well as the issues common to all LLW sites. Strategies for addressing the analytical difficulties arising in any complex hydrologic evaluation of the unsaturated zone are demonstrated.

Humid Site Example

The humid site example emphasized the analysis of the engineered components of the facility. The facility consisted of a series of concrete vaults topped by a multi-layer 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 composite geomembrane/compacted soil barrier, and a capillary break. The hypothetical facility was located in a humid environment (southeast U.S. coastal plain) characterized by high annual rainfall and short duration, high-intensity precipitation events. Hourly precipitation data and daily pan evaporation data were used in the analysis.

The analysis was simplified by performing two complementary simulations. The first was a one-dimensional, transient simulation limited to that portion of the cover above the geomembrane/compacted soil barrier. With this approach, near-surface processes such as precipitation and evapotranspiration could be modeled at a relatively short time-scale (one hour). In this humid environment, the temporal variability of precipitation has a strong influence on the flow of water through the upper layers of the cover. Below the composite barrier, however, temporal variability is less important; a steady-state analysis is appropriate. The geometry of the facility and the multidimensional flow it produces is of greater importance. The second part of the analysis was thus a three-dimensional, steady-state simulation limited to the capillary barrier and concrete vault.

The one-dimensional simulations illustrated the effect of averaging precipitation data. Using hourly averaged precipitation resulted in almost six times less net infiltration (and six times more runoff) than using daily averaged precipitation. This result has implications for the design of the surface layer (to prevent erosion), the surface drainage system, and the subsurface drainage layer. In addition, the amount and distribution in time of net infiltration will influence the potential for desiccation of the compacted soil barrier. The simulation using hourly data showed that the net infiltration occurred in short pulses with up to four years of very little net infiltration between pulses. Finally, the estimate of net infiltration is important because it may be used as an upper bound for the water flux through the facility in the event that the barrier layers become completely degraded.

An evaluation of uncertainty showed that the hydraulic parameters of the topsoil had a marked influence on runoff, evapotranspiration, and net infiltration. In this study, variations in the parameters K_S and α produced two orders of magnitude variation in net infiltration. The relationship between net infiltration and the hydraulic parameters was nonlinear. In addition, combined changes in the two parameters produced a greater effect than a change in either parameter alone. Both the nonlinearity and the combinatorial effect are important if the analysis is intended to bound the water flux through the facility.

The three-dimensional simulation assessed the performance of the capillary barrier. The assessment considered three capillary barrier slopes (1:5, 1:10, and 1:25) and three material property combinations for the sand and gravel of the capillary barrier. Simulations were carried out in two and three dimensions to explore the importance of dimensionality in predicting barrier effectiveness.

The hydraulic properties of the capillary barrier materials were shown to be the most important factor for capillary barrier effectiveness in diverting water. The slope of the capillary barrier was only mildly important for the hypothetical waste disposal facility design we analyzed. Achieving design hydraulic properties in the as-built condition is therefore crucial to the success of the disposal facility. These results were obtained for a numerical simulation under an assumption of stable slopes (no subsidence), which may not be true for actual waste site conditions.

The importance of dimensionality in evaluating a waste disposal facility design is, of course, strongly dependent on the design geometry. For the humid site design, several combinations of material properties and slope caused significant three-dimensional flow within 5 m of the corner of the vault. For capillary barrier effectiveness, the three-dimensional estimate of leakage through the barrier was always less than the two-dimensional estimate. The difference, however, was never more than 8% (absolute) of the flux input at the top of the barrier. Two-dimensional modeling, in this case, produces a reasonable and conservative result.

Arid Site Example

The hypothetical arid site facility consisted of a 4-m-deep trench backfilled with coarse, homogeneous soil. Underlying sediments were coarse and heterogeneous. The slope of the surface soil was less than 2% and no surface drainage systems were used. No barrier systems were employed and vegetation was expected to reestablish itself naturally after closure of the facility. The hypothetical facility was located in an arid environment (southwestern U.S., Mojave Desert) characterized by very low and infrequent precipitation. Meteorological and soils data from a USGS study site near Beatty, NV and from the Nevada Test Site were used in the analysis.

Transient, one-dimensional simulations of the hypothetical facility were conducted using the UNSAT-H and HELP computer codes. A simple one-dimensional, steady-state analysis was also used to demonstrate the potential significance of the geothermal gradient on deep percolation of water at the hypothetical arid site.

Simulations were conducted with the UNSAT-H code using hourly and daily averaged precipitation data to determine the effect of temporal averaging. No significant differences between the predicted water balance results were obtained. This is in contrast to the humid site, where significantly more runoff was obtained using hourly data than when using daily averaged data. This difference between humid and arid sites is apparently a result of the low and infrequent precipitation and high evaporative demand at the arid site.

The results of a 45-year simulation using UNSAT-H suggested that in the absence of vegetation, approximately 95% of precipitation is evaporated. These results also indicated that nonisothermal processes at the site have a significant influence on the predicted water balance and that vapor flow is the dominant mechanism controlling water movement at the site. The estimated net infiltration from the UNSAT-H simulations was very small (0.0002 mm/yr) and was primarily a result of the imposed lower boundary condition. Fluxes at the 5-m and 10-m depths were upward.

The 45-year HELP simulation predicted much less evaporation than the UNSAT-H simulations. The net infiltration estimated by HELP was 11.5 mm/yr., significantly larger than the UNSAT-H estimate.

The 45-year UNSAT-H simulations indicated a slow increase in water storage in the backfill material resulting from the initially dry condition and the absence of plants. UNSAT-H and HELP were also used in 500-year simulations to estimate the long-term flux through the facility under vegetated and nonvegetated conditions. Without plants, both UNSAT-H and HELP indicated that a quasi-steady state would be reached within 500 years. The long-term flux at a depth of 13-m predicted by UNSAT-H was about 2.5 mm/yr. The corresponding flux predicted by HELP was nearly ten times larger. When water uptake by plants was modeled, UNSAT-H predicted a flux of only 0.0002 mm/yr. at the 13-m depth. HELP predicted a much larger flux of 0.69 mm/yr. These results demonstrate the significant influence of plants.

The 500-year simulations also demonstrated the large variability that can occur in model predictions of recharge. This variability can arise from the particular processes simulated (e.g., including vapor-phase flow reduced the amount of stored water in the 45-year simulations) and from the sensitivity of the model results to the parameters of the model. The latter condition was illustrated for HELP by increasing the evaporative depth by about a factor of two. This resulted in more than a ten-fold reduction in the predicted flux at the 13-m depth.

The strong thermal gradients, dominant vapor flow, and proximity of waste disposal trenches to the ground surface all suggest that potential exposure to contaminants via the air pathway may be of greater concern than potential exposure via the groundwater pathway at the hypothetical arid site. Vapor-phase transport appears to be the dominant mechanism by which water movement occurs at this site. Advective gas transport in coarse sediments is a potential mechanism for the movement of several contaminants (e.g., ^{3}H, ^{14}C, and ^{222}Rn). This suggests that performance assessment evaluations of LLW disposal facilities that use shallow land burial of wastes in arid environments should consider and evaluate the potential risks associated with vapor-phase transport of contaminants.

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 (JCN L2466). The report presents a framework for evaluating infiltration, percolation, and redistribution of water through natural and geotechnical materials and components associated with the site and engineered systems at commercial low-level radioactive waste (LLW) facilities. Specific information is provided on technical issues, models, and analyses for numerical estimates of water movement through the various natural and engineered systems at a LLW facility. The report also discusses application of the Hydrologic Evaluation Methodology (a revision and extension of an "Infiltration Evaluation Methodology" previously documented in NUREG/CR-5523) to two hypothetical LLW disposal facilities, using both an arid and a humid setting. This work provides, in part, the technical bases for hydrologic evaluation analyses in support of the NRC staff development and testing of a performance assessment methodology for LLW facilities. The Hydrologic Evaluation Methodology was designed to provide assistance to technical reviewers with the Agreement States, NRC staff and interested parties. This report has been peer reviewed by technical experts and has been circulated for comment to other federal agencies before publication.

NUREG/CR-6346 is not a substitute for NRC regulation, 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.

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Abbreviations

ASTM	American Society for Testing and Materials
BTP	Branch Technical Position
cdf	cumulative distribution function
DOE	U.S. Department of Energy
EPA	U.S. Environmental Protection Agency
ET	evapotranspiration
GCL	geosynthetic clay liner
HDPE	high-density polyethylene
HELP	Hydrologic Evaluation of Landfill Performance (computer code)
HiQC	high quality control materials for the humid site example capillary barrier
LLW	low-level radioactive waste
LoQC	low quality control materials for the humid site example capillary barrier
MidQC	medium quality control materials for the humid site example capillary barrier
MSTS	Multiphase Subsurface Transport Simulator (computer code)
NOAA	U.S. National Oceanic and Atmospheric Administration
NTS	Nevada Test Site
NRC	U.S. Nuclear Regulatory Commission
NWS	U.S. National Weather Service
pdf	probability density function
RWMS	Radioactive Waste Management Site
SCS	U.S. Soil Conservation Service
UNSAT-H	(computer code)
USGS	U.S. Geological Survey
VAM3DCG	Variably Saturated Analysis Model in Three Dimensions with Pre-conditioned Conjugate Gradient Matrix Solvers (computer code)
VLDPE	very low-density polyethylene
WGEN	Weather Generation model (computer code)

Symbols

Roman Symbols

c	solute concentration of the fluid phase (M/L^3)
C_{cl}	measured Cl^- concentration in soil water (M/L^3)
D	deep percolation (L/T)
D	solute hydrodynamic dispersion coefficient (L2/T)
D_{cl}	Cl^- deposition rate (M/L2 T)
D_m	coefficient of molecular diffusion in the pore fluid (L^2/T)
D_o	osmotic fluid diffusivity (L^2/T per bar)
D_t	thermal fluid diffusivity (L^2/T °K)
ET	Evapotranspiration (L/T)
H	hydraulic head (L)
h_m	matric potential (soil water pressure head) (L)
h_{me}	parameter of the Brooks-Corey water retention relationship (L)
h_o	osmotic potential (L)
h_z	gravitational potential (L)
i	gradient (L/L)
J_r	net residual flux (L/T)
K	hydraulic conductivity (L/T)
K_S	saturated hydraulic conductivity (L/T)
l	depth below which ^3H concentration is negligible (L)
L	length (L)
m	parameter of the van Genuchten water retention relationship (dimensionless)
n	parameter of the van Genuchten water retention relationship (dimensionless)
P	precipitation (L/T)
q	vertical water flux ($L/T\ L^2$)
q^{barr}	flux through barrier (L/T)
q^{cap}	capacity flow rate of drainage layer per unit width (L^2/T)
q_i	average net infiltration; average flux of water percolating below the root zone and into drainage layer (L/T)
Q^{req}	required average flow rate of drainage layer per unit width (L^2/T)
R	solute retardation factor (dimensionless)
RG	recharge (L/T}
RO	runoff (L/T)
s	solute concentration associated with solid phase of soil (M/L^3)
S	soil moisture storage (L/T)

S_i	sensitivity coefficient (dimensionless)
S_{ni}	normalized sensitivity coefficients (dimensionless)
t	time (T)
T_K	absolute temperature (ºK)
T	thickness (L)
T_H	total quantity of ^3H stored in the soil profile (M)
T_{pi}	average ^3H concentration in precipitation for year i before sampling (M/L^3)
u	source or sink term used to account for water uptake by plant roots (M/T)
v	average pore water velocity (L/T)
W_i	weighting factor (dimensionless)
z	depth, measured positive downward from the soil surface (L)

Greek Symbols

α	parameter of the van Genuchten water retention relationship (1/L)
α_L	dispersivity (L)
β	angle of sloped layer
ϕ	source or sink for solute (M/T)
γ	semivariogram
λ	parameter of the Brooks-Corey water retention relationship (dimensionless)
λ_H	decay constant (1/T)
θ	volumetric water content, or volume of water per unit bulk volume of soil (L^3/L^3)
θ_r	residual water content (L^3/L^3)
θ_s	saturated water content (L^3/L^3)
θ_z	volumetric water concentration at depth z (L^3/L^3)
ρ	soil bulk density (M/L^3)
τ	tortuosity factor (dimensionless)

Other Symbols

∇	vector gradient operator (1/L)

1 Introduction

Near-surface disposal of low-level radioactive wastes (LLW) is permitted under the Code of Federal Regulations, 10 CFR Part 61. Analysis of water movement in unsaturated soils and the determination of soil and hydrologic parameters are therefore needed to support the U.S. Nuclear Regulatory Commission (NRC) and state regulatory authorities in licensing and regulating LLW disposal sites. How much water infiltrates and how fast it moves to the waste and subsequently mobilizes and transports contaminants to the underlying water table are integral questions in the performance assessment of a LLW disposal facility.

Regulatory acceptance of a proposed LLW facility depends, in part, on demonstrating that the water flux into the facility can be controlled or limited to levels that ultimately provide acceptable groundwater quality for long periods of time (e.g., 500 years and longer). This demonstration is compounded by the complexity of facility design; although the natural environment of the site plays a key role, an engineering solution is often necessary to limit water access to the waste (Bedinger and Stevens, 1990). In addition, the long-term nature of LLW disposal makes prediction of facility performance difficult. Sites that at one time were thought to be suitable for long-term disposal have been shown later to have significant groundwater contamination problems (Nativ, 1991).

It is clear that regulatory and technical issues related to the water pathway need to be integrated in order to determine the optimum engineering solution for LLW sites. In the following discussion we address the regulatory and technical issues that determine the level of hydrologic analysis that may be required for evaluating LLW sites.

1.1 Regulatory Issues

Safe disposal of LLW in near-surface facilities depends on our ability to rely on a combination of the natural system and suitable engineered barriers to isolate the waste from pathways to the biosphere. To this end, numerous concepts have been proposed. In France, Germany, and other countries, well engineered sites with suitable hydrologic conditions are being used for disposal with apparent success (Schwarz, 1990; Templeton et al., 1994). In Europe, there appears to be regulatory acceptance for and confidence in a variety of disposal options that are a product of both engineered and natural system performance, coupled with assurances of long-term institutional control over waste sites. In the U.S., careful consideration and analysis of engineered hydrologic controls and site suitability are required for LLW disposal facilities to be accepted.

1.1.1 Near-term vs. Long-term Perspective

A review of the technical issues raised by the NRC staff and its contractors reveals a set of issues that can apply to either a near- or a long-term perspective. Treatment of these issues in current performance assessments is skewed toward the long-term perspective; few treatments address the real confidence we have in the relatively near-term performance of systems in the next 500 years. More attention should be paid to this time period. This dilemma has arisen because our attention is often focused on the health threat posed by long-half-life inventory items such as Tc-99 and I-129 that move with water in the vadose zone and into the groundwater aquifer after they are released from the waste form and engineered system. Regarding this type or class of inventory item, 10 CFR Part 61 § 61.7 calls for the following;

> "For certain radionuclides prone to migration, a maximum disposal site inventory based on the characteristics of the disposal site may be established to limit potential exposure."

In NUREG-0782 (USNRC, 1981; Vol. 1, pg. 40) under the topic of waste classification, the NRC further clarifies their position on the issue of the mobile and long-half-life radionuclides in the inventory as follows;

> "... four radionuclides were identified that are of significance from the standpoint of migration. These are H-3, C-14, Tc-99, and I-129. These nuclides have been addressed on a site-specific inventory basis. That is, the total quantity of these four radionuclides acceptable for disposal at any particular site will be determined as part of the licensing process based on the specific hydrogeological conditions, facility designs, and operating procedures at the site."

In this report, we assume that the NRC is intent on limiting nuclide inventories at LLW facilities to safe levels, thus focusing on relatively short-term needs (less than 500 years). This viewpoint requires demonstrating that, for the current estimated inventory, a reasonable assurance exists for compliance with regulation. Under the inventory-limiting concept, conservative approaches can be taken to estimate the long-term performance of wastes (controlled by a combination of engineered barriers and natural systems). Society then has the opportunity to choose the lowest risk option at the expense of locating the long-half-life nuclides in another disposal site in which it has greater confidence. With this premise, we have chosen to address the short-term (<500 year) issue. If simple and conservative or worst case conceptual models and simulation methods do not provide the necessary assurance, then reasonable assurance may be achievable through progressively more sophisticated engineering barrier and environmental pathway conceptualizations and simulations. Such an approach is illustrated in the humid site example (Section 6.1), with an analysis that moves from relatively simple one-dimensional hydrologic models to more complicated three-dimensional models of a LLW disposal facility.

1.2 Technical Issues: Hydrology

Guidelines for conducting necessary research and for closure of LLW sites have been written (O'Donnell and Lambert, 1989; White et al., 1990). Three areas of research – source term (release rates), concrete structure performance, and hydrologic assessments – have been identified as key areas where studies have been needed for LLW (Fischer, 1986; O'Donnell and Lambert, 1989). This report focuses on hydrologic assessment, particularly the unsaturated zone.

The following questions have been raised by the NRC relating to engineered covers and their hydrology at LLW sites:

- How should infiltration, recharge, and seepage into waste be determined in humid and semi-arid or arid environments?
- How should spatial heterogeneity be incorporated into the analysis?
- How should constitutive properties of natural and engineered materials be determined?
- How should the analysis of infiltration and recharge in the natural setting be validated?
- What constitutes an appropriate cover design?
- How important is the geometry of the cover layers to limiting water movement?
- How will engineered covers perform over time?
- How should the engineered system be analyzed?
- How should the analysis of water flow in the facility be validated?
- Should there be a design goal for the cover (i.e., should it be designed to achieve a specific seepage flux?)
- If there is a design goal, what criteria should be used for determining the adequacy of the designed engineered system in limiting seepage?

These questions can be grouped into four major issues:

(1) Estimating the water balance at a site (i.e., infiltration, runoff, water storage, evapotranspiration, and recharge);

(2) Analyzing the hydrologic performance of engineered components of a facility;

(3) Evaluating the application of models to the prediction of facility performance; and

(4) Estimating the uncertainty in predicted facility performance.

There is a need for a summary of the information that is currently available for evaluating these hydrologic issues at LLW sites. We address these major issues and provide a review of current research in unsaturated zone hydrology that relates to these issues. Much of the research is ongoing. The methods needed to evaluate the hydrologic performance of engineered barriers, particularly in arid climates, remain largely untested.

1.2.1 Hydrologic Evaluation Methodology

The general objective of a hydrologic evaluation at a LLW site is to determine the flux of water into the disposal facility. While the particular flux value, or range of values, arrived at is important, the questions listed above indicate that the process by which the flux is estimated is equally important. Only when the process is justifiable can the result of the process be acceptable. This report presents a process, or methodology, for hydrologic evaluation of LLW facilities that is based on the best current technical understanding.

Figure 1.1 is a flowchart for the hydrologic evaluation methodology presented in this report. It serves as both a simple outline for the report and as a road map for the preparation or review of the unsaturated zone hydrology component of a LLW facility license application. The sequence of the flowchart reflects the organization of this report with one exception; identifying and characterizing sources of uncertainty is located early in the flowchart. This is an indication of our belief that uncertainty should be considered early in an investigation. Site characterization and design should consider the primary sources of uncertainty.

The first step in the flowchart is the identification of the processes and factors affecting recharge and seepage through the facility. Technical issues related to the estimation of water balance at a LLW site are discussed in Section 2.1, with a review of the factors controlling recharge contained in Section 2.2. Identification and characterization of the primary sources of uncertainty (Section 5.1) is the next step in the flowchart. With knowledge of the uncertainties, the natural recharge at the undisturbed site can be estimated; the most common estimation methods are reviewed in Section 2.3. The natural recharge estimate is used in the regional groundwater flow component of a LLW site performance assessment.

The flowchart continues with a description of the engineered components of the facility, including their classification according to function, their potential performance, applicable design criteria, and potential degradation mechanisms (Chapter 3). The next item in the flowchart describes the simulation of water flow in LLW facilities, including the modeling process (Section 4.1), criteria for use in the evaluation of model applications (Section 4.2), and a description with respect to these criteria of several representative models (Section 4.3). Methods for estimating the effect of uncertainty on model predictions are presented in Section 5.2. The flowchart concludes with a determination of the rate of water flow into the waste, the quantity we call seepage. The

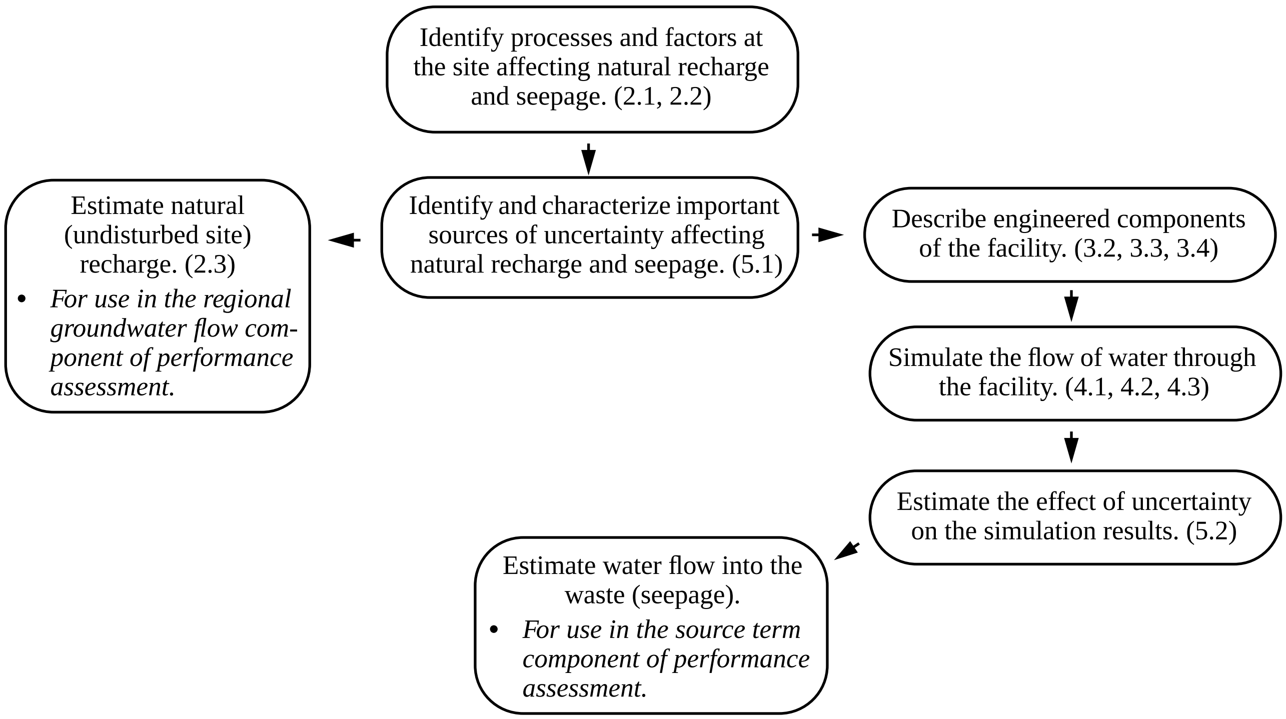


Figure 1.1 Flowchart for the Hydrologic Evaluation Methodology. Numbers indicate sections in this document in which the items are discussed.

source term component of LLW site performance assessment requires an estimate of seepage.

The methodology as outlined in the flowchart is applied using two example facilities, one in a humid environment and the other in arid site conditions. These examples are presented in Chapter 6 and illustrate both the methodology and many of the technical issues discussed in Chapters 2 through 5.

2 Fundamental Hydrologic Concepts

The first step in the hydrologic evaluation of a LLW facility is to identify the processes and factors that affect the water balance at the site. A number of potentially important processes are listed in Figure 2.1. The role these processes play in determining the water balance at a site is discussed in Section 2.1. Section 2.2 extends the discussion to include climate, soil, vegetation, and engineered barrier factors affecting water flow. The discussion of the issues related to water flow through an engineered barrier system is brief. Detailed discussion of engineered barriers is contained in Chapter 3. Section 2.3 addresses the estimation of recharge, including a discussion of the governing equations of water flow in unsaturated porous media. The typical methods for estimating recharge are described, with an assessment of their relative strengths and weaknesses. The chapter concludes with a brief discussion of hydrologic property measurement and the estimation of model parameters.

2.1 Water Balance

The essential hydrologic components of a water balance are precipitation, infiltration, runoff, water storage, and recharge. Figure 2.2 illustrates the components of water balance at a LLW site. Each of these components is discussed in this section.

2.1.1 Precipitation

Precipitation, occurring as either rain or snow, is the source term in a water balance and therefore must be accurately estimated. Precipitation at a potential LLW site can be relatively easily measured using automatic equipment. Unfortunately, several factors conspire to make estimates of long-term precipitation somewhat uncertain.

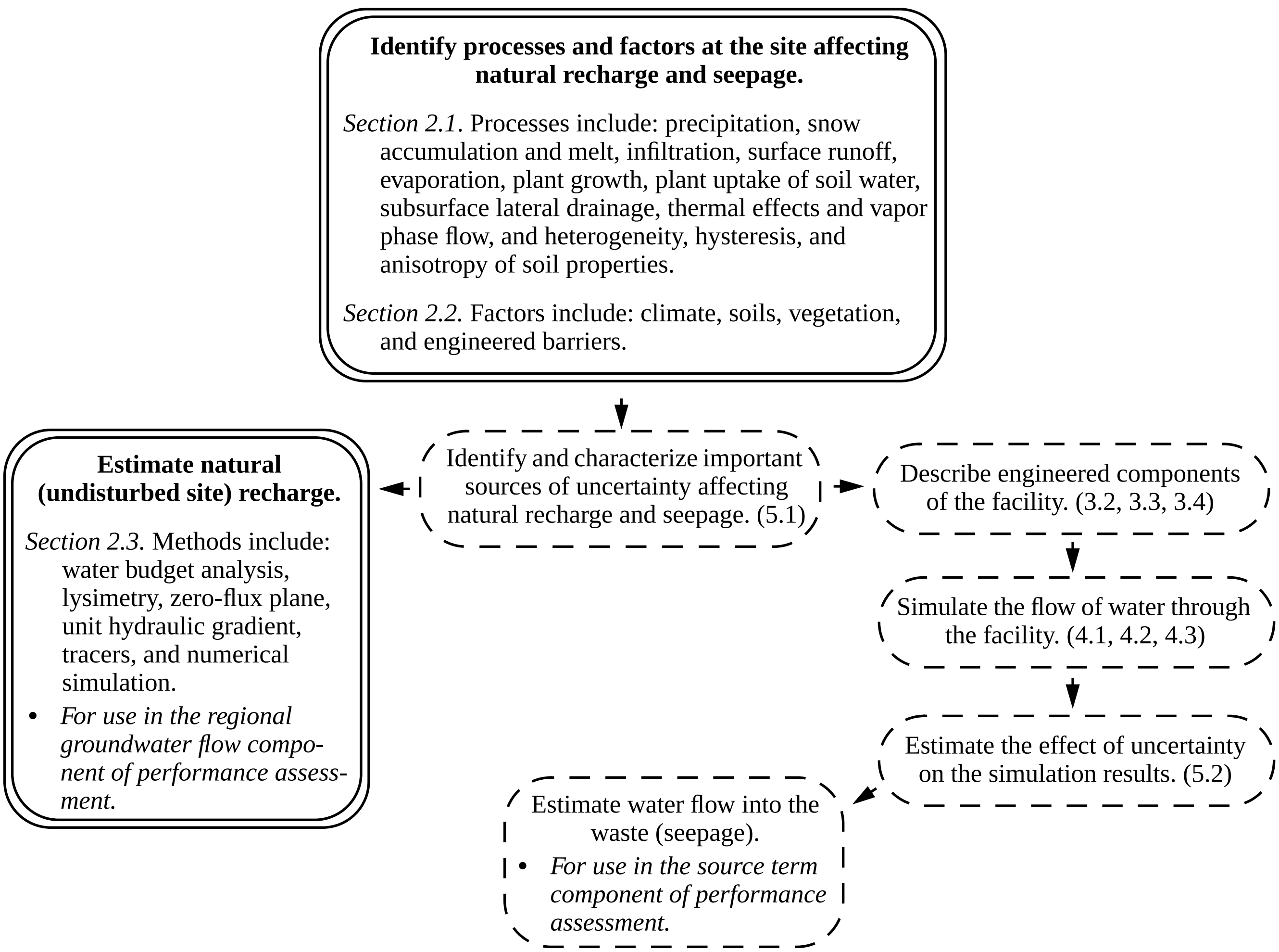


Figure 2.1 Flowchart for the Hydrologic Evaluation Methodology. Chapter 2 discusses the processes and factors affecting recharge and seepage as well as methods for estimating recharge. Numbers indicate sections in this document in which the items are discussed.

For many LLW sites, particularly in arid and semi-arid areas, site-specific precipitation records are often limited or absent. At such sites, estimates of precipitation are often made using records from sites located 10 to 20 km or more away from the site of interest. The spatial variability of climate at this scale is widely acknowledged and experienced by everyone. When data from a distant location are used, there is a high likelihood that the resulting precipitation estimates will not accurately represent the actual site-specific record.

Precipitation is also highly variable in time. Measurements that are averaged over hours, days, or months may poorly represent the actual, variable precipitation that occurs at the site. This can significantly affect recharge estimates (see Section 2.2.1 for an example). Snow precipitation can also contribute to the time variability of the water balance. An extreme, but not infrequent, example of snow-affected water balance is seen in the Pacific northwest climate where warm "chinook" winds cause rapid snowmelt. Rapid snowmelt may produce localized runoff, ponding, and subsequent deep percolation (and recharge) in coarse soils (Gee and Hillel, 1988).

Even when a precipitation record exists, it is likely to be of short duration relative to the operating life of a LLW facility. A short record will provide uncertain estimates of the probable maximum precipitation or other design events.

2.1.2 Infiltration

Infiltration is defined simply as the intake of water into surface soils (Hillel, 1982). In practice, infiltration is treated as a gross water balance parameter and never measured directly. A typical analysis of water infiltration requires an assessment of the infiltration capacity of soil, the instantaneous precipitation rate, and the runoff susceptibility (USDA, SCS, 1985). In a water balance analysis, infiltration would be defined as the difference between the precipitation and the runoff for a given time period (assuming interception by vegetation and surface evaporation during rainfall are negligible). While of importance in the analysis of water erosion potential for a LLW site, infiltration is seldom used as a defining parameter for subsurface water movement.

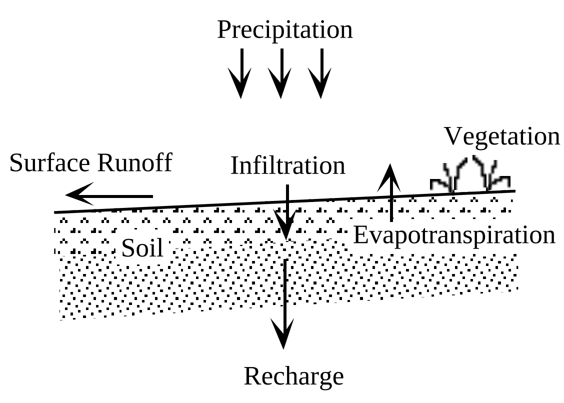


Figure 2.2 Water balance at a LLW site

The term "net infiltration" has been used to refer to the overall processes of net water intake into soils. In this context, net infiltration is computed as the difference between water applied (precipitation) and water lost from runoff and evapotranspiration. If computed over a sufficiently large time frame where annual storage change is negligible, net infiltration is synonymous with the term deep percolation. Under special circumstances, where lateral flow does not occur and there are no other water removal processes (e.g., deep plant root extraction, etc.) so that the downward percolating water enters the water table, net infiltration can also be called recharge. A quantitative method for transforming infiltration into recharge using a parametric transfer function approach is described by Besbes and deMarsily (1984).

Because infiltration has been used to refer to a number of different quantities, the following definitions are offered and will be consistently used throughout the text:

- infiltration – water entering the ground across the soil surface
- net infiltration – water passing beneath the zone of evapotranspiration
- recharge – water reaching the water table.

Since LLW disposal facilities are likely to have engineered components that control water flow, two additional terms will be used to refer to quantities of subsurface water flow:

- subsurface lateral drainage – water diverted laterally by some combination of engineered components
- seepage – water entering the part of the facility containing waste.

2.1.3 Runoff

Water lost from surface soils in overland flow is termed runoff (Hillel, 1982). Factors that affect runoff include precipitation rates, soil hydraulic properties, surface slope, and surface roughness. Short duration, high intensity storms are far more likely to cause runoff than gentle rains. Well vegetated, highly permeable, granular surfaces are less susceptible to runoff than bare, low permeable soils. Transient changes in runoff characteristics for surface soils relate to changes in soil water content, vegetation, soil freezing, and soil dispersion (from salt accumulation, etc.).

Details for calculating runoff using U.S. Soil Conservation Service (SCS) -type curves (based on soil texture, and plant cover conditions) are available in the National Engineering Handbook (USDA, SCS, 1985). It should be noted that these runoff curves have been developed over the years from data collected largely from agricultural fields. Just how well these type curves describe runoff potential at constructed waste sites has not been determined.

2.1.4 Soil Water Storage

Soil water storage is the total quantity of water in the soil zone of interest. For LLW sites with an engineered barrier, this generally refers to the water storage in the surface cover. Water storage changes are most pronounced near the soil surface and within the top two or three meters, where roots are active and evaporation processes are most effective. Of all the components of the water balance, water storage is one of the more easily measured parameters. This is accomplished by monitoring the soil water content and integrating over the soil depths of interest (Hillel, 1982). Changes in calculated storage over a selected time interval are usually of most interest.

There are a number of ways to monitor soil water. Several of these, including neutron probe and time domain reflectometry are described in detail in a recent NUREG report (Wierenga et al., 1993). Typical errors in measurement of water storage range from 2 to 4% of the total storage value. In a 2-m-deep soil profile, at an average water content of 20 volume percent, this translates to an error ranging from 8 to 20 mm. While this is a relatively small error, it can be significant for arid site water balance.

2.1.5 Evapotranspiration

Evapotranspiration (ET) is the combined evaporation from soil and plant surfaces (Hillel, 1982). In a water balance analysis, precipitation that is intercepted by vegetation and that subsequently evaporates is accounted for in ET. Sublimation of snow would also be a component of ET. ET can account for 50% or more of water losses at the soil surface at humid sites and generally accounts for most, if not all, water losses at arid sites. Measurement of ET is never direct and most often is calculated as a difference between precipitation and the remaining components of the water balance: runoff, storage change, and recharge.

Micrometeorological methods, such as Bowen ratio and eddy correlation, estimate ET by measuring transient temperature and humidity gradients near the ground surface and estimating latent heat fluxes from soil surfaces. For arid sites, these methods have met with limited success when measurements are made over hot, dry surfaces where latent heat fluxes are small (i.e., below 0.5 mm/day).

ET can also be estimated as some fraction of potential evapotranspiration (e.g., Thornthwaite and Mather, 1955; Saxton et al., 1974; Morton, 1983). Potential ET is a measure of the maximum amount of water that can be absorbed into the atmosphere given the atmospheric vapor density and radiant energy condition (Campbell, 1977). Various methods can be used to calculate potential ET, typically using solar radiation, wind speed, and other climate data (Doorenbos and Pruitt, 1977). Potential ET can be used to empirically estimate actual evaporation and transpiration without describing any controlling physical processes such as diffusion and convection. In the absence of plants, only evaporation is considered for the ET component.

Unfortunately, no approach short of very data-intensive energy balance methods accurately accounts for evaporation from dry surfaces. A very compelling discussion of this observation is given by Campbell (1977), who states, “Numerous attempts have been made to express non-potential [actual] ET as some fraction of potential ET. If the soil or soil-plant system (rather than atmospheric factors) is controlling water loss then such attempts are obviously futile because ET is not functionally related to potential ET.”

At arid and semi-arid sites, for a large portion of the year the soil-plant system, rather than the atmospheric variables, is controlling water loss from the surface. As an example, for the Hanford Site, a semi-arid site in southcentral Washington State, an annual potential ET value of 1600 mm was calculated, while for the same period, the actual evaporation from both bare and vegetated soils was measured to be less than 120 mm, or less than 10% of the potential ET (Gee et al., 1989).

Estimates of annual ET using any of these techniques are at best accurate to within 10% (Gee and Hillel, 1988). At humid sites, where annual precipitation may be 1000 mm or more and ET as much as 500 mm, errors of 50 mm in ET may be tolerable. At arid sites, however, where precipitation may be 160 mm and ET 150 mm or more, errors of 15 mm or greater become relatively more important.

2.1.6 Recharge

As discussed earlier, recharge is water that eventually reaches the water table. Of all the water balance components, recharge is perhaps the most difficult to estimate reliably. It can be estimated as a residual of the other water balance terms (precipitation, runoff, water storage, and ET), measured as drainage from lysimeters, or estimated from chemical tracer profiles and assumptions about chemical mass balances. These methods (and others) are discussed in some detail in Section 2.3.2. Errors of estimation are usually large for the recharge term, ranging from 20% at humid sites to 100% or more at arid sites.

2.2 Factors Affecting Recharge

Recharge and the related quantity, seepage, when coupled with the release rate of the contaminant provide one of the key input parameters needed in LLW performance assessments (used to predict long-term acceptability of subsurface disposal of LLW). Perhaps one of the greatest challenges currently faced in providing technically sound performance assessments is the quantification of recharge and the processes that lead to it (Rockhold et al., 1995). Because of the need to quantify recharge, it is important to understand the factors that affect the estimate of recharge at both humid and arid sites.

2.2.1 Climate

Climate is the dominant variable in controlling water flow and transport at LLW sites. Variations in precipitation amount, duration, and intensity, coupled with the energetics of solar radiation, temperature, and wind combine to dictate the water input at the surface of a LLW site. It is the complex interaction of these variables that create significant uncertainties in both infiltration and ET from the surface of a LLW site.

While weather records are often available for a given LLW site, they are generally of insufficient duration (and quality) to provide adequate statistics to estimate precipitation input or evaporation potential for extended time periods. At the present time, records obtained from the closest recording station in the NWS-NOAA (National Weather Service) network must be relied on. These data, coupled with extreme value statistics (Kinneson, 1983), can be used to predict the extreme weather conditions likely to be encountered over the life of the LLW disposal facility. While it is not possible to predict exact climatic variation with any accuracy, daily climatic variations can be estimated via stochastic weather generation models such as WGEN (Richardson, 1981; Richardson and Wright, 1984). An application of WGEN for generating a 500 year weather sequence is described in Section 6.2.

Climatic parameters such as precipitation and ET vary dramatically in space and time, and these variations cannot be ignored. In a recharge analysis, average values of these parameters are typically used. This can have a dramatic effect on recharge estimates as is illustrated in several examples provided here.

Meyer (1993) simulated the water balance for a hypothetical disposal facility located in a humid environment. The top meter of soil was simulated to estimate the amount of net infiltration (i.e., the amount of water passing below the zone of evapotranspiration). Meyer (1993) compared the use of average daily and average hourly precipitation. In the humid environment simulated, with many short-duration, high-intensity storms, the predicted net infiltration was significantly reduced by the use of hourly averaged data. Results of the two-year simulation are given in Table 2.1.

Table 2.1 Simulated water balance at a humid site (from Meyer, 1993)

	Water Balance [cm/yr.] (% of Precip.)	
	Daily Average Precipitation	**Hourly Average Precipitation**
Infiltration	112.1 (93.0)	76.3 (63.3)
Runoff	8.4 (7.0)	44.2 (36.7)
Storage	-0.2 (-0.2)	-1.6 (-1.3)
ET	76.9 (63.8)	72.9 (60.5)
Net Infiltration	35.5 (0.29)	4.8 (4.0)

A second illustration is found in the recharge study of the U.S. Geological Survey (USGS) at the Hanford Site. A model was developed by the USGS to calculate average annual recharge using input parameters that included dynamic (time-dependent) input for precipitation, and static (time-independent) soil type and vegetative cover input (Bauer and Vaccaro, 1986). The model was run in two ways. First, the actual daily climatic records (along with input parameters obtained from soil and plant data) were used to predict annual recharge using a 21-year record of precipitation. Second, the average daily climatic records were used to predict annual recharge for the same climatic record.

Table 2.2 Simulations of recharge at the Hanford Site using a 21-year climate record (from Bauer and Vaccaro, 1986)

	Recharge [mm/yr.]	
	Actual Daily Climate	**Average Daily Climate**
Maximum	58	31
Minimum	0.5	0
Average	12	2

Table 2.2 shows a dramatic difference in results between the two model runs. Input of actual daily precipitation resulted in prediction of an annual recharge rate six-fold higher than that predicted when precipitation was input as daily averages from the 21-year record.

2.2.2 Soil

Heterogeneity, anisotropy, and hysteresis in the hydraulic properties of natural and emplaced soils can have a significant effect on recharge. Recharge events are typically caused by extremes in precipitation (i.e., thunderstorms, rapid snowmelt events, etc.). When soils get sufficiently wet, pulses of water from these extreme events can flow through macropores (i.e., root channels, fissures, cracks, and other heterogeneities in soil profiles) and can cause water to recharge underlying aquifers more quickly than would occur if the soil were uniform and precipitation steady (Gee and Hillel, 1988). In addition, unstable flow (fingering) can be created in layered soils and in relatively uniform soils (e.g., coarse sands) when appropriate conditions on pore size distribution and water flux are met (Hillel, 1987; Gish and Shirmohammadi, 1991; Glass, 1992).

Because precipitation is high and surface soils often saturated, flow through preferred pathways is of greatest concern in humid environments. The surface soil is literally teaming with life (roots, earthworms, burrowing animals, etc.), all combining to promote preferred pathways of flow. Because most surface soils at humid sites contain large numbers of macropores of various sizes and configurations, and the distribution of these macropores is seldom well known, chances for accurately predicting water infiltration (and subsequent percolation and recharge) rates at a humid site are low. The dynamics and hydrologic significance of these preferred paths or channels, their formation, distribution and persistence, are just now being evaluated (Germann, 1988; van Genuchten et al., 1991a; Gish and Shirmohammadi, 1991; Gee, 1991). The major problem in the analysis of water infiltration and recharge at humid sites lies in the characterization of soil macropores.

Soil hysteresis has been shown to be an important factor in accurate predictions of seepage through an engineered cover at the semi-arid Hanford Site (Fayer, 1995). Six years of water storage and drainage data were collected in a weighing lysimeter filled with 1.5 m of silt loam overlying approximately 0.1 m of sand and a shallow gravel layer. This placement of materials constitutes a capillary barrier (see Section 3.2.3), increasing the storage capacity of the silt loam and delaying drainage. The lysimeter was kept free of vegetation. Drainage occurred only in the final year of operation.

Water flow in the lysimeter was modeled with UNSAT-H, Version 3.0 using a variety of approaches including the use of calibration, heat flow modeling, and hysteresis modeling. The results, shown in Table 2.3, demonstrate that although the four UNSAT-H models had comparable errors in storage, only the model that included hysteresis predicted the drainage that occurred. This model predicted 52% of the actual drainage and predicted drainage within one month of its actual occurrence. (Results using the HELP, Version 2.05 code are shown in Table 2.3 for comparison. HELP predicted drainage in all six years, probably due to its inability to model the physics of flow through the capillary barrier.)

Table 2.3 Modeling of lysimeter drainage at the Hanford Site over a six year period. Measured drainage was 29.6 mm. (Y indicates a process that was included in the model, N indicates one that was not.)

Code	Calibration	Heat Flow	Hysteresis	Storage RMS Error [mm]	Cumulative Drainage [mm]
UNSAT-H	N	N	N	23.6	0.0
UNSAT-H	Y	N	N	23.6	0.0
UNSAT-H	N	Y	N	23.4	0.0
UNSAT-H	N	N	Y	23.7	15.3
HELP	N	N	N	97.6	537.0

2.2.3 Vegetation

Large-scale changes in surface conditions at LLW sites can affect infiltration and recharge. Vegetation changes resulting from drastic disturbances such as fire, pest and disease, land-use changes, or extreme weather (tornadoes, hurricanes, etc.) can cause reductions in ET, ultimately increasing recharge rates. The removal of deep- rooted vegetation can have a particularly dramatic effect. Examples of the effect of changing land use on recharge are provided by Allison et al. (1994). Farming practices in Australia, which have removed native trees and replaced them with shallow-rooted pasture, have dramatically increased recharge along the Murray River drainage basin. The increased recharge has leached salts from the arid soils and has resulted in the salinization of the major fresh water resource in Australia.

Examples can also be found of the effect of vegetation changes on recharge at arid waste sites. An 18-m-deep, closed-bottom lysimeter at the Hanford Site was sampled gravimetrically for water content during filling in December 1971 and again in October 1985 (Fayer et al., 1986). No drainage occurred, and storage decreased over the 14 year period. During this time, vegetation (e.g., annual and perennial desert species including tumbleweed and scurf pea) became established on the lysimeter. After all plants were removed from the lysimeter in February of 1988, water storage increased more than 100 mm over a 3-year period. In spring 1991, subsequent reinvasion of vegetation on the lysimeter completely removed the excess water storage in just a few months (Gee et al., 1994). These data clearly show the impact of both the presence and absence of vegetation in controlling arid-site recharge.

2.2.4 Engineered Barriers

The term engineered barrier refers to those components of a waste disposal facility that are intended to improve the facility's ability to meet the performance objectives. (Chapter 3 discusses engineered barriers in detail.) The presence of an engineered barrier system will have a dramatic effect on recharge (and seepage). When operating as designed, a barrier system should significantly reduce the recharge rate. As the engineered system degrades, however, its presence may actually increase recharge over that of the natural preexisting (undisturbed) site. This is the worst possible consequence of an engineered system and must be avoided. Ways in which a failed engineered barrier system may enhance recharge include the following:

- Reduction of surface runoff: water, initially directed away from the site by engineered, surface-diversion features, can be rerouted by subsidence or other surface alterations so that water is ponded on, or adjacent to, the waste site.
- Reduction of ET: alteration of the natural (undisturbed site) vegetative community may reduce ET (e.g., replacing deep-rooted vegetation with shallow-rooted plants in a thin topsoil layer). This increases the proportion of water available for recharge in the event of barrier failure.
- Reduction of subsurface lateral drainage: lateral diversion drains can seal off in time through the process of siltation. In addition, subsidence could divert lateral drainage systems and potentially saturate soils above the waste.

Suter et al. (1993) have identified a variety of mechanisms that have caused water movement through covers at waste sites. These mechanisms include design and construction flaws, shrink-swell cycles, freeze-thaw cycles, erosion, subsidence, root intrusion, and animal intrusion. These failure mechanisms will be addressed in more detail in the following chapter. Suter et al. (1993) and others correctly conclude that the likelihood of long-term failure suggests that either perpetual care must be provided for buried wastes, or the waste site must be designed to withstand long-term threats to barrier integrity.

2.3 Estimating Recharge

A variety of methods are available for estimating natural groundwater recharge rates in undisturbed systems and recharge (or seepage) rates in systems involving engineered components. These methods are all based on quantifying water flow and solute transport processes in the unsaturated zone. In this section, the fundamental principles and governing equations used to describe unsaturated flow and solute transport are briefly reviewed, followed by descriptions of methods that have been used for estimating recharge rates. Portions of this section are taken from Rockhold et al. (1995).

2.3.1 Governing Equations

Water flow and solute transport processes in the unsaturated zone are complex and multidimensional and generally occur under nonisothermal conditions with multiple fluid phases (liquid water and water vapor). For brevity, the following discussion will be limited to the description of isothermal, single-phase (liquid water) flow and solute transport in one dimension (the vertical direction).

Water moves from regions of higher to lower potential energy, with the total potential generally taken to be the sum of the matric potential and the gravitational potential. (This assumes that the gas pressure and osmotic potentials are negligible.) Matric potential consists of hydrostatic pressure and the capillary and adsorptive forces that attract and bind water to the soil matrix. Gravitational potential is the energy associated with the location of water in the Earth's gravitational field, measured with respect to some reference point such as the ground surface or the water table.

This sum of the matric and gravitational potentials, when expressed on an equivalent height-of-water basis, is commonly referred to as the hydraulic head, or H. That is,

$$H = h_m + h_z \quad (2\text{-}1)$$

where

h_m = matric potential, and

h_z = gravitational potential.

The matric potential is also referred to as the soil water pressure head and is negative for unsaturated conditions. Corey and Klute (1985) provide a detailed discussion on the application of the potential energy concept to soil water equilibrium and transport.

For saturated systems, the vertical flux of water through soil can be determined using the Darcy flow equation

$$q = -K_s \frac{\partial H}{\partial z} \quad (2\text{-}2)$$

where

q = vertical water flux

K_s = saturated hydraulic conductivity

z = depth, measured positive downward from the soil surface

For unsaturated soils, the hydraulic conductivity is nonlinearly related to the pressure head or water content. Therefore, Eq. 2-2 is usually modified as

$$q = -K(\theta)\frac{\partial H}{\partial z} \tag{2-3}$$

where

K(θ) = hydraulic conductivity

θ = volumetric water content, or volume of water per unit bulk volume of soil.

To describe transient water flow in the vertical direction, Eq. 2-3 is combined with the equation of continuity,

$$\frac{\partial\theta}{\partial t} = -\frac{\partial q}{\partial z} \tag{2-4}$$

to give

$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial z}\left[K(\theta)\frac{\partial H}{\partial z}\right] + u \tag{2-5}$$

where

t = time, and

u = a source or sink term used to account for water uptake by plant roots.

Equation 2-5 is known as the Richards equation (Richards, 1931) and forms the basis for most process-based descriptions of water movement in the unsaturated zone. Equation 2-5 can also be expressed as

$$\frac{\partial\theta}{\partial t} = \frac{\partial}{\partial z}\left[K(h_m)\frac{\partial h_m}{\partial z} - K(h_m)\right] + u \tag{2-6}$$

To solve Equation 2-6, constitutive functions relating the unsaturated hydraulic conductivity and the water content to the pressure head are needed. The most commonly used relationships are those of van Genuchten (1980) and Brooks and Corey (1964), although other expressions are available (Mualem, 1992; Rossi and Nimmo, 1994; Fayer and Simmons, 1995). The van Genuchten water retention relationship is

$$\theta(h_m) = \theta_r + (\theta_s - \theta_r)[1 + (\alpha|h_m|)^n]^{-m} \tag{2-7}$$

where

α = curve fitting parameter related to air entry pressure

n,*m* = curve fitting parameters related to pore size distribution; the relationship, m=1-1/n, is often assumed

θ_r = residual water content

θ_s = saturated water content

The van Genuchten hydraulic conductivity relationship, based on the model of Mualem (1976) is

$$K(h_m) = K_s\frac{\{1-(\alpha|h_m|)^{n-1}[1+(\alpha|h_m|)^n]^{-m}\}^2}{[1+(\alpha|h_m|)^n]^{0.5m}} \tag{2-8}$$

The corresponding Brooks-Corey relationships are

$$\theta(h_m) = \theta_r + (\theta_s - \theta_r)\left(\frac{h_{me}}{h_m}\right)^{\lambda}; h_m < h_{me} \tag{2-9}$$

$$\theta(h_m) = \theta_s; h_m \ge h_{me} \tag{2-10}$$

and

$$K(h_m) = K_s\left(\frac{h_{me}}{h_m}\right)^{2+3\lambda}; h_m < h_{me} \tag{2-11}$$

$$K(h_m) = K_s; h_m \ge h_{me} \tag{2-12}$$

where

h_{me} = curve fitting parameter related to air entry pressure

λ = curve fitting parameter related to pore size distribution.

