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Information on Hydrologic Conceptual Models, Parameters, Uncertainty Analysis, and Data Sources for Dose Assessments at Decommissioning Sites

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Abstract

This report addresses issues related to the analysis of uncertainty in dose assessments conducted as part of decommissioning analyses. The analysis is limited to the hydrologic aspects of the exposure pathway involving infiltration of water at the ground surface, leaching of contaminants, and transport of contaminants through the groundwater to a point of exposure. The basic conceptual models and mathematical implementations of three dose assessment codes are outlined along with the site-specific conditions under which the codes may provide inaccurate, potentially nonconservative results. In addition, the hydrologic parameters of the codes are identified and compared. A methodology for parameter uncertainty assessment is outlined that considers the potential data limitations and modeling needs of decommissioning analyses. This methodology uses generic parameter distributions based on national or regional databases, sensitivity analysis, probabilistic modeling, and Bayesian updating to incorporate site-specific information. Data sources for best-estimate parameter values and parameter uncertainty information are also reviewed. A follow-on report will illustrate the uncertainty assessment methodology using decommissioning test cases.

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Executive Summary

This report addresses issues related to the analysis of uncertainty in dose assessments conducted as part of decommissioning analyses. The analysis is limited to the hydrologic aspects of the problem. For buried contaminants, this means that the analysis is limited to the pathway involving infiltration of water at the ground surface, leaching of contaminants, and transport of contaminants through the subsurface to a point of exposure.

This report discusses three particular dose assessment codes. The DandD code, with generic parameter values is intended to be used in a generic screening phase of the decommissioning framework. DandD was developed by the NRC specifically for their decommissioning analyses. With site-specific parameter values, DandD may also be applicable in the second, more site-specific phase of the framework for decommissioning. The other two codes discussed are RESRAD and MEPAS. While being applicable to the NRC decommissioning framework, these codes have also been applied to a wide variety of other problems.

The emphasis in this report is on parameter uncertainty, although this is not intended to downplay the importance of uncertainty arising from the suitability of the conceptual models embodied in the dose assessment codes discussed here. The essential simplifications of the conceptual model held in common by the three dose assessment codes examined are: use of a relatively simple model for the near-surface water budget to determine the net infiltration rate, steady-state, one-dimensional flow throughout the system, use of a small number of layers with uniform properties in each layer, and a simple model of mixing in the aquifer. The site-specific conditions under which the codes may provide inaccurate, potentially nonconservative results include: the presence of significant preferential flow in the near surface, significant temporal variation in net infiltration and water content, significant heterogeneity resulting in focused flow or fast transport pathways, and fractured or karst formations.

Although these codes have much in common conceptually, they can nevertheless produce different results when modeling the same problem. This is primarily because of differences in the mathematical implementations of the basic conceptual model shared by the codes.

The hydrologic parameters of DandD, RESRAD, and MEPAS were identified and found to have many similarities. The majority of differences between the parameters of the codes were due to the use of underlying quantities to derive a parameter instead of specifying the parameter directly. The greatest differences were in the physical parameters of the saturated zone related to the point of exposure: location of the well, well depth, and pumping rate.

The importance of a particular parameter in causing uncertainty in dose was defined as the product of the sensitivity of the code's predicted dose to the parameter value and the uncertainty in the parameter (as measured by its coefficient of variation). Under many conditions, it is expected that the distribution coefficients and the net infiltration (or parameters contributing to the net infiltration) will be the most important contributors to dose uncertainty. These results may vary, however, depending on the dose assessment code used and on the specific site conditions. Sensitivity analysis can be used to determine the impact of parameters on uncertainty in dose, but such analysis should include both a delineation of the dose response surface over a parameter's expected range of variation and a statistical sensitivity approach in which multiple parameters are varied simultaneously.

The relationship between best-estimate parameter values, parameter variability, and parameter uncertainty is discussed. Since many of the parameters represent a large scale, they require an average (effective) value and the uncertainty that should be considered in the analysis is the uncertainty of the average value. This is likely to be smaller than the small-scale variability of the parameter at the site. However, since data are often measured at a relatively small scale, while many of the hydrologic parameters represent a site-wide scale, additional uncertainty can be introduced in the process of upscaling from measurements to parameters. This contribution to parameter uncertainty should be considered.

Finally, a variety of data sources are reviewed. These data sources are available to provide estimates of parameter values in the absence of site-specific information. The large national databases can also be used to characterize parameter uncertainty. This is particularly appropriate when there are insufficient site-specific data on which to base parameter uncertainty estimates. Recommended distributions for soil hydraulic parameters are included in appendices and a method to update these distributions using site-specific data is reviewed.

Foreword

This technical contractor report, NUREG/CR-6656, was prepared by Pacific Northwest National Laboratory (PNNL) under their DOE Interagency Work Order (JCN W6933) with the Radiation Protection, Environmental Risk and Waste Management Branch, Division of Risk Analysis and Applications, Office of Nuclear Regulatory Research. The report provides information on hydrologic conceptual models, parameters, uncertainty analysis, and data sources for dose assessments at decommissioning sites. NUREG/CR-6656 is the first report in a series of three contractor reports documenting PNNL's uncertainty assessment methodology, its testing and applications to decommissioning sites.

The PNNL research study was undertaken to support licensing needs for estimating and reviewing hydrologic parameter distributions and their attendant uncertainties for site-specific dose assessment modeling as outlined in NUREG-1549. The PNNL research focuses on hydrologic parameter uncertainties in the context of dose assessments for decommissioning sites. Important hydrologic parameters are identified for commonly-used dose assessment codes (i.e., DandD, RESRAD and MEPAS). The information provided in the report supports the NRC staff's efforts in developing dose modeling guidance. Specifically the report provides: technical bases for estimating and reviewing hydrologic parameter distributions, and conceptual hydrologic model assumptions; understanding hydrologic parameter uncertainties; and identifying data sources for obtaining the "best-estimate" parameter values and uncertainty characterization.

NUREG/CR-6656 is not a substitute for NRC regulations, and compliance is not required. The approaches and/or methods described in this NUREG/CR are provided for information only. Publication of this report does not necessarily constitute NRC approval or agreement with the information contained herein. Use of product or trade names is for identification purposes only and does not constitute endorsement by the NRC or Pacific Northwest National Laboratory.

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Office of Nuclear Regulatory Research

1 Introduction

The final rule specifying radiological criteria for license termination is summarized in Table 1-1. This rule requires estimates of the peak annual dose over a 1000-year period for each site undergoing decommissioning. The analyses needed to evaluate such dose estimates involve some degree of predictive modeling (to estimate future dose). Such predictive modeling is referred to as dose assessment in this report.

U.S. Nuclear Regulatory Commission (NRC) staff have developed a decision-making framework for analyses carried out to comply with the NRC regulations on radiological criteria for license termination. This framework, shown in Figure 1-1, is intended to be a general one, applicable at sites where potential contamination is limited and exposure pathways are simple as well as at sites with greater potential contamination and complex exposure pathways.

It is anticipated that the decision framework will be used in a phased approach. Initial analyses will generally be screening-type analyses using pre-defined models and generic screening parameter values. These models and parameter values were selected to provide a reasonably conservative range of doses. If a site satisfies the license termination criteria using the screening analysis, no further analyses will be required.

If compliance cannot be demonstrated using the generic screening analysis, the models and/or parameter values may be modified. It is anticipated that the application of parameter values and models that reflect actual site conditions will result in less conservative, more realistic dose estimates. Site-specific data are required in this case to demonstrate the appropriateness of the models or parameter values chosen.

Analyses involving predictions of contaminant transport in the environment 1000 years from now are inherently uncertain. The complex exposure pathways of dose assessments adds to this uncertainty. In addition, limitations on the available site-specific data compound the issue. Including an analysis of the impact of this uncertainty on dose estimates seems prudent and is consistent with the NRC's use of a risk-informed approach.

This report addresses issues related to the analysis of uncertainty in dose assessments conducted as part of decommissioning analyses. The analysis is limited to the hydrologic aspects of the problem. For buried contaminants, this means that the analysis is limited to the pathway involving infiltration of water at the ground surface, leaching of contaminants, and transport of contaminants through the subsurface to a point of exposure.

This report discusses three particular dose assessment codes. The DandD code, with generic parameter values is intended to be used in the generic screening phase of the decommissioning framework. DandD was developed by the NRC specifically for their decommissioning analyses. With site-specific parameter values, DandD may also be applicable in the second phase of the framework. The other two codes discussed are RESRAD and MEPAS. While being applicable to the NRC decommissioning framework, these codes have also been applied to a wide variety of other problems. NRC needs with respect to dose modeling for decommissioning and the application of DandD, RESRAD, and MEPAS (as well as other codes) within the context of the NRC decommissioning framework (Figure 1-1) is discussed in Nicholson and Parrott (1998).

The emphasis in this report is on parameter uncertainty, although this is not intended to downplay the importance of uncertainty arising from the suitability of the conceptual models embodied in the dose assessment codes discussed here. Conceptual model uncertainty is the subject of an NRC research project being conducted elsewhere. The conceptual model elements held in common by DandD, RESRAD, and MEPAS are presented in Chapter 2. The purpose of reviewing the conceptual models of these codes is to identify some of the site conditions under which these codes would not be applicable.

Table 1-1. Summary of radiological criteria for license termination (10 CFR Part 20 Subpart E)

	Unrestricted Release[1]	Restricted Release	
Dose Criterion	25 mrem TEDE per year peak annual dose to the average member of the critical group	25 mrem TEDE per year peak annual dose to the average member of the critical group while controls are in place	100 or 500 mrem TEDE per year peak annual dose to the average member of the critical group upon failure of the controls
Time Frame	1000 years	1000 years	1000 years
Other Requirements	ALARA	ALARA, financial assurance, public participation	ALARA, financial assurance, public participation

[1] TEDE: total effective dose equivalent; ALARA: as low as reasonably achievable

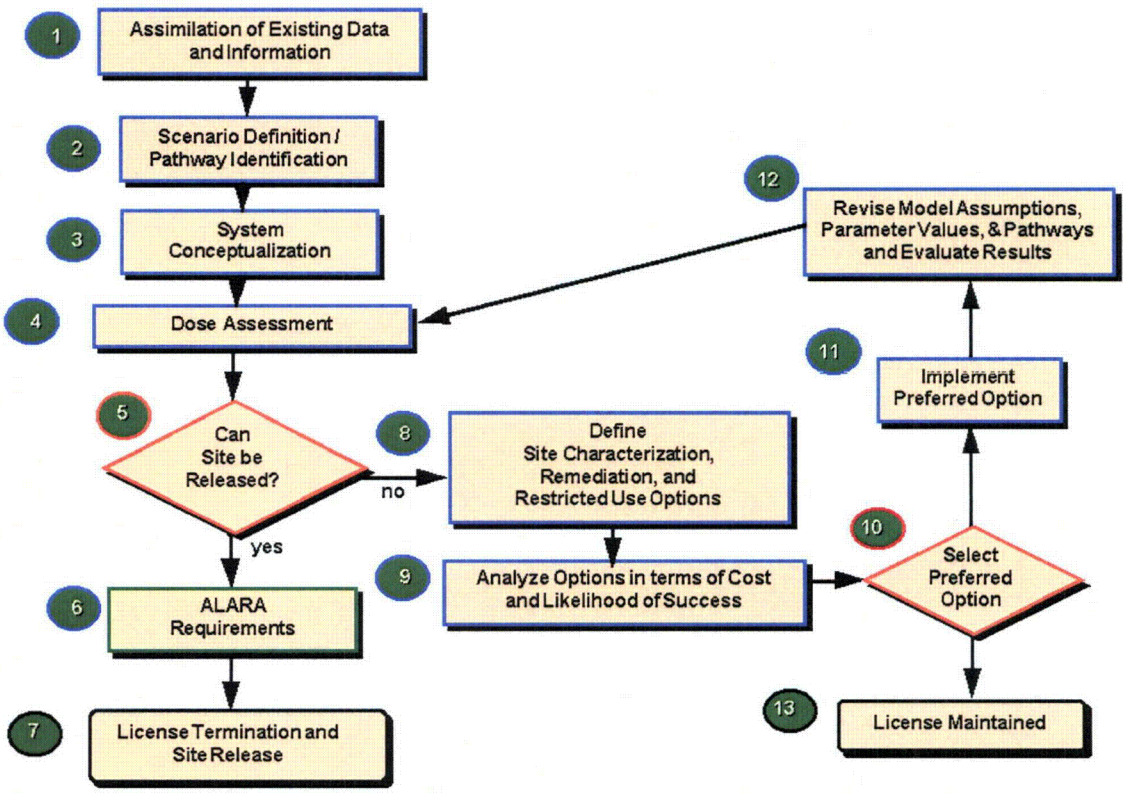

Figure 1-1. NRC decommissioning and license termination decision-making framework (from NRC, 1998)

The hydrologic parameters of the three dose assessment codes are reviewed in Chapter 3. As a result of the similarities in their conceptual models, the codes have many common parameters. Basic differences in parameterization are also identified. Chapter 4 discusses the potential sources of parameter uncertainty and procedures by which to identify those parameters that are likely to be the most important contributors to uncertainty in dose estimates. The report concludes by discussing available data sources for estimating parameter values and parameter uncertainty.

This report builds on methods presented in NUREG/CR-6565 (Meyer et al., 1997). Generic probability distributions for hydrologic parameters related to subsurface flow and transport were recommended in NUREG/CR-6565. In addition, a Bayesian updating method was developed to systematically modify generic probability distributions when site-specific data are available. This report places these methods within the larger context of an uncertainty assessment methodology for decommissioning analyses. This report is the first of two reports that describe and demonstrate the application of this methodology.

2 Summary of DandD, RESRAD, and MEPAS Groundwater Conceptual Models

This chapter discusses the groundwater conceptual models embodied in DandD, RESRAD, and MEPAS, three dose assessment codes that are currently used by NRC staff in their decommissioning analyses. Although the NRC does not require the use of these codes in decommissioning analyses, no other codes are discussed here. In addition to their use by NRC staff, RESRAD and MEPAS are widely used in dose/risk assessments by other federal agencies.

As discussed in the introduction, the NRC's decommissioning decision framework, described in NUREG-1549 (NRC, 1998), provides for an initial level of screening that uses DandD with default parameters and pathways and site-specific source information. The default parameters were chosen to provide calculated doses that are likely to be overestimates, but not necessarily worst-case estimates (Gallegos et al., 1998). In addition to the initial level of screening, DandD, or another code such as RESRAD or MEPAS, can be used with site-specific parameters and pathways to assess the dose. The analysis using site-specific parameter values should provide more realistic and less conservative dose estimates than the application of DandD with default parameters (NRC, 1998).

The code documentation reviewed for this report included NUREG-5512 (Kennedy and Strenge, 1992) containing the mathematical formulations for the DandD code; Gallegos et al. (1998), which discusses the use of DandD within the NRC decommissioning decision framework; Beyeler et al. (1998), which provides justification for the parameter distributions used to determine the default DandD parameters; and a draft version of NUREG/CR-5512 Vol. 3 (Beyeler et al., 1996), which contains the technical basis for identifying the default DandD parameters. The DandD code[1] itself was also reviewed.

For the RESRAD code, the user's manual for version 5.0 (Yu et al., 1993a) and the data collection handbook (Yu et al., 1993b) were reviewed. In addition, version 5.82 of the code and the uncertainty add-in were reviewed[2]. Version 5.91 of RESRAD became available during the preparation of this report. The uncertainty add-in is incorporated in this latest version of the code.

The technical documentation for MEPAS Version 3.2 that was reviewed included Whelan et al. (1996), containing the groundwater pathway formulations; Streile et al. (1996), containing the source term and near-surface hydrology formulations; Buck et al. (1995), a guide to application of the code, including sources of information for selecting parameter values; and Buck et al. (1997), which includes a description of modifications to the code made for the NRC. (Additional information on MEPAS is available at http://mepas.pnl.gov:2080/mepindex.htm.)

No comprehensive comparison of the codes was attempted here. See Cheng et al. (1995) for a benchmarking comparison of RESRAD and MEPAS. Cole et al. (1998) compared the DandD methodology to hybrid codes in which the unsaturated zone or saturated zone component of DandD is replaced with a numerical code. In addition, the NRC is currently conducting a comparison of DandD and RESRAD[3]. For additional comparisons involving RESRAD, see Gnanapragasam and Yu (1997) and Camus et al. (1999).

2.1 Conceptual Model Definitions

Because various definitions of a conceptual model have been proposed, this section takes a moment to describe the components of a groundwater conceptual model and the way in which a conceptual model is used in conjunction with a mathematical model.

The conventional definition of a groundwater conceptual model is a mostly qualitative and often pictorial description of the groundwater system, including a delineation of the hydrogeologic units, the system boundaries, inputs/outputs, and a description of the soils and sediments and their properties. An example of a component of such a conceptual model is shown in Figure 2-1. This figure provides a qualitative description of the geology beneath an underground tank at the Hanford Site. The natural system beneath the tank is complex, consisting of fine to coarse sediments deposited in a heterogeneous manner. Qualitative descriptions of these materials are given. The actual properties of these materials are only estimates derived from a relatively small number of small-scale measurements. The small-scale variations in materials are generally not represented. It is only the large-scale layering that appears in the conceptual model. In the saturated zone, the question marks indicate a high degree of uncertainty in the location of the boundaries between material layers.

Using the definition of a conceptual model given above, a mathematical model can be thought of as a quantitative representation of the conceptual model. Because the mathematical model is quantitative, it can be used to interpret site observations and to make quantitative predictions about the future conditions of the site. As a part of this process, the conceptual model, and consequently the mathematical model also, may be modified to account for new observations. The iterative relationship between field observations, the conceptual model, and the mathematical model is illustrated in Figure 2-2.

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1. DandD is available at http://techconf.llnl.gov/radcri/java.html.

2. The data collection handbook, a draft RESRAD user's guide, and version 5.91 of the code are available at http://web.ead.anl.gov/resrad/.

