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Title: MODELING OF AN EVAPOTRANSPIRATION COVER FOR THE GROUNDWATER PATHWAY AT LOS ALAMOS NATIONAL LABORATORY TECHNICAL AREA 54, MATERIAL DISPOSAL AREA G

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Acronyms and Abbreviations

1-D	One-dimensional
2-D	Two-dimensional
3-D	Three-dimensional
ET	Evapotranspiration
GIS	Geographic information system
HELP	Hydrologic Evaluation of Landfill Performance
ITP	Integrated Test Plots
Laboratory	Los Alamos National Laboratory
LANL	Los Alamos National Laboratory
MDA	Material Disposal Area
RCRA	Resource Conservation and Recovery Act
TA	Technical Area
TDR	Time domain reflectometry

Acknowledgements

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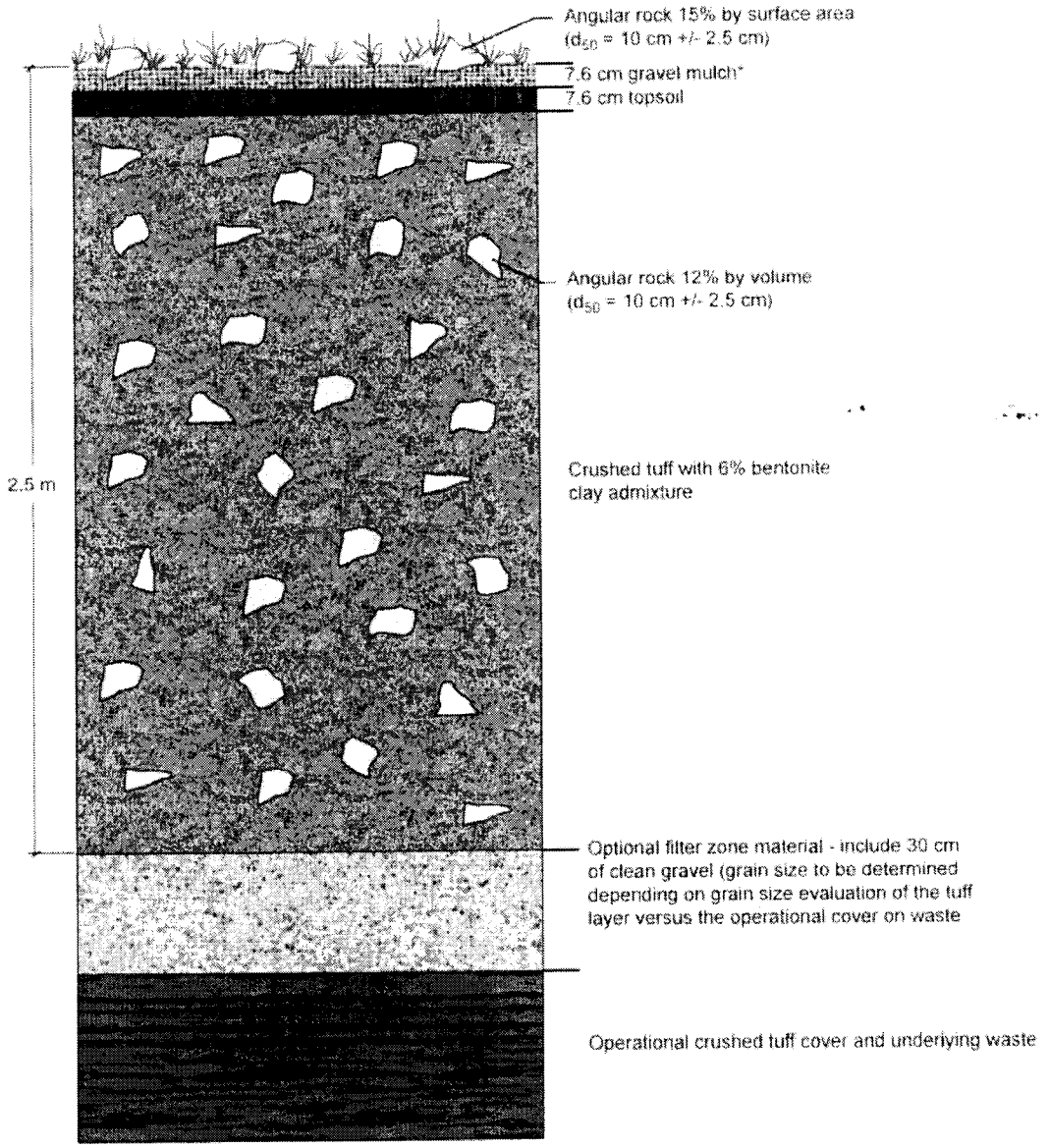
1.0 Introduction

A landfill cover system is being considered for installation as part of the closure process at the Los Alamos National Laboratory, Technical Area (TA-) 54, Material Disposal Area (MDA) G, Low-Level Radioactive Waste Site. Landfill covers are one of the most common management approaches for reducing risks from buried waste sites. Covers serve two primary risk reduction roles. First, they serve as a barrier between the waste and the surface environment, thus reducing the potential for waste exposure by erosion and transport of wastes to the surface by flora and fauna. Second, landfill covers reduce the downward movement of water into and below the waste zone. This decrease in downward flux is expected to reduce the rate of waste container degradation and downward transport of contaminants to the groundwater system. The modeling and analysis discussed in this report focus on estimating the downward flux of water through the cover and into the waste zone.

For this assessment, the performance of the monolithic evapotranspiration (ET) cover for MDA G described in Day et al. (2005) was examined (Figure 1). Evapotranspiration covers are intended to provide water storage sufficient to contain spring snowmelt within the cover until it is used through ET later in the year. The cover design proposed for MDA G has a variable thickness with a minimum 2.5-m (8.2-ft) thick cover over the waste. The cover is composed of crushed Bandelier Tuff mixed with 6 percent bentonite and 12 percent angular cobbles, and has a shallow surface zone designed to promote plant growth. Additional information on the general performance of ET covers can be found in Bonaparte et al. (2004), ITRC (2003), Nyhan (2005), and Scanlon et al. (2002).

The remainder of this report describes the approach, results, and conclusions of this study. An overview of the HYDRUS software package selected for the modeling, a discussion of the input data used to conduct the model simulations, and information about model sensitivity to variations in conditions are provided in Section 2. The results of the modeling are presented in Section 3; these results and the uncertainties related to the modeling are discussed in Section 4.



*Gravel mulch is 1/2" minus pea gravel intermixed with topsoil

Figure 1
Cross Section of Proposed Evapotranspiration Cover
Source: Day et al., 2005

2.0 Methods

Three major considerations for this study were the selection of an appropriate modeling package, the selection of representative input datasets, and the sensitivity of the model to variations in conditions such as cover thickness and initial soil pressure. This section explains why specific choices were made and discusses the efforts made to constrain model sensitivity.

2.1 Selection of the HYDRUS Model

Many software packages are available for evaluating landfill cover performance; the HYDRUS model (Simunek et al., 1998 and 1999) was selected for this study. The HYDRUS model is based on Richards' equation (the theoretical equation for vertical unsaturated flow) and allows for the analysis of water flow and solute transport in variably saturated porous media. The reasons for this selection and the basic characteristics of the HYDRUS package are presented below.

The Hydrologic Evaluation of Landfill Performance (HELP) model (Schroeder et al., 1994) is often used for landfill cover modeling. However, recent literature (Albright et al., 2002; Scanlon et al., 2002), the draft EPA alternative cover guidance (Bonaparte et al., 2004), and ITRC cover guidance (2003) all indicate that HELP is a poor choice for modeling ET and capillary-barrier covers, especially in semiarid environments. This is mainly because the HELP model is not based on Richard's equation and thus cannot properly represent the dynamics of water content changes and fluxes, particularly under dry climate conditions. Also, HELP is limited to one-dimensional (1-D) or pseudo two-dimensional (2-D) modeling.

Other landfill performance models based on the Richards' equation (e.g., UNSAT-H) could have been selected for this study; however, using HYDRUS offered several advantages. First, 2-D and three-dimensional (3-D) versions of HYDRUS (HYDRUS-2D and HYDRUS-3D) are available, and future studies at MDA G may require 2-D or 3-D modeling. In fact, HYDRUS-2D (Simunek et al., 1999) was used in an early phase of this study. Second, models are more easily developed and implemented using HYDRUS because of its graphical interface. Third, the opportunity existed to discuss the modeling approach and results directly with the author of the HYDRUS package (J. Simunek, University of California, Riverside). Finally, recent versions of the code have received excellent reviews by the scientific community (Selker, 2004).

