Section 5
Parameter Sensitivity Analysis: Hypothetical Modeling Scenario

The characteristics of a representative physical site are required to realistically study the sensitivity of the five models proposed in this report for simulating the transport and fate of radionuclides in the unsaturated zone. Such a site would be used to set the standards for base parameter choices in the sensitivity tests and for parameter range determination. The ideal candidate site should have well characterized soil properties, and should have sufficient chemical transport and fate data and climatological information for running the pertinent simulations. Once a site is chosen, a conceptual model of that site is required so that the site data, the five proposed modeling codes, and the intended application of the models are all consistent with one another. In what follows, we consider the site selection process, selection of the candidate site, characteristics of the Las Cruces Trench Site in New Mexico, development of a conceptual model, and the base parameter selection.

5.1 Site Selection Process

The sensitivity studies reported in this document are part of an overall evaluation of the general applicability of each model (i.e., HYDRUS, CHAIN 2D, FECTUZ, MULTIMED-DP 1.0, and CHAIN) for simulating the fate and transport of radionuclides. The radionuclides of interest are the following five elements/isotopes (U.S. EPA, 2000b):

Element/Isotope	***K_d Default Values in ml/g***
Plutonium (^{238}Pu)	5
Strontium (^{90}Sr)	1
Technetium (^{99}Tc)	0.007
Tritium (^{3}H)	0
Uranium (^{238}U)	0.4 ,

where K_d is the soil/water partition coefficient for the linear Freundlich isotherm. These five elements/isotopes are taken to be the parent species in the decay chains and the major segments of the chains are shown in Figure 5-1 along with the corresponding half-lives of the species.

The quantity, K_d, in all five models being studied, is a lumped parameter representing known and unknown phenomena. It tends to lose some of its meaning in the modeling world, while retaining its full meaning in the laboratory. In the laboratory K_d is determined under carefully controlled conditions, but the real world cannot be completely controlled or measured. Thus, the conditions surrounding the sorption phenomenon must be estimated, and these estimates will only represent localized conditions in the vicinity of the sampling. Consequently, the large heterogeneities of most, if not all, subsurface systems make it difficult to identify a single K_d value for the system. Further, unless the model has a geochemical component, K_d will also represent everything one does not know about the site's geochemistry. The relationships between K_d values, the chemical species, and a site's geochemistry are discussed in U.S. EPA (1999ab, 2000b). However, in the current report, the default K_d values, given above, are taken as the base values for the sensitivity analyses combined with an interval domain about these values, to partially represent the heterogeneity found in the vadose zone.

Based on the above radionuclides, the site selection process consisted of identifying three features: site listing, data availability, and existing field and modeling studies. By reviewing existing literature and databases, a ***list of candidate sites*** was developed, see Table 5-1. These candidate sites, in general, were either contaminated with radionuclides, or were current or future radioactive waste disposal sites. For example, Superfund sites with soil contaminated by one or more of the above five radionuclides were identified in the U.S. EPA's ***VISITT*** database (i.e., the Vendor Information System for Innovative Treatment Technologies, Version 6.0). Many of these radionuclide