These single-valued relationships (Equations 2-7 through 2-12) assume that hysteresis is not important.

The advective-dispersive solute transport equation can be written as

$$\frac{\partial}{\partial t}(\rho s) + \frac{\partial}{\partial t}(\theta c) = \frac{\partial}{\partial z}\left[\theta D\frac{\partial c}{\partial z} - qc\right] + \phi \tag{2-13}$$

where

s = solute concentration associated with the solid phase of the soil,

ρ = soil bulk density,

c = solute concentration of the fluid phase,

D = solute hydrodynamic dispersion coefficient,

ϕ = source or sink for solute.

If the source/sink terms in Eqs. 2-6 and 2-13 are neglected and the adsorbed concentration is related to the solution concentration through the linear sorption isotherm (i.e., s = k_dc), Eq. 2-13 reduces to the standard advection-dispersion equation

$$R\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial z^2} - v\frac{\partial c}{\partial z} \tag{2-14}$$

where

v = q/θ is the average pore water velocity, and

R = 1 + ρk_d/θ is the solute retardation factor.

The dispersion coefficient can be defined as

$$D = \tau D_m + \alpha_L|v| \qquad (2\text{-}15)$$

where

τ = a tortuosity factor,

D_m = the coefficient of molecular diffusion in the pore fluid [L^2/T], and

α_L = the dispersivity [L].

The dimensionless tortuosity factor can be written as a function of θ using a relationship such as that of Millington and Quirk (1961),

$$\tau = \theta^{10/3} / \theta_s^{\ 2}. \qquad (2\text{-}16)$$

Equations 2-3, 2-6, 2-13, and 2-14, or variants of these equations, form the mathematical basis for most of the methods used to estimate groundwater recharge. The most common of these methods are described in the following section.

2.3.2 Recharge Estimation Methods

Recharge is seldom measured directly. At humid sites a water budget analysis is generally used. Recharge is often simply estimated as the difference between precipitation and the sum of ET and runoff (Simmers, 1988). Estimates of recharge at humid sites rely on reasonable estimates of ET, which is generally about one-half of the precipitation. Estimation errors of 10% in ET and runoff give rise to errors in recharge that are generally less than 20%.

For semi-arid and arid sites, Allison et al. (1994)) have indicated that recharge can be estimated in several ways including water budget analysis, lysimetry, and tracer analysis. At these drier sites, ET is generally a much larger percentage of precipitation than at humid sites. This can lead to relatively large errors in estimates of recharge when using water budget analysis (see Section 2.3.2.1). Of the available methods, lysimetry and tracer analysis appear to be the most reliable and water budget modeling the least reliable for estimating recharge at semi-arid and arid sites.

2.3.2.1 Water Budget Analysis

Gee and Hillel (1988) discuss the use of a water budget to obtain recharge estimates. This is a well known and often used method of attempting to measure all components of the water balance including precipitation (P), runoff (RO), ET, and the change in soil moisture storage (ΔS). See Figure 2.2 for an illustration of these components. The remaining component, the deep percolation that eventually constitutes recharge (RG), can then be determined as the difference between precipitation and the sum of all other components:

$$RG = P - (RO + ET + \Delta S) \qquad (2\text{-}17)$$

The reliability of the recharge estimate thus calculated obviously depends on the accuracy and precision with which each of the other components is measured at a (presumably) representative site. The problem is that such measurements are seldom very accurate or precise; when the difference is taken between two nearly equal quantities, each of which is fraught with an appreciable measure of uncertainty, the resulting uncertainty easily becomes untenably large. This condition can be demonstrated by the following equation.

$$(X \pm x) - (Y \pm y) = (X - Y) \pm (x \pm y) \qquad (2\text{-}18)$$

As an example, if the mean difference between X and Y is 0.1X, and the range of uncertainty in each, ±x and ±y, is only 0.05X, then we obtain

$$(X \pm 0.05X) - (0.9X \pm 0.05X) = 0.1X \pm 0.1X. \qquad (2\text{-}19)$$

This shows that an uncertainty range of only 5% in the two values can magnify to an uncertainty of 200% in the difference between them. Precipitation measurements are hardly ever more precise than ±5% and ET measurements are almost never more precise than ±10%, so the resulting error in estimating recharge can be even greater than the example given. As the value of recharge becomes small, errors of several orders of magnitude are entirely possible.

Water budget models have serious deficiencies at arid sites for the following reasons: 1) water budget models often rely on generalized site characteristics that are derived from average values; 2) water budget models do not properly account for evaporation from dry surfaces, and they tend to estimate evaporation and transpiration more reliably at humid sites; 3) all water budget models (when used where runoff is negligible) calculate recharge as the difference between precipitation and ET. At arid sites, one can be very nearly equal to the other, so such a calculation has an inherently large error (often several orders of magnitude); 4) vegetation distributions change with time, potentially causing dramatic changes in rooting depths and water extraction rates (thus altering ET); 5) recharge can be transmitted from the soil surface to the water table by preferred pathways, thus bypassing much of the soil volume (Gee and Hillel, 1988).

2.3.2.2 Lysimetry

The water budget method is classified as an indirect physical method because recharge is not directly measured. The only method available for directly measuring recharge is lysimetry. One of the strengths of lysimetry is that it provides a control volume in which a number of water balance components can be measured directly, thus providing the necessary data to calibrate numerical models, which can then be used to forecast recharge.

The two principal types of lysimeters are drainage lysimeters and weighing lysimeters. Drainage lysimeters consist of soil-filled containers instrumented with neutron probe access tubes or other sampling means that allow for the measurement of water contents at different depths. Changes in water storage can be calculated from these measurements. Weighing lysimeters consist of soil-filled containers resting on platform scales. Weight changes in the lysimeter are measured and related to changes in storage. In either case, drainage is directly measured. If precipitation is also measured, ET can be calculated using Eq. 2-17. Lysimeters are generally built on relatively flat surfaces and have elevated edges. These features eliminate runon and runoff.

Although they provide the only direct means of measuring recharge, lysimeters have several disadvantages, compared to some indirect methods. Lysimeters are usually fixed in space and are therefore limited in their ability to quantify the effects of spatial variability. The soils filling the lysimeters may represent composite samples of the surrounding sediments; therefore, the natural stratification or layering is usually not preserved. For determining recharge at a LLW site, however, this may not be a disadvantage since the natural layering may not be representative of the final engineered disposal facility. Finally, the length of the data record available from lysimeters is often relatively short, so that meaningful long-term averages may be difficult to obtain from lysimeter records.

2.3.2.3 Zero-Flux Plane

The zero-flux plane method for estimating recharge relies on determining the location of a plane of zero hydraulic gradient in the soil profile (Wellings, 1984). The location of this plane can be determined using sensors to directly or indirectly measure soil suction or capillary pressure (e.g., tensiometers, thermocouple psychrometers, heat dissipation sensors, etc.). Recharge for a given duration is calculated by integrating water-content measurements below the zero-flux plane to determine the change in total water stored in the profile. A decrease in total storage below this plane over the time period is assumed to be recharge. Unfortunately, this zero-flux plane is not always stationary, and the method cannot be used during periods of high infiltration if the hydraulic gradient becomes positive downward throughout the profile. In a comparison of recharge estimation methods, Healy (1989) determined that the zero-flux plane method had such severe limitations that its use was inappropriate at the LLW site studied.

2.3.2.4 Unit Hydraulic Gradient

While studying drainage losses from lysimeters, Black et al. (1969) noted that a “unit gradient” condition often occurred. This condition arises for fairly uniform (homogeneous) soils when the water content is nearly constant with depth and results in $dH/dz \approx (-)1$. For unit gradient conditions, Eq. 2-3 reduces to $q = K(\theta)$, and the flux of water moving through the soil is equal to the unsaturated hydraulic conductivity of the soil. Unit gradient conditions have been observed in some lysimeters and at some water balance study locations on the Hanford Site (Rockhold, et al. 1988; Gee et al., 1989). For unit gradient conditions, recharge rates can be estimated from the measured volumetric water content and the estimated unsaturated hydraulic conductivity of the soil below the plant root zone (Nimmo et al., 1994).

Both direct and indirect methods are available for measuring or estimating unsaturated hydraulic conductivities (Klute and Dirksen, 1986; van Genuchten et al., 1992). However, no single method appears to be suitable for providing reliable estimates of unsaturated hydraulic conductivity over a wide range of soils.

2.3.2.5 Tracers

Various chemical and radioactive tracers can be used to estimate natural groundwater recharge rates in arid and semi-arid environments (Allison et al., 1994; Phillips, 1994). As noted by Phillips (1994), these tracers should possess several characteristics. Most importantly, the tracer must be conservative, meaning that it is not adsorbed onto the solid phase and it is not produced in the soil. The rate at which the tracer is introduced into the soil must also be known. The most common tracers used to estimate recharge include chloride (Cl^-), chlorine-36 (^{36}Cl), and tritium (^3H).

Tritium

Large quantities ^3H were released into the environment by atmospheric nuclear weapons testing, mostly during the early 1960s (Phillips, 1994). Some ^3H was also generated from sea-level nuclear weapons testing in the 1950s. This entered the hydrologic cycle as tritiated water vapor, which behaves almost identically to water vapor. Therefore, ^3H is an excellent tracer for water movement in both liquid and vapor phases (Phillips, 1994). The use of bomb-^3H as an environmental tracer is limited because its half-life is 12.4 yr. (Phillips, 1994).

Allison (1981) described two simple methods for estimating mean annual recharge using bomb-^3H profiles. In the first method, assuming steady-state (with constant water content) and piston flow (no dispersion) and that ^3H moves with the mass fluid flow, recharge is estimated by dividing the total amount of water stored in the profile above the ^3H peak by the time elapsed since the fallout peak. In the second method, local annual recharge or net residual flux, J_r, is estimated by evaluating the ^3H mass balance as

$$J_r = T_H/T_A \qquad (2\text{-}20)$$

where T_H is the total quantity of ^3H stored in the soil profile. T_H is calculated as

$$T_H = \int_0^l T_z \theta_z dz \qquad (2\text{-}21)$$

where

ℓ = the depth below which the ^3H concentration is negligible,

T_z = ^3H concentration at depth z,

θ_z = volumetric water content at depth z.

The term T_A is given by

$$T_A = \sum_{i=1}^{n} W_i T_{pi} e^{-i\lambda_H} \quad (2\text{-}22)$$

where

W_i = weighting factor that accounts for year-to-year variations in recharge,

T_{pi} = average ^3H concentration in precipitation for year i before sampling,

λ_H = decay constant for ^3H,

n = number of years considered before sampling.

Allison and Hughes (1978) tested different schemes for estimating the weighting factors, W_i, but determined that using a constant value of 1.0 was adequate. An application of this method for estimating natural groundwater recharge in a semiarid region of New Mexico is described by Mattick et al. (1987). Both of the methods described above require the 1962-1965 bomb-^3H peak to be clearly identified in the soil profile.

Chlorine-36

Chlorine-36 (^{36}Cl) is produced naturally in the atmosphere, but was also produced indirectly, as a by-product of nuclear weapons testing, by thermal neutron irradiation of chloride in sea water (Phillips, 1994). This bomb-^{36}Cl was released in measurable amounts only during the sea-level tests in the 1950's, rather than during the stratospheric tests of the 1960's (Bentley et al., 1982; Elmore et al., 1982). Therefore, the maximum fallout of ^{36}Cl preceded the maximum ^3H fallout by about 10 yr. (Phillips, 1994).

The ^{36}Cl fallout entered the hydrologic cycle as chloride anion dissolved in precipitation and as dry fallout (Phillips, 1994). ^{36}Cl is conservative, chemically stable, and nonvolatile. Therefore, unlike ^3H, it is a tracer for the transport of solutes only in the liquid phase. The half-life of ^{36}Cl is approximately 301,000 years (Phillips, 1994).

The methods used to estimate natural groundwater recharge from $^{36}Cl/Cl$ ratios are essentially the same as those described previously for ^3H. Since ^3H moves in both the liquid and vapor phases, it can move faster than ^{36}Cl. A major problem with the use of ^{36}Cl (and ^3H) to estimate recharge at low flux rates is the relatively short residence time of these tracers in soil (less than 40 years). In addition, plant uptake, macropore flow, and other near-surface processes can significantly affect ^{36}Cl (and ^3H) movement in the root zone. Tyler and Walker (1994) have shown that when recharge rates are below 20 mm/yr., estimates of recharge with ^{36}Cl are not reliable.

Chloride

Meteoric chloride (Cl^-) originates primarily from sea salts and is continuously deposited on the land surface by precipitation and as dry fallout. This Cl^- moves into the soil profile with infiltrating precipitation. Cl^- is conservative and non-volatile and is almost completely retained in the soil when water evaporates or is transpired by plants (Phillips, 1994). Therefore Cl^-, like many other tracers, may concentrate in the root zone as a result of ET. The Cl^- mass balance method has become a relatively popular method for estimating recharge rates. A brief description of this method is given below, after Phillips (1994).

Assuming one-dimensional piston flow (no dispersion), recharge or net residual water flux can be calculated from Cl^- measured in a soil profile as

$$J_r = D_{cl}/C_{cl} \quad (2\text{-}23)$$

where

J_r = the net downward residual water flux at the depth of measurement (L/T),

D_{cl} = the Cl^- deposition rate (M/L^2 T), and

C_{cl} = the measured Cl^- concentration in the soil water (M/L^3).

The value of C_{cl} can be determined by plotting cumulative Cl^- content with depth against cumulative water content at the same depths. The slopes of straight line segments correspond to C_{cl} for the depth interval (Phillips, 1994). Changes in the slopes of different line segments, corresponding to the different depth intervals, can represent temporal variability of recharge rates.

In soils with high pH and high adsorption of other anions, anion exclusion can result in faster movement of Cl^- than ^3H. Previous studies have shown a direct correlation between clay content and anion exclusion (Warrick et al., 1971). James and Rubin (1986) reported an increase in the velocities of Cl^- over pore water velocities of about 10% in columns containing sandy soils. This increase in velocities was directly attributed to anion exclusion.

Phillips (1994) suggests that systematic uncertainties in estimated Cl^- deposition rates (D_{cl}) can be as great as 20% if the Cl^- mass balance technique is extended to estimate recharge rates before the Holocene epoch (approximately 10,000 years before present). Errors in estimated deposition rates linearly propagate into the recharge estimates made using the Cl^- mass balance method.

Tracer Summary

During the past 20 years, estimates of recharge have been made using chemical tracers including ^{3}H, ^{36}Cl, and Cl^{-}. Of these tracers, Cl^{-} appears to be the most reliable for arid and semi-arid locations (Allison et al., 1994). A recent summary of tracer studies by Cook and Walker (1995) indicates that Cl^{-} is a more reliable indicator of recharge rate when the flux is less than 20 mm/yr. Above this value all three methods give similar results.

We emphasize at this point that tracers such as Cl^{-} and ^{3}H are a reliable way to estimate natural recharge at an undisturbed site. Such an estimate, however, may not be a conservative estimate either of recharge at the same site after it has been disturbed, or of seepage into an engineered facility at the site. This is because site surface conditions (e.g., soil and plant characteristics), which are always modified from their natural state, strongly control the flow of water into a waste disposal facility.

2.3.2.6 Numerical Simulation

If sufficient data are available, Eqs. 2-6 and 2-13 or variants of these equations can be used to simulate soil-water dynamics and solute transport in response to observed or estimated weather data and tracer deposition rates. Scanlon (1992) recently used simulations of this type to estimate natural recharge rates in the Chihuahuan Desert of Texas. Numerical simulation is the most data-intensive method for estimating groundwater recharge rates and probably yields recharge estimates that have the most uncertainty. Nevertheless, numerical simulation has several unique advantages over the other methods.

Numerical simulation is useful for investigating “what if” questions. For example, how do predicted recharge rates change if precipitation doubles or triples as a result of climate change? Also, how do predicted recharge rates change if the dominant vegetation changes from deep-rooted sagebrush to shallow-rooted grasses as a result of range fires? These types of questions either cannot be answered or require an impractical amount of data to answer using lysimetry or tracer techniques. Numerical simulation can also be used to evaluate the sensitivity of recharge estimates to different parameters. Such a sensitivity analysis can help focus future data collection activities on the areas or parameters that have the greatest influence on the system.

Although numerical simulation is the only practical tool for forecasting recharge rates for future climate and land use scenarios, it relies on the use of numerous parameters estimated from data to represent climate, soils, and vegetation characteristics. Lysimeter data are useful for testing numerical simulation models and for refining the mechanistic descriptions of various processes in these models.

Lysimetry, tracer techniques, and numerical simulation all have unique strengths and weaknesses. The use of several methods in combination provides the most defensible estimates of recharge for the performance assessment of a LLW disposal facility.

2.3.3 Hydrologic Property Measurement and Parameter Estimation

Developing defensible conceptual and mathematical models of recharge and seepage at a LLW disposal site requires the measurement or calculation of a number of physical and hydraulic properties of the natural soils and engineered materials used in the construction of the facility. These properties generally include, but may not be limited to:

- particle size distribution
- particle density
- bulk density
- total porosity
- water retention
- saturated hydraulic conductivity
- unsaturated hydraulic conductivity.

Description of several methods for measuring or calculating each of these properties can be obtained from numerous textbooks and references on this important subject (e.g., Klute, 1986; van Genuchten et al., 1992, Wierenga et al., 1993). A number of methods are also included in ASTM standards (ASTM, 1995).

As discussed in Section 2.3.1, methods for the solution of the equations describing flow in unsaturated porous media often use models of the water retention and unsaturated hydraulic conductivity (e.g., Equations 2-7 through 2-12). These models contain parameters that are commonly determined by fitting the chosen model to measured data. The parameters of the Brooks-Corey and van Genuchten relationships can be estimated using the optimization software RETC (van Genuchten et al., 1991b; Leij et al, 1992; Yates et al., 1992).

Since the quality of any hydrologic evaluation depends on the quality of the available data, careful consideration must be given to the collection of data. Locations of samples, collection methods, and descriptions of measurements should all be well documented. Replicate tests should be carried out whenever possible. Since all the hydrologic properties listed above are spatially variable, multiple samples should be collected to obtain a measure of spatial variability. We also emphasize that water pressure and hydraulic conductivity are highly non-linear functions varying by orders of magnitude as water content changes from saturation to air dry. Measurements must be carried out over a range of water content and pressure expected to occur during the life of the LLW facility. Other test conditions should also reflect expected site conditions. For instance, hysteresis in water retention and unsaturated hydraulic conductivity should be measured if the site will undergo wetting as well as draining conditions. Results of some tests may be a function of temperature or the chemical characteristics of water; this should be accounted for in the analysis.

The results of a hydrologic evaluation at a LLW disposal facility are highly dependent on how well the hydraulic properties and parameters reflect the actual site conditions. Failure to collect quality data at this point of an analysis may lead to failure in accurately predicting recharge, seepage, and subsequently contaminant transport and dose.

3 Engineered Barriers

To meet performance requirements, a LLW facility will generally require one or more engineered components to limit the amount of water reaching the waste. The analysis of the engineered components is provided in the hydrologic evaluation methodology (Figure 3.1). In this chapter, engineered components are classified according to their functions. The expected performance, design criteria, and degradation mechanisms of engineered components are discussed.

3.1 Overview

Several types of disposal facilities are typically considered for near-surface disposal of LLW. In the past, LLW has been disposed of via shallow land burial using a simple earthen cover to cap an open trench. While this type of disposal facility is still applicable in certain arid regions, its use in humid environments is problematic, requiring structurally stable waste forms. Alternative disposal methods for humid sites (and also arid sites) use a containment structure to isolate the wastes from the environment. Examples include

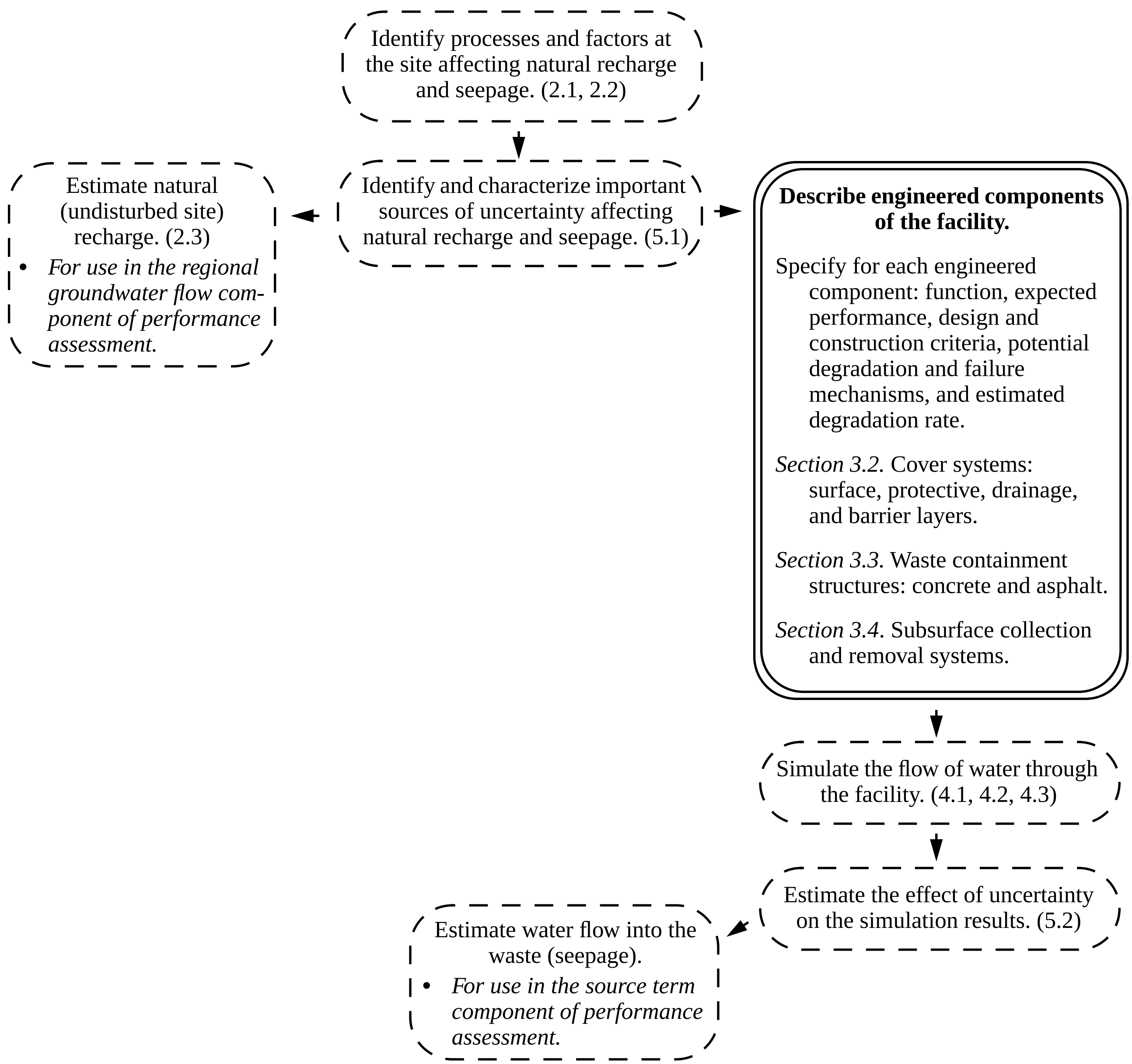


Figure 3.1 Flowchart for the Hydrologic Evaluation Methodology. Chapter 3 discusses the engineered components of the facility. Numbers indicate sections in this document in which the items are discussed.

below ground vaults, earth mounded concrete bunkers, and above ground vaults. Shaft disposal and mined cavity disposal have also been considered for LLW. In this report, the discussion is limited to shallow land burial and below ground vault disposal facilities, although most of the ideas presented also apply to earth mounded concrete bunkers.

A disposal facility typically uses one or more engineered barriers to isolate the waste from the environment. Engineered barriers are components of a waste disposal facility designed and built to improve the facility's ability to meet performance objectives (as specified in 10 CFR 61 Subpart C). For the purposes of this discussion, however, the term engineered barriers will refer only to those components that provide structural stability or limit the movement of water into the waste and the movement of contaminant from the disposal facility into the environment. The stabilized waste form is itself an engineered barrier but will not be discussed as such in this report. Chemical barriers, such as a sorbing backfill, are potentially very effective at limiting the release of contaminants (IT Corp., 1994) but also will not be discussed here. Engineered barriers are distinguished from natural barriers, such as groundwater divides and natural low-permeability formations, by the fact that they are composed of synthetic materials or of natural materials whose composition and placement have been engineered.

Engineered barriers fall into one of three major functional categories: cover systems, waste containment structures, and subsurface collection/removal systems. Cover systems overlie the waste and are intended to limit the amount of water that comes into contact with the waste. Cover systems are used in both humid and arid environments and are common to shallow land burial and below ground vault facilities. Waste containment structures provide structural stability, physical containment and separation of the waste, and potentially an additional barrier to water. Waste containment structures are used in both humid and arid environments. Subsurface collection and removal systems provide a means to collect and remove water that has percolated through the cover system and can therefore potentially come into contact with the waste. Subsurface collection and removal systems are not typically used in arid environments.

Figure 3.2(A) is a schematic for a below ground vault facility as it might be applied at a humid site. This facility contains all three of the functional categories of engineered barriers. The cover system consists of multiple layers of materials, each serving a particular purpose. The waste containment structure is a concrete vault. The subsurface collection and removal systems may have two parts: a primary drainage system, which collects water from inside the vault, and a secondary system, which collects water outside and below the vault. Figure 3.2(B) shows a schematic for a shallow land burial facility as it might be applied at an arid site. In this case, the only engineered barrier used is a multilayer cover system.

For an evaluation of unsaturated water movement, the most important engineered barrier is the cover system. For this reason, the discussion in this chapter emphasizes cover system components and their functions. Specific discussion of laboratory and field tests for cover systems can be found in Bennett and Horz (1991). The role of containment structures and collection and removal systems in limiting water movement into the waste is briefly discussed. For the application examples presented in Chapter 6, the analysis is limited to the cover systems.

3.2 Cover Systems

The primary objective of a LLW disposal facility cover system is to limit the amount of water that passes through the cover, thus limiting the amount of water potentially contacting the waste. There are only a few ways in which the cover can limit the passage of water: by evapotranspiration (ET) and by diverting water into runoff or subsurface lateral drainage. This is illustrated in Figure 3.3. Note, the particular cover design may allow subsurface drainage to occur in more than one layer. Assuming the total amount of water stored in the cover is constant (which is reasonable over long periods of time), a simple water balance yields:

Seepage = Precipitation - Surface Runoff -
Evapotranspiration - Subsurface Lateral Drainage

Since precipitation cannot be controlled, seepage can only be minimized by maximizing the sum of runoff, ET, and subsurface lateral drainage. Other objectives that have a direct impact on water flow through the cover are also often important. For instance, it is often necessary for the cover to minimize wind and water erosion and to prevent plant and animal intrusion. Which of these multiple objectives is emphasized may be site-specific. At an arid site, for example, proper control of ET and erosion may be all that is required to achieve a sufficiently small amount of seepage. At a humid site, control of runoff and subsurface lateral drainage may also be essential.

The cover must also remain stable for it to prevent seepage of water. Stability is strongly dependent on cover slope, the materials of the cover (both natural and synthetic), water content of the cover soils, and the foundation materials. Because of this dependence, a geotechnical stability analysis and an evaluation of unsaturated water flow are best carried out concurrently. U.S. EPA (1995) contains current guidance for stability analysis of covers. Stability analysis, however, will not be addressed in this report. The collection and controlled release of gases is a possible additional requirement of a cover system, but is outside the scope of this report.

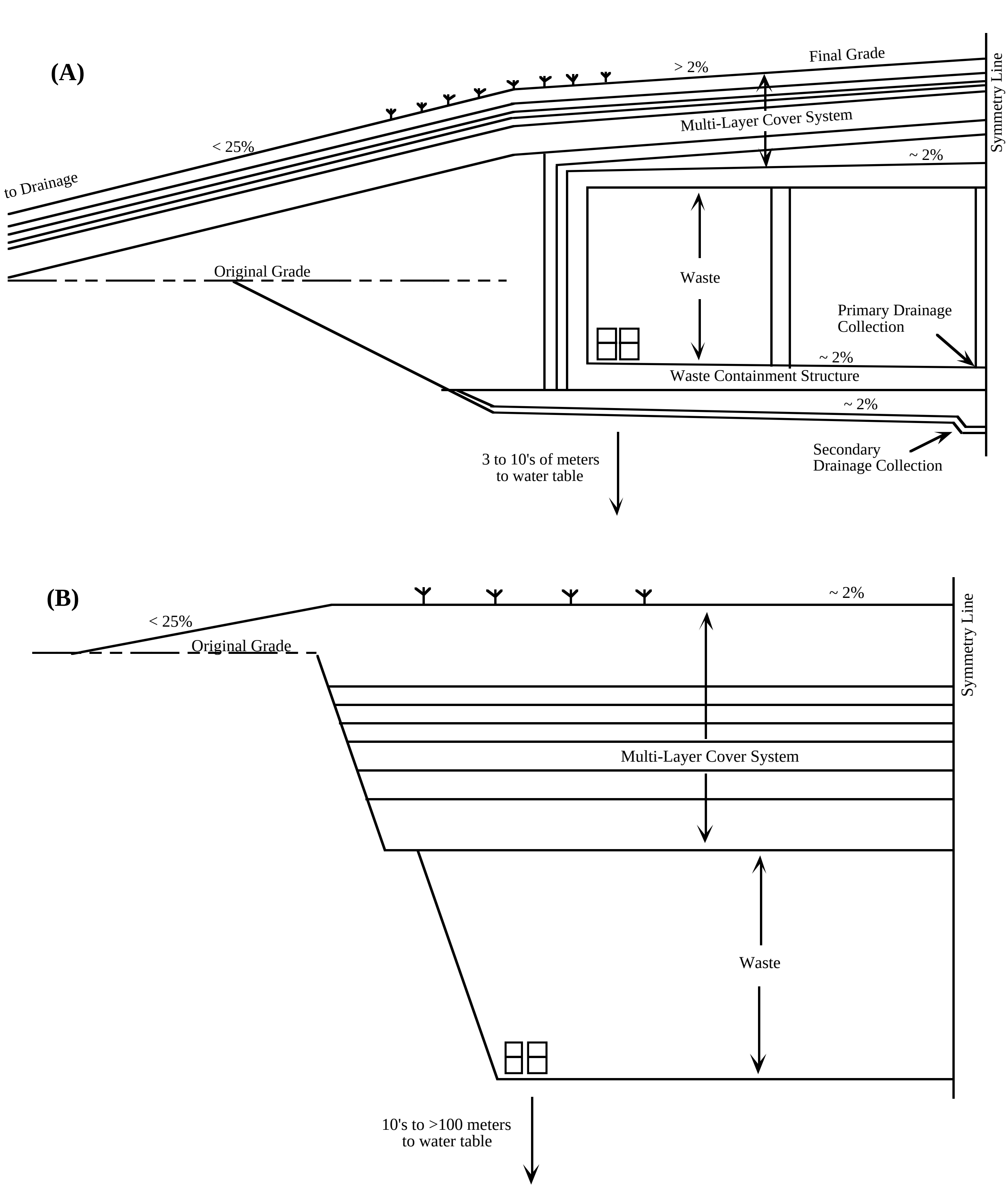


Figure 3.2 Illustrations of low-level waste disposal facility components. (A) Below ground vault typical of a humid site facility. (B) Shallow land burial typical of an arid site facility.

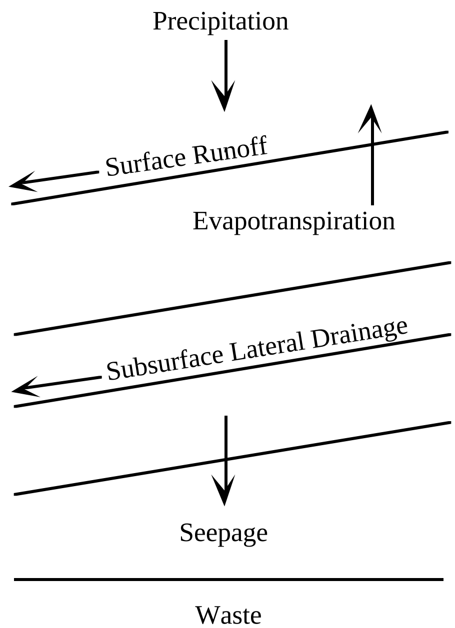


Figure 3.3 Illustration of a simple steady-state water balance in a cover system

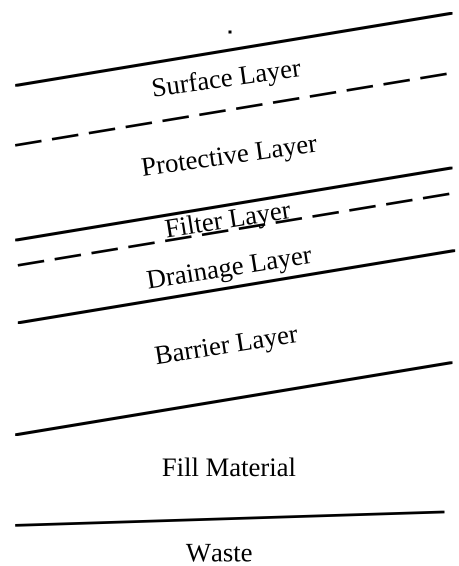


Figure 3.4 Illustration of cover system components

Following the categorization of Daniel and Koerner (1993), cover system components can be placed in one of the following four groups:

- surface layer
- protective layer
- drainage layer
- barrier layer.

A typical arrangement of component layers is illustrated in Figure 3.4. Not all layers are required at any given site; a drainage layer may not be required at an arid site, for example. In addition, each component of the cover system may serve more than one function. For example, a geomembrane placed above a compacted clay layer acts as a low permeability barrier and also serves to protect the clay from desiccation.

3.2.1 Surface and Protective Layers

3.2.1.1 Functions

The surface layer of a cover system is the component most exposed to the atmospheric and biotic processes acting on the cover. This exposure requires that the surface layer be carefully designed to perform multiple functions. The functions of the surface layer depend on the climatic conditions of the site but typically include the following:

- managing runoff
- minimizing erosion
- maximizing ET.

Note, the first two functions are not independent; a surface layer that produces large amounts of runoff may erode rapidly. Typically, some balance must be reached between runoff and erosion.

A protective layer is often placed directly beneath the surface layer. The combined layers function to protect underlying layers from degradation, which can occur through:

- repeated freeze/thaw cycles
- repeated excessive wetting/drying
- plant, animal, or human intrusion.

3.2.1.2 Options in Materials and Design

The design variables for the surface and protective layers include material type(s), slope, thickness, and vegetation.

Material Types

Natural materials that could be considered for a surface layer include the following:

- topsoil – supports the growth of vegetation by providing water storage capacity

- topsoil/gravel mixture – promotes vegetation while resisting wind erosion in dry climates (Ligotke and Klopfer, 1990)
- cobbles – minimizes erosion but does not limit infiltration and does not support vegetation.

Synthetic materials that might be considered for a surface layer include the following:

- a geosynthetic erosion control layer. This material may be used to prevent erosion while vegetation is becoming established. A geosynthetic would not be relied on to prevent erosion in the long term, however.
- paving materials (Daniel and Koerner, 1993) such as concrete or asphalt
- sheeting materials such as corrugated aluminum or fiberglass (Schulz et al., 1992).

Paving and sheeting materials can be relatively easily maintained since they lie directly at the surface and may therefore be applicable as a temporary cover during the period of waste subsidence. Because they require constant maintenance, however, these materials are not an adequate surface layer in the long term.

For the protective layer, two materials are typically considered:

- local soil – a relatively inexpensive choice to protect an underlying barrier layer from freezing and excessive drying. The local soil is placed directly beneath the surface layer.
- cobbles – placed deeper within the cover to minimize animal and inadvertent human intrusion. A cobble or gravel layer may also limit root intrusion somewhat. In some instances, a cobble layer at depth may serve as an erosion resistant layer in the event that all layers above are removed in a catastrophic event.

Slope

The slope of the surface layer plays an important role in determining runoff, erosion, and infiltration. Steeper slopes produce greater runoff, more erosion, and less infiltration. Typical slopes for that portion of the cover directly over the waste range from:

- 3-5% in humid environments – this range is chosen to produce runoff while limiting erosion, and
- 2% in arid environments, where runoff may be less important.

Side slopes may be steeper, up to 20% for humid environments and perhaps even larger in arid environments. Stability and erosion are concerns with such steep slopes. Daniel (1994) emphasizes that surface layer erosion is often underestimated in cover design. The Universal Soil Loss Equation (Wischmeier and Smith, 1965) is an empirical method available to determine rates of erosion. U.S. NRC (1990) recommends the use of the tractive force (or shear stress) method (Temple et al., 1987) in cover design because it can incorporate the effect of design storms and gully erosion. Bennett and Horz (1991) discuss methods that can be used to estimate rates of wind erosion. U.S. EPA (1989) recommends a rate of erosion no greater than 4.5 MT/ha/yr. (2.0 tons/acre/yr.) for hazardous waste landfill covers.

Thickness

The surface and protective layers commonly serve as protection against freezing and/or desiccation of a deeper barrier layer such as a compacted clay. It is the combined thickness of these layers (as well as any drainage layer above the barrier) that offers this protection. The depth of maximum frost penetration has been well mapped (see U.S. EPA, 1989, for example). The depth required to protect a compacted clay layer from desiccation is less certain. This issue will be discussed further in Section 3.2.3.

If vegetation is a component of the cover, it is the combined thickness of the surface and protective layers that provides the water storage capacity for plant growth and maintenance. Allowance must be made for plant requirements during periods of drought, which will tend to increase the required thickness. Anderson et al. (1993) estimated the capacity of three grasses and one shrub to remove water from the soil in a semi-arid environment. Combining these estimates with site-specific precipitation data and a measure of their cover soil's storage capacity, they recommended a cover layer of 200 cm.

A topsoil surface layer over a local subsoil protective layer is typical. Typical thickness for the combined topsoil/subsoil layers is:

- 60-100 cm in a humid environment, and
- 200 cm or more in an arid environment.

Note, these values are much less than the maximum rooting depths of plants that can be expected to develop on the cover if not maintained (see the following section).

The soil thickness required to support vegetation can be deduced by observing a natural plant community similar to that expected to develop on the cover. The climate and the surface soils of the natural community must be similar to the LLW site for this comparison to be valid. Additional thickness may be required for frost protection, as discussed above.

Vegetation

Vegetation on a cover has both benefits and risks. Vegetation will reduce the amount of runoff, thereby significantly reducing erosion of the surface layer. Although this will simultaneously increase the amount of infiltration, with appropriate soils in the surface and protective layer, the additional infiltration will be stored in the soil and subsequently removed by ET. The risk of vegetation, however, is that it may ultimately increase the amount of seepage if the roots penetrate a barrier such as a compacted clay or geosynthetic clay liner. Root channels provide a preferential flow path for water. By removing water from the soil column, plants may also contribute to the desiccation of a clay barrier. In addition, there is the potential for plants to take up contaminants if the roots penetrate deeply into the facility.

In humid environments, shallow-rooted (less than one meter) grasses are the preferred vegetation. Without continual maintenance, however, ecological succession will quickly change the plant community. Suter et al. (1993) estimate that at Oak Ridge, Tennessee the transition from grass to mature forest could take as little as 65 years without intervention. The average rooting depth of larger woody shrubs and trees may be three meters or more (Foxx et al., 1984b). Such plants are likely to have roots capable of penetrating compacted soil barriers. In addition, Suter et al. (1993) point out that trees allowed to reach maturity may be uprooted by high winds, which may have disastrous effects on the cover.

Reynolds (1990) studied three semi-arid grasses and one shrub and found that each plant species was able to penetrate a 0.6-m clay barrier in just three years. Reynolds also looked at the use of gravel/cobble and scoria (basalt) as barriers to root penetration. While these materials were more effective than the compacted soil in limiting the depth of penetration and the root density, Reynolds observed that instances of complete barrier penetration occurred for each plant species in each barrier type.

In semi-arid regions of the western U.S., grasses and shrubs are common vegetation types, with many areas devoid of trees (Rickard and Vaughan, 1988). Grasses common to the arid and semi-arid west, however, have maximum rooting depths greater than 2 m (Foxx et al., 1984a). Common shrubs have average rooting depths of 2-4 m, with roots extending to maximum depths of 5 m or more (Foxx et al., 1984a). Natural revegetation in arid environments may be unpredictable. At the Hanford Site, one area that was cleared remained free of vegetation 35 years later (Fitzner et al., 1979). In addition, there is some evidence that the plant community may be undergoing changes due to the relatively recent introduction of foreign species. The dominant shrub (sagebrush) may be unable to compete with the introduced species (mainly cheatgrass) after the occurrence of fires (Leopold, 1966). The replacement of deep-rooted shrubs with shallow-rooted grass will increase the seepage at this site.

An active revegetation program is preferable to natural revegetation. An unvegetated surface layer is susceptible to erosion, particularly in a humid environment. In addition, during the time it takes for vegetation to move back onto the cover, ET is greatly reduced. The resultant increase in stored water and, potentially, seepage may be significant. This is particularly true in arid environments due to the length of time required for natural revegetation and the relative importance of plant uptake of water.

3.2.2 Drainage Layer

3.2.2.1 Function

The function of a drainage layer is to collect water that has infiltrated and to divert this water laterally so it has no opportunity to contact the waste. Drainage layers are typically placed beneath the surface/protective combined layers and above the barrier layer(s). In this location, a drainage layer:

- reduces the head of water on the barrier layer, which limits the flow of water through the barrier, and
- reduces the water content of the surface and protective layers, improving the stability of these layers and increasing their storage capacity.

A drainage layer is generally susceptible to failure due to the transport of fine soil particles that can:

- fill the void spaces of the drainage layer material, thereby reducing its ability to transmit water, or
- clog the outlet of the drain, causing a backup of water in the drainage layer.

The potential movement of fine soil particles is usually addressed by placing a filter layer adjacent to the drainage layer. Failure of the drainage layer can still occur, however, if the filter itself becomes clogged with fine particles.

If the drainage layer or filter becomes excessively clogged, pore pressures within and above the drainage layer may rise to the point where the drainage layer or the overlying soils become unstable. A landslide may then occur leading to catastrophic failure of the cover. Failure of the drainage system in a cover system is particularly acute because there is no way to design a redundant system (unlike a barrier).

3.2.2.2 Options in Materials and Design

To fulfill its function, a drainage layer must be capable of transmitting whatever amount of water passes through the surface and protective layers. The flow capacity of a drainage layer is determined by the drainage layer material type, slope, and thickness as well as the applied normal stress.

Materials

Daniel and Koerner (1993) identify a number of alternative drainage/filter layer combinations, consisting of natural and synthetic materials. These include:

- Sand or gravel drainage layer with a soil filter
- Sand or gravel drainage layer with a geotextile filter
- Geosynthetic drainage options: a thick geotextile acting as both drain and filter, a geonet drain with a geotextile filter, or a geocomposite sheet drain (consisting of an encapsulated polymeric drainage core with an overlapping geotextile filter)

Geosynthetic drainage layers offer several advantages. They can be made with a very high in-plane transmissivity, especially geonets and geocomposites. Because they are lightweight, geosynthetics can be installed using light equipment that is less likely to puncture an underlying barrier layer (such as a geomembrane). In addition, they can be inexpensively shipped to any location.

One of the disadvantages of geosynthetics, particularly geonets and geocomposites, is that they introduce a potential plane of slippage between components of the drainage layer and between the drainage layer and an underlying geomembrane. The primary disadvantage of geosynthetic drainage layers, however, is that their long-term viability is uncertain. Koerner (1994) describes tests that have been used to estimate the effects on geosynthetic performance of clogging and various degradation mechanisms. Unfortunately, these tests are all relatively short-term and do not provide the required information on geosynthetic aging and long-term degradation. Several additional factors argue against the use of geosynthetics as drainage components in LLW disposal facility cover systems:

- There is a relatively short history of experience with geosynthetics.
- LLW disposal requires a long operating life.
- Geosynthetics with a high ratio of surface area to mass, such as geotextiles, tend to be shorter lived (Daniel, 1994).
- Disposal facilities cannot be designed with redundant drainage systems without great cost.

In sum, these factors provide a strong case for constructing a drainage layer of natural materials only, as recommended by Daniel (1994). For similar reasons, Daniel (1994) also cautions against the use of manufactured drains, such as pipes, at the toe of the slope (the outlet of the drainage layer).

The advantage of a sand filter and sand/gravel drainage layer is primarily the long history of application. The disadvantages of these natural materials are:

- Fine soil particles in the materials can be transported to a point where they clog the drainage layer or the drain outlet, resulting in failure as described above. The potential for this problem to occur can be reduced by washing the drainage materials before construction.
- A gravel drainage layer may puncture a geomembrane or geosynthetic clay liner if placed directly on top of it. Daniel and Koerner (1993) recommend restrictions on maximum particle size or the use of a cushioning layer if this is a concern.
- Potentially high cost if the natural materials are not available locally.

Slope and Thickness

Flow in a drainage layer occurs primarily under gravitational forces. In this case, a simple analysis using Darcy's Law can be used to evaluate the drainage layer design. The required average flowrate of the drainage layer is given by

$$Q^{req} = q_i \, L \qquad (3\text{-}1)$$

where the parameters are identified in Figure 3.5 and defined as follows:

Q^{req} = required average flowrate of the drainage layer per unit width [cm^2/s]

q_i = average net infiltration: the average flux of water percolating below the zone of ET and into the drainage layer [cm/s]

L = the (horizontal) length of the drainage layer [cm]

The capacity flowrate of the drainage layer must be greater than the required flowrate and can be estimated as

$$Q^{cap} = K_s \, T \, i \qquad (3\text{-}2)$$

where

Q^{cap} = capacity flowrate of the drainage layer per unit width [cm^2/s]

K_s = in-plane saturated hydraulic conductivity of the drainage material [cm/s]

T = thickness of the drainage layer [cm]

i = the gravitational gradient [= $\sin \beta \approx$ slope]

These terms are also illustrated in Figure 3.5.

If the average net infiltration at a site is 5.0×10^{-7} cm/s (12.6 cm/year) with a drainage length of 60 m, Eq. 3-1 results in a required flowrate of 0.003 cm^2/s. The U.S. EPA recommended drainage layer for hazardous waste disposal facility covers consists of 30 cm of soil with a saturated hydraulic conductivity of at least 10^{-2} cm/s, placed on a slope of at least 3%. According to Eq. 3-2, this yields a capacity flowrate of 0.009 cm^2/s, three times what is

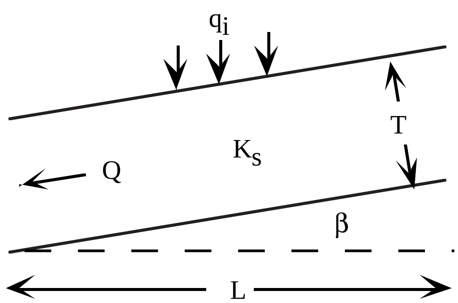


Figure 3.5 Parameters used in evaluating drainage

required. The appropriate factor of safety to apply in this case is a matter of engineering judgement but should consider the long required operating life of the cover and that the required flowrate will vary over time and may be significantly higher at any moment than the average value.

Flow in geosynthetic drainage materials can be similarly analyzed, although the flow is potentially turbulent, particularly in geonets and geocomposites. Koerner (1994) provides a discussion of the appropriate analysis in this case.

Applied Normal Stress

The transmissivity of a geosynthetic drainage layer may be a strong function of the applied normal stress (Koerner, 1994). A possible reduction in the drainage capacity due to a sustained load must be accounted for in this case. With proper compaction during construction, this is not an issue for sand and gravel drainage layers.

3.2.3 Barrier Layer

3.2.3.1 Function

Although each component of a cover system serves a purpose, the barrier layer is often the most critical component. This is because of the typical requirement that a waste disposal facility allow only a very small amount of water to contact the waste (on the order of a few cm/year or less: 10^{-7} cm/s ≈ 3.2 cm/yr.). It is very difficult for runoff and ET alone to limit seepage into the waste to such a small amount, even in dry climates. Barrier layers are typically located immediately beneath a drainage layer and, through their low permeability, are capable of successfully limiting seepage into the waste.

3.2.3.2 Options in Materials and Design

The most important considerations in the success of a barrier layer are the choice of materials and proper installation. Barriers fall into one of two broad classes – those that rely on the low intrinsic permeability of their materials:

- compacted soil
- geomembranes
- geosynthetic clay liner
- asphalt mixtures

and those that rely on a contrast in unsaturated hydraulic characteristics between two different materials, commonly known as capillary barriers.

Each of these materials is discussed below. Composite barriers (made up of a combination of materials) are discussed in Section 3.2.3.3.

Compacted soil layers

Compacted soil layers (composed of clay-rich soils or soil/bentonite mixtures) were once commonly used as the sole barrier component of disposal facility (hazardous and solid waste) covers. These materials were believed to be adequate because of their low permeability; under ideal conditions a compacted soil with high clay content can have a saturated hydraulic conductivity less than 1.0×10^{-7} cm/s (3.2 cm/yr.). In a cover with adequate drainage, the head of water driving flow through the barrier will be fairly small. Under such circumstances, the gradient is approximately one and the flux through the barrier can be calculated using Darcy's Law as

$$q^{barr} = K_s\, i = K_s \qquad (3\text{-}3)$$

where

q^{barr} = the flux through the barrier [cm/s]

K_s = the vertical saturated hydraulic conductivity of the barrier [cm/s]

i = the vertical gradient across the barrier [cm/cm], usually calculated as $(H + T) / T$; when H is small with respect to T, then $i \approx 1$

H = the head of water above the barrier [cm]

T = the thickness of the barrier [cm]

Under ideal conditions, the water flux through the compacted soil barrier is thus approximated by the saturated hydraulic conductivity of the barrier material.

It is now recognized that there are several mechanisms to which compacted soil layers are susceptible that may lead to a flux through the barrier much greater than that given by its saturated hydraulic conductivity. In addition, these mechanisms may produce failure of the barrier in a relatively short period of time. The mechanisms are:

- inadequate construction techniques
- freeze/thaw cycles

- desiccation
- root penetration
- differential settlement.

Inadequate construction techniques. U.S. EPA recommendations for hazardous waste covers are for a compacted soil barrier with a saturated hydraulic conductivity no greater than 1.0×10^{-7} cm/s. It is generally believed that such a requirement can be met using typical compaction methods (ASTM D698 or ASTM D1557; see also U.S. EPA, 1988a). The field-scale study of Krapac et al. (1991) demonstrated that proper attention to construction techniques can satisfy the EPA requirement. Depending on the method of measurement, their 90 cm thick compacted soil liner had an as-built hydraulic conductivity of 3.3×10^{-9} - 6.7×10^{-8} cm/s.

