Pacific Northwest National Laboratory

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Estimates of Deep Drainage Rates at the U.S. Department of Energy Pantex Plant, Amarillo, Texas

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Estimates of Deep Drainage Rates at the U.S. Department of Energy Pantex Plant, Amarillo, Texas

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April 1998

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Summary

In FY 1996, the Pacific Northwest National Laboratory (PNNL) provided technical assistance to Battelle Columbus Operations (BCO) in their ongoing assessment of contaminant migration at the Pantex Plant in Amarillo, Texas. The objective of this report is to calculate deep drainage rates at the Pantex Plant. These deep drainage rates may eventually be used to predict contaminant loading to the underlying unconfined aquifer for the Pantex Plant Baseline Risk Assessment. These rates will also be used to support analyses of remedial activities involving surface alterations or the subsurface injection/withdrawal of liquids or gases.

The scope of this report is to estimate deep drainage rates for the major surface features at the Pantex Plant, including ditches and playas, natural grassland, dryland crop rotation, unvegetated soil, and graveled surfaces. Areas such as Pantex Lake that are outside the main plant boundaries were not included in the analysis. All estimates were derived using existing data or best estimates; no new data were collected. The modeling framework used to estimate the rates is described to enable future correlations, improvements, and enhancements.

The scope of this report includes only data gathered during FY 1996. However, a current review of the data gathered on weather, soil, plants, and other information in the time period since did not reveal anything that would significantly alter the results presented in this report.

Infiltration volumes and rates were estimated for the channel bottoms and playas. The recommended infiltration rates for the playas ranged from 2.4 ft/yr for Playa 5 to 5.5 ft/yr for Playa 1. The recommended infiltration rates for the channel bottoms ranged from 10.5 to 21.9 ft/yr. Because field data to corroborate the model results were lacking, examples were provided to demonstrate the model's sensitivity to several input parameters.

Average long-term drainage rates were estimated for various combinations of major soil types and vegetation conditions at the Pantex Plant; the estimates provided a basis for recommending drainage rates for each soil-vegetation combination. Under grassland, the recommended rate is 0.1 mm/yr for all soil types. Under a typical dryland crop rotation, the recommended rates vary from 0.1 to 3.7 mm/yr, depending on soil type. With no plants on the surface, the recommended rates vary from 2.1 to 27.3 mm/yr, depending on soil type. Finally, the recommended rate for unvegetated surfaces with a gravel cover is 418 mm/yr.

For all the drainage estimates, the weather data were the most defensible on a site-specific basis. The only exception was rainfall intensity, which was limited to 0.5 cm/h, and probably underestimated the most intense storms. With this limit in place, runoff was significantly reduced and infiltration (and thus drainage) was significantly increased. The remainder of the modeling parameters (i.e., channel characteristics, hydraulic properties, plant behavior) were estimated from site, regional, or national information. The credibility of the drainage estimates presented herein could be improved by collecting site-specific hydrologic, soil, and plant data to parameterize and calibrate the models and to verify their predictive abilities. Of these data, rainfall intensity, ditch and playa calibration data, and actual site-specific soil hydraulic properties would probably provide the greatest improvement in the deep drainage flux estimates.

Acknowledgments

We thank the staff at the Battelle Columbus Operations office for their help in obtaining for us the information needed to analyze deep drainage rates at the Pantex Plant. We would also like to thank Bill Laseter of Battelle Pantex for providing much of the site-specific weather data. A draft of this report was reviewed by Bridgit Scanlon of the Bureau of Economic Geology, University of Texas, Austin, Texas, and Ken Rainwater and Dave Thompson of Texas Tech University, Lubbock, Texas; their comments were useful and greatly appreciated.

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1.0 Introduction

The Pantex Plant in northern Texas was built in the 1940s to machine parts for defense weapons. During plant operations, various contaminants entered the subsurface environment, including solvents, fuels, explosives, metals, and trace uranium-238. Some of these contaminants (i.e., explosives, chromium, and solvents) were observed in the perched aquifer that lies above the regional Ogallala aquifer, the major source of water for the City of Amarillo, Texas (DOE 1995).

Battelle Columbus Operations (BCO) is developing numerical groundwater flow models of the vadose zone, perched aquifer, and regional Ogallala aquifer at the Pantex Plant (hereafter referred to as the Plant). These models will provide a capability for evaluating contaminant issues. Such issues include

- evaluating groundwater recovery scenarios aimed at capturing contaminated groundwater and preventing further offsite migration of contamination
- the potential long-term migration and fate of contaminants residing in the vadose zone, to support decisions regarding the need to remediate
- the effectiveness, under site-specific conditions, of remedial alternatives aimed at removing/destroying contaminants residing in the vadose zone
- potential risks to human receptors resulting from the leaching of contaminants residing in the vadose zone to the groundwater aquifers beneath the plant
- predicting the possible extent of contamination in areas where deep vadose zone sampling is not cost effective
- evaluating the effects of alternative land uses and surface water disposal options on deep drainage rates, which could have important effects on the mobility of contaminants in the vadose zone.

Quantifying the spatial distribution of recharge to the groundwater aquifer depends on understanding the deep drainage rates for the various land uses. The analysis of deep drainage rates (i.e., the water flux beneath the zone of water withdrawal by plant roots) can be divided into two areas: 1) ditches and playas, and 2) all other areas, which are typically lumped together and called inter-playa areas. Deep drainage beneath the ditches and playas depends on operational discharges from the Plant, and on the runoff from precipitation and irrigation activities. Deep drainage in the inter-playa areas is connected with the infiltration of incident precipitation and irrigation water, and the nature of the site-specific surface soil and vegetation.

1.1 Background

Storm runoff and operational discharges to the ditches and playas were estimated based on computer modeling and interviews with Plant staff (Ramsey et al. 1995). The estimates of runoff are the

minimum (52,000 acre-inches to Playa 3) and maximum (835,000 acre-inches to Playa 5) infiltration amounts for the period from 1952 to 1991. The estimates of operational discharges were provided as average and maximum daily flow rates from various buildings. The highest estimate was 134,000 gal/d from Building 12-17. However, for numerical modeling of the vadose zone, a time series of runoff and operational discharges is needed.