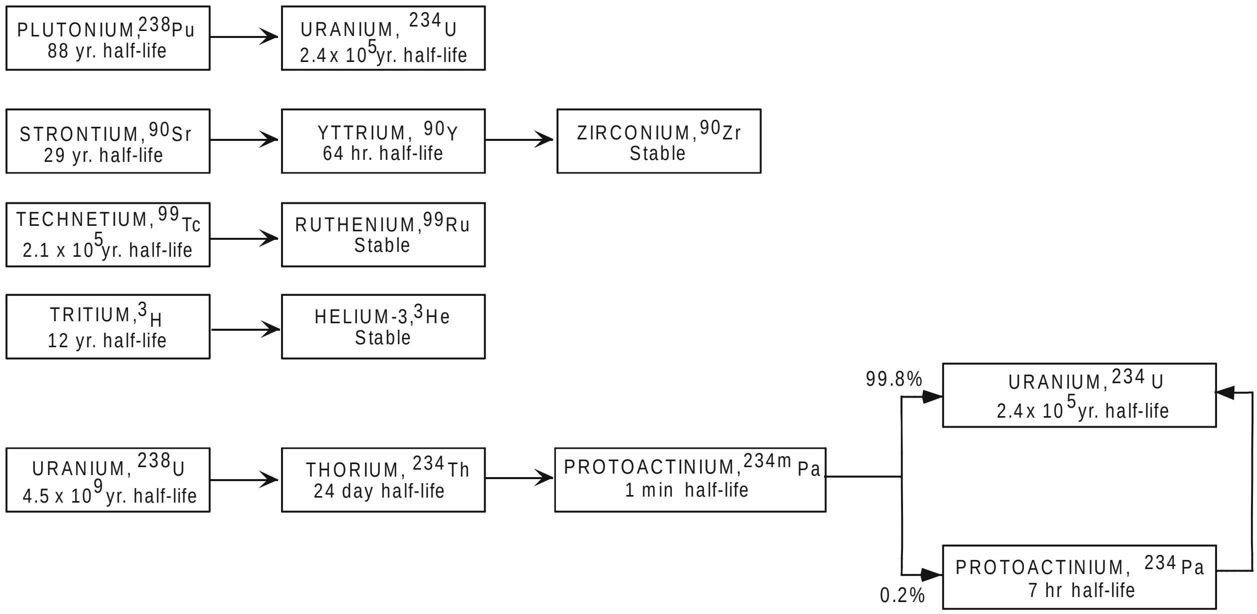

Figure 5-1. The major segments of the decay chains for the five elements/isotopes considered to be parents in these analyses (U.S. EPA, 2000b).

contaminated sites were a result of past nuclear production and related activities, and are currently under the environmental restoration program operated by the U.S. Department of Energy. With reference to low-level radioactive waste storage sites, the most attractive areas were those having low annual precipitation, high evapotranspiration, and thick unsaturated soils/sediments. An example of such a site is the Mojave Desert Waste-Burial Site near Beatty, NV. In addition, the Nevada Test Site is a radionuclide contaminated site from nuclear testing as well as an on-site/off-site low-level waste disposal facility. The only non-nuclear contaminated site and non-nuclear storage site considered in this evaluation was the Las Cruces Trench Research Site in New Mexico. The field studies at this site have been used to provide data to test deterministic and stochastic models for water flow and solute transport, Wierenga, et al. (1991), Hills, et al. (1991, 1994), and Rockhold, et al. (1996). The Las Cruces Trench Site was included in the list of candidate sites because it fit the above physical characteristics for waste disposal facilities and because many detailed site characterization studies and field experiments have been conducted at this location.

The ***availability of soil data and climatological records*** are essential for the proper simulation of water flow and radionuclide transport in unsaturated soils. From the twenty-some sites in the original candidate list, four sites that had the most available data were selected for further evaluation. These were the Las Cruces Trench Site, the Beatty Waste Storage Site, Idaho Falls National Laboratory and the Hanford Washington Site. In addition, the Perdido Alabama Site was placed on the list; this was the site that was analyzed in the earlier sensitivity study of Nofziger, et al. (1994). Actually, the Perdido Site, which is a benzene contaminated site in an area of high annual precipitation, was assigned soil properties obtained from another site having the same soil series. Thus, no site-specific soil properties were available for the Perdido site. This led to the elimination of the Perdido site from further consideration. The existing ***field/modeling studies*** for the four remaining sites were reviewed and summarized. The studies considered were water balance, recharge and infiltration experiments; tracer and radionuclide migration studies; laboratory and field measurements of bulk density, K_s, and soil water retention curve data; and model construction, testing, and simulation runs.

5.2 Selection of the Candidate Site

For the final four sites (Las Cruces, Beatty, Idaho Falls, Hanford), additional factors and options were considered in the choice of the best candidate site. Two of the important factors were the availability of required soil data for the five pre-selected transport models in this study and the attainability of transport parameters from the

Table 5-1. Partial List of Radionuclide Contaminated and Disposal Sites in the U.S. (U.S. EPA's VISITT Database).

	SITE NAME	*Location, City*	*State*	*Contaminants*	*Site Characteristics*
1	Rocky Flats Environmental Technology Site	Golden	Colorado	Plutonium, Uranium	Superfund Site. On-site waste disposal
2	Idaho National Engineering & Environmental Laboratory	Idaho Falls	Idaho	Radioactive Materials, Plutonium, Tritium	Radionuclide Contaminated Site: Radioactive Waste Management Complex was used for disposal site for low-level and transuranic radioactive waste
3	Ethyl Corporation	Baton Rouge	Louisiana	Uranium	Superfund Site
4	DOE FUSRAP St. Louis Site Treatability Study	St. Louis	Missouri	Uranium	Superfund Site
5	Nevada Test Site	Mercury	Nevada	Plutonium, Tritium	Hazardous Waste Site: Radionuclide contaminated site from nuclear testing: Low-level waste disposal facility for both onsite and off-site generated defense low-level waste
6	Mojave Desert Waste Burial Site	Beatty	Nevada	Various Radionuclides	Low-level radioactive waste and hazardous chemical waste disposal
7	NL Industries, Inc.	Pedricktown	New Jersey	Strontium	Superfund Site
8	Los Alamos Natl. Laboratory	Los Alamos	New Mexico	Plutonium, Uranium	Superfund Site
9	Las Cruces Trench Site	Las Cruces	New Mexico	None	Experimental Site
10	Sandia Natl. Lab.	Albuquerque	New Mexico	Uranium, Plutonium	Superfund Site
11	West Valley Nuclear	West Valley	New York	Strontium	Superfund Site
12	Mound Demonstration Project	Miamisburg	Ohio	Plutonium	Superfund Site
13	Portsmouth Gaseous Diffusion Plant (DOE)	Piketon	Ohio	Uranium, Technetium	Superfund Site
14	EPA SITE Demonstration	Alliance	Ohio	Uranium	Superfund Site
15	Fernald Feed Materials Production Center	Fernald	Ohio	Uranium, Technetium	Superfund Site
16	Apollo Fuel Conversion Plant	Apollo	Pennsylvania	Uranium	Superfund Site
17	Savannah River Site	Aiken	South Carolina	Uranium	Superfund Site
18	INEL Pit 9 Pilot Project	Clemson	South Carolina	Uranium	Superfund Site
19	K-25 Site	Oak Ridge	Tennessee	Technetium, Uranium	Superfund Site
20	Hanford Site	Richland	Washington	Uranium, Strontium	Superfund Site. On-site waste disposal.
21	DOE Morgantown Energy Tech. Center	Morgantown	West Virginia	Various Radionuclides	Superfund Site