Several authors have shown that standard laboratory measurements of hydraulic conductivity (ASTM D5084) of both undisturbed and recompacted samples may be more than 1000 times smaller than the actual average field value (Day and Daniel, 1985; Daniel, 1984; Rogowski, 1988). Elsbury et al. (1990) attribute this phenomenon primarily to the persistence of soil clods and to a failure to bond soil lifts. These conditions lead to macropore flow between clods and lifts. Daniel (1989) reviews options for measuring the hydraulic conductivity of compacted soil barriers. He recommends the use of sealed double-ring infiltrometers and pan lysimeters because they measure over an area sufficiently large to account for the effects of macropore flow and they provide reliable measurements of the low hydraulic conductivity values of a well-constructed barrier. These tests should be carried out on the actual barrier, or on a test pad representative of actual site construction practices.

Freeze/thaw cycles. Even a barrier that is carefully constructed to achieve a low field value of hydraulic conductivity can be quickly degraded by any of several mechanisms. All barrier layers must have a sufficient overburden thickness to prevent freezing of the pore water within the barrier, as discussed previously. The formation of ice lenses in the overburden, however, can contribute to desiccation of a barrier layer. When water in soil freezes, capillary pressures are reduced, thus producing a movement of liquid water from unfrozen soil to the frozen zone.

Desiccation is of great concern with compacted soil barriers because it generally causes the soil to shrink, potentially producing cracks that can significantly increase the overall hydraulic conductivity of the barrier. The problem is made worse by conventional construction practices in which the barrier is emplaced at fairly high water contents in order to produce satisfactory compaction and sufficiently low hydraulic conductivity. As Daniel and Wu (1993) point out, however, the potential shrinkage of the soil increases with the water content. This is particularly important for covers because a desiccation crack is more likely to reseal when inundated with water if the effective confining pressure is large (Boynton and Daniel, 1985). The thin layer of soil above the barrier in a typical cover will produce relatively low pressures.

Daniel and Wu (1993) present a method to determine the range of water content and compaction density to provide low hydraulic conductivity, minimal potential for shrinkage on drying, and adequate shear strength for stability. As Daniel and Wu state, however, there is currently very limited data to relate the degree of shrinkage to the significance of cracking (namely, Kleppe and Olson, 1985, a single study using three soils).

The effect of desiccation on compacted soil barriers is most convincingly illustrated by the results of a study carried out in Hamburg, Germany (Melchior et al., 1993, 1994) This large-scale field test examined several cover designs including one with a 60 cm compacted soil layer (17% clay, 26% silt, 52% sand, and 5% gravel; lab measured geometric mean saturated hydraulic conductivity of 2.4×10^{-8} cm/s) overlain by 25 cm of coarse sand and 75 cm of grass-vegetated topsoil. Two experimental covers were constructed with this design, one at a 20% slope and one at a 4% slope. The compacted soil layers began to pass significant quantities of water after only 20 months of operation. During the fifth year of operation, the leakage through the barriers was 14.3% (for the 20% slope) and 31.3% (for the 4% slope) of the water percolating into the overlying drainage layer (Melchior et al., 1994). Table 3.1 presents the results for the first five years of data.

A tracer study showed the existence of continuous preferential flow paths in the compacted soil barriers. Mechanisms other than shrinkage due to desiccation were ruled out as explanations for the presence of macropores. Upward capillary flow of water during the relatively dry summers and the removal of soil water by plant roots produced the desiccation of the barrier. The desiccation occurred despite careful construction procedures and minimization of shrinkage potential through appropriate choice of materials (clay composition was 50% illite, 30% smectite, and 20% kaolinite and chlorite).

Root penetration. High clay content and compaction to increase soil bulk density both impede plant root growth. In addition, the high water content of a compacted soil barrier prevents root growth by limiting oxygen availability. Nevertheless, an unprotected, compacted soil barrier is susceptible to root penetration in the long term. Desiccation cracks, areas of poor compaction, and worm holes provide potential avenues for root growth. The study of Reynolds (1990) discussed earlier demonstrates the potential for rapid root penetration in compacted soil barriers. (Although it should be noted that Reynolds [1990] gives no data describing the compaction.)

Table 3.1 Subsurface lateral drainage and leakage through a compacted soil barrier (after Melchior et al., 1994)

	20% Slope		4% Slope	
	Subsurface Lateral Drainage [cm/s]	**Leakage [cm/s] (% of potential leakage)**	**Subsurface Lateral Drainage [cm/s]**	**Leakage [cm/s] (% of potential leakage)**
1988	1.2×10^{-6}	6.0×10^{-9} (0.5)	1.2×10^{-6}	2.2×10^{-8} (1.9)
1989	7.8×10^{-7}	1.0×10^{-8} (1.3)	5.7×10^{-7}	2.5×10^{-8} (4.2)
1990	1.0×10^{-6}	4.2×10^{-8} (4.0)	9.2×10^{-7}	5.5×10^{-8} (5.7)
1991	5.6×10^{-7}	4.2×10^{-8} (7.1)	5.8×10^{-7}	2.7×10^{-8} (4.5)
1992	9.1×10^{-7}	1.5×10^{-7} (14.3)	7.1×10^{-7}	3.2×10^{-7} (31.3)

Differential settlement. Daniel and Koerner (1993) summarize the available data on the relationship between differential settlement and tension cracking in compacted soils. They conclude that compacted soil barriers will crack when their distortion due to differential settlement is greater than 0.05 to 0.1. Distortion is defined as the ratio of differential settlement to length of settlement (see Figure 3.6.) For a 10-m diameter crater, for example, this means that cracking can be expected for settlements greater than 0.25-0.5 m. In the experience of Daniel and Koerner (1993), this magnitude of distortion is common in municipal landfill covers in which the waste is typically quite compressible. They believe, however, that such large distortions are not likely in modern hazardous waste disposal facility covers. By analogy, differential settlement is unlikely to be an issue for LLW as long as disposal practices require stabilized and well packed-waste. Differential settlement is likely to be of greater concern with shallow land burial than with vault-type disposal.

Geomembranes

Geomembranes have become increasingly common as a component of cover systems and are currently recommended by the EPA for hazardous waste disposal facilities (U.S. EPA, 1989; U.S. EPA, 1988b). Koerner (1994) lists nine types of geomembranes currently in use and compares the properties of a number of these. For cover applications, high-density polyethylene (HDPE) seems to be the most popular.

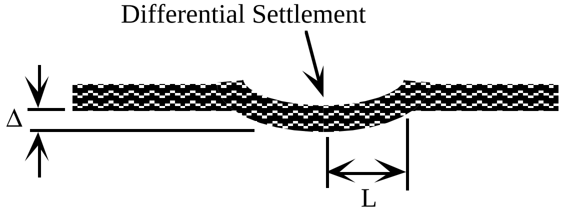


Figure 3.6 Definition of distortion, Δ/L, in a compacted soil barrier due to differential settlement (after Daniel, 1994)

Geomembranes have several advantages over compacted soil barriers. They are not susceptible to damage from freezing, desiccation, or root penetration. In addition, they are able to withstand much greater differential settlement. While compacted clays cannot sustain tensile strains larger than 0.1-1% (Daniel and Koerner, 1993), laboratory tests reported in Koerner (1994) indicate that HDPE can sustain axisymmetric strains in excess of 20% (corresponding to distortions in excess of 0.5). Other geomembranes with greater extensibility such as very low-density polyethylene (VLDPE), sustained strains greater than 70%. A final advantage of geomembranes is that their cost is not dependent on local availability, as is the case with natural clay soils.

The primary advantages of geomembranes are their extremely low permeabilities. The permeability of an intact geomembrane is so low, in fact, that standard water permeability measurement techniques are inadequate. Geomembrane permeability is typically measured instead by a water vapor transmission test (ASTM E96); resulting equivalent hydraulic conductivities are on the order of 1.0×10^{-11} to 1.0×10^{-13} cm/s (Giroud and Bonaparte, 1989a; Koerner, 1994). These values are much smaller than anything achievable with compacted soil barriers. (Note, flow in geomembranes is modeled using Darcy's Law even though this is not strictly correct. The resulting hydraulic conductivities are referred to as "effective" because the value obtained for a particular geomembrane is a function of the pressure gradient producing the flow [Giroud and Bonaparte, 1989a].)

Geomembranes are not the perfect barrier, however, particularly for LLW disposal. The primary failure mechanisms are:

- punctures produced during construction
- poor quality seams

- long-term degradation and aging of geomembranes.

The first two mechanisms cause increased flow through the geomembrane and generally result in reduced cover performance from the time of construction. Reduction in performance due to degradation and aging occur gradually over a much longer time period.

Giroud and Bonaparte (1989a) used the results of a simple model to estimate the flowrate through a geomembrane containing holes. A portion of their results are summarized in Table 3.2. As the table indicates, the presence of holes can have a dramatic effect on the flux through a geomembrane. These results assume an HDPE geomembrane with a thickness of 1.0 mm (40 mils) and that a coarse drainage material ($K_s \geq 0.1$ cm/s) lies above and below the geomembrane. The presence of less permeable materials adjacent to the geomembrane will reduce the flowrate through the holes.

Table 3.2 Estimated flux [cm/s] through a geomembrane with holes (after Giroud and Bonaparte, 1989a)

Hole Diameter [mm]	Water Depth on Top of the Geomembrane [cm]		
	0.3	**3.0**	**30**
0.0	1×10^{-14}	1×10^{-12}	1×10^{-10}
0.1	1×10^{-12}	1×10^{-11}	1×10^{-10}
2.0	1×10^{-8}	3×10^{-8}	1×10^{-7}
11.3	3×10^{-7}	1×10^{-6}	3×10^{-6}

Giroud and Bonaparte (1989a) also assumed the geomembrane had an average of one hole per 4000 m^2 (1 acre). This value was based on six case studies that documented the detection of seam defects and assumed adequate quality control and an independent quality assurance inspection followed by repair. The results presented in Table 3.2 could be multiplied by an appropriate factor if the frequency of defects was greater than one per 4000 m^2. Daniel (1994, personal communication) estimated that a defect frequency of a few holes per acre was achievable. Gilbert and Tang (1993) performed a probabilistic analysis of results from case studies of 16 hazardous waste landfills including primary and secondary liners. For the landfill cells examined, the estimated defect frequency after inspection and repair ranged from 3 to 52 defects per 4000 m^2 (including seam and panel defects). The average over all cells was 17 defects per 4000 m^2. Gilbert and Tang (1993) also estimated the mean defect size, which was found to range from 7 to 11 mm, with an average over all cells of 9 mm. This compares well with the largest hole diameter presented in Table 3.2.

Punctures can occur during construction due to the use of heavy machinery and the placement of the geomembrane adjacent to gravel layers. Preventing punctures is particularly important because they usually occur after the geomembrane is covered; detection is consequently difficult. Koerner (1994) discusses the available lab tests for measuring puncture resistance of geomembranes (ASTM D5494 and D4833). The results of these tests indicate that the resistance increases linearly with geomembrane thickness. Placing a cushioning geotextile on the geomembrane greatly increases its puncture resistance. Koerner (1994) also discusses several field-simulated performance tests that are under development for testing puncture resistance.

Seams are typically regarded as the weak point in geomembrane construction, especially when they are made in the field. Koerner (1994) provides an extensive discussion of factory and field seaming of geomembranes and the various tests (both destructive and continuous, nondestructive) available to determine the quality of the seams. Additional information can be found in U.S. EPA (1991) and U.S. EPA (1993a).

Koerner (1994) emphasizes the importance of proper seaming and seam testing. He argues for the use of seaming methods with features that can be controlled according to weather conditions and feedback from seam quality measurements. The hot wedge fusion system is one such method. Koerner (1994) also argues for the use of a nondestructive test that can assess the quality of 100% of the seams on a continuous basis. The current method preferred by design engineers and construction quality assurance inspectors (the vacuum box method) has serious deficiencies. One-hundred percent inspection is impractical using the vacuum box method, and this method cannot be used on slopes, in corners, and around details (e.g. sumps, vents, and patches), places where seaming problems are most likely. Koerner (1994) suggests that ultrasonic methods show particular promise.

Long-term degradation and aging. Koerner (1994) summarizes the available information on the endurance properties of geomembranes. The mechanisms discussed are ultraviolet, radioactive, biological, chemical, and thermal degradation. For a LLW cover application in which the geomembrane is covered with a meter or more of soil, the most important mechanisms are radioactive degradation (a concern mainly because of the lack of data) and biological degradation (mainly potential damage from burrowing animals). No established test procedures exist for either degradation mechanism.

Lifetime prediction techniques are also discussed by Koerner (1994). These techniques attempt to predict the lifetime of a geomembrane under field conditions by performing measurements of its strength (or some other property) at elevated temperatures. The tests assume that the high temperature results, which are obtained in a practical amount of time, can be extrapolated to low temperatures and correspondingly long lifetimes. Although the techniques discussed by Koerner (1994) are all applied to measurements of stress, it is possible that they could be applied as well to measurements of permeability, which may be of most concern in LLW cover applications. The consensus on lifetime is that an HDPE geomembrane as a component of a cover system can be expected to perform for a few hundred years (Daniel, 1994, personal communication).

Koerner (1994) expresses concern over the ability of a geomembrane to survive the packaging, handling, transportation, and installation processes. He summarizes the survivability requirements of geomembranes to provide a check on design and offers the following minimum requirements for cover applications:

- thickness as measured by ASTM D5199 – 0.88 mm (35 mils)
- tensile behavior using a 25 mm strip as measured by ASTM D882 – 10.5 kN/m (60 lb./in.)
- tear resistance as measured by ASTM D1004 Die C – 67 N (15 lb.)
- puncture resistance as measured by ASTM D4833 modified – 160 N (35 lb.)
- impact resistance as measured by ASTM D1424 modified – 15 J (20 ft.-lb.)

These requirements are all lab index tests. Koerner (1994) strongly recommends the use of field-simulated performance tests whenever available in addition to the index tests. A construction quality control/quality assurance program is an added requirement.

Geosynthetic Clay Liners

Geosynthetic clay liners (GCLs) are a relatively new addition to the world of geosynthetic barriers. The GCLs currently available consist of a thin layer of bentonite clay stitched, needled, or glued between two geotextile sheets or glued to a geomembrane. The amount of clay used is 4.9 kg/m^2 (1.0 lb./ft.^{2}), approximately 5 mm thick, measured as-received. The bentonite provides a low permeability barrier. Daniel (1993) summarizes the available data on the hydraulic conductivity of GCLs (see also Estornell and Daniel, 1992); values fall in the range of 2×10^{-10} to 6×10^{-9} cm/s. The geotextiles contribute shear strength to the GCL but mainly serve as a carrier for the bentonite.

GCL seams are formed by overlapping the sheets from 75 to 225 mm, spreading bentonite between sheets in certain cases (U.S. EPA, 1993b). Estornell and Daniel (1992) found only minor increases in hydraulic conductivity due to seams when the manufacturer’s recommendations were followed.

GCLs are relatively new and experience of their behavior under various conditions is currently limited. Several potential failure mechanisms resulting from their application in cover systems have been identified, however. These include:

- excessive shear stresses, in-plane and those due to differential settlement
- punctures
- desiccation and freezing
- root penetration.

Shear. Koerner (1994) states that the resistance to shear in a GCL is dominated by its geosynthetic component. He discusses several lab tests that can be used to measure GCL shear behavior. Daniel (1994) cautions that a GCL will undergo long-term shearing stresses (difficult to measure using lab index tests) that need to be considered in the design. Citing studies by LaGatta (1992) and Boardman (1993), Daniel (1994) concludes that GCLs can withstand distortions up to 0.5 without significant increases in hydraulic conductivity (approximately 5 to 10 times larger than for compacted soil layers). This amount of distortion corresponds to a tensile strain of 10 to 15%. As noted, most of a GCL’s resistance to shear comes from its geosynthetic components, not from the bentonite.

Punctures. The thinness of GCLs renders them susceptible to punctures. Because bentonite swells greatly when hydrated, however, minor punctures will reseal. Shan and Daniel (1991) punctured a dry, geotextile-encased, adhesive-bonded GCL and found that, when hydrated, punctures less than 25 mm in diameter resealed.

Desiccation and freezing. Few data exist on the effect of desiccation and freezing on GCLs. Shan and Daniel (1991) found no change in the hydraulic conductivity of a geotextile-encased, adhesive-bonded GCL after three wet/dry cycles, each of which produced severe desiccation cracking. Boardman (1993) desiccated a GCL buried under 60 cm of gravel and found that its hydraulic conductivity returned to its original value when rehydrated. Shan and Daniel (1991) also subjected a GCL to repeated freeze/thaw cycles and found that its hydraulic conductivity was unaffected. Daniel (1994) reports that similar results have been obtained in other unpublished studies.

Root penetration. There are no published studies on the ability of roots to penetrate GCLs and the resulting effect on GCL performance. When hydrated, the bentonite component of a GCL will resist root penetration. When desiccated, however, bentonite cracks severely. Combined with the thinness of GCLs, this suggests that the bentonite component may provide little protection against root penetration in the long term. The geotextile components are also unlikely to provide any significant barrier to root penetration. The geomembrane component of a geomembrane/bentonite GCL, however, will provide resistance to root penetration.

While the laboratory results on GCL performance are encouraging, no long-term studies of GCL performance under realistic field conditions have been carried out. Such studies are required to test the ultimate value of GCL's as components of LLW cover systems.

Asphalt Mixtures

Asphalt mixtures are an uncommon, but potentially effective and long-term barrier in covers. Natural asphalts are known to have survived in the subsurface for more than 5000 years (Forbes, 1955). Hydraulic conductivities as low as 10^{-9} cm/s have been measured using hot-mix asphaltic concrete material (Freeman et al., 1994). A large-scale field study of a cover system utilizing a sprayed asphalt barrier is currently underway at the Hanford Site in Washington State (Wing and Gee, 1994; Gee et al., 1994).

Capillary Barriers

In contrast to compacted soil, geomembrane, and GCL barriers, a capillary barrier does not rely on the low intrinsic permeability of its materials to be an effective barrier. In fact, capillary barriers must be constructed of materials that have rather high saturated hydraulic conductivities. The use of capillary barriers in cover systems has been suggested by Frind et al. (1977) and Johnson et al. (1983) among others. An illustration of a capillary barrier is shown in Figure 3.7. The actual barrier is formed by the interface of a fine material and a coarse material (e.g., sand over gravel). Water percolating from above (q in Figure 3.7) moves through the fine soil until it reaches the interface. At the interface, capillary forces hold the water in the smaller pores of the fine material thus preventing deeper percolation of water into the coarse material.

With a capillary barrier of slope, $\beta = 0$, water will accumulate above the interface, increasing the pressure head there. If the pressure at the interface becomes so high that it is insufficient to hold the water in the fine soil, the capillary barrier will fail as water moves into the coarse material. The barrier must thus be designed to remove water from the interface. This can be done in one of two ways. Plant roots will remove water from the fine layer if they are able to

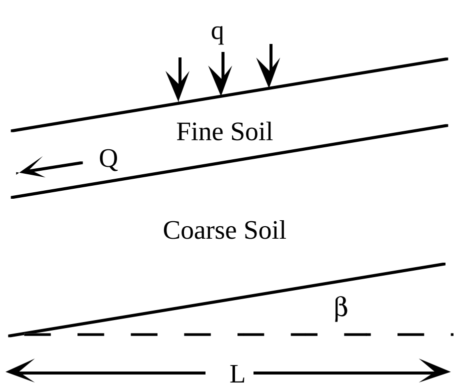


Figure 3.7 Illustration of a capillary barrier

grow within the barrier. This approach is applicable in relatively arid environments. An alternative approach, usually necessary in humid environments, is to construct the barrier with a slope $\beta > 0$. In this case, water reaching the interface will be able to drain laterally, thus increasing the pressure head at the interface.

There are several critical factors in the successful design and construction of a capillary barrier. These include:

- selection of materials
- limiting the input flux, q, in humid environments
- slope and thickness (and plant selection in horizontal barriers)
- proper construction.

The first three design variables can be evaluated using numerical models of unsaturated water flow (e.g., Oldenburg and Pruess, 1993; Meyer, 1993; Yeh et al., 1994). As a relatively simple check on design, however, the analytical solutions of Ross (1991, 1990) or Morel-Seytoux (1994) can be used.

Materials. The effective length of a capillary barrier is a nonlinear function of the properties of its materials. The selection of materials for a capillary barrier is therefore complex, requiring knowledge of the unsaturated hydraulic characteristics of both drainage and barrier layers. In a humid environment, a capillary barrier typically will consist of a coarse sand or gravel soil overlain by a drainage layer composed of a soil that is finer than the barrier layer. Although geotextiles can also be used for either component of the capillary barrier, their questionable longevity argues for the use of natural materials. In an arid environment in which lateral subsurface drainage is not a concern, the upper material may have a higher percentage of fines.

Figure 3.8 shows unsaturated characteristic curves for two soils that might be used to construct a capillary barrier. In this example, the coarse soil has a saturated hydraulic conductivity two orders of magnitude larger than the fine soil. At lower pressures, however, the hydraulic conductivity of the coarse soil is several orders of magnitude smaller than the fine soil. For the example shown in Figure 3.8(A), the critical pressure (the point at which the hydraulic conductivities of the two soils are equal) is approximately 0.7 cm. The capillary barrier will be successful as long as the pressure at the interface remains somewhat larger than this critical value.

It is commonly assumed that a capillary barrier will fail when the fine soil at the interface becomes saturated. This condition corresponds to the optimal situation and is illustrated by the water retention curves in Figure 3.8(B). However, some materials may function as a capillary barrier at low pressures yet fail well before the fine soil becomes saturated at the interface. A careful analysis that considers the

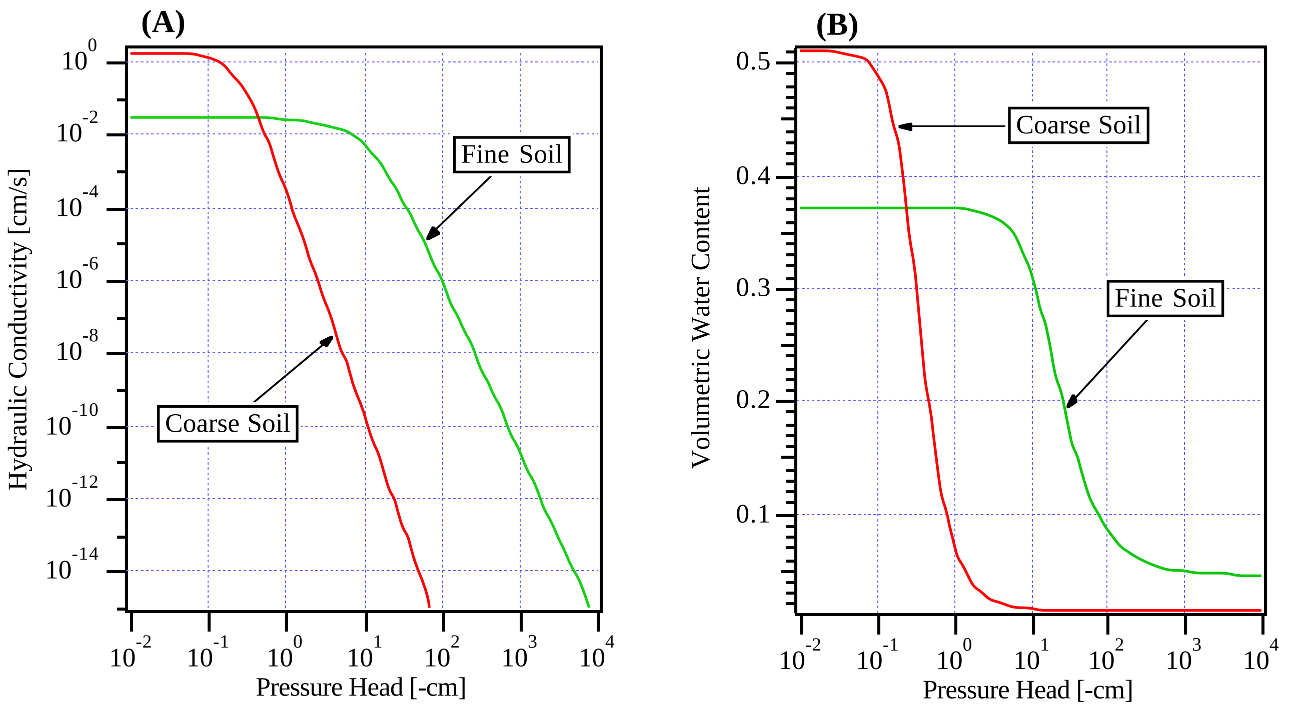


Figure 3.8 Unsaturated hydraulic conductivity (A) and water retention (B) characteristics in a capillary barrier

unsaturated flow characteristics is necessary to predict the performance of a capillary barrier.

Figure 3.8(A) also illustrates the low hydraulic conductivities that can be achieved with a capillary barrier. Coarse materials such as gravels, when dry, can have hydraulic conductivities that rival those of geomembranes. As explained above, these low conductivities can only be achieved if the pressure head at the interface is kept sufficiently low by choosing an appropriate fine soil.

Input flux. As discussed above, the success of a capillary barrier requires that the soil water pressure at the interface of the fine and coarse materials be relatively low. In an arid environment, this may not be an issue simply because precipitation is low and ET is high. Nyhan et al. (1990) illustrated the potential effectiveness of a capillary barrier in a semi-arid environment (Los Alamos, NM). Their capillary barrier field plots (3.0 m by 10.7 m) consisted of 71 cm of sandy loam topsoil over 5-10 mm gravel. The interface was maintained with a geotextile. The capillary barrier increased ET from approximately 88% of precipitation (in the control plots) to just over 96%. Seepage was 0.0 and 1.5% of precipitation in the two plots with capillary barriers and 6.1% in the control plots. These data were collected over three years under natural precipitation.

In a humid environment, a capillary barrier is not likely to be successful unless the input water flux to the top of the fine soil (q in Figure 3.7) is limited in some way. This can be done by placing a low permeability barrier such as a compacted soil layer, geomembrane, or GCL immediately above the fine soil layer of the capillary barrier.

In spite of the careful selection of materials, a capillary barrier will fail if there is a sufficiently large input of water. Unlike other barriers, however, this failure does not signal the end of the barrier's useful life. The capillary barrier will function again once the input of water is reduced and the materials dry out.

Slope. In an arid environment, a capillary barrier with no slope can be utilized. Such a design has been used in a prototype barrier constructed at the Hanford Site (Gee et al., 1993). Two meters of silt loam overlie coarse sands and gravels. The capillary barrier acts to hold water in the silt loam during the winters (when precipitation is high and ET is low). This water is subsequently removed from the fine soil during the spring and summer when evaporation and plant transpiration are both much higher. The success of this design requires that plants be able to extract soil water from the two meter depth and that the storage capacity of the silt loam, which is increased by the action of the capillary barrier, be sufficient to hold the winter precipitation (Gee et al., 1993).

In a humid environment, the capillary barrier must be sloped to drain the water that reaches the interface. Cost considerations will generally require that a cover system be constructed with each of its layers at approximately the same slope (as shown in Figure 3.2). The use of a relatively steep slope to increase the effective capillary barrier length must therefore be balanced against the design requirements of the surface and drainage layers. The solutions of Ross (1991) and Morel-Seytoux (1994) can facilitate this design analysis.

Construction. As is the case for barriers relying on their low intrinsic permeability, the performance of a barrier layer is sensitive to the quality of its construction. The interface between the fine and coarse materials must be fairly sharp. In addition, excessive movement of fine soil particles into the coarse layer may reduce the effectiveness of the barrier. A filter layer is sometimes used to limit fine particle movement. The presence of the filter layer may change the behavior of the barrier, however. This should be considered in the design.

The large-scale field experiment of Melchior et al. (1993, 1994) described above (in the Compacted Soil Layers section, page 25) included a study of a capillary barrier. In increasing depth from the surface, the experimental cover consisted of 75-cm of topsoil, a 25-cm coarse sand drainage layer, a 40-cm compacted soil barrier composed of the same material as described earlier, 60 cm of fine sand, and 25 cm of coarse sand/fine gravel. The last two layers comprise the capillary barrier. The barrier was constructed at a 20% slope.

Results of capillary barrier performance are given in Table 3.3, taken from Melchior et al. (1994). The capillary barrier performed perfectly for four years, successfully diverting 100% of the water passing through the compacted soil barrier. The amount of water leaking through the compacted soil layer increased each year, however. This layer was undergoing gradual degradation due to desiccation as described earlier. In the fifth year of operation, sufficient quantities of water passed through the compacted soil layer to cause leakage in the capillary barrier. However, the capillary barrier still diverted 87% of the water reaching it.

Stormont et al. (1994) have proposed the maintenance of a capillary barrier in semi-arid environments by blowing dry air through a coarse soil layer. Numerical simulations of a cover system incorporating such a dry barrier layer (Stormont et al., 1994) show that significant amounts of water can be removed from the coarse layer at certain times of the year. No field experiments of cover performance have been reported, however, and the numerical simulations did not include transient water input. Timing of precipitation may be critical since the greatest amount of water can be removed from a dry barrier during the summer, whereas the greatest need for removal may be in the winter (if precipitation is high and ET low at this time). The success of a dry barrier will also depend on cover thickness and the amount of available water storage, as does a passive capillary barrier.

3.2.3.3 Composite Barrier Designs

Because the barrier layer plays such a critical role in the success of the cover system, most cover designs incorporate redundant barrier layers, often utilizing more than one material to satisfy the permeability requirement in the long term. The benefit of this approach was illustrated in the examples of Melchior et al. (1994) discussed above (results in Tables 3.1 and 3.3). In these examples, the performance of a compacted soil/capillary barrier combination was much better than the performance of the compacted soil barrier alone. Barrier redundancy is particularly important given the long required period of safe performance of LLW disposal facilities.

Daniel and Koerner (1993) consider a variety of options for cover system barriers and summarize the relative performance of each with respect to a number of critical factors. For LLW disposal, the single-component options considered by Daniel and Koerner (1993) cannot be recommended. The multiple-component (composite) options they discuss are:

- geomembrane/compacted soil
- geomembrane/GCL
- geomembrane/compacted soil/geomembrane

Table 3.3 Subsurface drainage and leakage through a capillary barrier with a 20% slope (after Melchior et al., 1994)

	Subsurface Lateral Drainage above Compacted Soil Barrier [cm/s]	Subsurface Lateral Drainage within Capillary Layer [cm/s]	Leakage Through Capillary Barrier [cm/s] (% of potential leakage)
1988	1.2×10^{-6}	2.7×10^{-8}	0.0 (0.0)
1989	7.4×10^{-7}	4.5×10^{-8}	0.0 (0.0)
1990	1.0×10^{-6}	9.8×10^{-8}	0.0 (0.0)
1991	6.3×10^{-7}	1.0×10^{-7}	0.0 (0.0)
1992	8.8×10^{-7}	3.2×10^{-7}	4.8×10^{-8} (3.9)

- geomembrane/GCL/geomembrane.

Each of these options is briefly discussed below.

Geomembrane/Compacted Soil Barriers

This composite barrier is attractive because the weaknesses of the geomembrane (possible punctures, seaming defects, and uncertainty in lifetimes) are complemented by the strengths of the compacted soil. Likewise, the geomembrane limits the major degradation mechanisms of the compacted soil layer (desiccation from above and root penetration). In addition, the geomembrane withstands much larger differential settlements than the compacted soil.

Giroud and Bonaparte (1989b) derived expressions to estimate the flux through a composite geomembrane/compacted soil barrier. With an intact barrier, flow will be governed by the hydraulic conductivity of the geomembrane and the head above the barrier. If there are holes in the geomembrane, however, the flux through the composite barrier will also be a function of the size of the holes, the hydraulic conductivity of the compacted soil, and the spacing between the geomembrane and the compacted soil. A small spacing between the two components of the barrier tends to reduce the amount of flow. In deriving their results, Giroud and Bonaparte (1989b) relied on the laboratory experiments of Brown et al. (1987) and Fukuoka (1986).

The results of Giroud and Bonaparte (1989b) are summarized in Table 3.4. The field conditions refer to the ability to provide good contact between geomembrane and compacted soil. Good field conditions require a soil without ruts, clods or cracks and a flexible geomembrane without wrinkles. Good field conditions result in a small spacing between barrier components. Poor field conditions result in a large spacing. As in Table 3.2, the results of Table 3.4 assume an HDPE geomembrane thickness of 1mm, a hole frequency of one per 4000 m^2, and a 0.9-m-thick compacted soil layer with a saturated hydraulic conductivity of 1×10^{-7} cm/s. A comparison with Table 3.2 illustrates the advantage of a composite barrier.

Table 3.4 Estimated flux [cm/s] through a composite geomembrane/compacted soil barrier with holes (after Giroud and Bonaparte, 1989b)

Field Conditions	Hole Diam. [mm]	Water Depth on Top of the Geomembrane [cm]		
		0.3	3.0	30
Good or Poor	0.0	1×10^{-14}	1×10^{-12}	1×10^{-10}
Good	2.0	2×10^{-12}	2×10^{-11}	1×10^{-10}
	11.3	2×10^{-12}	2×10^{-11}	2×10^{-10}
Poor	2.0	1×10^{-11}	1×10^{-10}	7×10^{-10}
	11.3	1×10^{-11}	1×10^{-10}	8×10^{-10}

Melchior et al. (1993, 1994) constructed an experimental cover using a composite geomembrane/compacted soil barrier. This cover was identical to the compacted soil barrier discussed earlier except that an HDPE geomembrane was placed over the compacted soil. The flux results of this experiment are presented in Table 3.5 (taken from Melchior et al., [1994]) and illustrate the improvement in performance of the composite barrier.

The small discharges observed by Melchior et al. (1994) were believed to be moisture losses from the compacted soil layer driven by thermal gradients. This raises the issue of potential long-term desiccation of the compacted soil layer. Vielhaber et al. (1994) present confirmation that moisture loss in a geomembrane/compacted soil barrier can be driven by thermal gradients. Whether the loss of moisture can be large enough to cause cracking of the compacted soil is unknown. In any event, once the geomembrane decays, the

Table 3.5 Subsurface lateral drainage and leakage through a composite geomembrane/compacted soil barrier (after Melchior et al., 1994)

	20% Slope		4% Slope	
	Subsurface Lateral Drainage [cm/s]	Leakage [cm/s] (% of potential leakage)	Subsurface Lateral Drainage [cm/s]	Leakage [cm/s] (% of potential leakage)
1988	1.1×10^{-6}	1.9×10^{-9} (0.2)	9.4×10^{-7}	1.1×10^{-8} (1.1)
1989	7.5×10^{-7}	9.5×10^{-10} (0.1)	4.9×10^{-7}	1.9×10^{-9} (0.4)
1990	1.0×10^{-6}	1.6×10^{-9} (0.2)	8.5×10^{-7}	1.3×10^{-9} (0.1)
1991	6.0×10^{-7}	2.2×10^{-9} (0.4)	5.2×10^{-7}	1.6×10^{-9} (0.3)
1992	1.1×10^{-6}	3.2×10^{-9} (0.3)	9.9×10^{-7}	2.5×10^{-9} (0.3)

performance of the compacted soil can be expected to quickly degrade as well.

Geomembrane/GCL Barriers

This barrier requires the GCL to perform similarly to the compacted soil in a geomembrane/compacted soil barrier. Koerner (1994) and Daniel (1994) discuss GCL/compacted soil equivalency and conclude that a GCL can be equivalent or superior to a compacted soil layer in most respects. In terms of potential leakage, puncture resistance is the most notable area in which a GCL is clearly inferior. In addition, predicting the performance of compacted soil barriers may be more reliable because of their long history of use.

Daniel (1993) raises the issue of transmission of water through geomembrane holes and laterally within the geotextile component of the GCL. If significant, this would greatly reduce the composite action of the barrier just as a large spacing between geomembrane and compacted soil results in reduced performance of that composite barrier. Estornell (1991) provides evidence that the presence of the geotextile component produces potentially significant lateral flow. Because overburden pressure compresses the barrier and causes intrusion of clay into the geotextile, Koerner (1994) concludes that lateral flow is not a concern with woven geotextiles. For needle-punched, nonwoven geotextiles the concern can be eliminated by purposely fouling the geotextile with clay during manufacture of the GCL and by using a textured geomembrane that will physically intrude through the geotextile and into the clay component of the GCL.

The equations developed by Giroud and Bonaparte (1989b) for flow through a geomembrane/compacted soil barrier (including flow between the two barrier components) assumed that the hydraulic gradient in the soil was one. This assumption will only be valid when the hydraulic head acting on the soil is small compared to the thickness of the soil. Since a GCL is only a few millimeters thick, this assumption is not likely to be valid. The flux through a composite geomembrane/GCL barrier when the geomembrane contains holes will thus be larger than the values given in Table 3.4.

Because of these concerns, a composite geomembrane/GCL barrier does not appear as attractive for LLW disposal applications as a composite barrier using a compacted soil.

Geomembrane/Compacted Soil/Geomembrane Barriers

This three-component barrier addresses the potential problem of drying from below in a geomembrane/compacted soil barrier. The second geomembrane placed below the compacted soil severely limits the potential for desiccation. Daniel and Koerner (1993) point out the construction difficulties of this barrier, particularly the compaction of clay on a geomembrane. The multiple interfaces also increase the potential for stability failure. Daniel and Koerner (1993, p. 481) recommend this design only "for extremely sophisticated waste containment facilities where an extraordinary degree of redundancy in the design is required." It is possible that safe disposal of LLW in some humid environments can only be achieved with such redundancy.

Geomembrane/GCL/Geomembrane Barriers

This three-component design is also highly redundant and is relatively easy to construct. The multiple interfaces create potential stability problems, but these can be addressed using appropriate anchoring of the geosynthetic components. The addition of a lower geomembrane, however, does not address the principal concerns with the geomembrane/GCL composite barrier. This three-component barrier is still vulnerable to puncture during construction (although the redundancy reduces the probability of complete barrier puncture) and relies on components whose long-term field behavior is relatively uncertain.

3.3 Waste Containment Structures

3.3.1 Function

A waste containment structure may be designed to serve several functions by providing:

- structural stability
- physical separation of the waste from the surface
- a barrier to intrusion, whether by plants, animals, or humans
- physical and chemical containment of the waste, limiting the movement of mobile contaminants out of the structure
- an additional barrier to water flow.

The first two functions are particularly important when the waste must be located relatively close to the ground surface. This is most likely in humid environments where a shallow water table can restrict the depth of a disposal facility. The function of a waste containment structure of most relevance to an evaluation of unsaturated zone hydrology is the additional barrier to water flow that the structure provides. This is particularly important in a humid environment. At arid sites, a waste containment structure may be less important because the amount of water is naturally small and the waste can typically be buried quite deeply.

3.3.2 Options in Materials and Design

The typical materials considered for construction of waste containment structures are reinforced concrete and asphalt. Concrete provides much greater structural strength than asphalt, but is susceptible to cracking under sustained loads.

Asphalt can be used in two ways: as a component of an asphalt-cement mixture and as a coating for a concrete substructure. Asphalt tends to deform under load, but may be less likely to crack than concrete.

The ability of asphalt to deform without cracking was observed by Rogers et al. (1987) who used bench-scale models of buried vaults to examine the flow of water and the release of soluble salts through waste containment structures. Five vaults were constructed; two were concrete, one was an asphalt emulsion solids admixture (with concrete sand and chopped fiberglass), another was a "rubberized" asphalt, and one consisted of a concrete substrate coated with a thin layer of the rubberized asphalt. Rogers et al. (1987) applied gradually increasing loads and a constant infiltration rate to the vaults. Release of the salts from the concrete vaults increased significantly when the structures failed. The vault consisting of asphalt-coated concrete released far smaller concentrations of salts, even after structural failure, apparently because the asphalt deformed without cracking.

The primary issues involved in the analysis of concrete and asphalt as barriers are the hydraulic conductivity and the long-term durability of each material.

3.3.2.1 Hydraulic Conductivity

Concrete

The saturated conductivity of concrete is a function of many variables, including the water to cement ratio, cement additives, curing conditions, and age of concrete. In general, the saturated hydraulic conductivity of concrete can be reduced by using:

- low water-to-cement ratios
- additives such as slag, fly ash and silica fume (among others)
- humid curing conditions
- longer time periods for curing
- adequate quality control.

In addition to the conductivity of intact concrete, the ability of joints and sealants to limit the passage of water for long time periods needs to be considered.

Various methods are available for measuring concrete hydraulic conductivity. Mercury intrusion porosity can be used to relate pore size distribution to permeability (Young, 1988). Hydraulic conductivity can be measured directly using a permeameter-type device. Air permeability is often commonly measured. Tests that require less time and show good correlation with permeameter measurements are also available (Whiting, 1988). Laboratory measurements such as these indicate that concrete hydraulic conductivities of 1×10^{-10} to 1×10^{-11} cm/s are achievable.

Asphalt

There is very little information available on the hydraulic characteristics of asphalt. In a study carried out for the performance assessment of tank waste disposal at the Hanford Site, Clemmer et al. (1992) measured the permeability to nitrogen of cores taken from a field-placed asphalt barrier. The saturated hydraulic conductivity for water estimated from these measurements was 2×10^{-13} cm/s (Kincaid et al., 1994). The asphalt/aggregate mixture for this barrier consisted of 7.5 ± 0.5% asphalt by weight, compacted to a minimum of 96% of maximum density and to less than 4% by volume of air voids (Kincaid et al., 1994). Note, the design described in Kincaid et al. (1994) consists of a buried concrete vault surrounded by a (minimum) 1-m-thick asphalt barrier.

3.3.2.2 Long-term Durability

Concrete

The long-term durability of concrete is related to many factors, including its permeability. Reinforced concrete integrity can be compromised by chemical reactions with various ions, particularly sulfate and chloride, transported into the pore space of the concrete. A low-permeability concrete can thus be expected to survive intact a longer time. ACI (1984) discusses the mechanisms by which concrete is known to crack. Prominent failure mechanisms for buried concrete vaults include:

- shrinkage due to nonuniform drying
- thermal stress
- concrete chemical reactions
- rebar corrosion
- construction joint failure due to degradation of water seals
- structural loading.

Models for the failure of concrete structures have been proposed by Walton (1990), Clifton and Knab (1989), and Hookham (1991). It is difficult, however, to quantify concrete degradation such that changes in hydraulic characteristics over periods of 100s to 1000s of years can be accurately predicted. A qualitative approach such as that adopted by Winkel (1994) is more practical. Winkel (1994) evaluated the significance of various concrete cracking mechanisms as the product of two factors, the probability of occurrence (on a scale of 1-5) and the relative consequence (also on a scale of 1-5). Based on the significance factors, and utilizing engineering judgement, the location and sizes of cracks were predicted for time periods of 0-100, 100-1000, 1000-10^4, and 10^4-10^5 years from construction. Hydraulic properties were then modified in the location of the cracks to be equivalent to the properties of the surrounding backfill soil (Kincaid et al., 1994).

Asphalt

As mentioned earlier, natural asphalts have been observed to survive in the subsurface for at least 5000 years. Whether asphalt elements of engineered barriers can function as designed for similar time periods is uncertain, however. Several important mechanisms contributing to the degradation of subsurface asphalt structures are:

- hardening of the asphalt due to oxidation or other reactions
- shrinkage due to volatilization
- slumping due to deformation of the underlying concrete or waste form
- cracking due to seismic stresses on hardened asphalt
- thermally induced cracking
- biodegradation.

There are no models available for subsurface asphalt structure failure. Winkel (1994) used a qualitative, significance factor approach (identical to the concrete degradation approach described above) for the analysis of asphalt barrier failure.

3.4 Subsurface Collection and Removal Systems

Subsurface drainage components of the cover system (i.e., the lateral drainage layers above any barriers) should be designed to divert water away from the waste to a point where the diverted water cannot interact with the waste. Some (small) amount of water may percolate through the cover system and the waste containment structure (if it is used) and potentially leach contaminants. The purpose of a subsurface collection system below the emplaced waste is to collect any water that has potentially come into contact with the waste. This water is typically drained to a point where it can be removed from the subsurface. Subsurface collection and removal systems are not typically used in arid environments, nor should they be needed in humid environments after closure when the final cover is in place and functioning. Water backing up within the subsurface collection system after closure may adversely affect the performance of the facility.

The required capacity of a subsurface collection and removal system is determined by the performance of the cover and must consider that the performance of the cover is likely to change over time. Guidance on design of subsurface collection systems can be found in U.S. EPA (1985) as well as many hydraulics texts. Koerner (1994) discusses the use of geosynthetics in collection system applications. A typical design includes a composite geomembrane/compacted soil barrier with a sand/gravel drainage layer above.

Liquid collected by the subsurface system should be capable of being removed. Knowing the volume of liquid collected provides a measure of the performance of the cover system. In some designs, water from inside the waste containment structure is kept separate from water percolating through the cover system but not entering the waste containment structure. In this case, the quantity and quality of the liquid provides an indication of the performance of the waste containment structure and the waste packaging.

4 Evaluating Models

Before a LLW facility is approved or constructed, the subsurface hydrologic environment it will form must be characterized to ascertain the risk of water contact with the waste and subsequent opportunity for contaminant migration away from the facility. The time for which safety must be assured, usually more than 500 years, renders prototype or demonstration approaches infeasible. Consequently, predictive modeling is often performed to evaluate the subsurface hydrologic behavior. Simulation of water flow within a LLW facility enters the hydrologic evaluation methodology as indicated in Figure 4.1.

If an analyst relies on a model to predict water distribution in the subsurface environment of a LLW facility, the confidence in that prediction will depend on a judgement of the applicability and capability of the model. Model capability is judged based on its demonstrated accuracy, function, and reliability. Model applicability is judged on the degree to which the underlying assumptions of the model represent the real system being simulated. In Section 4.1, the modeling process is defined in a way that allows us to examine model capability and applicability in a systematic manner. In Section 4.2, criteria for evaluating model capability and applicability are developed and discussed. These criteria are used in Section 4.3 to compare several computer codes used in the applications of Chapter 6.

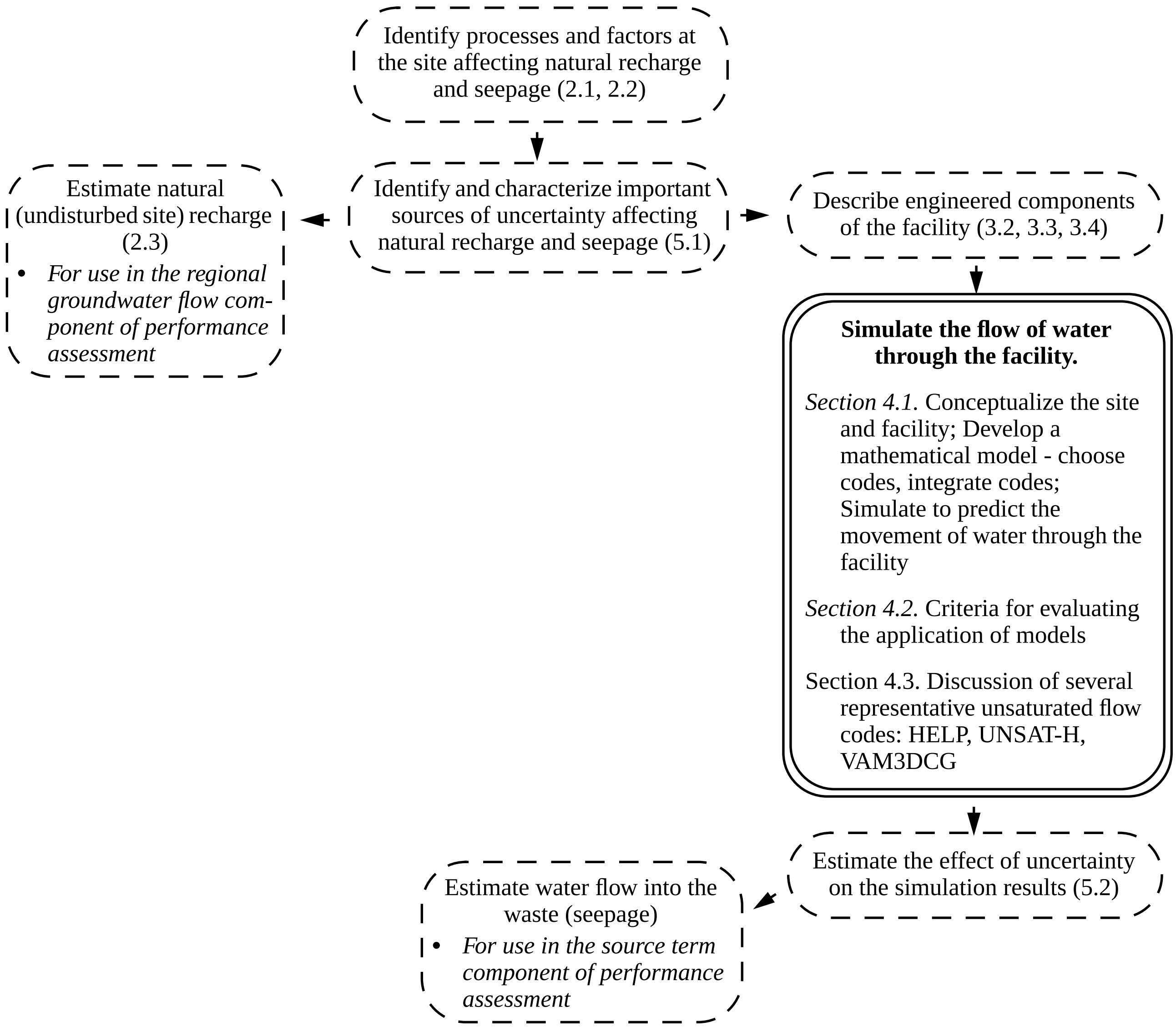


Figure 4.1 Flowchart for the Hydrologic Evaluation Methodology. Chapter 4 discusses the simulation of water flow through the facility and the evaluation of model application. Numbers indicate sections in this document in which the items are discussed.

4.1 Perspective on the Modeling Process

Fluid flow in porous media, as in most natural systems, is extremely complex. Our understanding of fluid flow processes is based on conceptualizations of the actual systems. We seek to develop a simplified model capable of sufficiently describing certain key aspects of the real system whose full complexity is beyond our perception. In doing so, there must be a balance between detail and perspective when selecting the resolution with which to model a real system. Since all models represent a simplification of the real system, the evaluation of a model must be based on the choice of simplifications and whether adequate evidence is provided to justify the simplifying assumptions.

To understand the modeling process and how to evaluate its use, we view the development of a physical model for evaluating hydrologic processes at a LLW facility as a three-step process:

(1) A conceptualization, or conceptual model, is developed from available regional and site-specific data, design specifications, and other pertinent information.

(2) A mathematical model that represents the key aspects (processes) of the conceptual model is developed, and simulations are conducted with this mathematical model to predict the behavior of the facility. This step often, but not always, involves the use of a computer code.

(3) Results obtained from simulation of the mathematical model are interpreted in terms of the conceptual model.

This general perspective of the modeling process provides a useful way to evaluate a model's capability and application. A systematic approach to the modeling process, similar to what is presented here, was previously suggested by Simmons and Cole (1985).

