DEVELOPMENT OF SITE CHARACTERIZATION SIMULATOR SPECIFICATIONS

THESIS

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AFIT/GEE/ENV/96D-07

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Jeffrey L. Heiderscheidt, Captain, USAF

Presented to the Faculty of the Graduate School of Engineering

of the Air Force Institute of Technology

In Partial Fulfillment of the

Requirements for the Degree of

Master of Science in Engineering and Environmental Management

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Jeffrey L. Heiderscheidt

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Abstract

The purpose of this study was to develop a tool for evaluating data quality when characterizing a potentially contaminated groundwater aquifer, and to provide a basis for developing a simulator to allow environmental managers and engineers to practice and learn about the site characterization process. Specifically, this study characterized the uncertainty, estimation block size, and cost for the various methods of determining the value of each geological, hydrological, and contaminant parameter necessary to characterize a site.

Research entailed identifying site characterization objectives and identifying parameters necessary to obtain those objectives. Methods of estimating each parameter were identified, then research was performed to characterize each method.

This research resulted in a list of site characterization objectives and matrices of process parameters, parameter estimation methods, method uncertainties, volumes, costs, applicable model boundary conditions, and references. Fifty transport, storage, and fate parameters were identified along with 85 different estimation methods. Of these methods, 61 were partially characterized and 24 were completely characterized (primarily pertaining to transport). Results were used to define the initial specifications for a site characterization simulator. Considering this research, more study is needed to characterize methods pertaining to storage (except equilibrium sorption) and all fate parameters.

I. Introduction

A. Background

Current methods of characterizing an uncontrolled hazardous waste site consist of estimating certain geological, hydrological, and contaminant parameters throughout the site. The only way to determine these parameters is by analyzing samples from the site. Since budget and time often restrict the number of samples that can be taken, it is important that the right kind of samples be taken from the optimal locations, and that the correct properties be analyzed. More importantly, the reason for acquiring these samples is so that the environmental manager, engineer, or scientist can develop an interpretation of the system. Interpreting this data is the most difficult part of the site characterization process. Due to the complexity of the subsurface environment, experience is the only way to become proficient at interpreting the sample data. A tool assessing the quality of site characterization data and for providing site characterization experience, in a safe and economical way, is needed. This study provides the basis for developing these tools.

B. Purpose

The purpose of this study was to develop a tool for site investigators to use to evaluate data quality, and to provide a basis for developing a simulator to allow environmental managers and engineers to learn and practice the site characterization process. Specifically, this study looked at the geological, hydrological, and contaminant parameters that must be determined to characterize a site. The methods of estimating those parameters (i.e., sampling techniques) and the uncertainty associated with each method was also addressed. In addition, an attempt was made to quantify the *estimation block* and cost of each parameter estimation. The sample estimation block is that volume of media in the actual aquifer site from which the sample is composed, and over which the parameter value, estimated by the sampling method, is averaged. For example, consider a five gram sample removed from a 1000 cm^3 soil core that has been thoroughly mixed after collection; this sample would have an estimation block volume of 1000 cm^3 because the parameter value determined from the sample would effectively be an average value taken from the entire soil core.

C. Research Questions

1. Main Question.

What are the parameters obtained by, and the uncertainties, estimation blocks, and costs associated with different sampling methods used to characterize a hazardous waste site?

2. Sub-questions.

a) What are the objectives to be attained by performing a hazardous waste site characterization (hereafter referred to as site characterization)?

b) What uncertainties are associated with various sampling and analysis techniques?

c) What estimation block volumes are associated with various sampling techniques? That is, what volume of the site does the sample represent?

d) What are the costs of the various sampling and analysis techniques?

e) How can these uncertainties, estimation block volumes, and costs be simulated using computer software in a site characterization simulator?

D. Scope of Study

This study researched the site characterization parameters of both the saturated and unsaturated zones of the subsurface environment. Since contaminants that enter the groundwater may come from sources in the vadose zone or above ground, it is important to model the parameters of the vadose zone when characterizing a site.

This study consisted of reviewing data and results of past experiments and studies. No experimentation was conducted to generate new data about the parameters of interest. This study identified potential areas of site characterization that require additional experimentation to properly quantify the associated uncertainties and estimation block volumes.

E. Significance of Study

The Air Force's Armstrong Laboratory/Environics Division is interested in developing a software application that will simulate the site characterization process. Air Force personnel will be able to gain experience in site characterization through training with this software. It will give environmental managers the opportunity to practice choosing where to sample, what types of samples to take, and how many samples should be taken, all within a constrained budget. Additionally, it will help personnel learn to interpret sample data into a conceptual model of the site, and into a quantitative, mathematical model that is necessary for testing the conceptual model.

However, before the software can be developed, this study must be completed to provide the data on the various parameter estimation methods so they can be modeled within the computer software. The data obtained by this study are the key to developing a realistic simulator. By incorporating realistic characteristics (i.e., uncertainty, estimation block, and cost) of common parameter estimation techniques, the simulator can provide useful, realistic experience to environmental managers.

Additionally, this data may be very useful to anyone modeling a site. The matrices of parameter estimation methods match parameters with contaminant fate and transport processes. They also provide valuable information about the approximate uncertainty and estimation block size of the various methods. This is important when determining how to apply a field data value to a model parameter. The approximate values of uncertainty may also be useful in providing a reasonable range over which to vary parameters during sensitivity analysis of the model. In general, the results of this study will be useful in helping investigators to interpret sampling data, by helping them to make determinations about the quality and representativeness of that data.

