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AN EVALUATION OF UNSATURATED FLOW
MODELS IN AN ARID CLIMATE

by

Jason Dixon

Bachelor of Science
Ohio Northern University
1997

Master of Science
University of Nevada, Las Vegas
1999

A thesis submitted in partial fulfillment
of the requirements for the

Master of Science Degree
Department of Civil and Environmental Engineering
Howard R. Hughes College of Engineering

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ABSTRACT

An Evaluation of Unsaturated Flow Models in an Arid Climate

by

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University of Nevada, Las Vegas

The objective of this study was to evaluate the effectiveness of two unsaturated flow models in arid regions. The area selected for the study was the Area 5 Radioactive Waste Management Site (RWMS) at the Nevada Test Site in Nye County, Nevada. The two models selected for this evaluation were HYDRUS-1D [Simunek *et al.*, 1998] and the SHAW model [Flerchinger and Saxton, 1989]. Approximately 5 years of soil-water and atmospheric data collected from an instrumented weighing lysimeter site near the RWMS were used for building the models with actual initial and boundary conditions representative of the site. Physical processes affecting the site and model performance were explored. Model performance was based on a detailed sensitivity analysis and ultimately on storage comparisons. During the process of developing descriptive model input, procedures for converting hydraulic parameters for each model were explored. In addition, the compilation of atmospheric data collected at the site became a useful tool for developing predictive functions for future studies. The final model results were used to evaluate the capacities of the HYDRUS and SHAW models for predicting soil-moisture movement and variable surface phenomena for bare soil conditions in the arid vadose zone. The development of calibrated models along with the atmospheric and soil data collected at the site provide useful information for predicting future site performance at the RWMS.

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LIST OF SYMBOLS

E	evaporation
PPT	point precipitation
RON	surface water run-on
ROFF	surface water runoff
ΔS	change in total lysimeter storage
θ	volumetric moisture content
θ_r	residual moisture content
θ_s	saturated moisture content
$\theta(h)$	volumetric moisture content as function of pressure head, moisture retention relationship
z	vertical depth (positive upward)
h	pressure head
α	inverse of the air-entry potential or bubbling pressure, also angle describing direction of flow
$K(h)$	unsaturated hydraulic conductivity as a function of pressure
$K(\theta)$	unsaturated hydraulic conductivity as a function of moisture content
K_s	saturated hydraulic conductivity
K_r	relative hydraulic conductivity
n	pore size distribution index
ι	pore-connectivity parameter
m	empirical constant in retention and hydraulic conductivity functions
S_e	effective moisture content
V	volume of water in a subregion
h_a	minimum pressure head at the soil surface
h_s	maximum pressure head at the soil surface
ε	absolute mass balance error in a flow domain
q	moisture flux
q_v	water vapor flux
q_{vp}	vapor flux due to water potential gradient
q_{vT}	vapor flux due to temperature gradient
R_n	net all-wave radiation
H	sensible heat flux
L_v	latent heat of evaporation (also written as λ)
G	ground heat flux
E	total evaporation
ψ	soil matric potential (also written as ϕ)
ψ_e	air-entry potential (also written as h_b)
ψ_f	suction head at the edge of a wetting front
b	inverse of the pore-size distribution parameter
C_s	volumetric heat capacity
ρ_l	liquid density
ρ_v	vapor density, also ρ_{vs}
ρ_a	density of air
ρ_{va}	atmospheric vapor density
ρ_{vs}	surface vapor density, also saturated vapor density
D_v	vapor diffusivity
h_r	relative humidity (also written as R_h)

s_v	slope of the saturated vapor pressure curve (also written as Δ)
ζ	an enhancement factor for vapor flux
k_s	thermal conductivity of the soil
c_s	volumetric heat capacity
c_l	specific heat capacity of water
m_j	weighting factor
M_w	molecular weight of water
R	universal gas constant
α_a	soil albedo
α_d	dry soil albedo
a_a	empirical coefficient for calculating albedo
f	is the infiltration rate
F_m	accumulated infiltration into layer m
$P(t)$	fitted periodic parameter as function of time
P_A	monthly average value
A	amplitude
ω	angular frequency
Γ	phase shift
$\hat{Y}_i$	simulated value
Y_i	observed value
n	number of observation points
E_{to}	total potential evaporation
e^o	saturation vapor pressure
γ	psychometric constant
C_p	specific heat of moist air
p	atmospheric pressure
W_f	linear wind coefficient
u_2	wind speed at 2 m above the ground
θ_p	midpoint moisture content
θ_T	tangent point moisture content
h_p	matric potential corresponding to θ_p
h_T	matric potential corresponding to θ_T
h_r	revised air-entry potential, also soil relative humidity
T_d	dew point temperature
p_s	saturated vapor pressure
T_{avg}	average daily temperature
S_{ni}	normalized sensitivity coefficient
$\overline{X}_i$	baseline or initial value
$F(\overline{X}_i)$	performance measure
ΔZ	change in the performance measure
ΔX_i	change in the design variable

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CHAPTER I

INTRODUCTION

The Area 5 Radioactive Waste Management Site (RWMS) is located in Frenchman Flat; approximately 130 km northwest of Las Vegas, Nevada, (Figure 1.1). The facility serves as a low-level waste disposal facility for the Nevada Test Site and off-site Department of Energy and Department of Defense waste generators. Frenchman Flat is an alluvium-filled closed basin, typical of the Great Basin Physiographic Province. The climate is extremely arid and characterized by low precipitation, high temperatures and low humidity which all result in high evaporation rates. Because the Area 5 RWMS receives low-level radioactive waste that is buried and covered in trenches and pits, a monitoring program was established to serve as the basis for ensuring the performance of the site. Just outside of the RWMS, a small plot has been set up to monitor specific climatic and near-surface processes in the alluvial sediments. The monitoring data collected at the site and used for this research included soil-water potential, moisture content, evaporation, storage and various meteorological data. These data made it possible to estimate soil water balance, and to calibrate unsaturated flow models that can be used to predict future performance of the site. This study combines field and laboratory measured data along with numerical simulations to provide an evaluation of the mechanisms affecting unsaturated flow at the site. The study period, as it is referred to in this work, is from March 1994 through December 1998.

The primary objective of this work was to evaluate the ability of two unsaturated flow models to simulate the physical processes in an arid climate. The HYDRUS-1D code [Simunek *et al.*, 1998], and the SHAW code [Flerchinger and Saxton, 1989], were selected for this evaluation. A secondary objective was to determine predictive methods for using the collected data from this research for future studies involving performance of disposal facilities in arid climates. This was accomplished by fitting field and laboratory measured data to analytical functions used by the computer models to predict important unsaturated flow processes. Model results were interpreted and compared to measured data to gain a better understanding of

the behavior of near-surface physical processes and moisture redistribution that accounted for storage changes below the near surface in this arid disposal facility. The models provided a tool for evaluating the magnitude and timing of moisture redistribution and buildup at specific depths, which is an important consideration at disposal facilities containing buried waste.

Figure 1.1 Location of the Area 5 RWMS

CHAPTER 2

SITE CHARACTERISTICS

2.1 Physical Setting

The Area 5 RWMS is located in the northern region of Frenchman Flat within the Nevada Test Site at the juncture of three coalescing alluvial fan systems [Synder *et al.*, 1995]. The RWMS elevation ranges from 969 to 975 m above mean sea level. A weighing lysimeter and atmospheric monitoring equipment are located approximately 400 m from the current southwest corner of the Area 5 RWMS.

2.1.1 Site Geology

Frenchman Flat is an intermontane basin typical of basin-and-range structure. The alluvium and tuff-filled valley is rimmed mainly by Proterozoic and Paleozoic sedimentary rocks and Cenozoic volcanic rocks. In the lowland areas of the basin, the Proterozoic and Paleozoic basement rock units are overlain with alluvium, volcanic, and Tertiary sedimentary rocks [Shott *et al.*, 1998]. The alluvial fans are comprised of interbedded gravel, sand and silt with varying degrees of cementation. These coarse-grained deposits grade to the predominantly clayey silt deposits of the playa, or dry lake, which lies approximately 4 km southeast of the site. Limited areas of wind-blown sand and silt are also present in portions of the lowland areas.

2.1.2 Near-Surface and Surface Characteristics

The near-surface stratigraphy displays features typical of lower-middle to distal alluvial fan deposition, including sheet-flood, stream channel and debris flows. A grain-size analysis reveals alternating sequences of fine- and coarse-grained sediments, with occasional lenses of very coarse channel

deposits [RSN, 1991]. The sediment contains variable assemblages of grain sizes and is considered to be geologically heterogeneous. However, the variability does not significantly affect subsurface water flow: thus, it is considered hydrologically homogeneous [Shott *et al.*, 1998]. The results of a 1996 soil characterization study at the Area 5 RWMS indicated that USDA particle size fractions in the near surface showed little variability. The ranges for percent sand, silt and clay were 84 - 87, 9 - 12 and 4 - 8 respectively, [Lee *et al.*, 1996].

The arid climate of Frenchman Flat limits the occurrence and movement of water on the surface. Runoff from storm events occurs intermittently in the basin washes, primarily during the summer local high-intensity thunderstorm activity of relatively short duration, commonly referred to as "summer monsoon season." Flooding and erosion caused by runoff in ephemeral channels affect the site's performance. Although runoff is limited on the alluvial fan material surrounding the site, small incised channels are capable of conveying storm waters near the boundary of the site during large storm events. The RWMS is currently surrounded by an engineered berm and drainage channel, which serve as flood protection and direct potential floodwaters away from the disposal cells.

2.1 Climatic Setting

The Nevada Test Site lies within a region of the southwestern United States known for its arid intermountain deserts. The climate is characterized by a large number of cloudless days, low precipitation, and high daily temperatures, especially in the summer.

The average annual precipitation in Frenchman Flat is approximately 12 cm from 1963 to 1994. The annual total rainfall is highly variable, ranging from 2.9 cm to of 23.4 cm over the same period. The rainfall varies widely with the seasons as well as with elevation. Rainfall during the winter months accounts for most of the moisture at the Nevada Test Site. Winter rains are typically longer in duration and less intense than their summer counterparts [Shott *et al.*, 1998]. Snowfall is rarely observed at the elevations at which the RWMS lies. Typical daily temperature ranges for the Area 5 RWMS are from -3° to 12°C in January, and from 17° to 36°C in July [Magnuson *et al.*, 1992].

Figure 2.1 shows the average amount of rainfall that occurred during the study period at the meteorological station near the two lysimeters. Winter rains accounted for approximately 43% of the average precipitation during the 5-year period.

Figure 2.1 Average seasonal rainfall measured from a tipping bucket and evaporation measured from a lysimeter at the study site (over the entire study period)

Evaporative demand is very high at the RWMS, particularly during the summer months when measured evaporation usually exceeds the precipitation. A side-by-side comparison of average monthly evaporation to precipitation at the site during the study period is also shown in Figure 2.1. The high evaporative demand can also be characterized by the use of micrometeorological measurements of evaporative demand, or the maximal potential evaporation (PE) rate which the atmosphere is capable of exacting water from a soil of given surface properties [Hillel, 1980]. PE was calculated from average daily values of air temperature, humidity, wind speed, and solar radiation using the Penman equation [Jensen *et al.*, 1990]. The Penman equation is described in Section 4.2.3. During the study period, average potential evaporation was much greater than actual rainfall during the summer months, but varied greatly with each season. Figure 2.2 illustrates the average moisture deficit that existed during the period of this research.

2.3

Field Instrumentation

The unsaturated soil-water properties were determined from the soil contained in a weighing lysimeter. The lysimeter consisted of a soil tank that measures 2 m by 4 m in cross-section and 2 m deep, supported on a sensitive scale and equipped with electronic load cells and data acquisition systems for the continuous measurement of soil-water storage, (Figures 2.3 and 2.4). The lysimeter soil was compacted at

each layer to the bulk densities that were taken from the same material measured in-situ. Therefore, the compacted lysimeter soil was considered a close representation of the material from the surface to a depth of approximately 200 cm. There are two lysimeters at the site; one lysimeter has been planted with native plant species, while the second lysimeter has a bare surface. Only data collected from the bare surface lysimeter was used for this study. The lysimeter surface lies on a flat grade and is protected from run-on and run-off by a small barrier.

Figure 2.2 Average potential seasonal moisture deficits at the Area 5 RWMS

Daily water content measurements are made with time domain reflectometry (TDR) probes at eight depths, while daily water potential and soil temperature measurements are made with thermocouple psychrometers (TCPs) at 10 depths. Placement of these sensors within the lysimeters is illustrated in Figure 2.4.

Atmospheric conditions are recorded at a nearby energy balance instrument stand located within a few meters of the weighing lysimeters. Measurements recorded at the stand include hourly averages of air temperature, relative humidity, wind speed, wind direction, net radiation, solar radiation, soil heat flux, soil temperature, and barometric pressure. Hourly totals of precipitation are also recorded with a nearby tipping bucket rain gauge [Levitt, *et al.*, 1996]. All of the monitoring described here continues at the site today.

Figure 2.3 Weighing lysimeter schematic

Figure 2.4 Measurement locations for soil water potential, temperature and moisture content within the weighing lysimeter

2.4 Monitoring Dataset Description at the Lysimeter Site

Meteorological data collection at the site began in March of 1994 and continues today.

Approximately five years of data beginning on March 15, 1994 and ending December 31, 1998 were used for this study. The monitoring data were used to develop a framework for predicting performance measures at the site using the HYDRUS and SHAW models.

2.4.1 Unsaturated Hydrologic Data

Core samples were collected from the lysimeters in 10-cm increments from 0 to 2 m depths to obtain a representative composite of the soil hydraulic properties. The physical property analysis included dry bulk density and porosity. The hydrologic property analysis included water retention relations,

saturated hydraulic conductivity and hydraulic conductivity-saturation relations. These data provide the physical and hydrologic characteristics required as input for computer models [Levitt *et al.*, 1996].

2.4.2 Atmospheric Data

The HYDRUS and SHAW models required descriptions of the atmospheric boundary conditions at the surface of the soil profile. Hourly values of soil temperature, wind speed, relative humidity and air temperature were collected at the site. All hourly data were either averaged for an approximate daily value, or the maximum and minimum daily values were used, depending on model requirements. Daily monitoring data were used to estimate PE demand at the site, and precipitation was totaled on a daily basis for use in the models.

Thermocouple psychrometers used for measuring soil temperature and matric potential in the soil were installed on 2/23/95, and the infrared temperature (IRT) sensors used to measure soil temperature at the surface, were installed on 12/15/94. Matric potential is a frequently used term in this work. It is also referred to as tension, and it describes a condition that occurs when hydrostatic pressures become subatmospheric which result in negative pressures or suction in the soil matrix. The first day for each model simulation was 3/15/94, therefore known values for soil temperature at the surface and in the profile were averaged over years '95 through '98 and used as estimates for unknown values at the beginning of the model simulations. Model input is described with more detail in Chapter 4.

2.4.3 Storage and Evaporation Data

Soil water storage and bare soil evaporation, in cm of water, was measured using the bare surface weighing lysimeter. All references to storage in this report are in terms of cm of water over the entire 2 m vertical dimension of the soil contained in the lysimeter. Lysimeter storage is considered the most accurate tool for measuring water balance at the study site. Changes in storage were measured with precision scales, and the initial storage was calculated on a volumetric basis from the initial moisture content integrated over the length of soil profile in the lysimeter. The lysimeter dataset is continuous since March 15, 1994. Evaporation for each day was calculated by accounting for the change in weight of the box (as measured from the precision lysimeter scales), measured precipitation and drainage. No drainage from the bottom of

the lysimeter has been measured to date. Evaporation was calculated according to the following water balance equation,

$$E = PPT + RON - ROFF - \Delta S \quad (2.1)$$

where:

E is the evaporation,

PPT is the point precipitation,

RON is the run-on,

ROFF is the runoff and

ΔS is the change in total lysimeter storage.

The lysimeter is protected from storm water run-on and runoff by barriers that surround the exposed horizontal surface of the lysimeter soil. Therefore, RON and ROFF in Equation (2.1) were left out of water balance calculations.

CHAPTER 3

NUMERICAL MODELS

3.1

Model Selection

The HYDRUS-1D computer model was obtained from Jirka Simunek of the U.S. Salinity lab in Riverside, California. The HYDRUS code has previously been used for investigations of water movement in protective barriers, craters and other areas at the Nevada Test Site, [Levitt and Sully, 1998, Levitt *et al.*, 1998, Albright *et al.*, 1997]. The code is capable of simulating several physical processes, but only infiltration, drainage, redistribution and evaporation were evaluated for this research. Additionally, the model is capable of simulating heat flow, but this component can only be turned on when a solute is introduced. The model was designed primarily for agricultural settings, and its applicability to a desert environment has not been fully evaluated.