3. A draft of the DandD/RESRAD code comparison can be found at http://techconf.llnl.gov/radcri/java.html.

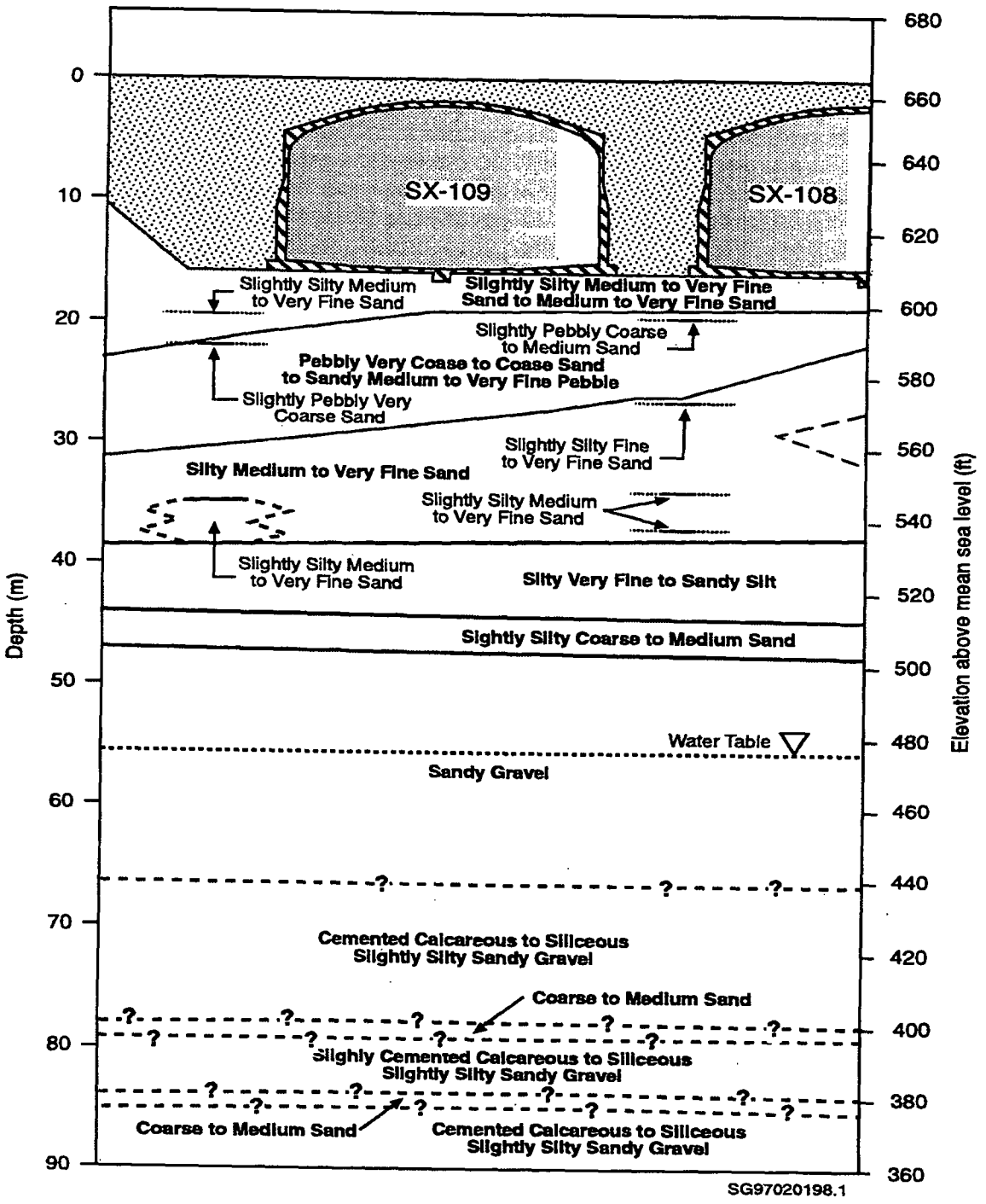

Figure 2-1. Conceptualization of the geology beneath an underground tank on the Hanford Site [taken from Ward et al. (1997), after Price and Fecht (1976)]

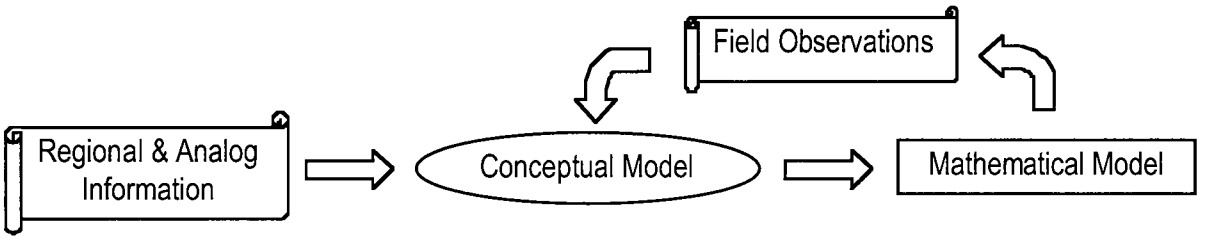

Figure 2-2. Iterative relationship between a conceptual and mathematical model

In translating a qualitative conceptual model into a quantitative mathematical model, it is inevitable that some amount of simplification and compromise will be required. Figure 2-3 provides an example of such simplification. This conceptual model of the geology beneath a Hanford tank farm included sloping interfaces between layers and potential inclusions and discontinuous layers. This conceptualization was represented in a mathematical model as a simplified, layered geology, with homogeneous layers.

A groundwater conceptual model has also been characterized as a hypothesis that describes the main features of the geology, hydrology, and geochemistry of a site, as well as the relationships between these components and the patterns of flow and contaminant transport (NAS, 1996). Figure 2-4 is an illustration of a variety of hypothesized sources and transport pathways potentially important in the transport of tank contaminants to the groundwater at the Hanford Site.

Using this definition of a conceptual model, mathematical modeling can be thought of as a process of hypothesis testing. In this process, the validity of the conceptual model can be evaluated by comparing measurements made at the site to predictions from a mathematical model of the site. Depending on the results of this comparison, the conceptual model (and subsequently the mathematical model) may be modified.

It is clear from these descriptions of conceptual models, that there is not a unique relationship between a conceptual model and its corresponding mathematical model. Given the available field observations and other information such as can be developed from regional data and/or analogous sites, it is possible (perhaps even likely) that a site could be conceptualized in more than one way. Each of these conceptual models could be implemented in a separate mathematical model that might provide significantly different assessments of dose. This concept is illustrated in the upper half of Figure 2-5.

As discussed above, simplifications may be made in implementing a conceptual model as a mathematical model. Decisions about how to simplify (or whether to simplify) the conceptual model could lead to the development of multiple mathematical models, each of which is consistent with the conceptual model. This concept is illustrated in the lower half of Figure 2-5.

As this discussion illustrates, a conceptual model is closely linked to its mathematical implementation. In fact, the underlying conceptual models of DandD, RESRAD, and MEPAS are very similar (as will be discussed in the following section). Their mathematical implementations are different, however, which can lead to significantly different dose estimates under some conditions. This has been illustrated in the comparison studies of the codes (see Cheng et al., 1995, for example).

2.2 Conceptual Model Simplifications of the Dose Codes

The basic conceptual models embodied in DandD, RESRAD, and MEPAS to model transport in the subsurface are discussed in this section, with an emphasis on the similarities between the codes. Specific comparisons with respect to hydrologic parameterization are discussed later in this report.

Each of the codes uses a fairly simplistic representation of flow and transport in the subsurface. A representation of the conceptual model of DandD is shown in Figure 2-6. The system is conceptualized as a series of compartments, one for the contaminated zone, up to ten for the unsaturated zone, and one for the saturated zone. Each compartment has uniform properties. In addition, the unsaturated zone is uniform throughout, regardless of the number of compartments used to model it. Mixing within each compartment is instantaneous. Water withdrawn from the aquifer is used for domestic purposes and is also reapplied to the surface as irrigation. Irrigation and natural infiltration occur at a constant rate.

A corresponding figure for the RESRAD conceptual model of subsurface flow and transport is shown in Figure 2-7. Like DandD, RESRAD uses a series of compartments to represent the contaminated, unsaturated, and saturated zones, with multiple compartments potentially making up

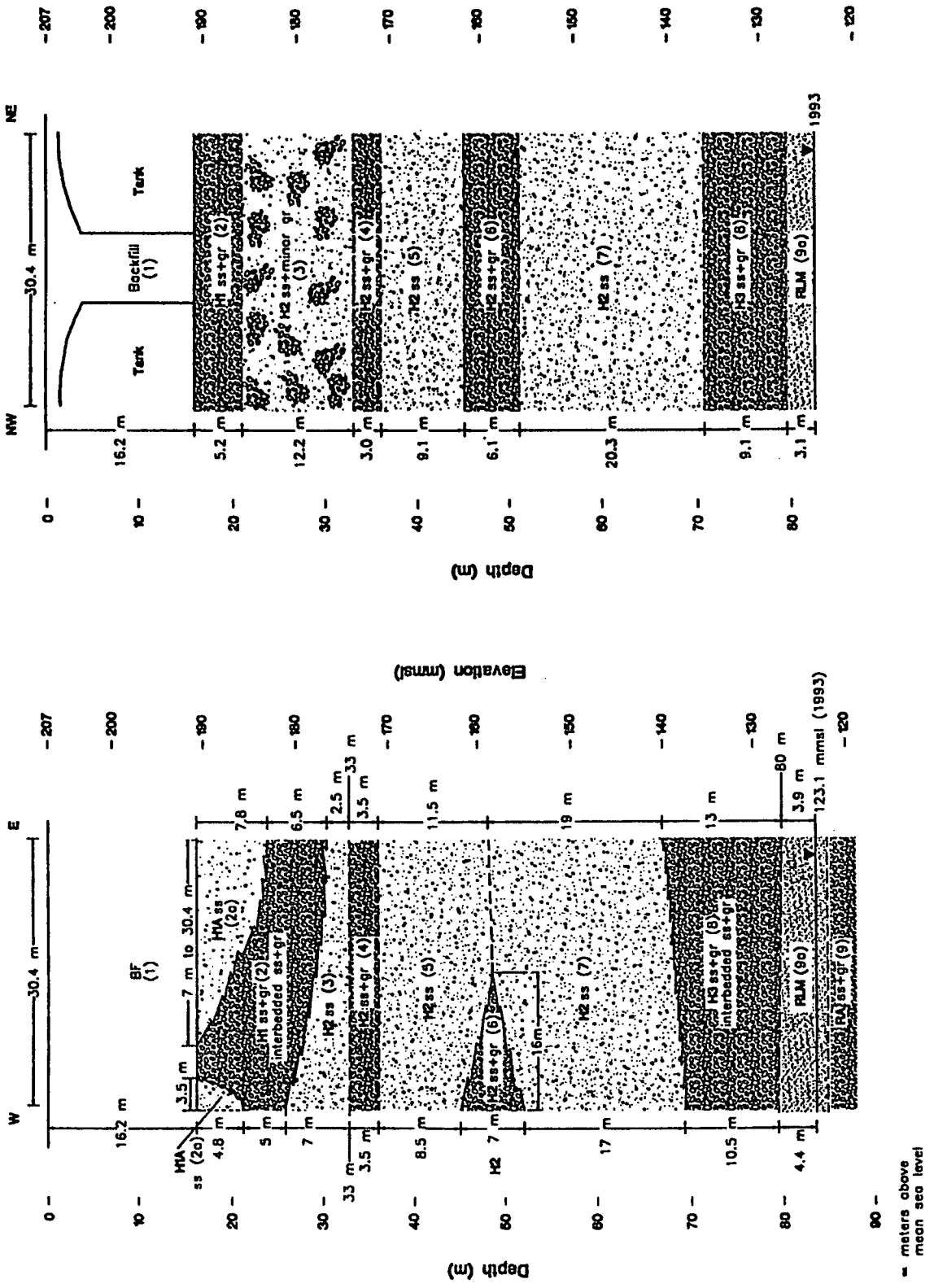

Figure 2-3. A relatively complex conceptual model of geology beneath a Hanford tank farm (left) represented as relatively simple geologic layering in a mathematical model [taken from JEGI (1998), after Piepho et al. (1996)]

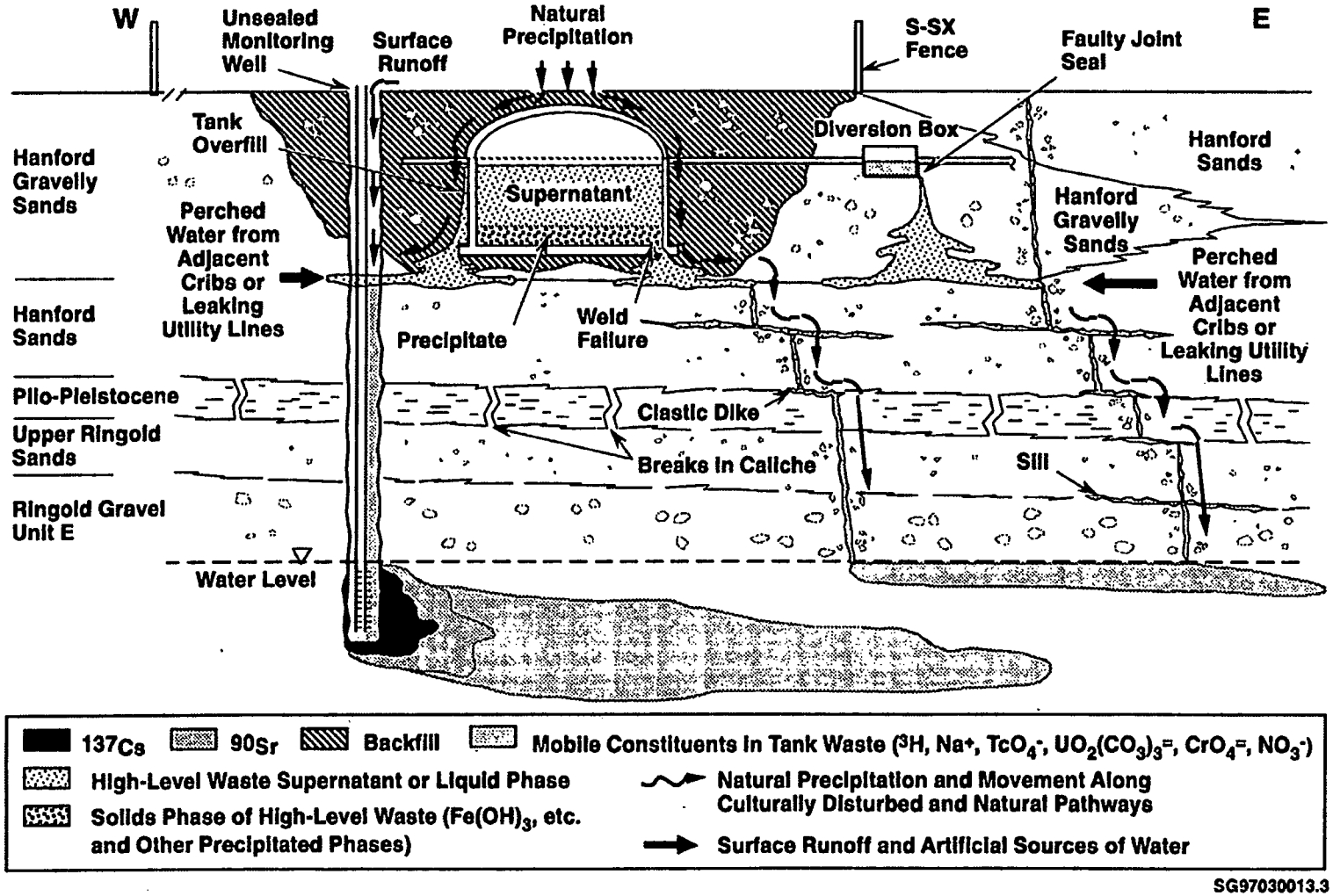

Figure 2-4. Illustration of hypotheses regarding subsurface transport mechanisms beneath one of the tank farms on the Hanford Site [from Ward et al. (1997) after Caggiano et al. (1996)]

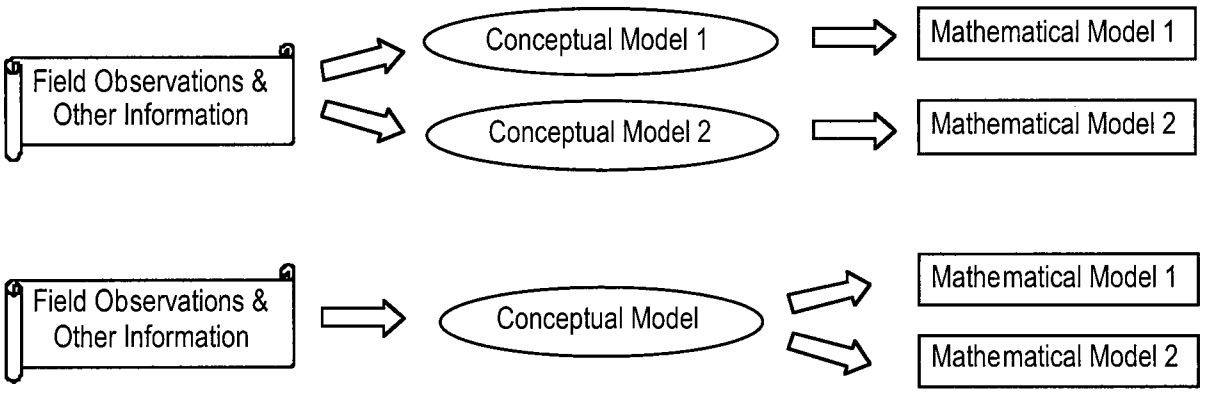

Figure 2-5. Alternative interpretations of field observations and other information may lead to multiple conceptual models (top) while a single conceptual model may be implemented as a mathematical model in more than one way

the unsaturated zone. Each compartment has uniform properties, although the unsaturated zone compartments in RESRAD may each have unique properties, thus allowing a layered model of the unsaturated zone. Transport through each compartment is explicitly modeled (i.e., mixing is not instantaneous) for the nondispersion model of RESRAD. The code also has the option of using a mass balance model in which mixing in the saturated zone is instantaneous and all contaminants are withdrawn through the well. In RESRAD, the withdrawal well is located at the edge of the contaminated area, although a version of RESRAD named RESRAD-OFFSITE is available for modeling a scenario in which the well is farther from the site.

A generalized conceptual model for MEPAS would look very similar to that in Figure 2-7. Like RESRAD, MEPAS allows multiple layers with independent properties in the unsaturated zone. Transport is explicitly modeled in each compartment of the unsaturated zone, including the effects of one-dimensional dispersion. One-dimension advective transport, with three-dimensional dispersion, is modeled in the saturated zone. MEPAS uses the concentration in the groundwater at a specified location as the concentration in water pumped from a well (i.e., there is no dilution due to pumping). The lack of dilution in the well and the use of dispersion are significant differences between MEPAS and RESRAD. Additional differences, such as the implementation of the contaminant source term, may also result in significant differences in predicted dose. Nevertheless, the underlying conceptualization of the two codes is similar.

2.2.1 Summary of Conceptual Model Simplifications Held in Common by the Dose Codes

To summarize, the common simplifying conditions used in DandD, RESRAD, and MEPAS related to flow and transport in the subsurface are listed here.

- Each code uses a relatively simple model for the near-surface water budget to determine the net infiltration rate, i.e., the flow of water through the system that drives the contaminant transport. In DandD the net infiltration is known, in RESRAD the water budget is based on average annual components (precipitation, evapotranspiration, and runoff), and for MEPAS the water budget is based on monthly average components.
- Steady-state flow throughout the system is imposed in each code. The net infiltration required by each code is a constant, average annual value.
- Flow throughout the system is one-dimensional. In addition, advective transport is also one-dimensional in all cases. (MEPAS includes the effect of dispersion, which can be three-dimensional in the saturated zone.)
- Only a small number of layers are allowed in the system and the physical, hydraulic, and chemical properties of each layer must be uniform. No other form of heterogeneity is allowed.
- A fairly simple model of mixing in the aquifer is used. In DandD mixing occurs instantaneously throughout the fixed aquifer volume. For RESRAD and MEPAS the aquifer has infinite lateral extent and a finite and constant thickness.