Most of the modeling work undertaken to evaluate cover performance at MDA G was conducted with HYDRUS-1D, version 3.0 (Simunek et al., 1998). HYDRUS-1D uses a finite-element approach for simulating the one-dimensional movement of water, heat, and multiple solutes in variably saturated media. Consequently, it is used extensively to address a wide variety of waste disposal and other hydrologic problems that require consideration of variably saturated porous media. HYDRUS numerically solves the Richards' equation for saturated-unsaturated water flow

and Fickian-based advection-dispersion equations for heat and solute transport. The water flow part of the model, which was the feature of HYDRUS used specifically for this study, can address constant or time-varying prescribed head or flux boundaries, boundaries controlled by atmospheric conditions, and free-drainage boundary conditions. The flow region in HYDRUS can include nonuniform soils. Unsaturated soil hydraulic properties can be described using a variety of analytical functions (e.g., van Genuchten-type parameters) and both evaporation and root water uptake (transpiration) can be modeled. The HYDRUS package has been extensively tested, used for regulatory-based assessments, and used for research. Additional information on the HYDRUS modeling package can be found in the HYDRUS-1D manual (Simunek et al., 1998).

2.2 Input Data

The HYDRUS model requires various input parameters to define the atmospheric boundary conditions for the simulations and to specify the hydraulic properties of the cover materials. This section discusses the data selected to characterize these parameters.

2.2.1 Atmospheric Input Data

The atmospheric input data (e.g., site-specific precipitation and potential ET time-series values) are important controls on how well a landfill cover model actually represents cover performance (Bonaparte et al., 2004; ITRC, 2003). These data can be a key source of uncertainty, especially in semiarid environments where the ET and precipitation are of similar magnitudes, and precipitation is highly variable in time and space. Because of the importance of the atmospheric input data to the modeling, substantial effort was spent in determining the best approach for constraining the atmospheric boundary in HYDRUS. The objective of this effort was to develop input data that accurately represented the site under current climatic conditions.

The paramount concern in developing atmospheric input data was to constrain ET, as this is often where the greatest uncertainty exists. Overestimation of ET leads to underprediction of downward fluxes (seepage) and vice versa. Four different approaches for estimating ET were examined by Simunek and McTiver (2004) using data from the ET cover studies of Nyhan (2005) and Nyhan et al. (1997); these evaluations are described below.

Nyhan (2005) and Nyhan et al. (1997) conducted a multiyear study of an ET cover design on Mesita del Buey at a location just west of MDA G. The general configuration of the cover design that was evaluated and some aspects of the experimental design are shown in Figure 2. The Nyhan and Nyhan et al. research provides an excellent basis for examining different approaches for predicting ET at the disposal facility because of the study location's close proximity to MDA G. Furthermore, experimental data were collected on a daily basis and, as such, provide a detailed record of site conditions.

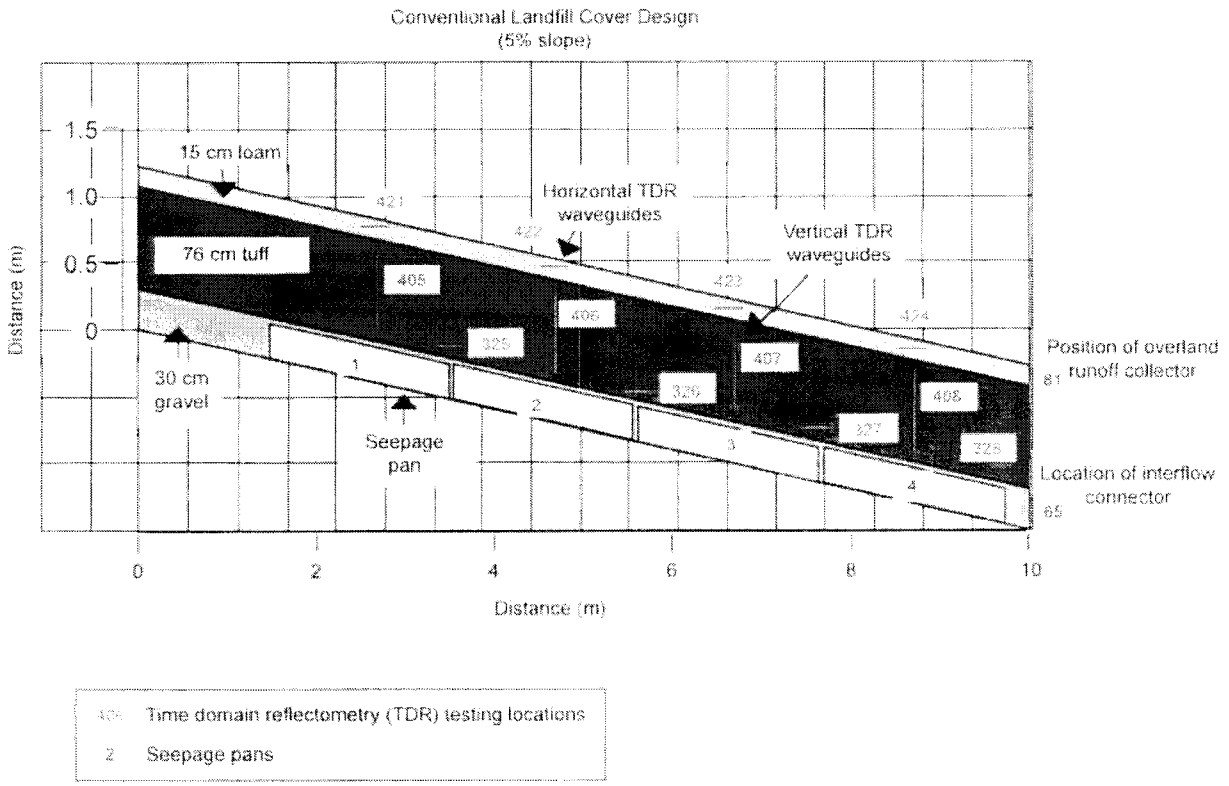


Figure 2
Cross Section of Conventional Landfill Cover Design with 5 Percent Slope

Source: Based on studies by Nyhan (2005) and Nyhan et al. (1997)

Using daily total precipitation and other meteorological data collected at the experimental site described in Nyhan (2005), Simunek and McTiver (2004) conducted simulations to determine which of four approaches to constraining ET yielded results that best matched the Nyhan water content profiles, seepage, and interflow (side drainage) data. The four approaches estimated daily ET using (1) the water balance equation to calculate ET directly from the 1993 experimental data (as reported in Nyhan, 2005), (2) the original version of the Penman-Monteith equation (Monteith, 1965 and 1981), (3) the combination Penman-Monteith formula (FAO, 1990), and (4) eddy covariance data collected at the Los Alamos, TA-6 meteorological station (see <http://weather.lanl.gov/>). The Penman-Monteith approaches calculate "potential" ET, or the maximum amount of water that can be lost to evapotranspiration under given atmospheric conditions. The other two methods yield "actual" ET values, which may be less than potential ET because of factors such as the depth of the evaporation front in the soil. Although each of the four approaches has associated problems (Simunek and McTiver, 2004), they currently represent the best means of constraining ET. For comparison purposes, cumulative ET values for 1993, determined with each of the four methods, are plotted in Figure 3.

Simunek and McTiver used HYDRUS-2D because the Nyhan experimental design had capillary barrier effects that caused interflow in addition to downward flow. Daily precipitation and other parameters were held constant to allow the effect of the different ET datasets to be readily seen. Direct (forward) and inverse modeling were used to evaluate the four ET approaches using the 1993 data reported in Nyhan (2005). For the direct simulations, the Nyhan experimental ET data (approach 1) yielded reasonable predictions of water content. However, the simulation did not predict seepage and, although it did predict interflow, the flux was underestimated. Both seepage and interflow occurred in the actual field experiment. The two Penman-Monteith approaches greatly underpredicted water contents, failed to predict seepage, and predicted only minor interflow. The eddy covariance approach severely overpredicted water contents, seepage, and interflow.

HYDRUS provides an inverse simulation option that allows the user to input certain properties while the program optimizes others. This option was used as an additional check on how well the four different ET estimation approaches could represent actual conditions. Under this option, HYDRUS estimates water contents and seepage and interflow fluxes using an initial set of hydrologic properties (taken from Nyhan, 1997) and compares predicted water content and fluxes to the observed values reported by Nyhan (2005). The program then varies the hydrologic properties until the sums of squares of the residuals between the observed and predicted water contents and fluxes are minimized. Thus, the model is run many times to find the "optimal" set of hydrologic properties that best fit the observed data. If the inverse simulation results for a given ET dataset show that only minor adjustments of hydrologic properties are needed and that seepage and interflow fluxes can be reasonably simulated, this provides additional evidence that a given ET dataset is likely a reasonable representation of actual ET values.