Interplaya deep drainage rates were evaluated around several playas located within 25 km of the Plant (Scanlon et al. 1996). The vegetation of these interplaya areas was most commonly short-grass prairie. The estimates of the deep drainage fluxes were generally less than 0.1 mm/yr based on chloride concentration profiles (Scanlon and Goldsmith 1997).

As part of a groundwater modeling exercise, the Bureau of Economic Geology (BEG) (1995) estimated the spatial distribution of natural recharge, to serve as the upper boundary condition for their model. The BEG took the regional estimate of recharge (6 mm/yr) and applied the total recharge integrated over the entire site to just the area (roughly 2.7%) encompassed by the playas. This was a steady-state approach that did not account for seasonal effects, playa differences, infiltration beneath ditches, or the impact of Plant facility discharges.

Xiang and Scanlon (1993) simulated preferential flow in the surface soils at a site about 5 km northeast of the Plant. They devised a method to incorporate the impact of macropores on the hydraulic conductivity function, then showed that the revised function caused water to move deeper into the profile than if the macropores were ignored. This study was not extended to the surface soils or the vadose zone at the Plant site, nor to situations involving contaminant transport.

No estimates of deep drainage rates were available for the various land uses within the Plant boundaries. These uses include farming (e.g., fallow, stubble, pasture, wheat, sorghum) and Plant facilities (e.g., parking lots, landfills).

1.2 Objectives and Scope

The objective of this report is to present a modeling framework for predicting deep drainage rates. These deep drainage rates will eventually be used to predict contaminant loading to the unconfined aquifer, and to support analyses of remedial activities involving surface alterations or the subsurface injection/withdrawal of liquids or gases.

The scope of this report is to estimate deep drainage rates for the major surface features at the Plant, including ditches and playas, natural grassland, dryland crop rotation, unvegetated soil, and graveled surfaces. Areas such as Pantex Lake that are outside the main plant boundaries were not included in the analysis. All estimates were derived using existing data or best estimates; no new data were collected. The modeling framework used to estimate the rates is described to enable future correlations, improvements, and enhancements.

The scope of this report includes only data gathered during FY 1996. However, a current review of the data gathered on weather, soil, plants, and other information in the time period since did not reveal anything that would significantly alter the results presented in this report.

2.0 Ditches and Playas

During past production operations at the Pantex Plant, contaminants were released in process waste discharges to a system of ditches (channels). The contaminated water flowed along the ditch system where it either infiltrated to the subsurface soil beneath the channel or was eventually conveyed to one of the playa lakes at the site. These operational discharges have ceased and were not considered in the following analyses of deep drainage rates. Stormwater runoff and effluent from the plant wastewater treatment facility continue to be routed through the channel systems to the playas. These two sources of water were used to calculate infiltration beneath the channels and playas. The infiltration water contributes a water flux to the vadose zone that can contribute to contaminant transport.

Although infiltration to the playa basins at the Plant was previously studied (Reed 1994; Greer 1994), this study did not include estimates of infiltration in the channel systems. In this current study, long-term simulations using available meteorological data were used to estimate the rainfall-runoff relationship. Runoff was conveyed either to a channel system or directly to a playa. Estimates of the amount of water infiltrated through the channel or playa bottoms were calculated using the simulation model.

2.1 Model Description

The simulation model is composed of three parts: a runoff model, a channel routing model, and a playa water balance model. The weather data used for these models is described in Chapter 3.0. The key features of each model are summarized in this section.

2.1.1 Storm Runoff

Daily runoff volumes were computed using the standard SCS (Soil Conservation Service) curve number (CN) method (Maidment 1993). This method is widely used for estimating floods on small to medium-sized ungauged drainage basins. The SCS method provides a non-linear relationship between accumulated precipitation and accumulated runoff, characterized by a dimensionless runoff CN. The value of CN depends on soil, cover, and the antecedent wetness condition of the basin. Three classes of antecedent moisture condition (AMC) are defined: dry, average, and wet. For a given depth of precipitation, runoff increases with CN and is greater under wet than dry AMC.

2.1.2 Channel Routing

Flows were routed through the channel system using the Muskingum hydrologic routing method (Maidment 1993) with a 1.2-h time step. The model has the capability to route flows in branched (tree-like) channel systems by dividing the system into a number of interconnected segments. The routing method accepts runoff volumes from both point discharges and lateral inflows along the channel. Water velocities and depths in each channel segment are computed using the Manning

equation by assuming that the flow is locally uniform at that time and location (Lane et al. 1985). In lieu of actual channel cross-sectional information, channel segments were represented with rectangular cross sections. Infiltration losses through the channel bottom were calculated with an infiltration rate and the wetted area of the channel. Note that the channel model does not include water losses from evapotranspiration (ET).

2.1.3 Playas

Daily infiltration and evaporation for playa lakes were calculated through an extension of the simple water balance approach described by Reed (1994) and Greer (1994). The daily change in surface water storage in the playa is equal to the difference between water input and water losses through infiltration and evaporation. The playa area is specified by the user and remains constant during the simulation. This area may be composed of two zones, an inner zone of surface water surrounded by an outer zone of unsaturated soils. The extent of the surface water zone changes with the amount of surface water stored in the playa through a unique user-defined relationship between storage and area. Precipitation falling on the outer unsaturated soil zone is infiltrated up to the limiting rate; the excess becomes runoff to the playa.

Input to the playa includes precipitation on the playa, direct runoff from adjacent land, and inflow from the channel flow model described above. Playa 1 receives discharge from the wastewater treatment plant via channel flow. The rate of evaporation from the playa surface is determined from daily meteorological conditions using the Penman equation (Doorenbos and Pruitt 1977).

2.2 Model Application to the Pantex Plant

The runoff, channel routing, and channel/playa infiltration models described earlier were applied to the Plant. Estimates of long-term average infiltration rates were developed by running the model for the entire period of meteorological record. A limited set of sensitivity tests was performed to assess how the infiltration rates would respond to changes in model parameters.

2.2.1 Storm Runoff

The Plant was divided into five major drainage basins, one for each playa lake. These basins were further divided into a total of 28 sub-basins based on the channel network and land use. Land use was classified as industrial or non-industrial. The work of Reed (1994) indicated little would be gained by a further subdivision of non-industrial areas based on soil and cover types. Summary information on the five major drainage basins is given in Table 2.1.

The model was run at a daily time step for each sub-basin using meteorological data from the Amarillo Airport for the years 1965 to 1995. Depending on the channel network, simulated runoff from a given sub-basin was either input to the appropriate channel reach for channel flow routing, or was input directly to the playa.