existing site modeling studies. Selection of the final candidate site was also dependent upon decision-making options. For example, when verification of modeling results is an important issue (i.e., comparison of modeling results with field and laboratory experimental data) in addition to data availability, the Las Cruces Trench Site was the best candidate. However, when reliable model input data is the only issue and model verification is less important (i.e., comparison among the SSG screening models is more important than model field verification or comparison of the screening models with more comprehensive modeling of the area), then the Beatty Waste-Burial Site is a good alternative candidate.

Four of the five proposed SSG models, HYDRUS, CHAIN 2D, MULTIMED-DP 1.0, and FECTUZ, require van Genuchten soil-water retention parameters (Table 2-1) These parameters plus dispersivities were available at the Las Cruces Site. For the Beatty Site, the van Genuchten parameters were not available and would have to be derived from the raw soil-water content/pressure head data (Andraski, 1996). Furthermore, a great amount of model testing at the Las Cruces Site has been conducted for the transport and fate of tritium, bromide and chromium in the unsaturated zone. Considering the location and climatological features of the site, and the abundance of existing field data in conjunction with significant modeling studies, the Las Cruces Trench Site was chosen as the candidate site for the model evaluation in the SSG for radionuclides.

5.3 Characteristics of the Las Cruces Trench Site in New Mexico

In the soil screening level (SSL) process, generic SSLs for radionuclides can be calculated based on a number of default assumptions chosen to be protective of human health for most site conditions. However, these are expected to be more conservative than calculated site-specific SSLs. When site-specific SSLs are of interest, a simulation using an appropriate model and site-specific data is required. Thus, in the current study, a typical physical site is required for the evaluation of the HYDRUS, CHAIN 2D, FECTUZ, MULTIMED-DP 1.0, and CHAIN Codes in the SSL process.

The Las Cruces Trench Research Site in New Mexico was chosen as the typical physical site because:

1. The site characteristics met the criteria of radioactive waste disposal areas (low annual precipitation, high annual evapotranspiration, and a deep water table);

2. The site had been subjected to extensive testing of its soil physical and chemical properties and soil-moisture distribution and movement in the unsaturated zone;

3. Results of tracer tests (chloride, bromide and tritium) and metal movement (chromium) were available.

This site lies in the Chihuahuan Desert Province of southern New Mexico (Bailey, 1980). This province is mostly desert and the Rio Grande and the Pecos River and a few of their larger tributaries are the only perennial streams. The area has undulating plains with elevations near 1200 m from which somewhat isolated mountains rise 600 m to 1500 m. There are washes which are dry most of the year that fill with water following a rain. Basins that have no outlets drain into shallow playa lakes that dry up during rainless periods. Extensive dunes of silica sand cover parts of the province, and in places, there are dunes of gypsum sand, the most notable being the White Sands National Monument near Alamogordo (a town 100 km northeast of Las Cruces).

The climate of the Chihuahuan Desert is distinctly arid and the spring and early summer are extremely dry. During July the summer rains usually begin, and they continue through October (Bailey, 1980). In general, these summer rains are local torrential storms. Average annual temperature in the province ranges from 10°C to 18°C. Summers are hot and long, and winters are short but may include brief periods when temperatures fall below freezing. The characteristic vegetation of the Chihuahuan Desert is a number of thorny shrubs. These shrubs frequently grow in open stands, but sometimes form low closed thickets. Short grass often grows in association with the shrubs. On deep soils, mesquite is usually the dominant plant; creosote bush covers great areas in its characteristic open stand and is especially common on gravel fans. Royo (2000) says the creosote bush is a desert plant "par excellence," a true xerophyte. It is a drought-tolerant shrub with small dark green leaves and has an extensive double root system – both radial and deep – to accumulate water from both surface and ground water. These plants can tolerate up to two years without precipitation. The leaves are coated with a varnish-like resin which reduces water loss by evaporation. The original creosote bush can live to about 100 years old, but it can produce clones of the parent as the bush ages. These clones are produced in a circular pattern of genetically-identical plants, expanding outward at the rate of about one meter every 500 years. The "King Clone" family on BLM land near Victorville, California, is estimated to be 11,700 years old.