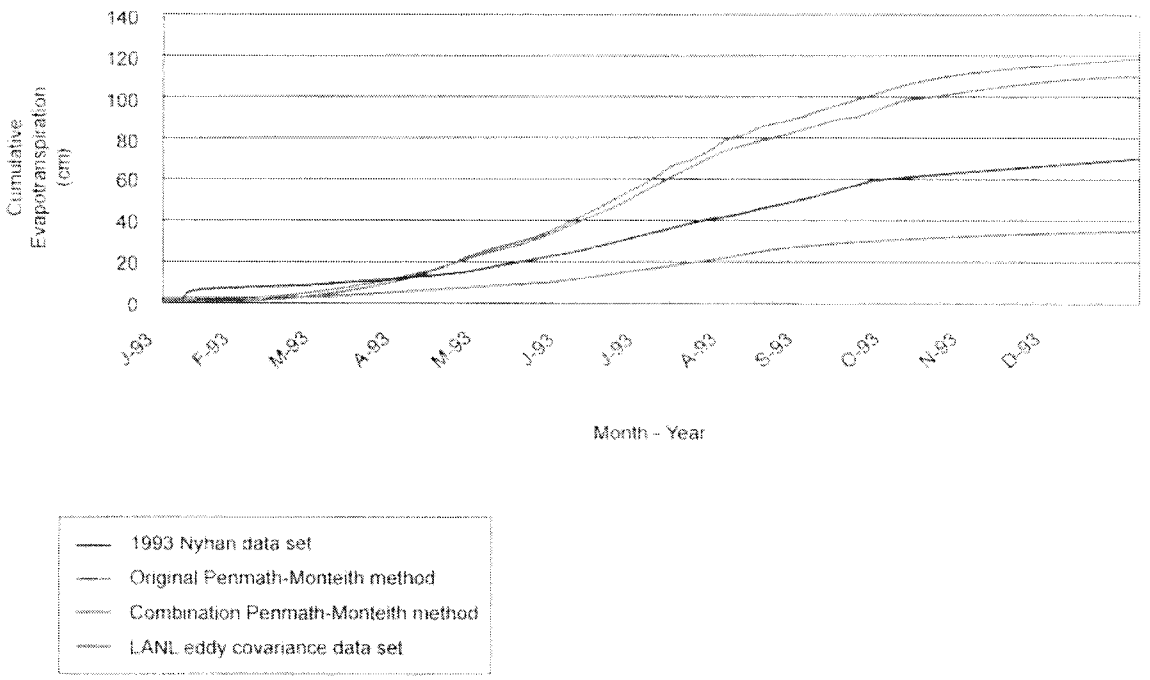


Figure 3
Comparison of Methods for Predicting Evapotranspiration Values at Material Disposal Area G (experimental cover data from 1993)

The inverse simulations using the Nyhan experimental ET data (approach 1) resulted in good matches for water content, cumulative seepage, and cumulative interflow (Figure 4) and the optimized parameters using the Nyhan experimental data were not significantly different than the measured hydraulic properties. The Nyhan-data inverse simulations did, however, underpredict water contents in the region just above the crushed tuff/gravel contact during the two wet periods, which occurred just after 200 and 400 days (Figure 4a). The inverse results for the two Penman-Monteith simulations were less successful in simulating the observed water contents and the optimized parameters for these approaches differed greatly from measured properties. The results from the original Penman-Monteith equation (approach 2) are shown in Figure 5; it is evident that the calculated and measured water contents do not match, especially during and after the two wet periods (Figure 5a). Also, although the occurrence of seepage and interflow were predicted (Figures 5b and 5c), the Penman-Monteith approach did not accurately simulate the timing of the flows as shown in Figure 5c. The results of the inverse simulation using the eddy covariance data showed the greatest discrepancy with the measured data (Figure 6). Water contents, seepage, and interflow were all overpredicted and optimized values were physically unrealistic. Additional discussion and details of the inverse modeling results can be found in Simunek and McTiver (2004).

The Penman-Monteith approach is commonly used to constrain ET for landfill-cover performance modeling. However, as shown by the forward simulations, this approach can result in overestimation of ET which, in turn, results in lower estimated downward and lateral fluxes. This is clearly not representative or conservative in terms of the groundwater risk pathway. In addition, the poor inverse modeling results suggest that this approach is problematic for use at MDA G.

Eddy covariance is considered to be one of the most accurate approaches for measuring ET if the energy balance error can be adequately reduced. It was hoped that the eddy covariance data would effectively constrain the atmospheric boundary condition because multidecadal atmospheric records including actual ET could be generated for Los Alamos. However, the HYDRUS modeling shows that the eddy-covariance-based ET data from Los Alamos are problematic and likely underestimate actual ET by significant amounts. The annual and monthly differences between measured precipitation and predicted ET were calculated and it was found that annual precipitation systematically exceeded annual ET, sometimes by a large amount. (data not shown). This difference is clearly not correct for a semiarid climate such as Los Alamos, and provides further confirmation that the ET values are probably underestimated. The possibility of correcting the ET values was considered, but consultation with a micrometeorologist indicated this is essentially an impossible task because of the nature of the errors in the latent heat determinations (Cooper, 2004).

Figure 4a Calculated and measured volumetric water contents

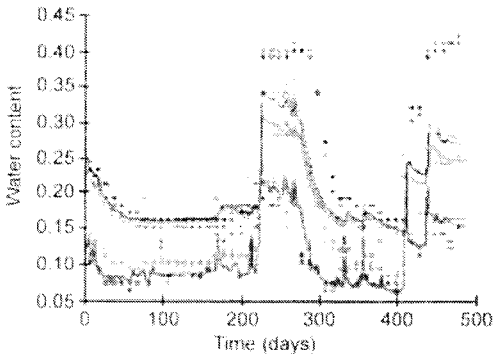


Figure 4b Cumulative seepage flux

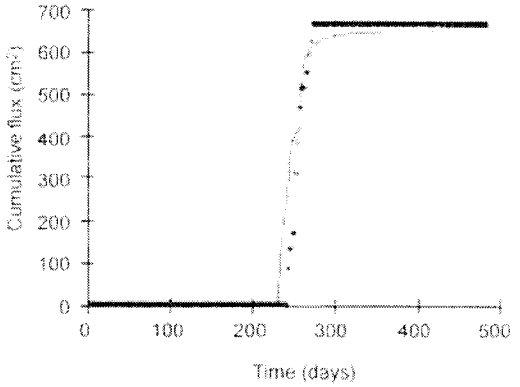
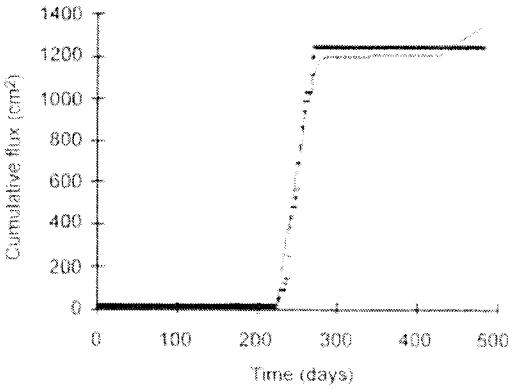


Figure 4c Cumulative interflow (side drainage)



•	= Observed values
———	= HYDRUS-predicted values
═══	= Values within the loam topsoil
·····	= Values in the middle of the crushed tuff layer
═══	= Values just above crushed tuff/gravel contact

Figure 4
Selected Results of Inverse Simulation for Evaluation of Evapotranspiration (based on data from Nyhan, 2005)

Figure 5a Calculated and measured volumetric water contents

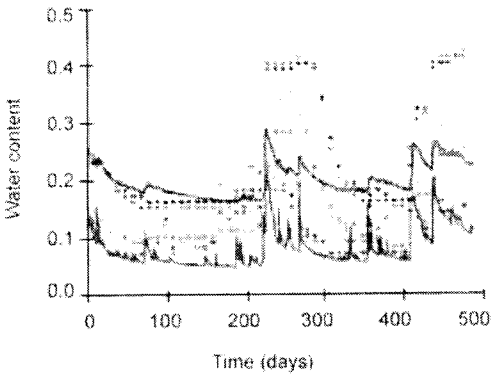


Figure 5b Cumulative seepage flux

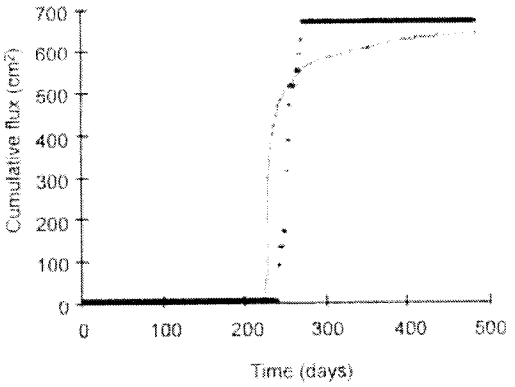
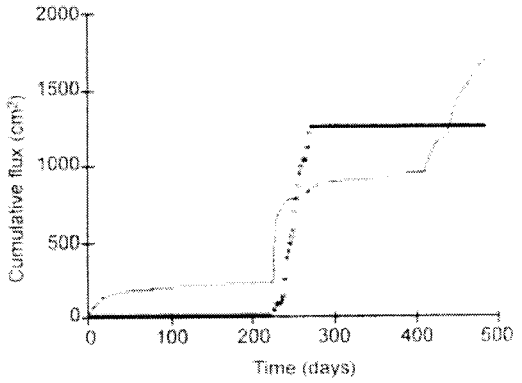