Table 2.1. Playa Basin Areas

Playa	Areas (acres)			
	Industrial	Non-Industrial	Playa	Total
1	590	2,860	109	3,560
2	251	2,060	102	2,420
3	0	1,070	44	1,110
4	411	3,590	161	4,160
5	0	1,220	144	1,360

2.2.2 Channel Routing

The channel systems selected for inclusion in the model correspond to those where significant contamination is present (Radian 1994a through e). Playas 1, 2, and 4 have distinct channel systems, whereas Playas 3 and 5 do not. The channel systems are shown in Figures 2.1, 2.2, and 2.3, respectively. The average channel widths and lengths were determined from topographic maps of the site. The channel permeability was assigned to the geometric mean of the infiltration rates reported by Ramsey et al. (1995) because there were not enough measurements to characterize the entire length of all channels adequately. A uniform value of 1.76 in/d was used in all simulations, except for those testing the sensitivity to the channel permeability parameter. Daily point and lateral inflows to the channel systems were provided by the runoff model. Outflow from the Wastewater Treatment Facility (WWTF) enters channel system 2 of Playa 1 at a point 900 ft upstream of Playa 1.

2.3 Results

A set of simulations was performed to examine the sensitivity of long-term playa infiltration to prescribed infiltration rates for various playa soils. In this case, a runoff curve number of 85 was used for non-industrial soils along with medium values for channel infiltration and width. The model was run with low, medium, and high prescribed values for unsaturated and saturated infiltration parameters (Table 2.2). Infiltration values were estimated from Greer (1994).

Long-term average annual infiltration from the five Pantex playa lakes is presented in Table 2.3. The results for each playa are expressed as an average volume of infiltration per year and as an average annual depth of infiltration per unit playa area. Annual infiltration depths were obtained by dividing the annual infiltration volume by the appropriate playa area listed in Table 2.1. Average annual infiltration depths for the playas are within a factor of three, ranging from a low of 1.64 ft/yr in Playa 5 to a high of 6.38 ft/yr in Playa 1.

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Figure 2.1. Playa 1 Channel Systems

Figure 2.2. Playa 2 Channel System

SG96090325.3

SG96090325.2

Figure 2.3. Playa 4 Channel Systems

Table 2.2. Model Parameters Used in Sensitivity Analysis

Case	Infiltration Rate (in/d)	
	Saturated	Unsaturated
Low	0.11	1.2
Medium	1.2	7.2
High	7.2	74.3

Table 2.3. Average Annual Playa Infiltration as a Function of Playa Soil Infiltration Rates (medium channel widths and infiltration, CN:85)

Playa Soil	Infiltration Units	Playa 1	Playa 2	Playa 3	Playa 4	Playa 5
Low	10 ³ ft ³ /yr	11,600	7,510	4,130	12,800	10,300
	ft/yr	2.45	1.69	2.16	1.82	1.64
Medium	10 ³ ft ³ /yr	26,200	12,800	8,270	24,500	15,100
	ft/yr	5.54	2.88	4.32	3.50	2.41
High	10 ³ ft ³ /yr	30,200	14,200	9,550	27,700	16,500
	ft/yr	6.38	3.19	4.98	3.95	2.63

A second set of simulations was performed to evaluate the sensitivity of long-term playa infiltration to prescribed runoff curve numbers. In this case, medium values were used for playa infiltration rates, channel infiltration, and channel width. The model was run with runoff curve numbers of 75, 85, and 90 for non-industrial areas. Industrial areas were assigned a curve number of 100. Results for these simulations are presented in Table 2.4. In this case, average annual infiltration ranges from a low of 1.50 ft/yr in Playa 5 to a high of 7.95 ft/yr in Playa 3. Playas 3 and 5 have the largest percentages of non-industrial land and exhibit the most sensitivity to changes in curve number. Runoff in the remaining playa basins is dominated by the industrial areas.

The parameter values used in the simulation model were estimated from the best available data. It must be stressed that the lack of reliable measurements of streamflow, playa water levels, infiltration rates, channel geometries, etc., introduces large uncertainties into the results presented in Tables 2.3 and 2.4.

Table 2.5 shows the average channel widths and permeabilities used for the channel simulations. Long-term average annual infiltration volumes and rates through the modeled channel bottoms are summarized in Tables 2.6 and 2.7, respectively. The results are expressed as an average volume of infiltration per year and as an average annual infiltration rate per unit channel bottom area. Base case infiltration rates varied between 10.5 and 21.9 ft/yr. Note that the infiltration rates are

Table 2.4. Average Annual Playa Infiltration as a Function of the Runoff Curve Number (medium playa soil infiltration rates, channel infiltration, and channel width)

Non-Industrial CN	Infiltration Units	Playa 1	Playa 2	Playa 3	Playa 4	Playa 5
75	10 ³ ft ³ /yr	24,600	12,000	3,180	23,700	9,420
	ft/yr	5.21	2.70	1.66	3.39	1.50
85	10 ³ ft ³ /yr	26,200	12,800	8,270	24,500	15,100
	ft/yr	5.54	2.88	4.32	3.50	2.41
90	10 ³ ft ³ /yr	28,000	13,800	15,200	25,300	22,700
	ft/yr	5.93	3.10	7.95	3.61	3.62

Table 2.5. Cases and Parameters for Channel Simulations

Case	Non-Industrial CN	Average Channel Width (ft)	Channel Permeability (in/d)
Base	85	5.0	1.76
High Runoff	90	5.0	1.76
Low Runoff	75	5.0	1.76
High Width	85	10.0	1.76
Low Width	85	2.5	1.76
High Perm	85	5.0	3.52
Low Perm	85	5.0	0.88

computed by dividing the average infiltration volume by the channel bottom area. Also note that channel system 2 for Playa 1 receives input from the WWTF.

A set of simulations was performed to demonstrate the effect of uncertainties in the channel model parameters and physical input data on the estimated infiltration volumes and rates through the channel bottoms. Table 2.7 shows that infiltration through the channel bottoms was not very sensitive to the different hydrologic input cases. This result occurred because the inflows to the modeled channels were primarily from industrial zones and the curve number for those areas did not vary from the base case. Lacking good estimates of confidence limits, we varied the channel bottom width and permeabilities by factors of 0.5 and 2.0 to test the sensitivity to these values. Nearly linear changes in average infiltration volumes and rates were obtained in response to doubling and halving the channel width and permeability.