The actual experimental site is located on the New Mexico State University college ranch some 20 or more kilometers due north of the city of Las Cruces, New Mexico. The site is on a basin slope of Mount Summerford at the north end of the Dona Ana Mountains (Wierenga, et al., 1991; Defense Mapping Agency, 1987). Geologically, these mountains are a domal uplift complex composed of younger rhyolitic and the older andesitic volcanics which were intruded by monzonite. The covered trench that provides horizontal access to the experimental plots and is used to provide soil samples for these plots is an evacuated earthen box with dimensions 26.4 m long, 4.8 m wide, and 6.0 m deep.

The published soil hydraulic properties for this site, given by Wierenga, et al. (1991), are listed in Table 5-2. Some pertinent site characteristics obtained by Gee et al (1994) are given on Table 5-3. Table 5-2 shows that the estimates for the hydraulic parameters were obtained for a uniform soil model and for a nine-layered soil model. The layers in the layered soil model correspond to the nine soil layers identified at the site. The saturated hydraulic conductivity for each soil layer was estimated by taking the geometric mean of the 50 laboratory-measured saturated hydraulic conductivities obtained from each soil layer. Likewise, the water retention data from all 50 samples from a given layer were used to estimate α,β,θ_r, and θ_s for a single water retention curve for that layer. For the uniform soil model, the geometric mean of 450 laboratory measured saturated hydraulic conductivities (nine layers with 50 per layer) was used to estimate a uniform soil saturated hydraulic conductivity value. Likewise, the water retention data for all 450 sample locations were simultaneously used to estimate single values for each of the parameters α,β,θ_r, and θ_s in a least squares sense (Wierenga, et al., 1991).

In Porro and Wierenga (1993), the solute transport dispersivity (cm) was determined for six layers ranging over $0 < z < 500$ cm. The values varied from 2.20 cm to 7.80 cm with an arithmetic average of 4.53 cm for the combined layer of 500 cm. Minor adaptations of some of these data have been made in the conceptual model developed for the sensitivity analyses. The details are given in the following subsection. Finally, Figure 5-2 shows the daily precipitation and potential evapotranspiration (PET) at the Las Cruces Site. The PET is calculated from daily climatic data using Penman's general equation for a well-watered grass reference crop (Jensen, et al., 1990):

$$\lambda E_{t0} = \Gamma \bullet (R_n - G) + 6.43\,(1 - \Gamma)\,W(e_0 - e)\ , \qquad (5\text{-}1)$$

where the terms in Equation (5-1) are defined as:

λ	=	latent heat of vaporization in mega-joules per kilogram,
E_{t0}	=	evapotranspiration rate (E_t) from a well-watered grass reference crop, in kilograms per meter squared per day,
λE_{t0}	=	latent heat flux density in mega-joules per meter squared per day,
Γ	=	dimensionless parameter dependent upon surface elevation and air temperature, Table 6-1 of Jensen, et al., 1990,
R_n	=	net radiation at the surface in mega-joules per meter squared per day,
G	=	heat flux density to the ground in mega-joules per meter squared per day,
W	=	$a + b\,u_2$ = wind function in meters per second,
a,b	=	positive constants,
u_2	=	wind speed at 2m above surface in meters per second,
e_0	=	saturated vapor pressure of air at some height z in kPa,
e	=	water vapor pressure in air at height z in kPa,
PET	=	potential evapotranspiration rate in mm/d, given by E_{t0} ÷water density in kilograms per meter squared per millimeter.

For the eighteen year period (1983-2000) shown in Figure 5-2, the annual precipitation ranged over the values from 11.5 cm/yr to 30.8 cm/yr, with an annual average of 22.5 cm/yr. For this same period, 28% of the precipitation came in the January to June period, and 72% came in the July to December period. This is consistent with the climatological description given by Bailey (1980).

5.4. Development of a Conceptual Model

The conceptual model for SSLs using detailed site-specific data is developed in a manner which is theoretically and operationally consistent with the simplified methodology described in Section 2 of the Soil Screening Guidance

Table 5-2. Soil Hydraulic Properties at the Las Cruces Trench Site for SSG Model Evaluation Study (reprinted from *Water Resources Research*, 1991, by P.J. Wierenga, R.G. Hills, and D.B. Hudson with the permission of the American Geophysical Union, Washington, DC).