The SHAW computer model was obtained from Gerald Flerchinger of the USDA-ARS Northwest Watershed Research Center in Boise, Idaho. During this study, the model was recompiled to allow for a more dense profile discretization and a correction was made to allow for extremely low clay contents. The SHAW model is also capable of simulating several physical processes that were not evaluated for this research. This study included an evaluation of the model's ability to simulate infiltration, drainage, redistribution, evaporation, heat flow, vapor phase flow and the surface energy balance. The model has not been extensively tested at the Nevada Test Site, but has produced reasonable results for an arid vegetated study site [Flerchinger *et al.*, 1998].

It was determined that both models could be used to create a realistic conceptualization of the site being studied. The models identify most of the significant hydrological and physical processes necessary to simulate unsaturated flow transport in a bare desert soil. HYDRUS and SHAW are widely used models and have been rigorously tested by the scientific community, [Simunek *et al.*, 1998, Flerchinger *et al.*,

1998]. Another important factor in selecting the two models was the adequacy in dimensionality of the models so that the behavior of the physical system in which they were used to simulate could be captured. In addition, the computational approach used to solve this complex problem was determined to be sufficient to the resolution in time and space.

3.2

The HYDRUS-1D Model

The HYDRUS-1D software package was developed to numerically simulate water, heat and solute movement in one-dimensional variably saturated media [Simunek *et al.*, 1998]. The model can also account for plant root uptake and hysteresis in the soil hydraulic properties. However, for the purposes of this research, only one-dimensional, non-hysteretic flow under bare soil conditions was considered. The heat model was tested, but proved ineffective when initialized with no solute present, and was therefore left out of the results.

The software consists of the HYDRUS (version 7.0) computer program, and the HYDRUS-1D interactive graphics-based user interface. The HYDRUS 7.0 program numerically solves the Richards equation for variably-saturated water flow and the convection-dispersion type equations for heat and solute transport. The flow equation incorporates a sink term to account for water uptake by plant roots. The heat transport equation considers transport due to conduction and convection with flowing water. The program may be used to analyze water and solute movement in unsaturated, partially saturated, or fully saturated porous media. The flow region itself may be composed of nonuniform soils having an arbitrary degree of local anisotropy. The water flow component of the model considers prescribed head and flux boundaries, boundaries controlled by atmospheric conditions and free drainage boundary conditions. The governing flow and transport equations are solved numerically using Galerkin-type linear finite element schemes. The version 7.0 of HYDRUS also includes a parameter optimization algorithm for inverse estimation of soil hydraulic and/or solute transport and reaction parameters from measured transient or steady-state flow and/or transport data [Simunek *et al.*, 1998]. The inverse modeling feature was not tested in this research.

3.2.1

Mathematical Model

HYDRUS-1D simulates unsaturated and saturated flow by numerical solution of the modified Richards' equation using assumptions that the air phase plays an insignificant role in the liquid flow process and that water flow due to thermal gradients can be neglected.

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[K \left(\frac{\partial h}{\partial z} + \cos \alpha \right) \right] - S \quad (3.1)$$

where:

h is the water pressure head.

θ is the volumetric water content.

S is a sink term.

t is time.

z is the spatial coordinate (positive upward).

α is the angle between the flow direction and the vertical axis and

K is the unsaturated hydraulic conductivity as a function of the pressure head.

All references to moisture content in this work are in terms of volumetric basis. In other words, the soil bulk density was used to convert water by weight to content by volume, where the volumetric moisture content is equal to the ratio of the mass of dry solids to bulk volume of soil multiplied by the (mass) moisture content (ratio of water to dry soil mass).

The unsaturated soil hydraulic properties, $\theta(h)$ and $K(h)$, in Equation (3.1) are nonlinear functions of the pressure head. HYDRUS permits the use of three different analytical models for the hydraulic properties [Brooks and Corey, 1964; van Genuchten, 1980; and Vogel and Cislerova, 1988]. The modified van Genuchten equations based on work by Vogel and Cislerova, 1988 were not evaluated in this study. Therefore, only two of the three models are described below.

The soil water retention, $\theta(h)$, and the hydraulic conductivity, $K(h)$, functions according to Brooks and Corey (1964) are given by

$$\theta = \theta_r + (\theta_s - \theta_r) * (\alpha|h|)^{-n} \quad (3.1)$$

$$K(h) = K_s \left(\frac{\theta - \theta_r}{\theta_s - \theta_r} \right)^{\frac{2}{n} + \iota + 2} \quad (3.2)$$

respectively, where:

the subscripts “s” and “r” with θ represent saturated and residual moisture content respectively,

h is the pressure head,

α is the inverse of the air-entry value, or bubbling pressure,

n is a pore size distribution index,

$K(h)$ is the hydraulic conductivity as a function of h , or unsaturated hydraulic conductivity and

ι is a pore-connectivity parameter assumed to be 2.0 in the original study of *Brooks and Corey, 1964*.

The parameters α , n and ι in HYDRUS are considered to be empirical coefficients affecting the shape of the hydraulic functions. The air-entry value ($1/\alpha$) can be defined as a critical point at which cohesive forces in the soil matrix can no longer hold onto water. When pressure becomes less (or more negative) than the air-entry potential, air will enter the soil pores because of the tension forces that develop.

HYDRUS also implements the soil-hydraulic functions of *van Genuchten, 1980* who used the statistical pore-size distribution model of *Mualem, 1976a* to obtain a predictive equation for the unsaturated hydraulic conductivity function in terms of soil water retention parameters. The expressions of *van Genuchten, 1980* are given by

$$\theta(h) = \theta_r + \frac{\theta_s - \theta_r}{\left[1 + (\alpha h)^n \right]^m} \quad (3.3)$$

where α , n and m are empirical constants affecting the shape of the retention curve and are not necessarily equal to the same parameters from Equation (3.1) and (3.2). Equation (3.3) along with the pore-size distribution model of *Mualem, (1976a)* are used to predict unsaturated hydraulic conductivity:

$$K(h) = K_s S_e^l \left[1 - \left(1 - S_e^{\frac{1}{m}} \right)^m \right]^2 \quad (m = 1 - 1/n, \quad n > 1) \quad (3.4)$$

where

$$S_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} \quad (3.5)$$

and S_e is the effective water content. The symbol, α , that appears in Equation (3.4) was thought to be about 0.5 as an average for many soils [Mualem, 1976a].

HYDRUS considers a wide variety of both system-independent and system-dependent boundary conditions, but for the purpose of this study, only boundary conditions that represented a realistic conceptualization of the study site were evaluated. HYDRUS describes the surface boundary condition with a soil-air interface exposed to atmospheric conditions. The potential fluid flux across this interface is controlled by external conditions. However, the actual flux depends also on the prevailing (transient) soil moisture conditions near the surface. The soil surface boundary condition may change from a prescribed flux to a prescribed head type condition (and vice-versa). The numerical solution of Equation (3.1) is obtained by limiting the absolute value of the surface flux by the following two conditions [Neuman *et al.*, 1974]:

$$\left| -K \frac{\partial h}{\partial z} - K \right| \leq E \quad \text{at } z = L \quad (3.6)$$

and

$$h_A \leq h \leq h_S \quad \text{at } z = L \quad (3.7)$$

where E is the potential rate of infiltration or evaporation under the current atmospheric conditions, and h_A and h_S are, respectively, minimum and maximum pressure head at the soil surface allowed under the prevailing soil conditions. The value for h_A is determined from the equilibrium conditions between soil water and atmospheric water vapor, whereas h_S is usually set equal to zero cm; if positive, h_S represents a small layer of ponded water which can form on top of the soil surface during heavy rains before initiation of runoff. One option in HYDRUS is to assume that any excess water on the soil surface above zero cm will be immediately removed. When one of the end points in Equation (3.6) is reached, a prescribed head boundary condition will be used to calculate the actual surface flux [Simunek *et al.*, 1998].

3.2.2

Numerical Solution

The one-dimensional water flow equation is solved by discretizing the soil profile into $(N-1)$ adjoining elements, with the ends of the elements located at the nodal points, and N being the number of nodes. A mass-lumped linear finite element scheme is used for discretization of the mixed form of the Richards Equation (3.1). The solution is based on a fully implicit discretization of the time derivative, and is solved with a Picard iterative solution scheme. Because of the nonlinear nature of this relationship, an iterative process must be used to obtain a solution of the global matrix equation at each new time step. For each iteration, a system of linearized algebraic equations is first solved, and after incorporation of the boundary conditions, is solved using the Gaussian elimination technique. The iterative process continues until a satisfactory degree of convergence is obtained. The first estimate (at zero iteration) of the unknown pressure heads at each time step is obtained by extrapolation from the pressure head values at the previous two time steps [Simunek *et al.*, 1998].

The atmospheric boundaries are simulated by applying either prescribed head or prescribed flux boundary conditions depending upon whether Equation (3.6) or (3.7) is satisfied [Neuman *et al.*, 1974]. If Equation (3.7) is not satisfied, boundary node n becomes a prescribed head boundary. If, at any point in time during the computations, the calculated flux exceeds the specified potential flux in Equation (3.6), the node will be assigned a flux equal to the potential value and treated again as a prescribed flux boundary.

The HYDRUS code performs water balance computations at prescribed times for several preselected subregions (defined by nodal spacing) of the flow domain. The water balance information for each subregion consist of the actual volume of water, V , in that subregion, and the rate, O , of inflow or outflow to or from the subregion. These variables V and O are evaluated in HYDRUS by means of

$$V = \sum_e \Delta z_e \frac{\theta_i + \theta_{i+1}}{2} \quad (3.8)$$

and

$$O = \frac{V_{new} - V_{old}}{\Delta t} \quad (3.9)$$

respectively, where:

θ_i and θ_{i+1} are water contents evaluated at the nodes defining element e ,

Δz , is the size of the element and

V_{new} and V_{old} are volumes of water in the subregion computed at the current and previous time levels, respectively. The summation in Equation (3.8) is taken over all elements within the subregion. The absolute error in the mass balance of the flow domain is calculated as,

$$\varepsilon = V_t - V_0 + \int_0^t (q_0 - q_N) dt \quad (3.10)$$

where q is the moisture flux and V_t and V_0 are the volumes of water in the flow domain, Equation (3.8), evaluated at times t and zero, respectively. The third term on the right-hand side of Equation (3.10) represents the net cumulative flux through both boundaries [Simunek *et al.*, 1998]. The results of Equation (3.10) were used as the basis to adjust the model's convergence tolerance and time step iteration criteria for this study so that an acceptable mass balance error could be achieved for the entire flow domain.

Acceptable criteria for mass balance error vary for specific model scenarios, but for this study, total errors that were less than 1 mm of water were considered acceptable. This represents a very small portion of the model domain (<0.05%).

3.3

The SHAW Model

The Simultaneous Heat and Water (SHAW) model is a detailed physical process model that simulates the effects of a multispecies plant canopy on heat and water transfer at the soil-atmosphere interface. The model consists of a one-dimensional profile extending from the vegetation canopy, snow, residue or soil surface to a specified depth within the soil. The system is simulated by integrating detailed physics of a plant canopy, snow, residue and soil into one simultaneous solution. Interrelated heat, water and solute fluxes are computed throughout the system and include the effects of soil freezing and thawing. Daily or hourly weather conditions of air temperature, wind speed, humidity, solar radiation and precipitation above the upper boundary along with soil conditions at the lower boundary are used to define heat and water fluxes into the system. Energy, moisture and solute fluxes are computed between nodes for each time step, and balance equations for each node are written in implicit finite-difference form [Flerchinger *et al.*, 1998]. For the purposes of this study, the plant canopy, snowpack and residue components of the natural system described here were not utilized. However, the effects of heat and vapor flux were evaluated. Furthermore, freezing water was not allowed to occur in the simulations, since soil

temperatures of zero °C are not observed at the Area 5 RWMS at depths greater than 10 cm. When freezing does occur near the surface at the study site, water rapidly thaws by midmorning.

The interrelated energy and water fluxes at the surface boundary are computed from weather observations of air temperature, wind speed, relative humidity and solar radiation. The surface energy balance may be written as

$$R_n + H + L_v E + G = 0 \quad (3.11)$$

where:

R_n is the net all-wave radiation,

H is the sensible heat flux,

$L_v E$ is latent heat flux,

G is soil or ground heat flux,

L_v is latent heat of evaporation and

E is total evapotranspiration from the soil surface and plant canopy [Flerchinger, 1998].

The energy balance equations for layers within the system are written in implicit finite difference form and solved using an iterative Newton-Raphson technique. Flux between nodes is calculated assuming linear gradients. Energy storage for each node is based on layer thickness. A balance equation is written in terms of unknown end-of-time step values within the layer and its neighboring layers. Partial derivatives of the flux equations with respect to unknown end-of-time step values are computed, forming a tri-diagonal matrix from which the Newton-Raphson approximations for the unknown values are computed. Iterations are continued until successive approximations for each layer are within a prescribed tolerance [Flerchinger et al., 1996].

3.3.1

Mathematical Model

The equation used by the SHAW model to simulate liquid and vapor flow through an unsaturated, heterogeneous, vertical soil profile with respect to soil type is

$$\frac{\partial}{\partial z} \left[K \left(\frac{\partial \psi}{\partial z} + 1 \right) \right] + \frac{1}{\rho_l} \frac{\partial q_v}{\partial z} + U = \frac{\partial \theta_l}{\partial t} \quad (3.12)$$

where:

K is unsaturated hydraulic conductivity,

ψ is the soil matric potential,

ρ_l is the density of liquid water (1000 kg/m³),

q_v is the water vapor flux and

θ_l is the volumetric liquid water content.

Each term represents respectively: net liquid flux into a layer, net vapor flux into a layer, a source/sink term (which includes root uptake) and rate of change of volumetric liquid content [Flerchinger and Saxton, 1989].

The relationship used to describe the moisture characteristic equation is [Brooks and Corey, 1966],

$$\psi = \psi_e \left(\frac{\theta_l}{\theta_s} \right)^{-b} \quad (3.13)$$

where:

ψ_e is the air-entry potential,

b is the inverse of the pore size distribution parameter,

θ_l is the volumetric liquid water content and

θ_s is the saturated volumetric water content.

Unsaturated hydraulic conductivity is described as a function of the moisture content and is computed from

$$K = K_S \left(\frac{\theta_l}{\theta_S} \right)^{(2+3b)} \quad (3.14)$$

where K_S is saturated hydraulic conductivity. The hydraulic conductivity function described by Equation (3.14) was determined from the work of Burdine, 1953.

Vapor transfer in the soil is calculated as the sum of the potential and temperature gradients,

$$q_v = q_{vp} + q_{vT} = -D_v \rho_{vs} \frac{dh}{dz} - \zeta D_v h_r s_v \frac{dT}{dz} \quad (3.15)$$

where:

q_{vp} and q_{vT} are vapor fluxes due to water potential gradient and temperature gradient respectively,

D_v is the vapor diffusivity of the soil,

ρ_{vs} is the saturated vapor density at soil temperature, T ,

h_r is the relative humidity within the soil,

h is the pressure head,

s_v is the slope of the saturated vapor pressure curve ($d\rho_v/dT$) and

ζ is an enhancement factor for vapor flux in response to the temperature gradient [Cass *et al.*, 1984].

The general heat flux equation for the soil matrix, considering convective heat transport by liquid and latent heat transfer by vapor in the soil is given by:

$$C_s \frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left[k_s \frac{\partial T}{\partial z} \right] - \rho_l c_l \frac{\partial q_l T}{\partial z} - L_v \left(\frac{\partial q_v}{\partial z} + \frac{\partial \rho_v}{\partial t} \right) \quad (3.16)$$

where the terms represent, respectively: specific heat term for energy stored due to a temperature increase; net thermal conduction into a layer; net thermal advection into a layer due to water flux; net latent heat evaporation within the soil layer. In the above equation,

t is time,

z is soil depth,

k_s is the thermal conductivity of the soil,

ρ_l is density of water,

c_l is specific heat capacity of water,

C_s is the volumetric heat capacity calculated as

q_l is liquid water flux,

L_v is latent heat of vaporization,

q_v is water vapor flux and

ρ_v is vapor density within the soil.