In summary, until field data are available to calibrate and validate the model, we recommend using the infiltration estimates provided here to calculate the transport of contaminants through the

Table 2.6. Average Annual Infiltration Volumes to the Channel Systems

Case	Infiltration Volumes (10^3 ft ³ /yr)					
	Playa 1			Playa 2	Playa 4	
	Channel System 1	Channel System 2	Channel System 3	Channel System 1	Channel System 1	Channel System 2
Base	2,250	372	412	322	1,050	406
High Runoff	2,250	372	417	322	1,050	406
Low Runoff	2,250	372	408	322	1,050	406
High Width	4,070	700	672	604	1,940	768
Low Width	1,220	203	248	178	595	227
High Perm	4,090	716	680	619	1,970	781
Low Perm	1,200	190	239	164	550	209

Table 2.7. Average Annual Infiltration Rates to the Channel Systems

Case	Infiltration Rates (ft/yr)					
	Playa 1			Playa 2	Playa 4	
	Channel System 1	Channel System 2	Channel System 3	Channel System 1	Channel System 1	Channel System 2
Base	14.8	21.9	10.5	16.3	15.5	15.5
High Runoff	14.9	21.9	10.6	16.3	15.5	15.5
Low Runoff	14.8	21.9	10.4	16.3	15.5	15.5
High Width	13.4	20.6	8.6	15.3	14.4	14.7
Low Width	16.1	23.9	12.6	18.0	17.6	17.4
High Perm	27.0	42.1	17.3	31.3	29.2	29.9
Low Perm	7.9	11.1	6.1	8.3	8.1	8.0

vadose zone. For infiltration in the playas, we recommend using the volumes and rates associated with the medium case in Table 2.3. For infiltration in the channel bottoms, we recommend using the volumes and rates associated with the base case simulations in Tables 2.6 and 2.7.

3.0 Interplaya Areas

The magnitude and timing of deep drainage at a particular location depends on the soil type, vegetation characteristics, and weather. Field methods can be used to measure deep drainage rates, but the expense of field work limits the application of these methods to no more than a few sites. One method that can be used to supplement the field methods is to conduct computer simulations. While such models need field data for parameterization and demonstration of credibility, their ease of use makes them ideal for studying a wide array of conditions quickly.

3.1 Methods

The UNSAT-H computer code was used to simulate deep drainage rates for a variety of surface soil and vegetation scenarios for the Plant. The UNSAT-H computer code is a one-dimensional water and heat flow code designed to simulate the water balance of soils and the deep drainage flux beneath the plant root zone. The code simulates liquid water flow using the Richards equation, vapor flow using Fick's law, and heat flow using Fourier's law (for this report, heat flow was not simulated). The code uses daily weather data to calculate the infiltration, evaporation, and transpiration fluxes, as well as soil water storage and deep drainage. Runoff is simulated as the difference between precipitation and soil infiltrability; the code does not address surface runoff or water detention. The code is fully documented in Fayer and Jones (1990). Examples of code applications are presented in Fayer et al. (1992), Fayer and Gee (1992), and Fayer and Walters (1995).

Simulations of the soil and vegetation scenarios were conducted for the years 1965 to 1995. This length of time, 31 years, was chosen to encompass the 30-year length of time used by the U.S. Weather Bureau to calculate weather statistics, thus allowing for a more accurate assessment of long-term drainage rates.

Two types of simulations were performed: transient and steady state. A transient simulation refers to a single simulation using the 31-year weather record and starting from the assigned initial conditions. A steady state simulation refers to repeated simulations using the same 31-year sequence of weather data until the change in the average drainage rate for that 31-year period is reduced to less than 0.1 mm/yr. Given sufficient time and assuming the 31-year weather sequence repeats indefinitely, the results of the steady state simulations yield the long-term average drainage rate and also indicate the annual variability in the rate.

3.2 Model Parameters

The parameters for each simulation include a description of the model domain and node spacing, soil hydraulic properties, initial conditions, boundary conditions, and vegetation information. The meteorological data were identical for all simulations.

3.2.1 Model Domain

In all cases, the model domain was 6 m deep. A test simulation with a 10-m-deep domain produced nearly identical results (less than a 1% difference in runoff and drainage), showing that a deeper domain was unnecessary. For each soil type, the node spacing within the model domain was varied from 0.2 cm at the surface to 50 cm at the deepest depth. At the interfaces of differing materials, the node spacing was gradually reduced to 2 cm. This level of discretization kept the average mass balance error at less than 0.2 mm/yr. A test simulation with node spacings reduced by half yielded a 5% decrease in drainage and showed that there was little value in decreasing the node spacing any further, especially given the computational time needed to solve a problem with twice as many nodes. The maximum time step size was limited to 1.0 h. A test simulation with a 0.5-h limit yielded nearly identical results to those based on a 1.0-h limit, showing that smaller maximum time steps were unnecessary.

3.2.2 Soil Hydraulic Properties

The soil map of the Plant indicates that four distinct soil types are present: Pullman clay loam, Estacado clay loam, Lofton clay loam, and Randall clay. Other soils were either identical to the four main soil types or of such small areal extent that they were considered to be insignificant. Changes in slope within a soil type were not addressed; all soils were analyzed as if their slopes were zero. Information was unavailable to describe the sediments beneath each soil type. For this study, we assumed a clay loam sediment occurred under all soils.

Retention data for the surface soils and the underlying Blackwater Draw formation at the Plant were unavailable. Limited water retention data were available for a site about 5 km northeast of the Plant. Soil water retention was measured in the matric potential range of 0.01 to 0.1 MPa on three soil samples that were collected in a single soil type at depths shallower than 1.0 m (Xiang and Scanlon 1993). Some limited onsite data were also available. *In situ* matric potentials and water contents were measured to depths of about 25 m in two boreholes in the northeast corner of the Plant (Scanlon et al. 1996). These retention data did not exhibit any clear pattern and did not sufficiently represent the matric potential range between 0.0 and 0.1 MPa. Other than these core and in situ data, no other retention data could be located for the surface soils or the Blackwater Draw formation in or near the Plant.