Layers	*Depth (cm)*	*Saturated Water Content (cm^3/cm^3)*	*Residual Water Content (cm^3/cm^3)*	*van Genuchten Alpha Coefficient, α, (cm^{-1})*	*van Genuchten Beta Coefficient, β, (—)*	*Saturated Hydraulic Conductivity, Ks, (cm/d)*
			Uniform Soil Model			
all	0 - 600	0.321	0.083	0.055	1.509	270.1
			Layered Soil Model			
1	0 - 15	0.348	0.095	0.042	1.903	539
2	15 - 140	0.343	0.091	0.062	1.528	250
3	140 - 205	0.336	0.085	0.060	1.574	267
4	205 - 250	0.313	0.071	0.068	1.537	300
5	250 - 305	0.302	0.072	0.040	1.550	250
6	305 - 370	0.294	0.090	0.070	1.711	334
7	370 - 460	0.310	0.073	0.027	1.418	221
8	460 - 540	0.325	0.083	0.041	1.383	172
9	540 - 600	0.306	0.078	0.047	1.432	226

Table 5-3. Characteristics of the Las Cruces Trench Site for SSG Model Evaluation Study (reprinted from *Soil Sci. Soc. Am. J.*, 1994, by G.W. Gee, P.J. Wierenca, B.J. Andraski, M.H. Young, M.J. Fayer, and M.L. Rockhold with the permission of *Soil Sci. Soc. Am. J.*, Madison, WI).

Annual Precipi-tation (cm/yr)	*Annual Potential (Pan) Evapora-tion (cm/yr)*	*Annual Potential Recharge (cm/yr)*	*Average Daily Max. Air Temper-ature (°C)*	*Average Daily Min Air Temper-ature (°C)*	*Elevation (m)*	*Depth to Water Table (m)*	*Geology*	*Typical Soil Type*	*Typical Vegeta-tion*
23	239	8.7	28	13	1357	60	Alluvial	Berino fine loamy sand	Creosote bush

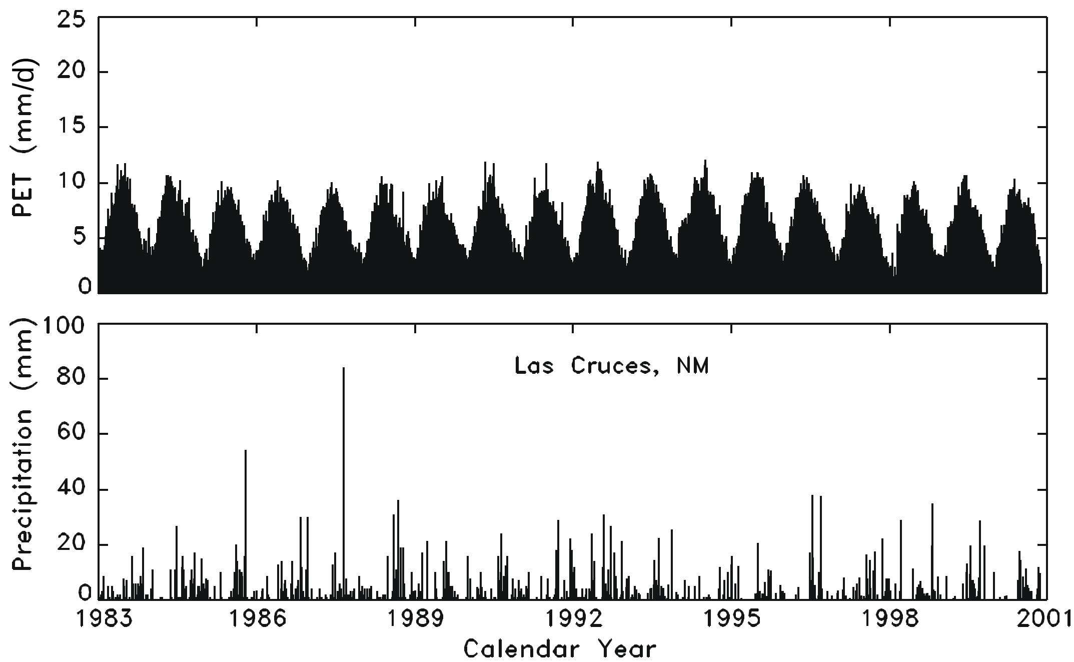

Figure 5-2. Daily precipitation and potential evapotranspiration (PET) at Las Cruces Site, NM. PET is calculated from daily climate data using Penman's equation (Jensen et al., 1990).

for Radionuclides: Technical Background Document (U.S. EPA, 2000b). In so doing, it is assumed that the Las Cruces Trench Site in New Mexico has been used as a waste disposal/storage facility where radionuclides from tank leaks or improper waste disposal were released to the soil surface for a period of time with a specified total amount of release set for each radionuclide (e.g., 10 mg/cm^2 of ^{238}U was released). Thus, a finite radionuclide contaminated source is assumed. The driving force to send this material on a downward migration to the water table is the infiltrated rainfall which produces a net annual recharge rate of 87 mm/yr. (Table 5-3). The site-specific soil hydraulic properties given in the "all-layer" row of Table 5-2 and the mean layer dispersivity of 4.53 cm, obtained for tritium transport through Berino fine loamy sand, are also used in the current analyses.