The first term in Equation (3.16), C_s , is the sum of volumetric heat capacities:

$$C_s = \sum \rho_j c_j \theta_j \quad (3.17)$$

where ρ_j , c_j , and θ_j are the density, specific heat capacity and volumetric fraction of the j^{th} soil constituent, respectively. Thermal conductivity of the soil is calculated using the theory presented by De Vries, 1963.

A fairly moist soil is conceptualized as a continuous medium of liquid water with granules of soil and pockets of air dispersed throughout. The thermal conductivity of such an idealized model is expressed as

$$k_s = \frac{\sum m_j k_j \theta_j}{\sum m_j \theta_j} \quad (3.18)$$

where m_j , k_j and θ_j are the weighting factor, thermal conductivity, and volumetric fraction of the j^{th} soil material, respectively. Net latent heat of vaporization occurring in the soil layer is computed from the rate of increase in vapor density minus the net vapor transfer into the layer. Vapor density in the soil is calculated assuming equilibrium with total water potential by:

$$\rho_{vs} = \rho_v' \exp\left(\frac{M_w g}{RT_K} \phi\right) \quad (3.19)$$

where:

ρ_v is vapor density,

ρ_v' is saturated vapor density,

M_w is the molecular weight of water,

g is acceleration of gravity,

R is the universal gas constant and

ϕ is the total water potential (*Flerchinger and Saxton, 1989*).

Important surface phenomena considered in the SHAW model include evapotranspiration and liquid infiltration. However, plant transpiration was not considered for the study of the bare site at the Area 5 RWMS. Sensible and latent heat flux components of the surface energy balance are computed from temperature and vapor gradients between the soil and atmosphere. Sensible heat flux is calculated from [*Campbell, 1977*]

$$H = \rho_a c_a \frac{(T - T_a)}{r_H} \quad (3.20)$$

where:

H is the heat flux at the soil surface,

ρ_a , c_a , T_a are the density, specific heat, and temperature of the air, respectively,

T is the surface temperature and

r_H is the resistance to heat transfer.

Latent heat flux is associated with transfer of water vapor from the exchange surface to the atmosphere, which is given by

$$E = \frac{\rho_{vs} - \rho_{va}}{r_v} \quad (3.21)$$

where:

ρ_{vs} and ρ_{va} are the surface and atmospheric vapor density and r_v is the resistance to vapor transfer. The resistances r_v and r_H are assumed equal and depend on atmospheric stability.

Daily solar radiation is input into the model directly, however the amount of radiation reflected at the surface is controlled by the soil's albedo (α_u) which varies with soil water content and is calculated from (Idso et al., 1975)

$$\alpha_u = \alpha_d \exp[-a_\alpha \theta_l] \quad (3.22)$$

where:

α_d is albedo of dry soil,

θ_l is the surface volumetric water content and

a_α is an empirical coefficient.

Rainfall and ponded water infiltrate into the soil at the end of each time step. Infiltration is calculated using a Green-Ampt approach for a multi-layered soil. The infiltration rate as a wetting front passes through layer m of a multi-layered system may be written as

$$f = \frac{dF_m'}{dt'} = \frac{\frac{F_m'}{\Delta\theta_l} + \psi_f + \sum z_j}{\frac{F_m'}{\Delta\theta_l K_{e,m}} + \sum \frac{z_j}{K_{e,j}}} \quad (3.23)$$

where:

f is the infiltration rate,

$K_{e,j}$ is the effective hydraulic conductivity of layer j ,

ψ_f is the suction head at the wetting front and assumed equal to the matric potential of the layer,

$\Delta\theta_l$ is the change in water content as the wetting front passes,

F_m' is the accumulated infiltration into layer m ,

t' is the time since the wetting front entered layer m and

z_j is the depth to the top of layer m .

Effective hydraulic conductivity for infiltration is determined by substituting the effective porosity, computed from $(\theta_s - \theta_f)$, for θ in Equation. (3.23), where θ_f is the water content ahead of the wetting front. Equation (3.23) may be integrated and written in dimensionless form as

$$t_* = (z_* - 1) \ln(1 + F_*) + F_* \quad (3.24)$$

Equation (3.24) is implicit with respect to F_* . By expanding the logarithmic term into a power series, *Flerchinger and Watts (1975)* developed the following explicit expression for F_* ,

$$F_* = \frac{1}{2} \left(t_* - 2z_* + \sqrt{(t_* - 2z_*)^2 + 8t_*} \right) \quad (3.25)$$

This expression is only valid if nearly-saturated flow exists behind the wetting front, which was shown to occur only if $z_* \leq 1$. When this criterion is not met, infiltration is calculated using Darcy's equation and assuming zero matric potential at the wetting front [*Flerchinger and Saxton, 1989*]. Darcy's equation can be written as

$$q = -K(\theta) \frac{\partial h}{\partial z} - K(\theta) \quad (3.26)$$

where $K(\theta)$ is the hydraulic conductivity as a function of moisture content.

3.3.2 Numerical Solution

As stated previously, the one-dimensional state equations that describe the energy balance for layers within the soil are written in implicit finite difference form and solved using an iterative Newton-Raphson technique. Finite difference approximation enables these equations to be applied to nodes representing layers of finite thickness. Flux between nodes is calculated assuming linear gradients. Energy storage for each node is based on layer thickness. A balance equation is written in terms of unknown end-of-time step values within the layer and its neighboring layers. Partial derivatives of the flux equations with respect to unknown end-of-time step values are computed, forming a tri-diagonal matrix from which the Newton-Raphson approximations for the unknown values are computed. Iterations are continued until successive approximations for each layer are within a prescribed tolerance [*Flerchinger and Saxton, 1989*].

CHAPTER 4

MODEL APPLICATION

4.1

Objectives

The task of establishing a conceptual model of the study site using the HYDRUS and SHAW models involved several steps that are explained in the following sections. The first step of the research was to analyze actual meteorological data along with the measured moisture retention and conductivity relationships to be used for input into the HYDRUS and SHAW models. During this process, methods were developed that could be used to apply monitoring data to the models in this study and future studies at similar sites. The two models underwent extensive testing using real monitoring data and actual input parameters. The ability of the models to predict total soil-water storage in the lysimeter under bare soil conditions was measured by comparing actual storage to predicted storage. The model input was adjusted to achieve calibration with actual site conditions, i.e. values of hydraulic parameters or site meteorological conditions. The physical processes in the models were evaluated, and suggestions were made for future applications of these models in arid climates. The HYDRUS and SHAW models were calibrated to allow for their future use at the Nevada Test Site for accurate prediction of moisture conditions near emplaced waste zones at the Area 5 RWMS.

4.2

Input Data Analysis

Several steps were taken to insure that an accurate conceptualization of the site was developed for input into the computer models. Time dependent data were compiled and arranged so that historical trends affecting site performance could be studied and used for the development of a representative model that incorporated the necessary flow parameters. Particular attention was paid to the components that account for water balance in the lysimeters. Atmospheric components contributing to liquid fluxes at the site were

closely examined, and these data was used to develop periodic functions that described measured data. In addition, a detailed procedure for estimating hydraulic properties of the soil for specific model input was developed.

4.2.1

Water Balance Data

Figure 4.1 is a summary of average monthly water balance data and potential evaporation measured at the study site compared to average lysimeter storage values in the same months. During the winter months, when precipitation is approximately 117% greater than evaporation, only a 24% average increase in storage was measured. The reason for such a small storage change is sharp upward-driving potential gradients that exist in the soil profile, especially during the spring and summer months. Upward driving forces cause redistributed moisture that infiltrates into the soil during the winter rains to migrate to the surface where it is removed by evaporation during the spring and summer months. This phenomenon is apparent from the plots in Figure 4.1, where a decreasing trend in storage exists during the spring and summer months followed by increases from the winter rains. Over the course of the study period, total evaporation and precipitation were relatively close in magnitude, as 93% of the precipitation was returned to the atmosphere based on measured storage changes in the lysimeter. Figure 4.1 also shows the average monthly evaporation to be greater than precipitation during the spring and summer months (March through September). For the entire study period, 66 cm of rain was recorded and the storage measured in the lysimeter increased from 11 to 16 cm. There was no measurable drainage, and the total calculated evaporation from the lysimeter measurements was 61 cm.

Figure 4.1 Average monthly water balance and calculated potential evaporation (cm of water), during the study period

4.2.2

Evaporation and Meteorological Data

Three main conditions contribute to the evaporation that was measured at the study site. Internally, evaporation is controlled by the soil texture and the amount of precipitation that becomes infiltration. Externally, there must be a continual supply of energy to the surface. Furthermore, there must be a vapor-pressure gradient between the soil surface and the atmosphere. The latter two conditions are external to the soil surface and are influenced by several meteorological parameters that were measured at the study site. Evaporation, and the components that describe it, are highly seasonal at the Area 5 RWMS. Measurements of air temperature, relative humidity, wind speed and solar radiation were plotted based on monthly averages. The data were continuous from December 1993 and were fit to periodic functions of the form

$$P(t) = P_{.t} + A \sin \omega t \pm \Gamma \quad (4.1)$$

or

$$P(t) = P_{.t} + A \cos \omega t \pm \Gamma \quad (4.2)$$

where:

$P(t)$ is the parameter being fit as function of time,

t is a number representing a particular month, (i.e. 1 for January, 2 for February and so forth),

P_A is monthly average value,

A is the amplitude of the parameter fluctuation, taken to be the result of the maximum value minus the average value,

$\omega = \frac{2\pi}{\tau}$ is the angular frequency,

τ is the period of the wave, where a full period was taken to be 12 months in most cases, and

Γ is a phase shift which was necessary to force the initial value that described the start of the wave to occur at the appropriate time.

The periodic functions that describe these measurements can be used in future studies utilizing computer models to predict various site performance measures at the Area 5 RWMS. Figures 4.2 - 4.5 show comparisons of actual data to the predicted data from the periodic functions representative of the actual conditions at the study site.

Equation (4.1) was used to fit the data for maximum wind speed, solar radiation and temperature, while Equation (4.2) was used to describe the relative humidity fluctuations. Table 4.1 is a summary of the values used to predict the atmospheric trends that control evaporation. Given the appropriate selection of Γ , only one of the two periodic functions is necessary, but both equations were used for this work. Equations (4.1) and (4.2) differ by a Γ equal to $(\pi/2)$.

Figure 4.2 Comparison between average monthly measurements of maximum wind speed and predicted maximum wind speed at 2 m height

Figure 4.3 Comparison between average monthly measurements of solar radiation and predicted solar radiation at 2 m height

Figure 4.4 Comparison between average monthly measurements of temperature and predicted maximum temperature at 2 m height

Figure 4.5 Comparison between average monthly measurements of relative humidity and predicted relative humidity at 2 m height

Table 4.1 Parameters Used to Fit Periodic Functions to Measured Data

	Maximum Wind Speed (m/s)	Avg. Solar Rad. (W/m^2)	Avg. Temp. (Jan-July) (deg.C)	Avg. Temp. (Aug-Dec) (deg.C)	Relative Humidity (Jan-July) (%)	Relative Humidity (Aug-Dec) (%)
Average	8.5	223.4	15.8		36.7	33.8
Maximum	10.1	330.1	28.9		61.6	49.8
Minimum	6.3	106.5	4.4		20.2	20.2
TA	8.5	223.4	15.8		36.7	33.8
A0	1.5	106.7	13.1		24.9	16.0
τ , (months)	11	12	16	12	12	14
Γ , (radians)	$.526\pi$	$.556\pi$	$.5\pi$	$.667\pi$	$.1\pi$	$.083\pi$
Root-mean-square error	0.06	0.06	0.11		0.21	

The observed values for maximum wind speed were more variable compared to other measured parameters, and the curve showed an upward trend in November. Therefore, a period of 11 months was selected for the function that predicted maximum wind speed. Solar radiation data was symmetric between the first and second 6-month periods, and could be described with a period of 12 months. The observed data for temperature and relative humidity reached their respective maximum and minimum values in July (month 7). Therefore, different values were used for the periodic functions to fit the data for the months from January through July and August through December, see Table 4.1. A normalized form of the root-

mean-square error (RMS) equation was used to demonstrate to relative goodness-of-fit obtained for each prediction.

$$\text{Normalized RMS error} = \left[\frac{1}{n} \sum_{i=1}^N \frac{(\hat{Y}_i - Y_i)^2}{(Y_i)^2} \right]^{1/2} \quad (4.3)$$

where:

n is the number of observation points,

$\hat{Y}_i$ is the predicted value and

Y_i is the observed value.

The RMS results are also shown in Table 4.1.

4.2.3 Estimation of Potential Evaporation

The HYDRUS model required input of the potential evaporation (PE) to perform surface flux simulations. PE at the Area 5 study site was calculated using the Penman equation, which required parameters collected at the micrometeorology station near the lysimeter. The Penman equation estimates the maximum PE at the soil surface from the temperature and vapor pressure of the evaporating surface. This method also accounts for the difference in energy flux at the surface, atmospheric pressure, and wind speed. A modified form of the Penman equation [Jensen *et al.*, 1990] was used,

$$\lambda E_{to} = \frac{\Delta}{\Delta + \gamma} (R_n - G) + \frac{\gamma}{\Delta + \gamma} 6.43 W_f (e_s^0 - e_a) \quad (4.4)$$

where:

E_{to} is the potential evaporation,

λ is the latent heat of vaporization (kJ kg^{-1}),

Δ is the slope of the saturation vapor pressure curve $(4098e^0)/(T + 273.3)^2$, ($\text{kPa } ^\circ\text{C}^{-1}$), [Tetens, 1930] and [Murray, 1967],

T is the dry bulb temperature ($^\circ\text{C}$),

e^0 is the saturation vapor pressure (kPa),

γ is the psychrometric constant $(C_p P)/(.622\lambda = 66.8 \text{ kPa } ^\circ\text{C}^{-1})$, ($\text{kPa } ^\circ\text{C}^{-1}$),

C_p is the specific heat of moist air at constant pressure ($1.013 \text{ kJ kg}^{-1} \text{ }^\circ\text{C}^{-1}$)

P is the atmospheric pressure (kPa),

R_n is the net radiation ($\text{MJ m}^{-2} \text{ d}^{-1}$),

G is the average daily sensible heat flux to the soil ($\text{MJ m}^{-2} \text{ d}^{-1}$),

$(R_n - G)$ is the difference between incoming solar radiation and outgoing long-wave radiation from the soil surface,

W_f is the linear wind coefficient or function (described below),

e''_z is the saturation vapor pressure over water (kPa),

e_z is the actual vapor pressure at level z above the ground surface (kPa) and

$(e''_z - e_z)$ is the vapor saturation deficit.

The linear wind coefficient or wind function is given by

$$W_f = (a_w + b_w u_2) \quad (4.5)$$

where:

for $R_n > 0$, $a_w = 0.27$ and $b_w = 0.526$

for $R_n \leq 0$, $a_w = 1.14$ and $b_w = 0.401$ (*Frere and Popov, 1979*), and

u_2 = wind speed at 2 m above the ground surface (km day^{-1}).

4.3

Procedure for Estimating Hydraulic Parameters

The most important factor for the successful application of unsaturated flow theory to actual field problems is obtaining the parameters for the governing transfer equations. Reliable estimates of the unsaturated hydraulic conductivity relationships are especially difficult to obtain, partly because of their extensive variability in the field, and because measuring these parameters is time-consuming and expensive. Several investigators have, for these reasons, used models for calculating the unsaturated conductivity from the more easily measured soil-water retention curve [*van Genuchten, 1980*].

The hydraulic parameters used in this study were based on laboratory measurements of $h(\theta)$ and K , for soil water retention characteristics and saturated hydraulic conductivity respectively [*Shott et al., 1998*]. These parameters provided the basis for quantitatively describing water flow throughout the lysimeter soil. Based on properties determined in the lab, soil from the lysimeter was determined to be

hydrologically homogeneous. Retention data from eight soil samples taken from various depths in the lysimeter soil were averaged (α was found by taking a log-average because it showed a log-normal distribution) and plugged into a computer program for curve fitting. Although different methods were available for fitting retention data and obtaining representative functions, the computer code RETC [van Genuchten *et al.*, 1991] was selected. RETC was developed specifically for estimating hydraulic properties of unsaturated soils. The program permits the user to fit analytical data simultaneously to observed water retention and hydraulic conductivity data. This is accomplished by specifying appropriate retention and conductivity functions in which to fit the observed data. The two options in RETC for empirically describing soil water retention curves are the equations of van Genuchten, 1980 and Brooks and Corey, 1964, which are Equations (3.3) and (3.13), further referred to as the VG and BC-equations, respectively. These two models can then be combined with either of the two hydraulic conductivity models from Mualem, 1976 and Burdine, 1953, which are Equations (3.4) and (3.14).