All three steps are crucial in the development of a capable model and its successful application. Notice that under this definition we distinguish between a model and a computer code. A computer code embodies only step two – the mathematics. A computer code may be restricted to a certain range of conceptualizations because of the code's specific capabilities or because it assumes a certain type of conceptualization, but that does not make it a complete model. The use of a computer code does not replace the human-oriented tasks of defining an acceptable conceptualization of the real physical system (step 1), or interpreting the results in light of the limiting assumptions made in the conceptualization (step 3). Therefore, we distinguish between a code, which can be used in the modeling process, and the model. Failure to recognize this difference risks the making of errors in steps one and three and therefore of making unwarranted conclusions. For example, choosing the computer code to use before the conceptual model is fully developed often leads to conceptualizing the physical system in ways the code can solve, not in terms of how the real system behaves. Therefore, we must insist upon a justification for code selection based on a realistic conceptualization.

Opportunity exists for the introduction of error in all three steps. Errors introduced in step one are termed conceptual errors and are highly subjective. Conceptual errors result from proposing a model that omits important processes, misrepresents the real system, or relies on unrealistic assumptions in translating concepts into mathematical terms. To accommodate the subjectivity of this judgement, the U.S. NRC in their Draft Branch Technical Position on Performance Assessment for LLW Disposal Facilities (U.S. NRC, 1994) advised that equally valid conceptualizations may be proposed, that all valid alternatives should be modeled, and that the worst results (not the average) be used as the basis for evaluation. Chapter 5 of this report takes up this concept in greater detail.

In contrast to subjective step one errors, errors in step two are very objective. This makes errors in step two easier to avoid. Technical training focuses intensively on this step and usually the correct application of the precise set of rules that constitute mathematics is carried out correctly. Also, because of the precise and consistent nature of mathematics, errors in step two are easier to detect than errors in steps one or three. Advances in computer technology have provided the opportunity to accomplish much more in step two; a computer's most notable ability is to manipulate numbers following a precisely defined set of rules very quickly and accurately. Although a computer code is not essential to modeling flow in porous media, one is commonly used. All of the concerns we have with modeling in general apply when using a computer code, and a few additional concerns specific to computer codes should be considered also.

Step three is the most difficult (and often most neglected) in the modeling process. Like step one, the errors in step three are typically subjective. Comparison of model results to laboratory or field data can be an important part of this step. Such data cannot verify (that is, prove) a model, but do act to build confidence in the results of a model for a given simulation. More important, conclusions reached in step three must be consistent with the limiting assumptions made in step one, developing a conceptualization. To repeat this point for emphasis: conclusions (step 3) reached based on simulation results (step 2) must be consistent with the assumptions made in developing the conceptualization of the problem (step 1).

4.2 Evaluating Model Capability and Applicability

Model capability is judged based on the demonstrated accuracy, function, and reliability of the model. Model applicability is evaluated based on the degree to which the underlying assumptions of the model represent the real system. To a large degree, capability and applicability are intricately linked: a model incapable of modeling a given phenomena is inapplicable to the problem. However, the capability to model a process does not, in and of itself, make the model applicable to the problem at hand. We will therefore consider how to evaluate applicability and capability together.

Models vary in type and solution techniques, which results in differing capabilities to consider. For computer codes, justifying the selection of a specific code requires some additional considerations. Judging the applicability of a model can be more subjective than judging capability. This document cannot provide an exhaustive list of applicability concerns. Instead, we'll discuss several critical applicability issues and encourage the use of active professional judgement to challenge specific models that exhibit a lack of applicability to the specific sites they are to represent. Table 4.1 provides a concise checklist of capability and applicability criteria as an evaluation aid. Each criterion in the checklist is discussed in more detail in this section to guide the evaluator in making an informed judgement about model application.

4.2.1 Comprehensive Conceptualization

As previously discussed, developing an acceptable conceptualization of a physical system is step one of the modeling process. The modeling process seeks to successfully balance detail and perspective: we cannot hope to simulate, or even understand, all processes occurring in a physical system at all scales. The conceptual model defines the specific processes the model will focus on; that is, how the system will be abstracted and simplified. The expectation is that the conceptualization will include all processes that have a significant effect on the results sought.

In the case of LLW facilities, there are numerous hydrologic processes that may be important in the conceptualization, including:

- precipitation
- snow accumulation and melt
- infiltration
- surface runoff
- evaporation
- plant growth
- plant uptake of soil water
- subsurface lateral drainage
- thermal effects and vapor phase flow
- heterogeneity, hysteresis, and anisotropy of soil properties.

A specific conceptual model may not include some of these hydrologic processes, but their omission should be based on site-specific and facility design information that clearly justifies an assumption of insignificance for that process. For example, snow accumulation and melt can safely be omitted from a conceptual model for sites located in climatic region where snow rarely or never occurs. Surface runoff may be unimportant in arid climates where infiltration rates are not limiting.

4.2.2 Conceptual Model Dimensionality

The actual world is three-dimensional, of course, but to simplify physical models conceptual models are often one or two dimensional. The geometry of the LLW facility design must be studied carefully, and the relevant hydrologic processes considered, to justify reducing the dimensionality of a conceptual model for convenience. If water infiltration at a site is essentially uniform and vertically-downward, a one-dimensional model is probably adequate. If, on the other hand, it is arguable that the flow has a significant horizontal component, a conceptualization that assumes one-dimensional flow or a computer code that accommodates only one dimension is inadequate and two or perhaps three dimensions must be included. Judgements with regard to the conceptualization may be arguable: there may be several equally valid conceptualizations of the system, as pointed out earlier. Nonetheless, the evaluator must make a judgement as to whether the model's dimensionality is applicable to the specific site in consideration.

4.2.3 LLW Facility Design Considerations

Any performance assessment model is based on the proposed design of a given facility as well as the site where it will be located. The conceptualization must therefore portray the geometry of the proposed design (thicknesses, slopes, layering) if it is to represent the response of the hydrologic system. Evidence that the conceptualization is based on the intended design should be provided. Some features of the design may not be hydrologically important and can be safely omitted from the conceptualization: e.g., a geotextile used to maintain a sharp discontinuity between soil layers is an important design feature, but is otherwise hydrologically unimportant.

4.2.4 Alternative Conceptualizations

The subjective nature of conceptual model formulation implies that there may be more than one equally valid conceptualization, each of which may fit the available site information. The U.S. NRC advised how to accommodate such

Table 4.1 Checklist for evaluating model application

	Criterion	Reference Section	Judgement
	Step One Issues: Conceptualization		
1.A	Does the conceptualization (conceptual model) identify all of the hydrologic processes significant to water distribution and movement in the subsurface environment at the site and facility? Processes to consider: precipitation, snowmelt, infiltration, surface runoff, evaporation, plant growth, plant uptake of soil water, subsurface lateral drainage, thermal effects, vapor phase flow, soil property heterogeneity, anisotropy, and hysteresis.	4.2.1	❐ Yes ❐ No
1.B	Is the dimensionality of the conceptualization adequate to capture the behavior of the real physical system?	4.2.2	❐ Yes ❐ No
1.C	Is the design of the LLW facility adequately represented by the conceptualization?	4.2.3	❐ Yes ❐ No
1.D	Were ALL valid, defensible conceptual models identified and proposed? Note: If alternative, significantly different conceptualizations that are supported by available information occur to the evaluator, they should be described to the analyst for consideration.	4.2.4	❐ Yes ❐ No
	Step Two Issues: Model Simulation		
2.A	Are the hydrologic processes simulated consistent with the conceptual model? If a process is part of the conceptualization but is not simulated, is adequate justification given for not including it?	4.2.5	❐ Yes ❐ No
2.B	Were the number of dimensions simulated consistent with the conceptualization?	4.2.5	❐ Yes ❐ No
2.C	Are the boundary conditions used consistent with the conceptualization? Is there adequate justification for the chosen boundary conditions?	4.2.5	❐ Yes ❐ No
2.D	Is the computational approach used adequate to the resolution in time and space required by the conceptual model? If there are limits on the temporal or spatial discretization (e.g., one day or one cell per layer), is there adequate justification that these limits will not adversely affect the results and that these limits are consistent with the conceptualization?	4.2.6	❐ Yes ❐ No
2.E	If a steady-state solution was used: Was sufficient justification provided that time-dependent processes are not significant to the problem? Also, was a steady-state analysis consistent with the conceptualization?	4.2.6	❐ Yes ❐ No ❐ N/A
2.F	If mechanistic approaches were used for any part of the model: Were the governing equations solved correctly and the computations consistent? (For widely reviewed computer codes, reference to documentation is sufficient to meet this criterion).	4.2.7	❐ Yes ❐ No ❐ N/A
2.G	If empirical approaches were used for any part of the model: Is adequate justification given that the conditions under which the empirical model was developed reflect the site-specific conditions being simulated? Are the assumptions of the empirical model consistent with the conceptualization?	4.2.7	❐ Yes ❐ No ❐ N/A
2.H	If empirical approaches were used for any part of the model: Was the empirical model calibrated to local site conditions and over the range of expected variation at the site? Were sufficient data available or collected to assure high confidence in the empirical parameter values used?	4.2.7	❐ Yes ❐ No ❐ N/A

Table 4.1 Checklist for evaluating model application

	Criterion	Reference Section	Judgement
2.I	If an analytic solution was used: Were the assumptions and approximations used to obtain the analytic solution consistent and reasonable with respect to the conceptualization?	4.2.8	❒ Yes ❒ No ❒ N/A
2.J	If a numerical solution was used: Was evidence of solution stability with respect to grid and time resolution provided? (i.e., an investigation of the errors due to the discretization and demonstration that the errors were sufficiently small?)	4.2.8	❒ Yes ❒ No ❒ N/A
2.K	If a numerical solution was used: Was the spatial grid refined enough to capture the hydrologic processes of concern, and reflect the complexity of the conceptual model?	4.2.8	❒ Yes ❒ No ❒ N/A
2.L	If a computer code was used: Was its selection justified by the applicant on the basis of a conceptual model developed for the specific site under consideration?	4.2.9	❒ Yes ❒ No ❒ N/A
	Step Three Issues: Model Interpretation and Confidence Building		
3.A	Was confidence in the model demonstrated either by conducting verification, benchmarking, and validation studies or by reference to supporting documentation of such studies? Do benchmarking and validation problems demonstrated or cited reflect important aspects of the actual site-specific problem? Note: Verification by users, rather than by reference to others' documentation, is preferable because it demonstrates the user possesses the basic ability to properly operate the computer code.	4.2.10	❒ Yes ❒ No
3.B	Was confidence in the model demonstrated by using site-specific data to history-match (calibrate) the simulation results? (For example, a comparison of measured and predicted water content over a period of time.)	4.2.10	❒ Yes ❒ No
3.C	Are the conclusions reached based on modeling results within the limitations imposed by the assumptions of the conceptual model?	4.2.11	❒ Yes ❒ No

subjectivity in their Draft Branch Technical Position on Performance Assessment for LLW Disposal Facilities (U.S. NRC, 1994). They advised that equally valid conceptualizations may be proposed, that all valid alternatives should be modeled, and that the worst results (not the average) should be used as the basis for evaluation. Therefore, the evaluator should accept multiple conceptualizations if proposed, see that each has been modeled, and use the worst results as the basis for evaluation. If other valid conceptualizations that could result in less favorable outcomes should occur to the evaluator, these alternative conceptualizations should be identified to the analyst for further consideration.

4.2.5 Consistency of Mathematical Model with Conceptual Model

An adequate conceptualization alone is not an assurance that the model will address all relevant hydrologic processes in the system. The mathematical implementation must be examined to ensure that all the processes identified by the conceptual model are actually simulated. If a process is not simulated, a justification must be provided for not doing so. The dimensionality of the mathematical model must also match the conceptual dimensionality. Finally, a mathematical model requires that boundary conditions be defined. The conceptual model may not explicitly define these boundaries, but the boundary conditions chosen for the mathematical model must at least be consistent with the conceptualization. Further, there must be some physical justification for choosing a boundary type (e.g., symmetry, physical divide, water table presence, etc.).

The dimensionality of computer codes illustrates how a mathematical model is chosen to meet the needs of the conceptualization. If water infiltration at a site is essentially uniform and vertically downward, a one-dimensional computer code such as UNSAT-H (Fayer and Jones, 1990) is applicable. Both the conceptualization proposed to describe the infiltration and the mathematical solution used are suitable to the process being modeled. If two or three dimensions are required to address lateral flow, an analyst may have to use a code that accommodates this, such as VAM3DCG (Huyakorn and Panday, 1993) or MSTS (White and Nichols, 1993; Nichols and White, 1993). Some codes may provide “quasi-” dimensionality as well. HELP (Schroeder et al., 1994a), for example, is a quasi-two-dimensional code in which horizontal runoff within layers is accounted for, but laterally-diverted water cannot cause different conditions downslope.

4.2.6 Time and Space Resolution

Many computational approaches discretize a physical system in time and/or in space. Such discretization treats the hydrologic processes of concern as if they occur in discrete, or finite, steps. If such an approach is used, the resolution of the discretization must be shown to be fine enough to ensure that the results are not affected by the discretization itself. A simple way this is sometimes accomplished is to increase the resolution (e.g., use twice as many grid cells in each dimension, or use a time step half as large) and repeat a simulation. If the results do not change appreciably, then the original resolution was adequate. In certain cases, grid Peclet and Courant number limitations provide an indication of numerical solution stability. Adherence to these limits should be demonstrated.

If the physical system is subject to large variation in conditions over time that could affect the assessment, the model should probably be time-transient. The alternative to transient analysis is to generate a steady-state solution, which presumes that variation in time is unimportant in the analysis. Steady-state solutions have several advantages, including faster solutions and reduced data requirements. These advantages are particularly appealing in stochastic simulation (refer to Chapter 5). However, use of steady-state solutions must be justified on a site-specific basis. A steady-state analysis is generally more applicable to simulations of water flow in deep soils (e.g., below the rooting zone and range of ET effects). Simulations in the near-surface soil profile involve time-dependent processes that must be evaluated with a transient analysis.

4.2.7 Model Types: Empirical to Mechanistic

Models range in type from empirical to mechanistic. Most models incorporate elements of both approaches to varying degrees. The empirical approach utilizes observation of relationships between various parameters and system responses to predict future response based on parameter values. The mechanistic approach relies on identifying the processes and fundamental laws that control the system and formulating these concepts in ways that allow prediction of future responses.

Mechanistic approaches are typically based on physical laws such as conservation of mass, conservation of energy, and Darcy's Law. These mechanistic descriptions of the fundamental physics do not change from one system to another and are often identified as the “governing equations” of the mechanistically-based model. Mechanistic approaches are generally preferred to empirical approaches, but in many cases we lack sufficient knowledge of the controlling processes or it may be too difficult to solve the governing equations. In these cases, we often rely on empirical approaches instead of, or in addition to, mechanistic ones. Because of the more universal nature of mechanistic approaches, the evaluator can have greater confidence in their use, assuming that the governing equations are correctly formulated and implemented. For existing, widely used computer codes, documents usually exist that can be cited to provide assurance of this. Any concern with a mechanistic model should be focused on the data quality and quantity used as input to the model.

Concerns with empirical models center on the fact that they must be developed and calibrated to each specific system modeled, and confidence can only be assured for the range over which the calibration was performed. This does not imply that empirical approaches are bad, only that greater caution in their application is necessary because, unlike the physical laws that mechanistic approaches are based upon, empirical models are not universal.

Many porous media flow models rely on a generally mechanistic approach but require empirical relations to complete the description. For example, many mechanistic computer codes such as UNSAT-H (Fayer and Jones, 1990), MSTS (White and Nichols, 1993; Nichols and White, 1993), and VAM3DCG (Huyakorn and Panday, 1993) solve the nonlinear Richards Equation (Richards, 1931), a mechanistic description of flow in unsaturated porous media in terms of water pressure. However, an empirical relationship, such as van Genuchten's (1980) function, is utilized in these codes to describe the relationship between fluid pressure and the degree of liquid saturation. A model's capability will be limited by the capability of such empirical relations to describe the physical system under consideration, and this in turn is limited by the site-specific data available to develop the empirical relationship.

To summarize, use of an empirical model requires the following:

- application of the model only to conditions that are similar to those under which the model was developed, and
- calibration of the empirical model to local conditions using adequate data collected across the range of expected variation.

An analyst is expected to demonstrate that these conditions have been satisfied to justify the use of an empirical approach in a model, including empirical components of primarily mechanistic codes.

4.2.8 Solution Types: Analytical to Numerical

Models may employ analytical and numerical solutions to the mathematical problems posed. An analytical solution is exact: the differential equations posed by the model have been solved so that for given input parameter values, the system response is directly computed from an equation. Unfortunately, most differential equations encountered are too complex, or even intractable, to solve by analytic means. To proceed in these cases, numerical approximation schemes are used to approximate the solution. Numerical schemes have become very powerful with the advance of computer technology. Hence, computer codes are widely used for solving the complex, highly nonlinear equations that describe unsaturated flow systems. Where possible, analytic solutions are desirable for exactness and speed, but numerical solutions offer a much broader range of application. When an analytical solution is used, only mathematical verification of the correctness of the solution and accuracy of the computations is necessary to provide full confidence in a solution. For a numerical solution, additional effort must be made to demonstrate that the solution meets stability criteria (e.g., adherence to Peclet and Courant number criteria, or demonstration that temporal and spatial discretization did not alter the solution).

4.2.9 Justifying Code Selection

The need to select a computer code to fulfill the requirements of a conceptualization was discussed above (Section 4.1). Again, the choice of a computer code must be based on the conceptualization and not vice versa. While this approach may result in a conceptual model that is beyond the ability of any computer code or computational technique to solve, this emphasis on the conceptual model's priority is necessary. When such solution difficulties arise, the problem might be addressed by using a number of simpler (tractable) models and linking these models together to represent the entire system. The conceptual model might also be revised to the least degree possible to allow simulation, recognizing that the interpretation of the simulation results must consider the full conceptual model. Either of these approaches is preferable to conceptualizing the site only in ways the preferred computer code can simulate while ignoring processes it cannot simulate. The evaluator is thus urged to be wary of conceptualizations developed to suit a specific computer code.

The combination of applicability demands on a code may be more than any single code can meet. For example, the need to evaluate infiltration in a time-dependent manner and simultaneously account for multidimensional flow requires a large computational effort. The combination realistically could be beyond the ability of any one code to accommodate. The humid site application example (Section 6.1) illustrates such a problem, where the surface cover layer requires daily or even hourly modeling to account for precipitation, evaporation, transpiration, and infiltration, while the barrier layers and the waste vault require multidimensional flow modeling to account for lateral subsurface flow. The solution in this example was to partition the problem, recognizing that the top layers of the cover could be modeled separately from the rest of the facility. The upper layers were modeled using a one-dimensional code, UNSAT-H (Fayer and Jones, 1990), which can account for all of the hydrologic processes in the near-surface in a time-varying manner. The lower region was modeled using a multidimensional code, VAM3DCG (Huyakorn and Panday, 1993), that handled the spatial discretization particularly well for the different sloping interfaces between soil types in the design. Neither of these codes would have been applicable to the other part of the analysis, but dividing the problem provided a compound model that fulfilled analysis needs.

4.2.10 Building Confidence in a Model

Building confidence in a model generally involves establishing confidence in the computer codes being used. Confidence in code capability is built by the processes of verification and benchmarking. Verification compares a code's results to analytical solutions for (usually) simple problems. Further confidence is built by contrasting the results obtained with a code to those obtained from other established codes. Such inter-code comparison is usually called benchmarking. While verification essentially ensures that the code is internally consistent and correctly solves the equations, benchmarking goes further by demonstrating that the equations embedded in the code compare well with other codes that have had a history of successful application to field problems.

Building confidence in a model by comparison with field and laboratory data has been called validation (Tsang, 1991). The use of this term is controversial (Oreskes et al., 1994; Konikow and Bredehoeft, 1992). Nevertheless, we will use it with the understanding that while verification and benchmarking are finite tasks, validation is never complete.

Thus, we speak of having verified and benchmarked a code, but we only point to greater levels of confidence building in validation, for we can never be certain a model will correctly predict a system's behavior under every set of conditions. All of these detailed processes (verification, benchmarking, validation) are not usually carried out as part of a site assessment, but the analyst should cite such studies to provide confidence in the code used.

The highest possible degree of confidence is, of course, to demonstrate that the model accurately predicts system response by comparing predictions with actual data from the specific site. As previously mentioned, this is not possible for the long time periods of concern in LLW disposal. Nevertheless, some history-matching (calibration) can be accomplished. For example, model results for an undisturbed site could be compared to lysimetry data to show that the model accurately predicts recharge for local soils and meteorological conditions over a period of a few years. In addition, data that are collected during the construction and operation of the facility can be used to test and refine the model of the site. Such evidence is direct, albeit limited, assurance of model capability and applicability.

4.2.11 Conclusions Constrained by Assumptions

The essence of step three in the modeling process as it was presented in Section 4.1 was to judge whether the conclusions reached based on simulation results were reasonable in light of the assumptions made in step one, the conceptualization. Evaluating this criterion requires the evaluator to apply careful scientific judgement in examining each conclusion to find if the conclusion is warranted or unwarranted in view of the limiting assumptions of the conceptualization.

4.2.12 User-Centered Reasons for Code Selection

There are other reasons for code selection that, while valid, are not important to the evaluator. These include the sophistication and ease-of-use of the user interface, the familiarity of users with the code, the license status of the code (proprietary or public domain), the quality of code documentation and code support, and other ease-of-use criteria. These are important factors to the code user, not just in terms of convenience but because they have direct implications for the user's ability to conduct a hydrologic assessment efficiently and without error. None of these ease-of-use factors outweighs the capability and applicability issues identified above, however. The applicability of a code to the site-specific conceptual model and demonstrated confidence in the code are the factors that concern the evaluator. The evaluator is concerned with the overall accuracy of the code, not the speed or ease with which it is used. Therefore, citing such criteria should not affect the evaluation of model application.

4.2.13 Data Issues

We have stressed the importance of selecting a computer code to meet the needs of a conceptualization and the dangers of reversing that order by modeling a system so that a particular computer code can be used. Data collection for hydrologic evaluation of a specific site follows this model-driven approach. Data requirements are defined by the needs of a model and the purposes for which the model is being used. If a site is not complex and a relatively simple model is required (as determined by the evaluation criteria discussed throughout Section 4.2), the data requirements may consequently be limited. We stress, however, that data availability is not a valid criterion for model selection. Intentionally choosing a model to suit an extremely limited data set is unjustifiable. Recognizing that data collection can be a lengthy, expensive process and that some data might not be obtainable (e.g., an 80-year meteorological record specific to the site), data adequate to meet the needs of the modeling process must still be identified and collected.

The data collection or site characterization program must be coupled to performance assessment modeling efforts. A data collection program that is not guided by the needs of the model(s) may collect unnecessary data and neglect to obtain critical information, thereby wasting time and resources. Even during construction and after closure of a LLW disposal facility, an ongoing data collection program should include among its purposes the collection of data necessary to verify the initial assessment by updating parameters to "as built" values. Dramatic changes from design conditions could then be evaluated to ensure that the facility still meets regulatory requirements as construction proceeds, or to guide reaction to unanticipated problems that might occur in the future.

4.3 Overview of Unsaturated Flow Computer Codes

The preceding discussion provided a general framework from which to evaluate any model applied to examine subsurface water movement at LLW facilities. Several applicable computer codes that are, in many ways, representative of the variety of codes available are discussed in this section. These codes were chosen because they are used in the applications presented in Chapter 6. No endorsement is implied by their being discussed here. We encourage the use of any code (currently available or that becomes available in the future) that can satisfy the evaluation criteria discussed above and summarized in Table 4.1. This discussion is not intended as a full critique of any code. Our purpose is not to evaluate any given code, but to provide an outline of the general features, capabilities, and applicabilities of several common codes to illustrate the general framework given above. For complete code evaluations, see Kozak et al. (1991) and Reeves et al. (1994), for example. Remember that model evaluation concerns not just evaluation of a computer code, but of the whole application of the modeling process to a specific site and facility design.

Two codes not discussed in this section were used in a previous, related study (Meyer, 1993), but were not used to obtain any of the results presented in Chapter 6. MSTS (White and Nichols, 1993; Nichols and White, 1993) is a three-dimensional, integrated-finite-difference code capable of simulating coupled water flow, air flow, heat transfer, and solute transport in variably saturated geologic media. The Two-Dimensional Princeton Unsaturated Code (Celia, 1991) simulates water flow using a finite element, mass conserving method (Celia et al., 1990).

4.3.1 The HELP Code

The computer code Hydrologic Evaluation of Landfill Performance, or HELP, has been developed by the U.S. Army Corps of Engineers (Vicksburg, Mississippi) for the Environmental Protection Agency (see Schroeder et al., 1984; Schroeder et al., 1994a,b). It was developed for conducting water balance analyses of landfills, cover systems, and solid waste disposal and containment facilities. HELP is used in the humid and arid site applications presented in Chapter 6.

4.3.1.1 Conceptualization Issues

Hydrologic Processes Simulated

HELP is capable of using meteorological data, including precipitation, to account for infiltration, surface storage, snowmelt, runoff, ET, plant growth, and lateral subsurface drainage. HELP does not account for thermal effects, vapor phase flow, or hysteresis or anisotropy of soil moisture retention relations. The dimensionality limitation of HELP makes the surface runoff and subsurface lateral drainage estimates of limited value. Refer to the discussion on dimensionality (below) for more information on this aspect of HELP.

HELP is inapplicable to the analysis of a capillary barrier. A capillary barrier is formed by the presence of a very coarse material below a very fine material under unsaturated conditions (see Section 3.2.3). HELP cannot be used to model this phenomenon because the code does not include capillary effects. The humid site application example (Section 6.1) illustrates the use of sloping capillary barrier in a hypothetical LLW design. This feature cannot be modeled with HELP because "the model [code] does not permit a vertical percolation layer to be placed directly below a lateral drainage layer" (Schroeder et al., 1994b), which is how a sloping capillary barrier is formed. Hence, if the design calls for this barrier, the analyst will have to use a multidimensional, more mechanistic code to model the facility.

Dimensionality and Geometric Configurations

HELP is a quasi-two-dimensional code. The principal, full dimension is aligned with that of infiltration (vertical). Multidimensional characteristics such as surface and subsurface lateral flow are accounted for indirectly. For example, surface runoff is predicted using the SCS curve number method, an empirically-based technique. The predicted surface runoff is a "point value" that does not include the true multidimensional effects of runoff water from higher slopes or the effect of runoff downslope. This is also true of subsurface lateral drainage predictions. Therefore, while lateral flow effects are accounted for, they are only applicable in cases where the runoff is routed away from the cover or barrier in question without an opportunity to resume vertical infiltration downslope.

4.3.1.2 Simulation and Mathematical Issues

Mechanistic and Empirical Approaches

Solution algorithms of the HELP code were initially based on the concept of fixed water extraction limits (Schroeder et al., 1984). Storage limits were assigned to each soil layer. In HELP Version 1.0, no vertical flow occurs when water storage drops below the "field capacity" (i.e., the hydraulic conductivity of the layer is assumed to be zero). Above this limit, water is allowed to flow at a rate controlled by the hydraulic conductivity value assigned to the average water content of the layer. Below field capacity water is extracted from the soil profile by ET until the wilting point is reached, then all water loss from the profile ceases. Water remains in the soil profile but is unavailable for either vertical flow or ET. In HELP Version 2.0, vertical flow is allowed to proceed below the field capacity in all layers. The flow rate is determined by the water content through the Brooks-Corey water retention relationship (Brooks and Corey, 1964). In the most recent version of HELP (3.0), vertical flow below field capacity is allowed only in the topsoil.

Field capacity and wilting point are often estimated using available soils data. Many surface soils have been analyzed for their water retention characteristics (i.e., water content data from samples that have been equilibrated on pressure plates at selected pressures). Water content at 0.3 bars (0.03 MPa) is often used to estimate field capacity while water content at 15 bars (1.5 MPa) is used to estimate the wilting point (Cassel and Nielsen, 1986). The difference between these two water contents when multiplied by the soil rooting depth is the "available water" in the profile. It should be noted that these limits are texturally dependent. For very coarse soils (sands and gravels), the field capacity is at a much lower tension (< 0.1 bars) while for very fine clays, it may be higher than 0.5 bars. Cassel and Nielsen (1986) discuss the issues related to these variable limits.

Water extraction by ET is initially controlled by climate variables (i.e., solar radiation, wind speed, and air temperature). As profile water content decreases below field capacity and further extraction continues to the wilting point, water loss is controlled mainly by soil factors (i.e., the unsaturated hydraulic conductivity).

Two of the three versions of the HELP code (Versions 1.0 and 3.0) predict that vertical flow in soil layers below the topsoil does not occur when moisture content is below field capacity. All versions of HELP predict that no water extraction occurs below the wilting point. In truth, water is always moving in a soil system (either as a liquid or a vapor). In general, the driving forces for water in an unsaturated system are gravity and capillarity. When soils are wet, gravity dominates the downward movement of water. As the soil dries, capillary forces begin to dominate. Soils being wetted experience the combination of gravity and capillarity. The HELP code only approximates these processes, and the errors involved in assuming flow-limit controls need to be quantified.

4.3.1.3 Confidence and Other Issues

Confidence Building

Barnes and Rogers (1988) found that the HELP code predicted water contents that were much less than actual in a field plot at Los Alamos, New Mexico over a three-year test period (1983-1985). The underestimate of water content was attributed, in part, to the inability to initialize soil water with field-measured values and also to excessive ET estimates predicted by HELP.

Martian (1994) reported on a HELP (v. 2.0) code analysis for the Hanford Site. A comparison was made between HELP results and measured water storage in weighing lysimeters. After an extensive calibration effort, Martian (1994) determined that HELP underestimated ET and overestimated drainage from the lysimeter. Martian (1994) concluded that HELP inadequately modeled the physics of flow in a shallow capillary barrier, particularly with an absence of vegetation. In addition, the evaporative depth parameter could not be predicted because it was time dependent.

Stephens and Coons (1994) used HELP Version 2.05 to estimate the recharge at a proposed landfill in southern New Mexico. They obtained a recharge value of 0.03 mm/yr. (9.66×10^{-11} cm/s), which compared favorably to the value of 0.02 mm/yr. (6×10^{-10} cm/s) obtained at the same site by the chloride mass balance method. Stephens and Coons (1994) modeled both runoff and plant transpiration in their application of HELP.

Predictions using the HELP code suffer from uncertainties in the water balance estimate which may overestimate recharge and seepage in some cases and underestimate them in others. Because the HELP code has gained wide regulatory acceptance, it is clear that knowing how well it performs is important. Estimation errors should be evaluated for the HELP code over a wide range of applications. To our knowledge, a systematic evaluation of estimation errors has not been undertaken for the HELP code.

For humid sites, where infiltration is often a large fraction of the total water budget, soils are often at field capacity or wetter. In terms of seepage, the error in assuming flow-limits (i.e., no vertical flow below field capacity) can lead to nonconservative predictions using HELP. This occurs because water does not actually cease to flow at field capacity. While flow rates at field capacity are small, they are not negligible. A typical rate of vertical flow at 0.3 bar water content for most medium and fine textured soils is 1-10 mm/day, which is well over 30 mm/yr.

For arid sites, underestimates of available water can lead to overestimates of seepage and recharge. Such underestimates are common for arid sites. The major reasons for this are improper accounting of the wilting point and the fact that soils in arid environments can dry substantially below the wilting point. Under desert (arid site) conditions, the soil profile dries by plant-water extraction to values drier than the 15-bar estimate since native plants generally do not wilt until water is extracted to a 50-bar or greater limit. In coarse sands, the water storage error is small since water extracted at 15-bars is only marginally greater than the water extracted at 50-bars (i.e, the water retention characteristic is very steep). However, in finer soils (silt and clay), water retention characteristics are such that the error is generally significant, amounting to a large fraction of the available water.

In arid climates, surface soils can dry to values that are in equilibrium with the surface humidity, which often is generally very low (equivalent to 1000 bars or greater; i.e., well below the wilting point). While evaporative drying seldom occurs below the top meter of a soil profile, this additional drying can have a measurable effect on the total water balance.

The result of these two processes (i.e., lower wilting point values for desert plants and accelerated surface drying in arid soils) is that the soil profile can become drier than predicted by HELP through extraction processes of evaporation and transpiration. Thus, in this situation the storage capacity of a soil is underestimated by HELP. Recharge and seepage under these conditions are overestimated because more infiltration is converted to recharge when the water storage capacity of the soil is exceeded. An example of such overestimation is suggested in a study by Nichols (1991), who compared HELP (v. 2.0) with UNSAT-H (v. 2.0) and found that HELP predicted higher seepage rates than UNSAT-H over a 10-year simulation period. Under the conditions of the simulations, the overestimation of seepage by the HELP code was small but potentially significant (4 mm).

Several other errors are possible with the HELP code, particularly in semi-arid or arid climates. One is the estimation of ET. HELP calculates surface water losses based on an estimate of the surface energy budget. Traditional energy budget estimates (e.g., based on Penman- or Thornthwaite-type formulas) of ET must be adjusted to account for dry-surface conditions that exist most of the time. As an example, potential ET at an arid site may be well over 1500 mm/yr., with precipitation seldom more than 150 mm/yr. Actual surface water losses (over extended time) cannot be more than precipitation, thus actual ET must be a small fraction of potential ET for arid sites. Calibration data (from direct or indirect measurement of ET) are required to make correct adjustments in ET estimates. Such calibration data are seldom available for a given site. Thus, the accuracy in ET estimates is generally poor, resulting in poor estimates of the water balance.

Ease-of-Use Issues

HELP is an attractive code to users for a number of reasons. The code is in the public domain and free to users. It is accepted or required by a number of regulatory agencies. HELP also uses many empirical input terms rather than data-derived mechanistic input. Empirical inputs (e.g., the evaporative depth) may be convenient in their simplicity but are often vague about the actual physical processes being simulated.

HELP features an interface that is easier to use than many comparable codes. A good interface is always desirable (although not a replacement for a good computational code). The interface to HELP can become quite difficult, however, if the user wishes to input their own (e.g., site-specific) climate data such as daily temperature and rainfall. The interface is considerably simplified when using default values, which HELP uses in many instances when actual data are not provided. Evaluation should focus suspiciously on this “advantage.” Such defaults are general values that might be useful for first-cut evaluations or learning purposes, but all too often their easy availability leads to their use in place of site-specific data. The analyst should be challenged to defend any use of a default value by demonstrating or providing a rationale that its use either will not affect the final results or that the default values are truly representative of the actual site and LLW facility being simulated.

4.3.2 The UNSAT-H Code

UNSAT-H was developed at Pacific Northwest Laboratory for the U.S. Department of Energy. It has been used primarily for predicting the near-surface water balance at waste disposal sites, including the analysis of cover systems (Fayer and Jones, 1990; Fayer et al., 1992a,b; Martian and Magnuson, 1994). The UNSAT-H code is used in the humid and arid site applications presented in Chapter 6.

4.3.2.1 Conceptualization Issues

Hydrologic Processes Simulated

The UNSAT-H code is deterministic and requires specific climate (e.g., precipitation, temperature, and solar radiation), soil, and plant data as input. It generates values for infiltration, evaporation, transpiration, redistribution, and recharge from these input data. Vapor flow in the soil is also incorporated in the code. Evaporation and transpiration are calculated, utilizing site-specific plant and soil data. Soil hydraulic properties (e.g., hydraulic conductivity and water content as functions of water potential) for individual soil horizons are inputs to the code as are detailed plant parameters such as plant rooting depth and density, and leaf area. UNSAT-H can compute water runoff and surface water detention but does not predict lateral routing of water.

Dimensionality and Geometric Configurations

UNSAT-H is strictly one-dimensional and does not predict lateral routing of water. As such, UNSAT-H is not suited to analyses of subsurface facilities or porous media structures that serve to route water laterally by design or circumstance. UNSAT-H utilizes daily or hourly precipitation data and daily meteorologic data to model surface fluxes of moisture and energy as well as plant interactions in the hydrologic processes of the near surface. This makes the UNSAT-H code most useful for highly mechanistic simulation of cover designs and ambient site conditions wherein water movement is well approximated by a one-dimensional (vertical) model, and surface fluxes are important.

4.3.2.2 Simulation and Mathematical Issues

Mechanistic Approaches

The UNSAT-H code is more mechanistic than the HELP code. Unlike the HELP code, UNSAT-H utilizes a water potential (head) formulation based on the Richards equation (Richards, 1931) to calculate water flow. While this mechanistic approach provides a better representation of the physics of unsaturated flow than the empirical approach of HELP, the computational demands of solving the Richards equation may make a code such as UNSAT-H less practical in certain cases. A judgement of which type of approach is most appropriate must be made on a site-specific basis. Often the use of more than one code is the best approach. This approach is illustrated in the example of section 6.1, in which UNSAT-H is used to estimate the potential errors in the water balance estimates of HELP due to the daily averaging (in HELP) of precipitation. The HELP code can then be used with greater confidence to make long-term predictions.

Empirical Approaches

Hydraulic parameters for the UNSAT-H code are obtained from both laboratory and field measurements. Water retention tests using hanging water columns, pressure plates, and vapor equilibrium techniques (Klute, 1986) provide the basic hydraulic property data for individual soil layers. Field-measured saturated and unsaturated conductivity (at water contents in the range from saturation down to drained water contents at or near field capacity) provide the best estimates of the conductivity (Rockhold et al., 1988). In the absence of these data, laboratory saturated conductivity values are combined with water retention data, and estimates of the hydraulic conductivity function can be made using Brooks and Corey (1964) or van Genuchten (1980) models.

Numerical Solutions

The UNSAT-H code, version 2.0, uses a finite difference method with a direct solver for the linear algebraic equations. A Picard iteration is used to linearize the Richards equation. Without careful user oversight, the methods used in UNSAT-H, Version 2.0 can result in unacceptably large mass balance errors, particularly when simulating arid environments. Codes utilizing mass conserving numerical methods (Celia et al., 1990; Kirkland et al., 1992) may be more appropriate in these cases.

4.3.2.3 Confidence and Other Issues

Confidence Building

A detailed sensitivity analysis of an early version of UNSAT-H was reported by Freshley et al. (1985), who used the code to simulate the water balance of a soil cover placed over an oil shale pile. Parametric analysis looked at the sensitivity of seepage and actual ET to precipitation, potential ET, saturated hydraulic conductivity, initial soil conditions, plant sink term, and rooting depth and density. Results of the sensitivity analysis demonstrated that the water flow model was most sensitive to precipitation, potential ET, initial soil conditions, rooting depth and density. The model was less sensitive to hydraulic conductivity and the plant root sink term.

UNSAT-H has been successfully tested against analytical solutions for infiltration (Fayer and Jones, 1990) and is currently being calibrated using Hanford Site lysimeters. The model has been tested against measured water storage and lysimeter drainage for a 1.5-year-period (Fayer et al, 1992a). The uncalibrated model, while agreeing with annual water balance measurements, diverged from both winter and summer water storage measurements (root-mean-square error as large as ± 22 mm, in a soil whose average storage was about 350 mm). Calibration, without optimization of the fit, reduced prediction error substantially (over 60% to about ± 8 mm).

Ease-of-Use Issues

UNSAT-H uses formatted input, which can make the preparation of correct input files somewhat more difficult than necessary. UNSAT-H Version 2.0 is in the public domain.

4.3.3 The VAM3DCG Code

The Variably Saturated Analysis Model in 3 Dimensions with Preconditioned Conjugate Gradient Matrix Solvers (VAM3DCG) was developed by Hydrogeologic, Inc. It simulates saturated-unsaturated ground-water flow and solute transport (Huyakorn and Panday, 1993). Use of the VAM3DCG code has been reported in Panday et al. (1993) and in the humid site application in this document (Section 6.1).

4.3.3.1 Conceptualization Issues

Hydrologic Processes Simulated

The VAM3DCG code accounts for heterogeneity, hysteresis, and anisotropy of soil properties, and has a limited ability to account for evaporation and infiltration boundaries and plant root water uptake. These capabilities are not simulated as mechanistically as in the UNSAT-H code but do nonetheless provide a multidimensional code with the ability to model these atmospheric-driven fluxes in a limited way. Infiltration and ET are handled in VAM3DCG by a iterative procedure adapted from Neuman et al. (1974). The parameters required for this procedure include wilting point (see discussion on the HELP code above for wilting point information), potential transpiration rate, and the relationship of root effectiveness function with depth. VAM3DCG does not account for thermal effects, vapor phase flow, or snow accumulation and melt.

Dimensionality and Geometric Configurations

VAM3DCG is a three-dimensional code. Either a rectangular or curvilinear orthogonal grid may be used with this code. The curvilinear grid provides greater flexibility to accommodate complex geometries such as the multilayered, sloping materials of LLW engineered barriers. Cylindrical and radial coordinate systems are not handled by VAM3DCG.

4.3.3.2 Simulation and Mathematical Issues

Mechanistic Approaches

The VAM3DCG code is deterministic, requiring specific hydrologic and dilute species data as input. It generates values for soil or rock continuum pressure, saturation, and flow velocities in liquid water phase only. The VAM3DCG code is highly mechanistic, solving the Richards equation for water flow in variably saturated soil.

Empirical Approaches

The relationship between liquid pressure and saturation are handled by empirical relationships, either the van Genuchten (1980) relationship or the Brooks and Corey (1964) relationship. Hysteresis in these functions can be modeled using the VAM3DCG code. The water retention parameters required by VAM3DCG include empirical curve-fitting parameter values for a van Genuchten (1980) or Brooks and Corey (1964) water retention function, saturated hydraulic conductivity values, porosity, and species diffusion coefficients if transport will be modeled.

Numerical Solutions

The VAM3DCG code uses a finite element method with a conjugate gradient numerical solver. Newton-Raphson and Picard iterations schemes are available as are other application-specific advanced numerical techniques.

4.3.3.3 Confidence and Other Issues

Confidence Building

Several verification problems are presented in the VAM3DCG User's Manual (Huyakorn and Panday, 1993) as well as some limited benchmarking. We are not aware of any more comprehensive verification and benchmarking studies of VAM3DCG, or of any validation studies.

Ease-of-Use Issues

The conjugate gradient and other advanced solvers used in VAM3DCG can shorten computer simulation time. The curvilinear grid can simplify the modeling of certain complex geometries such as layered soils. Preparation of input files and verification of their correctness can require substantial effort due to the use of formatted input and the complicated dependencies between input parameters. The code is copyrighted and is subject to a license agreement and fee.

5 Analysis of Uncertainty

The concept of reasonable assurance stated in 10 CFR 61 implies that the performance assessment of a LLW disposal facility must consider the uncertainty associated with model predictions. The objective of an uncertainty analysis is to determine the uncertainty in predicted performance as a function of the cumulative variability in the input data and model parameters. Uncertainty analysis is necessary because of the highly heterogeneous nature of most subsurface environments and the long time frames of interest for forecasting the performance of LLW disposal facilities.

As illustrated in Figure 5.1, the assessment of uncertainty enters into the hydrologic evaluation methodology at two points. Early in the analysis, the most important sources of uncertainty should be identified and characterized. Appropriate data must be gathered to sufficiently characterize the uncertainty. Examples of parameters that contribute to uncertainty in the hydrologic evaluation of the unsaturated zone at LLW disposal facilities are discussed extensively in Section 5.1.

Uncertainty analysis also enters the methodology after a simulation model has been developed. Several methods for evaluating the effect of uncertainty on the results of a simulation are reviewed in Section 5.2 along with the relative benefits and possible problems associated with these methods. Each of the methods discussed can be carried out with virtually any model, including all those discussed or mentioned in Chapters 3 and 4.

For the engineering design of a LLW disposal facility, performance measures of interest might include the amount of surface layer erosion, the required capacity of a subsurface lateral drainage layer, the fraction of percolating water diverted laterally by a barrier layer, and the water retention characteristics of the soil components of a capillary barrier. For an comprehensive facility performance assessment, the

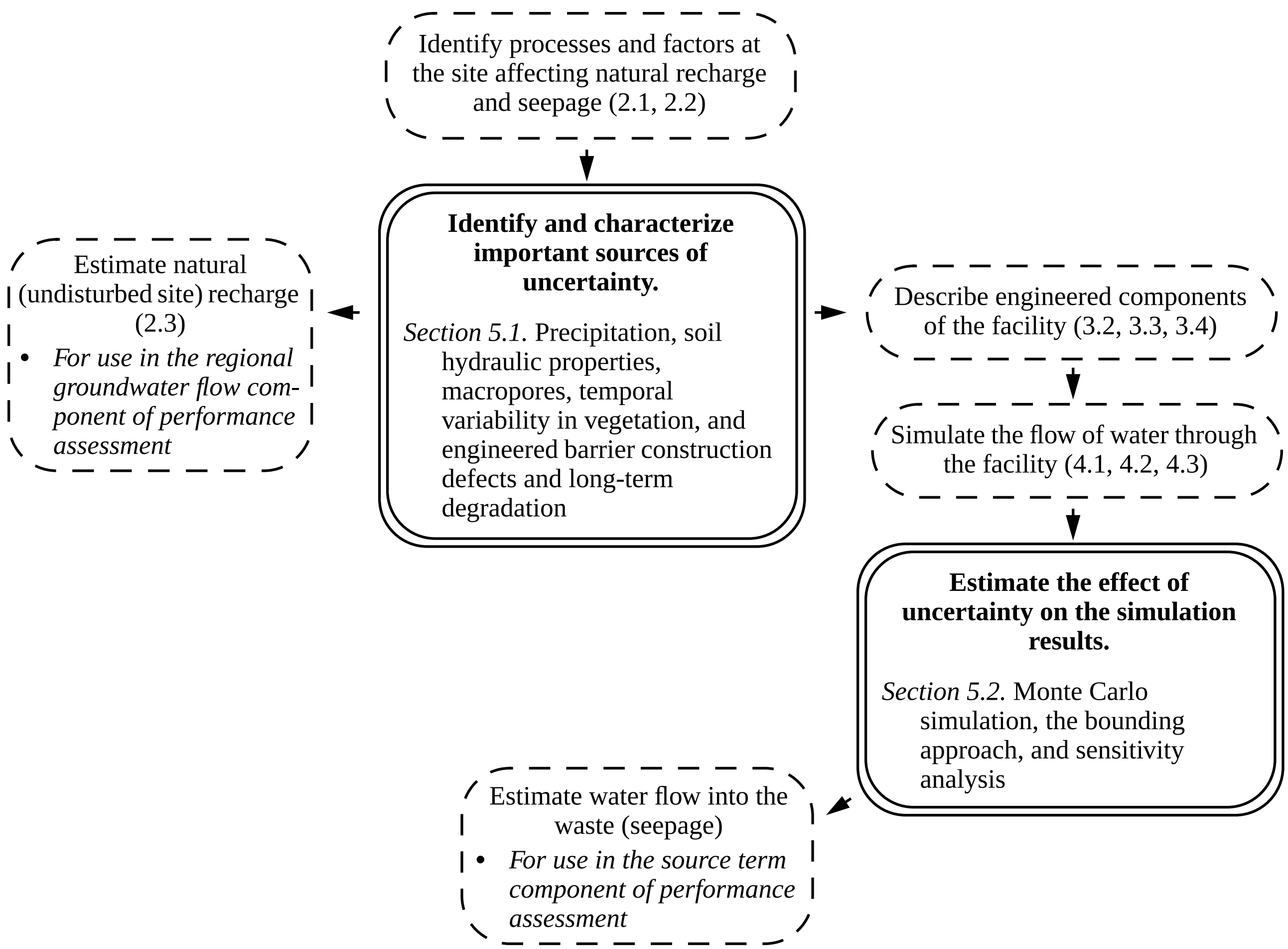


Figure 5.1 Flowchart for the Hydrologic Evaluation Methodology. Chapter 5 discusses sources of uncertainty and methods to estimate the effect of uncertainty on the results of simulations. Numbers indicate sections in this document in which the items are discussed.

most pertinent measure of performance with respect to the unsaturated zone water flow is the flux of water reaching the waste.

5.1 Types and Sources of Uncertainty

Uncertainty is classified here into three major types:

- random or systematic measurement error
- random variability inherent in many physical processes and measurable quantities
- imperfect knowledge of parameters, models, or underlying physical processes.

The first two types of uncertainty are exhibited in experiments that produce different (random) results under apparently identical conditions. Many processes and phenomena involved in the flow of water through a LLW disposal facility are characterized by randomness and are consequently unpredictable to some degree. Precipitation is an excellent example. The number of defects in a geomembrane liner is another. Predictions involving random processes and phenomena (seepage through a cover, for example) are naturally uncertain. The essential characteristic of random uncertainty is that it cannot be reduced by the collection of data (although data may help to better characterize random uncertainty).

In contrast to random uncertainty, the uncertainty arising from imperfect knowledge of parameters, models, and underlying physical processes can be reduced by the collection of additional data. Following Wu et al. (1991), we classify uncertainty due to imperfect knowledge into three types:

- Parameter uncertainty is associated with imprecise or inaccurate model input parameters that may result from estimating parameters using inaccurate, unrepresentative, or limited data. For example, the parameters of the van Genuchten water retention model may be estimated from one or two soil samples.
- Modeling uncertainty is a consequence of using imperfect representations of reality (models) to describe a physical system. Examples include use of a normal probability distribution to model variability in precipitation that may be better characterized as lognormal, and use of a one-dimensional model for a three-dimensional reality. Modeling uncertainty can also arise from the application of a model outside its range of validity; for example, extrapolating parameters determined from short-term experimental data to longer time frames.
- Completeness uncertainty arises from a failure to consider all the significant processes and potential future states (scenarios). The impacts of potential future scenarios such as land use change and climate change are examples of completeness uncertainty.

Of the three types of uncertainty due to imperfect knowledge, parameter uncertainty is the easiest to quantify. There is often insufficient data available (or it is simply too expensive to obtain) to reliably estimate the impact of model and completeness uncertainty.

Kozak et al. (1993) describe a comprehensive approach to uncertainty analysis in LLW disposal facility performance assessment that incorporates all the types of uncertainty discussed above. This approach attempts to deal with model and completeness uncertainty by enumerating and evaluating all plausible conceptual models (e.g., one- vs. two-dimensions, isothermal vs. nonisothermal conditions, macropore flow, and material degradation rates) and scenarios (e.g., climate and land use changes). The approach of Kozak et al. (1993) is depicted in Figure 5.2. For many applications, it may be sufficient to limit the analysis to a single scenario and even a single conceptual model. In this case, only parameter uncertainty and random variability would be considered (using one of the methods described in Section 5.2).

Section 2.2 discussed four broad factors that affect recharge at a LLW disposal facility: climate, soil, vegetation, and engineered barriers. Under each of these factors fall a number of processes or phenomena that exhibit inherent variability that can lead to uncertainty in recharge (and seepage) estimates. In addition, parameter estimation and modeling are an integral part of unsaturated zone hydrologic evaluation and contribute added uncertainty. The remainder of this section discusses specific sources of uncertainty in the hydrologic evaluation of the unsaturated zone at LLW disposal facilities.

5.1.1 Climate

Climatic processes and parameters that exhibit significant spatial and temporal variability include:

- precipitation amount, duration, and intensity
- air temperature
- wind speed and direction
- solar radiation.

While each of these climatic parameters is important, variability in precipitation is particularly important because of its direct effect on all water balance components. Air temperature, wind velocity, and solar radiation primarily affect ET. In addition, because the size of a LLW facility is small relative to the spatial variability of these climatic processes, the temporal variability is of greatest concern.