Figure 5c Cumulative interflow (side drainage)



•	= Observed values
———	= HYDRUS-predicted values
═══	= Values within the loam topsoil
·····	= Values in the middle of the crushed tuff layer
═══	= Values just above crushed tuff/gravel contact

Figure 5
Selected Results of Inverse Simulation for Evaluation of Evapotranspiration (based on original Penman-Monteith formulation)

Figure 6a Calculated and measured volumetric water contents

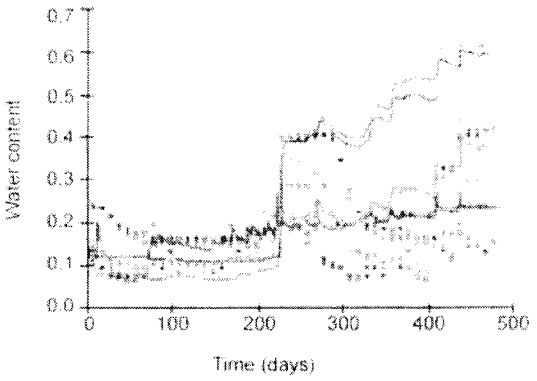


Figure 6b Cumulative seepage flux

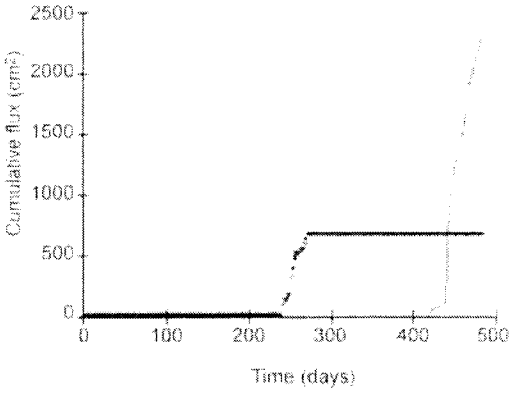
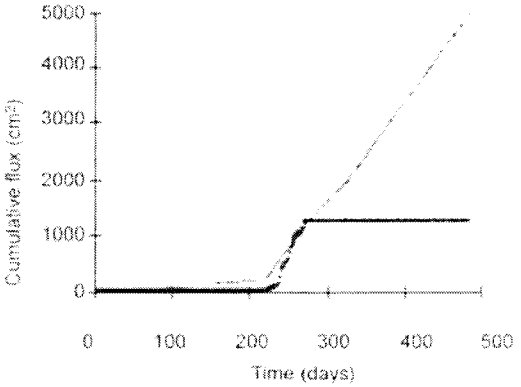


Figure 6c Cumulative interflow (side drainage)



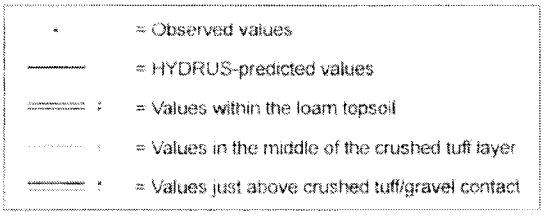


Figure 6
Selected Results of Inverse Simulation for Evaluation of Evapotranspiration (based on Los Alamos eddy covariance data)

In short, the 5-year-long, water-balance-derived ET dataset from Nyhan's cover demonstration plot (approach 1) appears to be the most representative for use at MDA G. Although not perfect, when compared to the data available for many other landfill-cover studies, these data are excellent for defining the atmospheric boundary conditions. The HYDRUS inverse modeling shows that these data can reasonably reproduce very complex cover behaviors including dynamic water content changes, interflow, and seepage. One disadvantage of using these data to model ET is that they cover only 5 years. Nevertheless, during this 5-year period, annual precipitation ranged from about 36 to 46 cm (14 to 18 in.) compared to the long-term average annual precipitation for MDA G of about 37 cm (15 in.) (Bowen, 1990). Although one of the years (1998) had precipitation that was slightly below average at 36 cm (14 in.), all other years had above average precipitation. Thus, even though the dataset does not adequately capture the local long-term variability in climate, it does appear to represent average or slightly above-average conditions. Another limitation to using the water-balance-derived approach is that it provides actual ET rather than potential ET. (The HYDRUS model is designed to use potential ET as input and then to calculate actual ET based on hydraulic properties.) Despite this inconsistency, however, the above analysis supports the use of the data from this approach.

As a further check on the influence of the atmospheric boundary data, simulations of the MDA G cover were conducted using experimental data from an earlier set of landfill cover experiments (Nyhan et al., 1990). These experiments, known as the Integrated Test Plots (ITP), were conducted over a 9-year period from 1985 through 1993. Daily precipitation records for the experimental period were obtained, but the ET data were available only as cumulative ET over 2-week periods. To build a daily time series, ET values were apportioned evenly for each of the 14 days. This led to an artificial step-type appearance to the data. However, over longer time scales, it was thought that this approximation would not severely affect the results.

Simulations based on the ITP data yielded higher ET rates than did the 1993 experimental data reported in Nyhan (2005). Thus, the ITP data appear to be slightly less conservative than the newer data. This result, in conjunction with the lower resolution of the ET data and water content measurements found in the ITP dataset, led to the adoption of the Nyhan (2005) cover-study data as the primary source for HYDRUS modeling of the MDA G cover. Thus, HYDRUS-1D simulations of the MDA G cover design were conducted using the 5-year atmospheric dataset supplemented by a few 9-year simulations using the ITP dataset. Additional 1,000-year simulations were conducted by repeatedly concatenating the 5-year dataset to build a 1,000-year-long time series.

2.2.2 Hydraulic Properties

The hydraulic properties (e.g., saturated hydraulic conductivity and the van Genuchten parameters) of the materials used in the cover are a major control on the rate at which water

flows through the disposal facility. Two cover materials were modeled in this study: a top layer that consists of crushed tuff with 6 percent bentonite, and a lower layer that consists solely of crushed tuff. The lower, crushed tuff layer was included to represent the operational cover placed over disposal units during interim closure and, in some cases, the underlying waste (Figure 1).

The values used for the hydraulic properties of the crushed tuff layer were reported in van Genuchten (1987). Unfortunately, no measurements are available for the 6 percent bentonite and crushed tuff mixture included in the MDA G cover design. Consequently, the properties for this layer were estimated using several approaches.

One of the interesting things that happens when crushed tuff is mixed with small percentages of bentonite is that the saturated hydraulic conductivity (K_s) decreases dramatically. A typical K_s value for crushed tuff is about 1×10^{-4} cm/s (3.3×10^{-5} ft/s). However, with the addition of 10 percent bentonite, the K_s can decrease by four orders of magnitude (Nyhan et al., 1997). In fact, a 10-percent-bentonite addition reduces the conductivity to such an extent that the resultant crushed tuff/bentonite material is equivalent to the "impermeable" clay layer used in the U.S. Environmental Protection Agency (EPA) Resource Conservation and Recovery Act (RCRA) cover design (Nyhan et al., 1997).

In terms of the current study, it was necessary to determine how the 6-percent-bentonite addition affects the hydraulic conductivity and other hydraulic properties of the upper layer of the modeled cover. Abeele (1984) conducted a laboratory and modeling study of crushed tuff mixtures with various proportions of bentonite and presents two models for predicting K_s at various compactions for a given percentage of bentonite. When used to estimate K_s for the 6-percent-bentonite admixture, these models yielded values ranging from 2.9×10^{-8} to 5.6×10^{-8} cm/s (9.5×10^{-10} to 1.8×10^{-9} ft/s). Nyhan et al. (1997) reported a K_s value of 6.3×10^{-8} cm/s (2.1×10^{-9} ft/s) for a 10-percent-bentonite/tuff mixture, which suggests that the Abeele (1984) estimates may be low. To examine this, a linear regression was fit between the K_s values for pure crushed tuff and the value for the 10-percent-bentonite mixture reported in Nyhan et al. (1997). The estimated result for the 6-percent-bentonite/crushed tuff mixture was 1.1×10^{-6} cm/s (4.3×10^{-7} in./s). Because this was the highest estimated K_s value, it was selected for use in the HYDRUS modeling.

This linear regression approach was also used to estimate the water content at saturation, the residual water content, and the van Genuchten α and n parameters. These parameters are used to estimate unsaturated hydraulic conductivities under varying water content conditions. The linear regression approach was pragmatic, given that there were data for only two crushed tuff/bentonite mixtures and that all of these properties are highly nonlinear. The approach was discussed with Rien van Genuchten from the George E. Brown, Jr. Salinity Laboratory (operated by the U.S. Department of Agriculture), who concurred that estimation using linear regression

was probably the best available approach given the lack of measurements (van Genuchten, 2004). The hydraulic properties used in the simulations are shown in Table 1.