F. Overview

This thesis consists of four more chapters. Chapter II is a review of the general literature concerning groundwater site characterization. Chapter III contains the methodology and results of obtaining characteristics of parameters and methods used in site characterization. Chapter IV contains the methodology and results of determining how to model the parameters and methods in a software simulator, along with the model specification to be used in the next step of developing the simulation software. Finally, Chapter V contains conclusions about this research, and recommendations for further study and development of the simulation software.

The appendices of this thesis contain a variety of data about site characterization. Appendix A contains a list of the titles and Standard numbers of those American Society for Testing and Materials standards that relate to site characterization (ASTM, 1996). Appendix B is a list of typical site characterization objectives. Appendices C through F contain matrices of parameter estimation techniques and their associated general references, uncertainties, estimation block sizes, and costs, respectively. Appendix G contains a matrix of possible boundary conditions that can be applied to a mathematical model of a site. Appendix H contains formulas for calculating the estimation block size for those methods where it is dependent upon method construction or existing parameter values at the sampling location. Finally, Appendix I contains formulas for calculating the cost for those methods where it is dependent upon method construction or existing parameter values at the sampling location.

II. Literature Review

The purpose of the literature review is to introduce the general process of site characterization, and to describe its inherent difficulties and the lack of research concerning its uncertainties. This review also covers the role that experience plays in reducing uncertainties, and the need for economical methods of obtaining experience.

A. Site Characterization Process

Melville et al. (1991) and Standard D5730-95a (ASTM, 1996) describe site characterization as the process of determining if a potential environmental problem exists at a particular site and, if so, obtaining enough data about the site to allow a detailed remediation design. Site characterization is an iterative process, as shown in Figure 1. There is no pre-established number of iterations to perform, and no pre-defined endpoint. Site characterization is a continuous process throughout the remediation of the site.

The top loop of Figure 1 is outlined in Standard D5730-95a (ASTM, 1996). The initial step is to determine why the site must be characterized. After clear objectives have been defined, existing data is gathered about the contaminant, the site hydrogeology, and the applicable fate and transport processes. This existing data is used to create a conceptual model of the site. The conceptual model is then compared to the objectives to ensure compliance with initial goals, and to identify data gaps. A sampling plan is created and implemented to fill any data gaps, and the conceptual model is updated. This process is repeated until there is enough data to create a mathematical model from the conceptual model.

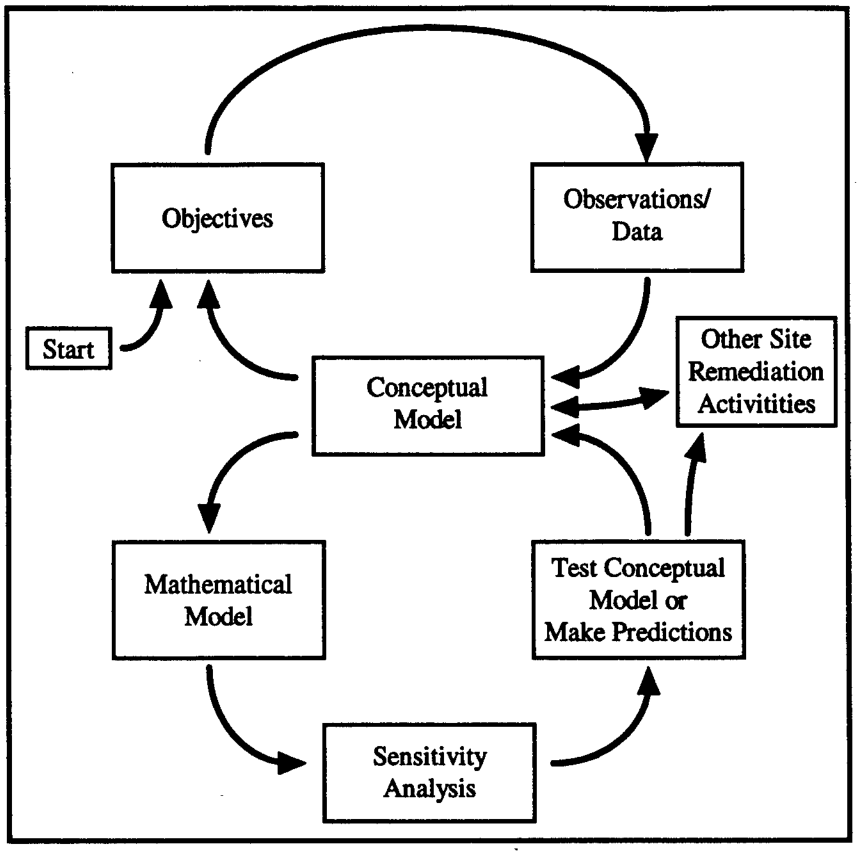

Figure 1: Site Characterization Process

Standard D5447-93 (ASTM, 1996) outlines the bottom loop of Figure 1. A mathematical model is created from the processes and parameter values defined in the conceptual model. After creating a mathematical model, an analysis is done to determine how sensitive the model is to the value of each parameter. This step gives the modeler a better understanding of how the modeled system behaves. Next, the modeler uses the mathematical model to test the conceptual model. This is accomplished by forming a hypothesis about how the system is believed to behave based on the conceptual model, and then comparing the response of the mathematical model to that hypothesis.