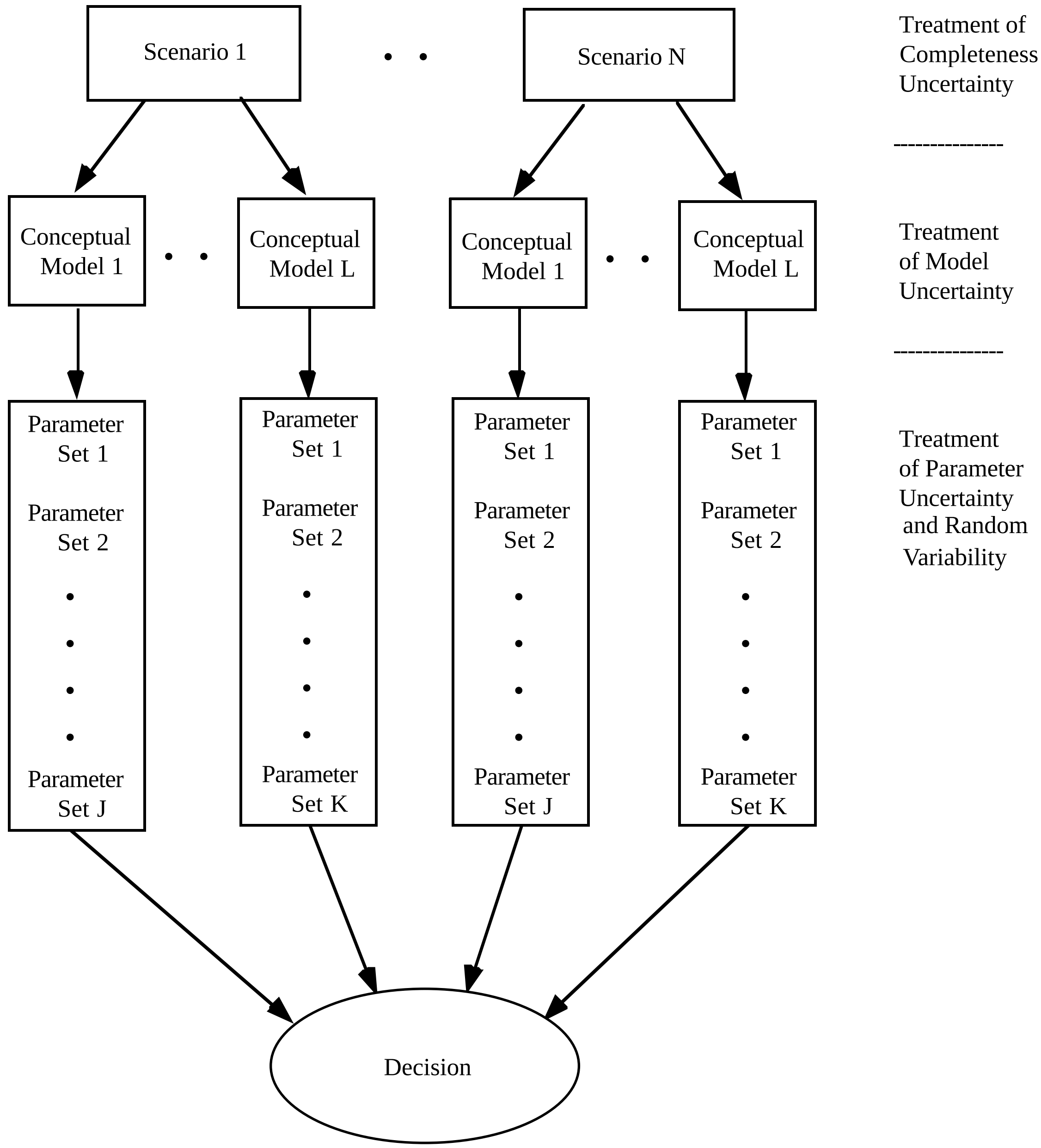


Figure 5.2 An approach to uncertainty analysis for low-level waste performance assessment (after Kozak et al., 1993)

Temporal variability in precipitation is illustrated in Figure 5.3, a histogram of the (log of) daily precipitation at a southeast (U.S.) coastal plain location for 1949-1991. Only those days on which precipitation was measured are included in the histogram. (Data for 1949-70 were collected in hundredths of an inch. In 1971, data began to be collected in tenths of an inch, resulting in the spike at -0.6.) Also shown is a gaussian fit to the data (excluding the spike). Daily precipitation is approximately lognormally distributed with a mean value of 1.26 cm/day (on those days when precipitation occurred) and a standard deviation of 1.58 cm/day. The maximum daily precipitation at this site over this 43-year period was 21.5 cm.

In many humid environments, rainfall intensity can vary dramatically in time, a phenomenon that is not captured by the average daily precipitation. Short duration, high intensity rainfall events increase runoff and erosion. Long duration, low-intensity rainfall leads to greater infiltration. This additional variability may be important in estimating recharge and should not be discounted without careful consideration. Figure 5.4(A) is a histogram of the (log of) daily net infiltration for the southeast coastal plain site mentioned above. Recall that net infiltration is the difference between precipitation and water lost to runoff and ET. The net infiltration represented in Figure 5.4(A) was obtained by simulation using hourly averaged precipitation data. The net infiltration was also obtained using the same precipitation data but distributing each day's precipitation over the entire 24-hour period (daily averaging). The histogram of the resulting daily net infiltration is shown in Figure 5.4(B). It is clear that the distribution of precipitation can have a marked influence on the character of the temporal variability of net infiltration.

5.1.2 Soil

The inherent variability of natural geologic formations and soils can be quite large. This variability is reflected in the parameters describing flow in the unsaturated zone, namely:

- saturated hydraulic conductivity
- water retention parameters (α and n in the van Genuchten parameterization, for example)
- porosity.

Studies of soils data gathered from 42 U.S. states (Carsel and Parrish, 1988) and from exhaustive sampling of a single experimental plot (Rockhold et al., 1994) indicate that the saturated hydraulic conductivity has the greatest variability of these parameters, as measured by the coefficient of variation. The water retention parameter related to the air entry pressure (van Genuchten's α) also exhibits significant variability. The porosity and the water retention parameter related to the pore size distribution have the least amount of variability.

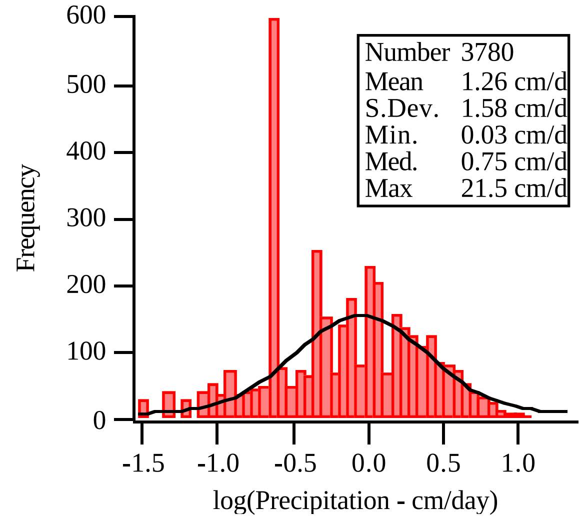


Figure 5.3 Histogram of daily precipitation data for a 43 year period

In addition to the parameters listed above, variability in unsaturated flow may be enhanced by:

- macropores (density, location, depth, size)
- unstable flow conditions.

Unfortunately, the variability of these phenomena is difficult to characterize. Nevertheless, these phenomena can have a

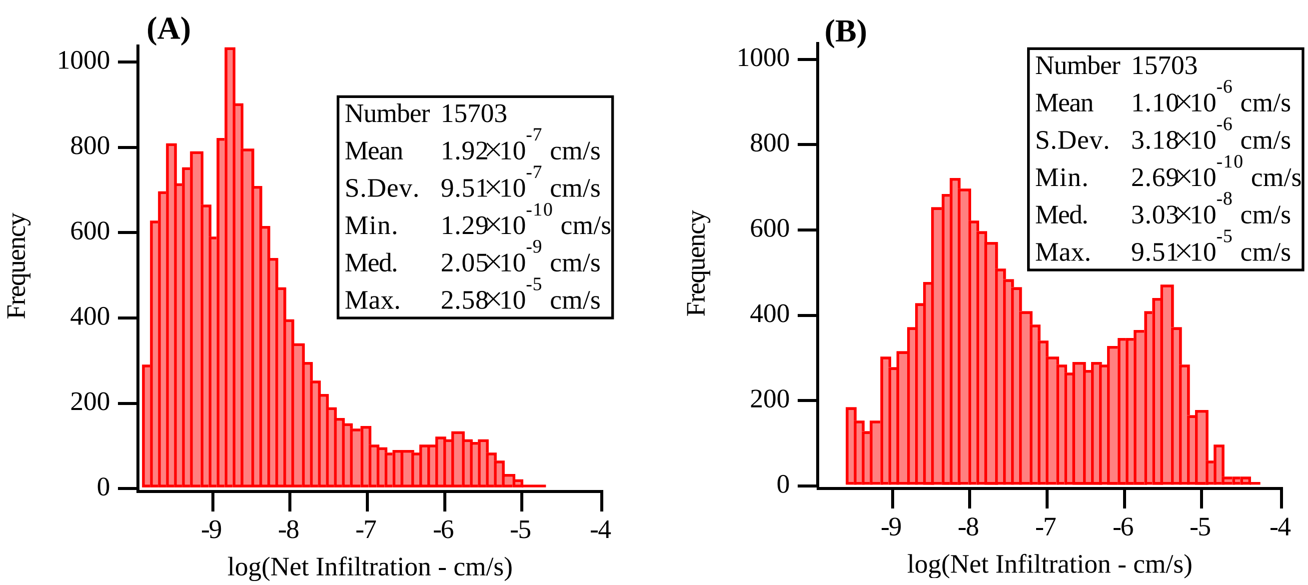


Figure 5.4 Histograms of simulated daily net infiltration for a 43 year period based on (A) hourly averaged precipitation and (B) daily averaged precipitation

dramatic effect on unsaturated flow and they should not be dismissed without consideration. Macropore flow is particularly important since it is likely to exist to some extent at the majority of LLW sites.

As an example of soil variability, Figure 5.5 shows a histogram of saturated hydraulic conductivities, K_s, for soils at the Las Cruces Trench Site in New Mexico (Wierenga et al, 1989). The data in Figure 5.5 represent a 25-m-long by 6-m deep, two-dimensional cross section of the sandy loam soil at the Las Cruces site. Note that the values of K_s shown in Figure 5.5 vary by more than three orders of magnitude and are log-normally distributed. This range of variability and probability-distribution type are typical for K_s in soils (Nielsen et al., 1973; Carsel and Parrish, 1988; Wierenga et al., 1989).

The probability density functions describing the statistical distributions of water retention parameters and other physical properties may or may not be well represented by normal or log-normal distributions. Hydraulic properties may also be cross-correlated with one another. Cross-correlation between parameters may have a significant effect on flow and should not be dismissed without consideration.

The inherent variability of physical and hydraulic properties is usually not entirely random but is more often spatially correlated. Values of measured properties that are close together in space are usually more similar than those measured farther apart. For example, Jacobson (1990) used

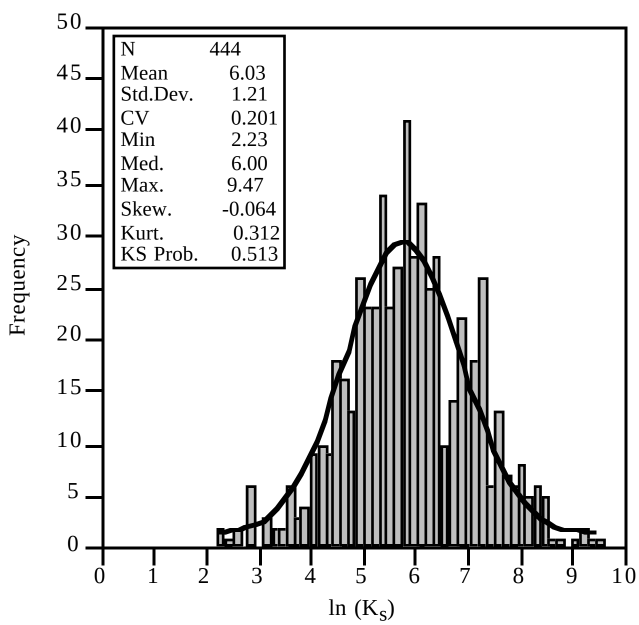


Figure 5.5 Histogram and probability density function for log-transformed values of in situ measurements of K_s from the Las Cruces Trench Site

directional semivariograms, γ, to analyze the spatial continuity of the log-transformed values of K_s shown in Figure 5.5. Using a two-dimensional, exponential semivariogram model, autocorrelation lengths of 2.5 and 0.5 m were estimated for the horizontal and vertical directions, respectively (Jacobson, 1990). The sample and theoretical semivariograms determined from this analysis are depicted in Figure 5.6. Isaaks and Srivastava (1989) provide an excellent description of different methods for quantifying spatial variability and structure.

If site-specific data are limited, a developer may be tempted to use literature-derived values of soil hydraulic properties that represent texturally-similar soils to simulate water movement at a proposed LLW disposal facility. Kool et al. (1990) simulated a field-scale, infiltration experiment conducted in spatially variable, unsaturated soil at the Las Cruces Trench Site in New Mexico (Wierenga et al., 1989) using hydraulic properties determined from site-specific data and properties obtained from the literature for a texturally similar soil (Carsel and Parrish, 1988). A spatial moment analysis was used to provide quantitative comparisons between the observed and simulated flow and transport behavior. Poor matches between the observed and simulated flow and transport behavior were obtained using literature-derived values of the van Genuchten model water retention parameters and K_s for a texturally-similar soil. The results of Kool et al. (1990) suggest that the use of literature-derived model parameters leads to predictions of infiltration and recharge that are more uncertain than predictions made using model parameters derived from site-specific data. This additional parameter uncertainty suggests that site-specific data are preferred for performance assessments of LLW disposal facilities.

5.1.3 Vegetation

Natural communities of vegetation are typically spatially heterogeneous. A LLW disposal facility, however, is likely to have a fairly homogeneous plant community, particularly during the period of institutional control. When active control of the facility ends, the plant community will evolve and become more heterogeneous. The spatial variability in ET resulting from a heterogeneous plant community is difficult to predict. The effect of this spatial variability on the average amount of net infiltration at the site is likely to be small, however.

Consideration of the temporal variability of vegetation is of greater importance in an uncertainty analysis than spatial variability. Previous discussions (Sections 2.2.3 and 3.2.1) have emphasized the dramatic effect that vegetation can have on the water balance and the effectiveness of an engineered cover system. Temporal variability in vegetation must be considered in an uncertainty analysis simply because a plant community on a LLW disposal facility will

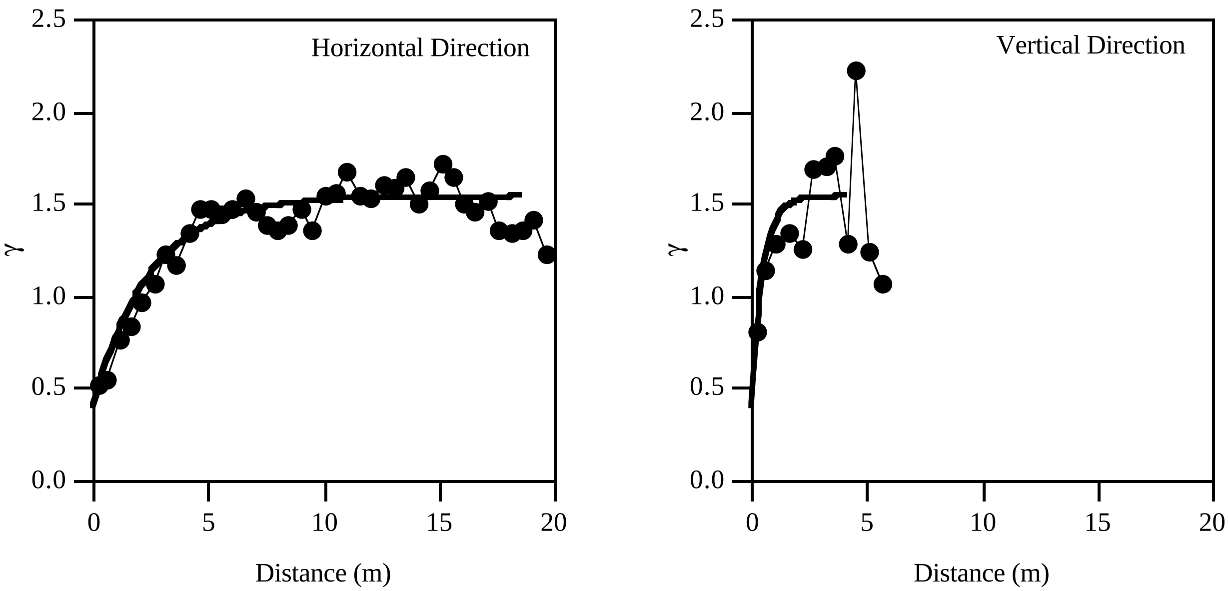


Figure 5.6 Exponential semivariograms determined from log-transformed, in situ measurements of K_s at the Las Cruces Trench Site (after Jacobson, 1990)

change over time, either through natural succession or through catastrophic events such as fires and large storms. Since changes in a plant community are difficult to predict, they should be considered using a bounding method and sensitivity analysis (see Sections 5.2.2 and 5.2.3).

5.1.4 Engineered Barriers

The long-term performance of engineered barriers is uncertain due to a number of causes (see Chapter 3), including:

- construction defects – punctures, faulty seams, etc. in geomembranes and geosynthetic clay liners; poor compaction of clay barriers; hydraulic conductivity variation in capillary barriers
- long-term aging and degradation – clogging of drainage layers; root penetration and desiccation of clay barriers; increased permeability of synthetic barriers; cracking of concrete vaults; differential settlement.

Engineering judgement and sensitivity analysis (see Section 5.2.3) can be used to estimate the relative importance of each of these processes. For those processes judged to be of greatest importance, their potential variability (spatial or temporal) can be characterized using literature-derived values (e.g., the geomembrane defect frequency data of Gilbert and Tang [1993]) and pilot studies (e.g., a construction test pad utilizing sealed double-ring infiltrometers to estimate the spatial variability in hydraulic conductivity of a clay barrier).

Literature reviews and pilot studies can provide bounds and probability distributions for parameters. In addition, such data can provide information about spatial and/or temporal autocorrelation and cross-correlation between parameters. In general, however, some amount of random variability in engineered components (as well as climate, soil, and vegetation) will remain no matter how much data are collected.

Engineered (and natural) components of a LLW disposal facility that are nonuniform and heterogeneous are often modeled as being uniform and homogeneous, or one-dimensional rather than multidimensional, to reduce the complexity and computational requirements of the analysis or simply because of insufficient data. Such simplifications may be necessary in some cases for practical reasons but can introduce additional uncertainty into estimates of water flow.

For example, GCLs can be evaluated in the laboratory to determine certain characteristics of the intact GCL such as permeability. However, the degradation of GCLs and other engineered components of a disposal facility over time may alter their permeability and water retention characteristics. The uncertainty associated with material degradation rates (or cracking) and the resulting changes in hydraulic properties adds uncertainty to long-term predictions of the effectiveness of engineered barriers.

5.2 Methods of Analysis

Numerous methods are available for analyzing uncertainty in performance assessment applications (Buxton, 1989;

Zimmerman et al., 1990; Zimmerman et al., 1991; Wu et al., 1991; Kozak et al., 1993; Robinson and Grinrod, 1994). For the purpose of evaluating water movement at a LLW disposal facility, we will focus on three primary methods:

- Monte Carlo simulation
- the bounding approach
- sensitivity analysis.

Several alternative approaches are also discussed.

Most methods of uncertainty analysis are not mutually exclusive. The type(s) of uncertainty analysis that is appropriate is usually determined by the complexity of the problem and the available data. Wu et al. (1991) also considered expert (engineering) judgement to be an uncertainty evaluation method. We acknowledge the use of expert judgement as being essential to a credible and defensible performance assessment and suggest that it should always be used in conjunction with one or more of the other approaches described below.

5.2.1 Monte Carlo Simulation

Monte Carlo simulation is the most comprehensive method of uncertainty analysis discussed here. Input uncertainties are represented as probability density functions (pdf's), such as that shown in Figure 5.7(A). In this example, the parameter varies between one and four and is more likely to take on lower values. Each pdf is sampled a number of times; the sampled parameter values are used as input to analytical or numerical models of performance. Figure 5.7(B) is an example of an analytical model of performance (a quadratic function). Each sampled parameter value, when simulated in a model, produces a value of performance. The collection of simulated performance values defines a pdf of performance (Figure 5.7(C)) that is used to estimate the average performance and the uncertainty in performance predictions. The approach described here and illustrated in Figure 5.7 for a single input parameter is easily generalized to complex models with multiple uncertain parameters, each described by its own pdf.

A number of methods for sampling parameter pdf's are available. Random sampling selects parameter values at random from the input pdf. This results in a large number of samples where the parameter value is most likely (1.25-2.0 in Figure 5.7(A)) and very few samples where the parameter value is unlikely (3.0-4.0 in Figure 5.7(A)). Stratified and Latin hypercube sampling (McKay et al., 1979; Iman and Shortencarier, 1984) ensure that all regions of the pdf are sampled. Importance sampling (Wu et al., 1991) is a type of stratified sampling where more samples are taken from the region of the input parameter pdf deemed most important (e.g., values corresponding to poor performance: 2.0-4.0 in Figure 5.7(B)). Kozak et al. (1993) recommend that parameter uncertainty analysis be addressed using a Monte Carlo simulation approach coupled with Latin hypercube sampling. Wu et al. (1991) caution, however, that latin hypercube sampling has not been shown to produce unbiased estimates or to be superior to stratified sampling when the input variables have a complex dependency structure. They recommend the use of stratified and importance sampling.

In general, Monte Carlo simulation may be computationally impractical, depending on the complexity of the models used, because it requires many simulations (or realizations) to ensure that the pdfs of input parameters and the pdf(s) of performance measure(s) are adequately described. Latin hypercube sampling, stratified, and importance sampling schemes can reduce the required number of simulations.

Even with improved sampling schemes, however, practical use of Monte Carlo simulation for evaluating uncertainty associated with the predicted performance of a LLW disposal facility may be limited to simplified analytical or steady-state solutions, and/or one-dimensional models, because of the large computational effort required to solve

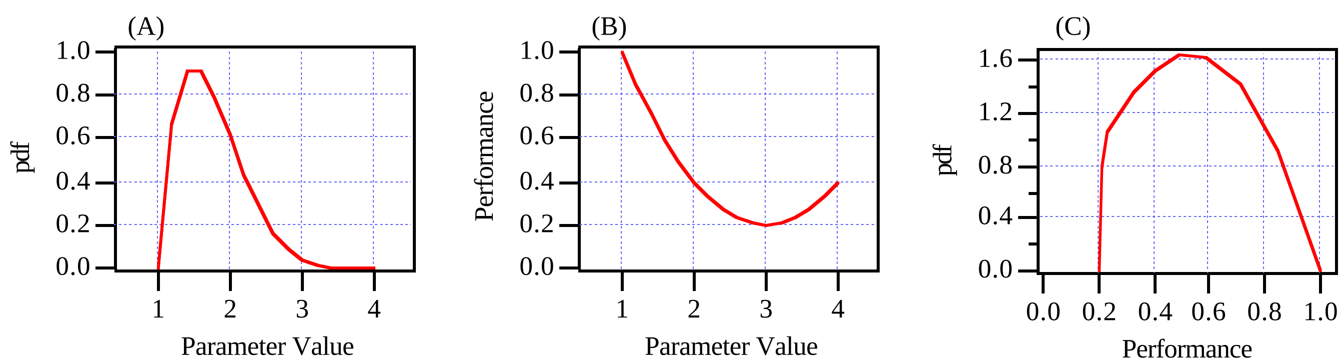


Figure 5.7 Hypothetical estimates of LLW disposal facility performance for different values of a model input parameter (pdf = probability density function)

the nonlinear, transient form of the governing equation (i.e., the Richards equation).

The efficacy of Monte Carlo simulation is also dictated by the quantity and quality of available data. Having sufficient data to accurately estimate the parameters in the probability density functions for the model input parameters will likely be a major problem for most LLW disposal facilities. Therefore, in order to use Monte Carlo simulation, a developer may be forced to make assumptions about model parameter distributions, or to rely on, for example, surrogate data or parameters for texturally similar soils. As noted previously, the use of literature-derived values of soil hydraulic properties, rather than site-specific properties for deterministic simulation is likely to result in inaccurate model predictions. However, when applied in a probabilistic framework, this approach may yield more reasonable results.

Given the fact that most performance assessment applications will be data-limited, it is useful to have other sources of data, parameters, and procedures that can be used to estimate model parameters from other related data. Van Genuchten et al. (1992) describe numerous indirect methods for estimating the hydraulic properties of unsaturated soils. Leij et al. (1994) also recently published a preliminary version of a soil hydraulic property data base that represents a compilation of hydraulic property data for soils from all over the world. The procedures described by van Genuchten et al. (1992) and the database of Leij et al. (1994) could conceivably be used to estimate parameter distributions for texturally similar soils if site-specific data are limited. Estimation of model parameters using indirect, related data and data from texturally similar soils can be used to establish reasonable bounds on the parameter space and measures of central tendency if this information cannot be reliably estimated from limited site-specific data. However, we will continue to emphasize that parameters estimated using site-specific data should be preferred over literature-derived values.

5.2.2 The Bounding Approach

Because of limited data, it is often not possible to specify the complete pdf and spatial correlation (see Figures 5.5 and 5.6) for all input variables. It is generally possible, however, to establish certain bounds on the input variables using a combination of the available data, theoretical considerations, and expert judgement. The estimated parameter bounds can then be used to bracket the expected performance of the LLW disposal facility.

If only sparse or generic data are available, it may be necessary to estimate the bounds as the minimum and maximum parameter values that are physically possible, or that have been measured for similar conditions. The extreme values used with this bounding approach can be modified later to reflect site-specific data as site characterization progresses and more information becomes available.

Although the bounding approach is probably the simplest approach that can be used to evaluate uncertainty, it has several drawbacks. The object of the method is to bound some measure of performance. Unfortunately, the minimum and maximum values of performance are not likely to correspond to minimum and maximum parameter values. This is illustrated in Figure 5.7(B) for the case of a single parameter. The minimum performance occurs at a value of 3 although the parameter bounds are 1 and 4. In the typical case, the performance measure(s) will be a complex function of several parameters, making it unlikely that simulations carried out for extreme parameter values will produce the bounding values of performance. Many additional simulations will need to be carried out for intermediate parameter values. In this case, the bounding approach loses some of its computational advantage over Monte Carlo simulation.

The bounding approach also does not provide any information about how probable any particular estimate of performance is. As discussed previously, Figure 5.7(A) illustrates a possible pdf for a parameter that is more likely to be near its minimum than its maximum value. This parameter pdf, when combined with the performance function depicted in Figure 5.7(B), results in a pdf of performance that looks like that in Figure 5.7(C). It is clear that the probability of performance is nonuniform; although two-thirds of the parameter range (2-4) results in a value of performance less than 0.4, the probability that the performance is less than 0.4 is only about 25%. This information would not arise from a bounding analysis.

If a bounding approach is used, it is recommended that some measure of the central tendency of the parameter distributions (i.e., the mean or median value) also be evaluated. The first order approximation of the mean performance is found by evaluating the performance measure at the mean parameter value(s). It is well known, however, that the first order approximation is appropriate only when the performance measure is a (nearly) linear function of the parameters or when the variance of the parameters is small with respect to the mean performance (Ang and Tang, 1975). These conditions are often not satisfied for unsaturated flow problems.

5.2.3 Sensitivity Analysis

Several different types of sensitivity analyses can be applied for engineering design and performance assessment. Sensitivity analysis is a useful tool for identifying key design variables, processes, and model parameters that contribute the most to uncertainty. This information can be used to direct future data collection and analysis activities, to focus on those areas that have the greatest influence on the system.

5.2.3.1 Deterministic Sensitivity Analysis

In a deterministic analysis, first-order sensitivity coefficients can be computed to quantify the effects of input parameter variability and the relative importance of different input parameters on a model output or performance measure (McCuen, 1973). The sensitivity coefficient, S_i, for a given performance measure, Z, can be determined by

$$S_i = \frac{\partial Z}{\partial X_i} \quad (5\text{-}1)$$

where X_i is a design variable or input parameter. (Examples of applicable performance measures were discussed in the introduction to this chapter.)

A perturbation approach can be used to calculate sensitivity coefficients with the following finite-difference approximation

$$S_i \cong \frac{Z_2 - Z_1}{X_{i2} - X_{i1}} \quad (5\text{-}2)$$

where the subscripts 1 and 2 correspond to negative and positive symmetrical perturbations, respectively, from an expected or baseline value. This approximation is only valid if S_i is approximately linear in the range of values considered. Therefore, the perturbations from the expected parameter values are usually (but not necessarily) taken to be relatively small.

Differences in the magnitudes of parameters can make direct comparison of sensitivity coefficients difficult. It is often more useful to compute normalized sensitivity coefficients, S_{ni}, as

$$S_{ni} = \left[\frac{\overline{X_i}}{F\left(\overline{X_i}\right)}\right]\left(\frac{\Delta Z}{\Delta X_i}\right) \quad (5\text{-}3)$$

where

$\overline{X_i}$ = is the initial or baseline value of the ith parameter and

$F\left(\overline{X_i}\right)$ = is the value of the performance measure when all parameters are equal to their baseline values.

If an input parameter is normally distributed, the mean value of the parameter should be used as the expected or baseline value. If a parameter is lognormally distributed, the median value is a more appropriate baseline value. The larger the value of the computed sensitivity or normalized sensitivity coefficient, the more sensitive the model output (or predicted performance measure) is to the particular parameter.

Deterministic sensitivity analysis has two potentially significant problems. First, the sensitivity of a model output may not be constant over the range of variability of a particular parameter. Second, the sensitivity of one parameter may not be independent of the value of another parameter. This second condition is an underlying assumption in the deterministic sensitivity analysis approach described above.

5.2.3.2 Probabilistic Sensitivity Analysis

As noted by Wu et al. (1991), for probabilistic performance assessment, probability/reliability sensitivity can be determined by measuring the change in probability/reliability relative to changes in the parameters representing the pdfs of the input variables (i.e., mean and standard deviation). The relative importance of the random variables can be evaluated by repeated probabilistic analysis in which one variable at a time is treated as a deterministic variable (with zero variance). This type of analysis results in a number of cumulative distribution functions (cdfs) or reliability curves that can be used to rank the relative importance of the input variables.

Wu et al. (1991) also discuss the extension of probabilistic sensitivity analyses to include all the major assumptions that are uncertain. These include such things as the types of probability distributions assumed for the input parameters (i.e., normal, lognormal, etc.), the process models (i.e., single-phase flow versus coupled, two-phase flow), and other empirical parameters (i.e., material degradation rates, etc.). In practice, Wu et al. (1991) recommend limiting probabilistic sensitivity analysis to only the most critical models and assumptions.

5.2.4 Other Uncertainty Analysis Methods

Several other methods are also available for evaluating uncertainty (Zimmerman et al., 1990; Wu et al., 1991, Robinson and Grinrod, 1994). Stochastic-perturbation and nested set/fuzzy logic methods are two alternative methods that may be well suited for evaluating the uncertainty associated with performance predictions. Brief descriptions of these methods are given below.

5.2.4.1 Stochastic-Perturbation Method

Early efforts at stochastic modeling of unsaturated flow are described by Dagan and Bresler (1979), Dagan and Bresler (1983), Yeh et al. (1985), and Mantoglou and Gelhar (1987), and others.

Polmann et al. (1988) summarize many of the early studies, and provide a detailed discussion of a stochastic-perturbation method developed by researchers at the Massachusetts Institute of Technology for modeling large-scale unsaturated flow and solute transport. This method extends the previous work of Mantoglou and Gelhar (1987).

The stochastic-perturbation method described by Mantoglou and Gelhar (1987) and Polmann et al. (1988) provides a way of deriving effective expressions for large-scale flow and transport processes in field soils. The theory presumes that local variations in hydraulic properties may be represented by spatially correlated random fields with known statistics (i.e., the mean and covariance). The effective parameters are propagated through a modified form of the Richards equation, using spectral representation techniques, to yield estimates of the mean flow behavior and the variances in pressure head and water content associated with small-scale fluctuations in the mean hydraulic properties. These variance estimates can be used to approximate the uncertainty associated with the predicted mean flow behavior. Complete details of the theory and numerical implementation are given by Polmann et al. (1988) and Polmann (1990).

Polmann et al. (1991) compared the results obtained using the stochastic-perturbation method with the results from a numerical experiment described by Ababou (1988). Luis and McLaughlin (1992) compared results obtained using this method with data from an infiltration experiment conducted at the Las Cruces Trench Site. In both cases, the observed flow behavior was predicted reasonably well by the effective flow parameters, and most of the observed values of pressure head and water content were bounded by the ±2 standard deviation confidence intervals that were estimated using the stochastic approach.

Gelhar et al. (1994) suggest that approximate expressions for the variance of small-scale fluctuations in travel time or solute concentration could be derived from a version of the stochastic theory. The resulting variances obtained using this type of analysis would not be as informative as the complete pdfs obtained by Monte Carlo simulation. Gelhar et al. (1994) suggest, however, that their variance estimates could provide some indication of the margin of error for a given application. At present, the stochastic-perturbation approach described above is limited to research applications.

5.2.4.2 Nested Set/Fuzzy Logic Approaches

As noted previously, there are several difficulties or potential problems associated with probabilistic methods for evaluating uncertainty. An alternative approach, based on nested set analysis and fuzzy logic is described by Robinson and Grinrod (1994). This approach is particularly well suited for incorporating subjective uncertainties based on expert judgement.

In this approach, groups of experts (or stakeholders) are requested to categorize different scenarios, conceptual models, and/or parameter sets according to their level of confidence in each choice. The choices are categorized using natural language expressions (rather than probabilities) that might range, for example, from “fully supported” or “very possible” to “completely unsupported” or “highly unlikely”. Different categories, or nested sets, are developed between these extremes. For example, an intermediate category/nested set of values might be referred to as “marginally supported”. The number of nested sets can also be determined by considering the proportion of experts who consider that each particular choice is possibly correct. This approach corresponds to a “membership” in fuzzy set theory.

The categories, or nested sets, define ranges of possibilities and their relative importance or likelihood of occurrence. A nested set of consequences is calculated for each set of values/models within each category. Consequence intervals are established from the results obtained using choices that have membership equal to or higher than that interval.

A nested set approach portrays the combinations of subjective uncertainties that arise in most performance assessments in a way that matches the intuition and expectation of nontechnical stakeholders. Stochastic variability can still be analyzed using an objective, probabilistic or Monte Carlo simulation approach embedded within a nested set analysis. The output distribution functions obtained with such a combined approach can be partitioned according to the consequence intervals described above to communicate the potential risks more effectively to nontechnical stakeholders.

6 Application Examples

This chapter presents two examples of the hydrologic assessment of the unsaturated zone at LLW facilities. The intent of the examples is to illustrate the issues raised in the preceding chapters and to demonstrate a methodology for analysis. One significant aspect of the analysis that is not addressed in these examples is the manner in which the hydraulic properties of the soil and engineered materials will change over time as the result of degradation and aging. The hydrologic assessment described here can be repeated using degraded properties that are estimated using engineering judgement and the results of laboratory and prototype testing.

The first example presented in this chapter is of a below ground vault located in a humid environment. The second example looks at a shallow land burial facility located in an arid environment. The examples utilize actual site-specific data and realistic facility designs. The two examples illustrate the issues unique to humid and arid sites as well as the issues common to all LLW sites. Strategies for addressing the analytical difficulties arising in any complex performance assessment are demonstrated.

6.1 Humid Site Example

The humid site application example is for a hypothetical below ground vault LLW disposal facility constructed in the humid climate regime representative of the southeast U.S. The site exhibits a shallow regional water table and a relatively high annual average precipitation. The example uses climate data from South Carolina and a facility design provided by the U.S. NRC. This humid site example application has been documented previously in Meyer (1993) and Nichols and Meyer (1996)[1], and the technical information presented here has been drawn extensively from those sources.

6.1.1 Problem Definition

The objective is to estimate the steady-state water distribution within a hypothetical LLW facility barrier designed for a humid site. The problem is defined by the site at which the facility is located (its soil types, climate, topography, etc.) and the specific design of the facility itself. Each of these is discussed in the following sections. An overview of the approach used to fulfill the objective follows.

1. Nichols, W. E. and P. D. Meyer, "Multidimensional water flow in a low-level waste isolation barrier," to appear in *Ground Water*, July-August or September-October, 1996.

6.1.1.1 Site Description

The hypothetical waste disposal facility is located in an environment typical of the southeast U.S. coastal plain region. The 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 nearby National Oceanic and Atmospheric Administration stations. Mean annual precipitation is approximately 111 cm/yr. based on 43 years of data (1949-1991). Rainfall is slightly higher than average during the summer months and slightly lower than average during the fall as illustrated in Figure 6.1. Precipitation during the spring and summer months frequently occurs as localized, intense thunderstorms. Winter precipitation tends to occur over a broader area. The regional mean annual snowfall is approximately 3 cm.

The mean monthly measured pan evaporation, also shown in Figure 6.1, varies significantly with the seasons. Mean annual evaporation based on 26 years of data (1964-1989) is approximately 137 cm/year. If potential ET is approximately equal to measured pan evaporation, then based on monthly averages, there is a precipitation excess during the winter months and thus an opportunity for significant recharge at that time.

The mean monthly maximum temperature ranges from approximately 60°F to 90°F. The mean monthly minimum temperature ranges from approximately 35°F to 70°F. The regional mean annual snowfall is approximately 3 cm, and the regional depth of frost penetration is less than 25 cm.

6.1.1.2 Facility Design

The hypothetical LLW disposal facility consists of an array of below-ground concrete waste containment structures, each overlain by a multilayer cover (see Figure 6.2(A)). The cover is sloped to promote runoff, which is collected by a surface drainage system located between each of the concrete vaults. A cross-section through one of the concrete vault/cover combinations appears in Figure 6.2(B). The cover system over each concrete vault uses many of the components discussed in Chapter 3 and is depicted in Figure 6.3.

The surface layer's functions are to promote runoff and maximize ET (by promoting plant growth). The surface layer is composed of 61 cm of topsoil classified as a silty sand (ASTM D2487). The surface layer thickness provides protection against frost damage and water storage for plant growth. Native, relatively shallow-rooted grasses are the anticipated vegetation. The relatively steep slope of the surface layer (20%) will produce significant runoff; erosion is thus a concern. Application of the Universal Soil Loss Equa-

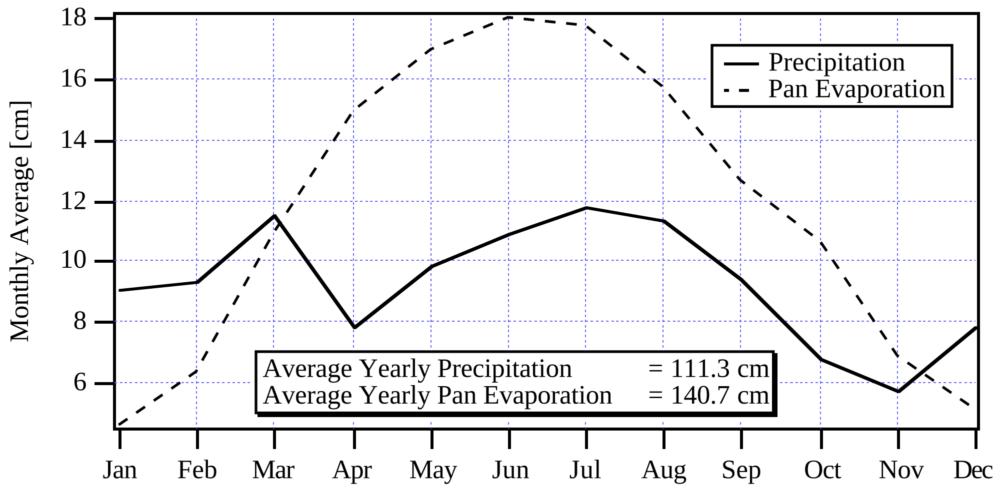


Figure 6.1 Average monthly precipitation and pan evaporation for the humid site application

tion (Wischmeier and Smith, 1965) suggests that soil loss from the surface layer due to water erosion is likely to be higher than 4.5 MT/ha/yr. (see Appendix A). Active erosion prevention measures could render a 20% slope acceptable. It is likely to be more cost-effective, however, to simply reduce the slope.

The facility uses filter and drainage layers composed of natural materials. The gravelly sand immediately beneath the topsoil functions as a filter layer to prevent small particles from entering the two layers beneath. The pea gravel and the underlying gravelly sand function as a drainage layer. This drainage layer directs water laterally to a point where the water enters the surface drainage system and is removed from the site.

The pea gravel is also intended to function as a protective layer, restricting root and animal penetration. The gravel layer is only 23 cm thick, however, and may provide little resistance to deep-rooted plants. Pea gravel is not likely to be large enough to be a significant barrier to burrowing animals. If protection against intrusion by plant roots and animals is of great concern, then evidence should be presented justifying the use of pea gravel as a barrier or a cobble layer should be used.

A redundant barrier system is used in this design consisting of a composite geomembrane/compacted soil barrier overlying a sand/gravel capillary barrier. Geomembrane/compacted soil composite barriers have been shown to be effective in limiting the seepage of water to very small values. The capillary barrier's function is to provide an additional barrier to water flow as the composite barrier degrades. The capillary barrier drains to a point beneath the concrete vault. Water can move from that point to the water table.

The concrete vault waste containment structure functions primarily to provide structural stability to the facility and to physically separate the waste. In addition, it acts as a barrier to water flow because of its low permeability. The top surface of the concrete vault is sloped at 2% to drain any water reaching it. The concrete is covered by bentonite panels whose primary purpose is to extend the life of the concrete as a water flow barrier.

There is no subsurface collection and removal system at this facility.

6.1.1.3 Overview of the Analysis

There are many processes and phenomena that could significantly affect water flow at the facility described above; precipitation, surface runoff, infiltration, ET, and subsurface lateral drainage are all important. At this facility, these processes are likely to exhibit significant temporal variability on the time scale of hours or even minutes. Snowmelt, nonisothermal processes, and vapor phase flow are not likely to have a major impact at this humid site. Long-term processes that will significantly affect flow are the degradation of the geomembrane/compacted soil barrier and of the concrete vault. These processes will take place over years or tens of years. Additional phenomena of unknown importance include macropore flow, soil spatial variability, anisotropy, and hysteresis.

The approach adopted for the analysis of unsaturated water flow at the humid site facility was to divide the problem into relatively independent pieces that could be analyzed separately. The problem was divided according to the time scale of the relevant transient processes. Above the composite geomembrane/compacted soil barrier, transient processes with temporal variability on the order of minutes, hours, and days will dominate the distribution of water. The analysis of this region must account for this transience. Below the composite barrier, the important transient processes occur on the scale of years or more. A steady-state analysis or a piecewise steady-state analysis is applicable in this region.

The illustrations of the site design (Figure 6.2) 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 composite barrier. The top four layers of the cover were thus modeled in one dimension. This simplification allows us to consider the short time-

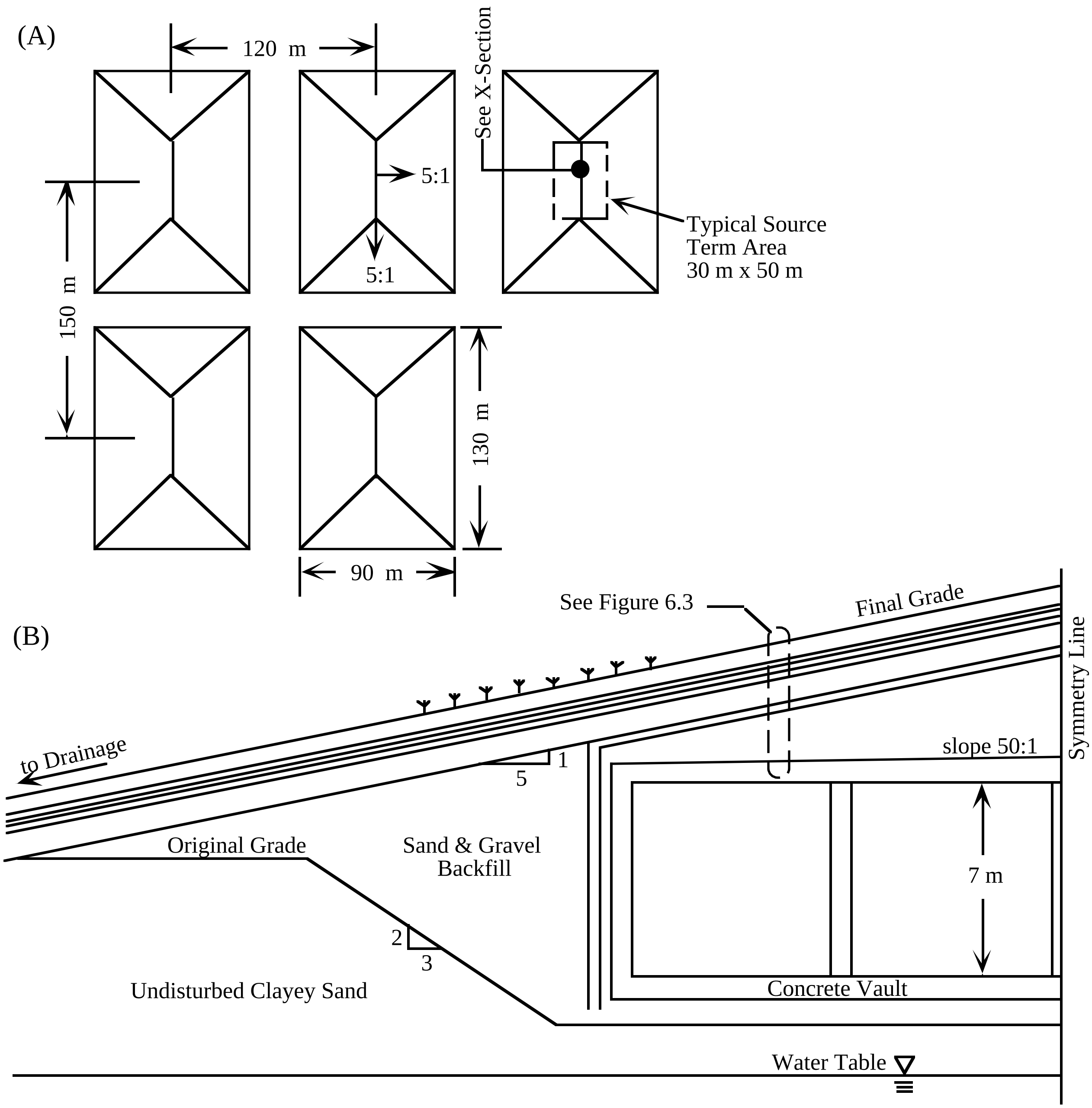


Figure 6.2 (A) Plan view and (B) cross-section of the hypothetical humid site facility

scale variability of the near-surface processes, a task that would be computationally difficult in two or three dimensions. This one-dimensional 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 results of the one-dimensional analysis were also used to determine the upper boundary condition of a two- and three-dimensional model of that portion of the facility below the composite barrier. This was a steady-state analysis. The multidimensional analysis addressed the design and performance of the capillary barrier and the ultimate flux (seepage) into the concrete vault.

6.1.2 One-Dimensional Analysis: Upper Cover

A number of simulation codes are applicable to the one-dimensional analysis of the humid site facility. We chose to use UNSAT-H (Fayer and Jones, 1990) and HELP (Schroeder et al., 1994a, 1994b). (See Chapter 4 for a brief description of these codes.) The results of these codes are discussed and compared in this section.

6.1.2.1 Climate and Vegetation Parameters

The physical processes modeled by UNSAT-H included precipitation, evaporation from the soil surface, infiltration, transpiration, and redistribution. Precipitation and ET inputs varied with time. Forty-three years of hourly precipitation data were used (see Section 6.1.1.1). These data are plotted as daily averaged precipitation in Figure 6.4(A). A histogram of this data was previously presented as Figure 5.3. Interception was assumed to be negligible.