Lacking sufficient information about the hydraulic properties of the soils and vadose zone at the Plant, we described each soil type using texture and permeability information from the soil survey for Carson County (USDA 1962) and the results of a recent resurvey of the county. A single average soil profile was defined for each soil type that was simulated. Variability within a given soil type was not addressed in this initial study.

The soil water retention properties of each texturally unique layer in the profile were described using the van Genuchten function (van Genuchten 1980). Table 3.1 lists the retention parameters, which were the mean values obtained from Carsel and Parrish (1988) based on the textural class of the individual layers. The only deviation from this strategy in the parameters was for the second layer in the Pullman soil. The UNSAT-H code had difficulty reaching a solution using the clay

Table 3.1. Parameters for the van Genuchten/Mualem Equations That Were Used to Describe Soil Hydraulic Properties in the Simulations. An asterisk shows where clay parameters were replaced with silty clay loam parameters.

Soil Type and Texture of Layers	Depth Intervals of Layers (cm)	θ_s m ³ /m ³	θ_r m ³ /m ³	a 1/cm	n –	K_s cm/h	USDA Permeability cm/h
Pullman clay loam (Pu)							
clay loam	0 to 15	0.410	0.095	0.019	1.31	0.26	1.016
clay	15 to 97	0.380*	0.068*	0.008*	1.18*	0.20	0.33
clay loam	97 to 132	0.410	0.095	0.019	1.31	0.26	0.33
silty clay loam	132 to 188	0.430	0.089	0.010	1.23	0.07	0.33
clay loam subsoil	188 to 600	0.410	0.095	0.019	1.31	0.26	0.33
Estacado clay loam (Es)							
clay loam	0 to 203	0.410	0.095	0.019	1.31	0.26	3.302
clay loam subsoil	203 to 600	0.410	0.095	0.019	1.31	0.26	0.33
Lofton clay loam (Lo)							
clay loam	0 to 23	0.410	0.095	0.019	1.31	0.26	2.794
clay	23 to 132	0.380	0.068	0.008	1.09	0.20	0.152
silty clay	132 to 203	0.360	0.070	0.005	1.09	0.20	0.33
clay loam subsoil	203 to 600	0.410	0.095	0.019	1.31	0.26	0.33
Randall clay (Ra)							
clay	0 to 147	0.380	0.068	0.008	1.09	0.20	0.152
clay	147 to 168	0.380	0.068	0.008	1.09	0.20	0.33
clay loam subsoil	168 to 600	0.410	0.095	0.019	1.31	0.26	0.33
Gravel cover							
(sand as surrogate)	0 to 15	0.430	0.045	0.145	2.19	29.7	–

parameters for that layer. There was insufficient opportunity to resolve the difficulty, therefore, the van Genuchten parameters for silty clay loam were successfully used instead. An additional soil type, called a gravel layer, is listed in Table 3.1 to represent those areas having graveled surfaces (DOE 1995). In lieu of actual data, the properties of the gravel layer were represented using the sand parameters from Carsel and Parrish (1988). This representation is more nearly like a gravel mix rather than a clean gravel, but it should indicate qualitatively the impact of a coarse layer on top of the soil surface.

Saturated hydraulic conductivity values were assigned to the different soils using the values reported by the USDA (1962). These values were assumed to be more representative than the conductivity values found in Carsel and Parrish (1998). Table 3.1 shows that, in general, the two sets

of conductivity values were quite similar. For three of the four surface soils, however, the USDA conductivity values were greater by a factor of 5 to 10. The higher USDA values may reflect the impact of preferential (or macropore) flow. However, no attempt was made to simulate macropore flow explicitly. The gravel conductivity value was represented using the Carsel and Parrish (1988) value of 29.7 cm/h for sand, because there was no USDA value for gravel. This value is small compared to other published values for gravel (e.g., 4×10^2 to 4×10^5 cm/h; Maidment 1993) and is more likely representative of a gravel layer mixed with site soils.

Unsaturated hydraulic conductivity values for the different soils were described using the Mualem conductivity model (Mualem 1976). This model was applied with a pore interaction term of 0.5 and the assumption that the van Genuchten parameter m is equivalent to $1-1/n$.

3.2.3 Initial Conditions

All of the simulations started in the year 1965. The matric potential profiles for each soil type and each vegetation scenario were unknown. Therefore, all simulations were initialized with a uniform matric potential profile of -0.1 MPa. This initial value corresponded to the matric potential profile observed by Scanlon et al. (1996) for borehole BEG1 in the northeast corner of the Plant. BEG2, a second borehole located in the south central part of the Plant, had much drier matric potentials. Starting with the BEG2 profile would affect the transient results but not the steady state results.

3.2.4 Boundary Conditions

The lower boundary of the model domain was at 6 m, which is well below the 2-m maximum depth of root penetration allowed in these simulations. The large depth interval between the deepest roots and the lower boundary allowed us to assume that the lower boundary was subject only to the drainage process. Therefore, the lower boundary condition was specified with a unit gradient condition (i.e., free drainage).

The upper boundary condition for these simulations was defined using a prescribed combination of daily precipitation and potential evapotranspiration fluxes. These fluxes were determined from meteorological information. Measured daily precipitation rates defined the water inputs (snowfall was treated as an equivalent rainfall). Daily potential evapotranspiration rates were calculated using the Penman method with daily values (either measured or estimated) of maximum and minimum air temperature, average dewpoint temperature, solar radiation, wind speed, and cloud cover (Doorenbos and Pruitt 1977).

A 31-year record of weather parameters was constructed for these simulations. Meteorological data were obtained to describe weather at the Plant since 1988, and at the Amarillo airport since 1965. The Plant data were collected every 15 minutes. The Amarillo data were reported for every day. The Pantex data set was the primary source of weather data. If the data were unavailable from the Plant, the data from the Amarillo airport were used as a supplement (with appropriate scaling between sites, as explained below). When data were missing from both sites on a particular date, data for the same date but in other years were used.

3.2.4.1 Maximum and Minimum Air Temperature

For each day, the 15-min air temperature data from the Plant were scanned to identify the maximum and minimum values for the day. When air temperature data for the Plant were unavailable, daily maximum and minimum air temperatures from the Amarillo airport were scaled to provide estimates for the Plant. Table 3.2 shows the regression equations used to transform the Amarillo data. Basically, Pantex and Amarillo temperatures are very similar at about 70°F. Pantex air temperatures tend to be slightly warmer than the airport when temperatures are lower than 70°F, and slightly cooler than the airport when temperatures are higher.