RETC is capable of fitting retention data and/or conductivity/diffusivity data. For this study, only retention data was measured in the lab, and the saturated hydraulic conductivity was measured directly for each of the eight soil samples from the bare surface lysimeter. Therefore, RETC could only be used to obtain the appropriate retention parameters, while the unsaturated hydraulic conductivity parameters were estimated from the resulting retention functions and the measured saturated hydraulic conductivity.

RETC was initialized by specifying which moisture retention and conductivity functions were to be used to empirically fit the observed data. The retention data were input with measured volumetric moisture content at tensions ranging from approximately zero to 1.5E+6 cm of water. The calculated output retention parameters given by RETC were residual moisture content (θ_r), n , and α . The n and α parameters are empirical constants that affect the shape of the retention curve, as described in Chapter 3.

Residual and saturated moisture content can sometimes be measured with a reasonable degree of accuracy in the lab, but should be examined carefully. Residual moisture content can usually be estimated from a measurement at very high tensions (>15,000 cm). The final fitted parameters were plugged into the VG or BC functions and compared to the measured retention curves for a final determination of the goodness-of-fit.

The current available version of SHAW simulates soil moisture with the BC retention equation, using the Burdine theory to describe the unsaturated hydraulic conductivity function. Equation (3.13) used in the SHAW model can be written in terms of the RETC nomenclature by:

$$S_e = \left(\frac{h}{h_b} \right)^{-mn} \quad (4.6)$$

where:

h_b is the air-entry value or bubbling pressure, whose inverse is often approximated as α from the VG function, and m is an empirical parameter described by the Burdine theory as

$$m = 1 - \frac{2}{n} \quad (4.7)$$

The exponent $(-mn)$, which appears in Equation (4.6), is the pore-size distribution parameter that is often written as λ . When combining Equation (4.7) with the exponent, $(-mn)$, from Equation (4.6), λ becomes $(n-2)$. The λ parameter is equal to the inverse of the (b) parameter from Equation (3.13) in the SHAW model.

Since the SHAW model uses the Burdine theory to describe the hydraulic conductivity relationship, Equation (3.14) can be written in terms of the RETC nomenclature described here as a function of pressure head,

$$K(h) = \frac{K_S}{(\alpha h)^{\lambda(t+1)+2}} \quad (4.8)$$

where:

$K(h)$ is the hydraulic conductivity as a function of pressure head and t is a pore-connectivity parameter estimated by many researchers to be 2.0 for Burdine-based conductivity models [van Genuchten *et al.*, 1991]. The SHAW model assumes this value constant at 2.0.

The BC equation has been shown to produce relatively accurate results for many coarse-grained textured soils characterized by relatively narrow particle-size distributions, i.e. large values for λ . This has not been the case for many fine-textured and undisturbed field soils because of the absence of a well-defined air-entry value for these soils [van Genuchten *et al.*, 1991].

Assumptions made by the Mualem theory differs from the Burdine theory for the above relationships in that ($m = 1 - 1/n$) and the parameter (ι) is commonly assumed to be 0.5 instead of 2.0. For this study, these restrictions were used to develop a hydraulic conductivity function from the fitted retention data, using Equation (3.4) in the HYDRUS model. One important difference between the two conductivity models presented here is that Burdine based equations hold only for ($n > 2$), while Mualem-based formulations are valid for all ($n > 1$). Since many soils have n -values that are less than 2, the Burdine-based models for unsaturated hydraulic conductivity have less applicability.

The HYDRUS model can use either the VG-Mualem or BC-Burdine functions to simulate flow transport. In order to estimate the appropriate input hydraulic parameters for HYDRUS, the retention data obtained from eight lysimeter soil samples were fit to the analytical expressions used by RETC, described here, to develop the predictive soil-moisture retention parameters. The data were fit using the VG-Mualem option in RETC, which was initialized and rerun with several different typical initial estimates to ensure that the process was converging to the correct final parameters. For comparative purposes, the RETC code was also run using both BC-Burdine and BC-Mualem options for the RETC curve-fitting process. Neither set of RETC output that used the BC function produced acceptable results, since both options yielded values of n that were less than 1.0. Only RETC output using the VG-Mualem option yielded parameters that accurately described the measured retention data (Figure 4.6). The VG-Mualem retention parameters determined from RETC were used as input for the HYDRUS model. Table 4.2 contains a description of the initial estimated parameters and output results from fitting the observed data to the retention functions. The values in Table 4.2 represent the averages for θ_r , θ_s , and n obtained from the results of the eight laboratory measured samples used as input for RETC. The α parameter was determined by taking the log-average value of the samples, since this value was shown to be log-normally distributed. The parameter output from RETC was plugged into the VG-equation and plotted for comparison to the actual observed retention data in Figure 4.6. The fitted curve produced a reasonable match, particularly for moisture contents greater than 0.1, or near saturation. However, the fitted curve deviated from the actual data near the residual moisture content predicted by RETC, which was 0.039. This value was questionable since the lowest average moisture content measured at 1.5E+6 cm tension in the laboratory was 0.01. The θ_r predicted by RETC seemed to be reasonable when compared to the lowest moisture content measured in

the field with the lysimeter. When the soil profile in the lysimeter was at its driest state of the study period, the measured storage was 9.36 cm of water in the entire profile. This value corresponded to an overall average moisture content of 0.047 for the entire 200 cm profile, which is slightly higher than the value predicted by RETC. The residual moisture content played a very important role in the determination of the proper retention values for the two models. In most cases, it is important to have an independent procedure, such as the one used here, for estimating the θ_r [van Genuchten, 1980]. Ultimately, a value of zero was used for this study, which produced an acceptable range of likely water contents under the given conditions for the HYDRUS and SHAW models. The issue of θ_r is discussed in more detail in Chapters 5 and 6.

Figure 4.6 Comparison between the predicted soil moisture retention curve and the curve representing the average of the eight samples from the lysimeter

Table 4.2 RETC Predicted Moisture Retention Parameters

Initial Estimates	θ_r	θ_i	α	n
Sand	0.032	0.352	0.044	0.541
Loamy Sand	0.032	0.352	0.044	0.541
Sandy Loam	0.065	0.410	0.075	1.890
Loam	0.078	0.430	0.036	1.560
Fitted Model	θ_r	θ_i	α	n
VG-Mualem	0.039	0.361	0.034	1.638
BC-Burdine	0.033	0.346	0.045	0.484
BC-Mualem	0.034	0.353	0.043	0.546

The SHAW model uses the BC function to describe soil moisture characteristics in conjunction with the Burdine model to describe the unsaturated hydraulic conductivity as a function of moisture. However, the parameters determined from the BC fitting option in RETC compromised the accuracy of the fit to the lysimeter soil data and could not be used. Therefore, the parameters used in HYDRUS had to be converted for SHAW BC input so as to generate a retention curve that matched as closely as possible to the measured retention curve and the curve predicted from the VG-Mualem functions. The objective in creating a set of hydraulic input for the SHAW model was to minimize the differences in the hydraulic functions based on the selected parameters so that the likelihood of any major discrepancies in the performance of the two models would be less likely a cause of the hydraulic parameters that were used as input. This facilitated a more complete evaluation of other flow processes that affected the results, such as the contributions of heat and vapor transport.

The VG-Mualem parameters used for HYDRUS were converted to equivalent BC parameters using the parametric VG (α and n) and BC (λ and h_b) relationships where $\lambda = n - 1$ and $h_b = 1/\alpha$. For the sake of brevity, the parameters determined with this method will be referred to as “converted parameters” throughout this work. As mentioned previously, this method is based on the theory of Mualem, where ($m = 1 - 1/n$). The parametric equivalences hold when the moisture content is sufficiently low. However, as shown in Figure 4.7, a large discrepancy was evident near saturation for the converted BC plot when compared to the VG plot. The results in Figure 4.7 also provide an illustration of why the Burdine assumption described by assumption of Equation (4.7) cannot be applied to the BC function for ($n < 2$). As the resulting retention curve for the BC-Burdine plot showed even larger discrepancies throughout the entire range of water contents. The method used here for converting from VG to BC has been shown to be best suited for sandy soils [Morel-Seytoux *et al.*, 1996]. However, it was apparent from Figure 4.7 that the BC function provided a poor fit near saturation, where the VG function yielded a smoother and more accurate fit to the measured data in this range (Figure 4.6).

A simple procedure was developed to improve the poor fit of the BC function near saturation while preserving the goodness-of-fit for lower moisture contents, thereby minimizing the impact that the poor fit of the BC function near saturation would have on the infiltration capacity of the soil. This was accomplished by taking advantage of the mild slope that existed near the midpoint of the VG and measured

curves. The mild slope near the middle of the range of water contents is commonly seen in sandy soils, and because of this, the procedure suggested here would not likely produce valid results for soil with high clay content. Clayey soils tend to have a steeper slope near the midpoint of the retention curve.

Figure 4.7 Comparison between the converted BC curve, BC-Burdine curve and the VG curve

Once the VG parameters were converted to the equivalent BC parameters, the α and λ values were revised and plugged back into the BC equation following these steps (shown graphically in Figure 4.8):

1. Calculate θ_p from $(\theta_s - \theta_r) / 2$. This point represents the midpoint over the predicted range of moisture contents.
2. Rearrange Equation (3.3) and use the RETC fitted VG parameters to solve for h_p in terms of n at θ_p from

$$h_p = \frac{\left[\left(\frac{\theta_s - \theta_r}{\theta_p - \theta_r} \right)^{\left(\frac{n}{n-1} \right)} - 1 \right]^{(-n)}}{\alpha} \quad (4.9)$$

(h_p is the matric potential corresponding to the moisture content at the midpoint in the range of moisture contents)

3. Locate the point of tangency on the VG curve approximately halfway between point (P) and θ_i and calculate h_T from θ_T at point (T) using Equation (4.9).
4. Find the slope of the VG curve between points (P) and (T) from,

$$S_{P-T} = \frac{\log(h_p) - \log(h_T)}{\theta_p - \theta_T} \quad (4.10)$$

5. Extend a line tangent to the VG curve at point (T) to meet the vertical line representing the air entry value at θ_i described by the converted BC curve. The intersection of the tangent line and the vertical line formed from the plot of the converted BC air-entry potential, $(h_h)_c$, represents the revised air entry potential, h_r . This value will always be less than the converted BC air entry potential, thereby minimizing the difference between the VG and BC curves near saturation.
6. Alternatively, the revised air entry potential (h_r) can be calculated by inserting h_T and θ_i into Equation (4.10) and rearranging to solve for h_r by,

$$h_r = 10^{\log(h_T) + S_{P-T}(\theta_T - \theta_s)} \quad (4.11)$$

7. The revised α_r is calculated by taking the inverse of h_r .
8. The final step is to determine an appropriate value for λ_r which can be done a number of ways. For this study, a reasonable fit was obtained by graphically fitting the curves and iteratively changing value for λ_r while holding α_r constant until a best-fit line is obtained. If an analytical measure of the goodness of fit is desired, an analysis using the root-mean-square difference between the BC and VG curves can be performed by,

$$\text{RMS error} = \left[\frac{1}{n} \sum_{i=1}^n (\hat{y}_i - y_i)^2 \right]^{1/2} \quad [\text{Flerchinger et al., 1998}] \quad (4.12)$$

where:

n is the number of observation points between the two curves,

$\hat{Y}_i$ is the fitted value, or the value of the corresponding value on the BC curve, for either moisture content or matric potential, and

Y_i is the baseline, or value of moisture content or matric potential based on an assumed value for λ_r that corresponds to the VG curve.

Figure 4.8 Graphical description for revising the converted BC parameters

Results of this revised conversion method were plugged into the BC retention equation, plotted, and compared to the VG retention equation in Figure 4.9. The revised parameters allowed for a closer match to the VG curve near saturation by spreading the curve differences out over the range of moisture contents near the midpoint of the curve. In this range, changes in moisture contents predicted by the VG and BC equation produce relatively small changes in matric potential. The revised curve also showed a very close match near the dry region of the plots. However, it is evident from the plots in Figures 4.6 and 4.7, that the VG retention function provides a more representative description of the soil moisture retention,

as the BC function predicts a well-defined air-entry value near saturation. Table 4.3 shows a summary of the parameters required to develop an acceptable retention curve for use in the HYDRUS and SHAW models. It should be noted that θ_r was assumed zero, and the SHAW model automatically sets this value to zero with no control given to the user for changing it.

The BC function assumes the moisture content is equal to the moisture at saturation for values of matric potential that are less than the air-entry potential. With θ_r equal to zero, the moisture retention curve will approach the matric potential axis asymptotically, thus never actually reaching zero. Figure 4.9 illustrates that the matric potential gradient rapidly steepens, or becomes asymptotic, around $(0.0\% < \theta \leq 10\%)$ because of the hydraulic parameters and the θ_r of zero used for this study. A steep potential gradient is common in arid unsaturated zones that consist of sandy material with low residual moisture contents. This steep negative pressure gradient is a characteristic of the site, which makes it challenging to model physically.

Table 4.3 Moisture Retention Parameters Used for HYDRUS and SHAW

Input Model	θ_r	θ_i	α	n	λ
VG-Mualem	0	0.361	0.034	1.638	-
BC-converted	0	0.361	0.034	1.638	0.638
BC-revised (for SHAW input)	0	0.361	0.091	2.5	0.5

Figure 4.9 Comparison between the retention curves used for the HYDRUS and SHAW models

Both models calculate unsaturated hydraulic conductivity as a function of pressure head. HYDRUS was evaluated using the Mualem model, Equation (3.4), while SHAW only uses the Burdine model, Equation (3.14). HYDRUS can also use the Burdine model with the BC function, but this option was only used in this study for comparative purposes. Equations (3.4) and (3.14) are functions for describing unsaturated conductivity based on measured and fitted retention parameters. Measured values of hydraulic conductivity as a function of pressure are difficult to determine in a laboratory and were not available for this work. The parameters used in these relationships are the same as those used in the moisture retention functions. Figure 4.10 indicates that the VG-Mualem functions provide a smoother

description of the unsaturated hydraulic conductivity for tensions less than 25 cm, or near saturation, when compared to the BC-Burdine function using the revised retention parameters.

Plots of the relative hydraulic conductivity versus the moisture content show another perspective of the difference between the VG-Mualem and BC-Burdine functions. The relative hydraulic conductivity is expressed as:

$$K_r = \frac{K(h)}{K_S} \text{ or } \frac{K(\theta)}{K_S} \quad (4.13)$$

Figure 4.11 illustrates that the two functions are very similar for most of the range of moisture contents for this particular soil. However, the Mualem and Burdine functions show the largest variations with respect to the predicted unsaturated hydraulic conductivity, for a range of matric potential from approximately zero (saturation) to 10 cm. Predicted $K(h)$ in this range have significant affects on the models' capacity to predict infiltration and the rapid moisture redistribution following a rain event.

Figure 4.10 Calculated curves for matric potential as a function of hydraulic conductivity for the VG-Mualem and BC-Burdine functions using the revised BC parameters

Figure 4.11 Calculated relative hydraulic conductivity as a function of moisture content for the VG-Mualem and the BC-Burdine model using revised BC parameters

4.4

Model Simulations

The modeling effort undertaken for this study attempted to simulate physical processes that were believed to have a significant effect on the results. This was accomplished by developing a comprehensive conceptualization of the physical system in and around the lysimeter. The approximately 5-year simulation is a much longer time period than those simulated in previous studies in arid environments, [Fayer *et al.*, 1992; Scanlon and Milly, 1994; Andraski, 1997]. This allowed for a more comprehensive view of flow processes with reduced dependence on initial conditions and diurnal variations in temperature, water potential, and heat and vapor fluxes.

4.4.1

Model Geometry

Model geometries for both HYDRUS and SHAW were one-dimensional. The model profile representing the lysimeter soil consisted of a 200 cm vertical column of unit width. The profile was

modeled as a homogeneous unit. Soil homogeneity was considered an accurate representation of the material contained in the lysimeter, which was a composite of the soil removed for construction of the underground chamber containing the soil instrumentation. In addition, results from the measurements of composite soil hydraulic parameters and the “*Soil Characterization Database for the Area 5 RWMS*,” [Lee *et al.*, 1997] indicate little variability in the alluvial soil properties near the surface at this study site.