Although the codes each use a simple model of mixing in the aquifer, there are substantial differences in the way they model aquifer mixing and calculate the exposure concentra-

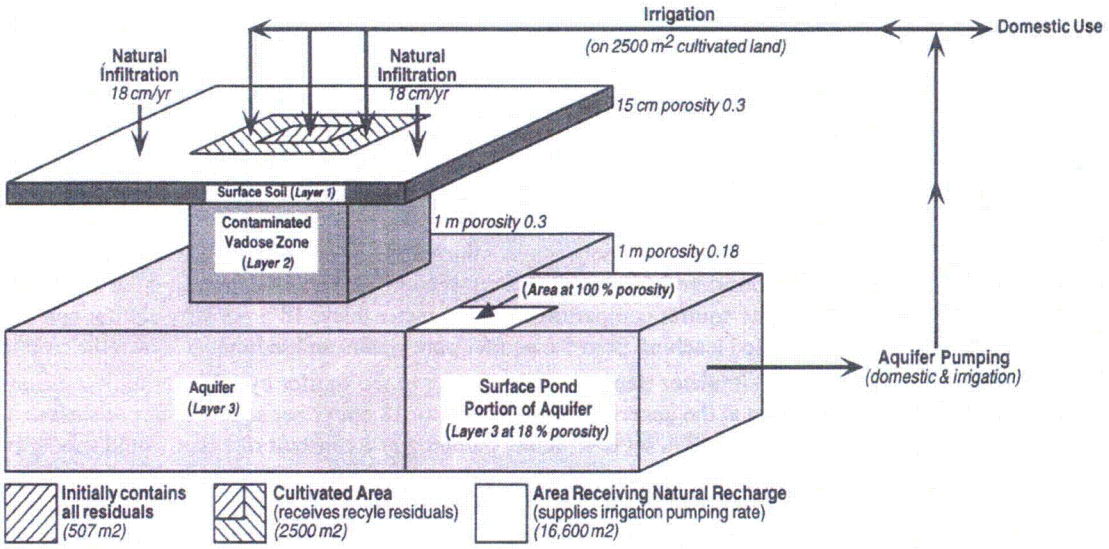

Figure 2-6. Conceptual representation of the hydrologic components of the DandD code for the residential farmer scenario (from Cole et al., 1998, after Kennedy and Strenge, 1992)

tion (i.e., the concentration in the well). These differences can lead to significant differences in the estimated doses.

There are many other simplifications embodied in each of the codes and the user is advised to review the appropriate code documentation for details. (See references given on page 3.)

2.2.2 Site-Specific Conditions Suggesting Cautious Application of the Dose Codes

As a consequence of the simplifications embodied in the dose assessment codes, there are site-specific conditions under which the codes may provide inaccurate, potentially nonconservative results. These conditions include the following.

- The presence of significant preferential flow in the near surface could lead to greater net infiltration than might be anticipated when relying on the simple water budget calculations of the dose codes.
- The imposed condition of steady-state flow will be violated to some degree at all sites. Net infiltration and percolation to the saturated zone vary in time as a result of intermittent precipitation and seasonal changes in evapotranspiration and precipitation. The contaminant flux may be affected as a result of temporal variation in net infiltration and water content. In addition, transient flow conditions may affect transport in the unsaturated zone.
- Significant heterogeneity in physical, hydraulic, or chemical properties may result in two- or three-dimensional flow patterns. Contrasting properties that result in focused flow and fast transport paths may produce conditions under which the dose codes predict nonconservative results.
- Subsurface conditions under which flow and transport are significantly influenced by fractures or karst formations clearly contradict the simplified conceptual models of the dose assessment codes. Because of the potential for fast transport of contaminants under these conditions, the codes may produce nonconservative results.

This list of conditions that run counter to the simplifications of the dose assessment codes is not intended to be all-inclusive. However, it does include the most prevalent conditions that are not represented in the conceptual models of DandD, RESRAD, and MEPAS and that could potentially result in nonconservative performance of these codes.

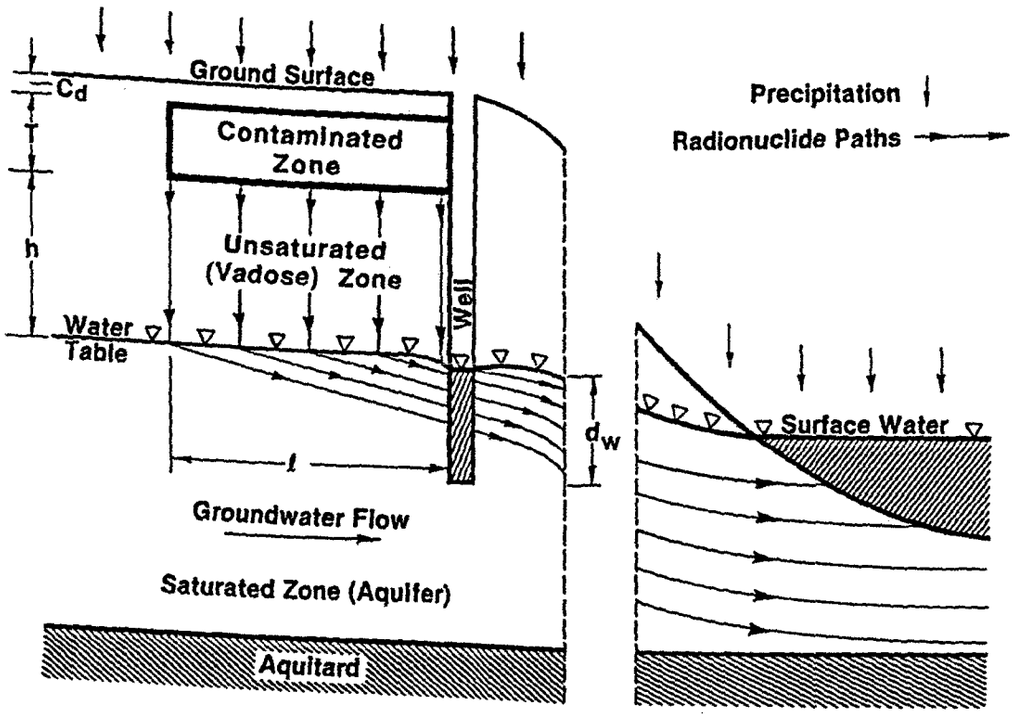

Figure 2-7. RESRAD conceptual representation of the subsurface transport pathways (from Yu et al., 1993a)

3 Hydrologic Parameters of the Dose Codes Related to the Groundwater Pathway

The previous chapter discussed similarities in the conceptual models of DandD, RESRAD, and MEPAS. This chapter looks at the parameters used by these codes as part of their calculation of transport through the groundwater pathway. Not surprisingly, the codes have many parameters in common.

Since this report is concerned primarily with the analysis of uncertainty in parameter values, one of the first steps is to identify the parameters of the dose assessment codes that potentially contribute to the uncertainty in dose. Since we are interested here only in the hydrologic aspects of the subsurface pathway, the parameter set is limited. These include near-surface hydrologic (i.e. water budget) parameters, which determine the flux of water into the subsurface; contaminated zone parameters, which determine the contaminant flux; and unsaturated/saturated zone flow and transport parameters. In addition, there are a number of physical parameters related to exposure scenarios, such as well depth, that interact with the hydrologic models. The hydrologic parameters of each dose assessment code are identified and discussed in the remainder of this chapter and are listed in Table 3-1.

3.1 Near-Surface Water Budget Parameters

The near-surface hydrologic parameters determine the flux of water through the contaminated and unsaturated zones. The codes refer to this as the infiltration rate, but it is more accurately called net infiltration since it is the rate of water flowing beyond the influence of the surface and plant roots. A basic water budget is solved:

$$I = P - (RO + ET) \quad (1)$$

where I is net infiltration, P is precipitation (potentially including irrigation), RO is runoff, and ET is evapotranspiration from plants (including evaporation from the soil surface).

For DandD, the annual average (net) infiltration is specified directly by the user and includes the contributions from precipitation and irrigation. Since the code models each zone of the site (contaminated zone, unsaturated zone, and saturated zone) as a well-mixed compartment (or up to ten compartments for the unsaturated zone), the irrigated area is also required to determine the total amount of water moving through the site on an annual basis. The irrigation rate is used to determine the amount of (possibly contaminated) groundwater applied at the surface and is also used in calculating the total volume of water in the aquifer (Beyeler et al., 1998).

For RESRAD, the user does not directly specify the annual average net infiltration. Rather, it is calculated as the sum of precipitation and irrigation minus some fraction of the total applied water allocated to evapotranspiration and runoff, as specified by the user through evapotranspiration and runoff coefficients. In other words, the runoff and evapotranspiration components of Equation 1 are specified by the user as fractions of the available water.

With MEPAS, the user may either directly specify the annual average net infiltration or have the code calculate it using an empirically-based water budget model. Monthly average precipitation is required. The average monthly maximum (potential) evapotranspiration is calculated using monthly average climatic parameters (air temperature, relative humidity, wind speed, percent cloud cover, and solar radiation). Actual evapotranspiration includes the effect of user-specified soil and vegetation parameters. The runoff component requires the Soil Conservation Service curve number.

Although MEPAS uses monthly average meteorological values in its water budget calculation, like the other three codes it uses an annual average net infiltration in its transport calculations.

At an actual decommissioning site, the presence of a surface cover, the properties of the soils comprising the cover, and the nature of the cover vegetation will have a marked influence on the net infiltration through the cover. Since DandD requires the direct input of the net infiltration, the effect of a cover on the infiltration rate needs to be estimated by the user in a process external to DandD. In a similar manner, the user of RESRAD is required to conduct an external analysis to estimate the effect of the cover on the water budget components of Equation 1. The cover-related parameters of RESRAD, such as the cover thickness and the rooting depth, influence the external radiation dose and the water-independent dose from plant ingestion, but they do not directly influence the water-dependent pathways. In MEPAS, the cover-related parameters (SCS curve number and top-soil water capacity) do affect the calculated net infiltration.

3.2 Contaminated Zone Parameters

The three dose assessment codes use similar models for leaching of contaminants due to infiltrating water. These models require the contaminated zone volume, bulk density, porosity, and water content. In addition, the distribution coefficient for each contaminant is required.

DandD uses a fixed area of contamination and thus the contaminated zone area is not included as an input parameter. DandD also uses the relative saturation of the contaminated zone instead of the water content. The relative saturation is the ratio of water content to saturated water content. In DandD, the saturated water content is equal to the porosity.

Table 3-1. Hydrologic flow and transport parameters of DandD, RESRAD, and MEPAS for residential farmer scenario, groundwater pathway

	DandD	RESRAD	MEPAS
Near-Surface Hydrology	annual infiltration annual irrigation area irrigated	annual precipitation annual irrigation evapotranspiration coefficient runoff coefficient	annual infiltration monthly precipitation monthly temperature monthly wind speed monthly maximum relative humidity monthly minimum relative humidity monthly cloud cover monthly number of days with precipitation SCS curve number top-soil water capacity
Contaminated Zone	thickness bulk density porosity relative saturation distribution coefficients	thickness area length parallel to flow bulk density porosity effective porosity saturated hydraulic conductivity soil-type exponent distribution coefficients	thickness length width bulk density porosity water content distribution coefficients
Unsaturated Zone	thickness bulk density porosity relative saturation # unsaturated zone layers distribution coefficients	thickness bulk density porosity effective porosity field capacity saturated hydraulic conductivity soil-type exponent # unsaturated zone layers distribution coefficients	thickness bulk density porosity field capacity saturated hydraulic conductivity soil-type exponent dispersivity (vertical) # unsaturated zone layers distribution coefficients
Saturated Zone		bulk density porosity effective porosity saturated hydraulic conductivity hydraulic gradient distribution coefficients (soil-type exponent, field capacity)	thickness bulk density porosity effective porosity Darcy velocity dispersivities (in 3 dimensions) distribution coefficients
Saturated Zone Physical Parameters Associated with Exposure	annual domestic water use volume of surface water pond	depth of well well pumping rate	depth of well distance to well well offset from plume centerline

RESRAD does not use the contaminated zone water content directly as an input parameter. Instead, the code calculates the water content using a relationship between water content and hydraulic conductivity presented by Campbell (1974). This calculation requires a soil-type exponent and also imposes the condition that unsaturated flow in the contaminated zone occurs solely due to gravity (i.e., the assumption of unit gradient flow).

Actual contaminant fluxes used by each code may vary due to the use of different models the dependence of the leaching rate on time.

3.3 Unsaturated Zone Parameters

The unsaturated zone parameters govern the rate of transport through the unsaturated zone. These parameters include the number of layers and the thickness of each layer. In addition a number of parameters are required for each layer. These are the bulk density, porosity, water content, and distribution coefficients for each contaminant.

DandD models the unsaturated zone as a series of well-mixed compartments. Although up to ten compartments can be used for the unsaturated zone, each compartment must have the same set of properties. As discussed in Cole et al. (1998), the number of unsaturated zone compartments is related to the effective longitudinal dispersivity. Cole et al. (1998) demonstrate that the approach used in DandD can reproduce results obtained using a numerical model for the unsaturated zone component (under homogeneous conditions). As in the contaminated zone, DandD uses the relative saturation instead of the water content.

RESRAD and MEPAS use semi-analytical solutions for contaminant transport in the unsaturated zone. Multiple layers with unique parameter values in each layer are allowed. RESRAD and MEPAS calculate the unsaturated zone water content using the relationship between hydraulic conductivity and water content developed by Campbell (1974). This requires specification of the saturated hydraulic conductivity and the soil-type exponent (and imposes unit gradient flow). The field capacity provides lower limit for the water content.

RESRAD does not model dispersion (the nondispersion model), while MEPAS allows longitudinal dispersion in the unsaturated zone.

RESRAD and MEPAS allow distribution coefficients to vary between each layer of the unsaturated zone. DandD requires that the distribution coefficient for each contaminant be constant throughout the unsaturated zone and that it have the same value it does within the contaminated zone.

3.4 Saturated Zone Parameters

The saturated zone parameters govern the transport of contaminants in the saturated zone. These parameters include the bulk density, porosity, effective porosity, the specific discharge (Darcy velocity), and the distribution coefficients for each contaminant.

DandD models the saturated zone compartment as another well-mixed compartment; this does not involve any transport modeling.

RESRAD has an option to use a Mass Balance model for the saturated zone, which imposes the condition that all of the contaminants reaching the saturated zone are withdrawn through a well. In this case, the concentration in the well is equal to the concentration in the aquifer. This option is similar to the model used in DandD.

For the nondispersion model, RESRAD represents the saturated zone in an essentially geometric manner, with the well (through which exposure occurs) located at the downgradient edge of the facility. The specific discharge is calculated as the product of the saturated hydraulic conductivity and the hydraulic gradient. (The code requires a soil-type exponent and field capacity for the saturated zone, but it is not apparent how these parameters are used.)

MEPAS solves a form of the three-dimensional advection-dispersion equation in the saturated zone, which allows the well to be placed at any location, although the solution is more accurate when the well is not too close to the facility. MEPAS uses the specific discharge as an input parameter (as the Darcy velocity). Three-dimensional dispersion in the saturated zone is modeled in MEPAS thus requiring longitudinal and two transverse dispersivity values.

3.5 Saturated Zone Physical Parameters

A number of parameters are required by the codes to translate contaminant concentrations in the aquifer into concentrations in the well. These parameters include the effect of mixing in the aquifer, well placement, and well pumping.

DandD uses the annual domestic water use and the volume of the surface water pond (along with the annual irrigation) to calculate the total volume of water in the aquifer. This is necessary to determine the concentration in the aquifer, which is also the concentration in the well.

The RESRAD nondispersion model places the well along the downgradient edge of the contaminated zone at the point of maximum contaminant concentration in the aquifer. RESRAD requires the depth of the well and the well pumping rate to determine dilution in the well and potentially the maximum travel time of contaminant in the saturated zone.

For the mass balance model of RESRAD, only the pumping rate is required to calculate the dilution since for this model all of the contaminated water is withdrawn through the well.

MEPAS allows the well to be placed at an arbitrary location in three dimensions, including at a point not on the centerline of the contaminant plume. This requires the user to input the well depth, the downgradient distance to the well, and the distance of the well from the plume centerline.

MEPAS does not dilute the aquifer concentration in the well, however, and therefore does not use the well pumping rate.

Differences in the way the codes model mixing in the aquifer and concentrations in the well can lead to substantial differences in estimated doses. This issue is not addressed in this report, but deserves further study.

4 Hydrologic Parameter Uncertainty

The NRC's criteria for license termination require an estimate of dose from a site (Federal Register, 1997). This dose will be estimated from site characteristics using a computer code that embodies source-term, environmental transport, and exposure models. In the context of decommissioning analyses, the NRC's risk-informed approach to regulatory decision-making suggests that an assessment of the uncertainty in the dose estimate produced by the code(s) is appropriate.

For decommissioning, the goal of an uncertainty analysis is to estimate the uncertainty of the desired code output, that is, maximum annual total effective dose equivalent within the first 1000 years after decommissioning (Federal Register, 1997). In addition, the relative contribution of uncertainty in the model input parameters to the overall uncertainty in dose should be determined. Those parameters that contribute the most to the uncertainty in dose can be targeted for site-specific sampling and a more detailed analysis of their uncertainty.

It is assumed in the discussion here that there are no site-specific measurements of contaminant concentrations in the vadose zone or groundwater. If such measurements are available, then a calibration exercise or a formal inverse procedure should be part of the process to estimate parameter values and uncertainties.

4.1 Relevance of Parameter Uncertainty

The importance of a particular parameter to the uncertainty in the results of a dose calculation depends on two factors: the actual uncertainty in the parameter value and the sensitivity of the code to the parameter value. The importance of a parameter will be the greatest when the value of the parameter is relatively uncertain and the dose predicted by the code is sensitive to the parameter's value. The importance of the parameter will be low when either the code's results are insensitive to the parameter value or the value of the parameter is known precisely. These intuitive concepts are consistent with the approach used for the proposed high-level waste repository (NRC, 1999) and can be described using the following relationship. [See Morgan and Henrion (1990) for a more complete discussion of these concepts.]

Importance of Parameter to Uncertainty in Dose	$\propto$	Uncertainty in Parameter Value	$\times$	Sensitivity of Code Results to Parameter Value

A graphical representation of this relationship is shown in Figure 4-1.