3.2.4.2 Dewpoint Temperature

For each day, the daily dewpoint was assigned a value equivalent to the average of the 15-min dewpoint temperature data from the Plant. If less than 78% of the 15-min data were available, the daily dewpoint was estimated from the minimum air temperature at the Pantex Plant. Table 3.3 shows the regression equation used to transform the data. Also included in Table 3.3 are two additional regressions that show a reasonably strong relationship between dewpoint temperature

Table 3.2. Regression Equations Relating Maximum ($T_{\max Am}$) and Minimum ($T_{\min Am}$) Air Temperature Data at the Amarillo Airport to the Same Variables at the Pantex Plant. The regressions were carried out using only those days from 1988 to 1991 for which at least 78% of the Pantex 15-min data were available.

Estimated Pantex Plant Daily Value	Equation	R^2	n	Std. Error (°F)
Maximum air temperature (°F)	$= 0.917 T_{\max Am} + 5.66$	0.932	1267	4.6
Minimum air temperature (°F)	$= 0.961 T_{\min Am} + 2.86$	0.974	1267	2.8

Table 3.3. Regression Equations Relating Minimum Air Temperature ($T_{\min Pan}$) and Dewpoint Temperature (T_{dewPan}) at the Pantex Plant and the Amarillo Airport. The regressions were carried out using only those days from 1991 to 1993 for which at least 78% of the Pantex 15-min data were available. There were no data for 1988 to 1990.

Estimated Pantex Plant Daily Value	Equation	R^2	n	Std. Error (°F)
Dewpoint temperature (°F)	$= 0.894 T_{\min Pan} - 3.06$	0.838	867	6.4
Dewpoint temperature (°F)	$= 0.968 T_{\text{dewAm}} - 0.220$	0.951	867	3.5
Dewpoint temperature at Amarillo airport (°F)	$= 0.893 T_{\min Am} - 0.365$	0.867	867	5.8

at the Plant and at the Amarillo airport. They also show a relationship between dewpoint and minimum air temperature at the Amarillo airport that is about as strong as the same relationship at the Plant.

3.2.4.3 Solar Radiation

No solar radiation data were available at either site. Potential solar radiation for the Plant was calculated using the latitude of the Plant (35°19') and Equation 12.5 on page 135 of Campbell (1985). Actual solar radiation was then estimated from potential solar radiation using the sunshine information (described below under cloud cover) and Equation 4.4.1 on page 4.31 of Shuttleworth (1993).

3.2.4.4 Wind Speed

For each day, the 15-min wind data from the Plant were averaged. When wind speed data for the Plant were unavailable, daily data from the Amarillo airport were used. These data were scaled from the 7-m measurement height at the airport to the 10-m measurement height at the Plant using the regression parameters in Table 3.4. When there was no wind data from either site for the years after 1983, the average wind speed of 12.4 mph during the period from 1988 to 1991 was used. There were no wind data for the years 1965 to 1983. For these years, the wind data for the period from 1985 to 1994 were used, with the last digit of the year determining which year would provide the data. For example, wind data from 1985 was used to represent wind in 1965 and 1975, 1986 for 1966 and 1976, and so on.

3.2.4.5 Cloud Cover

There were no cloud cover data for the Plant. The Amarillo airport provided sunshine data, both in the form of percent sunshine and total sunshine hours. The percent sunshine data were subtracted from 100 to estimate the percent cloud cover at the airport. That estimate was then used to represent cloud cover at the Plant. When only the total number of sunshine hours was provided, the percent sunshine was calculated by dividing the total number of sunshine hours by the potential number of daylight hours (which was calculated using Equation 4.4.1 on page 4.31 in Shuttleworth 1993).

Table 3.4. Regression Equation Relating the 7-m Wind Speed at the Amarillo Airport to the 10-m wind speed at the Pantex Plant. The regression was carried out using only those days from 1988 to 1991 for which at least 78% of the Pantex 15-min data were available.

Estimated Pantex Plant Daily Value	Equation	R ²	n	Std. Error (mph)
Wind speed (mph)	$= 0.977 \text{ Wind}_{\text{Am}} - 0.366$	0.772	1229	2.10

3.2.4.6 Precipitation

For each day, the 15-min precipitation data from the Plant were summed to calculate the total precipitation for the day. When precipitation data from the Plant were unavailable, daily data from the Amarillo airport were used to provide an estimate of the values for the Plant. For all years, daily precipitation was applied starting at 0000 h at a rate of 0.5 cm/h and continuing at that rate until all of the precipitation for the day was added. On several days during the 31-year period, that rate was insufficient to apply the total precipitation amount. On those days only, the hourly rate was increased to ensure that the total precipitation for the day was added. This method does not capture the impact of short intense storms, during which the runoff potential is much higher and infiltration is lower. In one test simulation (Pullman clay loam with no vegetation), increasing the maximum precipitation to 1.0 cm/h resulted in a 3-fold increase in runoff and 40% less drainage.

3.2.5 Vegetation Information

Two vegetation scenarios were studied for this report: natural grassland and crop rotation. Natural grassland consists of a variety of species including *Bouteloua gracilis* (blue grama), *Bouteloua curtipendula* (sideoats grama), and *Buchloe dactyloides* (buffalo grass), with blue grama being the dominant species on most soils (USDA 1962 and subsequent revisions). Therefore, the simulations representing natural grassland were conducted using blue grama parameters. The second vegetation scenario was a typical 3-year crop rotation, consisting of winter wheat and sorghum separated by fallow periods.

Vegetation information consisted of 1) the method to partition potential evapotranspiration, 2) active season, 3) bare fraction of soil, 4) root length density, 5) maximum root depth during the year, and 6) the effectiveness of plant water withdrawal as a function of matric potential. Literature parameters or reasonable estimates of parameters for each plant were chosen and used. The plant parameters were held constant for each simulation year. Variations in plant responses due to yearly precipitation and temperature variations, fire, diseases, nutrient cycling, grazing, and land use changes, were not addressed.