The geometry was discretized so that the number of vertical nodes, or grid cells, was fine enough to ensure that the results were not affected by the discretization itself. SHAW is currently limited to a maximum of 50 input nodes. Based on a sensitivity analysis of the number of nodes and spacing with the HYDRUS model, a 50-node profile was considered sufficient. Nodal spacing for both models was extremely fine at the surface and gradually increased with depth. Distance between nodes ranged from 0.1 to 1 cm near the surface, and gradually increased to a maximum of 20 cm near the center of the profile. A finer nodal spacing, 1 to 2 cm, was input near the bottom of the profile. It was necessary to implement an extremely fine mesh near the top boundary to capture the rapid moisture redistribution caused by steep potential gradients and large variations of atmospheric variables measured near the surface. Although not as fine as the near-surface, close spacing near the bottom of the profile was implemented to achieve more detailed representations of any potential wetting fronts that could advance to the bottom of the profile and be affected by the bottom boundary condition. Also, finer spacing near the boundaries lowers the likelihood of potential mass and energy-balance errors that could develop under extreme dry or wet conditions.

4.4.2 Initial and Boundary Conditions

Initial conditions were based on the average measured moisture content of the soil placed inside the lysimeter on March 15, 1994, the first day for the simulations. The measured initial volumetric moisture content used to initialize both models was 0.056, which corresponded to pressure values of -560 and -458 cm for the HYDRUS and SHAW models, respectively. The difference in these initial calculated pressures is indicative of the different retention functions used by the two models. The initial moisture content was assumed constant for the entire profile at the beginning of each model run, and was used to approximate the initial lysimeter storage of 11.2 cm (0.056×200). Although the initial condition may not

accurately represent the actual moisture content at each node in the profile, the 5-year simulation period allowed for a more comprehensive view of flow processes with a reduced dependence on the initial conditions at each node, as mentioned earlier.

The HYDRUS model has a built-in heat transport model that was briefly tested but produced no change in hydraulic properties or predicted storage in lieu of temperature gradients. Furthermore, during this study it was discovered that the heat model does not work unless a solute is present. SHAW considers both vapor and heat transport so it was necessary to specify initial temperature conditions. The initial temperature profile was taken from the buried TCP readings in the lysimeter soil at depths between 10 and 170 cm (Figure 2.4). Linear interpolations were made for nodes between measurement depths. A thermal gradient of zero was assumed between 170 and 200 cm for the initial profile, because no TCPs were installed at these depths. The initial temperature at the top node was taken from measured infrared temperature (IRT) readings on the bare soil surface. The TCPs were not installed until 2/23/95, and the IRT gage was installed on 12/15/94. Since the simulation period began on 3/15/94, average soil and surface temperature values for a time period consisting of 10 days before and after March 15 from subsequent years through 1998 were used to provide initial temperatures for SHAW.

Boundary conditions at the soil surface for both models were system-dependent and required measurements of actual weather conditions from the study site. The surface boundary condition for HYDRUS required knowledge of daily precipitation, potential evaporation estimated from Equation (4.4) and values for the critical pressure at the surface node for each time record. The critical pressure, "HcritA", at the soil surface describes the minimum allowable pressure head that the surface node can reach. "HcritA" was set at the default value of (-100,000) cm for this study. HYDRUS also allows the user to specify a maximum allowable pressure at the surface, "HcritS", to account for ponding conditions. This value was set to zero cm to prevent any ponding. No ponding has been observed at the study site to date. The actual surface flux in HYDRUS depends on the transient soil moisture conditions near the surface and is determined from the equilibrium conditions between the soil water and atmospheric water vapor [Simunek *et al.*, 1998] (see Section 3.2.1 for more details).

The surface boundary for the SHAW model also varies daily, however, it combines heat, water and vapor transport equations to estimate actual evaporation rates at the surface. The surface processes are

simulated by using actual weather data to determine sensible heat flux components of the surface energy balance and the latent heat flux associated with the transfer of water vapor. The time dependent weather input consisted of precipitation, maximum and minimum daily air temperatures, average daily solar radiation, dew point temperature and the daily wind run. The total daily wind run was estimated by converting the maximum wind speed measured on a particular day to a total run length for the day (wind velocity x time). The daily dew point temperature, or temperature at which the air just becomes saturated at a given specific humidity, was calculated from [Chow, 1988],

$$T_d = \frac{237.3 \ln\left(\frac{\rho_v}{611}\right)}{17.27 - \ln\left(\frac{\rho_v}{611}\right)}, \quad (4.14)$$

$$\rho_v = R_h(\rho_s) \quad \text{and} \quad (4.15)$$

$$\rho_s = 611 \exp\left(\frac{17.27 T_{avg}}{237.3 + T_{avg}}\right) \quad (4.16)$$

where:

T_d is the daily average dew point temperature,

ρ_v is vapor pressure of water vapor,

R_h is the relative humidity,

ρ_s is saturated vapor pressure and

T_{avg} is the average daily temperature.

In addition, the SHAW model required a ponding depth to be input, and this value was set at zero cm.

The lysimeter was designed to allow vertical drainage under a buildup of moisture at the bottom of the soil profile. Therefore, a free-drainage boundary condition was used to describe the bottom node in HYDRUS. Free drainage represents a unit-gradient condition, which typically describes situations where the water table lies far beneath the model domain. The bottom boundary condition for the SHAW model was tested using both a unit gradient and a “user-specified” moisture content for water flow at the bottom of the profile. When a “user-specified” moisture content was used for the bottom boundary condition, the model required a known moisture profile for the last time step in the run to perform a linear interpolation at

the bottom node between times for which the user provided moisture content data. A unit gradient condition means the hydraulic gradient becomes (-1) and the vertical flux is then equal to the unsaturated hydraulic conductivity, $K(h)$. The unit gradient boundary condition provided better results and was determined to be an excellent representation of the soil profile in a lysimeter, since the measured and simulated suction head near the bottom never decreased to near zero. Selection of the unit gradient boundary condition was further justified based on work by researchers at water balance study sites on the Hanford Site in Richland, Washington [Rockhold *et al.*, 1988; Gee *et al.*, 1989]. Unit gradient conditions were observed in many of their lysimeters.

4.4.3

Simulation Controls

HYDRUS and SHAW differ greatly in the amount of control given to the user for time steps and iteration criteria. Time steps for HYDRUS were internally varied between $1.0\text{E}-5$ and 1.0 day, depending on the mass-balance and convergence criteria. A maximum time step of one day was specified to match the time-dependent input data. The selection of an initial time step was based on past experience with the model and the extremely dry conditions that develop at the study site. High-pressure gradients that develop during infiltration into an initially very dry soil profile require relatively small time steps to achieve convergence. The iteration criteria in HYDRUS were controlled by a specified tolerance in water content, which described the maximum desired change in the value of the water content between two successive iterations during a particular time step. The moisture content tolerance was a fairly sensitive parameter, and was adjusted according to the particular situation being modeled for this study. As stated previously, for most runs, 1 mm of water was considered acceptable an water balance error.

The only input parameter required by SHAW for control of the predicted modeling error and convergence, was a single value representing the error tolerance. This value was used for convergence criteria for energy balance and the fraction of change in matric potential or vapor density for water. The tolerance factor was adjusted according the particular model situation being evaluated, but was set at 0.01 for most of the runs in this study.

4.4.4

Additional Input

Additional input required by the SHAW model was included in a model file that described the site characteristics. These input variables were determined from either direct measurements or other sources and are summarized in Table 4.4.

Table 4.4 Additional Input Required for the SHAW Model

Input Variable	Value	Comments
Latitude	36°51"	
Slope of the study site	0°	
Aspect of slope	0°	
Time of solar noon	11.5	Default value for the eastern part of a time zone.
Site elevation above sea level	972.9 m	
Albedo of dry soil	0.36	<i>Levitt and Sully, 1998</i>
Moist soil albedo exponent	0.0	See Equation (3.22)
Wind-profile surface roughness	0.2 cm	Bare soil estimate based on <i>Scanlon, 1992</i>
Measurement height for air temperature, wind speed and humidity	3.0 m	
Bulk density of soil layer	1618 kg/m ³	(assumed constant for entire profile), <i>Lee et al., 1996</i>
Percent sand	85.3	(assumed constant for entire profile), <i>Lee et al., 1996</i>
Percent silt	10.4	(assumed constant for entire profile), <i>Lee et al., 1996</i>
Percent clay	4.3	(assumed constant for entire profile), <i>Lee et al., 1996</i>
Percent organic matter	0.0	(assumed constant for entire profile), <i>Lee et al., 1996</i>

CHAPTER 5

RESULTS

5.1 Sensitivity Analysis

Most of the physical parameters used for this study were considered accurate descriptions of the site. However, not all parameters necessary for model input could be directly measured or collected. Furthermore, the uncertainty of the interaction between all input parameters and physical processes of the two models made it necessary to perform a detailed sensitivity analysis. The purpose of this sensitivity analysis was to accomplish three goals:

1. Provide a means to show that the models were correctly simulating the underlying transport equations.
2. Provide a means to estimate specific parameters that could not be measured directly in the field or inferred from other measured parameters.
3. Provide an initial estimate of which parameters should be adjusted to achieve the desired results, or calibration to actual measurements.

While evaluating the parameters to be tested, care was taken to minimize the selection of input variables that were dependent on other parameters. This is a common error made in many deterministic sensitivity analyses, which produces unrealistic results. The deterministic approach taken for this study compared differences in the normalized sensitivity coefficients, S_{ni} , calculated from

$$S_{ni} = \left[\frac{\overline{X_i}}{F(\overline{X_i})} \right] \left(\frac{\Delta Z}{\Delta X_i} \right) \quad (5.1)$$

where:

$\overline{X_i}$ is the initial or baseline value of the i^{th} parameter,

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

ΔZ is the change in the performance measure and ΔX_i is the change in the design variable.

The larger the value of the computed normalized sensitivity coefficient, the more sensitive the model output was to the particular parameter tested [Meyer *et al.*, 1996]. The sensitivity of a particular parameter was tested by holding all variables described in the “Baseline Model” constant, and changing only the variable of interest for each condition tested. Summaries of the sensitivity results are shown in Tables 5.1 and 5.2 for HYDRUS and SHAW, respectively. It should be noted that the sensitivity coefficients were determined using different performance measures for HYDRUS and SHAW and therefore should not be compared with each other.

The results of this sensitivity analysis indicated that both models seemed to accurately reproduce or reflect the mathematics used to describe the natural phenomena being simulated. The performance measure used for the HYDRUS model was the average daily storage, which was essentially a summation of the results of several physical processes in the model (Table 5.1). Two baseline models were used in HYDRUS. The Initial Baseline Model (IBM) was initiated with typical retention parameters of sandy loam material with a 50-node profile. These parameters were used for the IBM because at the time this research had begun, the measured moisture retention properties had not been completely analyzed. The Final Baseline Model (FBM) was initialized with the revised retention parameters that were numerically fit from the measured retention data that incorporated the RETC program described in Chapter 4. Some of the most important findings related to the performance of the HYDRUS model included:

- Using the estimated initial baseline parameters, the model seemed to be most sensitive to an order-of-magnitude increase and decrease in the saturated hydraulic conductivity. An increase in the hydraulic conductivity produced higher surface fluxes out of the profile, thereby significantly decreasing the average storage. Typically, the saturated hydraulic conductivity is a reasonable parameter to adjust for calibration since its values usually show large ranges of spatial variability when compared to other hydraulic parameters.
- By lowering the pore-connectivity value from 0.5 to zero in simulation #3 (Table 5.1), the storage showed a slight decrease during the summer months. The decrease in storage was expected, since the theoretical effect of lowering the pore-connectivity value to zero is lower unsaturated

hydraulic conductivities, $K(h)$, as a function of decreasing pressure heads for dry conditions. For lower pore-connectivity values, unsaturated conductivities tend to yield sharper decreases as the profile becomes drier, particularly during the summer months.

- The residual moisture content used in HYDRUS was tested with both baseline models, and the sensitivities were different by one order of magnitude. This result illustrates the importance in selecting or measuring the appropriate hydraulic parameters, as slight changes in these variables can produce considerably different results. The residual moisture content seemed to have a large effect on the model's ability to predict storage as the moisture content decreased or pressures became more negative.
- The "HcritA" parameter tested for simulation #9 (Table 5.1) is an adjustable parameter in the time-dependent boundary conditions that can be input for each day. "HcritA" represents the minimum value of pressure head at the surface, or the driest state in which the surface node is allowed to reach. The model default value is -100,000 cm, which is input as +100,000 cm in tension. Storage results indicated that by increasing this value to 150,000 cm for the entire time domain, "HcritA" parameter had little effect on the model.
- Another important result from the HYDRUS sensitivity simulations is the lack of sensitivity to the number of nodes in the profile for both baseline conditions. This result verified that 50 nodes in the FBM and calibrated models were sufficient in simulating a realistic conceptual flow domain.

Table 5.1 HYDRUS Sensitivity Summaries

Simulation Description	Baseline Value	Tested Value	Average Daily Storage (cm)	Sensitivity Coefficient
1. Initial Baseline Model	-	-	<u>17.05</u>	-
2. Avg. Potential Evaporation (cm)	0.439	0.878	15.28	0.104
3. Pore-Connectivity (t)	0.5	0	16.29	0.044
4. Saturated Hydraulic Conductivity (cm/hr)	334.1	3341	15.30	0.114
5. Saturated Hydraulic Conductivity (cm/hr)	334.1	33.4	18.30	0.081
6. Residual Moisture Content	0	0.039	18.39	0.027
7. # of Nodes in Profile	50	30	16.95	0.015
8. # of Nodes in Profile	50	100	16.77	0.016
9. HcritA (cm)	100,000	150,000	17.04	0.0015
10. Final Baseline	-	-	<u>12.01</u>	-
11. Residual Moisture Content	0	0.039	16.86	0.139
12. # of Nodes in Profile	50	100	12.02	0.0007
13. Pore-Connectivity (t)	0.5	0.75	13.95	0.161

Table 5.2 shows a summary of the SHAW sensitivity results. The SHAW model provided more complete output tables showing results of direct calculations of components that make up the total water and energy balances in a very user-friendly format. Therefore, the SHAW model allowed for a more descriptive testing of the model's sensitivity based on a combination of individual water balance components. The performance measure used for the SHAW model was the total water balance over the length of the study period, which was calculated based on an initial storage of 11 cm, total precipitation, drainage and evaporation. Just as with HYDRUS, the SHAW model was also tested with two different baseline models. The IBM, simulation #1, was modeled with 30 nodes and retention parameters that were converted (for BC model) from the initial estimates used in the HYDRUS IBM. The FBM, simulation # 7, was modeled with 50 nodes, and the calibrated parameters were calculated using the procedure outlined in

section 4.3. Important insight into the performance of the SHAW model was gained based on the following results:

- An order-of-magnitude increase in the saturated hydraulic conductivity produced only slightly lower storage results, but significantly increased drainage and evaporation. Based on the calculated sensitivity coefficient, the model was much more sensitive to a 1 order of magnitude decrease in conductivity.
- The bulk density parameters of 1623 (kg/m³) and 1649 (kg/m³) were selected based on results from *Lee et al.*, (1996), where these values represent averages near the surface and at a depth near 2 m, respectively. Based on the small change in storage it was concluded that bulk density had little effect on the model results.
- The SHAW model was very sensitive to the number of nodes selected, which lead to the selection of the maximum allowable value of 50. The increase in nodes produced a simulated positive flux into the profile via the bottom boundary. This incoming flux condition, albeit small in relative magnitude, was probably an artifact of the numerical model and the resulting limitations of the bottom boundary conditions. More importantly, the increase in nodes from 30 to 50 along with a more dense spacing near the bottom eliminated the predicted model drainage out of the profile.
- The atmospheric parameters tested with the FBM indicated that the SHAW model was very sensitive to solar radiation and changes in the maximum daily air temperature. Solar radiation and air temperature make up the major components in the relationship used to describe evaporation, and by doubling the input in each case, the total evaporation was substantially increased as expected.