After testing the conceptual model, the process moves back to the top loop to either refine the conceptual model, if testing was unsuccessful, or to ensure that the original objectives have been met. At this point, the investigator repeats the entire process (gathering new data, refining both models, testing the conceptual model, and reviewing the objectives) as necessary. Only after the conceptual model represents the real system to the degree required by the objectives, can other site remediation activities proceed (Domenico and Schwartz, 1990). However, even after other site remediation activities begin, site characterization does not end. Remediation activities could affect the parameters or processes of the system making the models invalid. Additionally, an investigator can continue to learn more about the site by perturbing the model and analyzing the response of the modeled system. Therefore, the conceptual and mathematical models need to be updated as other site remediation activities occur.

B. Objectives of Site Characterization

The initial step is to determine the objectives of the site characterization. In order to scope and direct the sampling and subsequent modeling efforts, it is important to know why the site needs to be characterized and to understand what knowledge is hoped to be learned from it. For this reason, a complete set of well-defined objectives is critical to the success of the site characterization. Examples of some general, starting objectives are:

- Has contamination occurred? (Ford and Turina, 1985)
- Where is the contamination located? (Ford and Turina, 1985; Domenico and Schwartz, 1990)

- What is the source of the contamination? (Ford and Turina, 1985; Domenico and Schwartz, 1990)
- What are the properties of the contaminant? (Domenico and Schwartz, 1990; Bedient et al., 1994)
- What are the site-specific environmental characteristics? (Domenico and Schwartz, 1990; Bedient et al., 1994)
- Where is the contaminant likely to go, and how will it get there? (Ford and Turina, 1985; Domenico and Schwartz, 1990; Bedient et al., 1994)

As examples, some of these objectives are rather general. In an actual site characterization the more specific the objectives, the more efficient the characterization process and the more useful the result will be.

C. Importance of Modeling

Once the objectives are clearly defined, the remainder of the process involves modeling the site and all applicable processes. There must be at least a preliminary model of the site before any drilling or sampling can occur; therefore, site characterization always results in the creation of a conceptual model (Preslo and Stoner, 1991). A conceptual model represents an understanding of the current state of the real-world system being modeled (Dagan, 1986). It is a clear, qualitative, physical description of the operation of the system and incorporates all properties and processes of the system that are relevant to the objectives of the study. A well-defined conceptual model clearly shows what the system looks like today, and identifies the processes that will affect how the system looks in the future (van Genuchten et al., 1988). It provides an understanding of the potential contaminant plume migration within the subsurface environment (Franke et al., 1987; Domenico and Schwartz, 1990; Bedient et al., 1994).

However, the conceptual model is essentially qualitative. It describes the dominant processes of a system and may contain values for various subsurface parameters; but there is no way to test the conceptual model by itself to determine if it adequately represents the processes of the real site. To test the conceptual model, a quantitative, mathematical model must be created (Dagan, 1986; van Genuchten et al., 1988; Fogg et al., 1995).

A mathematical model represents the real system through a series of mathematical equations and procedures (Franke et al., 1987). Processes and parameter values identified in the conceptual model are used to create the mathematical model. By comparing the response of the mathematical model to the expected behavior of the real system, the investigator can determine if the processes and parameters identified in the conceptual model are valid. The actual values determined by the mathematical model (e.g., hydraulic head or contaminant distribution) may not match true values in the site. However, the general behavior of the mathematical model should match the expected behavior of the real system, if the conceptual model adequately represents the important processes.

Along with testing the conceptual model, van Genuchten et al. (1988) state that mathematical models are becoming a useful tool for predicting the response of a system to future stresses, such as those that might occur as a result of remedial actions such as pumping. The usefulness of such predictions depends on the degree to which the modeled processes, parameters, and boundary conditions represent the significant characteristics of the system (van Genuchten et al., 1988; Rogers, 1992). Fogg et al.

(1995) agree that the major constraint on the application of a mathematical model is the calibration, and suggest that most predictions are inaccurate.

Konikow (1986) argues that although mathematical models may not provide accurate predictions, their primary value is in "providing a disciplined format to improve one's understanding of the aquifer system." By performing a sensitivity analysis on the model parameters, one can gain a better understanding of the processes involved in a particular system. The sensitivity analysis will also help determine which parameters have the most significant effects on the behavior of the model, and therefore the real system (Fogg et al., 1995). This analysis improves the site characterization process by pointing out what parameters should have resources allocated to their estimation.

D. *Difficulties in Site Characterization*

Before beginning to allocate scarce resources toward a site characterization effort, it is important to understand the uncertainties and difficulties inherent to the site characterization process. In an extensive review of the literature, only one systematic review of factors leading to uncertainty in groundwater data was found. The study was qualitative in nature, because there was scarcely any published data upon which to base qualitative estimates of sample uncertainty and bias (Gillham et al., 1983). Therefore, the study reviewed the various procedures used to acquire groundwater samples and described the sources of uncertainty for each. Since that time, there have been a few efforts to quantify some of these uncertainties; however, the results have not been collected and compiled into a single study.