Potential evapotranspiration was partitioned into potential evaporation and potential transpiration using the leaf area method (Ritchie and Burnett 1971). For each of the plants, leaf area throughout the growing season was constrained using its active season (defined below) and the maximum leaf area. For both vegetation scenarios, the maximum leaf area was based loosely on yield data for winter wheat. Musick et al. (1994) report that dryland winter wheat produces roughly 34% of the yield of irrigated wheat. Irrigated wheat and sorghum can achieve leaf area indexes of 4 to 5 during a growing season. For dryland wheat and sorghum, 34% of the average of these values gives a maximum leaf area index of 1.5. This value was assumed to apply to blue grama also. When used to partition potential evapotranspiration, a leaf area index of 1.5 results in 65% of the potential evapotranspiration being attributed to transpiration. Figure 3.1 shows the leaf area variation throughout the three years.

Figure 3.1. Leaf Area Index During the Three-Year Crop Rotation

The active season of the plants is used to determine when to calculate transpiration and when roots started or stopped growing. The active season was specified with starting and ending days of the year. Blue grama was started on February 1 (day 32) and ended on June 15 (day 166). For the crop rotation scenario, Table 3.5 shows the start and end days for each of the three years of the rotation based on the cultural practices outlined in Steiner et al. (1987).

The bare fraction of soil is used to scale the potential transpiration based on the amount of soil surface covered by the vegetation. For both vegetation scenarios, the bare fraction was set to zero, meaning that the vegetation covered 100% of the ground surface and thus potential transpiration was not reduced.

Root length density (RLD) for each species was described using the exponential model

$$RLD = 0.19 \exp(-0.02 z)$$

where z is soil depth in cm. The maximum annual rooting depth was determined as the maximum depth of roots reported in USDA (1962) for each soil type. These values were 132 cm for the Pullman clay loam, 200 cm for the Estacado clay loam, 23 cm for the Lofton clay loam, and 51 cm for the Randall clay. Seasonally, the roots of all three species were allowed to grow at the rate of 1 cm/d for their entire growing season.

Table 3.5. Simulation Parameters for a Three-Year Crop Rotation

Year	Simulation Parameters		
	Months	Vegetation Status	Start and End Days
1	Jan to Aug	fallow	1 to 243
	Sep to Dec	winter wheat	244 to 365
2	Jan to May	winter wheat	1 to 151
	Jun to Dec	fallow	152 to 365
3	Jan to Apr	fallow	1 to 120
	May to Sep	sorghum	121 to 274
	Oct to Dec	fallow	275 to 365

The plant water uptake function was defined with three matric potential parameters: HN, HD, and HW. The parameter HN is the matric potential above which oxygen is limiting and plant water withdrawal ceases. For all species, the parameter HN was set to -0.006 MPa for the clay loam, -0.014 MPa for the silty clay loam, and -0.03 MPa for the clay and silty clay. The criteria for specifying the HN value was that potential above which the air content of the soil is less than 0.05 cm³/cm³, or the value -0.03 MPa, whichever is greater. The parameter HD, which is less than HN, is the matric potential below which plants begin to have difficulty withdrawing water from the soil. Between HN and HD, plants can withdraw water at the optimal rate. For all soil types and plant species, HD was set to -0.1 MPa. The parameter HW can be thought of as the wilting point, which is the matric potential below which plants can no longer withdraw water. For all soil types and plant species, HW was set to -1.5 MPa. Between HD and HW, ease of water withdrawal decreases with decrease in matric potential.

3.3 Results

The deep drainage rates determined in the simulations are presented in two formats: transient and steady state. For the transient results that exhibit an increase in drainage above the initial conditions, the drainage rate is plotted as a function of time from the start of the simulation. The initial drainage rate of 0.4 mm/yr is a function of using the initial condition of -0.1 MPa throughout the profile.

3.3.1 Transient Rates

Simulations of natural grassland on the Pullman clay loam and Estacado clay loam showed that drainage rates after 31 years were <0.4 mm/yr (which was the initial condition). Thus, the initial conditions were wetter than could be sustained by the 31-year weather record. For all soils, this result is consistent with estimates provided by Scanlon and Goldsmith (1997) for natural grasslands.

Figure 3.2 shows the impact of a 3-year crop rotation on deep drainage rates for two soil types. For the Estacado clay loam, the rates varied between 0.45 and 0.51 mm/yr for the entire 31-year period. In contrast, rates under the Pullman clay loam begin to rise above the initial rates seven years after the start of cropping. For both soils, there is very little year-to-year variability in the rates. Crops on Lofton clay loam and Randall clay were not simulated because there was no indication that these two soils were cropped at the Plant. If these soils were farmed, we expect that the deep drainage rates would be less than or equal to drainage rates under the Estacado clay loam.

Figure 3.3 shows significant drainage rates following the start of no vegetation in 1965. However, it takes 8 to 10 years before the lack of vegetation is reflected in the drainage rates at the 6.0-m depth. For Pullman clay loam, drainage rates increase more quickly than for the other soils. This behavior continued later in the simulation, where peaks observed in the drainage rates under Pullman clay loam were not observed in the other soils. Drainage rates are highest for the Pullman clay loam. This result is important because Pullman clay loam is the dominant soil type at the Plant. Of all four soils, the Randall clay has the lowest drainage rates. Even after 31 years without plants, drainage rates at 6.0 m under Randall clay are only 0.9 mm/yr.

All of these soils have a large capacity to store water between depths of 2 and 6 m. If vegetation was allowed, the soils would continue to have excess deep drainage for many years. The drainage water would originate from the 2 to 6 m zone, where plant roots typically do not reach.

Figure 3.2. Transient Deep Drainage Rates Under a Three-Year Crop Rotation

Figure 3.3. Transient Deep Drainage Rates in the Absence of Plants

Figure 3.3 shows that the drainage rates without plants are higher than with plants roughly by a factor of 10. This demonstrates the ability of dryland agriculture to utilize most of the precipitation. Because the rates are so much higher, the drainage pulses seen in Figure 3.3 (each spanning several years) are not apparent in Figure 3.2.

Whether cropped or not, the soil drainage results in Figures 3.2 and 3.3 show that fluxes at the 6.0-m depth did not increase significantly until seven or more years after the start of the simulations. This indicates that the response of deep drainage to surface alterations may not show up at deeper depths, say in the perched aquifer at 80 to 100 m, for 100 years or more. The actual length of time will depend on the initial conditions (e.g., drier initial conditions will increase the time required for a surface alteration to be manifested as a change in flux at a particular depth).