Table 1
Hydraulic Properties Used in the HYDRUS-1D Simulations

Material	Residual Water Content	Saturated Water Content	van Genuchten Parameters		Saturated Hydraulic Conductivity (m/d)
			α	n	
1- Crushed Tuff with 6% Bentonite	0	4.0E-01	5.6E-02	3.0E+00	9.3E-04
2- Crushed Tuff	1.0E-02	3.3E-01	1.4E+00	1.5E+00	2.5E-01

The hydraulic properties developed for the crushed tuff/bentonite layer are highly uncertain, the impacts of which are discussed in Section 4. A series of crushed tuff/bentonite mixtures has been submitted for analysis to the George E Brown, Jr. Salinity Laboratory for hydraulic properties analysis. However, the data will not be available until late 2005.

Gravel and cobble are also included in the cover design (Figure 1) and may affect the hydraulic behavior of the cover. However, the effects of the gravel and cobble additions were not modeled. Approaches do exist that allow hydraulic properties to be adjusted for the addition of gravel, but given the large uncertainties related to the values for the basic properties of the 6-percent-bentonite cover, the examination of the effects of gravel mixtures was deferred until the laboratory analyses of the crushed tuff/bentonite mixtures become available.

A topsoil and optional gravel layer are also shown in Figure 1. These features were not included in the HYDRUS modeling for several reasons. First, these layers were not included in the landscape evolution model for the MDA G performance assessment and composite analysis (Wilson et al., 2005), and the decision was made to preserve consistency between the surface and cover modeling efforts. In addition, the topsoil layer is identical to the crushed tuff/bentonite material in the main cover layer except that it is amended with soil "pep," a ground bark material to support plant establishment. Thus, the topsoil layer should be more similar hydrologically to the crushed tuff/bentonite mixture that was modeled than to topsoil. Once the laboratory analysis of the crushed tuff/bentonite mixture is completed, subsequent HYDRUS modeling will include the topsoil layer. Simulations with and without the optional gravel layer can also be run; however, this will require 2-D modeling because of the strong potential for capillary barrier effects and interflow generation.

2.3 Simulations Using Variable Conditions

Simulations were run to explore the effect of variations in the crushed tuff/bentonite layer thickness, total profile thickness, initial pressure head, and plant uptake on downward flux. To predict the effect of cover thickness on flux, both the thickness of the crushed tuff/bentonite layer and of the total profile were varied. Thicknesses of 1 and 5 m (3.3 and 16 ft) were selected to represent the topmost (crushed tuff/bentonite) layer of the modeled cover. This range was chosen on the basis of the cross section of a long slope length cut from the geographic information system (GIS) cover model (Wilson and Crowell, 2005) and is expected to generally encompass the remaining thicknesses of this cover layer at the site after 1,000 years of surface erosion. The total profile thickness was varied between 2 and 15 m (6.6 and 16 ft) to assess the impact of variable backfill conditions at the site. Simulations for 5- and 1,000-year periods were performed using the daily atmospheric boundary data collected by Nyhan (2005), as described in Section 2.2.1. In addition, 9-year simulations were made using the ITP data.

Because of the large uncertainties associated with hydraulic properties at present, no sensitivity analysis of the effect of these properties was performed; such analysis has been deferred until measured hydraulic properties of the crushed tuff/bentonite material are available from the George E Brown, Jr. Salinity Laboratory. The effects of two different initial pressure head conditions were determined by conducting simulations with a -1 m (-3.3 ft) initial condition (representing wet, but not saturated conditions) and a -10 m (-33 ft) initial condition (representing a drier condition).

Most simulations involved removal of water through ET directly from the surface of the cover. However, because plants will also cause water removal to occur within the cover, a few simulations were made using the HYDRUS root uptake feature (Simunek et al., 1998). The Feddes root uptake model was used to represent a generic grass cover; this model was recommended by J. Simunek over the S-shaped model (the other root uptake model included in HYDRUS; see Simunek et al., 1998 and 1999 for more information) as more appropriate for the MDA G simulations (Simunek, 2005). As a starting point for the plant uptake simulations, 50 percent of the total ET was arbitrarily assigned to evaporation and 50 percent to transpiration.

3.0 Results

The HYDRUS modeling included short-term (5- and 9-year) and long-term (1,000-year) simulations, as described above. The 5-year simulations use the ET data documented in Nyhan (2005); these data were concatenated repeatedly to build the 1,000-year time series. The 9-year simulations use ET data from the ITP experiment of Nyhan et al. (1990). The results of the simulations are described below.

3.1 Short-Term Simulations

Average annual fluxes for the 5- and 9-year simulations are shown in Table 2. Fluxes range from 0.05 to 0.19 cm/yr (0.02 to 0.075 in./yr) and were determined by dividing the cumulative amount of water leaving the bottom of the profile by the number of years that the simulation was run (in this case, 5 or 9 years). The 9-year results, conducted using the ITP dataset, were comparable to the 5-year results, but the flux was slightly lower (Table 2, simulations 1 and 4). This difference can be attributed to the slightly lower precipitation-to-ET ratio that was observed in the ITP data.

Table 2
Average Annual Flux for 5- and 9-Year Simulations

Simulation [a]	Thickness (m)		Flux (cm/yr)
	Cover (6% bentonite)	Cover Plus Underlying Crushed Tuff	
5-Year Simulations			
1	1	2	7.0E-02
2	5	15	1.9E-01
3 [b]	1	2	7.0E-02
9-Year Simulations			
4	1	2	5.0E-02
5	1	3	1.0E-01
6	1	6	1.6E-01

[a] *All simulations run with an initial pressure head of -10 m*

[b] *Simulation 3 included root uptake modeling*

Typical results for the 5-year simulations are shown in Figures 7 through 9. These results, plotted from the simulation 1 data shown in Table 2, represent a 1-m (3.3-ft) thick layer of crushed tuff/bentonite overlying 1 m (3.3 ft) of crushed tuff. The effects of the time-varying atmospheric boundary condition can be seen in Figure 7. This figure represents the daily net flux through the surface (top) of the profile, with negative flux indicating the removal of water from the cover. Values oscillate around zero depending on whether precipitation or ET was greater on a given day. Variations in water content through time are shown in Figure 8, in which the effect of the two different cover materials is clear from the sharp transition at a depth of 1 m (3.3 ft). Cumulative water at the bottom of the profile (i.e., total water passing through the bottom boundary of the profile over the simulation period) during the 5-year simulation is shown in Figure 9. The nonlinear cumulative water plot indicates that steady-state conditions (i.e., a near constant flux over time) were not quite reached.

3.2 *Long-Term Simulations*

The compliance period of the MDA G performance assessment and composite analysis is 1,000 years. Consequently, a series of 1,000-year simulations was conducted; the atmospheric data series for these simulations was generated by concatenating the 5-year datasets as discussed in Section 2.2. The average annual flux results for these simulations are shown in Table 3. Values were generally lower than fluxes for the 5-year simulations, ranging from 0.003 to 0.07 cm/yr (0.001 to 0.03 in./yr).

Table 3
Average Annual Flux for 1,000-Year Simulations

Simulation	Thickness (m)		Initial Pressure Head (m)	Flux (cm/yr)
	Crushed Tuff / Bentonite Layer	Crushed Tuff / Bentonite Layer Plus Underlying Crushed Tuff		
7	1	2	−10	3.0E−03
8	5	6	−10	5.0E−03
9 [a]	1	2	−10	8.0E−03
10	1	6	−10	9.0E−03
11	1	2	−1	1.2E−02
12	5	6	−1	1.8E−02
13	1	6	−1	7.0E−02

[a] *Simulation 9 included root uptake modeling*

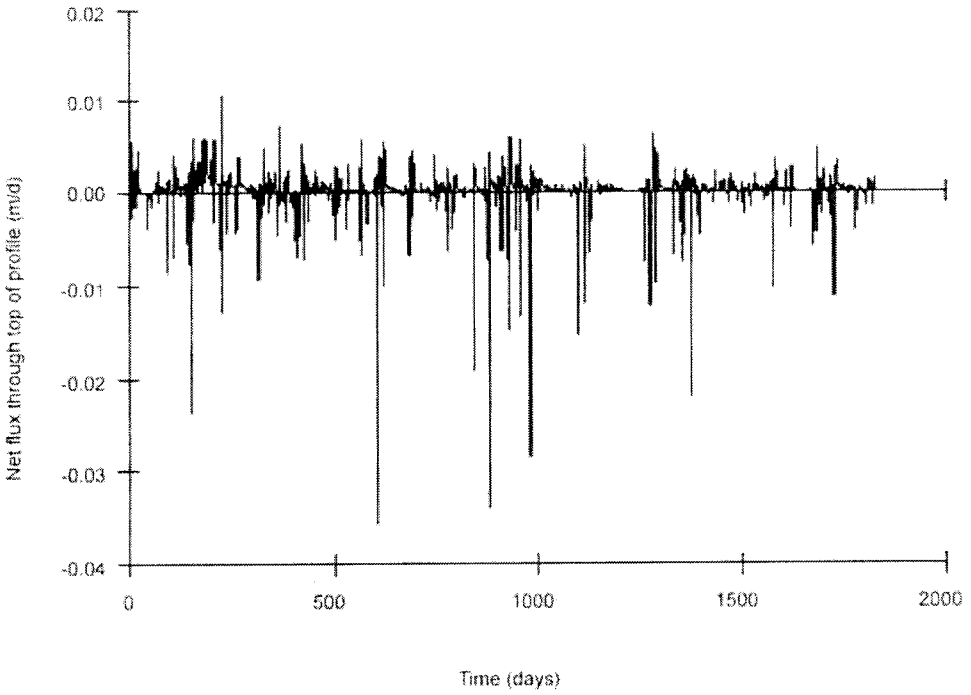


Figure 7
Daily Surface Fluxes for HYDRUS Simulation 1
(5-year simulation)