Site characterization is a very difficult process. The subsurface environment is generally very heterogeneous; hydrogeologic properties usually vary dramatically through space (McLaughlin et al., 1993; Wolf, 1994). Besides site heterogeneity, there are a number of other factors that make site characterization a difficult process:

- The contaminant source flux can vary with time (Mercer and Faust, 1980; Wolf, 1994).
- The location, time, and composition of the source are often unavailable due to a lack of records about the source (Mercer and Faust, 1980; Mackay et al., 1986b; McLaughlin et al., 1993).
- Aquifer recharge can vary with time (McLaughlin et al., 1993: Wolf, 1994).
- Chemical reactions can affect contaminant transport (McLaughlin et al., 1993: Wolf, 1994).
- Sorption of the contaminant can affect its transport (McLaughlin et al., 1993).
- Determining hydrogeologic properties and contaminant concentrations can be cost prohibitive (McLaughlin et al., 1993).
- Parameter properties can usually only be observed at relatively few sampling locations, because the site being characterized is underground (Konikow, 1986; Mackay et al., 1986b; McLaughlin et al., 1993).
- Dominant fate and transport processes may be poorly understood (Mercer and Faust, 1980; Mackay et al., 1986b)

Additionally, a mathematical model, which is required for testing the conceptual model or attempting to predict future system responses, requires that parameter values be specified for all points in the model. Traditionally this was done by determining a parameter value at some point in the system, assuming the system to be homogeneous and isotropic, and then applying the parameter value to all points of the model (Yeh, 1986).

Modeling techniques have had to be improved to consider real world heterogeneities. Yeh (1986) discusses various modeling techniques that allow specification of parameter values at every point in the system, as required by the mathematical models, based on values obtained at relatively few sampling locations throughout the site. Different methods use different statistical techniques to estimate parameter values. Yeh (1986) found that method performance varied significantly under different scenarios, indicating that the method chosen to estimate parameter values has a large impact on the results obtained from the mathematical model.

Another requirement for creating a mathematical model is to define boundary and initial conditions. Identifying appropriate boundary conditions and choosing proper values for initial conditions is essential to modeling groundwater systems; it is also the part where modelers are most prone to make serious errors (Franke et al., 1987). The importance of parameter values and boundary conditions can best be illustrated by some examples.

Sudicky et al. (1983) performed a field tracer study at the Canadian Forces Base, Borden, Ontario that has been extensively studied and characterized. The goal of the study was to experimentally examine the scale dependence of dispersion. Following the tracer experiment, a computer model was used to simulate the experimental results. During the tracer experiment, the plume unexpectedly split into two distinct halves moving at different rates. Sudicky et al. (1983) were not able to determine the nature of the heterogeneity that caused the split from field data obtained before, during, or after the experiment. To model the experimental results, they had to use a "parameter fitting procedure that is itself somewhat inconsistent with the basis of the underlying theory" (Sudicky et al., 1983).

Konikow (1986) evaluated a model created in 1965 to predict the response of an aquifer in the Salt River and lower Santa Cruz River basins of central Arizona to continued high volume pumping. Konikow (1986) compared ten years worth of data (1965-1974) to the predictions made in 1965 by the original model. He found the predictions of the original model were drastically different from the data of the next ten years. Konikow (1986) attributed the discrepancy to the use of incorrect boundary conditions in 1965.

McLaughlin and Johnson (1987) compare three independent studies, commissioned with the same objectives, for the same region of the San Juan basin of New Mexico. The three studies resulted in significantly different results, with estimated aquifer drawdown differing by as much as 183 meters. Although the three studies had access to the same site data, they each determined different boundary conditions and aquifer parameter values from that data.

Finally, Freyberg (1988) had groups of graduate students at Stanford University calibrate a numerical groundwater flow model to a set of perfectly observed head data. All groups used the same model and identical sets of observed data. The groups differed in how they used this data to estimate aquifer parameters throughout the model. After calibrating the model, each group used their calibrated model to predict the response of the aquifer to a new pumping well. Again each group used the same data about the pumping well. Results showed that the predicted response varied significantly between groups. The group whose calibrated model most closely matched the initial head distribution, resulted in the worst prediction. On the other hand, the group whose model resulted in the best prediction, had one of the poorest matches to the initial head distribution.

E. Need for Experience

The previous sections demonstrate that much of the site characterization process relies on the judgment of the investigator. The process of site characterization, and concurrent modeling of the site, requires the investigator to make many assumptions at every stage of the process. Some of those assumptions include: what the dominant processes are, what parameters should be estimated, and how those parameters should be estimated. Ultimately, these assumptions must often be based on the modeler's subjective interpretation of very limited amounts of uncertain field data (McLaughlin and Johnson, 1987). How an investigator interprets the field data will affect how the model responds. Therefore, the modeling process (and the site characterization process in general) is very dependent on the judgment of the investigator. A person's judgment, in turn, is quite dependent upon that person's experience. Faust and Mercer (1980) remind us that even the "selection of the 'truest' model is a subjective task that must be done by the modeler." There are many types of models available; selection depends upon which processes are assumed to dominate. The investigator must recognize what is happening at the site to be able to choose the best model.

The group with the best prediction in Freyberg's (1988) study had actually done one of the best jobs of estimating the value of the hydraulic conductivity throughout the model. Successful prediction relied on proper characterization of site parameters, not on correctly calibrating the model to match observed initial heads in the unmodified aquifer. Conversely, closely matching the observed heads did not mean that the site parameters had necessarily been estimated correctly. Considering the results of most of the student groups, this fact was not intuitively obvious. The experience gained by these students, through simulation, ought to be invaluable when they must characterize a real site.

Gillham et al. (1983) point out that the subsurface is generally heterogeneous with extreme variations in conditions from one site to another; therefore, there can be no automatic method of defining the appropriate sampling scale for a particular investigation. Initial judgments must be based on experience and available information about a particular problem (Gillham et al., 1983). Clearly there is a need for investigators to gain experience in site characterization. However, there is currently no fail-safe, economical way of doing so. While universities and continuing education can provide some training, on-the-job experience is the primary mechanism for gaining experience in site characterization. On-the-job experience is a very valuable, but expensive and potentially dangerous way to learn from mistakes.