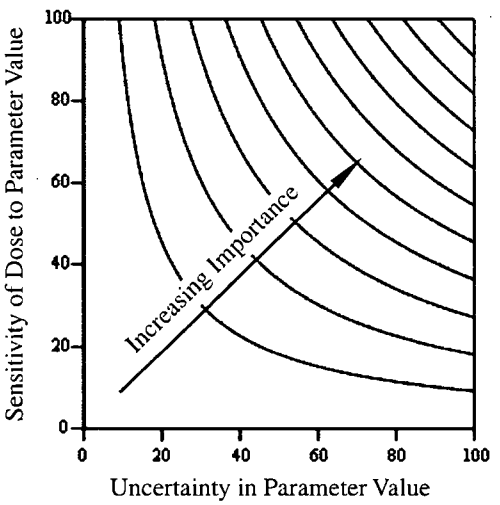

Figure 4-1. Relationship between parameter uncertainty, sensitivity, and the importance of the parameter to uncertainty in dose predictions

Dependencies between parameters and nonlinear relationships between parameters and the output(s) of a dose code may make it difficult to apply the above relationship in a quantitative manner. Note also that the importance of a parameter may be a function of which pathways are included in a dose assessment. These caveats notwithstanding, the relationship is at least useful in a qualitative sense.

4.1.1 Sources of Uncertainty

There are potentially many sources of uncertainty when conducting dose assessment modeling and the reader should consult a general reference such as Morgan and Henrion (1990). In this section we are concerned only with the primary contributors to the uncertainty in the hydrologic parameters of the dose codes discussed in Chapter 3. These primary sources of uncertainty can be classified as variability and lack of knowledge.

4.1.1.1 Variability

The natural variability of many hydrologic properties is a primary contributor to parameter uncertainty. This variability may be spatial as is the case with many soil hydraulic parameters. Figure 4-2 is a histogram of the natural logarithm of saturated hydraulic conductivity measured on 92 samples from several boreholes and shallow excavations at a site in Nevada (Andraski, 1996). On the relatively small

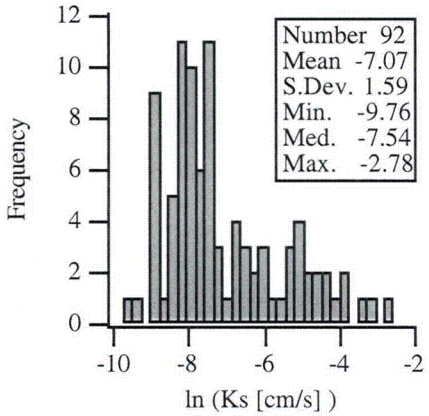

Figure 4-2. Spatial variability of saturated hydraulic conductivity at the Amargosa Desert Research Site near Beatty, Nevada as reported by Andraski (1996)

scale of these measurements, this parameter varies over several orders of magnitude.

A hydrologic process or parameter may also vary in time. Figure 4-3 shows the temporal variability in drainage (net infiltration or percolation) as measured in four lysimeters at a site near Coshocton, Ohio. Yearly drainage varied from 0 to more than 60 cm/yr over this 50-year period. This variability in drainage can be attributed to temporal variability in precipitation and other meteorological conditions as well as changes in vegetation. Although the four lysimeters are located adjacent to each other, the yearly drainage also exhibits spatial variability due to differences in vegetation and soil properties.

4.1.1.2 Lack of Knowledge

In addition to natural variability, parameter uncertainty may arise from the presence of inaccurate, unrepresentative, or limited data. This source of uncertainty can be characterized, in general, as a lack of knowledge. As an example, consider the distribution of saturated hydraulic conductivity values measured at the site in Nevada (see Figure 4-2). If only three or four measurements were made at this site, it would not be difficult to arrive at inaccurate values of the average value of hydraulic conductivity at the site and its variance. Similarly, if lysimeter measurements were only available from 1960-1970 for the site in Figure 4-3, the variability of the drainage at this site would likely be underestimated.

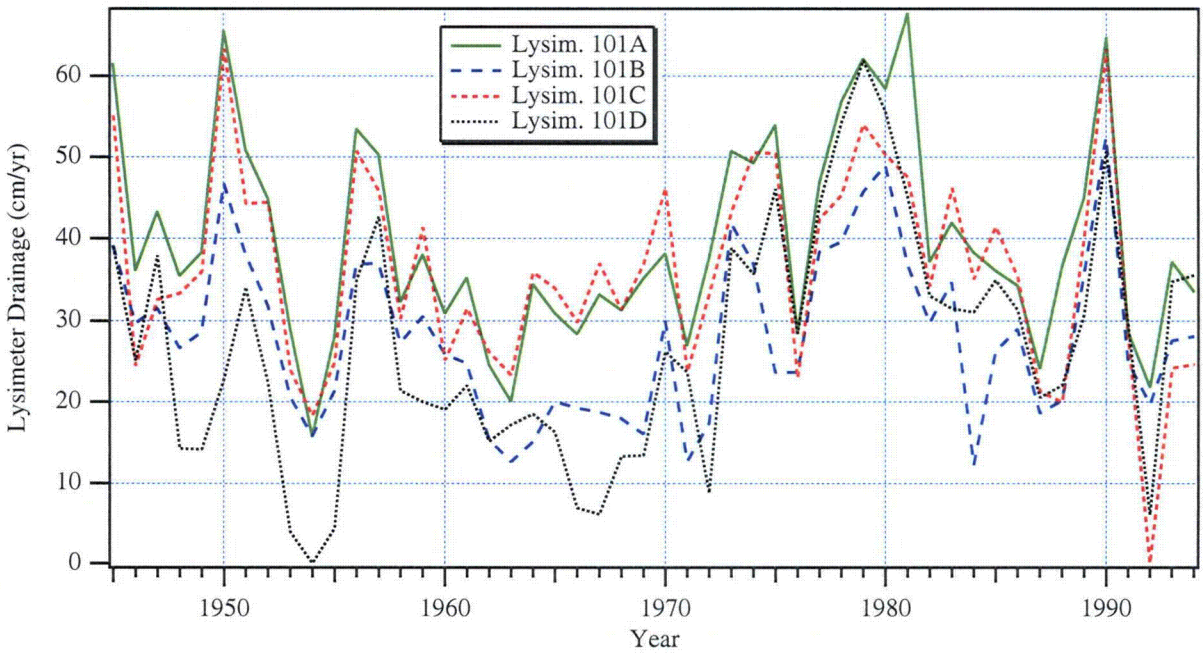

Figure 4-3. Yearly drainage measured in four lysimeters at a site on the North Appalachian Experimental Watershed near Coshocton, Ohio

4.1.2 Sensitivity Measures

The results of a dose assessment code (as measured by peak dose in 1000 years, for example) can be expected to vary as a function of the values of the input parameters. This reflects the fact that the actual contaminant transport behavior depends on the properties of the soil/groundwater system. In general, sensitivity refers to the magnitude of this dependency, that is, the degree to which the results of a code depend on the value of its input parameter(s).

The relationship between the results of a code and the value of its input parameter(s) is referred to as a response surface (Myers and Montgomery, 1995). An example of a single-parameter response surface from RESRAD is shown in Figure 4-4. This figure shows the results for peak (total) dose from all pathways as a function of the plant rooting depth for a realistic (but hypothetical) decommissioning analysis. (Note that the dose occurs via water-independent pathways in this example.) The response surface was derived by calculating the peak dose for a range of rooting depths (indicated by the open circles). This concept is generalizable to multiple input parameters, although for more than two input parameters, a response surface is difficult to depict graphically.

The most common measure of sensitivity evaluates the slope of the response surface at a given point. For example, the sensitivity of peak dose to rooting depth at point A in Figure 4-4 could be written as

$$Sensitivity = \left.\frac{\partial(PeakDose)}{\partial(RootingDepth)}\right|_A \qquad (2)$$

When multiple parameters with widely varying magnitudes are included in a sensitivity analysis, the output and input parameters in Equation 2 can be normalized by their values at the point where the sensitivity is calculated. This makes the sensitivities calculated for multiple input parameters more comparable.

The calculation of sensitivities using Equation 2 provides a local measure only and the results should not be interpreted to apply over the entire potential range of the input parameter. In Figure 4-4, for example, the local sensitivity at point A is nearly zero, while at point B the sensitivity is significant. With multiple input parameters this effect is compounded because the sensitivity of dose to a particular input parameter such as rooting depth may also depend on the values of the other input parameters. A typical analysis that calculates sensitivity to each input parameter while holding all remaining parameters at their nominal (baseline) values will not discover these dependencies.

The effect on dose calculations of interactions between input parameters can be seen by simultaneously varying the values of multiple parameters. This can be done systematically by selecting a set of values for each parameter and calculating the dose for all combinations of parameter values. The simplest version of this method is a bounding analysis in which the set of values for each parameter consists of the upper and lower bounds. The calculations required increase quickly with the number of parameters and parameter values included in the analysis.

As an alternative to enumerating all combinations of parameter values, a statistical approach could be used. Parameter values and their combinations can be randomly generated

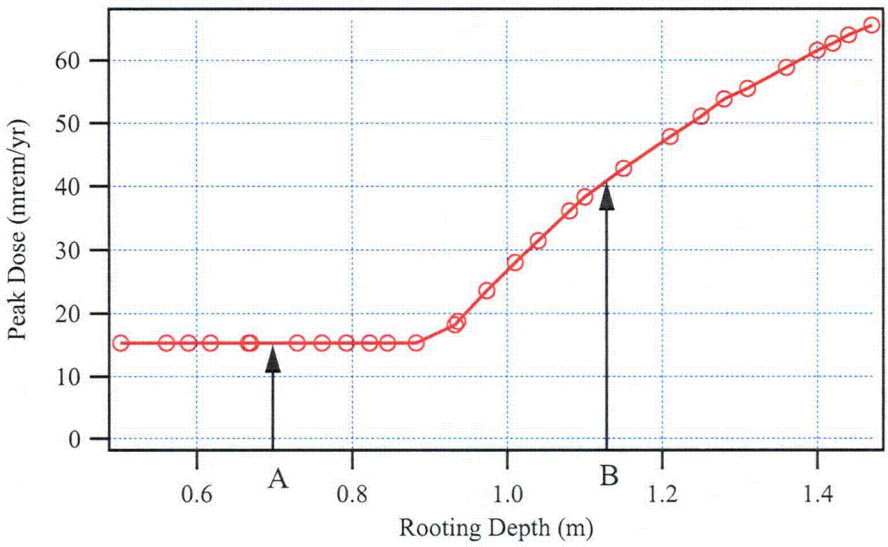

Figure 4-4. Response surface for a RESRAD calculation showing peak dose as a function of rooting depth

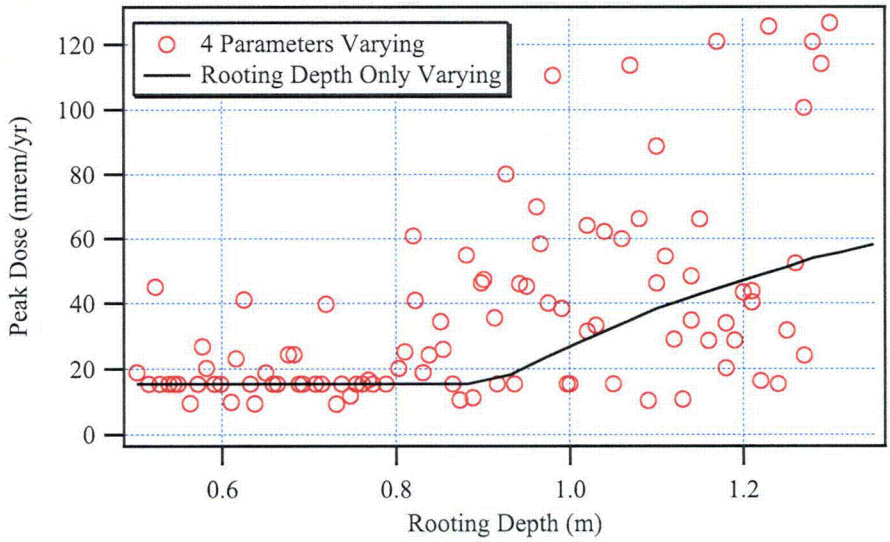

Figure 4-5. Example RESRAD results for a Monte Carlo simulation with four input parameters varying. The results from Figure 4-4 with only the rooting depth varying are shown for comparison.

using the Monte Carlo simulation capabilities of RESRAD and MEPAS. Iman et al. (1978) developed a method in which a linear response surface model was fit to the Monte Carlo simulation results, with the fitted parameters of this linear model (the standardized partial regression coefficients) representing measures of sensitivity. Doctor et al. (1990) adopted this approach for a sensitivity analysis of MEPAS, but used the partial R^2 (partial coefficient of determination) values calculated from the Monte Carlo simulation to estimate relative sensitivities. The partial R^2 for an input parameter is a measure of the fraction of the total variance of the output attributable to that input parameter. When using its Monte Carlo simulation feature, RESRAD reports partial correlation coefficients. These measure the correlation (linear relationship) between dose and each individual input parameter and also provide a relative measure of parameter sensitivity.

Figure 4-5 shows the results from the RESRAD example of Figure 4-4, with an additional three parameters varying simultaneously (^{14}C distribution coefficient, cover erosion rate, and cover depth). The results from Figure 4-4 are included for comparison. The inclusion of the additional parameters results in a scattered relationship between peak dose and the rooting depth. The partial correlation coefficient for this relationship is 0.54, reflecting a moderate linear relationship. As observed in Figure 4-4, however, the relationship between dose and rooting depth is nonlinear. This nonlinearity causes a reduction in the partial correlation coefficient for the rooting depth. Other measures of sensitivity that rely on a linear model, such as the partial R^2 values and the standardized partial regression coefficients, can have the same problem. For this reason, it is always instructive to understand the single parameter relationship as represented in Figure 4-4.

The results shown in Figure 4-5 illustrate the potential effect of interactions between input parameters. When multiple parameters are included in the analysis, the peak doses follow the same general pattern as the results obtained while varying only the rooting depth. That is, the dose tends to be lower and relatively constant when the rooting depth is less than about 0.9 and the dose tends to increase with larger rooting depths above this point. The actual values of the peak dose, however, can be significantly different (both larger and smaller). For this example, this is primarily because the peak dose is also sensitive to the cover depth (partial correlation coefficient of -0.65). In this example, the cover depth and rooting depth were uncorrelated. Correlation among these input parameters may modify their combined effect on dose.

Combining the use of probabilistic and deterministic measures of sensitivity, such as described in this section, is consistent with the analyses conducted for the proposed high level waste repository at Yucca Mountain, Nevada (NRC, 1999).

4.2 Evaluation of DandD, RESRAD, and MEPAS Hydrologic Parameters

For any given analysis, the actual parameters that will exhibit the greatest uncertainty at a particular site and the

sensitivity of the dose to parameter values will vary. It is thus impossible to conclusively identify the parameters that will be the most important to include in an uncertainty analysis conducted as part of a dose assessment. Nonetheless, some general observations can be made.

4.2.1 Relative Uncertainty of Parameters

Based on a review of the literature and available databases, it is possible to identify the relative magnitude of uncertainty for the hydrologic parameters identified in Chapter 3. The measure of uncertainty used here is the coefficient of variation, defined as the standard deviation divided by the mean value.

Distribution coefficient values are often highly uncertain due to their strong sensitivity to site-specific conditions and the fact that the use of a linear equilibrium adsorption model may represent an oversimplification of a number of complex processes. The net infiltration rate will also often have a high degree of uncertainty as a result of its temporal and spatial variability and its dependence on a variety of complex processes (climate, runoff, plant growth). Saturated hydraulic conductivity is generally highly uncertain due to its spatial variability. Dispersion (as represented by the dispersivity) is often highly uncertain, but due primarily to a lack of knowledge. The saturated zone physical parameters associated with exposure (see Table 3-1) are also highly uncertain due to a lack of knowledge regarding the future exposure scenarios.

Parameters that generally exhibit a moderate degree of uncertainty include the Darcy velocity, water content in the unsaturated and contaminated zones, the soil-type exponent, and the field capacity. Parameters with a relatively low degree of uncertainty (due to a limited range of variability) include porosity, effective porosity, bulk density, and the unsaturated zone thickness. Under some circumstances, such as a shallow, fluctuating water table, uncertainty in the unsaturated zone thickness may be greater.

4.2.2 Relative Sensitivity of Parameters

The sensitivity of the dose codes to their parameter values will be a function of the specific site conditions and exposure scenarios. The techniques discussed in Section 4.1.2 should be used in each application to understand the code response and sensitivities. This section reviews results from generic sensitivity analyses that have been performed on DandD, RESRAD, and MEPAS. Although the results of a generic sensitivity analysis may not apply to a site-specific application, it is nonetheless instructive to review the available studies.

Cole et al. (1998) examined the sensitivity of the NUREG/CR-5512 formulations to a variety of hydrologic parameters. The largest and most consistent sensitivity (over all contaminants examined) was to the infiltration rate, irrigation rate, the irrigated area, and the unsaturated zone thickness. The code also exhibited a significant sensitivity to the number of unsaturated zone layers, particularly for thicker unsaturated zones. Beyeler et al. (1998) looked at the sensitivity of the DandD code to a variety of parameters. The greatest sensitivity was to the distribution coefficients, the infiltration rate, the unsaturated zone thickness, and the unsaturated zone porosity, bulk density, and relative saturation.

Cheng et al. (1991) conducted a sensitivity analysis using an early version of RESRAD. The dose predicted by the code for an example problem was shown to be sensitive to a number of hydrologic parameters, including the precipitation and irrigation rates, the evapotranspiration and runoff coefficients, the thickness of the unsaturated zone, porosity, effective porosity, bulk density, distribution coefficients, and the depth of the well.

Doctor et al. (1990) conducted a sensitivity analysis using an early version of the MEPAS code. The Hazard Potential Index was calculated for an example problem and was found to be most sensitive to distribution coefficients, precipitation, saturated zone Darcy velocity, unsaturated zone thickness, contaminated area, and unsaturated zone bulk density, soil type, and porosity.

4.2.3 Relative Importance of Parameters in an Uncertainty Analysis

The relative importance of the dose assessment code hydrologic parameters in an uncertainty analysis is represented qualitatively in Table 4-1. As discussed in Section 4.1, the most important parameters to consider in an uncertainty analysis are those that (1) are most uncertain and (2) can significantly impact the dose calculations within their range of possible variation. Table 4-1 is a generalized representation of uncertainty importance and may not be applicable to a site-specific analysis. A similar table could be developed for any site-specific analysis, however, along with the technical references and analyses used to justify the importance of each parameter.

Table 4-1. Generalized relative importance of dose assessment code parameters in an uncertainty analysis. Results for a specific application may vary.

		Uncertainty Due to Variability and/or Lack of Knowledge		
		Low	**Medium**	**High**
Model Sensitivity	**High**	UZ Thickness		Distribution Coefficients Net Infiltration Rate
	Medium	Effective Porosity Bulk Density	Darcy Velocity Unsaturated Water Content	SZ Exposure Parameters SZ Hydraulic Conductivity
	Low	Porosity	Soil-Type Exponent Field Capacity	UZ Sat. Hydraulic Conductivity Dispersivity

5 Data Sources for Best-Estimate Parameter Values and Uncertainty Characterization

This chapter discusses the potential sources of information that can be used to provide best estimates of parameters and also to characterize parameter uncertainty.