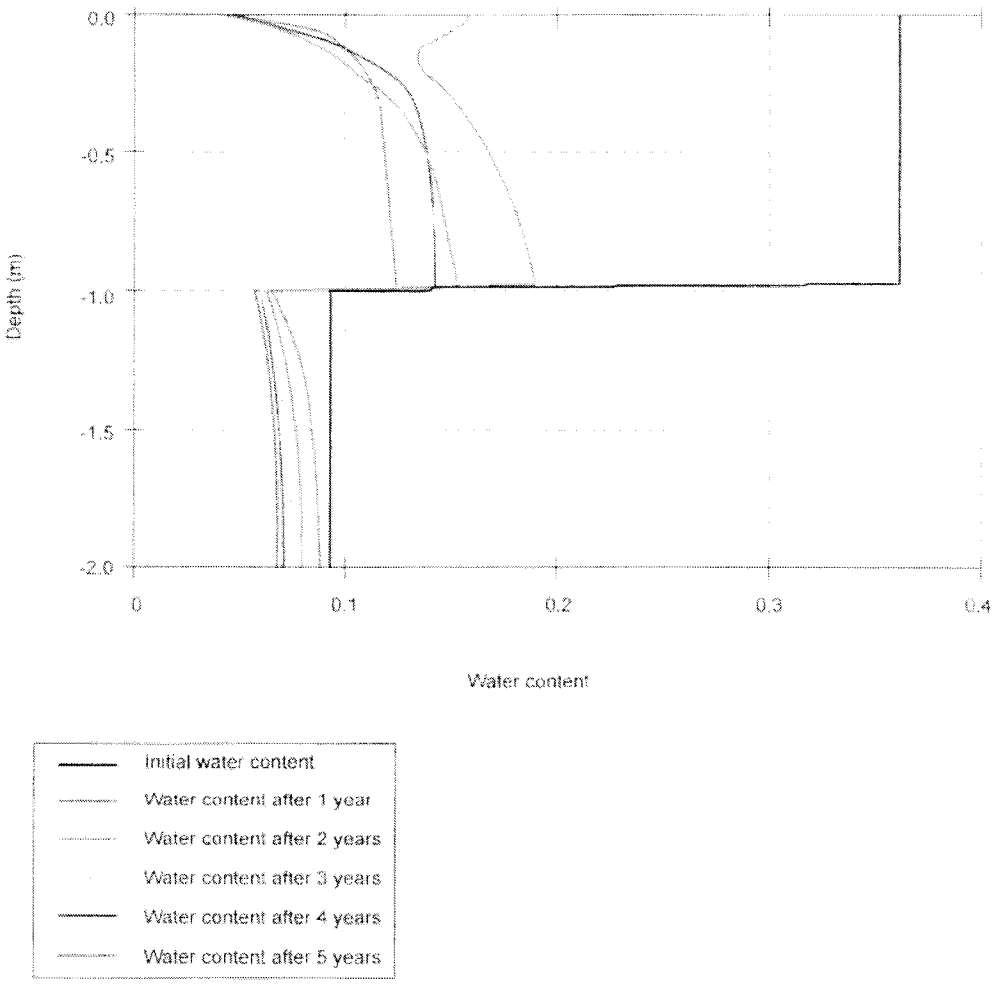


Figure 8
Water Content Profiles for HYDRUS Simulation 1
(5-year simulation)

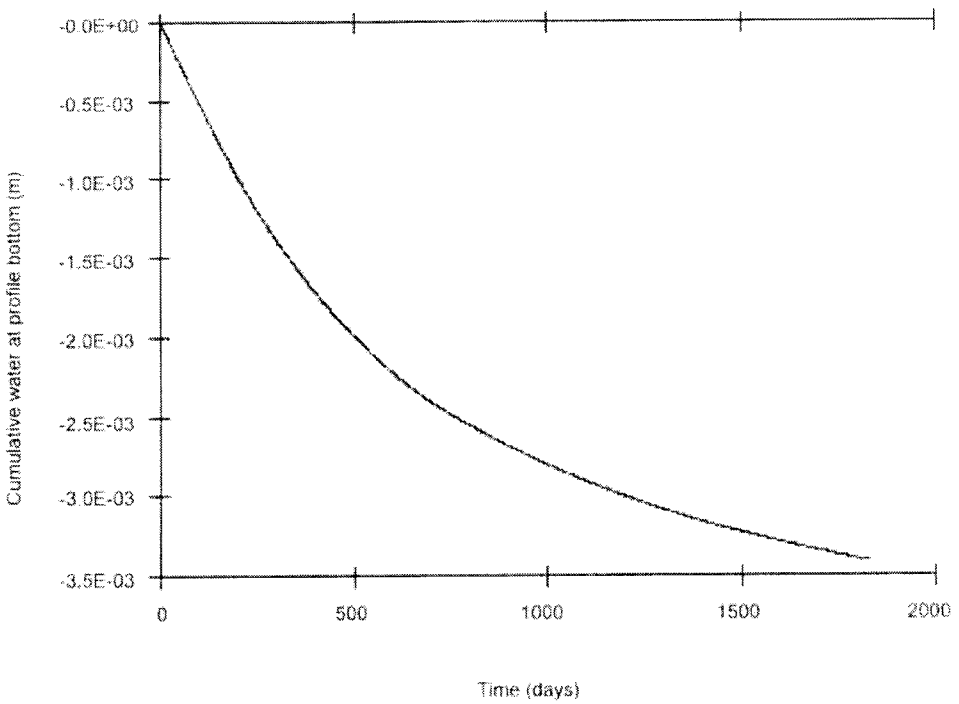


Figure 9
Cumulative Water at Bottom of Profile for HYDRUS Simulation 1
(5-year simulation)

Typical results for the 1,000-year simulations, based on data from simulation 11 (Table 3), are shown in Figures 10 through 12. Simulation 11 represented a 1-m (3.3-ft) thick cover overlying 1 m (3.3 ft) of crushed tuff. The effects of the time-varying atmospheric boundary condition on surface fluxes can be seen in Figure 10. Variations in water content through time are shown in Figure 11; as with the 5-year simulation shown in Figure 8, this figure shows a marked contrast in water content at the interface between the crushed tuff/bentonite layer and the underlying crushed tuff/waste. Cumulative water at the bottom of the profile over the 1,000-year simulation period is shown in Figure 12. This cumulative water plot indicates that steady-state conditions (near-linear changes in water leaving the bottom of the profile over time) were achieved over most of the simulation period. Because a low steady-state flux was reached, the average annual fluxes tended to be lower than in the 5-year simulations (Table 3). In other words, the 5-year simulations were dominated by the higher fluxes during the initial drainage phase of the profile, whereas the 1,000-year simulations were more influenced by the long-term, steady-state conditions.

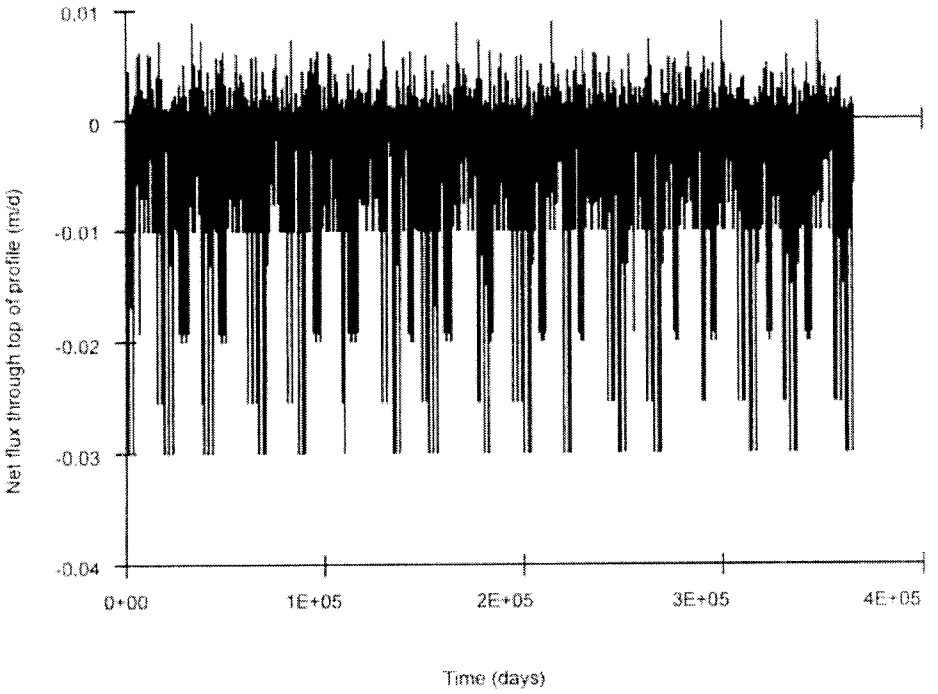


Figure 10
Daily Surface Fluxes for HYDRUS Simulation 11
(1,000-year simulation)