The results from Freyberg's (1988) exercise illustrate the need and potential usefulness of a site characterization simulator. Experience gained by using such a simulator would almost certainly improve the degree to which an investigator's conceptual and mathematical models correspond to the actual site. The development of better models leads to more effective use of limited site characterization funds. Creating better models forces investigators to gain a better understanding of the systems. A better understanding helps the investigators spend money on samples that are more useful and are obtained from more suitable locations than would otherwise be possible (Bedient et al., 1994). Additionally, better models would improve remediation system designs and increase the effectiveness of remediation efforts.

III. Results: Characteristics of Parameter Estimation Methods

A. Methodology

This part of the study consisted of an extensive literature search. Data were acquired from peer-reviewed journal articles, EPA manuals, ASTM standards, conference proceedings, reports (e.g. Pacific Northwest Laboratory, U.S. Geological Survey, American Petroleum Institute, U.S. Army Corps of Engineers Waterway Experiment Station, U.S. Air Force Civil Engineer and Services Agency), and hydrology textbooks. Information was collected regarding the objectives of site characterization and various methods for estimating the values of aquifer hydrogeological parameters and contaminant characteristics; including method specific measurement uncertainties, sample estimation block size, and approximate costs. If no information could be found pertaining to the uncertainty, estimation block, or cost of a particular estimation method for a parameter, that parameter estimation method was indicated as a candidate for further study

The articles were used to determine common site characterization objectives and to create a series of matrices of subsurface parameters and methods of estimating those parameters. The parameters were categorized by the hydrologic processes that they influence. The first matrix lists general references for each parameter estimation method. If studies have determined that a parameter's uncertainty is based on the estimation method, the uncertainty of that method is listed in the second matrix along with the references used to determine that uncertainty. The estimation block for each method of estimating each parameter is listed in the third matrix along with references regarding the estimation block. The fourth matrix lists an approximate cost (or cost function, if the cost depends on soil or sampling method construction parameters) for each parameter estimation method along with the references pertaining to the cost. The estimation block and cost of a particular parameter estimation method are often a function of hydrogeologic parameters other than that being estimated; they can also be a function of the construction parameters of the estimation method (e.g., monitoring well screen length). The estimation block or cost, for those estimation methods, is listed as a mathematical function instead of an absolute range or value. The final matrix contains common boundary conditions, used in modeling a site, along with reference describing the application of each boundary condition.

If no information could be found that discussed estimation block size for a given method of estimating a parameter, an attempt was made to calculate a reasonable estimation block volume for that method. The estimation block volume was calculated in terms of other parameters as necessary, such as porosity or sampling well screen length.

B. Summary of Data Found

Approximately 85 sources were used to obtain the data found in Appendices C through F; 72% of these sources were peer-reviewed. In addition, 23 separate ASTM standards were used, but are included in the above numbers as one source. Table 1 indicates for which parameter estimation methods data was obtained. Each method for which estimation block data was found has a reference number assigned in the last column, corresponding to the x-axis (rank) of Figure 2 in Chapter IV, Section B.

Table 1: Summary of Estimation Method Found

Parameter	Sym.	Estimation Method	Data Found			E.B.
			Uncert.	E.B.	Cost	Ref.
Water Content in Vadose Zone	θ_v	Gravimetric analysis of soil core		x		13
		Drying soil sample	x	x	x	14
		Neutron probe	x	x	x	23
		Tensiometry (in-situ)	x	x	x	2
Darcian Flux (vertical)	q_z	Infiltration rate, from historical data				
		Double-ring infiltrometer		x	x	20
		Water balance				
Hydraulic Conductivity (z)	K_z	Column test on soil core (steady-state head control)	x	x	x	13
		Unsaturated flow apparatus (UFA™) test on soil core	x	x		1
		Estimate from soil parameters and soil/water retention curves	x			
Soil Type (Classification)		Soil core		x	x	14
Subsurface Lithology		Soil core		x	x	15
		Cone penetrometer (resistivity)	x	x	x	11
		Electrical conductivity (direct-push)		x	x	7
Average Soil Grain Size		Soil core (sieve analysis)		x	x	14
Depth to Water Table		Monitoring well installation or soil boring		x	x	24*
		Cone penetrometer (dynamic pore pressure)		x	x	3
		Advanced geophysical techniques			x	
Depth to Confining Layer		Soil boring		x	x	24*
		Cone penetrometer (resistivity)		x	x	11
		Advanced geophysical techniques			x	
Water Content in Saturated Zone	θ_W	Estimate from soil type		x	x	14
		See above, under Water Content in Vadose Zone				
Effective Porosity (equals Water Content in Saturated Zone, if no separate phase)	n	Soil core (drainable porosity combined with grain size)	x	x	x	14
		Tracer experiment (soil core)		x		4
		Two-well tracer experiment (field)		x	x	28*
		Single-well tracer (drift and pumpback)		x	x	26*
Darcian Flux (x-direction)	q_x	Water balance				
Hydraulic Head	h	Wells (piezometers), drilled installation	x	x	x	24*
		Wells, direct push installation		x	x	19
		Cone penetrometer (dynamic pore pressure)		x	x	3
Isotropic 1-D Hydraulic Conductivity (x and y-directions)	K_r	Slug test	x	x	x	27*
		Single-well pump test with impeller flowmeter in borehole	x	x		22*
		Single-well tracer (drift and pumpback)		x	x	26*
		Lab column permeameter test on soil core (based on K_Z)	x	x	x	10
		Cone penetrometer (dynamic pore pressure)		x	x	3
		Qualitative based on soil type	x	x	x	18*
		Regression on grain size distribution	x	x	x	14
Anisotropic 1-D Hydraulic Conductivity (x-direction)	K_x	Pump test with observation wells aligned in x-direction	x	x	x	30*
		Field tracer test with observation wells in x-direction		x	x	28*
		History matching (parameter estimation model, based on hydraulic heads)	x	x		29*