Table 5.2 SHAW Sensitivity Summaries

<u>Simulation Description</u>	Baseline Value	Tested Value	Total Precipitation (cm)	Total Drainage¹ (cm)	Total Evaporation (cm)	Total Water Balance (cm)	Sensitivity Coefficient
1. Initial Baseline (30 nodes)	-	-	66.44	-1.42	61.68	<u>17.19</u>	-
2. Sat. Hydraulic Cond. (cm/hr)	13.92	139.2	66.44	-8.76	69.17	17.03	0.001
3. Sat. Hydraulic Cond. (cm/hr)	13.92	1.392	66.44	-0.26	60.00	17.71	0.034
4. Bulk Density (kg/m³)	1649	1623	66.44	-1.44	61.70	17.18	0.022
5. Wind Surface Roughness Parameter (cm)	0.2	2.0	66.44	-1.82	62.33	16.94	0.002
6. # of Nodes in Profile	30	50	66.44	1.57	61.55	14.32	0.308
7. Final Baseline (50 nodes)	-	-	66.44	0.44	62.15	<u>14.85</u>	-
8. Avg. Daily Dew Pt. Temp. (°C)	-9.27	-2.69	66.44	0.43	62.23	14.78	0.007
9. Avg. Daily Solar Radiation (W/m²)	129.44	454.41	66.44	0.34	63.51	13.60	0.034
10. Avg. Daily Wind Run (miles)	237	118.5	66.44	0.87	61.59	14.98	0.018
11. Moist Soil Albedo Exponent	2.6	0	66.44	0.43	62.19	14.82	0.002
12. Dry Soil Albedo	0.15	0.36	66.44	0.47	61.93	15.05	0.009
13. Avg. Daily Max. Temp. (°C)	25.03	50.06	66.44	0.34	63.19	14.02	0.063

¹ A negative value for drainage indicates a moisture flux out of the modeled soil profile, and a positive value indicates moisture pulled up from below the profile. Realistically, moisture entering the soil at the bottom of the profile will not occur, because the lysimeter is essentially sealed off from the soil below by an open space that contains measurement equipment.

5.2

Storage Comparisons

Ultimately, storage changes in the lysimeters provided a comprehensive measurement of the performance of the HYDRUS and SHAW models. Actual storage in the lysimeter was taken to be a very accurate measurement of the sum of several physical processes at the site. Changes in storage were controlled mainly by pressure gradients in the soil profile, which were greatly affected by the soil properties and the interaction of atmospheric and surface processes that affect the moisture redistribution throughout the soil. After assemblage of all the measured parameters and several complex calculations, the storage was predicted numerically using the HYDRUS and SHAW models. In the field, daily changes in storage were measured with precision load cells, which were enclosed in a space below the lysimeter and sheltered from external climate effects. The changes in storage measured in the field provided an excellent tool for achieving model calibration.

5.2.1

HYDRUS Storage

The HYDRUS model was evaluated using two sets of baseline parameters, as discussed earlier in Chapter 5.1. The IBM was established using typical retention parameters for a loamy sand material. These initial estimates were made because the measured retention parameters from the laboratory data were not available when this research began. Furthermore, the results from two different retention parameter sets gave important insight into the importance of accurate estimates of the hydraulic properties. The retention properties used for both baseline models are summarized in Table 5.3. The same saturated hydraulic conductivity, 334 cm/day, was used for both baseline models, as this parameter was directly measured in the lab using a constant head procedure before this study began.

Table 5.3 Retention Parameters Used in the Baseline HYDRUS Models

	θ_r	θ_s	α	n
Initial Baseline	0.0	0.369	0.067	1.318
Final Baseline (from actual measurements and fitting procedure)	0.0	0.361	0.034	1.638

The results of the IBM indicated an over prediction of storage as shown in Figure 5.1. The model appeared to be severely underpredicting evaporation during dry-down periods, particularly following the large rainfall events late in the winter of 1995. The results of increasing the daily potential evaporation, “PE x 2”, only lowered the storage by a small amount. However, by increasing the saturated hydraulic conductivity one order of magnitude from $3.34\text{E}2$ to $3.34\text{E}3$ (cm/day), the storage was significantly lowered to a much closer match until February 1998. As indicated in the sensitivity analysis an increase in the saturated hydraulic conductivity produced a large increase in fluxes out of the soil profile. Figure 5.1 also shows the results of using a RETC-fitted θ_r of 0.039 instead of zero. Overpredicted storage from the simulation, “residwc”, further justified the use of zero for θ_r .

Figure 5.1 Storage comparison with the initial baseline model for the HYDRUS sensitivity analysis

Figure 5.2 illustrates the results of the storage output from the FBM tests. The results obtained by only changing the retention parameters to fitted parameters that were based on measured values were significant. In general, the FBM tended to underpredict storage during the dry-down summer months followed by closer comparisons during the wet winter months. Also, the model appeared to overpredict storage during the summer following the beginning of the simulation. However, this result was probably due to the fact that the model was still coming into equilibrium with the surrounding conditions. Several other modeling scenarios were simulated and are summarized in Tables 5.4 and 5.5.

Figure 5.2 Predicted storage comparisons of the HYDRUS Final Baseline Model with measured storage

Table 5.4 provides a description of the modeling scenarios that were tested in HYDRUS using the different retention models and the different methods for determining the parameters for these models. All simulations described in Table 5.4 assumed a pore-connectivity value of 2.0, which is consistent with the original Brooks-Corey theory [Brooks and Corey, 1964]. The saturated hydraulic conductivity was left at a constant value of 334 cm/day for all simulations, which was the value measured in the laboratory. Since HYDRUS has the option to select the BC retention model, three different scenarios were tested using the theory of Burdine and Mualem, as described in Chapter 4.3, to predict the retention parameters for use with the BC function in HYDRUS. The retention parameters used in the "BC-Mualem" model described in Table 5.4 are the same parameters obtained through the parametric equation conversion process between the VG and BC parameters. A comparison was made between the revised parameters that were determined using the procedure described in Chapter 4.3, and the parameters that were converted from VG to BC using both the Burdine, ($m = 1 - 2/n$), and Mualem, ($m = 1 - 1/n$), theories. The conversion using the Mualem theory was explained in Chapter 4.3 and is suggested for many types of soils. Here the conversion using the Burdine theory was considered for comparative purposes only. The model with the parameters converted using the Mualem parametric equations, "BC-Mualem", produced superior results when compared to the other BC model runs as shown in Figure 5.3. The "BC-SHAW" model severely

overpredicted storage with the same retention parameters that were used in SHAW. As described in Section 5.2.2, these same parameters produced reasonable results using the SHAW model. The results shown in Figure 5.3 indicate that the VG retention relationship yields far superior model predictions of storage for the HYDRUS model.

Table 5.4 HYDRUS Simulations Based on Different Retention/Hydraulic Theories

Model Name	Description
<BC-Burdine>	<ul style="list-style-type: none"> - Brooks-Corey option selected as the hydraulic model - θ_r, θ_i, α were set equal to the values used in the FBM, 0.0, 0.361, 0.034 respectively - λ was set at 0.362 from the Burdine theory, ($\lambda = n - 2$), see Table 4.3, where ($n = 1.638$) - Initial pressure head conditions were based on the starting moisture content of .056, and were calculated using the BC equation as it is applied in HYDRUS, $S_e = \alpha h ^{-n}$
<BC-Mualem> (converted parameters)	<ul style="list-style-type: none"> - Brooks-Corey option selected as the hydraulic model in - θ_r, θ_i, α were set equal to the values used in the FBM, 0.0, 0.361, 0.034 respectively - λ was set at 0.638 from The Mualem theory, ($\lambda = n - 1$), see Table 4.3, where ($n = 1.638$) - Initial pressure head conditions were based on the starting - moisture content of 0.056, and were calculated using the BC equation as it is applied in HYDRUS, $S_e = \alpha h ^{-n}$
<BC-SHAW> (revised, converted parameters)	<ul style="list-style-type: none"> - Brooks-Corey option selected as the hydraulic model - θ_r, θ_i were set equal to the values used in the FBM, 0.0 and 0.361 respectively - The two curve fitting parameters, α_r and λ_r were set at 0.091 and 0.5 respectively (same as SHAW FBM) - Initial pressure head conditions were calculated based on moisture content of 0.056 and plugged into the BC equation as it is applied in HYDRUS, $S_e = \alpha h ^{-n}$

Figure 5.3 Storage predictions from simulations using various hydraulic parameter estimations which applied the Brooks-Corey retention model compared to the HYDRUS FBM

Figure 5.4 Comparisons between various sensitivity tests and the calibrated HYDRUS model

Table 5.5 Summary of Modeling Scenarios Tested for Calibration

Model Name	Description
<resid. vmc = .039>	<ul style="list-style-type: none"> - All retention/hydraulic parameters were set equal to FBM except θ_r, - $\theta_r = 0.039$, from the RETC curve fitting analysis based on measured retention properties - Initial pressure head conditions were based on the starting moisture content of 0.056, and were calculated using the VG Equation (3.3)
<pore con. = 1 >	<ul style="list-style-type: none"> - All retention/hydraulic parameters were set equal to the FBM except the pore-connectivity value, ι - ι was changed from the default value of 0.5, to 1.0
<calibrated>	<ul style="list-style-type: none"> - All retention/hydraulic parameters were set equal to the FBM, except the pore connectivity value, ι - ι was changed from the default value of 0.5 to 0.75

Table 5.5 is a summary of the simulations that were used to arrive at a final calibrated model. Based on the storage results in Figure 5.4, the calibrated HYDRUS model appeared to be in excellent agreement with actual storage measured in the field. However, the storm event that occurred in February 1998 caused noticeable underprediction of storage for the remainder of the study period. The results indicated that storage was underpredicted during and immediately following this storm event. The effects of this storm are significant to the results of this study, and are discussed in more detail in Chapter 6. Predicted storage changes for the remainder of 1998 plotted parallel to the actual storage changes, which indicated that the model predicted less infiltration than was measured by the lysimeter only during this period of what was defined to be excessive precipitation (4.7 cm over 27 hours). In addition, initial overpredicted storage during late 1994 can probably be owed to the model not being in equilibrium with the surrounding conditions. The calibrated storage plot in Figure 5.4 is from a model run with the maximum allowable number of print times of 100 (points on the graph), for water balance information. The calibrated model was also run using sequential runs with 100 print times for each run, by importing the final conditions of a completed run for the initial conditions of a subsequent run. This process was continued until a predicted storage was available for each day of the study period. This allowed for a more complete

view of storage changes (Figure 5.5). Total water balance error for the entire calibrated simulation was only -0.0039 cm.

Figure 5.5 Daily storage predictions from the calibrated HYDRUS model compared to measured storage

5.2.2

SHAW Storage

As stated earlier, the SHAW model was evaluated using two sets of baseline parameters from which all comparisons were made. The hydraulic parameters for the IBM in SHAW were based on the same parameters as the IBM used in HYDRUS, which were converted using the VG and BC parametric equations based on the Mualem theory. The FBM SHAW parameters were also based on the same parameters used in the HYDRUS FBM. However, for the SHAW FBM, retention parameters were converted using the revised method suggested for this research to obtain the appropriate BC retention relationship that could be used for the SHAW model. The saturated hydraulic conductivity was left at 334 cm/day, as measured in the laboratory, for all simulations. All other hydraulic parameters used in the two baseline models are described in Table 5.6. The final calibrated model was developed by adjusting all time-variant input in the FBM according to the results of the sensitivity analysis described in Chapter 5.1.

Table 5.6 Retention Parameters Used in the Baseline SHAW Models

	θ_r	θ_s	α	λ
Initial Baseline	0.0	0.369	0.091	0.299
Final Baseline (based on revised conversion method)	0.0	0.361	0.091	.5

The SHAW model simulates storage changes by solving the coupled energy and mass balance relationships to estimate a total water balance in the soil profile. Actual evaporation is estimated from the available moisture and resulting heat and vapor transport predictions. For this study, daily storage changes were predicted and compared to actual storage measurements in the lysimeter. When this research began, SHAW only had the capability to handle 30 nodes in a profile. However, an updated version was compiled that allowed for up to 50 nodes. The IBM for SHAW had only 30 nodes and after adding 50 nodes to the profile, a sensitivity analysis revealed that SHAW was very responsive to an increase in nodes from 30 to 50. The resulting changes in storage are shown in Figure 5.6. The IBM with 30 nodes overpredicted storage during the dry-down periods following winter precipitation. Evaporation was increased as a result of applying a denser nodal discretization of 50 nodes to the model profile.

Figure 5.6 Comparison between 30 and 50 node profiles using the Initial Baseline Model

A calibrated model was achieved after using the BC retention parameters determined using the revised method developed for this research (Section 4.3). Furthermore, a few slight adjustments were made to parameters that had a limited overall effect on the results, such as dry and moist soil albedo. The bare soil albedo, or soil reflectivity, had a very small effect on the model output, but a final determination of the appropriate values was based on the work of *Levitt and Sully, 1998*, where a bare-soil value of 0.36 was used at the Area 5 RWMS. The SHAW model also required a value for the exponent in Equation (3.22) that was used to determine the moist soil albedo. This exponent was set to zero so that moist and dry soil albedo were equal, since over a long period of time, the bare soil remained relatively dry due to the high evaporative conditions at the study site. As mentioned in Section 4.4.2, the selection of an appropriate bottom boundary condition was very important. Simulations were made with a specified moisture content at the final input time for interpolation of moisture at the bottom of the profile between times for which moisture content profiles were known. Although moisture profiles were known for portions of the simulation period, a major goal of the evaluation process was to test SHAW's ability to predict moisture. Therefore, this option was not a valid choice for this study. Fortunately, SHAW provided an option to

specify a unit gradient for a bottom boundary condition. A unit gradient boundary condition is typically a valid choice to model lysimeters when the bottom of the modeled profile does not approach saturation, as was the case for this particular study site. Using the calibrated parameters, a comparison was made between the two choices for boundary conditions (Figure 5.7). The storage results in Figure 5.7 support the findings for the sensitivity analysis in which a specified moisture boundary condition produced significantly higher moisture contents near the bottom of the profile following wetter periods, which lead to significant amounts of predicted drainage after advancements of large wetting fronts.

The final calibrated SHAW model compared very well to observed storage in the lysimeter (Figure 5.8). Early on, predicted storage was higher than the actual storage as a result of underpredicted evaporation, but as the simulation period continued the differences in predicted and actual storage became less. The initial overprediction of storage was probably a result of the model not being in equilibrium with the atmospheric conditions, which appeared to be the case for HYDRUS also. Like HYDRUS, the SHAW model badly underpredicted storage during and immediately following the large precipitation event in February of 1998, but predicted storage plotted parallel to measured storage for the remainder of the simulation period. This occurrence appeared to be a result of less simulated infiltration during the event than what actually occurred at the lysimeter site. Similar results indicate further evidence of underprediction of infiltration during other large rain events in the late spring of 1995 and winter of 1997. Water balance error for the calibrated SHAW model was simulated to be a total of -0.203 cm.

Figure 5.7 Comparison of the effects of the bottom boundary conditions in the SHAW model

Figure 5.8 Calibrated SHAW model storage predictions compared to actual measured storage

CHAPTER 6

DISCUSSION

6.1 Effects of a Nonisothermal Flow Regime

Several researchers have reported that thermal and vapor effects play a significant role in transport processes at arid sites. *Scanlon and Milly, (1994)* studied a site in the Chihuahuan Desert in Texas, and observed that, "below 30 cm, attenuation and phase shift of water potentials and temperatures were similar." It was also suggested that, "water potential variations may be controlled by temperature fluctuations, with little influence from changes of water content." *Andraski, (1997)* presented results from a multiple-year field study in the Mohave Desert in Nevada, which suggested nonisothermal vapor flow was significant enough to warrant consideration above depths of 1 m at that arid site. However, a few researchers have indicated that a relatively high degree of model accuracy can be obtained in simulations that ignore nonisothermal vapor transport under certain conditions. For example, *Meyer et al, 1996*, modeled a site in a climate similar to that of the Area 5 RWMS on the NTS. Their site was located in Beatty, Nevada, approximately 80 km from the Area 5 location. They concluded that isothermal simulations appeared to be "a practical alternative to conducting nonisothermal simulations." However, they added that, "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."

The field data and modeling results of this study suggest that the thermal gradients and vapor transport may not play a significant role in the physical processes involved with unsaturated flow simulations for the extremely arid climate studied. HYDRUS is an isothermal model that ignores vapor flow and the results obtained during this study were remarkably consistent with field measured data and the SHAW model, which incorporates nonisothermal vapor flow. It appeared that a nonisothermal setting had very little effect below the near-surface at the study site. In the active surface zone near the top 15 cm

of the soil profile, predicted matric potential data suggested that pressure gradients were strongly influenced by seasonal temperature variations. It is likely that the soil at the Area 5 RWMS often reached low enough water potentials to become desiccated, especially near the surface. When the soil becomes desiccated, vapor transfer can become the dominant mechanism of water movement [Hillel, 1980]. However, this near-surface process had very little overall effect on the models' capabilities to accurately predict moisture storage at the site.