Further assumptions are:

- The unsaturated zone is homogeneous although HYDRUS, CHAIN 2D, FECTUZ and MULTIMED-DP 1.0 are capable of simulating layered soils and the hydraulic properties for layered soils are available at the site.
- There is no significant vapor pressure for most radionuclides (except for radon, which is not considered in this study) and the dimensionless Henry's Law constant is assumed to be zero.
- Only vertical flow and transport are considered; horizontal flow and transport are ignored, even though CHAIN 2D is capable of simulating two-dimensional flow and transport.
- There is no chemical or biological degradation in the unsaturated zone.
- There is radioactive decay (Figure 5-1) in the unsaturated zone; however, since the published data on decay rates (or half-lives) for radionuclides are reasonably accurate and precise, no sensitivity analysis will be made on decay rates.
- Complexation, oxidation-reduction, dissolution and precipitation, and ion-exchange are not considered because these processes are not implemented in the five models being evaluated.
- There is no facilitated transport (e.g., colloidal transport, preferential flow in fractures or root channels, fingering pathways) of the radionuclides in the unsaturated zone.
- The aquifer lying below the unsaturated zone is unconsolidated and unconfined. However, flow and transport of the radionuclides in the saturated zone are not considered and only leachate contributions to the ground water at the center of the disposal area are of interest.
- Initial concentrations of radionuclides in the soil are zero.

In order to specify a total amount of radionuclide and a reasonable level of a radionuclide concentration release from the waste source, a literature survey of radionuclide contamination in soils was conducted. Based on the survey information, the radionuclide concentration released from the hypothesized waste source and the duration of radionuclide release were determined. Thus, the total amount of radionuclide release can be obtained from the product of the recharge rate, source concentration, and the duration time of waste release. The depth of radioactive contaminated soil at the termination point of waste release from the source can be determined from the product of the pore velocity times the duration time of waste release.

The decay series of the radionuclides in the sensitivity analyses in this report are based on the chain segments given in Figure 5-1. The chain segments for plutonium-238 and uranium-238 are not complete but are sufficient for current purposes because of the long half-life of uranium-234. Further, due to the time discretization in the five models and the relatively short half-lives of the intermediate species in the strontium-90 and uranium-238 chains, the following parent-daughter chains are only of importance in this report:

$$^{238}\mathrm{Pu} \longrightarrow {}^{234}\mathrm{U} \qquad {}^{90}\mathrm{Sr} \longrightarrow {}^{90}\mathrm{Zr}$$

$$^{99}\mathrm{Tc} \longrightarrow {}^{99}\mathrm{Ru} \qquad {}^{3}\mathrm{H} \longrightarrow {}^{3}\mathrm{He}$$

$$^{238}\mathrm{U} \longrightarrow {}^{234}\mathrm{U}$$

5.5 Base Parameter Selection

Table 5-4 provides the base values of selected input parameters to be used in the sensitivity analyses given in later sections. These values are those that are basically used in the analyses of HYDRUS and CHAIN 2D. Subsets of these values will be used in the analyses of FECTUZ, MULTIMED-DP 1.0 and CHAIN. Justification and rationale for the use of these specific base parameters are presented in the following paragraphs.

The area of the ***disposal facility*** is arbitrarily taken as 400 m^2, whose length and width are both 20 m. The one-dimensional vertical models are assumed to be located at the center of the square, thus eliminating edge effects in the unsaturated zone simulation. The ***total duration*** of the release of the radionuclide mass was arbitrarily chosen to be 1000 days; however, this value was reasonably consistent with the survey information mentioned in the previous subsection.

The ***potential evapotranspiration (PET)*** from the surface of well-watered short grass was calculated from Las Cruces climatic data using Penman's equation (Jensen, et al. 1990). The weather/climatic data required for this equation are temperature, relative humidity, wind speed, and solar radiation, along with the estimated albedo coefficient of 0.21 and the 1357 m elevation of the site. Using the daily climatic data for the years 1983 to 2000, the estimated value of PET is 204 cm/yr and the average precipitation at the site is 22.5 cm/yr. These values are consistent with those reported by Gee, et al. (1994), see Table 5-3; thus, we use the ***annual potential recharge*** of 8.7 cm/yr given by Gee, et al. In Table 5-2, the all-layer ***residual moisture content*** is given as 0.083 and the all-layer ***saturated moisture content*** is given as 0.321. It is expected that the "uniform" annual recharge of 8.7 cm/yr will produce a soil moisture somewhere between θ_r and θ_s. Thus, we arbitrarily chose an ***initial water content***, θ, equal to the geometric mean of θ_r and θ_s, $(\theta_r \theta_s)^{1/2}$. This value to two significant figures is $\theta = 0.16$.