5.1 Best Estimates and Uncertainty

"Best estimate" is a descriptive term and is used here to refer to the parameter values that best represent the actual site properties. The best-estimate parameter values should, in the judgement of the analyst, provide the most accurate representation of the flow and transport behavior of the site.

Since the DandD, RESRAD, and MEPAS codes use simplified representations of flow and transport processes (with lumped parameters), the available site-specific data generally require some interpretation to arrive at best-estimate parameter values. This is often the case with soil properties. Most soil property measurements are made on a relatively small scale, while the codes referenced above require lumped parameter values on a much larger scale. This situation is illustrated in Figure 5-1, which is a representation of the DandD residential scenario conceptual model. The process of scaling up from small-scale measurements to the large-scale effective parameter values appropriate for use as best-estimates is not straightforward in all cases (Renard and de Marsily, 1997; Dagan, 1997).

As discussed in Chapter 4, natural variability and a lack of knowledge can result in significant parameter uncertainty, including uncertainty in the best-estimate values. Conditions such as the disparity between the scales of measurement and parameters contribute additional uncertainty. As a result of this uncertainty and to fulfill specific objectives of the analysis, the best-estimate parameter values may not be the most appropriate values, even when the analysis is a deterministic one. This is the case, for example, when conservative values of parameters are required to avoid underestimating the actual dose.

When a probabilistic analysis is carried out, estimates of uncertainty are required in addition to the best-estimate parameter values. Information that characterizes the uncertainty of a parameter can be presented in a variety of ways, including:

- a qualitative description of uncertainty
- maximum and minimum limiting values
- conservative values
- reasonable bounding values
- variance or standard deviation about the mean value
- quantiles or percentiles of a probability distribution
- a complete probability distribution.

These categories are listed in increasing order of specificity and completeness, although the best and least ambiguous characterization of a parameter's uncertainty involves sev-

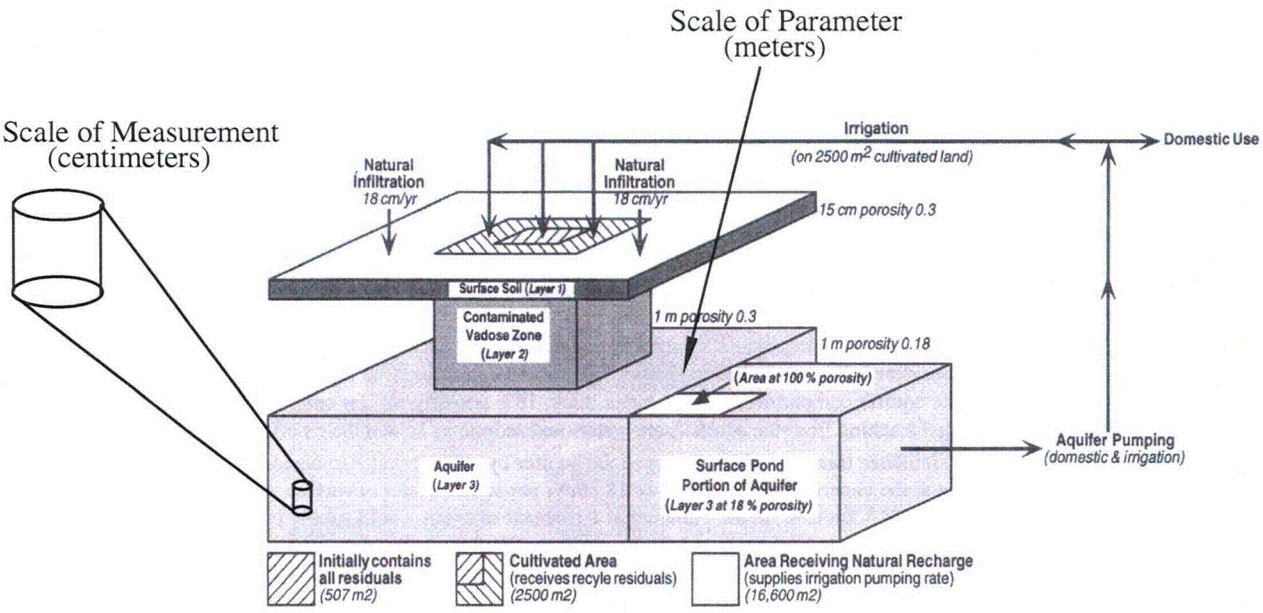

Figure 5-1. DandD conceptual model illustrating the contrast between the scale of the required parameters and the scale of typical measurements of soil properties

eral of these categories with a description of the data and analyses on which they are based.

As discussed in Chapter 4, many of the parameters required by the codes used in dose assessment analyses exhibit spatial and/or temporal variability. It is necessary to distinguish between this variability and the appropriate uncertainty characterization when applying DandD, RESRAD, and MEPAS (or similar codes). This issue is a matter of differences in scale and requires the correct interpretation of model parameters. Soil properties vary on both a small and large scale. Likewise, variability in meteorological processes such as rainfall can be characterized on the scale of hours to years. The soil parameters in these relatively simple codes represent average (effective) values over the entire site. The precipitation required as an input parameter is the long-term average value. When conducting an uncertainty analysis, it is therefore the uncertainty of the average values that must be characterized.

The expected form of the relationship between parameter variability and uncertainty in the average parameter value is given in Figure 5-2. This figure shows the relative form of the probability density functions and represents the intuitive concept that the uncertainty in an average parameter value is less than the variability of that parameter. This result is also reflected in the classical statistical relationship for the variance (uncertainty) of a sample average obtained from a random sample of parameter values,

$$Var(\bar{X}) = \sigma^2/N \qquad (3)$$

where σ is the variance of the parameter (a measure of its variability) and N is the number of samples. For a sample size greater than one, the uncertainty in the average value will be less than the variability of the parameter.

5.2 Data Sources

A hierarchy of data and information may be available to determine best-estimate parameter values and their uncertainties. A general characterization of these data and information types is provided in the left column of Figure 5-3. Information sources based on national data (i.e., data from across the United States) can be applied in a generic manner, without regard to a specific location. Data from these national or regional databases are also frequently related to a specific location, and thus can be used to provide more local information. Local information refers to a relatively small area (such as the county in which the site of interest is located). Local (and perhaps even site-specific) information may also be available from local experts. Finally, site-specific measurements of parameters may be available. These are data obtained directly from the site of interest. This characterization of data sources is consistent with MARSSIM (1997), which discusses acceptable methods for conducting final radiation status surveys for soil.

Identified sources of information are listed in Figure 5-3 and are briefly described here

- UNSODA (Leij et al., 1996) is a database of soil physical and hydraulic property measurements compiled from a variety of international sources. UNSODA is available from the USDA-ARS U.S. Salinity Laboratory (http://www.ussl.ars.usda.gov/). UNSODA contains soil property measurements, but some analysis may be required to obtain soil parameters for use in dose assessments. Two related databases, compiled from U.S. sources, are summarized in Schaap and Leij (1998). The distribution of samples by soil textural class for these three databases is shown in Figure 5-4.
- In NUREG/CR-6565 (Meyer et al., 1997) generic probability distributions for soil parameters were presented for use directly in RESRAD and MEPAS. These parameter distributions were based on the work of Carsel and Parrish (1988) who used data from both the National Soil Characterization Database and a national database similar to the RAWLS database of Figure 5-4.
- The National Soil Characterization Database is a large collection of soil properties available from the USDA Natural Resources Conservation Service (NRCS) (see http://www.nrcs.usda.gov/). This database consists of standard soil survey measurements on small-scale soil pedons generally obtained near the surface. Some analysis may be required to derive parameter values from the measured soil properties. The distribution of samples by soil textural class for this database is shown in Figure 5-5 for those samples with measured sand, silt, and clay

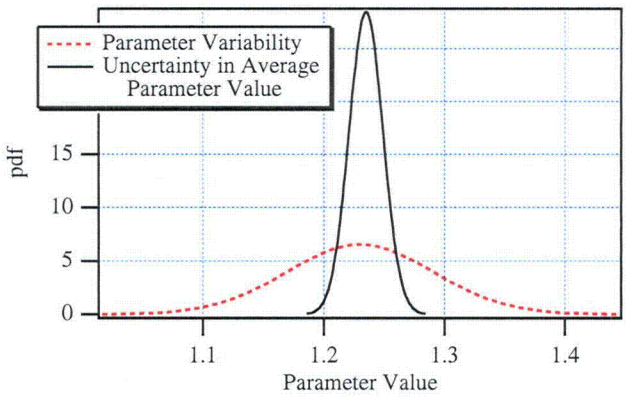

Figure 5-2. Expected relationship between parameter variability and uncertainty in the average parameter value (pdf = probability density function)

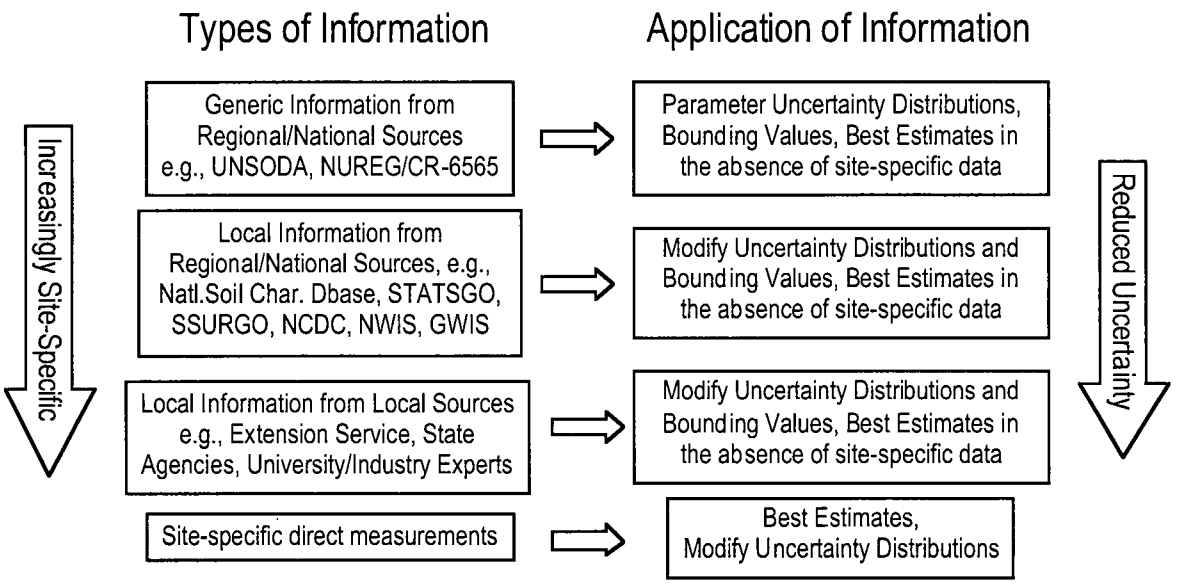

Figure 5-3. Types and uses of data sources and information

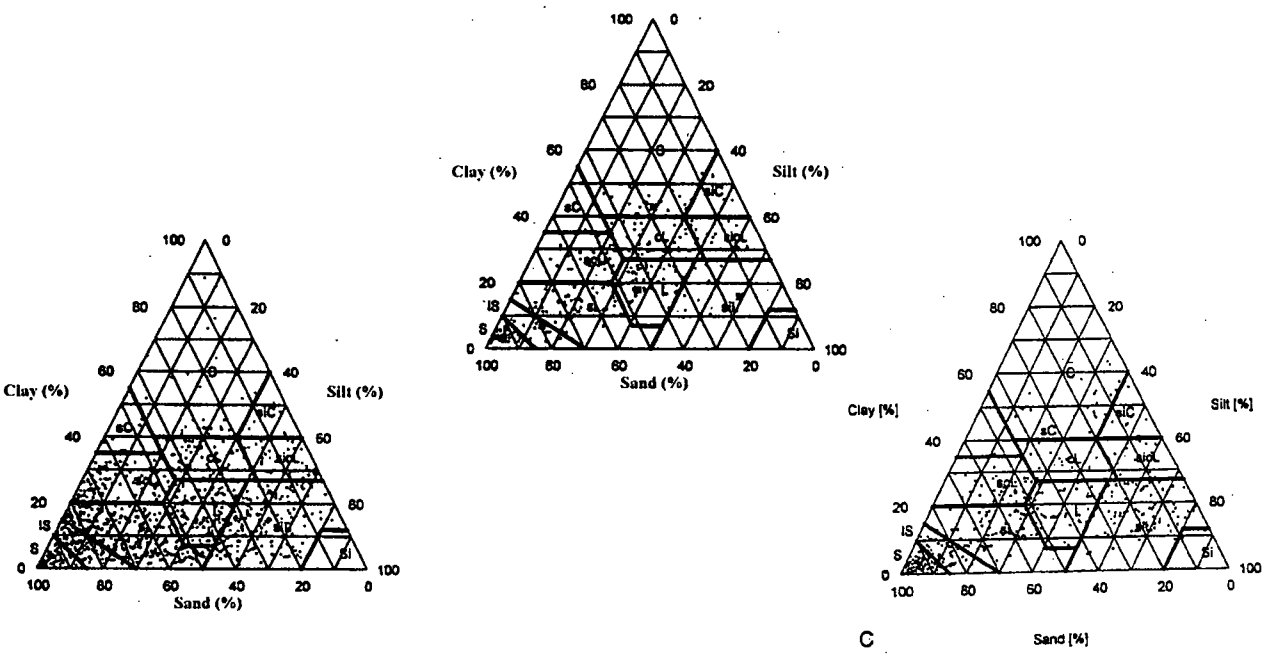

Figure 5-4. The distribution of samples by soil textural class for the UNSODA database and two related databases as reported in Schaap and Leij (1998)

percentages, bulk density, and water content at a soil water pressure of 1/3 bar (approximately 340 cm of water).

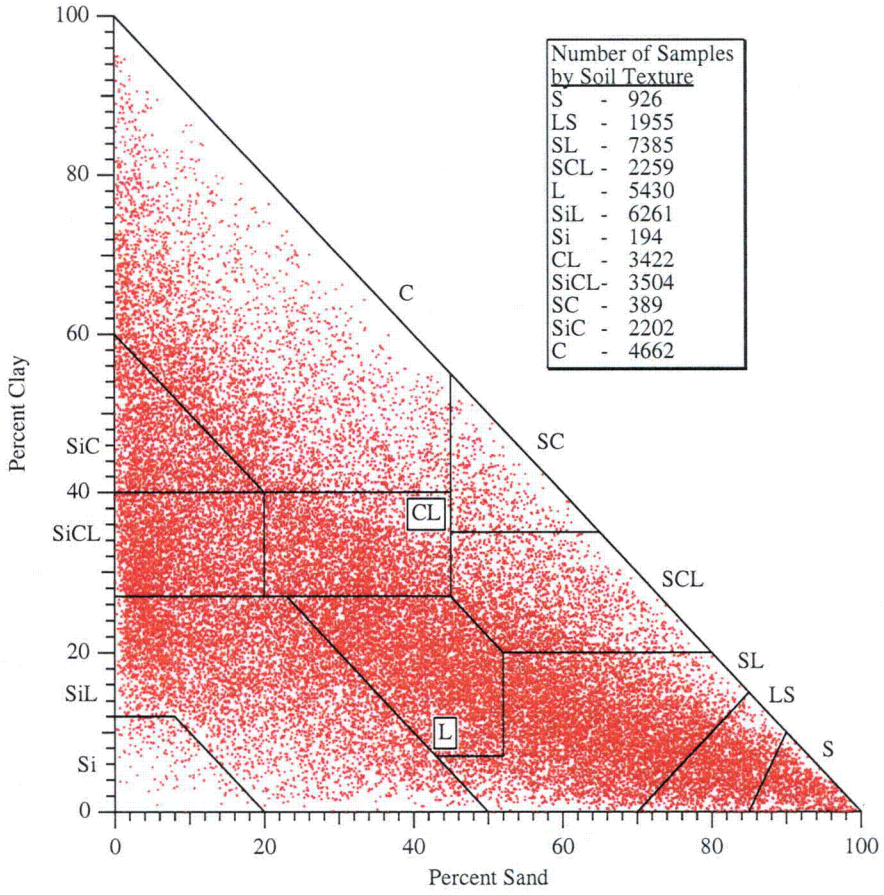

Figure 5-5. Distribution of samples by textural class for the National Soil Characterization Database for those samples with measurements of sand, silt, and clay percentages, bulk density, and water content at a soil water pressure of 1/3 bar (340 cm of water)

- SSURGO is a database of the original NRCS soil surveys digitized for use with Geographic Information System (GIS) software. These are the most detailed soil survey data available from the NRCS and are currently available for limited areas of the United States. SSURGO data are at a sufficiently small scale to be useful for parameter estimation in decommissioning analyses. Additional analyses may be required to derive parameter values from the soil property measurements in the database. More information and data are available at http://www.nrcs.usda.gov/.
- The STATSGO database is an NRCS product that generalizes the detailed soil survey data to a larger scale. This database is also intended for use with GIS software. The scale of STATSGO data is generally too large to be of significant use in estimating parameter values for decommissioning analyses, although it may be useful in characterizing uncertainty. The STATSGO database, interpreted to a regular, 1-km square grid was the basis of soil parameter distributions used in DandD (Beyeler et al., 1996).
- The National Climatic Data Center (NCDC) provides meteorological data measured at locations throughout the United States. Many of these data are available at http://www.ncdc.noaa.gov/, although it may require some analysis to derive the parameter values required for dose assessment analyses. The use of this data in evaluating uncertainty in net infiltration estimates was described by Meyer et al. (1997).

- The NWIS is a database of surface water information available from the U.S. Geological Survey (USGS) at http://water.usgs.gov/. The GWIS is a database of groundwater information currently in development by the USGS. The GWIS will be an easily available source of information on depth to groundwater when it is completed.
- Extension Service agents; state, county, and municipal staff; and university or industry personnel with experience in local conditions may be excellent sources of information and data related to a site. Information related to specific soil types, land use patterns and climatic data are often readily available from extension offices and other local sources. Water table depths, percolation tests (which give some indication of soil hydraulic properties) can be obtained in areas where septic tank systems are used. Local county or city files are often the source for such information.

Additional information on data sources for dose assessment codes can be found in Yu et al. (1993b), and Buck et al. (1995).

5.2.1 Uses and Abuses of Database Information.

Figure 5-3 provides a summary of the use of available databases and the application of data sources and their relationship to uncertainty distributions. It is clear that reduction in uncertainties occur as more site specific, direct measurements are made. Frequently, however, the site-specific data are unavailable and there must be reliance on estimates from generic, regional or local data sources that act as surrogate for site specific information. There is some caution that must be exercised in applying the local, regional, or generic data bases to site-specific cases. Under these conditions, the following issues related to applicability should be considered.