Nonisothermal effects at the study site were evaluated by comparing attenuation and phase shift of water potentials and temperature with depth for the duration of the study period. The first step in this process was to evaluate SHAW's ability to predict temperature with depth. Measured temperature data collected at site was only available at 10 vertical locations between 10 and 170 cm and at the surface (Figure 2.4). The SHAW model predicted temperatures that were in good agreement with measured temperatures between the surface and 10 cm. At 20 cm depth, predicted summer temperatures were in good agreement, but winter temperatures were overpredicted by an average of 4.5 °C. Below 40 cm depth, phase shifts were in good agreement, but the temperatures were progressively underpredicted with depth during the summer months. At 170 cm depth, average summer predicted temperatures were underpredicted by approximately 13.5 °C. It is not known whether these differences can be attributed to errors in the prescribed properties or to inaccuracies in the handling of the heat simulation by the SHAW model. Simulations were evaluated with varying bulk densities and particle sizes to evaluate the effects of the corresponding changes in thermal conductivity, but the differences in storage were negligible. Furthermore, the differences could also be related to the artificial boundary conditions created by the steel walls of the lysimeter. Comparisons between measured and predicted temperatures at depths of 10 and 170 cm are shown in Figures 6.1 and 6.2.

The next step was to construct plots of daily matric potential data from both HYDRUS and SHAW along with predicted temperatures from the SHAW model. These plots, Figures 6.3 – 6.4, gave valuable insight into the possible dependencies of pressure on seasonal temperature fluctuations at various depths. Predicted soil temperatures from the SHAW model were used because measured temperature records were not available in 1994, and it was shown that SHAW accurately predicted phase shift at all depths. The model also predicted soil temperatures that were in good agreement above 20 cm for all

seasons. It was observed that matric potential was indeed highly dependent on temperature variations at the very near surface. This relationship is clearly shown in Figure 6.3, where potentials at 0.1 cm were estimated to be in excess of 100,000 cm tension during much of the study period. Based on the modeled pressure head dependency on temperature, nonisothermal vapor flow appeared to be the dominant transport mechanism only between the surface and 1 cm. It is important to note that because of the boundary condition in HYDRUS, which allowed a minimum pressure at the surface of -100,00 cm, comparisons with the HYDRUS model in this region could not be made. Near-surface matric potentials in the SHAW model were allowed to reach extremely high values ($>100,000$ cm). Predicted potentials from HYDRUS and SHAW at depths below 1 cm were in good agreement. Below 1 cm, attenuation and phase shift were significantly reduced and consequently, the matric potentials appeared to become less dependent on temperature. Figure 6.4 illustrates that matric potential at 15 cm was still slightly affected by seasonal temperature fluctuations. Below 15 cm, fluctuations in matric potential became less affected on the variation in soil temperature and more dependent on the available moisture and the advancement of wetting fronts. Downward thermal fluxes during the summer and upward thermal fluxes during the winter seemed to have had little effect on moisture movement at greater depths. During periods of low moisture storage in the lysimeter, particularly the summers of 1996 and 1997, matric potentials were out of phase with the seasonal temperature attenuation during these dry-down periods. At 90 cm, matric potentials showed very little fluctuation as a result of seasonal temperature changes (Figure 6.5)

Figure 6.1 Comparison between daily predicted temperatures from SHAW and actual measured temperatures at 10 cm

Figure 6.2 Comparison between predicted daily temperatures from SHAW and actual measured temperatures at 170 cm

Figure 6.3 Near surface relationship between predicted temperature and predicted matric potential from the SHAW model at 0.1 cm

Figure 6.4 Relationship between temperature and predicted matric potential from the HYDRUS and SHAW models at 15 cm

Figure 6.5 Relationship between temperature and predicted matric potential from the HYDRUS and SHAW models at 90 cm

Predicted and measured water potential profiles were compared to gain a better understanding in the overall behavior of matric potential during the winter and summer seasons. Actual potentials measured with the installed thermocouple psychrometers (TCP) were not used because of large errors in the readings. However, the time domain reflectometer (TDR) probes that were installed at the same depths as the TCP, predicted storage changes that showed relatively close matches to the storage changes measured by the lysimeter scales for most of the study period. However, there were several days throughout the study period when malfunctions in the TDR produced erroneous data. Therefore, it should be noted that a definite but unknown degree of uncertainty existed in the TDR measurements presented for this study. Also, because the TDR probes malfunctioned for most of 1997, data from that year were not considered in the seasonal averages. For the plots in Figure 6.6, measured moisture contents were converted to potentials for comparison to model predictions using the same van Genuchten relationship that was used to calculate the parameters for the calibrated HYDRUS model.

Predicted potential gradients from the HYDRUS and SHAW models in Figure 6.6 were in good agreement throughout the simulation period. This result could be further evidence that nonisothermal

transport had little effect on a model's ability to predict storage. Average predicted matric potentials during the winter months showed little change in the directions of driving forces below 40 cm for both models. Potential data that was converted from measured moisture contents showed large variations in the near surface. However, the same general trend existed below 20 cm that was predicted with HYDRUS and SHAW models. During the summer months, potential gradients showed little change below 70 cm for measured and predicted profiles in Figure 6.6. Strong upward driving forces were consistent with the large decreases in storage due to high evaporative demand, particularly during the summer. Throughout the study period, both models indicated that above the simulated 200 cm profile, on average, the direction for isothermal liquid flow was upward.

A comparison between measured and predicted temperature profiles in Figure 6.7 illustrates the large variations in average seasonal temperatures profiles during the study period. The differences between the temperature profiles predicted by SHAW and the measured temperatures are consistent with the differences in daily temperature plots shown in Figures 6.1 and 6.2. It appeared that an increasingly larger discrepancy with depth existed below 30 cm during the summer months; while predicted and measured winter temperatures were in good agreement for the same depths. Near the surface, the sharp decrease in measured temperatures during both winter and summer seasons was determined to be a result of diurnal cooling that was not accounted for in the SHAW model. Because SHAW was run with daily input, diurnal variations in temperature were not captured. However, since the objective of this study was to evaluate long-term seasonal effects, diurnal atmospheric fluctuations were not considered to have a large overall effect on the results.

Predictions from the SHAW model plotted in Figures 6.6 and 6.7 indicated that water potentials and temperature gradients were in the same direction during the summer and diametrically opposed during the winter. These findings are consistent with those reported by *Andraski, (1997)*, in which a nearby waste disposal site in the Mohave Desert was studied. However, for this study, opposing temperature and potential gradients had little overall effect on storage predictions in the profile.

Figure 6.6 SHAW model seasonal matric potential profiles. HYDRUS profiles were in good agreement SHAW predictions, but are not depicted here in order to provide a less congested plot area

Figure 6.7 Comparison between average predicted and measured temperature profiles

The effectiveness of the HYDRUS and SHAW models in predicting unsaturated flow in an arid environment was evaluated by comparing measured storage from the lysimeter to the predicted storage results from the two calibrated model simulations. Changes in storage, as measured in the lysimeter, were controlled by the amount of evaporation that withdrew moisture from the soil profile. Both models predicted storage changes that were generally in good agreement with measured storage changes in the lysimeter. However, a large amount of precipitation was experienced during February of 1998, which caused significant underpredictions of storage from both models.

Approximately 93% of the actual precipitation measured at the study site was returned to the atmosphere as evaporation. The HYDRUS and SHAW models predicted, over the course of the study period, that respectively 94% and 89% of the precipitation was returned to the atmosphere as evaporation. The SHAW model overpredicted evaporation immediately following precipitation events, and usually underpredicted evaporation following the times when the initial high evaporation rates over-dried the near-surface soil. Over the course of the simulation, cumulative evaporation predictions were very close to the measured evaporation (Figure 6.8). The likely cause of the overpredicted evaporation from the SHAW model during precipitation events could be the weakness of the Brooks-Corey function near saturation, explained in Chapter 4.

An estimation of the relative accuracy of the models was made by calculating the root-mean-squared, RMS, error of the simulated storage compared to the measure storage using the Equation (4.3). For the calibrated simulations, prior to February 1998, the RMS error of the HYDRUS and SHAW models was 0.63 and 0.81 respectively. For the entire study period, the RMS error for HYDRUS and SHAW was 1.69 and 1.83 respectively. It is interesting to note the remarkable similarities between the calibrated HYDRUS and SHAW models in Figure 6.9. The similarities between the storage output of the two models could be another indication that nonisothermal vapor transport is an unnecessary consideration for accurate unsaturated flow predictions at the Area 5 RWMS.

Figure 6.8 Predicted model evaporation compared to measured evaporation and precipitation

Figure 6.9 Calibrated model storage comparisons

6.2.1

February 1998 Precipitation

Approximately 4.7 cm of precipitation was measured in a 27-hour period in February 1998. On February 23 and 24, the Area 5 RWMS experienced what was estimated to be a 25-year, 24-hour storm event. Furthermore, another 5.6 cm of precipitation fell between 1/29/98 and 2/20/98. To put this in perspective, the 10 cm of precipitation that was measured during this period was 2 cm more than the total

amount that was measured during every month of January over the entire study period. It was only 1 cm less than what was measured for all the combined spring seasons (March - May) from the entire study period! HYDRUS and SHAW both overpredicted evaporation between 2/14/98 and 2/24/98 by almost 79%. The predicted moisture profiles from the models indicate lower than expected moisture contents at the end of the time step representing the day of the storm. The moisture profile in Figure 6.10 indicated that infiltration rates were lower than what might be expected based on accumulated storage near the surface considering the extreme amount of water available for infiltration at that time step. Unfortunately, comparisons between the predicted moisture profile and measured profile could not be used because of a malfunction in the TDR probes during most of 1997 and the beginning of 1998. Nevertheless, two possible hypotheses were developed to explain the underpredicted model storage:

1. Daily times steps were inadequate for capturing infiltration during times when precipitation intensities were the highest. In addition, larger times steps could be a possible cause for the lack of moisture redistribution in the near-surface profile and the overprediction of evaporation.
2. In arid environments, hysteresis of the soil hydraulic properties may play a significant role in the redistribution of moisture. Hysteresis was not considered in this study and was an obvious weakness.

To evaluate the potential results of using hourly time steps, the HYDRUS and SHAW models were set up using hourly time steps and measured hourly meteorological input during February 1998 only. However, predicted storage remained unchanged during this period. Although hourly times steps did not provide the expected results, there was assurance that daily time steps sufficiently captured the necessary physical processes for accurate predictions of moisture movement over long periods.

Figure 6.10 Predicted and measured moisture profile for 2/24/98

Soil in arid environments is often subjected to large pulses of infiltration followed by rapid dry-periods from high evaporative demand and sharp pressure gradients in the near-surface, making hysteresis of hydraulic properties an important process to consider. Hysteresis, as it applies to soil hydraulic properties, is a phenomenon that is commonly observed in unsaturated soils when changes in moisture content (with decreasing pressure as the soil dries) are different than when the same soil is being wetted (increasing pressure). Hysteresis is dependent upon factors such as wetting and drying history, entrapped air and soil structure. The hydraulic parameters used for this study were measured in sorption or wetting phase, but in order to properly evaluate hysteresis, desorption or drying phase hydraulic parameters must also be measured. Hysteresis of hydraulic properties is often neglected because of the difficulties in obtaining accurate field and laboratory measurements. HYDRUS has the capabilities to model hysteresis of the conductivity and retention functions, but no measured data was available to distinguish between wetting and drying soil properties for accurate input. A simulation was attempted using HYDRUS, by assuming the soil was initially drying, and the original α value used in the calibrated model was assumed to be equal to the α_d for describing the drying retention curve. The wetting α_w was assumed equal to $(2\alpha_d)$

[Simunek *et al.*, 1998], while all other parameters were left unchanged. Unfortunately, the model produced large mass balance errors and would not run properly. No other attempts were made to run HYDRUS under hysteretic conditions since accurate estimates of soil sorption properties were not available. However, by lowering the saturated hydraulic conductivity by one order of magnitude in the calibrated HYDRUS model, the resulting storage predictions closely resembled the storage measured in the lysimeter during the heavy rainfall in February 1998. This was an indication that hysteresis of the soil hydraulic properties may play a significant role in the conductivity of the soil. Preceding the storm in February 1998, the soil profile was near its driest state of the study period. It is possible that the soil could have become desiccated to the point that the initial measured hydraulic conductivity was no longer representative of the soil conditions. At the point of the February 1998 storm, the soil had been in the lysimeter for over 4 years. It is possible that during this time, hydraulic properties were slightly altered from measurements of the composite soil initially placed in the lysimeter due of possible cementation and buildup of more porous top layers from heavy infiltration. During the summer prior to this event, lysimeter storage was near the lowest amount of the study period at 5% volumetric moisture content averaged over the entire profile. At such low moisture contents, the soil is likely to become desiccated based on the corresponding matric potentials, particularly near the surface. These phenomena provide likely explanations for the underpredicted model storage during this brief portion of the simulations.

The moisture contents shown in Figure 6.10 exemplify conditions that describe a hydraulic conductivity at the time of the storm that was lower than the value used in the models. In other words, a modeled hydraulic conductivity that is too high would likely produce an overestimation of evaporation as the moisture redistributes.

Even if measurements and an accurate model of hysteresis in the water retention function were available, the saturation history of the profile must be determined, such as whether the system was initially drying or wetting, or whether different sections of the profile were drying or wetting, before the natural system can be simulated [Scanlon and Milly, 1994].

6.3

Importance of Input Parameters

Input parameters used for this study were carefully examined and selected so as to produce a representative conceptual model of the lysimeter soil. The HYDRUS and SHAW models were relatively insensitive to the meteorological input, but very sensitive to soil parameters. It was apparent that different hydraulic properties affect the ability of modeled soil to absorb the heaviest rainfalls. Initial overprediction of storage indicated that the selection of initial conditions had a large effect on the models' ability to come into equilibrium with the surrounding conditions. However, this is only true for the soil below the near surface-active zone. Deeper liquid fluxes were highly sensitive to the estimated hydraulic properties and initial moisture conditions. This observation came as a consequence of noting that deeper water potential profiles remained nearly frozen at the initial conditions until the passing of a wetting front. Later in the simulations, water potential returned to near initial conditions at deeper depths. The sensitivity of fluxes to variations in initial water potential suggested that accurate information on initial water potential is important, particularly below the shallow subsurface active zone. The same observation was made by *Scanlon and Milly, 1994*.

Modeling water flow in an arid environment requires accurate representation of the soil water retention characteristics near saturation and in the very dry range ($>15,000$ cm of tension) [*Rockhold et al., 1988*]. It is very difficult to obtain an accurate fit of retention curves near saturation when the BC function is used. However, the method suggested for this research for converting from VG to BC enabled an improved description near saturation for the BC parameters used as input for the SHAW model. Other parameters that had a large effect on the simulation results included the residual moisture content and the pore-connectivity value.

6.3.1

Residual Moisture Content

In order to ensure a reasonably good representation of the water retention behavior at low water contents, the residual moisture content, θ_r , was assumed to be zero for the HYDRUS model. The SHAW model allows no control of this value, but is automatically set to zero according to the BC function used by the model, Equation (3.13). The residual moisture content is a very important parameter that refers to the region of $h(\theta)$ where adsorptive forces are dominant and h is decreasing rapidly with little change in θ [*Jury*

et al., 1991]. HYDRUS was tested using a θ_r value of 0.039, which was determined from the RETC curve fitting process. This value corresponded well to the minimum storage measured in the lysimeter during the study period. Over time, the minimum storage may be closely related to the θ_r or the driest state of the soil profile. However, using a θ_r greater than zero caused the HYDRUS model to severely underpredict evaporation during dry-down periods as indicated in Figures 5.1 and 5.4. This was likely a cause of the misrepresented retention function at higher values of matric potential. Therefore, a θ_r of zero was determined to be appropriate for this study.

6.3.2 Pore-Connectivity

The pore-connectivity, ι , parameter, which appears in Equation (3.14) for the Burdine conductivity function and Equation (3.4) for the Mualem conductivity function, is typically assumed to be equal 2.0 and 0.5 according to the Burdine and Mualem theories, respectively. In reality, this parameter may be highly variable, and it plays a major role in extremely dry soil conditions. It is also possible that this value can change over time if cementation is occurring. The ι parameter was estimated by *Mualem, 1976a* to be 0.5 as an average for some 45 soils, but values for different soils ranged from about -5 to +5. Mualem's database consisted primarily of repacked soils, many of them being relatively coarse-textured [*Mualem, 1976b*]. The SHAW model uses the Burdine hydraulic conductivity function where ι is assumed to be 2.0 according to the Burdine theory used in the original work of *Brooks and Corey, 1964*. This is not an adjustable parameter in the SHAW model, but it can be adjusted in the HYDRUS model.