As stated in the previous subsection, the total mass of the individual radionuclides released from the hypothetical Las Cruces disposal/storage site was chosen to be consistent with radionuclide releases from real sites throughout the country. The relationship between the ***mass released*** and the ***concentration of the radionuclide in the recharge water*** from the waste source is given by:

$$\begin{aligned} \text{Mass (mg/cm}^2\text{)} &= \text{Recharge (cm/yr)} \bullet \frac{\text{Duration (d)}}{\text{365 (d/yr)}} \bullet \frac{1}{\text{1000 (cm}^3\text{/L)}} \bullet \text{Concentration (mg/L)}\,, \\ &= (8.7)\left(\frac{1000}{365}\right)\left(\frac{1}{1000}\right)\text{Concentration (mg/L)}\,, \qquad (5\text{-}2) \\ &= 0.024\ \text{(Concentration, mg/L)}\,, \end{aligned}$$

Table 5-4. Base Values of Input Parameters for Unsaturated Zone Radionuclide Models (from Wierenga, et al., 1991; Gee, et al., 1994; U.S. EPA, 2000ab; and U.S. EPA VISITT Database).

Parameters	***Values***
Source-Specific Parameters	
Area of disposal facility (m^2)	400
Width of disposal facility (m)	20
Length of disposal facility (m)	20
Mass release of Radionuclide ^{238}U (mg/cm^2)	10
Concentration of ^{238}U in recharge water from waste source (mg/L)	417
Mass Release of Radionuclide ^{99}Tc (mg/cm^2)	3×10^{-4}
Concentration of ^{99}Tc in Recharge Water from Waste Source (mg/L)	1.25×10^{-2}
Mass Release of Radionuclide ^{90}Sr (mg/cm^2)	4.8×10^{-3}
Concentration of ^{90}Sr in Recharge Water from Waste Source (mg/L)	0.2
Mass Release of Radionuclide ^{238}Pu (mg/cm^2)	2.4×10^{-9}
Concentration of ^{238}Pu in Recharge Water from Waste Source (mg/L)	1.0×10^{-7}
Mass Release of Radionuclide ^{3}H (mg/cm^2)	2.6×10^{-9}
Concentration of ^{3}H in Recharge Water from Waste Source (mg/L)	1.1×10^{-7}
Duration of Waste Source Being Completely Released (days)	1000
Potential Recharge Rate (mm/yr)	87
Initial Water Content (cm^3/cm^3)	0.16
Soil Properties in Unsaturated Zone	
Saturated Hydraulic Conductivity, K_s, (cm/d)	270.1
Porosity (–)	0.358
Residual Water Content (cm^3/cm^3)	0.083
Saturated Water Content (cm^3/cm^3)	0.321
Bulk Density (g/cm^3)	1.70
van Genuchten Alpha Coefficient, α, (cm^{-1})	0.055
van Genuchten Beta Coefficient, β, (–)	1.509
Depth to Water Table (m)	6
Solute Transport Parameters	
Decay Coefficient for Parent Product ^{99}Tc (1/d)	9×10^{-9}
Decay Coefficient for Daughter Product ^{99}Ru (1/d)	Stable
Distribution Coefficient for ^{99}Tc (ml/g)	0.007
Distribution Coefficient for ^{99}Ru (ml/g)	5.0
Dispersivity (cm)	4.53
Diffusion Coefficient in Free Water (cm^2/d)	1.73
Apparent Molecular Dispersion Coefficient (cm^2/d)	0.33
Dispersion Coefficient (cm^2/d)	1.01

or

$$\text{Concentration (mg/L)} = 41.7\ (\text{Mass, mg/cm}^2). \tag{5-3}$$

Using Equation (5-3) and the mass releases of ^{238}U, ^{99}Tc, ^{90}Sr, ^{238}Pu and ^{3}H in Table 5-4 results in the corresponding concentrations of these species given in the table.

In order to keep the initial concentration and the total amount of the radionuclide entering the soil fixed for varying recharge rates, q, in the sensitivity analyses, the duration of the source emissions in Equation (5.2) was allowed to vary. That is, the following product in Equation (5-2) was held fixed at its base value as the time duration of the source varied with the recharge rate, q:

$$(\text{Duration}) \times (\text{Recharge Rate}) = 8700 \text{ cm-d/yr} . \tag{5-4}$$

For the range of q used in the sensitivity analyses, 5.11 cm/yr $\leq$ q $\leq$ 10.95 cm/yr, the source duration ranges over the interval 795 d $\leq$ duration $\leq$ 1703 d. However, for the species considered in this report, the differences in source time duration have a negligible effect on the output values of concern in this report. That is, since the total mass of a radionuclide and its initial concentration are held fixed, the differences produced by the total release times (i.e., the pulse width of release) have sufficient time to smooth out in the soil column before the major parts of the breakthrough curves (BTCs) are seen at the bottom, the 6 m depth, of the soil columns.