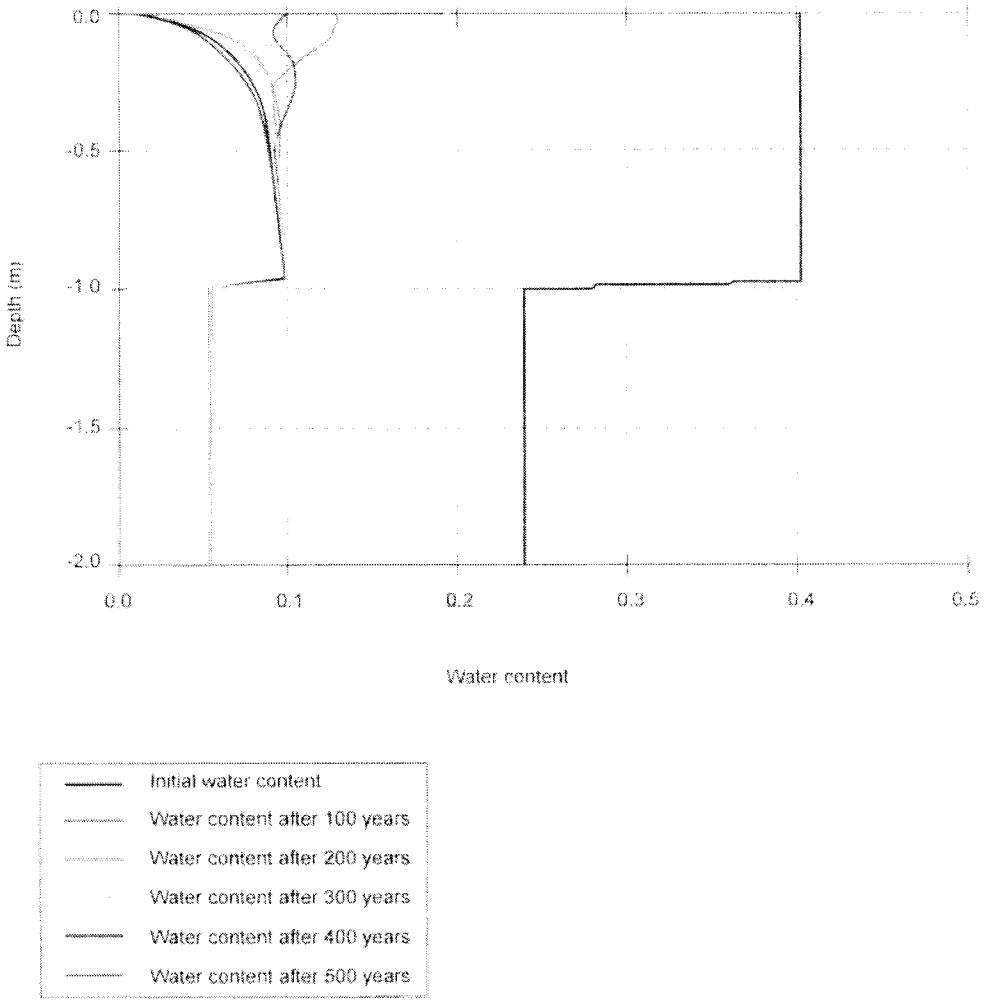


Figure 11
Water Content Profiles from HYDRUS Simulation 11
(1,000-year simulation)

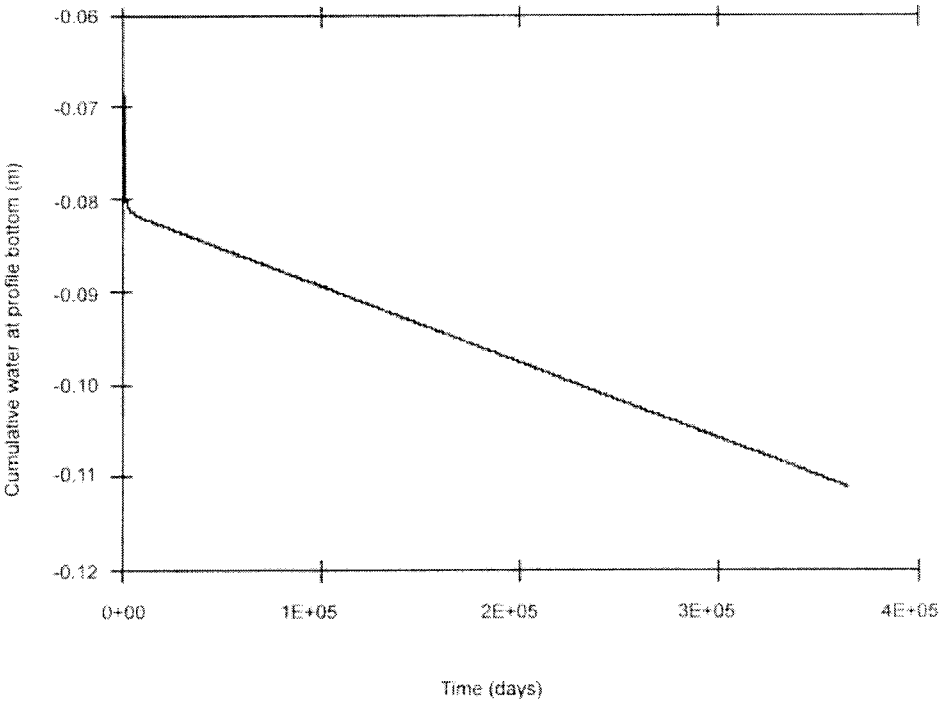


Figure 12
Cumulative Water at Bottom of Profile for HYDRUS Simulation 11
(1,000-year simulation)

4.0 Discussion

In general, the fluxes for all simulations are quite low. Results indicate expected average annual fluxes will be less than 0.2 cm/yr (0.079 in./yr), and possibly as low as a few thousandths of a centimeter per year. This section discusses the effect of varied conditions on downward flux as well as the uncertainties inherent in this modeling effort.

4.1 Effects of Variable Conditions

Projected fluxes appear to be sensitive to initial pressure conditions, as shown in Table 3 by the long-term simulations in which flux is greater with an initial pressure of -1 m (-3.3 ft) than with an initial pressure of -10 m (-33 ft). For example, simulation 7, which had an initial pressure of -10 m (-33 ft) showed a flux of 0.003 cm/yr (0.0012 in./yr); in contrast, simulation 11, which had parameters identical to simulation 7 except for an initial pressure of -1 m (-3.3 ft), yielded a flux of 0.012 cm/yr (0.0047 in./yr). As noted above, the -1 m (-3.3 ft) initial pressure represents a fairly wet condition, while the -10 m (-33 ft) initial pressure is more representative of soils with volumetric water contents of around 10 percent, which is similar to those commonly observed in the shallow subsurface at MDA G.

The thickness of the layer of crushed tuff/bentonite shown in Figure 1 has relatively little effect on flux values. For simulations 7 and 8, both of which had an initial pressure of -1 m (-3.3 ft), flux increased from 0.003 to 0.005 cm/yr (0.0012 to 0.002 in./yr) when the thickness of the crushed tuff/bentonite layer was increased from 1 to 5 m (3.3 to 16 ft). Simulations 11 and 12, which had a higher initial pressure head, also showed minor changes in flux when the thickness of this cover layer was varied. The flux for simulation 11, which had a crushed tuff/bentonite layer thickness of 1 m (3.3 ft), was 0.012 cm/yr (0.0047 in./yr); the flux for simulation 12, in which the same layer had a thickness of 5 m (16 ft), was slightly higher at 0.018 cm/yr (0.0071 in./yr).

The effect of total profile thickness on infiltration characteristics is also relatively small. For example, a total profile thickness of 1-m (3.3-ft) resulted in a flux of 0.01 cm/yr (0.0039 in./yr) (simulation 11). When the crushed tuff layer was increased to 5-m (16-ft) thick, the flux increased to 0.07 cm/yr (0.028 in./yr) (simulation 13). In short, variations in cover thickness and overall profile thickness result in flux changes that are less than an order of magnitude. Flux does increase with thickness, but this is probably related to the larger volume of initial drainage that occurs in the thicker profiles. The small variation in flux in response to changes in thickness is probably related to the fact that even the thinnest profile examined (1 m [3.3 ft] of crushed tuff/bentonite overlying 1 m [3.3 ft] of crushed tuff) appears to have ample storage to contain infiltrating water until it is removed by ET.