Figure 3.4 shows that the highest drainage rates of any scenario are for a soil with a gravel cover and no vegetation, such as surfaces prepared for parking lots, roadways, and storage areas. Under this scenario, fluxes at the 6.0-m depth increase dramatically after only one year. The implication is that drainage at deeper depths could begin increasing in as little as 10 to 15 years.

Figure 3.4. Transient Deep Drainage Rates Under a Gravel Cover in the Absence of Plants

3.3.2 Steady State Rates

The transient simulations that indicated drainage rates higher than the initial 0.4 mm/yr were repeated until the results did not change by more than 0.1 mm/yr. Table 3.6 shows that the Pullman clay loam without plants has the highest long-term average rate (27.3 mm/yr), while the Estacado clay loam under the 3-year crop rotation has the lowest (0.8 mm/yr). Table 3.6 also shows that the soils with higher average drainage rates generally also have greater variability in annual rates as evidenced by the difference between the maximum and minimum annual values. Figure 3.5 shows this result graphically.

Table 3.7 summarizes the estimates of steady-state deep drainage rates for each combination of soil type and surface condition. The grassland simulations indicated that rates are less than 0.4 mm/yr for two of the soils (Estacado and Pullman clay loams); similar behavior is expected for the other two soil types. It was therefore assumed that, for grasslands on all soils, the long-term rate can be represented as 0.1 mm/yr (Scanlon and Goldsmith 1997) report that the rates are ≤ 0.1 mm/yr). Crop rotation simulations were not performed for the Lofton clay loam and Randall clay soils. These soils showed low drainage rates when plants were absent, and the rates were lower than those for the other two soil types. Therefore, we assumed that the rates for the Lofton and Randall soils under cropping would be lower than for the other soils. As Table 3.7 indicates, we set the rates at 0.1 mm/yr. Finally, only one soil with a gravel cover was simulated. That result was used

Table 3.6. Summary of Estimated Steady-State Deep Drainage Rates for 1965-1995 (steady state refers to repeating the 31-year simulation with the same weather data until the initial and final conditions match)

Soil Type	Surface Condition	Simulated Drainage Rates (mm/yr)		
		Minimum	Average	Maximum
Estacado clay loam	bare soil	6.4	9.2	17.5
	3-yr crop rotation	0.7	0.8	0.9
Lofton clay loam	bare soil	5.0	6.4	8.8
Pullman clay loam	bare soil	17.7	27.3	62.4
	3-yr crop rotation	2.6	3.7	5.7
Randall clay	bare soil	1.6	2.1	2.8

Figure 3.5. Steady-State Deep Drainage Rates in Absence of Plants

Table 3.7. Recommended Steady-State Deep Drainage Rates for the 6-m Depth. Grassland values listed as "0.1" mm/yr are based on observations by Scanlon and Goldsmith (1997). An asterisk indicates the estimated rate is based on inference from another soil type rather than on direct simulation.

Surface Scenario	Recommended Drainage Rates (mm/yr)			
	Estacado Clay Loam	Lofton Clay Loam	Pullman Clay Loam	Randall Clay
Grassland	0.1	0.1	0.1	0.1
3-year crop rotation	0.8	0.1	3.7	0.1
No plants	9.2	6.4	27.3	2.1
Gravel cover	418	418*	418*	418*

to represent drainage for the other soils when covered with gravel. The assumption was that the gravel layer decouples the underlying soil from the atmosphere and thereby controls the loss of water by evaporation. Therefore, all four soils were assigned the same steady-state deep drainage rate.

Within the context of a geographical information system (GIS), Table 3.7 can be used to prepare a map of steady-state deep drainage rates at the Plant. The GIS must have at least two coverages: soil type and land use. The GIS can then be used to identify combinations of these two coverages and assign the rates in Table 3.7 to the combinations. If the coverages contain soil types or land uses not reflected in Table 3.7, the closest associated soil type or land use should be used. For example, the land use map of the Plant shows industrial areas. These areas are complex and existing information is inadequate to delineate surface conditions for this type of analysis. As an alternative, the industrial areas can be treated as if they were the underlying soil type but with no plant cover. This assumption was used by Fayer and Walters (1995) to prepare the deep drainage map of the Hanford Site, a U.S. Department of Energy facility that is located in Richland, Washington.

4.0 Summary of Analysis

The objective of the vadose zone modeling effort is to develop a modeling framework with which to predict contaminant loading to the unconfined aquifer and to support analyses of remedial activities. One aspect of this framework is the estimation of drainage beneath major surface features at the Plant, including ditches and playas, natural grassland, dryland crop rotation, unvegetated soil, and graveled surfaces.

Infiltration volumes and rates were estimated for the channel bottoms and playas. The estimated infiltration rates for the playas ranged from 2.4 ft/yr for Playa 5 to 5.5 ft/yr for Playa 1. The estimated infiltration rates for the channel bottoms ranged from 10.5 to 21.9 ft/yr. Because there was a lack of field data to corroborate the model results, further simulations were conducted to demonstrate model sensitivity to several input parameters.

Average long-term drainage rates were estimated for various combinations of the major soil types and vegetation conditions at the Plant. For grassland, the estimated drainage rate is 0.1 mm/yr for all soil types. Under a typical dryland crop rotation scenario, the estimated rates vary from 0.1 to 3.7 mm/yr, depending on soil type. With no plants on the surface, the estimated rates vary from 2.1 to 27.3 mm/yr, depending on soil type. Finally, the estimated rate for unvegetated surfaces with a gravel cover is 418 mm/yr.

In all the drainage estimates, the weather data were the most defensible on a site-specific basis. The only exception was rainfall intensity, which was limited to 0.5 cm/h, and probably underestimates the most intense storms. With this limit in effect, runoff is reduced significantly and infiltration (and thus drainage) is increased significantly. The remainder of the modeling parameters (i.e., channel characteristics, hydraulic properties, plant behavior) were estimated from site, regional, or national information. The credibility of the drainage estimates presented in this study could be determined by collecting site-specific hydrologic, soil, and plant data to both parameterize and calibrate the models and to verify their predictive abilities. Of these data, rainfall intensity, ditch and playa calibration data, and site-specific soil hydraulic properties would probably provide the greatest value in improving the deep drainage flux estimates. In addition, ongoing characterization activities can provide distributions of contaminant or environmental tracers that can be used to calibrate the models and establish the credibility of the predictions.

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