ET can be calculated in UNSAT-H from either daily weather data or potential ET values that are input by the user. For the hypothetical site, daily potential ET values for each year of the 43-year simulation (1949-1991) were set equal to the average daily pan evaporation as measured over the period 1964-1989 (see Figure 6.1). Each year of the simulation

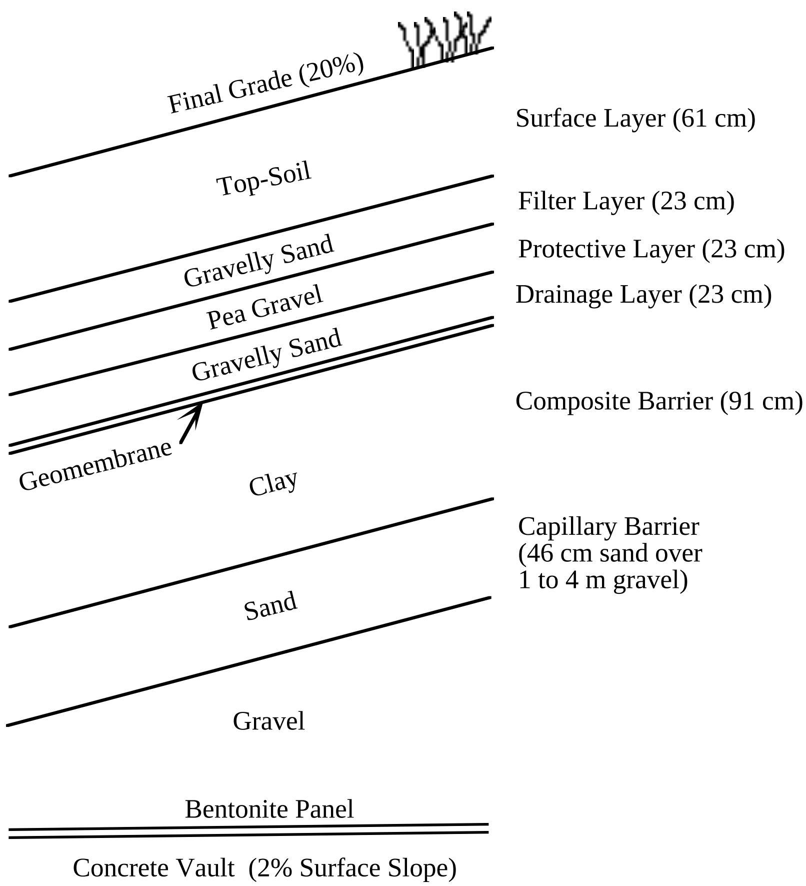


Figure 6.3 Details of the multilayer cover system for the humid site facility

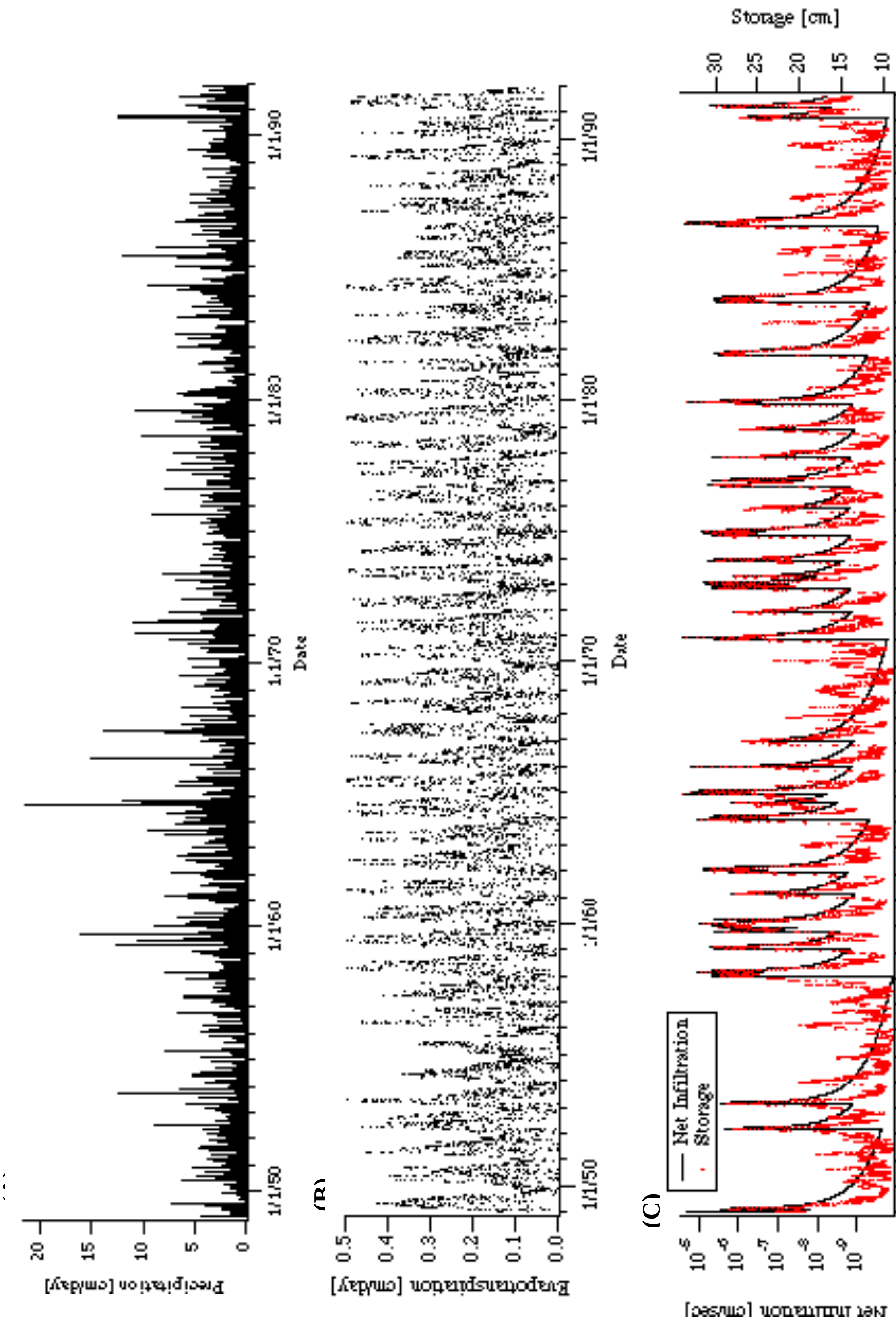


Figure 6.4 Daily water balance for the humid site facility over a 43-year period: (A) Precipitation data, (B) ET simulation results, and (C) Net infiltration and storage simulation results. Simulation results are from UNSAT-H.

thus used identical potential ET values (but different precipitation values) to calculate actual ET.

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 topsoil 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. Runoff is not allowed to infiltrate at a later time. This method may result in a greater amount of runoff than would occur under actual conditions, since vegetation slows the rate of overland flow and may allow water that runs off the upper slope to infiltrate farther downslope. In this case, UNSAT-H may underpredict the amount of net infiltration.

The transpiration component of ET (water uptake by plants) is represented in UNSAT-H as a sink at nodes within the root zone. The potential (maximum) transpiration is calculated as a fraction of potential ET and is a function of the leaf area index. The leaf area index used to model the hypothetical site varied over the year such that potential transpiration constituted 98% of potential ET during June, 95% of potential ET during July and August, and 100% of potential ET during the rest of the year (see Figure 6.5(A)).

UNSAT-H distributes potential transpiration 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 topsoil layer. Figure 6.5(B) shows the root length density function used.

Actual transpiration at each node will be less than the potential, depending on the node's volumetric water content, θ. Above $\theta=\theta_n$, plants cease to transpire because of anaerobic conditions. At very low water content, plants have difficulty drawing water from the soil. The point at which transpiration begins to be reduced is denoted as θ_d. The water content below which plants wilt and all transpiration ceases is denoted as θ_w. Representative values for θ_n, θ_d, and θ_w were chosen as 0.369, 0.115, and 0.113, respectively (corresponding to pressure heads of -30 cm; -10,000 cm; and -14,000 cm). Figure 6.5(C) illustrates the transpiration fraction as a function of the water content.

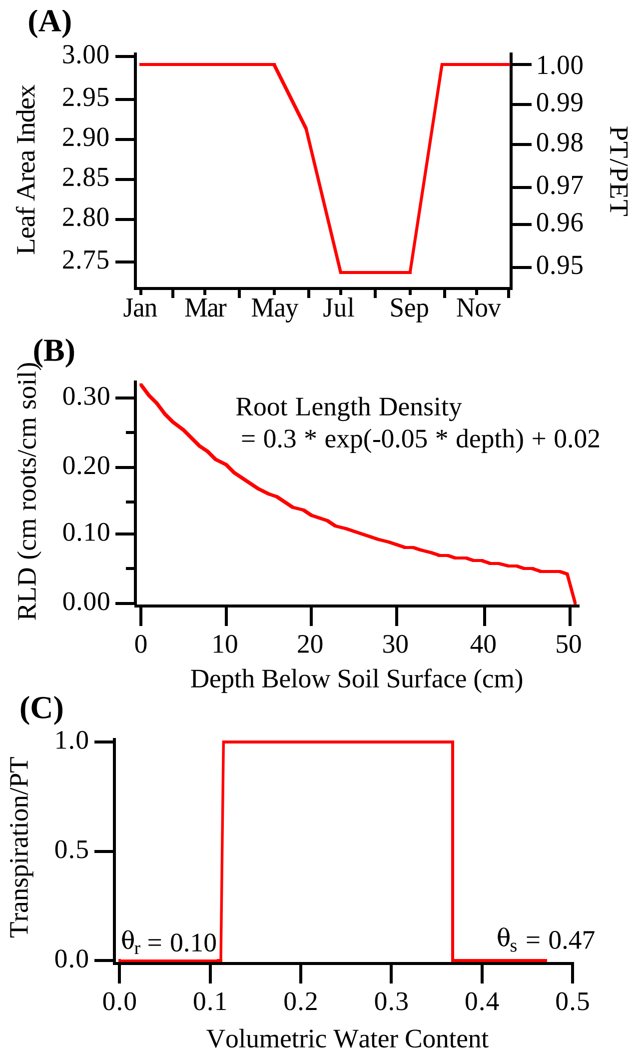


Figure 6.5 Plant relationships used in the UNSAT-H simulation (PT - potential transpiration; PET - potential ET)

6.1.2.2 Soil Parameters and Model Specification

The UNSAT-H code solves Richards equation for unsaturated flow (Equation 2-6) using the van Genuchten constitutive relationships (Equations 2-7 and 2-8). The parameter values required for the van Genuchten model are listed in Table 6.1 for each of the materials of the facility. Only the top four layers were simulated using UNSAT-H. The remainder of the materials are presented for completeness.

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 precipitation, 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 precipitation events. If the pressure fell below the minimum allowable value of -15.3 m, the surface node was held constant at this value. The

Table 6.1 Hydraulic parameters of the humid site facility materials

Material Name (refer to Figure 6.3)	Water Content		van Genuchten Parameters		Saturated Hydraulic Conductivity (cm/s)
	Residual	Saturated	α (cm^{-1})	n	
Topsoil	0.10	0.47	0.0440	1.523	1.00×10^{-4}
Upper Gravelly Sand	0.02	0.32	0.1008	2.922	1.00×10^{-2}
Pea Gravel	0.03	0.26	4.6950	2.572	1.00
Lower Gravelly Sand	0.02	0.34	0.1008	2.922	1.00×10^{-2}
Clay	0.0001	0.36	0.0016	1.203	1.00×10^{-7}
Sand (Capillary Barrier)	0.045	0.37	0.0683	2.080	3.00×10^{-2}
Gravel (Capillary Barrier)	0.014	0.51	3.5366	2.661	1.85
Concrete	0.08	0.40	0.0063	1.080	1.00×10^{-8}
Undisturbed Clayey Sand	0.21	0.30	0.0035	3.000	1.40×10^{-7}

bottom boundary was specified to have unit hydraulic head gradient.

6.1.2.3 UNSAT-H Simulation Results

Table 6.2 summarizes the results of the 43-year simulation of the upper four layers of the humid site facility. Results are given as the fraction of precipitation allocated to each term of the water balance over the entire 43-year period. Note, interception losses are assumed to be negligible and all evaporative losses occur from the soil surface after infiltration. The first column of data lists the water balance resulting from the use of hourly averaged precipitation. Almost one-third of the precipitation becomes runoff and only 5% is net infiltration.

ET represents the single largest sink of water at 62% of precipitation. Most of the ET is attributable to plant uptake; of the total predicted ET, approximately 88% occurs as transpiration. Figure 6.4(B) illustrates the daily ET as a function of time. The annual variation in ET is evident. The peak ET is relatively constant from year to year as a consequence of using the long-term average daily potential ET for each year (see Section 6.1.2.1). There is considerable day-to-day variability, however, as plant uptake responds to soil water conditions. Since the plant model parameters described in Section 6.1.2.1 were not based on site-specific data, the estimated ET is considered to be relatively uncertain.

Net infiltration tends to occur in short pulses over the 43-year simulation period. This is shown in Figure 6.4(C). Net infiltration increases rapidly over a very short period of time and then decreases more slowly. These pulses usually occur

Table 6.2 Simulated water balance at the humid site as a fraction of precipitation

	UNSAT-H		HELP
	Hourly Precipitation	Daily Precipitation	Daily Precipitation
Infiltration	0.675	0.944	0.901
Runoff	0.325	0.056	0.099
Δ Storage	-0.001	0.000	0.001
ET	0.621	0.633	0.732
Net Infiltration	0.054	0.312	0.168

early in the year when precipitation is relatively high and transpiration quite low. The peak flux of net infiltration varies and occasionally exceeds 10^{-5} cm/s. The histogram of the net infiltration was presented previously as Figure 5.4(A), which illustrates its highly skewed nature. There are several instances where the average daily net infiltration exceeds 10^{-6} cm/s for two weeks or more. For a calculation of the required subsurface lateral drainage capacity, this larger flux is more appropriate than the mean flux of 1.92×10^{-7} cm/s. Application of Equation 3-1 using a net infiltration rate of 5×10^{-6} cm/s and a length of 60 m yields a required subsurface lateral drainage flowrate of Q^{req} = 0.03 cm^2/s. The capacity flowrate of the lower gravelly sand alone is $Q^{cap} = (10^{-2}$ cm/s) (23 cm) (0.2) = 0.046 cm^2/s. Since the pea gravel will contribute to the lateral drainage during periods of high flow, the drainage layer appears adequate for this environment.

As Figure 6.4(C) shows, a pulse of net infiltration does not occur every year. For most of the simulation, including stretches of three to four years, the net infiltration is very small (< 10^{-8} cm/s). During such extended periods of low net infiltration, the compacted soil barrier would be susceptible to desiccation without the protection of the overlying geomembrane.

The humid site facility was also simulated using daily averaged precipitation. That is, each day's precipitation was distributed evenly over its 24 hours. The results of the 43-year simulation, with all other parameters the same as described above, are presented in the second column of Table 6.2. Using daily precipitation produces significantly more net infiltration and much less runoff. The amount of ET remains approximately the same. A histogram of the net infiltration from this simulation was shown in Figure 5.4(B). Net infiltration is still highly skewed, but significantly more days have a value greater than 10^{-6}.

The amount of ET predicted by UNSAT-H represents just 50% of the potential ET. Transpiration is limited by two factors. First, during rain events no transpiration (or evaporation) occurs. The results presented in Table 6.2 suggest, 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 θ_w, θ_d, and θ_n. Obtaining accurate values for the plant parameters is thus crucial to accurately predict ET with this type of model.

6.1.2.4 HELP Simulation Results

The 43-year simulation was also carried out using HELP Version 3.0. All parameters were selected to be as close as possible to the parameters of the UNSAT-H simulation. Field capacity and wilting point were calculated from the van Genuchten water retention function (Equation 2-7) evaluated at 340 and 15,300 cm (0.33 and 15 bars), respectively, using the parameters from Table 6.1. Runoff is calculated in HELP using the SCS curve-number method (USDA, SCS, 1985). A curve number of 85 was used here with a runoff length of 50 m. The evaporative zone depth was 50.8 cm, and the maximum leaf area index was 2.99. The growing season was 255 days. Temperature and other meteorological data were synthetically generated by HELP using data from Columbia, South Carolina. The precipitation data used were identical to the daily averaged data used in the UNSAT-H simulations.

Water balance results for the 43-year HELP simulation are presented in the third column of Table 6.2. They are qualitatively similar to the UNSAT-H results using daily averaged precipitation. HELP predicts somewhat higher ET and approximately one-half the net infiltration of the UNSAT-H daily precipitation simulation. In this example, the greatest discrepancy in the results of the two codes appears to be the time-scale over which precipitation is averaged. Knowing this, the HELP code, which is computationally faster, could be used to perform a more extensive uncertainty evaluation than would be possible with UNSAT-H. Very long-term simulations that might require an excessive amount of time using UNSAT-H may also be more feasible using HELP.

6.1.2.5 Uncertainty Evaluation

The results of the one-dimensional UNSAT-H and HELP simulations presented above provide an estimate of the long-term average net infiltration and illustrate how the net infiltration can be expected to vary over time. These results were obtained using a single set of plant and soil parameters. To illustrate the uncertainty in the water balance estimates presented in Table 6.2, a sensitivity analysis was carried out. The hydraulic parameters of the topsoil were varied in this case, although a similar analysis could be performed on the plant parameters. The UNSAT-H model with hourly precipitation was used in this sensitivity analysis.

The topsoil was chosen for this analysis simply because the hydraulic parameters of the topsoil will have a much greater influence on the water balance than the parameters of the underlying sand and gravel layer. As was previously discussed (see Section 5.1.2), of the parameters listed in Table 6.1 the saturated hydraulic conductivity K_S and the van Genuchten parameter α possess the greatest variability as measured by the coefficient of variation. Carsel and Parrish (1988) determined the variability of soils based on soil types. The parameters of the topsoil used here most closely matched the mean parameters of the silt loam data they examined. The coefficients of variation in their silt loam data were 2.751 for K_S and 0.647 for α. Carsel and Parrish (1988) also found that the best fit for the distribution of these parameters was lognormal in each case.

Table 6.3 Sensitivity of the simulated water balance at a humid site to the hydraulic parameters of the topsoil. Results are presented as a fraction of precipitation. Units of α are cm^{-1}. Units of K_S are cm/s.

	Infiltration	Runoff	Δ Storage	ET	Net Infiltration
Base Case: α=0.044, $K_S=10^{-4}$	0.675	0.325	-0.001	0.621	0.054
Case 1: α=0.044, $K_S=10^{-3}$	0.951	0.049	-0.001	0.833	0.119
Case 2: α=0.044, $K_S=10^{-5}$	0.235	0.765	-0.003	0.238	0.001
Case 3: α=0.018, $K_S=10^{-4}$	0.789	0.211	-0.003	0.761	0.030
Case 4: α=0.018, $K_S=10^{-3}$	0.978	0.022	-0.002	0.882	0.096
Case 5: α=0.018, $K_S=10^{-5}$	0.397	0.603	-0.003	0.399	0.001
Case 6: α=0.111, $K_S=10^{-4}$	0.552	0.448	0.000	0.299	0.254

The values used for the two parameters were the base case value (given in Table 6.1) plus or minus approximately 1.5 standard deviations (of the log-transformed parameter). The standard deviation for each parameter was based on the coefficients of variation given above. Appendix B describes the procedure used to arrive at the following values:

K_S = $\{10^{-5}, 10^{-4}, 10^{-3}\}$ cm/s

α = $\{0.018, 0.044, 0.111\}$ cm^{-1}.

The 43-year simulation described above was carried out using various combinations of these two parameters. The parameter combinations and the results of the simulations given in terms of the water balance are presented in Table 6.3 (including the base case for comparison). These results illustrate the relatively large differences in the predicted water balance that can result from moderate changes in the hydraulic parameters of the topsoil. The predicted net infiltration varied over two orders of magnitude from an inconsequential 0.1% of precipitation to more than 25%.

The results presented in Table 6.3 also illustrate the nonlinear nature of the problem. Comparing the base case to cases 1 and 2, it is clear that an increase in K_S from 10^{-5} to 10^{-4} cm/s results in a much larger increase in the net infiltration (54 times) than does an increase in K_S from 10^{-4} to 10^{-3} cm/s (2.2 times). The parameter α exhibits a similar relationship. An increase in α from 0.018 to 0.044 cm^{-1} results in an increase in net infiltration by a factor of 1.8 (compare the base case to case 3), while an increase in α from 0.044 to 0.111 cm^{-1} results in an increase in net infiltration by a factor of 4.7 (compare the base case to case 6).

A further consideration is the combined effect of parameters. Consider case 5, which results in a net infiltration of just 0.1% of precipitation. Increasing just α to 0.044 cm^{-1} (case 2) results in no increase in net infiltration. Increasing just K_S to 10^{-4} cm/s (case 3) increases net infiltration by a factor of 30. When both parameters are increased, however, the net infiltration is increased by a factor of 54 (base case). Thus if the bounding values of net infiltration are of interest, combinations of parameter values must be examined.

6.1.3 Multidimensional Analysis: Capillary Barrier

The one-dimensional simulation of the top four layers of the cover incorporated the transient processes of most importance at the site: precipitation and ET. These transient processes produce a transient net infiltration. The net infiltration exhibits less variability on a day-to-day basis than either precipitation or ET, however (see Figure 6.4). This temporal variability is expected to be even further attenuated by the passage of water through the clay barrier. The analysis presented in this section assumes that the fluctuations in net infiltration have little effect on the flow of water within and below the clay barrier. With this assumption in mind, the purpose of the multidimensional analysis was to estimate the performance of the capillary barrier and the steady-state flux (seepage) into the concrete vault.

The design of the capillary barrier will produce two-dimensional and perhaps three-dimensional water flow as the capillary barrier diverts water around the concrete vault. One of the questions that arises in this case is whether a two-dimensional analysis is sufficient. This question was answered by comparing the results of a three-dimensional simulation and an approximately equivalent two-dimensional simulation. Each simulation was carried out for a number of capillary barrier designs to provide some indication of the sensitivity of the results. The computer code used for these simulations was VAM3DCG (see Chapter 4).

6.1.3.1 Conceptualization

For the multidimensional analysis, we simplified the humid site facility design to a conceptual model that captured the three-dimensional geometry and salient features related to the capillary barrier and concrete vault. Our conceptual

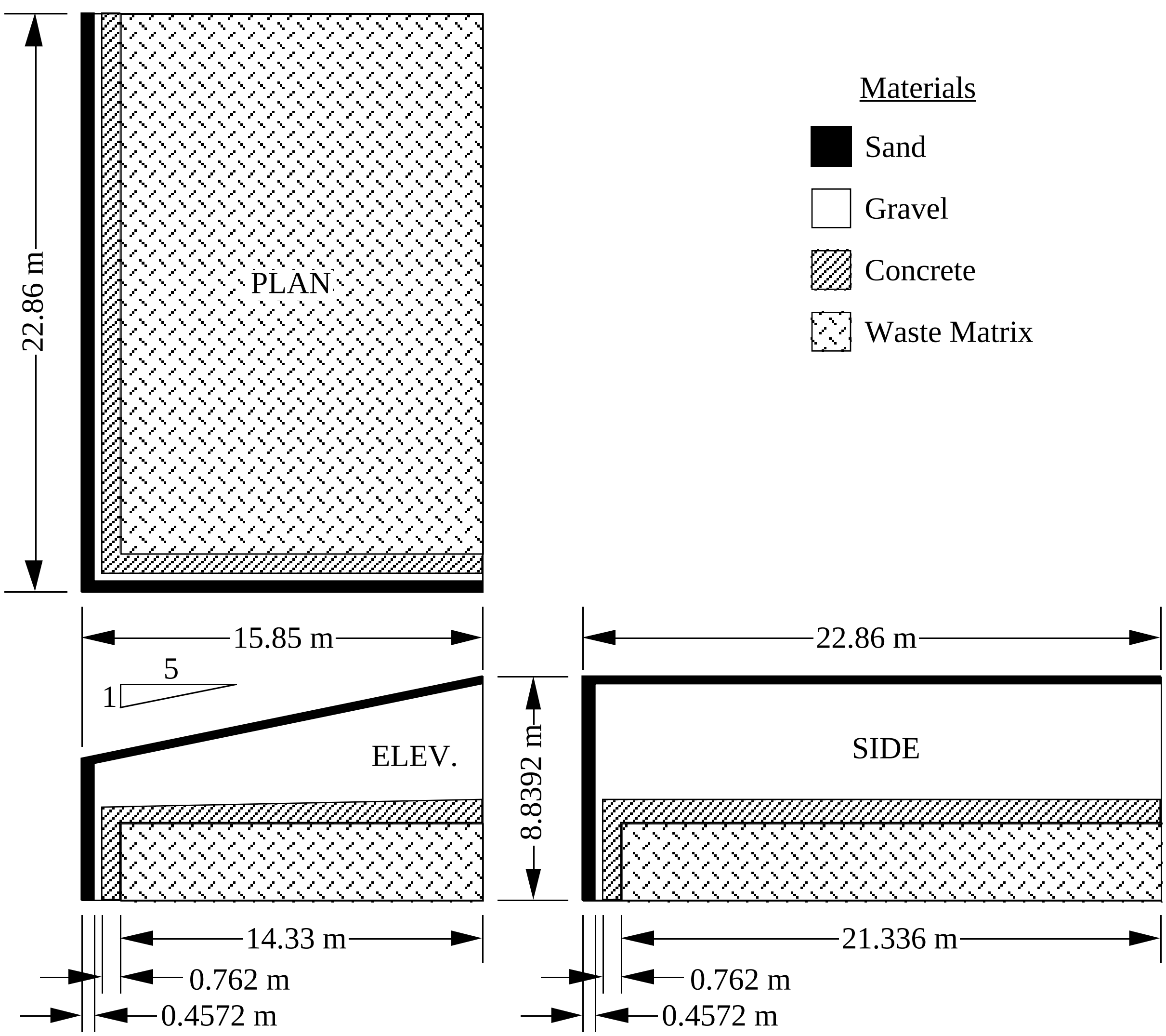


Figure 6.6 Elevation, plan, and side views of 1:5 slope configuration three-dimensional model.

model is illustrated in Figure 6.6, which depicts the elevation (XZ), plan (XY), and side (YZ) perspectives of one-quarter (from symmetry considerations) of a single vault in the facility (see Figure 6.2). Figure 6.6 also shows the arrangement of barrier soils and materials; note, the capillary barrier surrounds the concrete vault on the top and all sides, though it only slopes in the XY direction. Three-dimensional flow can occur because of the (cross-slope) capillary force induced by the presence of the sand on the sides of the vault.

6.1.3.2 Design Parameters and Uncertainty Evaluation

The two most important aspects of the capillary barrier design, from a hydrologic perspective, are the slope of the barrier and the hydraulic properties of its materials. Several values of these design parameters were simulated to estimate the sensitivity of the capillary barrier performance to its design. Three barrier slopes were considered: 20%, 10%, and 4% (1:5, 1:10, and 1:25). Elevation views for all three slope configurations are depicted in Figure 6.7, with the numerical grid discretization used in the VAM3DCG simulation superimposed on each.

Three sets of sand and gravel properties were also simulated. Following the nomenclature of Meyer (1993), we identify the first of these as a high quality control (HiQC)

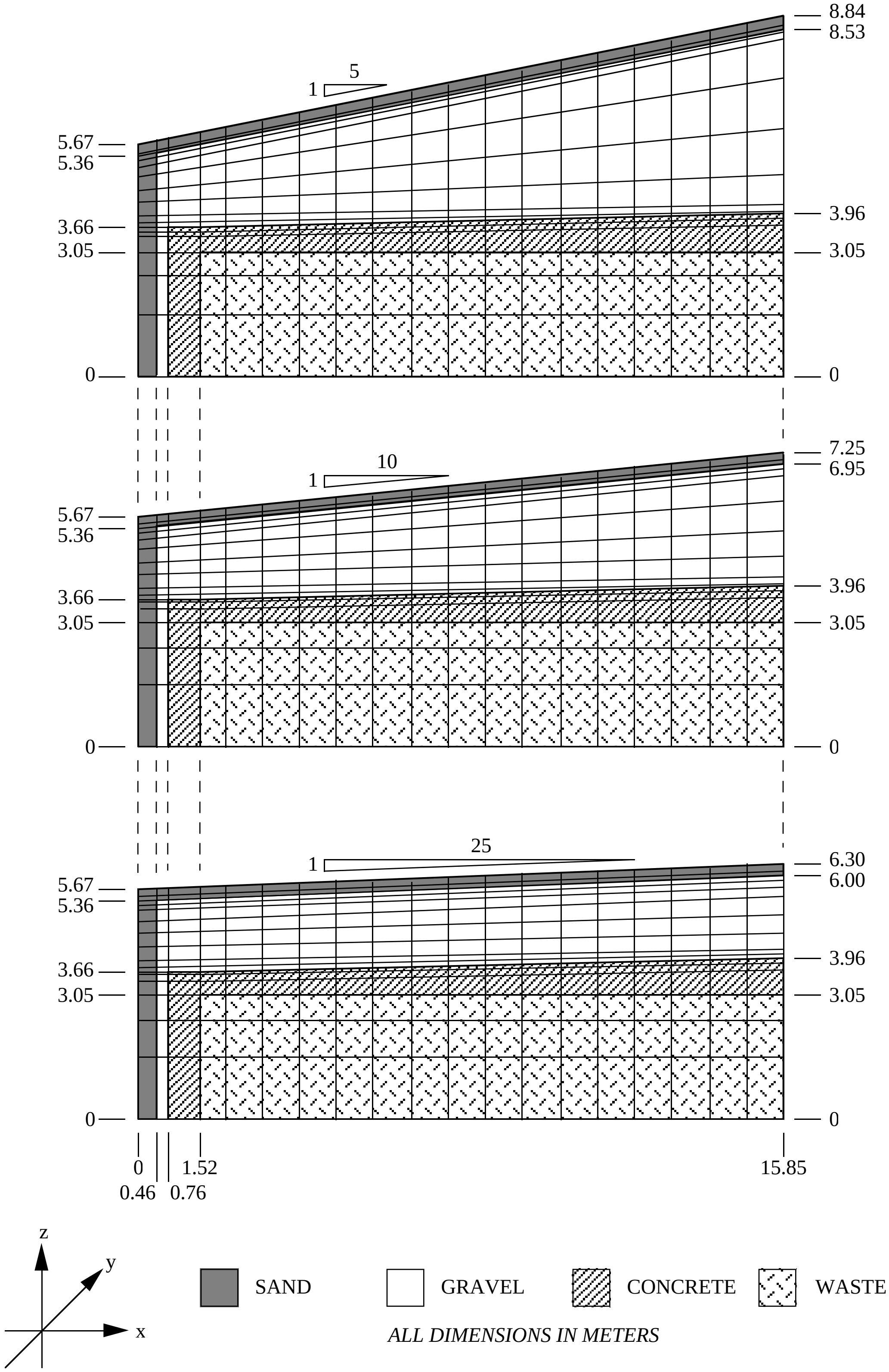


Figure 6.7 Elevation (XY) perspectives of the three-dimensional model for three capillary barrier slopes.

material property set that represents the base case design values for coarse sand and gravel (see Table 6.1). For a low quality control (LoQC) set, properties of silty sand were substituted for coarse sand, and properties of gravelly sand were substituted for gravel. The LoQC property set represents possible mixing between coarse and fine materials during cover construction and/or potential degradation with time resulting from migration of fine particles into the pore spaces of underlying coarse materials. A MidQC property set represents an intermediate condition.

Each slope configuration was combined with each set of material properties, which resulted in nine cases to simulate. To explore dimensionality effects, all nine cases were simulated in two- and in three-dimensions.

VAM3DCG solves a three-dimensional form of Equation 2-6. Van Genuchten's (1980) relationships between pressure head, water content, and unsaturated hydraulic conductivity (Equations 2-7 and 2-8) were used. The discretized grid included 304 elements for the two-dimensional simulations and 7904 elements for the three-dimensional simulations. The boundary conditions applied for the simulations included a lower boundary at saturation (atmospheric pressure), no flow conditions at all vertical faces (symmetry condition), and a constant input flux of 10^{-6} cm/s uniformly distributed over the upper boundary. Based on results presented in Chapter 3 (Tables 3.1, 3.4, and 3.5) and on the one-dimensional simulation results presented above, a flux of 10^{-6} cm/s through a composite geomembrane/compacted soil barrier would represent a severely degraded state of the barrier. This input flux thus provides a reasonably conservative test of the capillary barrier performance.

The values of the hydraulic parameters for the materials of the capillary barrier are listed in Table 6.4. (The HiQC parameters were previously listed in Table 6.1.) For convenience, we set the hydraulic parameters of the waste to those of the gravelly sand (drainage) layer specified in Table 6.1 (specific waste properties were unimportant because water did not infiltrate through the concrete in any of the simulations performed for this study). The water retention and hydraulic conductivity curves for the HiQC, MidQC, and LoQC sands and gravels are shown in Figure 6.8 (curves marked with an "S" distinguish sand from unmarked curves that represent gravel).

6.1.3.3 Dimensionality

The question of dimensionality is important from a computational standpoint. It is simpler and faster to model such a barrier design in two dimensions (in our case, the XZ, or elevation, cross sections shown in Figure 6.7). However, if water flow is three-dimensional, using a two-dimensional model may yield a significantly different prediction of barrier performance than would be obtained using a three-dimensional model. To test the importance of this effect for the hypothetical LLW design, we simulated the nine cases in both two and three dimensions. The two-dimensional model was actually a three-dimensional simulation with only one element in the Y-direction, whose Y-length was equal to the total Y-dimension of the three-dimensional model (22.86 m). This made flux predictions of the two-dimensional model directly comparable to those of the three-dimensional model. The two-dimensional model neglects the presence, and hence the effect, of the vertical columns of sand, gravel, and concrete that extend along the bottom of the plan view in Figure 6.6.

6.1.3.4 Multidimensional Simulation Results

The capillary barrier's function is to divert water downslope and around the waste vault. Figure 6.9 is a compound vector plot and grayscale image of elemental fluxes for the plane of computational elements just above the capillary barrier interface (XY plane 15) from the 1:5 slope and HiQC properties. This figure illustrates how water is diverted over the capillary barrier and downward around the concrete vault. The grayscale image shows the magnitude of downward vertical fluid velocities (light for low velocity over the capillary barrier, dark at the draining edges), while the superimposed vector plot depicts the relative magnitude of velocity

Table 6.4 Three sets of hydraulic parameters for the humid site capillary barrier materials

Material Name	Water Content Parameters		van Genuchten Parameters		Saturated Hydraulic Conductivity, K_s (cm/s)
	Residual, θ_r	Saturated, θ_s	α (1/cm)	n	
Sand (HiQC)	0.045	0.37	0.068	2.080	3.0×10^{-2}
Sand (MidQC)	0.098	0.35	0.044	1.523	3.0×10^{-2}
Sand (LoQC)	0.098	0.35	0.044	1.523	1.0×10^{-4}
Gravel (HiQC)	0.014	0.51	3.537	2.661	1.85
Gravel (MidQC)	0.020	0.34	0.400	2.922	1.00
Gravel (LoQC)	0.020	0.34	0.101	2.922	1.0×10^{-2}

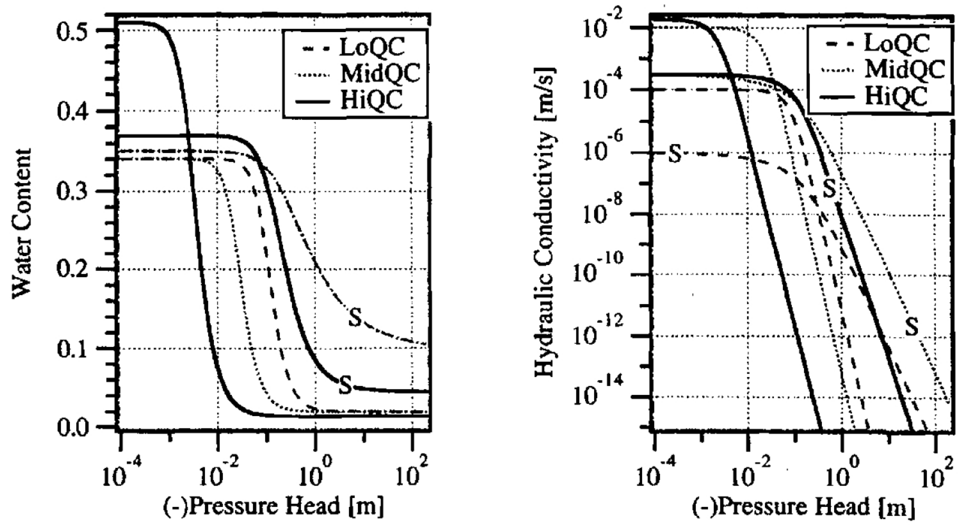


Figure 6.8 Water retention and hydraulic conductivity curves for Hi-, Mid-, and LoQC sand and gravel materials. Curves labeled with an "S" are sand, and the others are gravel (MidQC and LoQC water retention curves for sand coincide).

down and across the capillary barrier slope. Because the barrier only slopes in the X-direction, any significant Y-direction velocity components are due to the capillary force of the sand "drain" (the vertical column of sand elements at the far left of the XZ views shown in Figure 6.7) in the third dimension. Significant Y-direction velocities only occurred within 5 m of the cross-slope drain in all simulations.

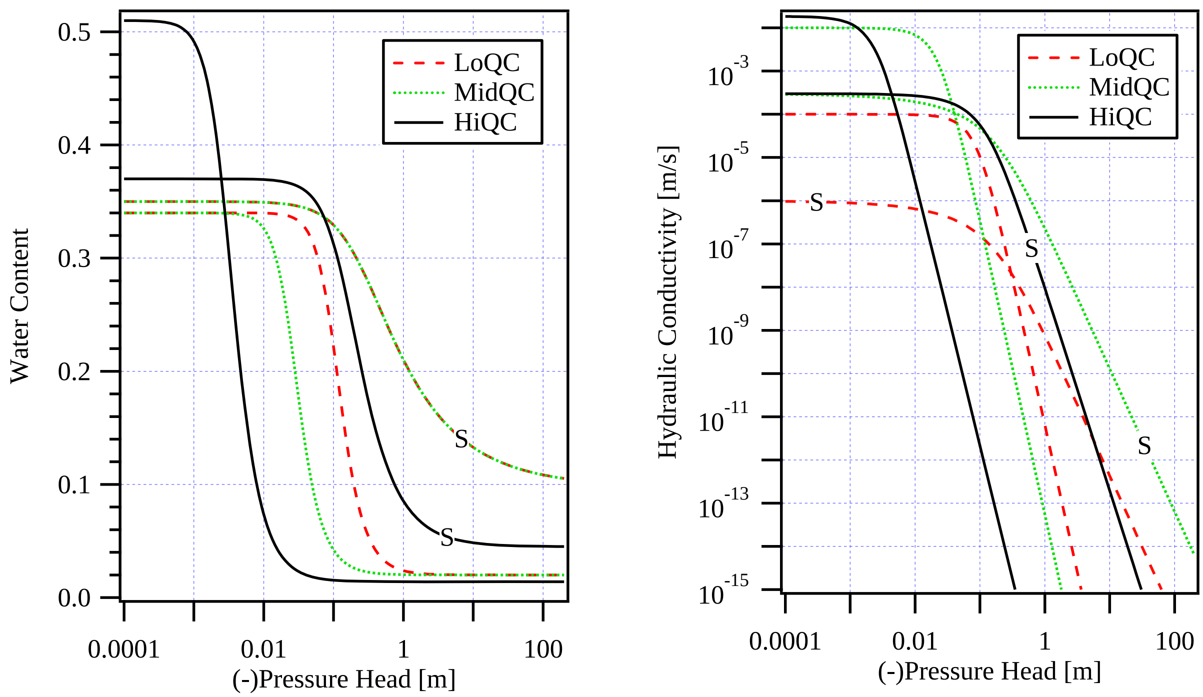
The effectiveness of a particular capillary barrier design can be measured by comparing the portion of water that crosses the barrier interface into the gravel (leakage) to the amount that flows through the upper conductive sand layer (lateral drainage). The results of the simulations for all parameter combinations are presented in Table 6.5. The results show that our simulations captured a range of barrier performances, from 100% effective cases in which all water is diverted around the waste vault (HiQC properties, any slope) to cases where the barrier is only about 5% effective (LoQC properties, any slope). Clearly, the material properties of the sand and gravel that compose the capillary barrier are much more important as a factor in barrier effectiveness than the slope of the capillary barrier. This does not imply that no slope is necessary in the design, rather that the degree of slope is not as critical as the properties of materials used to construct the barrier.

The importance of dimensionality is revealed by comparing the predictions of capillary barrier effectiveness obtained from the two- and three-dimensional simulations (Table 6.5). For HiQC properties, there were no differences because all HiQC simulations resulted in 100% effectiveness. For MidQC and LoQC materials, however, the estimate of leakage from the two-dimensional simulation was greater than the estimate produced by the three-dimensional simulation. In all cases the absolute difference in leakage was less than 8% (although relative differences for the MidQC materials were significant). Two-dimensional predictions in this case are conservative, since any acceptable result obtained with a two-dimensional model would only be made more acceptable by using a three-dimensional model.

6.1.4 Humid Site Conclusions

The humid site example of a hydrologic evaluation at a LLW disposal facility emphasized the analysis of the engineered components of the facility. 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 composite geomembrane/compacted soil barrier, and a capillary break. The hypothetical facility was located in a humid environment (southeast U.S. coastal plain) characterized by high annual rainfall and short duration, high-intensity precipitation events. Hourly precipitation data and daily pan evaporation data were used in the analysis.

The analysis was simplified by performing two complementary simulations. The first was a one-dimensional, transient simulation limited to that portion of the cover above the



0.5
0.4
0.3
0.2
0.1
0.0
Water Content
0.0001
0.01
1
100
(-)Pressure Head [m]
LoQC
MidQC
HiQC
S
S
10-3
10-5
10-7
10-9
10-11
10-13
10-15
Hydraulic Conductivity [m/s]
0.0001
0.01
1
100
(-)Pressure Head [m]
LoQC
MidQC
HiQC
S
S
S

Figure 6.8

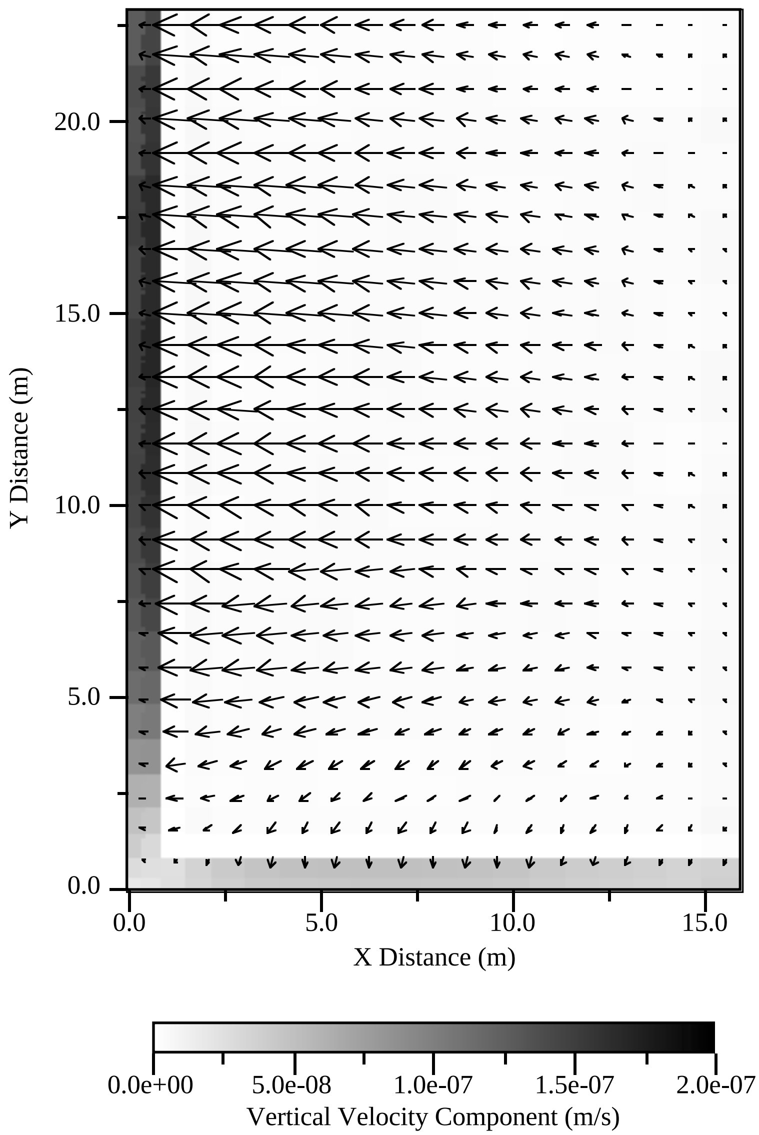


Figure 6.9 Velocity vector plot for three-dimensional model, 1:5 slope, HiQC materials in XY plane 15 (the plane immediately above the capillary barrier). The vectors depict the velocity components in the X and Y directions (parallel to the capillary barrier), while the grayscale raster image depicts the magnitude of the element vertical (Z-direction) velocity components.

geomembrane/compacted soil barrier. With this approach, near-surface processes such as precipitation and ET could be modeled at a relatively short time-scale (one hour). The temporal variability of precipitation has a strong influence in this humid environment on the flow of water through the upper layers of the cover. Below the composite barrier, however, temporal variability is less important; a steady-state analysis is appropriate. The geometry of the facility and the multidimensional flow it produces is of greater importance. The second part of the analysis was thus a three-dimensional, steady-state simulation limited to the capillary barrier and concrete vault.

The one-dimensional simulations illustrated the effect of averaging precipitation data. Using hourly averaged precipitation resulted in almost six times less net infiltration (and six times more runoff) than using daily averaged precipitation. This result has implications for the design of the surface layer (to prevent erosion), the surface drainage system, and the subsurface drainage layer. In addition, the amount and distribution in time of net infiltration will influence the

Table 6.5 Comparison of two- and three-dimensional simulations of capillary barrier performance for each of the barrier material properties and slopes

		Two-Dimensional Results		Three-Dimensional Results	
Material	**Slope**	**Subsurface Lateral Drainage** [m^3/s]	**Leakage** [m^3/s] (% of potential leakage)	**Subsurface Lateral Drainage** [m^3/s]	**Leakage** [m^3/s] (% of potential leakage)
HiQC	1:25	3.62×10^{-6}	-1.12×10^{-10} (0.0)	-3.62×10^{-6}	-5.09×10^{-11} (0.0)
	1:10	3.60×10^{-6}	-1.55×10^{-11} (0.0)	-3.60×10^{-6}	-9.00×10^{-12} (0.0)
	1:5	3.55×10^{-6}	-3.76×10^{-12} (0.0)	-3.55×10^{-6}	-2.87×10^{-12} (0.0)
MidQC	1:25	3.19×10^{-6}	-4.34×10^{-7} (12.0)	-3.45×10^{-6}	-1.69×10^{-7} (4.7)
	1:10	3.54×10^{-6}	-6.94×10^{-8} (1.9)	-3.58×10^{-6}	-2.24×10^{-8} (0.6)
	1:5	3.54×10^{-6}	-1.28×10^{-8} (0.4)	-3.55×10^{-6}	-4.14×10^{-9} (0.1)
LoQC	1:25	1.96×10^{-7}	-3.42×10^{-6} (94.6)	-3.64×10^{-7}	-3.26×10^{-6} (89.9)
	1:10	-2.08×10^{-7}	-3.40×10^{-6} (94.2)	-3.77×10^{-7}	$-3.23 \times 10–6$ (89.5)
	1:5	-2.29×10^{-7}	-3.32×10^{-6} (93.6)	-3.96×10^{-7}	-3.16×10^{-6} (88.8)

potential for desiccation of the compacted soil barrier. The simulation using hourly data showed that the net infiltration occurred in short pulses with up to four years of very little net infiltration between pulses. Finally, the estimate of net infiltration is important because it may be used as an upper bound for the water flux through the facility in the event that the barrier layers become completely degraded.

An evaluation of uncertainty showed that the hydraulic parameters of the topsoil had a marked influence on runoff, ET, and net infiltration. In this study, variations in the parameters K_S and α produced two orders of magnitude variation in net infiltration. The relationship between net infiltration and the hydraulic parameters was nonlinear. In addition, combined changes in the two parameters produced a greater effect than a change in either parameter alone. Both the nonlinearity and the combinatorial effect are important if the analysis is intended to bound the water flux through the facility.

The three-dimensional simulation assessed the performance of the capillary barrier. The assessment considered three capillary barrier slopes (1:5, 1:10, and 1:25) and three material property combinations for the sand and gravel of the capillary barrier. Simulations were carried out in two and three dimensions to explore the importance of dimensionality in predicting barrier effectiveness.

The hydraulic properties of the capillary barrier materials were shown to be the most important factor in terms of capillary barrier effectiveness in diverting water. The slope of the capillary barrier was only mildly important for the hypothetical waste disposal facility design we analyzed. Achieving design hydraulic properties in the as-built condition is therefore crucial to the success of the disposal facility.

These results were obtained for a numerical simulation under an assumption of stable slopes (no subsidence), which may not be true for actual waste site conditions.

The importance of dimensionality in evaluating a waste disposal facility design is, of course, strongly dependent on the design geometry. For the humid site design, several combinations of material properties and slope caused significant three-dimensional flow within 5 m of the corner of the vault. In terms of capillary barrier effectiveness, the three-dimensional estimate of leakage through the barrier was always less than the two-dimensional estimate. The difference, however, was never more that 8% (absolute) of the flux input at the top of the barrier. Two-dimensional modeling, in this case, produces a reasonable and conservative result.

6.2 Arid Site Example

Evaluation of net infiltration at LLW disposal facilities located in arid and semi-arid environments generally requires other considerations in addition to those that were addressed in the humid site example. The application example presented below represents a hypothetical facility located in an arid climate regime. The example uses climate data from Beatty, Nevada, soil hydraulic property data from a USGS study site near Beatty, and a disposal facility design appropriate for the extremely arid environment. The trench design consists of a backfill cover overlain by a vegetated soil layer. The cover does not utilize any geosynthetic materials. The arid site facility design also does not use a waste containment structure or a subsurface collection system.

6.2.1 Problem Definition

The objective is to estimate net infiltration and the flux of water below a backfilled trench. As with the humid site example, the problem is defined by the site at which the facility is located (its soil types, climate, topography, etc.), and the specific design of the facility. Each of these is discussed in the following sections.

6.2.1.1 Site Description

The hypothetical waste disposal facility is located in an arid environment typical of the southwestern U.S. Mojave Desert area. The topography in the region is characterized by long, broad valleys bounded by block-faulted mountains composed primarily of lower Paleozoic and Tertiary volcanic rocks. The hypothetical disposal facility is located in a relatively flat part of the valley, several kilometers away from the closest mountains. The valley sediments are coarse-textured gravelly sands and loams underlain by more than 170 m of alluvial fan, fluvial, and ephemeral lake deposits. The depth to the water table is approximately 85 m.

The climate is characterized by very hot, dry summers and mild winters. Climate data were obtained from weather stations operated by the U.S. Geological Survey (USGS) near Beatty, Nevada. Mean annual precipitation in the area varies from about 11.4 cm at Beatty (altitude 1,005 m), 17.4 km north of the hypothetical site, to 7.4 cm at Lathrop Wells (altitude 817 m), 30 km southeast of the site (Nichols, 1986). Thus, the mean annual precipitation is more than one-order-of-magnitude less than that at the hypothetical humid site described previously. About 70% of the precipitation falls during October through April. For the period 1949-79, the mean daily maximum temperature exceeded 32˚ C from June through September (Nichols, 1986). The mean daily maximum temperature in July is 37˚ C. Mean daily minimum temperatures fall below 0˚ C during December, January, and February, but snow is infrequent. Vegetation in the area is sparse; the dominant vegetation is creosote bush.

6.2.1.2 Facility Design

The hypothetical LLW disposal facility consists of several shallow (2 to 15 m deep), backfilled trenches similar to that depicted previously in Figure 3.2(B). For the purposes of this example, the hypothetical facility is represented as a 4-m-deep backfilled trench shown in Figure 6.10. This design does not use a geomembrane or an engineered waste containment structure. The coarse-textured nature of the sediments, and the fact that precipitation at the hypothetical arid site is very low and infrequent, suggests that runoff at the facility is negligible. Therefore, the slope of the surface soil is less than 2% and no surface drainage systems are used.

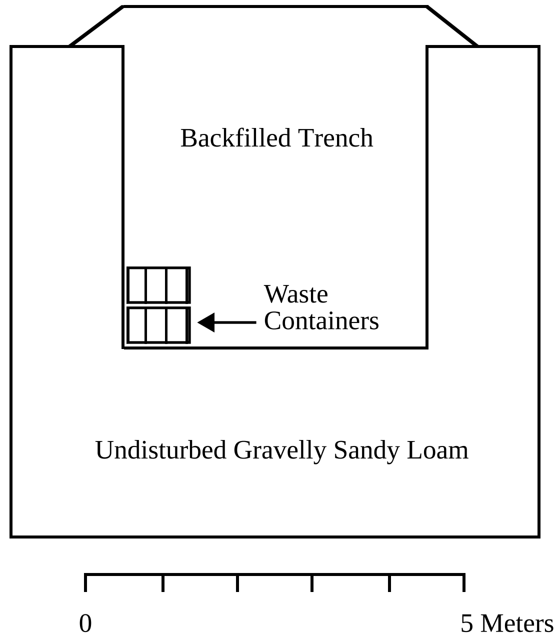


Figure 6.10 Cross-section of hypothetical arid-site LLW disposal facility

The trenches at the hypothetical facility are backfilled with common fill material obtained during excavation of the trenches. No capillary barriers or other barrier systems are employed. Vegetation is expected to reestablish itself naturally after closure of the facility.