5.2.1.1 Application of Near-Surface Data to Describe Subsurface Hydrologic Properties

All of the available databases on soils are biased toward surface soil characterization. With few exceptions, all soil profile descriptions are confined to the top two meters of soil (see Buol et al., 1973, USDA-SCS, 1982). Thus data bases such as SSURGO, STATSGO, UNSODA, etc., reflect soil properties that are strongly influenced by the topmost soil, usually dominated by the highest amount of organic matter and lowest density materials in the soil profile. Subsurface soils and sediments, on the other hand, tend to be massive (high density) and void of organic matter. At waste sites there is often a removal of topsoil and a significant disturbance and mixing of the subsoil. In such cases, pedon descriptions, soil series and the defining physical and chemical properties associated with them are less important than onsite characterization. Thus, in general, the common approach of using soil physical data from surficial soils and sediments to estimate hydraulic properties of deeper sediments is at best qualitative and should be used with caution.

5.2.1.2 Application of Surrogate Climatic Data

Generally, most sites do not have extensive records of climatic data. Seldom will there be any onsite records, or, if available, they will not extend back more than a few decades at most. Our experience with climate data used for water balance calculations suggests that the records often must be supplemented for completeness.

As an example, Meyer et al (1996) provided an assessment of yearly average precipitation for Beatty, Nevada. To assess the impact of precipitation variations on water balance over a 45-year period, a 5-yr record available from the US Geological Survey (USGS) had to be supplemented. Data extending back to 1949 were obtained from weather stations located at the Nevada Test Site (NTS), a distance less than 20 km away from Beatty. The record was complicated by a move of NTS stations in 1972 to higher ground. Meyer et al. (1996) merged the data but observed a shift in the post-1972 record of about 56% (more precipitation at the higher NTS site). Only by adjusting the post-1972 record downward by 56% was there agreement with the USGS record and the NTS data. The study illustrates that significant uncertainty in precipitation can result from using data that represent only slightly different elevations of topographic settings.

A second example of the use of surrogate precipitation data illustrates the potential effect on the water balance of the data's temporal scale. In this study (Meyer, 1993), the water balance at a waste site in South Carolina was simulated using weather data taken from two small towns in South Carolina (Wagener and Blackville) located about 30 km apart, but at about the same elevation and orographic setting. Table 5-1 shows the resulting water balance for a two-year simulation, reported in terms of a percentage of the total precipitation. Note that the total precipitation was nearly the same (120 cm/yr) at both sites for the two-year simulation period (1984-85).

The simulations suggest that variation between the two towns has much less effect than the impact of the precipitation time scale. Differences in the water balance when using daily precipitation from Blackville or Wagener are modest. Runoff differs by a factor of two while drainage differs less than 15%. In contrast, using hourly precipitation resulted in much higher runoff and significantly less drainage than using daily average data. Differences between the water balance using hourly and daily precipitation are likely due to a better accounting of the low soil infiltration capacity at the site. Precipitation distributed evenly over the day does not correctly account for storm intensities and their interaction

Table 5-1. Simulated water balance results using precipitation data from two site in South Carolina (water balance given as a percent of total 1984-85 precipitation)

	Blackville Precipitation (Daily Only)	Wagener Precipitation	
		Daily	Hourly
Runoff	2.9	7.0	36.7
Infiltration	97.1	93.0	63.3
Evapotranspiration	62.2	63.8	60.5
Storage Change	0.0	-0.2	-1.3
Drainage	35.0	29.5	4.0

with soil infiltration capacity. When the precipitation exceeds the soil infiltration capacity more runoff occurs resulting in low drainage. In this case, drainage estimates using daily values are highly conservative and surface cover designs to reduce drainage at this site would be correspondingly more expensive.

A final example illustrating the use of non-site-specific data for water balance calculation is from the Hanford Site in Washington State as reported by Gee (1987). The USGS (Bauer and Vaccaro, 1987) used a regional model that required soil characteristics plus plant and climatic data to estimate recharge for the Hanford Site. The area simulated was over 1200 km^2 in extent, with grid spacing varying from 0.64 to 2.6 km^2. Plant cover was estimated from aerial photography and land-use maps. Soil survey data (Hajek, 1966) were used to delineate the variations in soil texture over the area. Climate records from the onsite weather station were used to model variations in precipitation and evaporative potential. Historical climate records for 21 years (1957-1977) were used to provide the water and energy inputs. Recharge estimates were made in two ways: actual daily values were used in one set of simulations and average daily values were simulated in another set. Table 5-2 shows the results of the two simulations.

Table 5-2. Simulated recharge at the Hanford Site using actual and average daily climates for a 21-year period (1957-1977)

	Recharge Based on Actual Daily Climate (mm/yr)	Recharge Based on Average Daily Climate (mm/yr)
Maximum	58	31
Minimum	0.5	0
Average	12	2

The water balance simulations illustrate the differences that can be obtained when average daily weather records are used instead of actual daily values. At this arid site, the averaging process tends to dampen the effect of extremes and the result is an apparent non-conservative (under) estimate of the recharge. In this study there was no assessment of the impacts or uncertainties in using regional soils data and the attendant estimated hydraulic properties. Nor was there an assessment of the reliability of uncertainty in the plant cover estimates and the impact of the estimates on actual plant water uptake, so it is difficult to assess the accuracy or reliability of either recharge estimate. However, it is clear that the averaging of climatic inputs, which is commonly done in water balance calculations, may be inappropriate and lead to under-estimates of recharge at arid sites.

In summary, the use of non-site-specific data is always a risk. While use of surrogate databases (regional or national) for assessment of uncertainties generally will provide a larger uncertainty than is obtained when using site-specific data, the impacts of temporal variations are not captured in the analysis. Accounting for time averaging and its impact on the water balance and net infiltration is an issue that should be addressed in the future.

5.3 Applications of Information

The right column of Figure 5-3 identifies a number of applications for the various information and data sources discussed in Section 5.2. In summary, the applications are:

- Characterize parameter uncertainty (as probability distributions, bounding values, etc.)
- Modify the uncertainty characterization
- Provide best-estimate parameter values.

In the ideal case, site-specific, direct measurements of the parameters required by a dose assessment code could be used exclusively for each of these applications. Figure 5-6 illustrates the expected relationship between the variability of a parameter at a decommissioning site and the variability of that same parameter when measured on a national scale. We expect the site-specific variability to be smaller. In addition, the average value at the site may be different than the national average. If enough site-specific data could be collected, we would thus expect that the best-estimate parame-

ter value would be both more accurate and also less uncertain than if we relied on a national database. Unfortunately, in many cases cost or time constraints preclude the collection of sufficient amounts of site-specific data to (1) define best-estimate parameter values with no uncertainty, or (2) adequately characterize parameter uncertainty.

Data covering a national (or extensive regional) scale are best suited to characterizing parameter uncertainty. In the absence of site-specific data, national or regional data sources can also be used to determine best-estimate parameter values. Local information can be used in a similar manner although in many cases it may be too limited to fully characterize parameter uncertainty. In this case it is better suited as a means to modify the parameter uncertainty established with the national databases. When available, site-specific data should be relied upon to establish best-estimate parameter values and modify parameter uncertainty estimates.

5.3.1 Soil Parameter Distributions from National Databases

Probability distributions characterizing the variability of soil hydraulic parameters on a national scale were presented in Meyer et al. (1997). The parameters for which distributions were given included those used in the RESRAD and MEPAS codes. Distributions were based on those provided by Carsel and Parrish (1988), but were modified to restrict the form of the distributions to normal, lognormal, and beta probability density functions. This allowed the distributions to be used without restriction in MEPAS; the beta distribution is not allowed in RESRAD, however. These parameter distributions and their correlations are presented in Appendices A and B and are recommended for use in decommissioning analyses.

Carsel and Parrish (1988) used bulk density and percent sand and clay data from the National Soil Characterization Database. Bulk density was not used directly, but was used to infer the porosity, which was assumed to be equal to the saturated water content. They derived soil hydraulic parameters from the saturated water content and percent sand and clay data using regression equations from Rawls and Brakensiek (1985). These regression equations were obtained using a set of data described in Rawls et al. (1982) with a distribution of samples similar to that shown in Figure 5-4 (Rawls database).

Schaap and Leij (1998) assembled the three databases represented in Figure 5-4 and compiled the mean and standard deviation for the parameters of the van Genuchten water retention function and the saturated hydraulic conductivity as a function of soil textural class (see Appendix C for the definition of the functions). Measured water retention data were used to fit the parameters for each sample. Schaap and Leij (1998) also derived neural networks using these databases that can be used to estimate hydraulic parameter values from basic soil survey measurements such as percent sand, silt, and clay, bulk density, and water content at soil pressures of 1/3 and 15 bars (approximately 333 and 15,000 cm of water). These neural network relationships have been shown to be superior to regression relationships, such as those used by Carsel and Parrish (1988) (Schaap et al., 1998). Meyer et al. (1999) examined the use of these neural networks with soils data from the NRCS Soil Characterization Database. This work is ongoing and may be used to modify the distributions presented in NUREG/CR-6565 (Meyer et al., 1997).

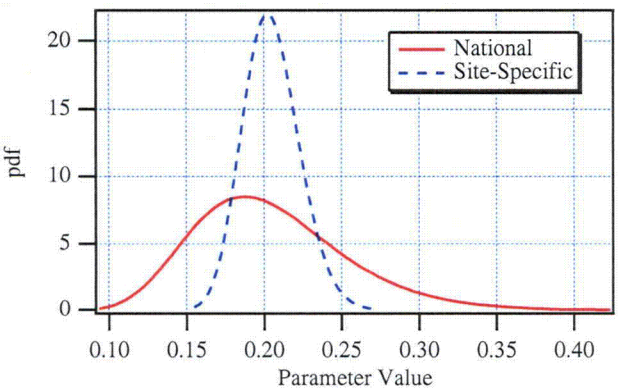

Figure 5-6. Expected relationship between the variability of a parameter on a national scale and on a site-specific basis

5.3.2 Updating Probability Distributions Using Site-Specific Data

In the absence of site-specific information, the effective value of a parameter at a site could conceivably be any reasonable value. Consider Figure 5-6. With no site-specific information to use, the distribution based on the observed national data defines the range and relative likelihood of values the parameter can reasonably be expected to assume at the site. That is, the value of 0.18 is most likely, but a value of 0.10, while unlikely, cannot be dismissed since it has been observed. It is thus appropriate to use the national distribution to represent the probability distribution of the effective (average) parameter value at the site, again, assuming that there is no site-specific information. As discussed previously, this will tend to overestimate the uncertainty of the parameter value both because the variability of the national data is likely to be greater than the variability at the site (see Figure 5-6) and because the variability of the national data is being used to represent the uncertainty of

the parameter (an effective or average value, see Figure 5-2).

When site-specific measurements of a parameter become available, this data can be combined with an existing parameter probability distribution, such as a distribution based on national data. Combing the two types of information should result in a modification of the existing parameter probability distribution. The expectation is that the best-estimate parameter value (as measured by the average of the distribution, for example) will be closer to the average of the site-specific measurements, and that the variance of the distribution will be reduced.

A procedure for combining an existing parameter probability distribution with site-specific parameter measurements was demonstrated by Meyer et al. (1997). This procedure uses Bayesian statistics and assumes that the parameter follows a normal distribution (or can be transformed to one). An example application of the procedure is illustrated in Figure 5-7. In this figure, the National Variability represents the parameter distribution that would be used in the absence of site-specific data. The variance of this distribution is quite large and the mean value is about 0.35. The Site Variability is the actual distribution of parameter values at the site. The variance of this distribution is smaller than that of the national distribution and the mean is significantly smaller (about 0.29). The site-specific data values shown in the figure were randomly selected from the site variability distribution.

The result of combining the national variability distribution with the site-specific data values is shown as probability distributions for the effective value (i.e., the parameter value required by the dose codes). As expected, the site-specific data reduce the variance of the effective value and shift the mean effective value towards the actual mean at the site. After four samples, the mean effective value is about 0.30. In spite of the large variance of the national data, after only four samples the variance of the effective value is very close to the variance that would be calculated using Equation 3 (on page 22). Note that this variance is less than that of the actual site value (denoted by the Site Variability curve). The Bayesian procedure thus reproduces the expected behavior discussed throughout this chapter.

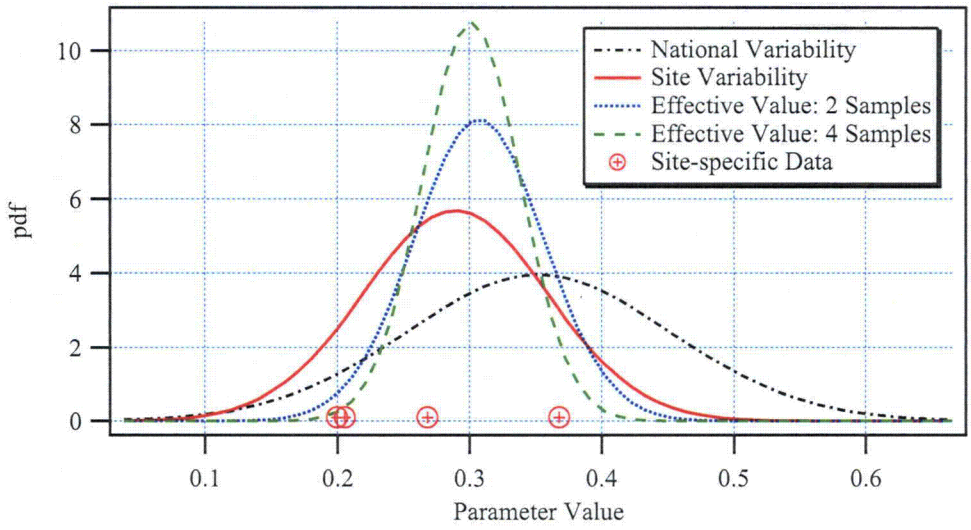

Figure 5-7. Example results of a procedure for combining a probability distribution representing parameter variability on a national scale and site-specific data. The average of the effective value approaches the actual site average while the effective value variance (uncertainty) is reduced.

6 Conclusions

This report has presented a variety of information that can be used to evaluate the impact of uncertainty in dose assessments for decommissioning analyses.

The role of conceptual model uncertainty in a dose assessment has not been discussed here. This is not meant to convey the impression that conceptual model uncertainty is unimportant. In many cases, it is likely that conceptual model uncertainty may dominate the overall magnitude of uncertainty. However, there are currently no general procedures for decision-making in the presence of conceptual model uncertainty, other than to examine alternative conceptual models as distinct cases. The NRC is sponsoring research elsewhere that has a goal of providing guidance on incorporating conceptual model uncertainty in the decommissioning framework.

Some of the basic similarities between the conceptual models of DandD, RESRAD, and MEPAS were outlined. These codes have much in common conceptually, but can nevertheless produce different results when modeling the same problem. This is primarily because of differences in the mathematical implementations of the basic conceptual model shared by the codes.

The essential simlifications of the conceptual model held in common by the three dose assessment codes examined are: use of a relatively simple model for the near-surface water budget to determine the net infiltration rate; steady-state, one-dimensional flow throughout the system; use of a small number of layers with uniform properties in each layer; and a simple model of mixing in the aquifer.

As a consequence of these conceptual model simplifications, there are a number of site-specific conditions under which the codes may provide inaccurate, potentially nonconservative results. These conditions include: the presence of significant preferential flow in the near surface, significant temporal variation in net infiltration and water content, significant heterogeneity resulting in focused flow or fast transport pathways, and fractured or karst formations.

The hydrologic parameters of DandD, RESRAD, and MEPAS were identified and compared. As a result of the similarity in the conceptual models used by the codes, there are many similarities in the parameters as well. The majority of differences between the parameters were due to the use of underlying quantities to derive a parameter. For example, DandD uses the relative saturation in the contaminated zone, which is the ratio of the water content to the porosity. MEPAS uses the water content and porosity directly. RESRAD calculates the water content using a simple model of flow.

The greatest differences in parameters were in the physical parameters of the saturated zone related to the point of exposure: location of the well, well depth, and pumping rate. Further study is required to evaluate the models of mixing in the aquifer and the well to provide a technical basis for comparing the codes and making recommendations on the appropriate parameters for this aspect of the dose modeling.

The importance of a particular parameter in causing uncertainty in dose was defined as the product of the sensitivity of the code's predicted dose to the parameter value and the uncertainty in the parameter (as measured by its coefficient of variation). Although the most important parameters are likely to vary depending on the dose assessment code used and on the specific site conditions, generic sensitivity analyses and available information on parameter uncertainty were used to draw some general conclusions. In many cases, it is expected that the distribution coefficients and the net infiltration (or parameters contributing to the net infiltration) will be the most important contributors to dose uncertainty (but likely not the only ones).

The various ways in which sensitivity can be measured were discussed. It was argued that the best approach is to conduct two analyses. First, delineate the dose predicted by the code as a function of a parameter's value over its expected range of variation. This is conducted while keeping the remaining parameters at their best-estimate values. In addition, a statistical sensitivity approach in which multiple parameters are varied simultaneously can serve to identify important interactions between parameters.

The relationship between best-estimate parameter values, parameter variability, and parameter uncertainty was discussed. One of the important issues raised was that of the difference in scale between many data sources (including site-specific measurement of parameters) and the scale of the parameters required in DandD, RESRAD, and MEPAS. Data are often measured at a relatively small scale while many of the hydrologic parameters represent a site-wide scale. The process of scaling up from the small to the large scale can introduce additional uncertainty that is generally not considered, and currently difficult to quantify in many cases.

Since many of the parameters represent a large scale, they require an average (effective) value and the uncertainty that should be considered in the analysis is the uncertainty of the average value. This is likely to be smaller than the small-scale variability of the parameter at the site.

Finally, a variety of data sources were reviewed. These data sources are available to provide estimates of parameter values in the absence of site-specific information. The large national databases can also be used to characterize parameter uncertainty. This is particularly appropriate when there are insufficient site-specific data on which to base parameter uncertainty estimates. Recommended distributions for soil hydraulic parameters were presented and a method to update these distributions using site-specific data was reviewed.

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Appendix A: Recommended Soil Parameter Distributions

Probability distributions of three types (normal, lognormal, and beta) were used to approximate the soil hydraulic parameter distributions generated from the Carsel and Parrish (1988) statistics. This appendix provides a summary of these distributions and presents tables of recommended distributions for selected soil hydraulic parameters. The information provided in Sections A.1 – A.3 can be found in many good probability or statistics textbooks (e.g., Ang and Tang, 1975). Definitions of parameters can be found in Appendix C.

This appendix was originally presented in NUREG/CR-6565 (Meyer et al., 1997).