The addition of plant uptake also had a relatively small effect on flux values. The 5-year simulations 1 and 3, which were identical except for root uptake, showed no significant difference in flux values (Table 2). There was, however, a slight (but insignificant) increase in estimated flux when root uptake was added to the 1,000-year simulations. Simulation 7, with no plant uptake, had a flux of 0.003 cm/yr (0.0012 in/yr) in contrast to a flux of 0.008 cm/yr (0.0032 in./yr) for simulation 9, which included plant uptake (Table 3). This increase was somewhat surprising, but is probably related to the grass uptake parameters that were used, which do not allow transpiration to occur if the cover material becomes too dry. In other words, the root uptake parameters can shut down transpirative removal of water under some conditions, resulting in more water that can move downward through the profile compared to simulations without root uptake. In any case, the root uptake results are considered exploratory in nature; additional work is required to better implement root uptake for MDA G, as discussed in Section 4.2.

4.2 Modeling Uncertainties

There are major uncertainties that should be addressed in any future modeling of the ET cover, and there is a real possibility that revised modeling results could differ substantially from what is reported here. This section discusses major uncertainties relative to possible future modeling work.

As explained in Section 2, the atmospheric-boundary-condition time series (e.g., precipitation and ET) is a critically important aspect of the cover modeling. This study used an internally consistent set of data that was collected at Mesita del Buey, the mesa on which MDA G is located. However, while these data represent near-average conditions, they do not capture the wide variation in climatic conditions that exist at Los Alamos. One means of addressing this variation would be to model a 1,000-year, stochastically generated time series as was done for MDA H (LANL, 2005). However, this would require using an approach such as the Penman-Monteith for ET, and the comparisons performed in this study indicate the Penman-Monteith method may overpredict ET and, consequently, underpredict downward flux. It is possible that the Penman-Monteith approach could be adjusted or calibrated to the cover demonstration data and used to generate ET for the 1,000-year stochastic weather predictions.

A few simulations were made to account for plant uptake using generic grass parameters; as discussed above, the introduction of plant uptake did not alter the results significantly. However, for these simulations the ratio of evaporation to transpiration was set arbitrarily to 1:1, even though this ratio is actually dynamic over time. In addition, a generic grass cover may not accurately reflect the characteristics of MDA G's native grass or any trees that could invade the site. Thus, it would certainly be worthwhile to explore how the evaporation-to-transpiration ratio and the inclusion of more representative vegetation parameters might impact the simulation

results. Future work could include a more refined plant uptake model using more site-specific grass and tree uptake parameters, and a more dynamic ratio of evaporation to transpiration.

Hydraulic properties of the crushed tuff-bentonite mixture are a major uncertainty, especially since the hydraulic conductivity estimated here contrasts so dramatically with pure crushed tuff. When the laboratory data become available, it will be important to rerun the simulations. This will allow the sensitivity to hydraulic properties to be examined in a meaningful way, and will provide a basis for determining the effect of the gravel and cobble additions to the cover.

The HYDRUS simulations showed a marked contrast in water contents at the contact between the crushed tuff/bentonite layer and underlying crushed tuff/waste (Figures 8 and 11). Measured hydraulic properties for the crushed tuff/bentonite layer will help to verify this strong demarcation in values. If the contrast remains when measured values are used, it is possible that capillary barrier effects and interflow along the edges of the cover may be observed. HYDRUS-2D or possibly HYDRUS-3D simulations would be required to examine capillary barrier effects and possible interflow generation. Examination of slope length effects would also need to be considered. A capillary barrier is often viewed as a design asset and is intentionally incorporated in some cover designs. However, it is important to determine if interflow will occur, because engineering controls may be needed to manage this water and route it away from the site. The optional filtration layer shown in Figure 1 is another area were capillary barrier effects might occur; if this layer is incorporated in the final design, it should be evaluated also.

A final uncertainty that may require future assessment is the issue of preferential flow. The modeling presented here used porous media (matrix) type flow throughout the 1,000-year period and did not assume any evolution or degradation of the cover. However, the addition of bentonite may make the cover prone to cracking, which has been a significant failure route in RCRA-type clay-layer covers. The percentage of clay may be low enough to prevent cracking, but the possibility should be assessed because cracks can route water quickly through the cover. In addition, the potential for tree invasion indicates that stemflow and macropore flow in root channels may be important preferential flow considerations. HYDRUS-2D is currently being used to examine ponderosa pine root channel preferential flow (Guan, 2005); similar simulations could be conducted for MDA G.

Finally, it should be noted that field experiments and studies could be performed to support or complement future HYDRUS modeling. This applies not only to preferential flow questions, but to the testing of cover materials. Small- or intermediate-scale field experiments would be very useful as a test on expected behaviors and performance and would help identify unanticipated effects and build confidence in model results.

Given the variety of uncertainties, one question is whether the HYDRUS-predicted fluxes obtained in this study are reasonable. To examine this question, the distribution of HYDRUS fluxes were plotted against fluxes measured independently at MDA G using the chloride mass-balance approach described in Newman et al. (2005). This plot, shown in Figure 13, indicates that the HYDRUS and chloride-based fluxes span a similar range, and consequently, that the HYDRUS results are "reasonable" values for the MDA G environment. It should be noted, however, that the chloride-based fluxes represent long-term average values for current conditions at MDA G and do not account for the addition of the proposed cover design modeled here. Nevertheless, the comparison is useful for evaluation purposes.

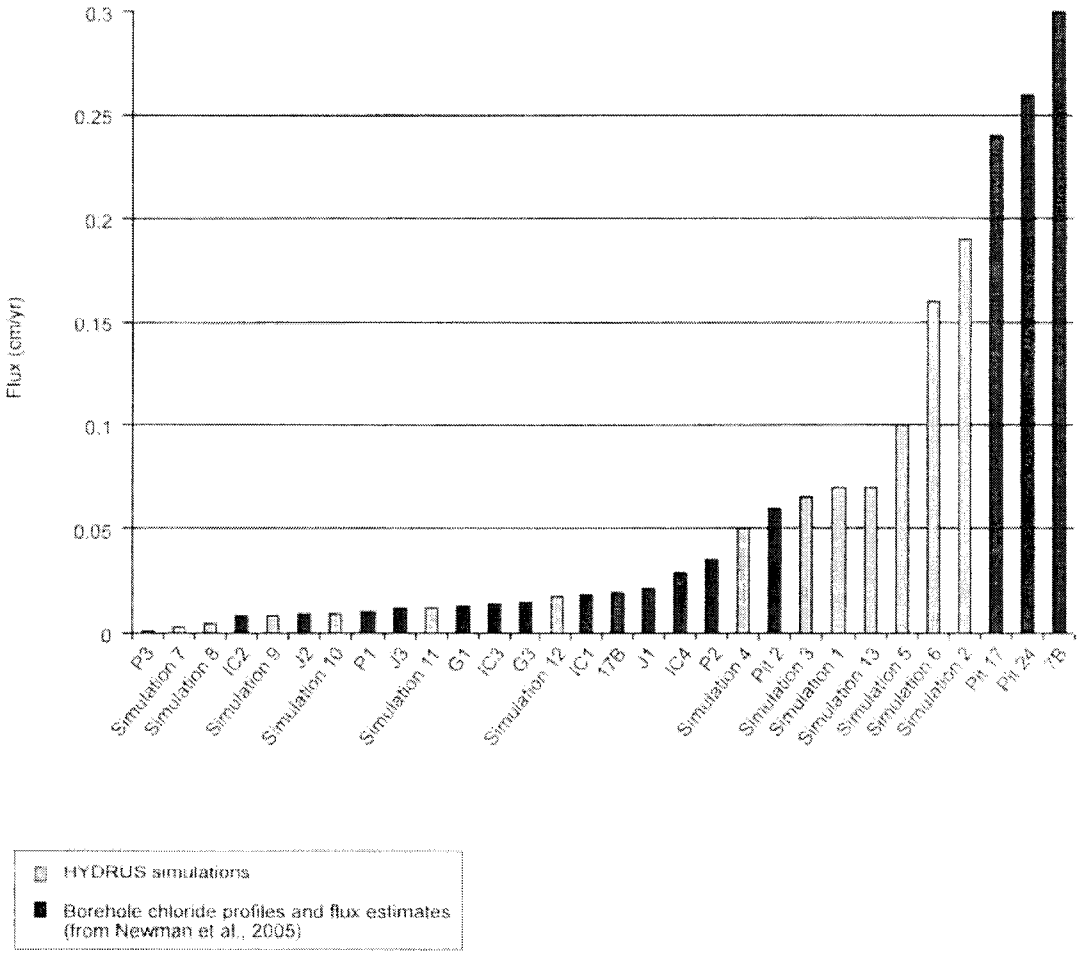


Figure 13
Comparison of HYDRUS Flux Estimates and Chloride Mass Balance Estimates for Material Disposal Area G

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