6.2.1.3 Overview of the Analysis

As with the humid site example, there are many processes that could significantly affect water flow at the arid site disposal facility. Given the arid climate, coarse sediments, and topographic setting, processes such as snowmelt and runoff will probably be insignificant. However, nonisothermal processes and vapor phase flow are likely to have a very significant affect on water movement. Since no manufactured materials and no waste containment structure are used in the facility design, the long-term degradation of these materials is not of concern. The effects of soil spatial variability, preferential flow, anisotropy, and hysteresis in water retention characteristics are of unknown importance. Since nonisothermal processes, vapor phase flow, and water uptake by plants are likely to have a significant effect on water movement at the site, the analysis presented here will focus on evaluating the significance of these processes.

6.2.2 One-Dimensional Analysis

A one-dimensional model was chosen for this application because, except for the slightly sloped surface (which may generate runoff from an extreme precipitation event), there are no features of the trench design that create lateral flow. There are numerous computer codes that may be applicable to a one-dimensional analysis of the facility. Very few documented computer codes are available in the public domain, however, that account for water flow in both the liquid and vapor phases under nonisothermal conditions, compute surface energy balance using a mechanistic approach based on actual hourly or daily meteorological data, and account for water uptake by plants. An analysis of all of these components may be required to provide defensible estimates of deep drainage or recharge at LLW disposal sites located in arid or semi-arid environments. The UNSAT-H code (Fayer and Jones, 1990) was selected for this example because it has these capabilities. Although the HELP code cannot model nonisothermal processes or vapor-phase flow, it was also used in the arid site application. HELP was chosen because it is widely used and we felt its comparison to a more mechanistic model (UNSAT-H) at an arid site would illustrate a number of issues raised earlier in this report (e.g., see Section 4.3.1).

The governing equations in UNSAT-H are based on a modified form of the Richards equation for liquid water flow, Fick's law of diffusion for the isothermal or thermal flow of water vapor, Fourier's law of heat conduction, and the theory of coupled water and heat flow in soils proposed by Philip and de Vries (1957). UNSAT-H does not directly solve the coupled equations for two-phase (liquid water and water vapor) flow, but instead uses a modified form of the single-phase Richards equation that includes a vapor conductivity term. This approximation is valid as long as the air pressure in the soil-water system is not significantly different from atmospheric pressure. The modified water and heat flow equations are solved sequentially using an iterative numerical scheme. For brevity, the governing equations used in UNSAT-H are not included here. Complete details on the theory and numerical implementation of the governing equations are provided by Fayer and Jones (1990).

Several important issues should be considered when simulating water and heat flow in soils under dry, nonisothermal conditions. These issues are related primarily to the numerical approximations of the governing equations, and the constitutive relations used to represent relative permeability, saturation, and capillary pressure. These issues are discussed briefly below.

One of the issues that should be considered when evaluating water infiltration into dry soils that are typical of arid sites is the accuracy of the numerical methods used to solve the governing flow equation. Celia et al. (1990) demonstrated that conventional pressure-head-based numerical approximations of the Richards equation are not necessarily mass conservative, especially when simulating water infiltration into dry soils. They proposed a mixed-variable form of the Richards equation with a Picard iteration scheme, which they referred to as the modified-Picard iteration method. This formulation was shown to provide superior mass conservation relative to standard pressure-head based formulations when simulating water infiltration into dry soils. In order to avoid potential mass balance problems, a modified version of UNSAT-H (Version 3.0) that uses a mixed form of the Richards equation with modified-Picard iteration was used for the arid site example application presented here. Kirkland et al. (1992) have proposed several other numerical approximations for the Richards equation that are superior to standard pressure-head-based formulations in terms of both mass conservation and speed of execution.

Another issue that should be considered is the numerical scheme used to approximate the flow of water in the liquid and vapor phases under nonisothermal conditions. Experimental evidence suggests that Fick's law of diffusion may underpredict thermal water vapor flux by as much as a factor of two (Philip and DeVries 1957, Cass et al. 1984). It has been suggested that actual vapor diffusion in soils is greater than that predicted by Fick's law because the measured thermal gradient underestimates the actual thermal gradient within the air phase, and the latter would be a more appropriate value to use in Fick's law. An alternative explanation is that water vapor is effectively transported through the liquid phase by condensation and evaporation processes operating within individual pores. This would effectively increase the cross-sectional area available for vapor diffusion to a value larger than the air-filled porosity and would effectively decrease the tortuosity, or path length for diffusion. Philip and de Vries (1957) proposed adding an enhancement factor to the thermal vapor diffusion term in the governing equation used to describe the nonisothermal transport of water to account for these processes. This enhancement factor is a function of the temperature gradient and the soil water content, and typically ranges in value from 0 to 2 (Cass et al. 1984). Jury and Letey (1979) and Cary (1979) attempted to measure values of this enhancement factor, but generated somewhat contradictory results.

A thermal vapor diffusion enhancement factor is implemented in UNSAT-H. This enhancement factor was not used for the nonisothermal simulations that are reported here because no data were available from the Beatty Site for estimating the parameters that describe the functional relationship between the enhancement factor, soil water content, and the temperature gradient. It should be noted, however, that not including this thermal vapor diffusion enhancement factor should result in underpredicted evaporation rates, which would eventually lead to more water stored in the soil profile and higher predicted recharge rates. Thus, neglecting this thermal vapor diffusion enhancement factor should be conservative in terms of predicted recharge rates.

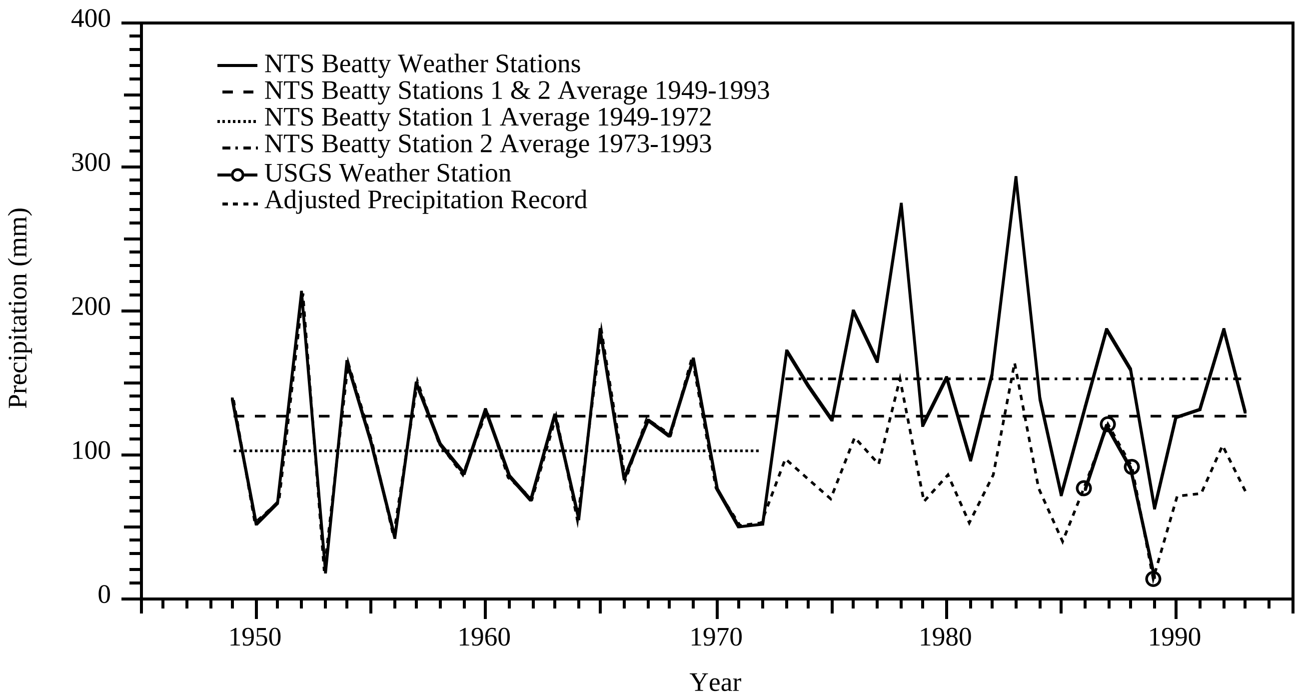


Figure 6.11 Yearly average precipitation data used for the arid site application

6.2.2.1 Climate Data

The USGS collects micrometeorological data from several locations near Beatty, Nevada. Hourly precipitation, air temperature, wind speed, and solar radiation data for 1986 through 1989 were obtained from USGS records (Wood and Fischer, 1991; Wood and Fischer, 1992; Wood et al., 1992; Wood and Andraski, 1992). These data were supplemented with a longer daily record of precipitation and air temperature data from two other weather stations near Beatty that are operated as part of a micrometeorological monitoring network for the Nevada Test Site (NTS). This longer daily weather record extends from mid-1948 through the present.

The NTS weather station near Beatty was moved to a higher elevation in December 1972. Consequently, the long-term average yearly precipitation recorded after 1972 is greater than that recorded up through 1972. The yearly average precipitation values recorded at the NTS and USGS weather stations are shown in Figure 6.11. The total precipitation recorded for 1986 through 1989 at the USGS weather station is approximately 56% of that recorded at the current NTS weather station. However, the trends in yearly average precipitation at the two sites are similar over this time period. Although the NTS and USGS weather stations are less than 20 km apart, the differences in observed precipitation at the sites are significant. Figure 6.11 illustrates the uncertainty in precipitation that can result from using data that represent different locations with slightly different elevations or topographic settings.

The precipitation data recorded after 1972 from the current NTS weather station were adjusted (i.e., reduced by 44%) to compensate for the apparent elevation-induced change in precipitation between the locations of the NTS and USGS weather stations in order to provide a more consistent, long-term record of precipitation for use in model simulations. The mean annual precipitation for the adjusted 45-year record is 9.54 cm.

Hourly data from the USGS station were used directly in 4-year model simulations for 1986 through 1989. These simulations examined the importance of using hourly precipitation data instead of daily averaged precipitation data. Simulations using the 45-year adjusted NTS precipitation record were also performed (see Section 6.2.2.8). These simulations examined the importance of nonisothermal processes and vapor-phase flow. Since no solar radiation or wind speed data were available from the longer-term daily NTS weather station records, daily average values of solar radiation and wind speed were computed from the hourly USGS observations for 1986 through 1989 and used as estimates of the daily solar radiation and wind speed for all other years in the 45-year model simulations.

As noted previously, one of the issues of concern when evaluating the performance of LLW disposal facilities in both arid and humid environments is their long-term performance. Since climate is the dominant variable controlling

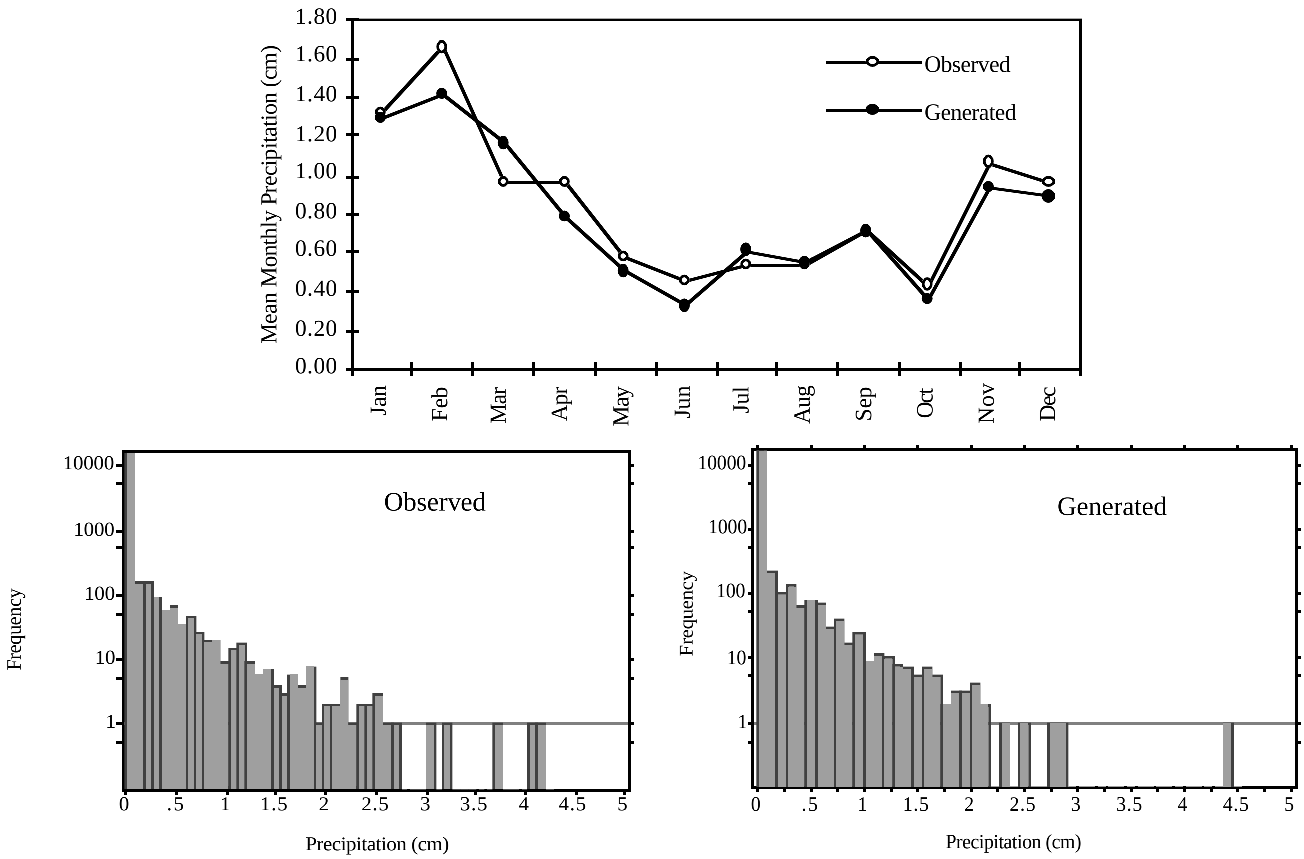


Figure 6.12 Monthly average precipitation (top) and histograms of daily precipitation for the arid site example (Observed: 45-year adjusted record; Generated: the first 45 years of WGEN simulated precipitation)

water flow and transport at LLW sites, it is of interest to generate longer-term climate data for use in simulation models to forecast this long-term performance. For this arid site application example, the WGEN code (Richardson, 1981; Richardson and Wright, 1984) was used in conjunction with the modified, 45-year record of data from USGS weather stations near Beatty to generate a stochastic realization of daily weather data for a 500-year period. 500-year simulations were then conducted with UNSAT-H and HELP using these synthetic weather data (see Section 6.2.2.9).

Monthly averages of the weather data generated using WGEN (precipitation, minimum and maximum temperatures, and solar radiation) matched the observed data reasonably well. Average monthly precipitation (observed and generated) for the initial 45-year period is shown in Figure 6.12. Since the WGEN code does not generate values of wind speed, daily average values of wind speed were computed from the 4 years of record obtained from the USGS study site near Beatty, and used for all 500 years in the model simulations.

6.2.2.2 Soil Hydraulic Properties

Two sources of data for the hydraulic properties of sediments in the vicinity of the hypothetical arid site were identified. Istok (1994) reported hydraulic property data representing sediment core samples collected from more than 140 locations on 183-m-long transects established along the exposed face of two excavations at a Radioactive Waste Management Site (RWMS) in Area 5 of the NTS. The RWMS is located approximately 60 km west of Beatty, just north of Mercury, Nevada. The 45-year simulations discussed in Section 6.2.2.8 used hydraulic properties determined using data from Istok et al. (1994). Andraski (1991) and Andraski (1996)[1] reported physical and hydraulic property data representing approximately 92 sediment samples collected from several boreholes and shallow excavations at a USGS study site near Beatty. The 500-year simulations discussed in Section 6.2.2.9 used hydraulic properties determined from the data reported by Andraski (1996).

1. Andraski, B. J., "Properties and variability of soil and trench fill at an arid waste-burial site," *Soil Sci. Soc. Am. J.* (in press), 1996.

The parent materials and sediment types at the RWMS and USGS Beatty site are similar, and the two sites are in relatively close proximity. However, the sediments near Beatty generally have a larger percentage of gravel and larger-sized particles. This difference can be attributed to different depositional environments. The RWMS is located on an alluvial fan in a closed topographic basin. Hence, the sediments are primarily alluvial deposits. Nichols (1986) suggested that the sediments near Beatty are largely fluvial deposits associated with the Amargosa River.

The hydraulic properties of the sediment samples from the RWMS were determined from whole sediment samples, including the gravel fraction, using standard methods (ASTM D2216, D2325, D2434). Therefore, no corrections for gravel were required for these data. The hydraulic properties of the sediments from the USGS study site were determined on the less-than-2-mm size fraction. Therefore, corrections were made to these data to account for the reduced cross-sectional area for flow and the lower porosity caused by the gravel and larger-sized particles (Andraski, 1996). Mehuys et al. (1975), Bouwer and Rice (1983), and Gardner (1986) describe procedures that can be used to correct the hydraulic properties determined on the less-than-2-mm size fraction to account for gravel.

Modeling water flow in arid and semi-arid environments requires an accurate representation of soil water retention characteristics near saturation and in the very dry range (>15,000 cm of tension). The dry range is usually less of a concern in humid environments or for agricultural applications where the soils are typically relatively wet. Rossi and Nimmo (1994) and Fayer and Simmons (1995) recently proposed modifications to the standard Brooks and Corey (1964) and van Genuchten (1980) water retention models that better approximate soil water retention behavior in the very dry range and still provide excellent fits to data in the wet range. The modified van Genuchten function proposed by Fayer and Simmons (1995) can also utilize previously determined parameters, thus allowing for the extended use of existing parameter sets. As an alternative to using the modified functions described above, the residual water content term in the standard van Genuchten or Brooks-Corey models can simply be set to zero, and the m parameter in the van Genuchten model can be fit, rather than relying on the usual assumption that m=1-1/n, in order to obtain better representations of water retention characteristics over the full range of water contents.

For this study, we used the Brooks-Corey water retention and the Burdine (1953) relative permeability models (Equations 2-9 to 2-12) to represent the sediment hydraulic properties. The water retention data for all of the samples collected from the USGS Beatty site are shown in Figure 6.13(A). (A plot of the RWMS data is similar but is not shown.) The water retention data were simultaneously fit with a common pore size distribution parameter, λ, using multiple linear regression by the method of dummy variables (Draper and Smith, 1981). Only the data representing less than -20 cm of pressure head were used (-60 cm for the RWMS data). The residual water content, θ_r, was assumed to be zero for each sample to ensure a reasonably good representation of water retention behavior at low water contents. The λ parameter in the Brooks-Corey model is equal to the slope of a straight line fit to the log(θ) versus log(h_m) data pairs. Evaluation of the Brooks-Corey model at θ_s using the fitted model parameters yields the air entry parameter, h_{me}. The saturated water content values, θ_s, were

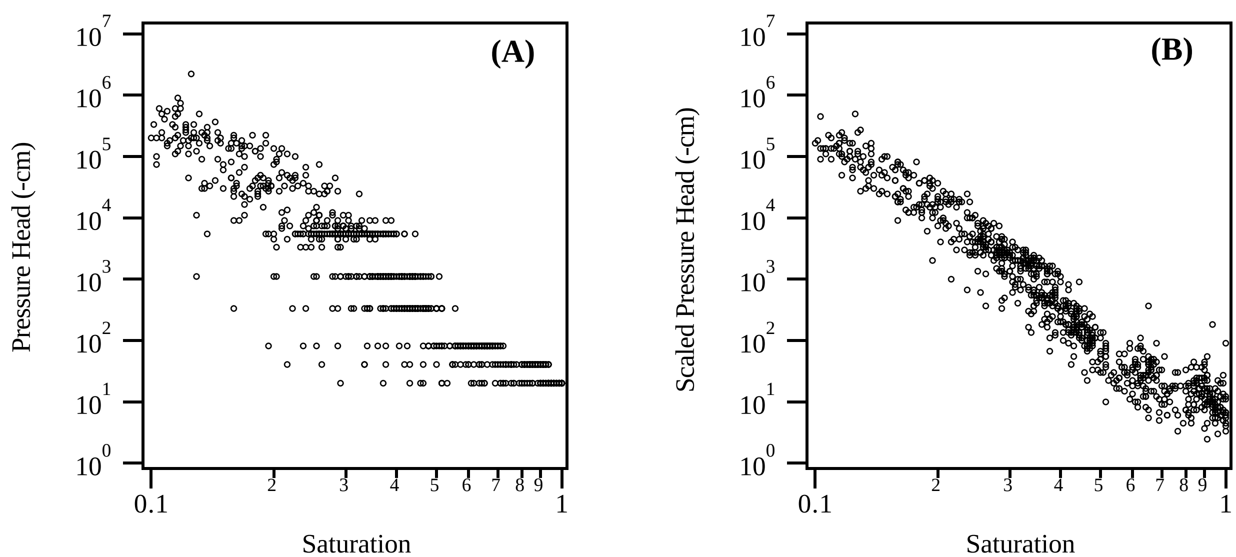


Figure 6.13 Pressure-saturation data from the Beatty Site used to estimate the Brooks-Corey model water retention parameters: (A) Unscaled data, (B) Scaled data

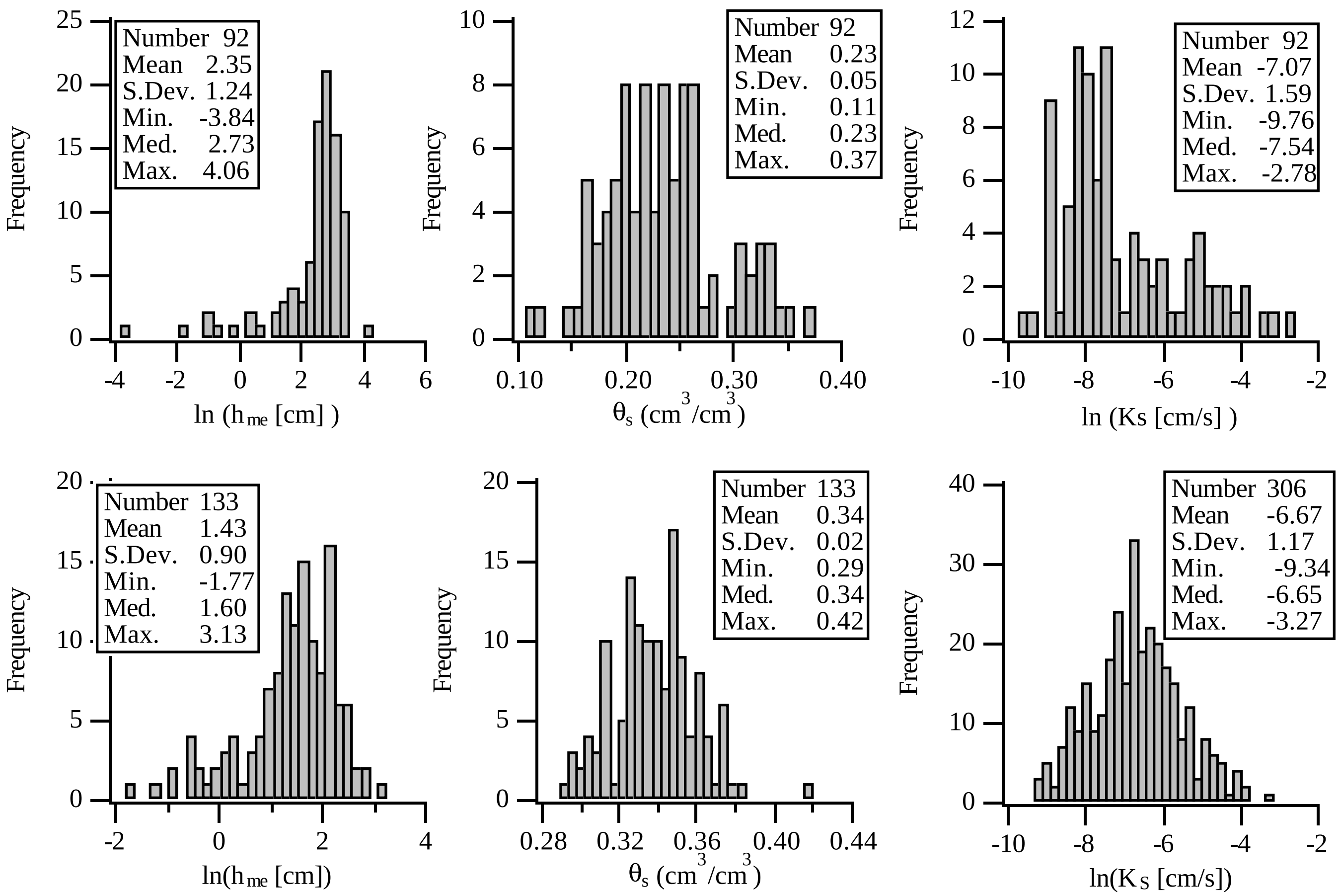


Figure 6.14 Histograms of the arid site soil hydraulic parameters derived from the USGS Beatty Site data (top) and the RWMS data (bottom)

assumed to be equal to the measured value of porosity for each sample.

Histograms of the log-transformed values of h_{me}, θ_s, and K_s are shown in Figure 6.14. (Beatty site data is across the top and RWMS data is across the bottom.) The parameter θ_s may be relatively well represented by a normal distribution. Note that θ_s at the Beatty site is significantly lower than at the RWMS. Although K_s at the RWMS appears to be log-normally distributed, K_s at the Beatty site and h_{me} at both sites are not well represented by either a normal or log-normal distribution. Transformations other than the log-normal may be applicable for h_{me} and K_s (Carsel and Parrish, 1988). Standard tests can be used to justify a particular statistical model (but were not used in this example).

Pressure-saturation data were scaled and fit with an average or scale-mean water retention curve. The unscaled and scaled pressure-saturation data for the USGS Beatty site are shown in Figure 6.13. For all simulations, the trench backfill material was assumed to be homogeneous and was represented using the fitted parameters for the scaled data (shown in Figure 6.13(B) for the Beatty site). The Brooks-Corey parameters derived from the Beatty site data and the RWMS data are listed in Table 6.6. The water retention and hydraulic conductivity relationships for the Beatty site data (used to represent the backfill material in the 500-year simulations) are depicted in Figure 6.15. (A corresponding figure

TABLE 6.6 Brooks-Corey parameters derived from the soil hydraulic data at the two arid sites

	Beatty Site	RWMS
θ_r	0.0	0.0
θ_s	0.232	0.34
h_{me} (cm^{-1})	14.768	4.95
λ	0.227	0.198
K_s (cm/s)	5.354×10^{-4}	1.294×10^{-3}

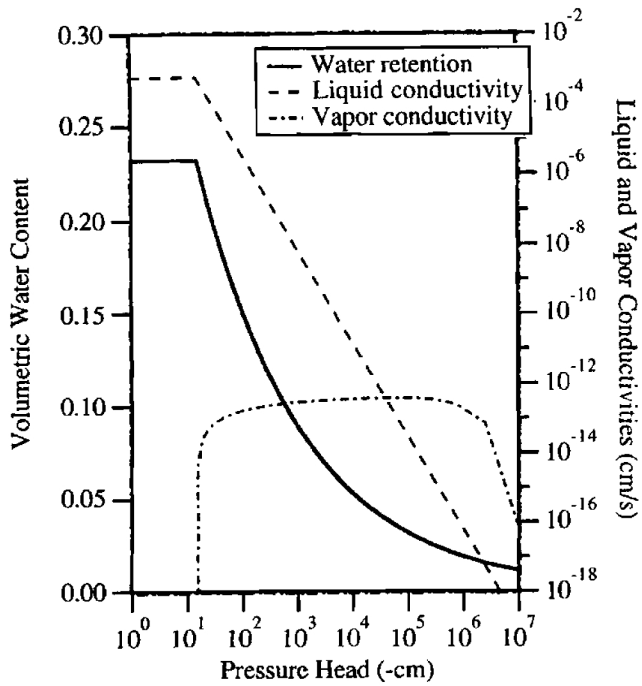


Figure 6.15 Water retention, liquid conductivity, and isothermal vapor conductivity (20°C) relationships for the backfill material estimated from Beatty site data

for the RWMS data, used to represent the backfill material in the 45-year simulations, is not shown.)

Driller's logs and neutron probe data indicate that the sediments underlying the trench are relatively heterogeneous. For the UNSAT-H simulations, these sediments were assumed to be scale-heterogeneous (Russo, 1991) and their hydraulic properties were estimated using the conditional simulation procedure described by Rockhold et al. (1994). This procedure for the conditional simulation of soil hydraulic properties has been tested using data from the Las Cruces Trench Site in New Mexico. Very good matches between the observed and simulated flow and transport behavior were obtained for the latest experiment conducted at that site using this method, without any model calibration (Rockhold et al. 1994). A brief summary of the conditional simulation procedure is given in Appendix C.

Soil hydraulic properties for the HELP simulations were homogeneous and are listed in Section 6.2.2.6.

6.2.2.3 Soil Thermal Properties

Two independent thermal properties are required for a quantitative description of heat transfer by conduction. These properties are the thermal conductivity and the heat capacity, which are functions of soil water content. The quotient of these two is referred to as the thermal diffusivity. Fischer (1992) used thermocouple psychrometer data from a USGS study site near Beatty to estimate a single, average value of thermal diffusivity equal to 6.8×10^{-7} m^2/s over a volumetric water content range from approximately 0.03 to 0.11. No other information pertaining to the thermal properties of sediments in the vicinity of the hypothetical arid site are available.

Information on the thermal properties of various minerals, soils, and rocks can be obtained from the literature (De Vries, 1963; Koorevaar et al., 1983). Koorevaar et al. (1983) note that at low water contents, the thermal conductivity of most mineral soils is less than 0.5 J/m-s K. The maximum theoretical value of thermal conductivity is reached at water saturation. For most mineral soils, this value is generally between 1.5 and 2.0 J/m-s K (Koorevaar et al.; 1983). De Vries (1963) also provides estimates of the thermal properties of several different minerals, soils, and rock materials at different temperatures and water contents.

Due to the paucity of site-specific thermal property data, the thermal conductivity parameters and heat capacity reported by Fayer and Jones (1990, p.D.37) for a silty gravel were adjusted to obtain an approximate match to the diffusivity value reported by Fischer (1992). The estimated thermal properties are shown in Figure 6.16. The parameters representing the estimated thermal properties fall within the range of parameters that appear in the literature for similar media (De Vries, 1963; Koorevaar et al., 1983).

6.2.2.4 Plant Properties

Plants are expected to eventually reestablish themselves naturally on the surface cover at the hypothetical disposal site. The timing of plant reestablishment is unknown, however. As noted previously, vegetation in the area is sparse, with the dominant vegetation being creosote bush. The creosote bush in the vicinity of the site generally has relatively shallow roots (< 1 m), and is known to be extremely drought tolerant (Wallace and Romney, 1972; Barbour et al. 1977). Simulations that included water uptake by plants were carried out to demonstrate the potential effectiveness of plants such as creosote bush in removing water from the soil cover and trench backfill material.

As noted previously, the transpiration component of ET (water uptake by plants) is represented in UNSAT-H as a sink term at nodes designated to be within the root zone. The potential (maximum) transpiration is calculated as a fraction of potential ET and is a function of the leaf area index. The assumed leaf area index used to model creosote bush is shown in Figure 6.17.

UNSAT-H distributes potential transpiration over the root zone according to the root density, which is represented as an exponential function of depth. The maximum depth of

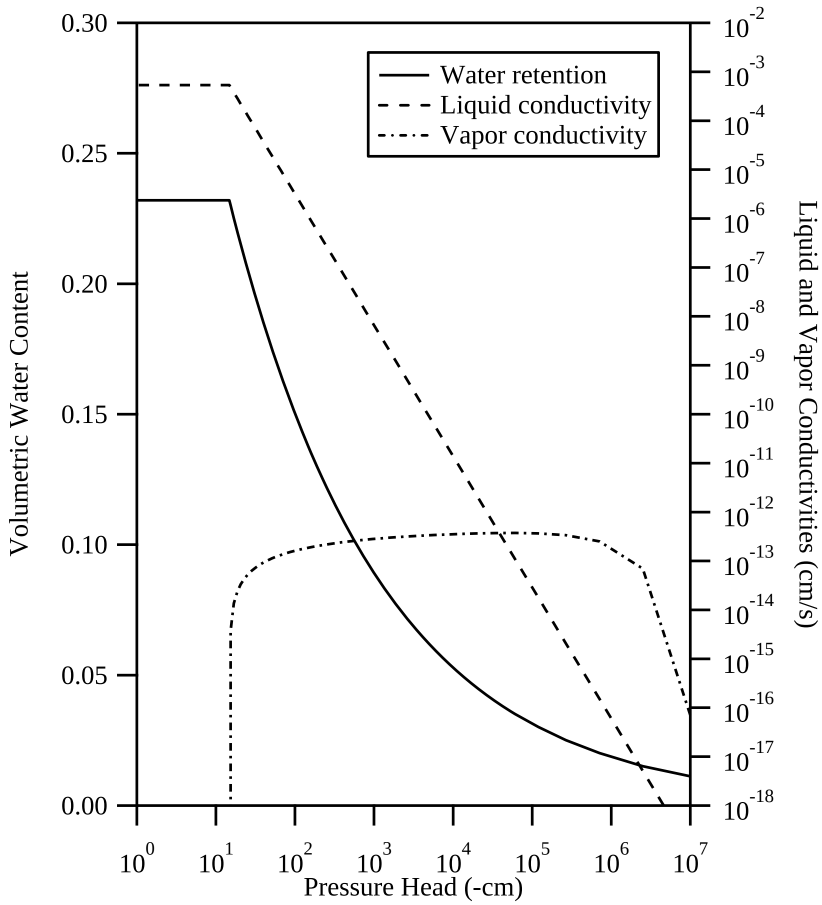

Water retention
Liquid conductivity
Vapor conductivity
0.30
0.25
0.20
0.15
0.10
0.05
0.00
Volumetric Water Content
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
10^{-12}
10^{-13}
10^{-14}
10^{-15}
10^{-16}
10^{-17}
10^{-18}
Liquid and Vapor Conductivities (cm/s)
10^0
10^1
10^2
10^3
10^4
10^5
10^6
10^7
Pressure Head (-cm)

Figure 6.15

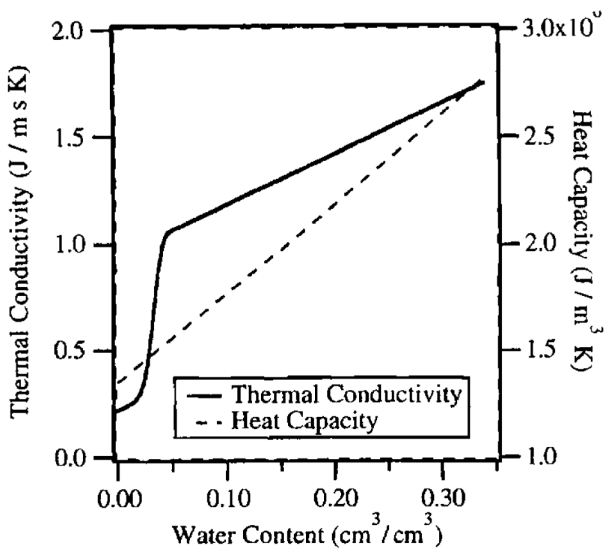


Figure 6.16 Estimated soil thermal properties for the arid site example

root penetration at the hypothetical site was assumed to be one meter. The root length density function that was used is shown in Figure 6.18.

Actual transpiration at each node within the root zone will generally be less than the potential transpiration and is a function of the soil water content, θ. The transpiration fraction as a function of water content used to represent creosote bush in the UNSAT-H model is shown in Figure 6.19.

Two parameters were specified in HELP to model water uptake by plants: leaf area index and evaporative depth. The particular values used are listed in Section 6.2.2.6.

6.2.2.5 UNSAT-H Model Configuration

A one-dimensional conceptual model was developed based on the cross section of the hypothetical trench shown in Figure 6.10. Thermocouple psychrometer data reported by

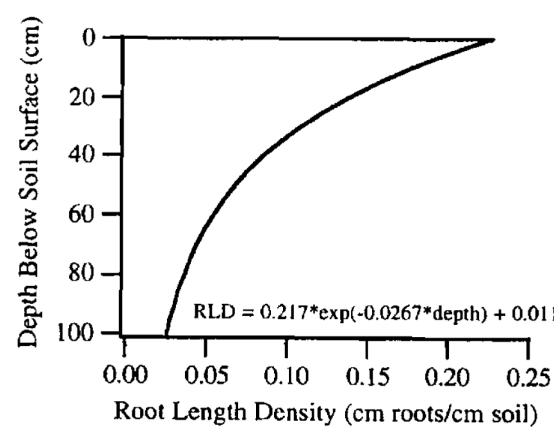


Figure 6.18 Root length density for the arid site

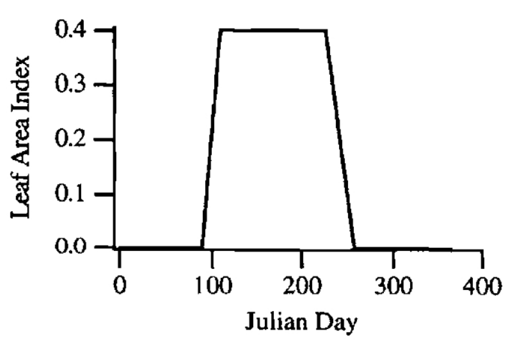


Figure 6.17 Leaf area index for the arid site

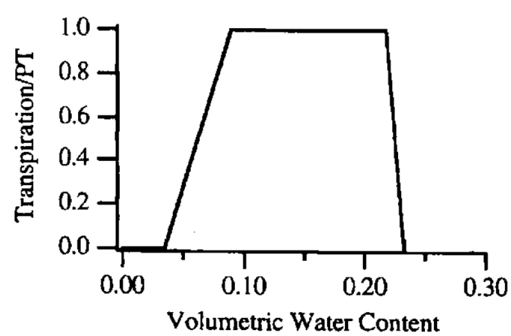
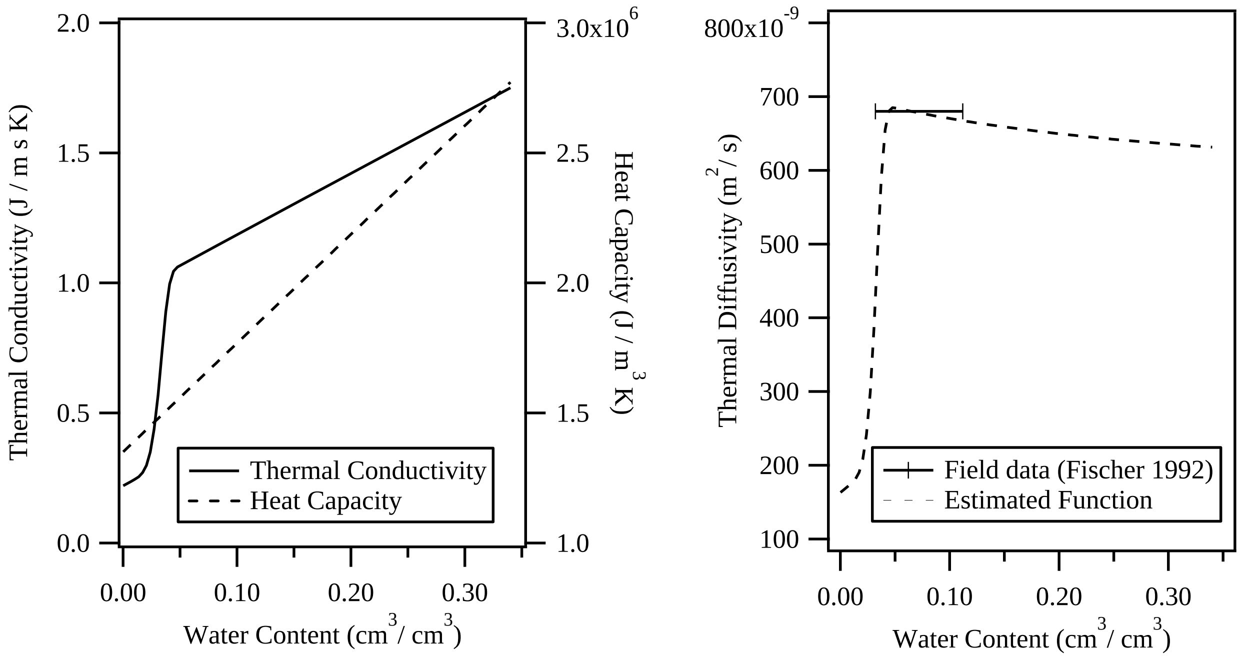


Figure 6.19 Transpiration as a fraction of potential transpiration (PT) for the arid site



Thermal Conductivity (J / m s K)
Heat Capacity (J / m3 K)
3.0x10^6
Thermal Conductivity
Heat Capacity
Water Content (cm3 / cm3)
Thermal Diffusivity (m2 / s)
800x10^-9
Field data (Fischer 1992)
Estimated Function
Water Content (cm3 / cm3)

Figure 6.16

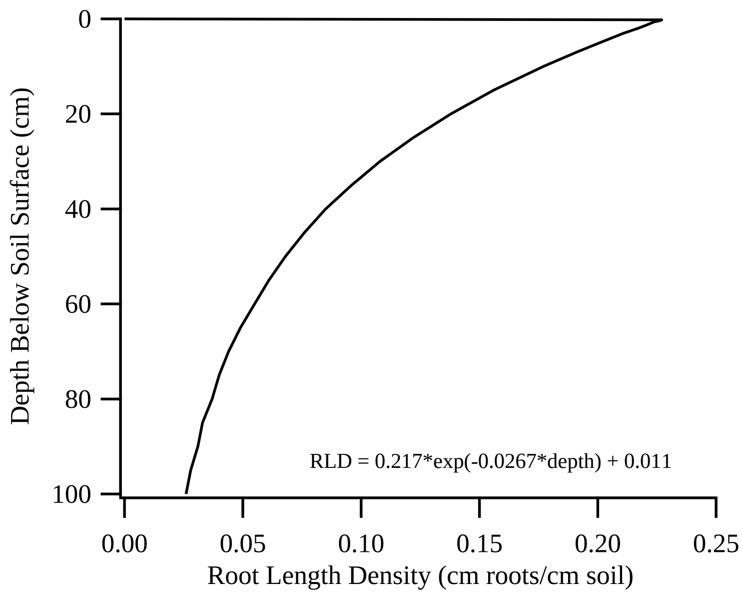

0
20
40
60
80
100
Depth Below Soil Surface (cm)
RLD = 0.217*exp(-0.0267*depth) + 0.011
0.00
0.05
0.10
0.15
0.20
0.25
Root Length Density (cm roots/cm soil)

Figure 6.18

Fischer (1992) indicate that the thermal pulse from annual temperature changes near Beatty propagates to below the 9-m depth. In order to minimize boundary condition effects in the numerical simulations, a 13-m-deep model domain was adopted, extending from the surface of the trench cover to the 13-m depth.

The hydraulic and thermal properties of the surface cover and backfill material were assumed to be uniform from the surface to the base of the trench. A uniform initial water content of 0.045 was used for the backfill soil and cover material. The hydraulic properties of the underlying sediments were assumed to be scale heterogeneous and were estimated using the conditional simulation procedure described in Appendix C. The hydraulic properties were conditioned on the initial water content and pressure head data reported by Fischer et al. (1992, p.40) for January 6, 1987. For the nonisothermal simulation, the temperature data reported by Fischer et al. (1992, p.40) for January 6, 1987 were used as initial conditions.

Data reported by Nichols (1986) and Fischer (1992) indicate that the water content distribution below the 4-m depth has remained more or less invariant in time since monitoring at the site began. The temperature of the sediments below the 10-m depth has also remained relatively constant. The thermal properties used to represent the sediments below the trench were the same as those used to represent the trench cover and backfill materials.

The 13-m-deep model domain was discretized using non-uniform node spacings ranging from a minimum of 0.2 cm at the surface to a maximum of 20 cm at depth. A total of 94 nodes were used to discretize the domain. Simulation results obtained using finer spatial discretizations yielded results that were not significantly different, suggesting that these node spacings were adequate for minimizing spatial discretization errors.

A 4-year simulation from 1986 through 1989 using hourly weather data from the USGS Beatty site and soil hydraulic properties from the RWMS was conducted to compare the use of hourly and daily averaged weather data. Three 45-year simulations were conducted, from 1949 through 1993, using RWMS soil hydraulic properties and the adjusted weather data discussed in Section 6.2.2.1. Two additional simulations were conducted for a 500-year period, using the synthetically generated weather data output by the WGEN model and soil hydraulic properties from the Beatty site. The upper boundary condition for the model simulations was varied with time, corresponding to the evaporative fluxes and infiltration rates that were calculated by UNSAT-H using the daily or hourly climate data. The lower boundary at the 13-m depth was specified to be at a constant temperature with a unit hydraulic gradient.

6.2.2.6 HELP Model Configuration

The 45-year and 500-year simulations performed with UNSAT-H were also carried out using HELP Version 3.0. A single layer of backfill material, 13-m in depth, was modeled (the heterogeneity of the underlying sediments could not be modeled with HELP). Soil hydraulic properties were derived from the RWMS data for the 45-year simulation and from the Beatty site data for the 500 year simulations (see Table 6.6). Hydraulic properties for the HELP simulations are listed in Table 6.7. Field capacity was determined by evaluating the Brooks-Corey water retention function (Equation 2-9) at a pressure head of -340 cm (-0.33 bars). Wilting point was determined by evaluating the same function at a pressure head of -1.53×10^5 cm (-15 bars). The initial water content throughout the profile was set to the wilting point value for all simulations. The slope was set to the minimum permissible value with HELP 3.0 (1%). The SCS curve number used was 88.6. For the simulations without plants, the evaporative depth was set to the default value for Las Vegas, NV for a bare soil (46 cm), and the leaf area index was set to zero. For the simulations with plants, the evaporative depth was set at 1 m, and the maximum leaf area index was set to 0.4.

TABLE 6.7 Hydraulic properties for the HELP simulations

	45-Years	500-Years
Porosity	0.34	0.232
Field Capacity	0.147	0.114
Wilting Point	0.069	0.048
K_S (cm/s)	1.294×10^{-3}	5.354×10^{-4}

6.2.2.7 4-Year Simulation Results

Only four years of hourly weather data were available for the arid site (1986-1989). Nonisothermal UNSAT-H simulations using this hourly data and daily averages of this data for the four-year period indicated that the predicted water balance results were not a function of the time-scale averaging of weather. This is apparently a consequence of the very low and infrequent precipitation at the arid site. This result is in contrast to the humid site example in which significantly more runoff, and less net infiltration, was predicted when using hourly data than when using daily data. Based on this four-year simulation of the arid site, the remainder of the UNSAT-H simulations reported in this chapter were conducted using daily average weather data.

6.2.2.8 45-Year Simulation Results

Table 6.8 summarizes the results from the three 45-year UNSAT-H simulations and the single (isothermal, no vapor

TABLE 6.8 Simulated 45-year water balance for the arid site as a fraction of precipitation

	UNSAT-H Version 3.0			
	Isothermal		Nonisothermal	
	No Vapor Flow	Vapor Flow	Vapor Flow	HELP Version 3.0
Infiltration	1.0000	1.0000	1.0000	0.981
Runoff	0.0000	0.0000	0.0000	0.019
Δ Storage	0.071	0.051	0.026	0.143
Evaporation	0.929	0.949	0.974	0.717
Net Infiltration	2×10^{-6}	2×10^{-6}	2×10^{-6}	0.121

flow) HELP simulation. The results in Table 6.8 are given as the average fraction of precipitation allocated to each term of the water balance for the 45-year period. Note that interception losses are zero and all evaporative losses from the trench cover occur after infiltration.