A.1 The Normal Distribution

The normal distribution has a density function given by

$$f(x) = \frac{1}{\sqrt{2\pi}\sigma'}\exp\left[\frac{1}{2}\left(\frac{x-\mu'}{\sigma'}\right)^2\right] \quad \text{(A-1)}$$

where x is the soil parameter being modeled and μ' and σ' are the parameters of the distribution. The mean, μ, and the variance, σ^2, are related to the parameters of the normal distribution as follows.

$$\mu = \mu' \quad \text{(A-2)}$$

$$\sigma^2 = \sigma'^2 \quad \text{(A-3)}$$

Although the normal distribution is unbounded, soil parameters modeled by a normal distribution often have physical limits. These limits can be enforced by specifying that the soil parameter values fall between given quantiles of the normal distribution. In the tables below, the lower (A) and upper (B) limits of each normal distribution are the 0.001 and 0.999 quantiles calculated as follows.

$$A = \mu' - 3.09\sigma' \qquad B = \mu' + 3.09\sigma' \quad \text{(A-4)}$$

A.2 The Lognormal distribution

The lognormal distribution has a density function given by

$$f(x) = \frac{1}{\sqrt{2\pi}\zeta x}\exp\left[\frac{1}{2}\left(\frac{\ln(x)-\gamma}{\zeta}\right)^2\right] \quad \text{(A-5)}$$

where γ and ζ are the parameters of the distribution. The mean and variance of the lognormal distribution are related to the parameters as follows.

$$\mu = \exp(\gamma + \tfrac{1}{2}\zeta^2) \quad \text{(A-6)}$$

$$\sigma^2 = \mu^2[\exp(\zeta^2) - 1] \quad \text{(A-7)}$$

These relationships can also be inverted.

$$\gamma = \ln\mu - \tfrac{1}{2}\zeta^2 \quad \text{(A-8)}$$

$$\zeta = \sqrt{\ln\left(\frac{\sigma^2}{\mu^2} + 1\right)} \quad \text{(A-9)}$$

The lognormal distribution is thus completely specified by either its parameters or its mean and variance.

The lognormal distribution is bounded below by zero, but has no upper bound. In the tables below, the lower and upper bound for the lognormal distributions are the 0.001 and 0.999 quantiles calculated as follows.

$$A = \exp(\gamma - 3.09\zeta) \qquad B = \exp(\gamma + 3.09\zeta) \quad \text{(A-10)}$$

A.3 The Beta Distribution

The beta distribution has a density function given by

$$f(x) = \frac{1}{\beta(q,r)}\frac{(x-A)^{q-1}(B-x)^{r-1}}{(B-A)^{q+r-1}} \quad \text{(A-11)}$$

where q and r are parameters controlling the shape of the distribution and A and B are the lower and upper limits of the distribution. $\beta(q,r)$ is the beta function, calculated through its relationship to the gamma function.

$$\beta(q,r) = \frac{\Gamma(q)\Gamma(r)}{\Gamma(q+r)} \quad \text{(A-12)}$$

where $\Gamma(\,)$ indicates the gamma function.

The mean and variance of the beta distribution are related to the parameters as follows.

$$\mu = A + \frac{q}{q+r}(B-A) \quad \text{(A-13)}$$

$$\sigma^2 = \frac{qr}{(q+r)^2(q+r+1)}(B-A)^2 \quad \text{(A-14)}$$

With some algebraic manipulation, these relationships can be inverted to provide the shape parameters as a function of the mean, variance, and limits.

$$q = \left(\frac{(B-\mu)(\mu-A)}{\sigma^2} - 1\right)\left(\frac{\mu-A}{B-A}\right) \quad \text{(A-15)}$$

$$r = q\left(\frac{B-\mu}{\mu-A}\right) \quad \text{(A-16)}$$

The beta distribution can thus be completed specified by its lower and upper limits and either its mean and variance or its shape parameters.

In the tables below, the lower and upper limits for the beta distributions are the actual limits, A and B.

A.4 Recommended Probability Distributions for Soil Hydraulic Parameters by Soil Texture

Tables A-1 to A-12 contain the recommended distributions for the selected soil hydraulic parameters. Each table represents a particular USDA soil textural classification. Observed correlations between parameters are given in Appendix B.

Table A-1. Recommended distributions for Sand

Parameter	Distribution[1]	Mean	Std. Deviation	Lower Limit[2]	Upper Limit[2]
θ_s	Normal	0.430	0.0600	0.245	0.615
θ_r	LN(-3.09,0.224)*	0.0466	0.0106	0.0228	0.0907
p_e	Normal	0.383	0.0610	0.195	0.572
f_c	LN(-2.83,0.241)	0.0607	0.0150	0.0280	0.124
w_p	LN(-3.09,0.224)	0.0466	0.0106	0.0227	0.0907
awc	LN(-4.34,0.387)	0.0141	6.12E-03	3.95E-03	0.0431
α [cm^{-1}]	Normal	0.147	0.0255	0.0687	0.226
n	LN(0.978,0.0998)*	2.67	0.267	1.95	3.62
h_b	LN(1.93,0.183)	7.02	1.38	3.92	12.1
λ	LN(0.502,0.161)	1.67	0.267	1.00	2.72
b	LN(-0.0253,0.216)	0.998	0.226	0.501	1.90
K_s [cm/s]	Beta(1.398,1.842)	8.22E-03	4.39E-03	3.50E-04	0.0186

Table A-2. Recommended distributions for Loamy Sand

Parameter	Distribution[1]	Mean	Std. Deviation	Lower Limit[2]	Upper Limit[2]
θ_s	Normal	0.410	0.0900	0.132	0.688
θ_r	Normal	0.0569	0.0145	0.0121	0.102
p_e	Normal	0.353	0.0913	0.0711	0.635
f_c	LN(-2.55,0.281)	0.0809	0.0224	0.0327	0.186
w_p	Normal	0.0570	0.0146	0.0119	0.102
awc	LN(-3.85,0.491)	0.0239	0.0125	4.65E-03	0.0966
α [cm^{-1}]	Normal*	0.125	0.0404	2.03E-04	0.250
n	LN(0.816,0.0910)	2.27	0.209	1.71	3.00
h_b	LN(2.15,0.401)	9.58	8.59	2.48	29.5
λ	LN(0.226,0.164)	1.27	0.209	0.756	2.08
b	LN(0.305,0.258)	1.40	0.397	0.610	3.01
K_s [cm/s]	Beta(0.7992,1.910)	3.99E-03	3.17E-03	3.90E-05	0.0134

Table A-3. Recommended distributions for Sandy Loam

Parameter	Distribution[1]	Mean	Std. Deviation	Lower Limit[2]	Upper Limit[2]
θ_s	Normal	0.410	0.0899	0.132	0.688
θ_r	Beta(2.885,2.304)	0.0644	0.0169	0.0173	0.102
p_e	Normal	0.346	0.0915	0.0629	0.628
f_c	LN(-2.21,0.314)	0.116	0.0369	0.0417	0.291
w_p	Normal	0.0659	0.0179	0.0106	0.121
awc	LN(-3.12,0.489)	0.0498	0.0256	9.75E-03	0.200
α [cm^{-1}]	Beta(1.816,3.412)	0.0757	0.0368	8.72E-03	0.202
n	LN(0.634,0.0818)*	1.89	0.155	1.46	2.43
h_b	LN(2.71,0.538)	17.7	12.0	2.85	79.4
λ	Normal	0.892	0.155	0.412	1.37
b	LN(0.632,0.282)	1.96	0.597	0.786	4.50
K_s [cm/s]	LN(-7.46,1.33)	1.17E-03	1.37E-03	9.62E-06	0.0347

Table A-4. Recommended distributions for Sandy Clay Loam

Parameter	Distribution[1]	Mean	Std. Deviation	Lower Limit[2]	Upper Limit[2]
θ_s	Normal	0.390	0.0700	0.174	0.606
θ_r	Beta(2.202,2.010)	0.101	6.09E-03	0.0860	0.114
p_e	Normal	0.289	0.0703	0.0723	0.507
f_c	LN(-1.59,0.254)	0.212	0.0568	0.0933	0.449
w_p	LN(-2.14,0.158)	0.120	0.0214	0.0724	0.193
awc	Beta(1.890,3.817)	0.0920	0.0393	0.0204	0.237
α [cm^{-1}]	LN(-3.04,0.639)	0.0572	0.0337	6.62E-03	0.343
n	LN(0.388,0.0858)*	1.48	0.127	1.13	1.92
h_b	LN(3.04,0.639)	26.2	21.3	2.92	151.
λ	Normal	0.479	0.127	0.0865	0.872
b	LN(1.41,0.275)	4.27	1.39	1.75	9.57
K_s [cm/s]	LN(-9.30,1.75)	3.23E-04	5.98E-04	4.12E-07	0.0202

Table A-5. Recommended distributions for Loam

Parameter	Distribution[1]	Mean	Std. Deviation	Lower Limit[2]	Upper Limit[2]
θ_s	Normal	0.430	0.0998	0.122	0.738
θ_r	Beta(3.639,2.652)	0.0776	0.0127	0.0374	0.107
p_e	Normal	0.352	0.101	0.0414	0.663
f_c	LN(-1.68,0.300)	0.194	0.0609	0.0735	0.468
w_p	LN(-2.40,0.250)	0.0935	0.0246	0.0418	0.196
awc	LN(-2.40,0.462)	0.101	0.0454	0.0218	0.380
α [cm^{-1}]	Beta(1.576,3.625)	0.0367	0.0202	3.51E-03	0.113
n	LN(0.442,0.0730)	1.56	0.114	1.24	1.95
h_b	LN(3.470,0.598)	38.9	29.3	5.05	203.
λ	Normal	0.560	0.114	0.209	0.911
b	LN(1.08,0.271)	3.07	0.900	1.28	6.82
K_s [cm/s]	LN(-9.26,1.66)	2.92E-04	4.91E-04	5.51E-07	0.0159

Table A-6. Recommended distributions for Silt Loam

Parameter	Distribution[1]	Mean	Std. Deviation	Lower Limit[2]	Upper Limit[2]
θ_s	Normal	0.45	0.0800	0.203	0.697
θ_r	Beta(3.349,2.566)	0.0670	0.0142	0.0243	0.0998
p_e	Normal	0.383	0.0813	0.132	0.634
f_c	Normal	0.252	0.0776	0.0119	0.491
w_p	LN(-2.22,0.397)	0.117	0.0471	0.0318	0.368
awc	Normal	0.135	0.0402	0.0107	0.259
α [cm^{-1}]	LN(-4.10,0.554)*	0.0193	0.0115	2.99E-03	0.0919
n	LN(0.343,0.0851)	1.41	0.120	1.08	1.83
h_b	LN(4.10,0.554)	70.3	41.9	10.9	335.
λ	Normal	0.414	0.120	0.0417	0.786
b	LN(1.28,0.334)	3.80	1.42	1.28	10.1
K_s [cm/s]	LN(-10.4,1.49)*	9.33E-05	2.24E-04	3.12E-07	3.11E-03

Table A-7. Recommended distributions for Silt

Parameter	Distribution[1]	Mean	Std. Deviation	Lower Limit[2]	Upper Limit[2]
θ_s	Normal	0.456	0.110	0.1206	0.799
θ_r	Beta(1.717,1.072)	0.0352	8.97E-03	0.0131	0.0490
p_e	Normal	0.425	0.110	0.0839	0.766
f_c	Normal	0.236	0.0578	0.0575	0.415
w_p	LN(-2.46,0.295)	0.0890	0.0268	0.0342	0.212
awc	Normal	0.147	0.0395	0.0252	0.269
α [cm^{-1}]	Normal*	0.0178	5.73E-03	3.91E-05	0.0355
n	Normal*	1.38	0.0369	1.27	1.49
h_b	LN(4.10,0.403)	68.1	74.8	17.3	209.
λ	Normal	0.380	0.0369	0.266	0.494
b	LN(1.16,0.140)	3.21	0.465	2.06	4.89
K_s [cm/s]	LN(-10.0,0.475)*	4.89E-05	2.76E-05	9.95E-06	1.87E-04

Table A-8. Recommended distributions for Clay Loam

Parameter	Distribution[1]	Mean	Std. Deviation	Lower Limit[2]	Upper Limit[2]
θ_s	Normal	0.410	0.0900	0.132	0.688
θ_r	Normal	0.0954	9.68E-03	0.0655	0.125
p_e	Normal	0.315	0.0905	0.0349	0.594
f_c	LN(-1.27,0.297)	0.292	0.0862	0.112	0.700
w_p	LN(-1.84,0.257)	0.164	0.0468	0.0714	0.350
awc	Beta(2.986,4.318)	0.128	0.0497	9.34E-03	0.301
α [cm^{-1}]	LN(-4.22,0.719)*	0.0190	0.0153	1.59E-03	0.136
n	Normal	1.32	0.0973	1.02	1.62
h_b	LN(4.22,0.719)	88.0	71.3	7.37	628.
λ	Normal	0.318	0.0973	0.0170	0.618
b	LN(1.73,0.323)	5.97	2.37	2.08	15.3
K_s [cm/s]	LN(-11.3,2.17)	9.93E-05	2.51E-04	1.42E-08	9.76E-03

Table A-9. Recommended distributions for Silty Clay Loam

Parameter	Distribution[1]	Mean	Std. Deviation	Lower Limit[2]	Upper Limit[2]
θ_s	Normal	0.430	0.0699	0.214	0.646
θ_r	Normal*	0.0880	9.00E-03	0.0602	0.116
p_e	Normal	0.342	0.0705	0.124	0.560
f_c	Normal	0.347	0.0710	0.127	0.566
w_p	LN(-1.61,0.233)	0.205	0.0508	0.0970	0.410
awc	Normal	0.142	0.0333	0.0387	0.245
α [cm^{-1}]	LN(-4.72,0.563)	0.0104	6.08E-03	1.57E-03	0.0508
n	Normal*	1.23	0.0610	1.04	1.42
h_b	LN(4.72,0.563)	132.	81.4	19.7	638.
λ	Normal	0.230	0.0610	0.0416	0.418
b	LN(1.96,0.265)	7.13	2.34	3.02	15.5
K_s [cm/s]	LN(-12.3,1.59)	1.54E-05	3.38E-05	3.44E-08	6.49E-04

Table A-10. Recommended distributions for Sandy Clay

Parameter	Distribution[1]	Mean	Std. Deviation	Lower Limit[2]	Upper Limit[2]
θ_s	Normal	0.380	0.0500	0.226	0.534
θ_r	Beta(4.000,1.487)	0.0993	0.0116	0.0508	0.117
p_e	Normal	0.281	0.0513	0.122	0.439
f_c	LN(-1.23,0.210)	0.299	0.0623	0.153	0.559
w_p	Beta(1.142,4.640)	0.165	0.0344	0.121	0.346
awc	Normal	0.134	0.0356	0.0238	0.244
α [cm^{-1}]	LN(-3.77,0.562)*	0.0270	0.0164	4.06E-03	0.131
n	LN(0.241,0.0653)*	1.28	0.0834	1.04	1.56
h_b	LN(3.77,0.562)	50.7	30.5	7.64	246.
λ	Normal	0.275	0.0834	0.0177	0.533
b	LN(1.89,0.260)	6.90	2.27	2.97	14.8
K_s [cm/s]	LN(-12.2,2.02)*	3.55E-05	1.48E-04	9.59E-09	2.50E-03

Table A-11. Recommended distributions for Silty Clay

Parameter	Distribution[1]	Mean	Std. Deviation	Lower Limit[2]	Upper Limit[2]
θ_s	Normal	0.360	0.0698	0.144	0.576
θ_r	Normal*	0.0706	0.0228	1.47E-04	0.141
p_e	Normal	0.289	0.0735	0.0623	0.517
f_c	Normal	0.334	0.0678	0.124	0.543
w_p	LN(-1.49,0.220)	0.230	0.0512	0.114	0.444
awc	Normal	0.103	0.0303	9.63E-03	0.197
α [cm^{-1}]	LN(-5.66,0.584)*	4.13E-03	2.60E-03	5.73E-04	0.0211
n	LN(0.145,0.0430)	1.16	0.0499	1.01	1.32
h_b	LN(5.66,0.584)	340.	216.	47.3	1743.
λ	Beta(2.591,3.268)	0.157	0.0499	0.0404	0.304
b	LN(2.29,0.259)	10.2	2.96	4.43	22.0
K_s [cm/s]	LN(-13.9,1.31)*	2.19E-06	4.08E-06	1.64E-08	5.37E-05

Table A-12. Recommended distributions for Clay

Parameter	Distribution[1]	Mean	Std. Deviation	Lower Limit[2]	Upper Limit[2]
θ_s	Normal	0.380	0.0900	0.102	0.658
θ_r	Beta(1.501,1.580)	0.0685	0.0344	8.36E-04	0.140
p_e	Normal	0.311	0.0963	0.0138	0.609
f_c	Normal	0.340	0.0893	0.0638	0.615
w_p	Beta(2.751,4.921)	0.263	0.0770	0.0939	0.567
awc	LN(-2.66,0.429)	0.0761	0.0299	0.0186	0.263
α [cm^{-1}]	LN(-5.54,0.893)	6.18E-03	7.59E-03	2.50E-04	0.0621
n	Beta(0.8857,2.400)	1.13	0.0697	1.04	1.36
h_b	Beta(0.8002,1.546)	353.	257.	14.1	1007
λ	Beta(0.8854,2.399)	0.127	0.0697	0.0397	0.365
b	Beta(1.751,11.61)	14.1	6.24	4.93	75.0
K_s [cm/s]	LN(-12.36,2.269)	3.65E-05	1.08E-04	3.87E-09	4.76E-03

1. LN(,) = Lognormal(γ,ζ); see Section A.2. Beta(,) =Beta(q,r); see Section A.3.

2. Lower Limit and Upper Limit are 0.001 and 0.999 quantiles for Normal and Lognormal distributions.

* Indicates that the recommended distribution is the same type as used by Carsel and Parrish (1988). This applies to the parameters θ_r, α, n, and K_s only.

A.5 References

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Appendix B: Soil Parameter Correlation Coefficients

The correlation coefficient is a measure of the strength of a linear relationship between two random variables (i.e., soil parameters), X and Y. Sample correlation coefficients were calculated as follows [e.g., Ang and Tang (1975)].

$$\hat{\rho} = \frac{1}{N-1}\frac{\sum_{i=1}^{N} x_i y_i - N\bar{x}\bar{y}}{s_x s_y} \qquad \text{(B-1)}$$

where

$\hat{\rho}$ = sample correlation coefficient

x_i, y_i = sample values for parameters X and Y

$\bar{x}$, $\bar{y}$ = sample mean values calculated as

$$\bar{x} = \frac{1}{N}\sum_{i=1}^{N} x_i \qquad \text{(B-2)}$$

s_x, s_y = sample standard deviations calculated as

$$s_x^2 = \frac{1}{N-1}\sum_{i=1}^{N}(x_i - \bar{x})^2 \qquad \text{(B-3)}$$

N = the number of sample values

Correlations between parameters were induced by applying the correlations between θ_r, α, n, and K_s given in Carsel and Parrish (1988). The rank correlation method of Iman and Conover (1982) as embodied in the Latin hypercube sampling code of Iman and Shortencarier (1984) was used. Note that the correlations given in the tables below do not necessarily appear to be the same as those of Carsel and Parrish (1988) since their correlations were calculated after the parameters were transformed to normal distributions. The correlations given below were calculated on the untransformed parameters. Definitions of parameters in the tables can be found in Appendix C.

This appendix was originally presented in NUREG/CR-6565 (Meyer et al., 1997).