Table 5-3 lists the depth to water table at the Las Cruces Test Site as 60 m. However, the detailed soil moisture data are given only for the first 6 m, as listed in Table 5-2. Thus, for the hypothetical modeling scenario of this report, we chose the 6 m depth to be the top of the water table in our sensitivity analyses. It is felt that this assumption will meet the project's objectives. As stated in the previous subsection, this 6 m layer is taken to be homogeneous with the ***soil properties*** listed in the all-layer row of Table 5-2, namely: $\theta_s = 0.321$, $\theta_r = 0.083$, VG-α = 0.055 cm^{-1}, VG-β = 1.509, and K_s = 270.1 cm/d.

Wierenga, et al. (1991) found that the ***bulk densities*** of the nine soil layers in Table 5-2 range in values from 1.66 to 1.74 g/cm^3, thus giving a geometric mean of the end points of 1.70 g/cm^3. In Table 5-3, Gee et al. (1994) stated that the typical soil type at the Las Cruces Trench Site is a Berino fine loamy sand. With these two pieces of information and two "rules of thumb" used by Eagleson (1970), we can roughly determine the ***porosity*** (n) and the ***effective porosity*** (n_e) at the site. The following "rules of thumb" were used by Eagleson to analyze the properties of a Touchet silt loam (ρ_s = 2.60 g/cm^3), a Columbia sandy loam (ρ_s = 2.67 g/cm^3), and an unconsolidated sand (ρ_s = 2.71 g/cm^3), where ρ_s is the density of the solid matrix and ρ is the bulk density:

$$n = 1 - \rho/\rho_s , \tag{5-5}$$

$$n_e = n - \theta_r . \tag{5-6}$$

Thus, using a density, ρ_s, of 2.65 g/cm^3 for Berino fine loamy sand and a bulk density of 1.70 g/cm^3 gives a porosity of 0.358 and an effective porosity of 0.275 for the all-layer soil column in Table 5-2.

The radionuclide used in the sensitivity analyses reported in Section 6 and 7 is technetium (^{99}Tc). This species possesses a rather long half-life and is highly mobile in the soil column, as seen by its default value for K_d (0.007 ml/g, as given in U.S. EPA 2000b). The decay coefficient for ^{99}Tc in Table 5-4 is derived from the radionuclide half-life given in Figure 5-1 The daughter product of ^{99}Tc (i.e., ruthenium, ^{99}Ru) is stable, and its decay coefficient is zero. The default values of K_d for ^{99}Ru is 5 ml/g, which indicates that this radionuclide is not very mobile in the soil column. Because of ^{99}Tc's high mobility and long half-life, it possesses many of the characteristics of a conservative species as it moves through the soil column. Conversely, a species such as plutonium (^{238}Pu), with a shorter half-life and a low mobility, may decay before reaching a receptor if the soil column is sufficiently long and facilitated transport does not exist.

The ***dispersion coefficient***, *D*, in the unsaturated zone is given by Hills, et al. (1991) as (also see Equations 2-22 and 2-23):

$$D = \tau_w D_w + D_L |q| / \theta , \tag{5-7}$$

where θ is taken as the initial water content of 0.16 and $|q|$ is the infiltration rate of 8.7 cm/yr. Taking the dispersivity of 4.53 cm given for tritium transport at the Las Cruces Site by Porro and Wierenga (1993), and the above values of θ and $|q|$, gives a value of 0.68 cm^2/d for $D_L |q| \theta^{-1}$. The ***diffusion coefficient in free water*** is assumed to be 1.73 cm^2/d and the tortuosity factor τ_w is taken as 0.19 (Tomasko, et al., 1989). Thus, the value of $\tau_w D_w$ in Equation (5-7) is given as 0.33 cm^2/d. Consequently, the sum of the two terms in Equation (5-7) is given as 1.01 cm^2/d, the value of the dispersion coefficient in Table 5-4.

The HYDRUS and CHAIN 2D Codes have the capacity for accounting for water uptake by plant roots, while the other three models do not have this feature (see Table 2-1). Therefore, ***root water uptake*** was only considered in Appendix F to show its impact on radionuclide movement using the HYDRUS Code. As we have previously stated, the creosote bush (Larrea tridentata) is the dominant plant at the Las Cruces Site. Gile, et al. (1998) indicated that the root depth system of this plant varies with the soil environment and the slope of the terrain; the depth of roots can extend 5 m, or so. Jenkins, et al. (1988) reported that the creosote bush roots at the Las Cruces Site have a vertical distribution over a range of 0.5 m to 3 m. Thus, for demonstration purposes, a ***root distribution*** of 0.5 m to 2.5 m was used in the current study (see Appendix F).