Table 1 (Continued): Summary of Estimation Method Found

Parameter	Sym.	Estimation Method	Data Found			E.B.
			Uncert.	E.B.	Cost	Ref.
Anisotropic 1-D Hydraulic Conductivity (y-direction)	K_y	Pump test with observation wells aligned in y-direction	x	x	x	30*
		Field tracer test with observation wells in y-direction		x	x	28*
		History matching (parameter estimation model, based on hydraulic heads)	x	x		29*
Horizontal Longitudinal Dispersion Coefficient	D_L	Laboratory column experiment (electrical conductivity)		x	x	6
		Tracer experiment (soil core)		x		4
		Tracer experiment (field)		x	x	28*
		Moment analysis of plume data (if plume is well known)		x		29*
		Estimate from textbook using grainsize and v_X				
Horizontal Transverse Dispersion Coefficient	D_T	Laboratory column experiment (electrical conductivity)		x	x	6
		Tracer experiment (soil core)		x		4
		Tracer experiment (field)		x	x	28*
		Moment analysis of plume data (if plume is well known)		x		29*
		Estimate from textbook using grainsize and v_Y				
Vertical Transverse Dispersion Coefficient	D_Z	Laboratory column experiment (electrical conductivity)		x	x	6
		Tracer experiment (field)		x	x	28*
		Moment analysis of plume data (if plume is well known)		x		29*
		Textbook value based on grain size				
Water Velocity in x-direction (q/n)	v_X	Tracer experiment	x	x	x	28*
		Heat sensor groundwater velocity detector (in-situ Perm. Flow Sensor)	x	x	x	16
Water Velocity in z-direction (q/n)	v_Z	Heat sensor groundwater velocity detector (in-situ Perm. Flow Sensor)	x	x	x	16
Tortuosity	τ	Look up in table based on soil type and grain size				
Diffusion Coefficient	D	Look up for free liquid and adjust by tortuosity				
		Tracer experiment		x	x	28*
		UFA™ analysis of soil core (for vadose zone D)	x	x		9
Retardation Factor	R	Partitioning tracer experiment	x	x	x	28*
		Moment analysis of plume data	x	x		29*
		<<< or calculate using parameters for each process below >>>	x			
Soil Bulk Density	ρ_B	Laboratory analysis of soil core	x	x	x	14
Sorption Coefficient	K_d	Laboratory batch experiment (isotherm)	x	x		14
		Laboratory batch experiment (1-point)	x	x		14
		Column experiment or box model		x		5
Fraction Organic Content	f_{OC}	Laboratory analysis of soil core	x	x		14
		Literature value based on soil type				
Concentration in Water	C_W	Cone penetrometer (membrane sensor)	x	x	x	3
		HydroPunch® sample	x	x	x	17*
		BAT® sampler	x	x	x	8*
		Monitoring well, via pumping	x	x	x	25*
		Monitoring well, via bailer	x	x	x	25*
		Monitoring well, via thief sampler	x	x	x	12*
		Multi-level sampler	x	x	x	25*

Table 1 (Continued): Summary of Estimation Method Found

Parameter	Sym.	Estimation Method	Data Found			E.B.
			Uncert.	E.B.	Cost	Ref.
Concentration in Air	C_A	Soil gas		x	x	21*
		Cone penetrometer	x	x	x	21*
		Fixed gas sampling well		x	x	21*
Concentration in Soil	C_S	Soil core, via drilling		x	x	14
		Soil core, via direct push		x	x	15
		Estimate from historical data				
Concentration in NAPL	C_N	Estimate from historical data and contaminant properties				
Effective Dispersion Coefficient	D_{eff}	Moment analysis of plume data (see D_T, D_L, and D_Z)		x		29*
		Literature value				
Desorption Rate Coefficient	k_2	Laboratory column experiment				
		Regression equation				
Fraction of Fast Sorption Sites	F	Laboratory column experiment				
Effective Diffusion Coefficient	D_S	Laboratory batch experiment		x		14
		Literature data based on diffusion coefficient (D), tortuosity, and average				
Air Content	θ_A					
Henry's Constant	H	Look up in table				
NAPL Content	θ_N	Partitioning tracer experiment		x		28*
		Neutron probe	x	x	x	23
		Advanced geophysical techniques			x	
		Estimate from historical records				
Water/NAPL Partition Coefficient	K_{NW}	Laboratory batch experiment		x		14
		Calculate from $\underline{v}_N$ and S_{SCL}				
Avg Molar Volume of NAPL	$\underline{v}_N$	Estimate from chemical make-up of NAPL, if known				
Hypothetical Super-Cooled Liquid Solubility	S_{SCL}	Look up in table				
Decay Rate in Aq. Phase	k	Experimentally derived (batch studies)	x			
		Zero moment analysis of field data				
		Conservative tracer experiment			x	
		Microbial counts				
Correction Factor	b	Non-linear regression on field or experimental data				
O_2 (e- acceptor) Solubility		Look up in table				
O_2 (e- acceptor) Flux Into System		Estimate				
O_2 (e- acceptor) Concentration		Water sample			x	
		Estimate				
Irreversible Sorption		Experimentally derived isotherms				
Oxidation State of Metal	Z	Look up in table				
		Estimate				
Solubility Product	K_{SP}	Look up in table				
		Estimate				
Water Flow to/from System		Estimate flow from surface water and to lower aquifer				
Volatilization		Measure concentration profile in vadose zone				
		Measure flux at ground surface directly				
		Look up in literature				

An asterisk in the last column of Table 1 indicates that installation or site parameters had to be assumed to calculate a typical estimation block volume for comparison. The various assumptions used are listed below.