Table B-1. Correlation coefficients for Sand

	θ_s	θ_r	p_e	f_c	w_p	awc	α	n	h_b	λ	b	K_s
θ_s	1	-0.01	0.99	0.15	-0.01	0.38	0.00	0.00	-0.02	0.00	-0.29	0.00
θ_r		1	-0.18	0.94	1	0.59	0.12	-0.84	-0.12	-0.84	0.91	-0.50
p_e			1	-0.02	-0.18	0.27	-0.02	0.15	0.01	0.15	-0.44	0.08
f_c				1	0.94	0.82	-0.11	-0.91	0.11	-0.91	0.89	-0.67
w_p					1	0.59	0.12	-0.84	-0.12	-0.84	0.91	-0.50
awc						1	-0.49	-0.79	0.49	-0.79	0.59	-0.78
α							1	0.29	-0.97	0.29	-0.09	0.73
n								1	-0.28	1	-0.88	0.84
h_b									1	-0.28	0.09	-0.68
λ										1	-0.88	0.84
b											1	-0.65
K_s												1

Table B-2. Correlation coefficients for Loamy Sand

	θ_s	θ_r	p_e	f_c	w_p	awc	α	n	h_b	λ	b	K_s
θ_s	1	-0.01	0.99	0.27	0.00	0.49	0.00	0.01	-0.03	0.01	-0.50	0.01
θ_r		1	-0.16	0.85	1	0.34	-0.29	-0.58	0.16	-0.58	0.71	-0.34
p_e			1	0.13	-0.16	0.42	0.05	0.10	-0.05	0.10	-0.60	0.07
f_c				1	0.85	0.79	-0.53	-0.76	0.33	-0.76	0.57	-0.58
w_p					1	0.35	-0.30	-0.58	0.17	-0.58	0.72	-0.35
awc						1	-0.60	-0.68	0.39	-0.68	0.19	-0.63
α							1	0.38	-0.57	0.38	-0.29	0.88
n								1	-0.22	1	-0.64	0.65
h_b									1	-0.22	0.17	-0.38
λ										1	-0.64	0.65
b											1	-0.41
K_s												1

Table B-3. Correlation coefficients for Sandy Loam

	θ_s	θ_r	p_e	f_c	w_p	awc	α	n	h_b	λ	b	K_s
θ_s	1	0.00	0.98	0.38	0.03	0.54	0.01	0.00	0.01	0.00	-0.44	0.01
θ_r		1	-0.19	0.72	1	0.34	0.14	-0.79	-0.17	-0.79	0.77	-0.22
p_e			1	0.24	-0.16	0.46	-0.02	0.15	0.04	0.15	-0.57	0.05
f_c				1	0.78	0.90	-0.35	-0.85	0.35	-0.85	0.51	-0.51
w_p					1	0.42	0.08	-0.82	-0.10	-0.82	0.77	-0.25
awc						1	-0.56	-0.65	0.57	-0.65	0.20	-0.56
α							1	0.36	-0.77	0.36	-0.11	0.82
n								1	-0.28	1	-0.78	0.60
h_b									1	-0.28	0.05	-0.51
λ										1	-0.78	0.60
b											1	-0.33
K_s												1

Table B-4. Correlation coefficients for Sandy Clay Loam

	θ_s	θ_r	p_e	f_c	w_p	awc	α	n	h_b	λ	b	K_s
θ_s	1	0.00	1	0.48	0.21	0.58	-0.01	0.00	-0.02	0.00	-0.43	-0.01
θ_r		1	-0.09	-0.02	0.23	-0.16	0.37	-0.11	-0.36	-0.11	0.21	0.16
p_e			1	0.48	0.19	0.59	-0.04	0.01	0.01	0.01	-0.45	-0.03
f_c				1	0.88	0.97	-0.67	-0.81	0.66	-0.81	0.42	-0.50
w_p					1	0.73	-0.51	-0.81	0.68	-0.81	0.65	-0.33
awc						1	-0.69	-0.73	0.58	-0.73	0.24	-0.54
α							1	0.77	-0.70	0.77	-0.49	0.82
n								1	-0.65	1	-0.76	0.71
h_b									1	-0.65	0.57	-0.39
λ										1	-0.76	0.71
b											1	-0.38
K_s												1

Table B-5. Correlation coefficients for Loam

	θ_s	θ_r	p_e	f_c	w_p	awc	α	n	h_b	λ	b	K_s
θ_s	1	0.00	0.99	0.55	0.18	0.63	0.03	0.00	0.04	0.00	-0.46	0.03
θ_r		1	-0.13	0.29	0.79	-0.03	-0.04	-0.70	0.07	-0.70	0.67	0.14
p_e			1	0.50	0.08	0.63	0.03	0.09	0.03	0.09	-0.54	0.01
f_c				1	0.75	0.93	-0.63	-0.71	0.70	-0.71	0.28	-0.41
w_p					1	0.47	-0.42	-0.87	0.56	-0.87	0.69	-0.16
awc						1	-0.62	-0.49	0.63	-0.49	0.00	-0.46
α							1	0.60	-0.73	0.60	-0.37	0.82
n								1	-0.55	1	-0.79	0.41
h_b									1	-0.55	0.39	-0.42
λ										1	-0.79	0.41
b											1	-0.21
K_s												1

Table B-6. Correlation coefficients for Silt Loam

	θ_s	θ_r	p_e	f_c	w_p	awc	α	n	h_b	λ	b	K_s
θ_s	1	-0.01	0.98	0.48	0.20	0.70	-0.02	-0.01	-0.02	-0.01	-0.20	-0.02
θ_r		1	-0.18	0.50	0.66	0.18	-0.29	-0.59	0.27	-0.59	0.63	-0.25
p_e			1	0.39	0.08	0.66	0.03	0.10	-0.06	0.10	-0.31	0.03
f_c				1	0.91	0.87	-0.72	-0.80	0.73	-0.80	0.63	-0.45
w_p					1	0.58	-0.63	-0.89	0.73	-0.89	0.86	-0.36
awc						1	-0.65	-0.50	0.54	-0.50	0.20	-0.44
α							1	0.74	-0.75	0.74	-0.56	0.80
n								1	-0.69	1	-0.88	0.48
h_b									1	-0.69	0.68	-0.39
λ										1	-0.88	0.48
b											1	-0.31
K_s												1

Table B-7. Correlation coefficients for Silt

	θ_s	θ_r	p_e	f_c	w_p	awc	α	n	h_b	λ	b	K_s
θ_s	1	-0.02	1	0.90	0.52	0.97	0.00	0.00	0.03	0.00	-0.39	0.02
θ_r		1	-0.10	0.25	0.57	-0.02	-0.19	-0.60	0.04	-0.60	0.70	-0.21
p_e			1	0.88	0.48	0.96	0.01	0.05	0.03	0.05	-0.44	0.04
f_c				1	0.81	0.92	-0.35	-0.37	0.16	-0.37	-0.03	-0.30
w_p					1	0.51	-0.60	-0.72	0.48	-0.72	0.44	-0.45
awc						1	-0.10	-0.06	-0.09	-0.06	-0.35	-0.14
α							1	0.55	-0.49	0.55	-0.41	0.89
n								1	-0.20	1	-0.84	0.44
h_b									1	-0.20	0.13	-0.29
λ										1	-0.84	0.44
b											1	-0.34
K_s												1

Table B-8. Correlation coefficients for Clay Loam

	θ_s	θ_r	p_e	f_c	w_p	awc	α	n	h_b	λ	b	K_s
θ_s	1	0.00	0.99	0.65	0.38	0.76	-0.02	0.00	-0.04	0.00	-0.40	0.01
θ_r		1	-0.11	-0.50	-0.46	-0.43	0.73	0.58	-0.74	0.58	-0.35	0.51
p_e			1	0.69	0.43	0.80	-0.10	-0.06	0.04	-0.06	-0.36	-0.04
f_c				1	0.89	0.90	-0.60	-0.71	0.55	-0.71	0.23	-0.42
w_p					1	0.60	-0.55	-0.84	0.75	-0.84	0.57	-0.33
awc						1	-0.52	-0.45	0.26	-0.45	-0.13	-0.42
α							1	0.79	-0.62	0.79	-0.42	0.89
n								1	-0.80	1	-0.73	0.58
h_b									1	-0.80	0.70	-0.36
λ										1	-0.73	0.58
b											1	-0.26
K_s												1

Table B-9. Correlation coefficients for Silty Clay Loam

	θ_s	θ_r	p_e	f_c	w_p	awc	α	n	h_b	λ	b	K_s
θ_s	1	0.00	0.99	0.73	0.46	0.85	-0.01	0.00	0.00	0.00	-0.19	-0.03
θ_r		1	-0.13	-0.42	-0.46	-0.21	0.72	0.55	-0.71	0.55	-0.37	0.47
p_e			1	0.77	0.51	0.87	-0.10	-0.07	0.10	-0.07	-0.15	-0.09
f_c				1	0.90	0.75	-0.62	-0.65	0.58	-0.65	0.35	-0.45
w_p					1	0.40	-0.68	-0.84	0.79	-0.84	0.69	-0.42
awc						1	-0.29	-0.11	0.02	-0.11	-0.30	-0.32
α							1	0.86	-0.75	0.86	-0.57	0.83
n								1	-0.84	1	-0.82	0.60
h_b									1	-0.84	0.80	-0.41
λ										1	-0.82	0.60
b											1	-0.32
K_s												1

Table B-10. Correlation coefficients for Sandy Clay

	θ_s	θ_r	p_e	f_c	w_p	awc	α	n	h_b	λ	b	K_s
θ_s	1	0.00	0.97	0.58	0.35	0.68	0.02	0.00	0.01	0.00	-0.23	0.05
θ_r		1	-0.23	-0.70	-0.82	-0.42	0.75	0.88	-0.92	0.88	-0.78	0.28
p_e			1	0.72	0.53	0.75	-0.15	-0.20	0.22	-0.20	-0.05	-0.02
f_c				1	0.89	0.89	-0.70	-0.78	0.68	-0.78	0.44	-0.33
w_p					1	0.58	-0.67	-0.85	0.87	-0.85	0.74	-0.24
awc						1	-0.58	-0.55	0.35	-0.55	0.05	-0.35
α							1	0.87	-0.74	0.87	-0.59	0.58
n								1	-0.86	1	-0.79	0.44
h_b									1	-0.86	0.83	-0.26
λ										1	-0.79	0.44
b											1	-0.23
K_s												1

Table B-11. Correlation coefficients for Silty Clay

	θ_s	θ_r	p_e	f_c	w_p	awc	α	n	h_b	λ	b	K_s
θ_s	1	0.00	0.95	0.94	0.74	0.84	-0.01	-0.01	-0.01	-0.01	-0.31	0.02
θ_r		1	-0.31	-0.29	-0.49	0.19	0.89	0.79	-0.88	0.79	-0.46	0.64
p_e			1	0.98	0.86	0.74	-0.28	-0.25	0.26	-0.25	-0.15	-0.18
f_c				1	0.91	0.70	-0.32	-0.33	0.24	-0.33	-0.07	-0.24
w_p					1	0.34	-0.50	-0.64	0.52	-0.64	0.32	-0.34
awc						1	0.14	0.33	-0.36	0.33	-0.70	0.03
α							1	0.84	-0.72	0.84	-0.47	0.86
n								1	-0.78	1	-0.77	0.64
h_b									1	-0.78	0.63	-0.44
λ										1	-0.77	0.64
b											1	-0.31
K_s												1

Table B-12. Correlation coefficients for Clay

	θ_s	θ_r	p_e	f_c	w_p	awc	α	n	h_b	λ	b	K_s
θ_s	1	0.00	0.93	0.88	0.73	0.76	0.00	-0.01	0.00	-0.01	-0.26	-0.01
θ_r		1	-0.36	-0.38	-0.50	0.13	0.70	0.79	-0.85	0.79	-0.52	0.53
p_e			1	0.96	0.85	0.66	-0.25	-0.29	0.31	-0.29	-0.06	-0.20
f_c				1	0.95	0.55	-0.38	-0.45	0.36	-0.45	0.08	-0.30
w_p					1	0.25	-0.47	-0.63	0.57	-0.63	0.33	-0.32
awc						1	0.09	0.28	-0.38	0.28	-0.63	-0.06
α							1	0.82	-0.61	0.82	-0.46	0.86
n								1	-0.78	1	-0.73	0.64
h_b									1	-0.78	0.67	-0.37
λ										1	-0.73	0.64
b											1	-0.30
K_s												1

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Appendix C: Summary of Water Retention and Conductivity Models

This appendix defines the parameters appearing in the tables of Appendices A and B. The information in this appendix was taken from NUREG/CR-6565 (Meyer et al., 1997).

Richards equation (Richards, 1931) forms the basis for most process-based descriptions of water movement in the unsaturated zone. Richards equation can be expressed as

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left[-K(h)\frac{\partial h}{\partial z} - K(h)\right] + u \qquad \text{(C-1)}$$

where

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

h = soil water tension, $h \geq 0$

z = depth, measured positive downward from the soil surface,

t = time,

$K(h)$ = hydraulic conductivity, and

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

To solve Richards equation, constitutive functions relating the unsaturated hydraulic conductivity and the water content to the pressure head are needed. The most commonly used relationships are those of van Genuchten (1980), Brooks and Corey (1964), and Campbell (1974), although other expressions are available (Mualem, 1992; Rossi and Nimmo, 1994; Fayer and Simmons, 1995).

C.1 Van Genuchten Model

The van Genuchten water retention relationship is

$$S_e(h) = [1 + (\alpha h)^n]^{-m} \qquad \text{(C-2)}$$

where

S_e = effective saturation = $\frac{\theta - \theta_r}{\theta_s - \theta_r}$, $0 \leq S_e \leq 1$

α = curve fitting parameter related to air entry pressure

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

θ_r = residual water content

θ_s = saturated water content

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

$$K(S_e) = K_s\sqrt{S_e}\left[1 - \left(1 - S_e^{1/m}\right)^m\right]^2 . \qquad \text{(C-3)}$$

or

$$K(h) = K_s\frac{\{1 - (\alpha h)^{n-1}[1 + (\alpha h)^n]^{-m}\}^2}{[1 + (\alpha h)^n]^{0.5m}} \qquad \text{(C-4)}$$

where

K_s = saturated hydraulic conductivity

C.2 Brooks-Corey Model

The Brooks-Corey water retention relationship is

$$S_e(h) = \left(\frac{h_b}{h}\right)^{\lambda} \quad \text{for } h \geq h_b \qquad \text{(C-5)}$$

$$S_e(h) = 1 \quad \text{otherwise.} \qquad \text{(C-6)}$$

When combined with the relative permeability model of Burdine (1953), Brooks and Corey derived the following hydraulic conductivity relationship.

$$K(S_e) = K_s(S_e)^{3+2/\lambda} \qquad \text{(C-7)}$$

or

$$K(h) = K_s\left(\frac{h_b}{h}\right)^{2+3\lambda} \quad \text{for } h \geq h_b \qquad \text{(C-8)}$$

$$\text{and } K(h) = K_s \text{ otherwise.} \qquad \text{(C-9)}$$

where

h_b = curve fitting parameter related to air entry pressure

λ = curve fitting parameter related to pore size distribution.

Carsel and Parrish (1988) used the following equivalence between the Brooks-Corey and van Genuchten parameters:

$h_b = \alpha^{-1}$ and $\lambda = n - 1$.

C.3 Campbell Model

Campbell (1974) adopted a water retention relationship similar to Brooks and Corey's, but with $\theta_r = 0$.

$$\frac{\theta}{\theta_s} = \left(\frac{h_b}{h}\right)^{1/b} \quad \text{for } h \geq h_b \qquad \text{(C-10)}$$

$$\frac{\theta}{\theta_s} = 1 \quad \text{otherwise.} \qquad \text{(C-11)}$$

Note that because $\theta_r = 0$, $b \neq 1/\lambda$. Campbell (1974) derived a corresponding hydraulic conductivity relationship.

$$K(\theta) = K_s\left(\frac{\theta}{\theta_s}\right)^{2b+3} \quad \text{(C-12)}$$

or

$$K(h) = K_s\left(\frac{h_b}{h}\right)^{2+3/b} \quad \text{for } h \geq h_b \quad \text{(C-13)}$$

$$\text{and } K(h) = K_s \text{ otherwise.} \quad \text{(C-14)}$$

where

b = curve fitting parameter related to pore size distribution.

Note that all of these single-valued relationships (Equations C-2 through C-14) assume that hysteresis is not important.

C.3.1 Calculation of Campbell's b Parameter

An expression for b in terms of θ_s, θ_r, and λ is derived by assuming that the Brooks-Corey model (Equation C-7) and the Campbell model (Equation C-12) predict the same hydraulic conductivity for a given value of water content. In this case, the water content used is that corresponding to an effective saturation of 0.5. Assuming $S_e = 0.5$ and using the definition of effective saturation given above, it follows that

$$\frac{\theta}{\theta_s} = \frac{0.5(\theta_s - \theta_r) + \theta_r}{\theta_s} = 0.5(1 + \theta_r/\theta_s) \quad \text{(C-15)}$$

Substituting this expression in Equation C-12 and equating this with Equation C-7 leads to

$$(0.5(1 + \theta_r/\theta_s))^{3+2b} = 0.5^{3+2/\lambda} \quad \text{(C-16)}$$

Equation C-16 can be solved for b,

$$b = 0.5\left\{\frac{\ln(0.5)(3 + 2/\lambda)}{\ln[0.5(1 + \theta_r/\theta_s)]} - 3\right\} \quad \text{(C-17)}$$

C.4 Additional Parameters

Several additional soil hydraulic parameters may be required by dose assessment codes. These parameters and the methods by which they were calculated are discussed here.

- Effective porosity, $p_e = \theta_s - \theta_r$
- Field capacity, $f_c = \theta(K = 10^{-8}$ cm/s)

  Field capacity is generally interpreted as the water content at which drainage from a field soil becomes negligible (see the discussion by Hillel, 1980). Field capacity is often calculated as the water content at a specified tension, usually taken to be 340 cm (1/3 bar). Hillel (1980) argues, however, that the field capacity should be based on the drainage rate considered negligible (which is a function of the intended application). Field capacity was calculated here as the water content at which the unsaturated hydraulic conductivity equals 10^{-8} cm/s using the van Genuchten model (10^{-8} cm/s ≡ 3 mm/yr).The value of 10^{-8} cm/s was chosen because it represents a water flux at which contaminant transport is likely to be insignificant. This value also results in somewhat larger field capacity values and a more realistic available water capacity for very coarse textured soils than using the water content at 1/3 bar soil pressure. See Meyer and Gee (1999) for a more detailed discussion of field capacity.
- Wilting point, $w_p = \theta(h = 15{,}300$ cm)

  Wilting point is the minimum water content (or maximum tension) at which plants can extract water from the soil. Wilting point was calculated as the water content at a tension of 15,300 cm (15 bars).
- Available water capacity, $awc = f_c - w_p$

  Available water capacity represents the amount of water available for plant uptake.

C.5 References

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