Many researchers have ignored this parameter due to the difficulties in measuring values of $K(h)$. *Fayer, (1992)* explored the effects of the pore-connectivity value in storage predictions at an arid disposal site and showed that the results were significant. For this research, unsaturated hydraulic conductivities were not available to guide the selection of an appropriate value for ι . Therefore, it was decided to test the effects that this value would have on HYDRUS' ability to predict storage. Initially, the default value of 0.5 was used for ι , but storage was underpredicted with this value. Storage results in Figure 5.2 indicated that the HYDRUS model was underpredicting storage during dry periods, particularly in the summer, when the near-surface tensions reached very high values. It followed then, that this value should be increased to

yield higher values of storage when high matric potentials developed near the surface. Based on Equation 3.4, if α is too low, a higher value of $K(h)$ is calculated, progressively more so as the soil dries, which increases evaporation. Therefore, with a higher value for α (0.75), simulated storage increased since evaporation decreased during the dry periods. The predicted storage results with ($\alpha = 0.75$) are shown in Figures 5.4 and 5.5 for the calibrated model, and described in Table 5.5. The reason for the seasonal effect is that the winter water contents were sufficiently high that $K(h)$ values were minimally affected by the change in α . In contrast, in the summer, water contents were sufficiently low that $K(h)$ was significantly affected by the change in α [Fayer, 1992].

6.4

Moisture Profiles

An important consideration for showing regulatory compliance at disposal facilities is the timing and magnitude of wetting fronts that could migrate to depths near the waste emplacement zones. The ability of a computer model to predict moisture movement is very important at these sites. Potential gradients were the dominant transport process of the soil profile as a whole, causing liquid flow to generally move in the direction of decreasing potential. The strength of the potential gradient driving force is largely a function of the arid climate and, to a lesser degree, the soil properties. The driving force is greatest near the surface and at the downward-leading edge of the wetting fronts. The maximum depth that a wetting front can be expected to reach is an important characteristic in judging the performance and design of landfill covers. Both HYDRUS and SHAW provided adequate representations of wetting fronts during this study. However, the magnitudes of the simulated wetting fronts were affected by the different methods in which the models handled infiltration and the inherent moisture retention functions of the models. For this study, the maximum wetting front depth was assumed to occur at a point just above the depth at which the water content returned to roughly the initial moisture condition before the wetting front entered the region.

For this study, 3 major wetting fronts developed in the lysimeter soil profile as a result of winter and early spring precipitation. The first period of elevated storage was measured during the winter of 1995 and studied here in detail. The second major wetting front occurred during the winter and spring months of 1997, but was much smaller in magnitude and advancement depth than the first. The third and largest

wetting front occurred during the storm of February 1998 but caused inaccurate model predictions during and immediately following the event. Moisture profiles from measured data along with the modeled profiles showed that the wetting front from the February 1998 event had a significant impact near the bottom of the profile. Because of the magnitude and accurate model performance during the relatively wet winter of 1995, this wetting front was studied in more detail to gain a better understanding of the depth and timing of a large wetting front followed by intense dry-down conditions.

On December 24, 1994, 2.4 cm of precipitation was measured at the study site. The wetting front from this event was tracked by plotting the moisture content profiles from the day before the event to the day at which the wetting front reached a maximum depth according to the definition of wetting front described earlier. The profiles in Figures 6.11 - 6.14 show the results of this advancing wetting front with comparisons between the HYDRUS and SHAW predicted moisture contents from the day before the storm event, 12/23/94, through the final day of moisture advancement as predicted by the two models. Measured moisture profiles are not shown in Figures 6.11 - 6.14 because TDR probes from 10 to 50 cm were not operational until 2/1/95. The profile on the day just before the precipitation, 12/23/94, was a typical dry moisture profile representative of the strong upward driving forces at the site. Both models were in excellent agreement with moisture measured by the TDR probes for that day. However, an obvious difference existed between the two models when infiltration initially penetrated the near surface. Moisture contents predicted by SHAW are considerably higher than the predictions from HYDRUS near the surface during infiltration. The moisture profile for 12/24/94, Figure 6.12, is indicative of the different methods by which the HYDRUS and SHAW models predict infiltration and describe the moisture retention relationship. Since the SHAW model uses the BC function to describe moisture retention, moisture contents for this particular soil remain constant near the saturated moisture content (0.361) when the predicted matric potential is between zero cm and the air-entry potential, (11 cm). The SHAW model also uses a modified form of the Green-Ampt approach if the flow conditions are near saturation behind the wetting front [Equations (3.23) through (3.25)], [*Flerchinger and Watts, 1975*]. Otherwise, infiltration is calculated using Darcy's equation. The shape of the wetting front in Figure 6.12 had the squared shape, emblematic of a Green - Ampt infiltration model. Another explanation for the higher moisture content predictions by SHAW could be the fact that the model assumes a zero matric potential at the wetting front.

According to the SHAW predictions, the initial penetration of the wetting front was 10 cm on 12/24. Because the HYDRUS model predicts infiltration by Darcy's equation and the VG retention function, the result was a noticeably smoother profile of the advancing wetting front with significantly lower moisture contents at the near-surface (Figure 6.12). The HYDRUS model predicted an initial penetration depth of 30 cm on 12/24. On the following day, 12/25, another 0.9 cm of precipitation was measured at the lysimeter. By the end of this time-step, the moisture profiles from HYDRUS and SHAW were closer together in their predictions, and the bottom edge of the wetting front was predicted at approximately 45 cm for both models. The major wetting front pulse reached a maximum depth of approximately 80 cm on 1/2/95 and 1/8/95 as predicted by HYDRUS and SHAW respectively (Figure 6.14). The maximum depth and timing of this wetting front was objectively determined by noting the time at which the downward driving force appeared to cease and the onset of the upward driving forces caused a decrease in moisture content at the depth corresponding to the edge of the wetting front. The HYDRUS wetting front reached its maximum depth slightly before the prediction of the SHAW model. The difference in timing of the moisture advancements is a direct result of the different moisture retention and conductivity models used by the two models. For example, it was observed during this study that the matric potential equivalent to the lower edge of advancing wetting fronts was in the range of 200 to 300 cm. According to the retention curves in Figure 4.9, this range of matric potential corresponds to moisture contents ranging from 0.07 to 0.09. In this range of moisture contents, the unsaturated hydraulic conductivity function based on the Mualem model is greater than that of the Burdine model. Therefore, HYDRUS should be expected to predict slightly faster moving wetting fronts compared to SHAW, as indicated in Figure 6.14. When compared to actual measured moisture profiles, the VG-Mualem functions provide superior predictions.

Moisture Profile, 12/23/94

Figure 6.11

Moisture Profile, 12/24/94

Figure 6.12

Moisture Profile, 12/25/94

Figure 6.13

Maximum Wetting Front Advancement

Figure 6.14

Following the time at which the wetting front from the December, 1994 storm had reached its maximum depth of penetration, very slow moisture redistribution produced a progressive increase in moisture content below 80 cm. This was most likely a result of the continued precipitation measured during the winter and early spring of 1995, and the relative strength of the downward-forcing potential gradient below the zone of elevated moisture content. As shown in Figure 6.15, the elevated moisture contents with depth continued to redistribute until the bottom moisture content had increased from the initial condition of 0.056 to nearly 0.075 around 8/20/95. Figure 6.15 only shows HYDRUS predictions, but it should be noted that the SHAW predictions matched very closely to both HYDRUS and actual measurements. This observation indicated that a buildup of moisture from repeated infiltration can create storage accumulation to depths at or below the 200 cm profile modeled at the study site, which is an important consideration for the design of landfill cover thickness. However, at the time of the storm of February 1998, moisture contents near the bottom of the profile had returned to near initial conditions in both models and the measured profiles (Figures 6.15 and 6.16). This is also an important observation, which indicates that a strong influence from surface processes can cause strong upward-driving potential gradients steep enough to effect moisture contents at or below 200 cm. TDR measured moisture profiles shown in Figure 6.16 were in good agreement with the model profiles above 70 cm, but were inconsistent with the models below 70 cm. The cause or causes of these differences below 70 cm are not completely understood.

Figure 6.15 Predicted moisture profiles following the winter of 1995, which illustrate the effects of the dry conditions at the site

Figure 6.16 TDR measured moisture profiles following the winter of '94 - '95

The results of this research indicated that the HYDRUS and SHAW models could effectively be used in arid environments to predict soil-water storage with a relatively high level of confidence.

Assurance of model performance was achieved by calibrating the model to measured storage in the lysimeter. Although a significant amount of measured data were available to support the findings, the effort was subjected to a limited number of assumptions that were made due to bounding limits of the measured parameters, model capabilities and lysimetry.

Uncertainties in the unsaturated hydraulic conductivity function, $K(h)$, make it difficult to assess the relative importance of liquid and vapor transport in arid environments and this parameter is extremely difficult to measure directly. If $K(h)$ values had been available for this research, the unsaturated hydraulic conductivity and pore-connectivity could have been fitted to $K(h)$ by using RETC and graphical adjustment procedures such as the one outlined in Chapter 4 for the retention properties. However, the unsaturated hydraulic conductivity could only be estimated using the Mualem and Burdine functions based on the measured and fitted retention parameters. The unsaturated hydraulic conductivity can also be estimated from the $K(h)$ relationship. A rough estimate of the $\theta(h)$ relationship can be made by measuring in-situ moisture content and corresponding matric potentials with TDR and TCP respectively. However, the potential data obtained from the TCP measurements for this study were unreliable. Because of the high tensions that developed near the surface, TCP measurements are usually out of measurement range near the surface, therefore measurements were only taken at and below 10 cm. The TDR data presented here are questionable due to unknown lengths of time in which the probes malfunctioned. Furthermore, the potential effects of the steel sidewalls are also unknown.

A lack of knowledge of the effects of hysteresis of the hydraulic properties was an obvious weakness in this study. Soil moisture retention curves from the lysimeter soil were only measured in the lab for desorption properties. In order to obtain estimates of retention properties related to hysteresis, the main wetting, or sorption functions should be measured in conjunction with drying or desorption properties. Although different procedures exist to measure hysteresis, it is very difficult to accurately measure it in a laboratory. The results of the storage predictions during the latter portion of the

simulations, post February 1998, indicated that hysteresis of the hydraulic properties is likely to be an important consideration in arid climates.

Another source of uncertainty could actually be the lysimeter used to compare simulated storage results. The lysimeter used in this study is a weighing lysimeter that is capable of accurately measuring changes in storage as a result of evaporation, with a bare surface that is level and protected from run-on and runoff. Lysimetry provides probably the most accurate method available for directly measuring recharge and evaporation from soil surfaces [*Meyer et al., 1996*]. However, the disadvantages of lysimeters are the artificial boundary conditions created by enclosing the soil in a box (usually steel), with only the surface exposed to the surrounding conditions. The largest potential for error with the lysimeter measurements is the effect that the steel sides surrounding the soil may have on the temperatures measured within the lysimeter soil.

Many researchers have argued that lysimeters produce unrealistic flow patterns as a result of the disturbed conditions. Disturbing the soil and inputting the measured parameters into a model to simulate unsaturated flow predictions could be problematic. However, if the model is to be used to make predictions for evaluating the performance of a closure cap, the soil used for the cap is always disturbed during construction. Therefore, in this situation disturbance can be considered negligible and possibly even more reliable than measurements on samples from an undisturbed site if the study site is to be used to estimate landfill cover performance. The problems in evaluating landfill cap performance may lie in the researchers ability to accurately measure the unsaturated soil properties and create a conceptual model that effectively describes the site.

6.6

Conclusions

A research facility at the Area 5 RWMS located in the Nevada Test Site was established to collect long-term meteorological and soil water data. Atmospheric data were collected from a micrometeorology tower stationed above a bare surface weighing lysimeter. Approximately 5 years of data from March 1994 through December 1998 were used to evaluate two unsaturated flow models. The monitoring data were analyzed to gain a better understanding of seasonal climate effects on unsaturated flow prediction in bare-surface soil profiles. The atmospheric data were used to develop predictive periodic trends that could be

used for future site performance modeling. Laboratory measurements of the hydraulic properties of the soil used in the weighing lysimeter were analyzed and tested in the HYDRUS and SHAW models. A method was developed for converting soil retention properties from the van Genuchten function used in the HYDRUS model to the Brooks-Corey function used in the SHAW model. The input parameters were tested and adjusted until calibrated models were developed. Both models were capable of simulating the dynamic changes in soil moisture and surface atmospheric effects typical of arid environments. The calibrated models provide a useful tool for demonstrating future performance measures at low-level waste disposal facilities in arid, unsaturated soils.

The HYDRUS and SHAW models were evaluated by performing a sensitivity analysis on the measured and estimated input parameters. The results were compared to the storage changes measured in the lysimeter. The HYDRUS model was used to predict one-dimensional water flow, while the SHAW model predicted one-dimensional transport by considering liquid, heat and water vapor flow processes.

After both models were calibrated, the results were analyzed to gain a better understanding of the flow processes at the study site. It was discovered that nonisothermal vapor flow had little effect on the models' overall ability to predict storage. Upward winter temperature gradients and downward summer temperature gradients below 15 cm were estimated to be relatively unimportant considerations in the flow processes. Isothermal liquid fluxes from potential gradients dominated over thermal vapor fluxes throughout most of the simulation period below the near-surface. Storage results from the HYDRUS and SHAW models produced almost identical predictions that agreed reasonably well with actual lysimeter storage and measured moisture profiles. The models were sensitive to the large seasonal fluctuations in meteorological parameters. It was determined, however, that hourly data were not necessary to capture the important long-term physical processes.

Model results indicate that hydraulic parameters such as saturated hydraulic conductivity (K_s), residual moisture content (θ_r) and pore-connectivity (τ) should be carefully evaluated even if the parameters show reasonable agreement with measured data. Residual moisture content and pore-connectivity were important parameters that required slight adjustments to achieve a calibrated HYDRUS model. These parameters could not be adjusted in the SHAW model, but θ_r is assumed to be zero in the code. Model results during the relatively wet winter of 1998 provided evidence that hysteresis in terms of moisture

retention and conductivity may play a significant role in the prediction of unsaturated flow in arid climates. It is also likely that a change in the hydraulic conditions over the duration of the study period had a significant effect on K_r .

6.7

Recommendations

During this research, major issues related to the evaluation of water flow in the unsaturated zone at the Area 5 RWMS disposal facility were considered. Recommendations were made for evaluating soil properties and using unsaturated flow models at the site. Specific recommendations regarding future needs for hydrologic evaluations at this and other low-level disposal facilities in arid environments include the following:

- *Evaluate the effects of vegetation using data from the vegetated lysimeter using the HYDRUS and SHAW models.* Surface vegetation has been shown to significantly increase surface fluxes via evapotranspiration processes [Levitt et al., 1998]. Landfill covers with vegetation could be effective in preventing moisture from reaching buried waste. The vegetated weighing lysimeter adjacent to the bare surface lysimeter, along with the unsaturated flow models used for this study, could be used to determine appropriate surface vegetation and root parameters. Storage plots over the approximately 5-year study period, have shown significantly lower moisture conditions for the lysimeter with vegetation.
- *Obtain measurements of hydraulic conductivity as a function of pressure.* Few reliable methods are available for measuring $K(h)$, but it can be done. Without these data, the unsaturated hydraulic conductivity must be indirectly estimated and plugged into an empirical function based on the calculated retention properties in order to obtain a relationship for $K(h)$.
- *Obtain measurements of hysteretic properties of the moisture retention and conductivity relationships.* Limited information is available describing model behavior of soil moisture movement when hysteresis is considered in simulations. Model results following the February 1998 storm suggest that hysteresis is an important consideration in arid environments. Hysteresis can be approximated in a laboratory by measuring main desorption (drying) and sorption (wetting)

curves. For this study, only data from desorption curves were collected to determine appropriate hydraulic properties. It would also be useful to obtain more measurements of hydraulic conductivity relationships at various depths during both drying and wetting conditions. This information would be useful for determining the relative accuracy of theoretical functions typically used to estimate these parameters. It is possible that repeated drying and wetting cycles have altered the soil structure and hydraulic properties from the original disturbed soil placed in the lysimeter.

APPENDIX

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