Hydraulic conductivity = 0.0072 cm/s
Hydraulic gradient = 0.04
Porosity is 0.30
20 m thick aquifer
10 m thick vadose zone
Wells penetrate 20 m below ground
10 cm diameter wells
2 m screened interval
10 m between wells
4 wells used for history matching (equally spaced at corners of square)
Soil type determined by taking a 61.0 cm tall soil core every 5 m vertically
Multi-level sampler (MLS) has eight 25 cm screened sections
Pump rate for multi-level sampler is 5 cm^3/s
MLS is pumped for 30 min (purge + sample)
Air content at point of soil gas samples is 0.20
10,000 cm^3 of soil gas removed for soil gas samples (purge + sample)
Pump rate for pump test is 633 cm^3/s (10 gpm)
Pump rate for borehole flowmeter method is 633 cm^3/s (10 gpm)
Time length of a borehole flowmeter sample is 30 sec
Vertical distance between borehole flowmeter readings is 15 cm
Volume of tracer injected for tracer tests is 500,000 cm^3
Extraction rate for two-well tracer test is 633 cm^3/s (10 gpm)
Time before extracting tracer in single-well tracer test is 5 days

C. Results

1. Objectives of Site Characterization

Determining the objectives is the most important step of the site characterization process. The objectives are what will guide what questions are to be answered, what types of samples are needed to answer those questions, and how many samples are needed to reduce uncertainty to an acceptable level. The possible objectives of any given site characterization effort are unlimited. Choosing the right objectives is very important since it will result the most effective use of limited site characterization funds.

According to Curtin (1996) and Standard E1689-95 (ASTM, 1996), there are four main objectives that the site characterization process must answer:

- What contaminant exists and where it is coming from (the source)?
- How could the contaminant pose a threat (the exposure pathways)?
- How will the contaminant get there (the transport)?
- What are the initial and boundary conditions for modeling the site?

These must be further broken down into more specific questions. Appendix B contains a list of the four general objectives, along with examples of more specific sub-questions. The specific sub-questions shown are some of the more common objectives that drive many site investigations. The data required to answer these questions are essential to developing a clear understanding of what processes and parameters are significant.

2. Uncertainty of Estimation Methods

a) Sources of Uncertainty

According to Zemo et al. (1995), sources of uncertainty in estimates of parameter values can be broken into four categories:

- Variability due to sample location (spatial)
- Variability due to the act of sampling (sampling)
- Variability due to the subsequent analysis of the sample (analytical)
- Variability due to the sampling method (method)

(1) Spatial Uncertainty

The effect of spatial variability varies dramatically from one site to another, as illustrated by comparing the results of three studies performed to determine the hydraulic conductivity at three different subsurface sites. All three studies used the same laboratory permeameter method to estimate hydraulic conductivity from intact soil cores obtained from the respective sites. Two of the study sites, Borden (Sudicky, 1986) and Otis Air Force Base on Cape Cod, Massachusetts (Hess et al., 1992), are considered to be quite homogeneous. The third study site, the macrodispersion experiment (MADE) site of Columbus Air Force Base, Mississippi, is considered to by very heterogeneous. The results of these three studies are summarized in Table 2.

Table 2: Effect of Spatial Variability on Hydraulic Conductivity

Site	Geometric Mean K (cm/s)	Mean of ln(K) (cm/s)	Variance of ln(K)	Total CV (%)	Reference
Borden	0.0072	-4.934	0.29	+/- 10.9	Sudicky, 1986
Cape Cod	0.035	-3.352	0.14	+/- 11.2	Hess et al., 1992
Columbus	6.13×10^{-5}	-9.7	5.5	+/- 24.2	Rehfeldt et al., 1992

The coefficient of variation (CV) is essentially a relative standard deviation that accounts for differences in the magnitude of the mean. The equation for calculating the coefficient of variation is $CV = (\sigma/\mu)*100\%$. Where σ is the standard deviation and μ

is the mean value (Skoog and Leary, 1992). In this case, the standard deviation and mean values are of the natural log of the hydraulic conductivities.

Both the Borden and Cape Cod site are considered quite homogeneous and resulted in very similar coefficients of variation. To get an idea of how much larger the spatial variability is at the Columbus site, take sampling and analytical uncertainties to account for half the total uncertainty for the Borden and Cape Cod sites. Then, if the inherent uncertainty of the laboratory permeameter method contributes half of the total uncertainty for these two sites (approximately +/- 5.5%), it can be seen that spatial variability at the Columbus site accounts for over four times as much of the total uncertainty as compared to the Borden and Cape Cod sites.

Sudicky (1986), Hess et al. (1992), and Rehfeldt et al. (1992) reported the geometric mean and the variance of the natural logs of the hydraulic conductivities because statistical analyses supported the hypothesis that the data came from lognormally distributed populations. This is typical of environmental parameters estimated without excluding spatial uncertainty. Gilbert (1987) points out that environmental data usually can not have a value less than zero and is often skewed to the right when graphed, with a long tail toward high values. The largest source of uncertainty is usually due to spatial variability, which is a result of the heterogeneity of the subsurface environment (Dagan, 1986, Yeh, 1986). Therefore, when spatial variability is included in the total uncertainty, it often overpowers the other sources of uncertainty and results in a lognormally distributed population for total uncertainty.