As shown in Table 6-6, no runoff is predicted for any of the UNSAT-H arid site simulation cases. Hence, infiltration is 100% of precipitation. For the UNSAT-H nonisothermal simulation case with vapor flow, evaporation accounts for the largest sink of water at 97.4% of precipitation. The results from this simulation case are considered to be the most realistic since more of the physics of the problem are

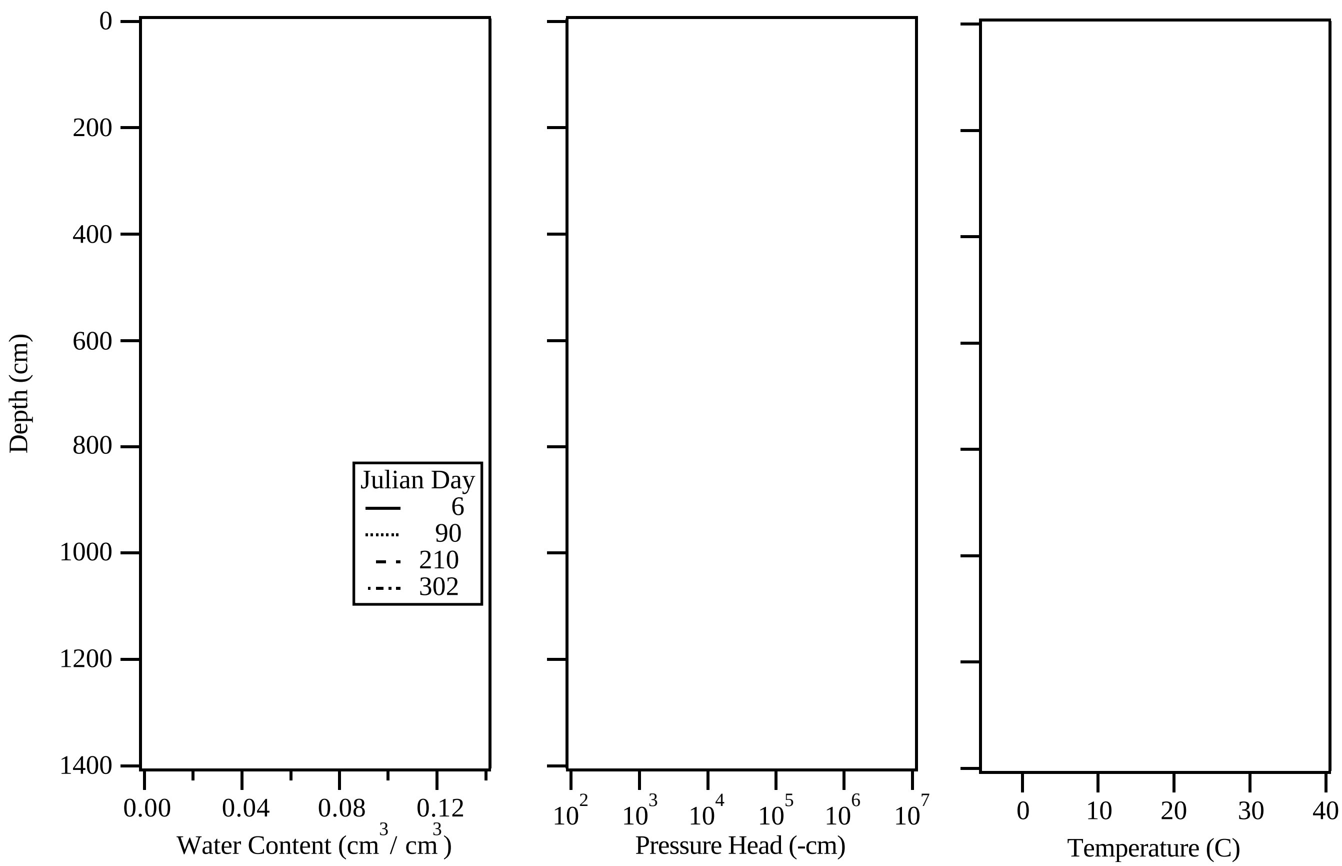


Figure 6.20 Simulated water content, pressure head, and temperature profiles for the first year of the 45-year nonisothermal simulation

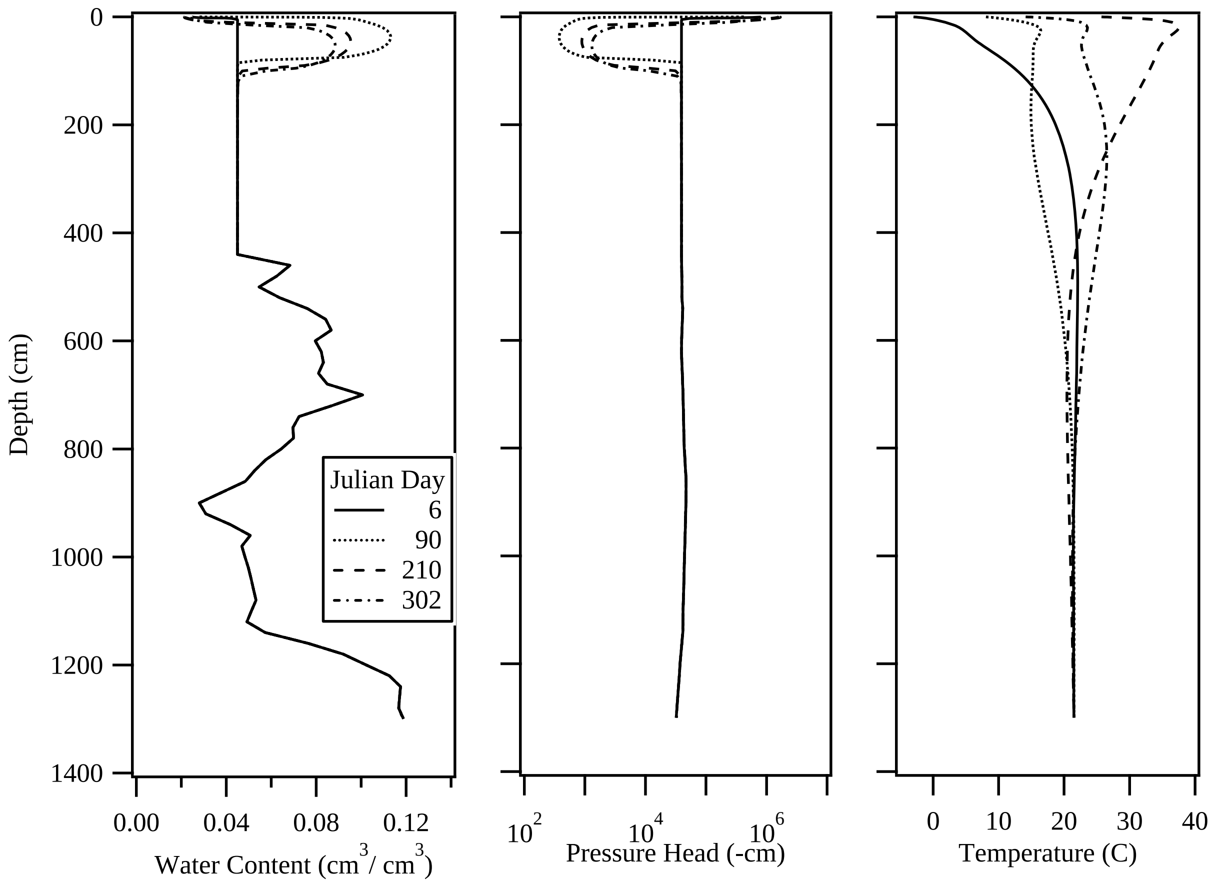

0
200
400
600
800
1000
1200
1400
Depth (cm)
Julian Day
6
90
210
302
0.00
0.04
0.08
0.12
Water Content (cm3 / cm3)
10^2
10^4
10^6
Pressure Head (-cm)
0
10
20
30
40
Temperature (C)

Figure 6.20

represented. If thermal vapor diffusion enhancement were considered, the evaporative losses predicted by UNSAT-H in nonisothermal mode would likely be greater. For the isothermal case with vapor flow, evaporation accounts for 94.9% of precipitation. If neither vapor flow nor the nonisothermal conditions are considered, the evaporation predicted by UNSAT-H is 92.9% of precipitation. Although these differences in predicted evaporation are small, the magnitude of net infiltration rates at arid sites may be low enough that these differences are significant. A very small amount of net infiltration was predicted for the 45-year simulations. Virtually all precipitation that was not evaporated was accumulated in the storage term.

The water balance results for the HELP simulations are also shown in Table 6.8 as a fraction of precipitation. HELP predicted that just under 2% of the precipitation would become runoff. HELP predicted significantly less evaporation than any of the UNSAT-H models. Net infiltration predicted with HELP is several orders of magnitude greater than that predicted by UNSAT-H and accounts for 12% of precipitation. The value of net infiltration predicted by HELP corresponds to a potential recharge of 11.5 mm/yr. (3.64×10^{-8} cm/s).

This value is about five times larger than the estimated natural recharge at Beatty obtained by Prudic (1994) using chloride mass balance (2 mm/yr.), and is several orders of magnitude larger than the value obtained by Nichols (1986) at the same site (0.04 mm/yr.). The value of Nichols (1986) is believed to be more representative of recent conditions (see Section 6.2.2.10).

Figure 6.20 shows simulated water content, pressure head, and temperature profiles on different days of the first simulation year for the UNSAT-H nonisothermal case. Simulated water contents and pressure heads in the top meter of the profile fluctuate in response to precipitation. The soil-water storage in the trench backfill material increases slowly from the initially dry conditions. The temperature profiles indicate that the simulated seasonal temperature pulse propagates to below the 10-m depth. These results are generally consistent with observations by the USGS at the Beatty study site.

Figure 6.21 shows predicted daily water fluxes at the 5- and 10-m depths as a function of time for the three 45-year UNSAT-H simulation cases. The predicted fluxes at these

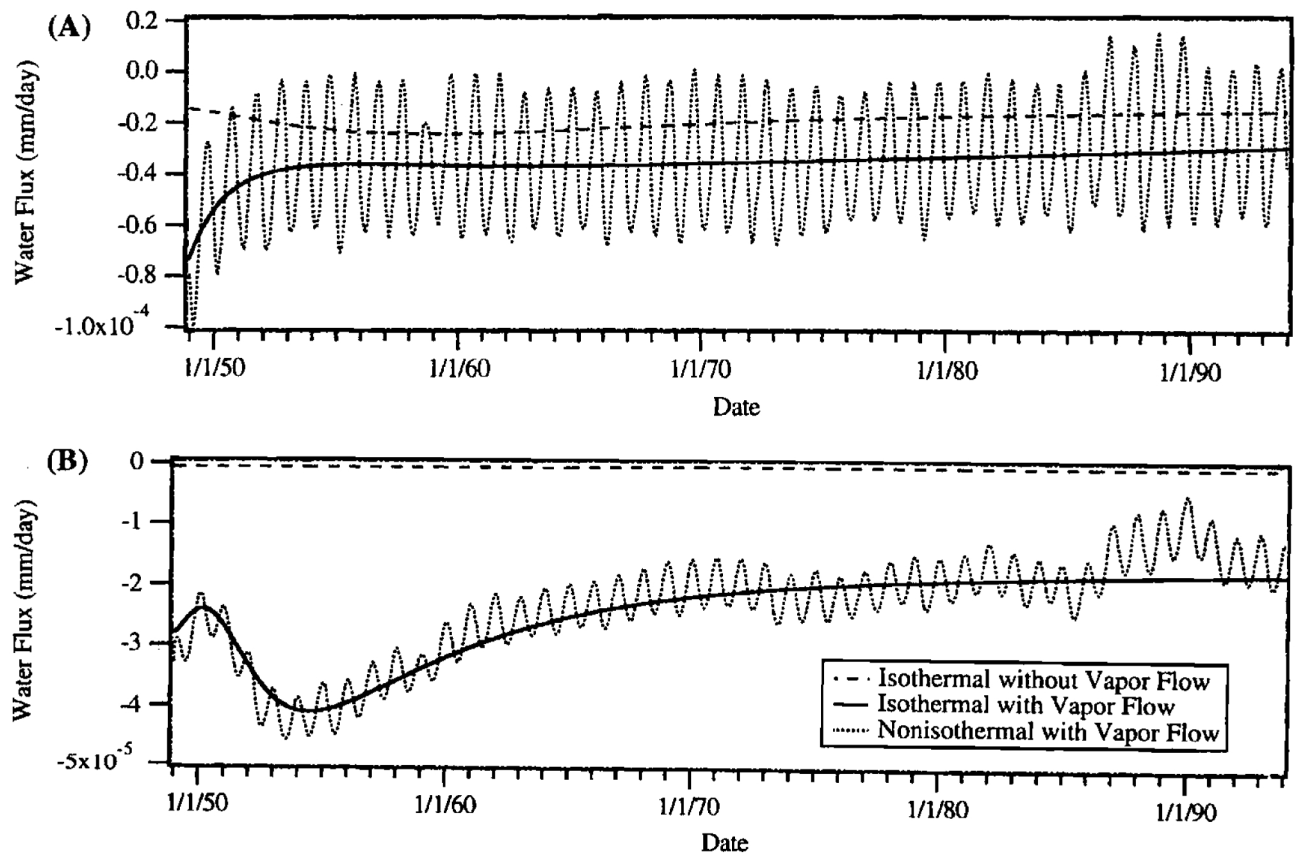


Figure 6.21 Simulated water flux at (A) 5-m and (B) 10-m depths for the arid site example

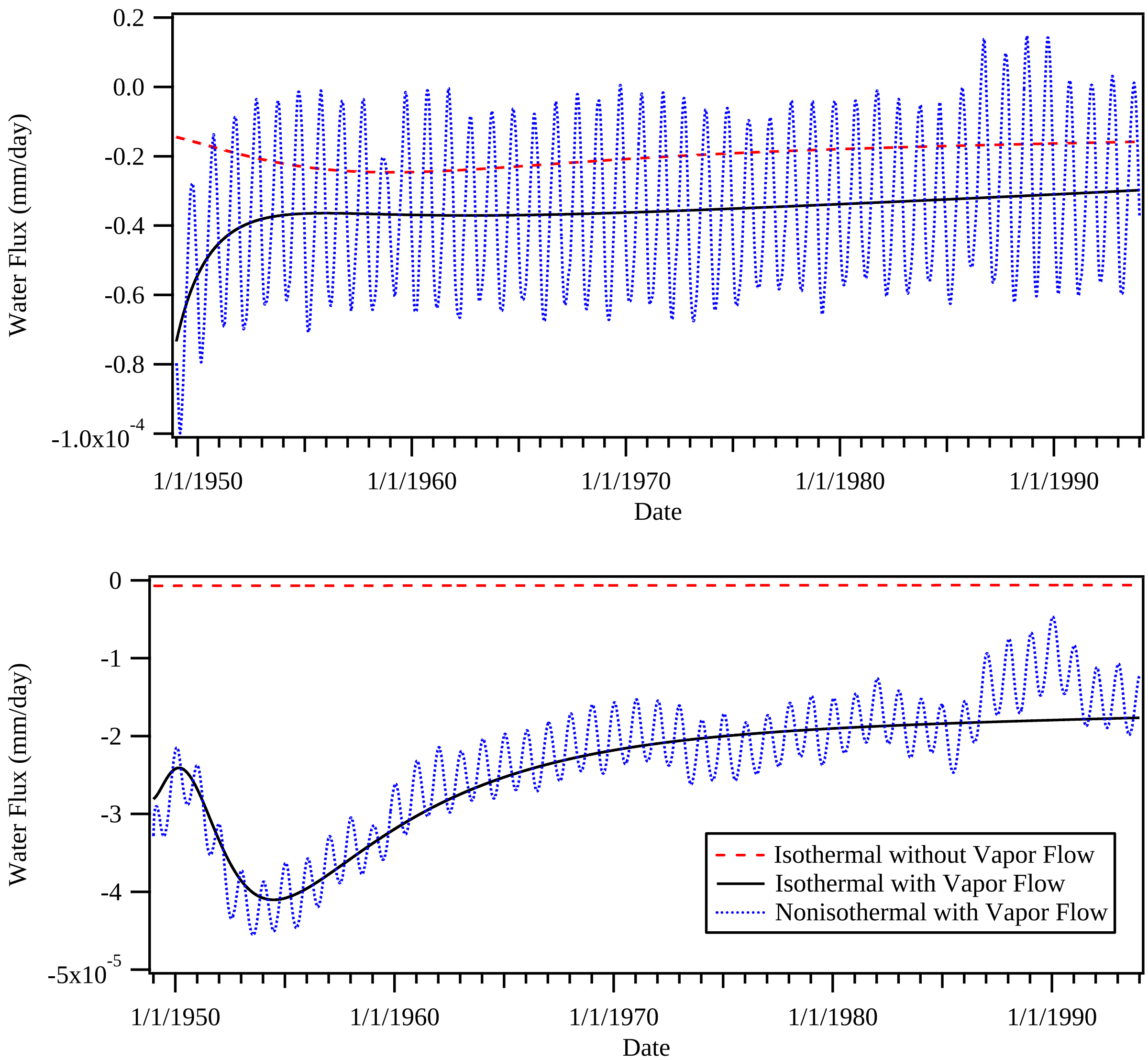

0.2
0.0
-0.2
-0.4
-0.6
-0.8
-1.0x10-4
Water Flux (mm/day)
1/1/1950
1/1/1960
1/1/1970
1/1/1980
1/1/1990
Date
0
-1
-2
-3
-4
-5x10-5
Water Flux (mm/day)
Isothermal without Vapor Flow
Isothermal with Vapor Flow
Nonisothermal with Vapor Flow
1/1/1950
1/1/1960
1/1/1970
1/1/1980
1/1/1990
Date

Figure 6.21

depths are mostly negative, indicating upward water flow. The fluxes predicted for the nonisothermal case cycle up and down in response to seasonal temperature variations. The fluxes predicted from the isothermal case with vapor flow follow a trend similar to the nonisothermal simulation results. The simulation results for the isothermal case without vapor flow remain relatively constant in time. Although the predicted fluxes at the 5- and 10-m depths are mostly upward, the predicted fluxes at the 13-m depth (the bottom of the model domain) are downward for all simulation cases. This is largely a result of the unit hydraulic gradient lower boundary condition that was specified for the model simulations.

The drainage fluxes predicted by UNSAT-H at the 13-m depth at the end of 45 years are approximately 0.0002 mm/yr. for all three cases. The results for all UNSAT-H simulation cases indicate a slow increase in soil-water storage in the trench backfill material. This is the result of having initially dry backfill sediments and no vegetation. Therefore, longer simulations are warranted to determine the impact of the increased water storage at later times.

Although the nonisothermal simulation case with vapor flow is considered to provide the most realistic representation of the actual processes occurring at the site, this case required 50 to 60 times the computational effort (CPU time) of either of the isothermal cases. The results obtained for the isothermal case with vapor flow closely follow the trends in the results generated for the nonisothermal case and only required from 2 to 3 minutes of CPU time per simulated year on a DEC Alpha workstation. Therefore, conducting isothermal simulations with vapor flow appears to be a practical alternative to conducting nonisothermal simulations. This approach should still yield reasonable and realistic water balance predictions for this arid site. The isothermal simulation case without vapor flow yielded the least evaporation and eventually would result in larger increases in storage and more net infiltration. Thus, using an isothermal model that does not account for vapor flow may yield a conservative, but not necessarily accurate, prediction of net infiltration for this arid site.

6.2.2.9 500-Year Simulation Results

Two 500-year UNSAT-H simulations were conducted (in isothermal mode with vapor flow) using synthetically generated weather data from WGEN. These simulations estimated the long-term flux through the hypothetical facility resulting from using a vegetated surface cover and a cover free of vegetation. The plant parameters used in the simulations were discussed in Section 6.2.2.4.

Water content profiles at selected times for the two UNSAT-H simulations are shown in Figure 6.22. For the simulation without plants, the water content increases slowly and the wetting front eventually reaches the bottom of the profile. For the simulation with plants, the water content remains relatively constant in time below the 1-m depth.

The fluxes at the bottom of the model domain for the two 500-year UNSAT-H simulations are given in Table 6.9. The results shown are for the end the indicated year. For the simulation without plants, the fluxes slowly increase as the water contents in the profile increase. A quasi-steady-state flux of about 2.5 mm/yr. is reached after 400 to 500 years. For the simulation with plants, the fluxes at the bottom of the profile remain very low and relatively constant for the entire 500-year simulation period.

Two 500-year HELP simulations, comparable to the UNSAT-H simulation, were carried out. The parameters for the HELP models were discussed in Section 6.2.2.6. The 500-year HELP simulations used the same WGEN-generated meteorological record as the UNSAT-H simulations. Fluxes at the 13-m depth predicted by HELP are shown in Table 6.9. The result given for each indicated year is the average daily flux over the 100-year period ending at that year.

At all times, the flux predicted by HELP is larger than that predicted by UNSAT-H. Without plants, HELP appears to reach a quasi-steady-state flux after approximately 100 years. The steady-state value is about 10 times larger than the UNSAT-H prediction. When the presence of plants is simulated, HELP predicts that the flux at a depth of 13 m is still increasing after 500 years. The value of 0.69 mm/yr. is much larger than the corresponding UNSAT-H prediction.

The results obtained from the long-term simulations demonstrate the potentially significant impact that plants can have on soil-water balance in arid climates. Given the uncertainty associated with the extent and timing of natural revegetation in arid climates, the results of this study suggest that it may be worthwhile to revegetate surface covers after closure of LLW disposal facilities rather than relying on natural revegetation.

6.2.2.10 Steady-State Analysis

Given the small fluxes predicted by the UNSAT-H simulation results and the large depth to the water table, an analysis of the influence of the geothermal gradient on flow at greater depths may be warranted. Enfield et al. (1973) used the following equation to estimate the steady-state water flux, q, in the deep unsaturated zone at the Hanford Site:

$$q = -K\nabla(h_m - z) - D_t\nabla T_K - D_o\nabla h_o \qquad (6\text{-}1)$$

where

K = unsaturated hydraulic conductivity [L/T]

∇ = vector gradient operator [1/L]

h_m = matric potential [L]

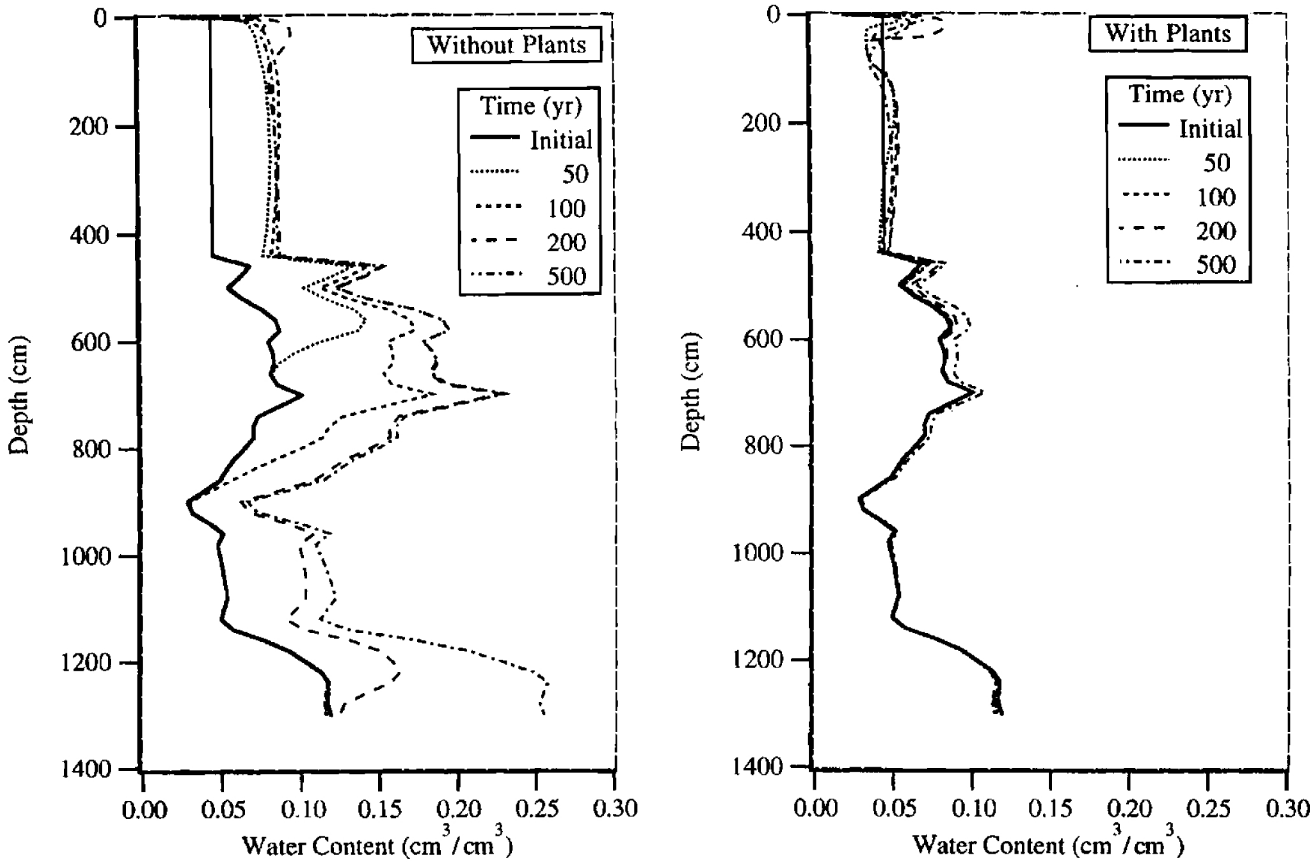


Figure 6.22 Water content profiles using UNSAT-H for the arid site example with and without plants

z = depth [L], measured positive downward

D_t = thermal fluid diffusivity, or the sum of thermal liquid diffusivity and the thermal vapor diffusivity [L^2/T °K]

D_o = osmotic fluid diffusivity [L^2/T per bar]

h_o = osmotic potential [bars]

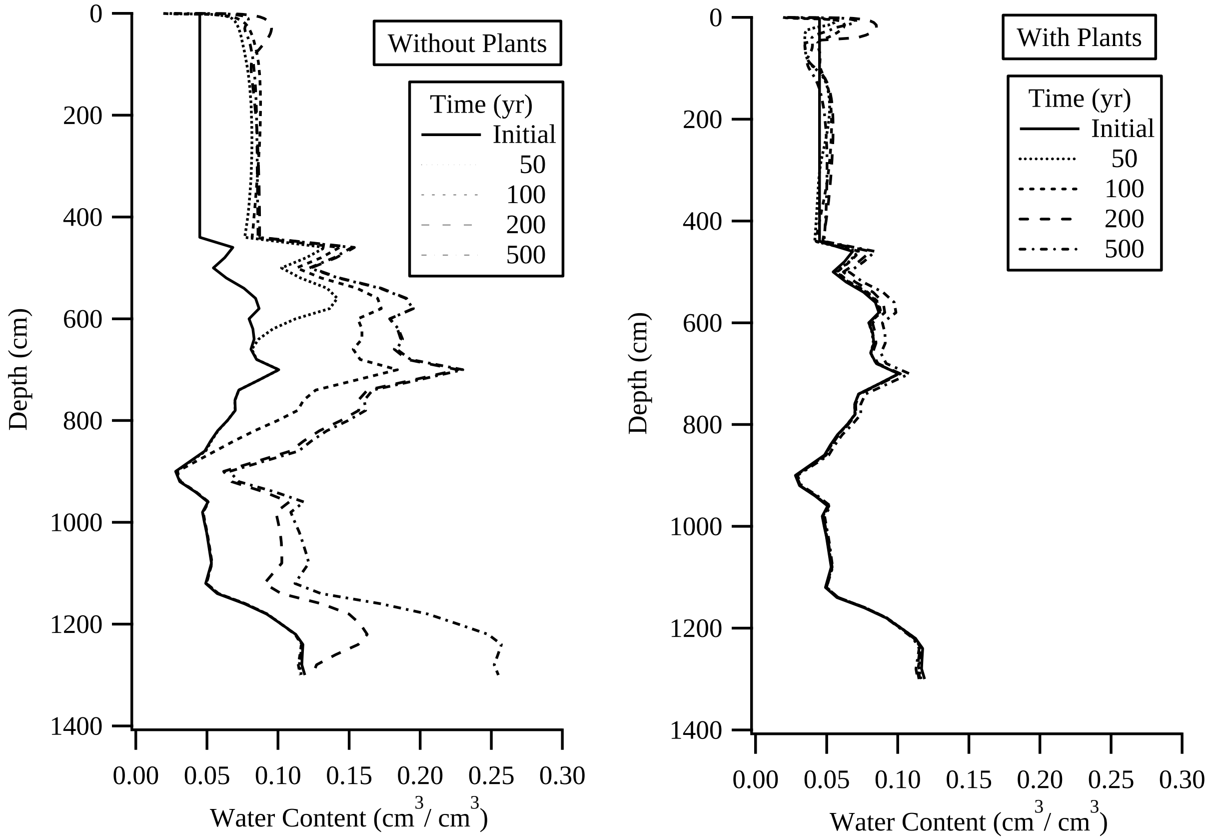
T_K = absolute temperature [°K].

As noted previously, Fischer (1992) reported an average value of thermal fluid diffusivity of 6.8×10^{-7} m^2/s for sediments at the USGS study site near Beatty. The thermal gradient below the 13-m depth at the USGS study site is approximately 0.05 °C/m (data provided by Dave Prudic, USGS, Carson City, Nevada). After making the appropriate

TABLE 6.9 Simulated fluxes (mm/yr.) at the 13-m depth with and without plants

	UNSAT-H Version 3.0		HELP Version 3.0	
Time[a] (yr.)	**Without Plants**	**With Plants**	**Without Plants**	**With Plants**
100	0.0002	0.0002	13.94	0.00
200	0.0005	0.0002	19.46	0.01
300	1.39	0.0002	18.52	0.04
400	2.69	0.0002	21.14	0.25
500	2.45	0.0002	22.43	0.69

[a] UNSAT-H results given as the flux at the end of the indicated year. HELP results given as the average flux over a 100-year period ending at the indicated year.



Without Plants
Time (yr)
Initial
50
100
200
500
Depth (cm)
0
200
400
600
800
1000
1200
1400
0.00
0.05
0.10
0.15
0.20
0.25
0.30
Water Content (cm3 / cm3)
With Plants
Time (yr)
Initial
50
100
200
500
Depth (cm)
Water Content (cm3 / cm3)

Figure 6.22

unit conversions, substituting these values into Equation 6-1 yields a water flux of -0.1 mm/yr. (upward) due to the thermal gradient. If flow induced by osmotic potential gradients is neglected, the estimated flux due to matric and gravitational potential gradients can be combined with the flux due to the thermal gradient using Equation 6-1, to yield the net water flux.

If the flux due to matric and gravitational potential gradients at the hypothetical site is 0.0002 mm/yr. (500-year UNSAT-H simulation with plants), the net estimated water flux below the 13-m depth is approximately -0.0998 mm/yr. (upward). Data from the USGS study site near Beatty suggest that this is a reasonable estimate for current site conditions. If the flux due to matric and gravitational potential gradients is 2.5 mm/yr. (500-year UNSAT-H simulation without plants) then the net estimated water flux is 2.4 mm/yr. (downward). This is likely to be a conservative estimate and is probably somewhat unrealistic since plants should be able to reestablish themselves naturally over the course of 500 years. These calculations assume steady-state flow and negligible osmotic potential gradients. These results suggest that the magnitude of the water fluxes below the 13-m depth may be small enough that the geothermal gradient could overcome the matric and gravitational potential gradients so that the net flux of water at the hypothetical site is actually upward.

The USGS has conducted detailed investigations since about 1976 to assess the potential for deep percolation and groundwater recharge from meteoric water at a commercial LLW disposal facility near Beatty. Nichols (1986) used psychrometer and neutron probe data from the USGS study site and estimated a flux of water below the 10-m depth of 0.04 mm/yr. (downward). Additional studies were initiated by the USGS in 1986 to 1) determine the effects of site disturbance on soil-water dynamics in simulated waste disposal trenches, 2) estimate the rates of subsidence and erosion for the trench covers, and 3) develop and evaluate methods for measuring physical and hydraulic properties of very dry, gravelly soils (Andraski, 1991; Andraski et al., 1991). More recent psychrometer and neutron probe data from the USGS studies are reported by Fischer (1992).

Prudic (1994) used the chloride mass balance method to estimate percolation rates and ages of water below the 10-m depth near Beatty. The chloride data suggest a long-term average recharge rate of 2 mm/yr. However, Prudic (1994) notes that the more recent neutron probe data and thermocouple psychrometer data indicate upward water flow above the 10-m depth. He suggests that the higher recharge rate estimated using the chloride mass balance method may be more representative of a period during the late Pleistocene when the climate at the site was cooler and wetter.

6.2.2.11 Uncertainty Evaluation

The results of the one-dimensional UNSAT-H and HELP simulations presented above provide estimates of the average net infiltration and illustrate how water fluxes vary over time and depth. These results were obtained for a single set of parameters for the backfill soil material and one realization of scale-heterogeneous sediments below the trench for the UNSAT-H simulations. At an arid site, it is not difficult to produce estimates of recharge that vary several orders of magnitude – this variation can be produced using realistic combinations of parameters. A simple sensitivity analysis using HELP illustrates this for the hypothetical arid site.

Previous discussions have pointed out the potential difficulties with the application of HELP in arid environments (see Sections 4.3.1.2 and 4.3.1.3). Parameters that have no basis in physics (e.g., field capacity) and those that are difficult to define or measure (e.g., wilting point and evaporative depth) may contribute a significant amount of uncertainty to the estimate of recharge. The 500-year results presented in Table 6.9 were obtained using an evaporative depth of 46 cm and a saturated hydraulic conductivity, K_S, of 5.3×10^{-4} cm/s. Table 6.10 presents the average flux predicted by HELP when the evaporative depth is increased to 1 m. As shown, approximately doubling the evaporative depth reduces the flux at 13 m by more than an order of

TABLE 6.10 Average flux (mm/yr.) predicted by HELP, Version 3.0 at the 13-m depth (without plants)

	Evap. Depth = 1 m	**Evaporative Depth = 46 cm**		
Time[a] (yr.)	**$K_S = 5.3\times10^{-4}$ cm/s**	**$K_S = 5.3\times10^{-4}$ cm/s**	**$K_S = 5.3\times10^{-3}$ cm/s**	**$K_S = 5.3\times10^{-2}$ cm/s**
100	0.00	13.94	21.75	34.70
200	0.04	19.46	25.96	37.91
300	0.85	18.52	24.84	35.07
400	1.52	21.14	27.96	39.63
500	1.73	22.43	29.73	41.38

a. Results given as the average flux over a 100-year period ending at the indicated year.

magnitude. The leaf area index was zero in both cases. Table 6.10 also presents the average flux predicted by HELP when the saturated hydraulic conductivity is increased by factors of 10 and 100. Increasing K_S by a factor of 100 causes the predicted flux at 13 m to approximately double.

A more comprehensive uncertainty analyses should be conducted for any genuine site application. For the hypothetical arid site, UNSAT-H or HELP (or both models) could be used in a comprehensive uncertainty analysis. In addition, a simple Monte Carlo simulation could be quickly carried out using Equation 6-1, with the assumption of steady-state flow below the 13-m depth. The point of an uncertainty analysis is not necessarily to demonstrate that a particular model is poor. Rather, any model application, using any code, should explore the range of reasonable predictions that can be produced.

6.2.3 Arid Site Conclusions

Results of simulations and steady-state calculations reported here for the hypothetical arid site demonstrated a wide range of estimated net infiltration, from a net upward flux for a vegetated surface to as much as 22mm (23% of annual precipitation) for a bare soil. UNSAT-H simulations provided the lowest estimates under all conditions tested and, in general, were in better agreement with USGS estimates of net infiltration at the Beatty site. HELP consistently gave the highest values for net infiltration. For bare soil, results comparable to UNSAT-H were achieved by (arbitrarily) increasing the evaporative depth parameter in HELP by about a factor of two over the default value

Although the results reported here should provide reasonable estimates of net infiltration for the simulated conditions, insufficient data from the USGS studies were available for calibrating the models or for critically evaluating the accuracy of the simulation results. Therefore, the net infiltration rates estimated for this application example should not be considered definitive estimates of the actual net infiltration (or exfiltration) rates for the Beatty site. This example simply serves to demonstrate some of the issues of concern when evaluating water infiltration for LLW disposal facilities located in arid or semi-arid environments.

The UNSAT-H simulation results obtained for this application example suggest that net infiltration at the hypothetical site can be very small. For undisturbed, vegetated conditions, the net infiltration may actually be negative, indicating net upward water flow. Dramatic increases in water content and recharge were observed when bare soil (i.e., no vegetation) was simulated. Nonisothermal conditions and vapor-phase transport appear to have a significant effect on water movement at the hypothetical arid site.

It should be cautioned that the effects of extreme events and preferential flow were not investigated in this example. The potential for heterogeneity-induced preferential flow after extreme precipitation events cannot be realistically evaluated using a one-dimensional model. Given the arid conditions, the type of sediments, and the great depth to the water table, however, the potential for significant exposure to contaminants leached from LLW via the groundwater pathway appears to be quite small.

The strong thermal gradients, dominant vapor flow, and proximity of waste disposal trenches to the ground surface all suggest that potential exposure to contaminants via the air pathway may be of greater concern than potential exposure via the groundwater pathway at the hypothetical arid site. Vapor-phase transport appears to be the dominant mechanism by which water movement occurs at this site. Advective gas transport in coarse sediments is a potential mechanism for the movement of several contaminants (e.g., ^{3}H, ^{14}C, and ^{222}Rn). This suggests that performance assessment evaluations of LLW disposal facilities that use shallow land burial of wastes in arid environments should consider and evaluate the potential risks associated with vapor-phase transport of contaminants.

7 Recommendations

In this report we have described the major issues related to the evaluation of water flow in the unsaturated zone at LLW disposal sites. We presented a methodology for this evaluation and provided examples of its use at hypothetical LLW disposal sites in humid and arid climates. Specific recommendations regarding future needs for hydrologic evaluations include the following:

- *Improve computational capabilities for flow and transport in the unsaturated zone.* Currently available numerical simulation codes are satisfactory for most LLW site hydrologic evaluations. Multidimensional simulations of complex processes such as vapor phase transport under thermal gradients remains computationally demanding, however. Further code development and the application of advanced numerical methods may improve the efficiency of these simulations. Improved computational capabilities are especially important in the effective analysis of uncertainty.

- *Address issues related to the use of limited data sets.* Limited data sets are a characteristic of hydrologic evaluations of the unsaturated zone. This can be attributed, in part, to (1) a site characterization period that is generally much shorter than the time scale of hydrologic process variability and (2) the spatial variability of soil hydraulic properties. Creative use of ancillary data can often be used to supplement site-specific data. Suitable ancillary data includes (1) long-term or spatially dense data from appropriate analog sites and (2) data such as particle size distributions that may be correlated with desired hydraulic properties. In addition, the effect of limited data sets on the uncertainty of model predictions should be quantified.

- *Collect data to support models of engineered barrier performance and degradation.* Engineered components of LLW facilities are often critical in achieving satisfactory hydrologic performance. In many cases, however, there are inadequate data to support reliable models of engineered barrier degradation and failure mechanisms and their associated probabilities. The collection of such data through laboratory and prototype studies as well as through the analysis of existing engineered facilities should be a priority.

- *Apply state-of-the-art site characterization and monitoring methods.* Characterization instruments and methods continue to be developed and refined. To provide the most defensible hydrologic evaluations, state-of-the-art instrumentation and data analysis methods must be employed during the characterization and monitoring of LLW disposal sites.

- *Integrate site characterization and performance assessment.* The best use of resources will occur when site characterization activities are integrated with performance assessment analyses. In addition, site characterization and assessment of the hydrologic performance of a LLW facility should continue throughout the period of institutional control. This can be facilitated by integrating long-term monitoring instruments into the facility design. Successful long-term monitoring will provide not only evidence of a facility's continued performance, but also a valuable data set to improve the design of future facilities at other sites.

- *Use the experience gained at current LLW sites to benefit future sites.* Several of the recommendations listed here mirror those made by the National Research Council in a review of issues raised at the Ward Valley, California LLW site (National Research Council, 1995). The Ward Valley experience and the experience gained at other LLW sites should be used to benefit future LLW site assessments.

As a final comment, we note that while this report focused on the hydrologic evaluation of LLW disposal facilities, the methodology discussed is suitable for decommissioning sites and other applications that require a near-surface hydrologic analysis.

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Appendix A

A.1 Application of the Universal Soil Loss Equation to the Humid Site Example

The Universal Soil Loss Equation (USLE) is written as

$$A = RKLSCP$$

where

A = soil loss (tons/acre/year)
R = rainfall erosivity index
K = soil erodibility index
L = hillslope-length factor
S = hillslope-gradient factor
C = cropping-management factor
P = erosion-control practice factor.

Values for the indices and factors were derived from the figures and tables presented in Dunne and Leopold (1978). Similar figures and tables can be found in many references including Lutton et al. (1979) and Stewart et al. (1975). Because the USLE is based on average values, there is a large degree of uncertainty associated with the estimated erosion rates. Additional uncertainty was contributed in this case by the fact that there was limited site-specific data on the soil parameters and the future vegetation for the example site. Because of the uncertainty, a range of values for the soil loss was estimated.

The range of values for each of the parameters was

$$250 \leq R \leq 350$$

$$0.1 \leq K \leq 0.37$$

$$LS = 5.8$$

$$0.013 \leq C \leq 0.1$$

$$0.45 \leq P \leq 0.9$$

The silty sand surface layer was assumed to be composed of 38% silt and very fine sand (grain size less than 0.1 mm) and 55% sand (grain size 0.1 to 2.0 mm). The soil structure rating was assumed to be 1.5 (very fine granular to fine granular). The percent organic matter was unknown (range 0-4) as was the permeability rating (range 1-6). These uncertainties resulted in the given range for K.

The LS factor was based on a slope of 20% and a hillslope length of 61 m (200 ft.). The factor C assumed no appreciable canopy with 40-80% grass ground cover. The greatest variability lies in the parameter C.

The resulting range of soil loss rates was

$$0.85 \leq A \leq 67.6$$

with a best estimate of

$$A = (300)(0.22)(5.8)(0.013)(0.45) = 2.2 \text{ tons/acre/year}$$

(= 4.9 MT/ha/yr.).

This value lies near the bottom of the expected range and may not be conservative in the long term.

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Appendix B

B.1 Parameter Distributions and Sensitivity Analysis for the Humid Site TopSoil

If

$$Y = \ln(X) \qquad \text{(B-1)}$$

follows a normal distribution, then we say that the parameter, X, is lognormally distributed. The relationships between the mean and variance of X and Y are given by (Ang and Tang, 1975)

$$\mu_X = \exp(\mu_Y + \sigma_Y^2/2) \qquad \text{(B-2)}$$

$$\sigma_X^2 = \mu_X^2(\exp(\sigma_Y^2) - 1) \qquad \text{(B-3)}$$

$$\mu_Y = \ln\mu_X - \sigma_Y^2/2 \qquad \text{(B-4)}$$

$$\sigma_Y^2 = \ln(1 + \sigma_X^2/\mu_X^2) \qquad \text{(B-5)}$$

where

μ_X, σ_X^2 =mean and variance of X

μ_Y, σ_Y^2 =mean and variance of Y.

For the humid site sensitivity analysis involving the hydraulic parameters of the topsoil, the saturated hydraulic conductivity, K_S, and the van Genuchten α parameter were assumed to be lognormally distributed. The mean of the natural logarithm for each parameter was taken to be the log of the basecase values given in Table 6.1, namely,

$\mu_{\ln(K_s)}$ =ln(10^{-4}) = -9.21

$\mu_{\ln(\alpha)}$ = ln(0.044) = -3.12.

The coefficient of variation, given by $COV_X = \sigma_X/\mu_X$, was taken for each parameter as the value determined by Carsel and Parrish (1988) for silt loam, namely,

COV_{K_S} =2.751

COV_α = 0.647.

These values were substituted in Equation B-5 to determine the variances of the logarithm of the parameters:

$\sigma^2_{\ln(K_S)}$ =ln(1 + 2.751^2) = 2.15

$\sigma^2_{\ln(\alpha)}$ =ln(1 + 0.647^2) = 0.350.

Two values were chosen for the sensitivity analysis, (μ_Y + 1.56 σ_Y) and (μ_Y - 1.56 σ_Y). These are the 0.94 quantile and the 0.06 quantile, respectively, and represent 88% of the parameter variability. The values of the untransformed parameters were then determined using Equation B-1. Thus, including the basecase, simulations were carried out using three values for K_S and α:

K_S = {10^{-5}, 10^{-4},10^{-3}} cm/s

α. = {0.018, 0.044, 0.111} cm^{-1}.

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Appendix C

C.1 Conditional Simulation of Soil Hydraulic Properties using Soft Data

The conditional simulation method described here was used previously by Rockhold et al. (1994) for estimating soil hydraulic properties for numerical simulations of a field-scale flow and transport experiment conducted at the Las Cruces Trench Site in New Mexico. Brief descriptions of the method and its application for the Las Cruces Trench Site and the hypothetical arid site example presented in Section 6.2 of this document are given below.

The conditional simulation method of Rockhold et al. (1994) is based on the concept of microscopic geometric similitude and scaling of soil hydraulic properties as described by Miller and Miller (1956). The application of this concept to scaling of soil hydraulic properties is founded on the physical relationship between the effective pore radius, r [L], and the soil-water pressure head, h_m,

$$h_m(r) = 2\sigma/\rho g r, \qquad \text{(C-1)}$$

where σ [M/T^2] is the surface tension at the air-water interface, ρ [M/L^3] is the mass density of the liquid water, and g [L/T^2] is the gravitational acceleration. Two porous media or two locations in a porous medium are said to be "Miller-similar" if a scaling length λ_s [L] can be found for each, such that identical values of the dimensionless ratio r/λ_s are obtained (Jury et al., 1987).

If a porous medium obeys the microscopic transport laws governing surface tension (the Laplace equation) and viscous flow (Stokes equation), and if the particle and pore structures at different locations are similar, then the transport coefficients that appear in the equations describing macroscopic flow (Darcy's law and the Richards equation) should be related by known functions of their scaling lengths. The dependence of scaled transport coefficients on the microscopic characteristic lengths is removed by relating the transport coefficients at a given location to the coefficients at an arbitrary reference point by scaling of the length ratios, $\alpha_s = \lambda_s/\lambda^*_s$, where α_s is a scaling factor, and λ^*_s denotes the scaling length at the reference location. Scale relations for pressure head and hydraulic conductivity are defined by

$$h^*_m(\theta) = \alpha_h h_m(\theta) \qquad \text{(C-2)}$$

and

$$K^*(\theta) = K(\theta) / \alpha_K^2 \qquad \text{(C-3)}$$

where h^*_m and K^* represent scale-mean values of pressure head and hydraulic conductivity, respectively (Miller and Miller, 1956). Note that the subscript s on α_s has been replaced by the subscript h or K in (C-2) and (C-3) to distinguish between the scaling factors estimated from water retention and hydraulic conductivity data, respectively.

Miller similitude requires that the scaling factors α_h and α_K be equal, which implies that the porosity is uniform. These scale relations have been used successfully to describe well-sorted sands, such as those typically used in laboratory column experiments, but have been shown to poorly describe field soils containing a broad range of particle sizes. Warrick et al. (1977) extended the range of application of scaling by estimating scaling factors relative to the degree of saturation, $s = \theta/\theta_s$, rather than θ. Effective saturation, $s_e = [(\theta - \theta_r)/(\theta_s - \theta_r)]$, can be used instead of s if soil-water retention data are characterized using non-zero θ_r values.

Scale-mean or reference values of pressure head and hydraulic conductivity are defined by the requirements that α_h and α_K have unit mean value and that $\lambda_s = 1$ at some reference location. After substituting s for θ in (C-2) and (C-3), this definition results in the conditions

$$h^*_m(s) = \left\{ \int_{-\infty}^{0} \left[h_m(s)\right]^{-1} f\left[h_m(s)\right] \mathrm{d}h_m \right\}^{-1} \qquad \text{(C-4)}$$

and

$$K^*(s) = \left\{ \int_{0}^{\infty} \left[K(s)\right]^{1/2} f\left[K(s)\right] dK \right\}^{2} \qquad \text{(C-5)}$$

where $f[h_m(s)]$ and $f[K(s)]$ are the probability density functions of h_m and K, respectively (Jury et al. 1987). Scale-mean values of pressure head and hydraulic conductivity can be approximated from (C-4) and (C-5) as

$$\widehat{h_m}^*(s) = n\left[\sum_{i=1}^{n} \frac{1}{h_m^i(s)}\right]^{-1} \qquad \text{(C-6)}$$

and

$$\widehat{K}^*(s) = \left\{\frac{1}{n}\sum_{i=1}^{n}\left[K_i(s)\right]^{1/2}\right\}^{2} \qquad \text{(C-7)}$$

where n is the sample size (Peck et al., 1977; Simmons et al., 1979). Several alternative definitions for the scale-mean hydraulic properties have also been proposed (Warrick et al., 1977; Hopmans, 1987).

Jury et al. (1987) analyzed soil hydraulic properties representing two different fields and concluded that Miller similitude ($\alpha_h = \alpha_K$) is not strictly valid for most field soils. Nevertheless, Miller similitude continues to be a premise for many recent numerical simulation studies (Russo, 1991; Tseng and Jury, 1994; Roth 1995). Jury et al. (1987) suggested that a complete description of the spatial variability of soil hydraulic properties will generally require at least three stochastic variates - K_s, α_h, and η, where $\eta = d\{\log[K(h_m)/K_s\} / \mathrm{d}[\log(-h_m)]$. They also noted that since their scaling factors were functions of water saturation, application of the scaling factors should be limited to the same range of water saturation as was used to estimate the scaling factors.

Rockhold et al. (1994) analyzed the hydraulic properties of the soils at the Las Cruces Trench Site and determined that the water retention characteristics of 448 core samples collected from the site could be represented almost as well using a single value of the Brooks-Corey model λ parameter ($r^2 = 0.97$) as using separate values of λ for each sample ($r^2 = 0.99$). The expressions for the scale-mean pressure head and hydraulic conductivity in (C-6) and (C-7) become independent of saturation for a single, common value of the Brooks-Corey model λ parameter. Being able to adequately represent the hydraulic properties of a spatially-variable soil using a single value of the Brooks-Corey model λ parameter is problematic, and will depend on the particular soil. Rockhold et al. (1994) also noted that the coefficients of variation for the Brooks-Corey model λ and θ_s parameters were significantly smaller than the coefficients of variation for K_s and h_{me}.

No measurements of the soil hydraulic properties were made on the experimental plots at the Las Cruces Trench Site where the field-scale flow and transport experiments were conducted. Measurements of the soil hydraulic properties were only made on core samples collected during excavation of an adjacent trench. Therefore no data were available for direct conditional simulation of the soil hydraulic properties used for simulation of the flow and transport experiments conducted at the site. Rockhold et al. (1994) used a simple conditional simulation method with soft data and the scale relations shown in (C-2), (C-3), and (C-6) to estimate hydraulic properties for simulations of the latest field-scale flow and transport experiment conducted at the Las Cruces Trench Site. The soft data consisted of the initial, field-measured water contents measured prior to the start of the experiment using a neutron probe, and an initial, depth-averaged pressure head distribution determined using measurements made just prior to the start of the experiment using tensiometers installed in the face of the trench.

The conditional simulation method consisted of the following steps. For each initial field-measured water content, a scaled pressure head, h^*_m, was calculated using a set of scale-mean water retention parameters corresponding to (C-6). A scaling factor, α_h, was then computed for each value of h^*_m, from the ratio

$$\alpha_h = \frac{h_m^*}{\widehat{h_{mi}}(z)} \qquad \text{(C-8)}$$

where h_{mi} (z) is the average initial pressure head for the measurement depth. Values of h_{me} and K_s were then estimated from the calculated scaling factors and the scale-mean hydraulic parameters, using (C-2) and (C-3), with uniform values of θ_s and the Brooks-Corey model λ parameter. Note, using uniform values of the θ_s and λ parameters facilitates application of the conditional simulation method but is not a necessary requirement.

Rockhold et al. (1994) showed that, although Miller similitude is not strictly valid for the soils at the Las Cruces Trench Site, the spatial correlation structures of the α_h and α_K scaling factors are quite similar. Using the assumption of Miller similitude in conjunction with the simple conditional simulation method described above resulted in a 40% reduction in the root-mean-squared (RMS) error for the observed versus predicted water content distributions relative to previous simulation results reported for the experiment (Hills and Wierenga, 1994). No model calibration was necessary to achieve these results.

The conditional simulation method described above was also used to estimate hydraulic properties for the arid site application example presented in Section 6.2. The water retention data from 92 samples reported by Andraski (1995) were fit simultaneously using a common value of the Brooks-Corey model λ parameter using multiple linear regression by the method of dummy variables (Draper and Smith 1981). The residual water content, θ_r, was assumed to be equal to 0 in order to obtain a reasonably good representation of the soil hydraulic properties at low water contents.

Field-measured water content and pressure head data from the USGS study site near Beatty, Nevada were used in conjunction with the set of scale-mean parameters determined from Andraski's (1995) data to condition the hydraulic properties used to represent the sediments underlying the hypothetical waste disposal trench. The initial water content and pressure head data were obtained from neutron probe and thermocouple psychrometer measurements made at the USGS study site near Beatty (Fischer, 1986). The psychrometer data were corrected for osmotic potential to obtain pressure head (unpublished data from Dave Prudic, USGS, Carson City, Nevada).

Rather than using a single, uniform value of θ_s, separate values of θ_s were estimated for each depth using the following optimization procedure. Values of h_m were first calculated that corresponded to the initial field-measured water contents using the values of h_{me} that were estimated using the conditional simulation method described above, with a single, uniform value of θ_s equal to the geometric mean value of θ_s determined from Andraski's data. If the calculated values of h_m did not match the measured initial value of h_{mi} for the measurement depth, θ_s was optimized to obtain a match (within a prescribed error tolerance) using Newton's method. It should be noted that care should be taken when using this optimization step to ensure that the optimized values of θ_s fall within the range of measured values used to estimate the scale-mean parameters. Values of K_s were estimated from (C-3) using the geometric mean value of K_s determined from Andraski's data as the scale-mean value.

C.2 References

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