(2) Sampling and Analytical Uncertainty

Uncertainties due to the act of sampling and laboratory analysis (excluding spatial variability) are generally due to random human errors or instrument fluctuations; these types of errors are typically distributed normally (Skoog and Leary, 1992). They can be a result of disturbing or contaminating a sample while obtaining and analyzing it. Another common source of these types of uncertainties is the analytical uncertainties associated with the analytical equipment; analytical equipment has an associated detection limit, accuracy, and precision.

(3) Method Uncertainty

Uncertainty due to the sampling method is actually a combination of the other three. Each sampling method estimates the parameter value based on an average obtained over a different volume of the site (estimation block). Additionally, each method physically disturbs the sample in a different way, or is affected by other hydrogeologic factors, which can have varying effects on the estimated value. Finally, each method has different analytical detection limits and uncertainties depending on the equipment involved.

b) Representation of Uncertainty Sources in this Study

All four sources of uncertainty have been quantified in the matrices located in the appendices of this study. Spatial variability is accounted for by knowing the estimation block of each parameter estimation method. Sampling and analytical uncertainties are combined in the value for uncertainty listed for each method. Uncertainty due to a particular method then is a combination of the listed estimation block and uncertainty for that method.

Breaking the total uncertainty up this way makes sense because it closely matches reality. Uncertainty due to sampling and analysis is random and can therefore be reduced by making multiple estimations from a single sample. Spatial uncertainty is more a function of the site and how much of the site a particular method sees at one time. More readings from the same location with a particular method will not reduce the size of the estimation block, so it will not reduce the spatial uncertainty. Hereafter, the term uncertainty will mean the combined sampling and analytical uncertainties. Spatial uncertainty will be referred to as such. Total uncertainty (or method uncertainty) will refer to a combination of all three.

c) General Results

Studies were identified that had determined uncertainties for different parameters using different sampling methods. Ideally, studies were found that had performed multiple estimations on each sample or made multiple parameter estimations at the same location, so that spatial uncertainty was removed and only sampling and analytical uncertainties were included.

Additionally, many studies looked at a particular parameter for multiple analytes within a sample (e.g., concentrations of different chemicals). Other studies used the same method to estimate a parameter value on multiple substrates (e.g., hydraulic conductivity of different soil types). In many cases, the uncertainty of a particular method depended on specifically what the analyte or substrate of interest was. For example the method may be very precise at determining the hydraulic conductivity in sandy soils, but not so precise in clayey soils. Most studies assumed a normal distribution and reported mean values and standard deviations.

For the purposes of this study, uncertainties from previous studies had to be averaged. The result is a tool reporting approximate uncertainties, making the tool more useful by being general instead of very site specific. To allow the averaging of results, the uncertainties from all studies were converted to coefficients of variation. This was done for each analysis within each study. The coefficients of variation for multiple analyses using the same method, within the same study, were then averaged. Finally, the coefficients of variation from all studies that looked at the same method for the same parameter were averaged to obtain an estimate of the uncertainty for that method. In some cases, the uncertainties determined in different studies varied dramatically; in these cases a range of uncertainty is reported. The differences are typically a result of using slightly different equipment or a slightly different experimental setup while still using basically the same parameter estimation method. The results are shown in Appendix D, where uncertainty generally refers to the coefficient of variation.

An estimate of the absolute uncertainty for a particular sample can be determined by assuming the measured value is the mean and multiplying it by the uncertainty shown in Appendix D. The result is an estimate of what the standard deviation would be, if multiple measurements were made.

d) Analysis of Uncertainty Data

Four types of uncertainty data were obtained to be used in estimating the uncertainty of each parameter estimation method. The types, and the percentage of methods for which data was found of that type, are:

- Single source stating an actual value for uncertainty of a method (excluding spatial) (11%)
- Multiple studies in good agreement with each other (36%)
- Multiple studies in poor agreement with each other (17%)
- Single study (36%)

There were a few estimation methods for which a source was found that provided an actual value for the uncertainty of the method. In these cases, nothing was done to the data; it is merely reported in Appendix D. Sources of this type included ASTM standards and articles about new estimation methods that have been tested for the express purpose of determining the uncertainty. Methods falling in this category are Unsaturated Flow Apparatus (UFA) for dispersion coefficient, neutron probe, cone penetrometer (resisitivity), and vadose zone water content via drying soil sample.

When multiple studies were found to be in good agreement about the uncertainty of an estimation method, an average value was determined and recorded in Appendix D as the uncertainty for that method. Additionally, when only a single study could be found, the uncertainty from that study was recorded in Appendix D. Methods for which these types of data were used can be identified in Appendix D as having a single value for uncertainty and multiple references or a single reference.

There were some cases where multiple studies were located but found to have considerably different values for the uncertainty of the estimation method being examined. In these cases, there were two approaches taken. First, if there were only two studies or if the values were pretty well spread out over a large range, the high and low values were recorded in Appendix D to represent the range of possible uncertainties for that method. Second, if the uncertainties from the various studies appeared to fall in groups (e.g., a couple low ones close together, and a couple high ones close together), the lowest group was averaged and the highest group was averaged. These two average values were then recorded in Appendix D to represent the range of possible uncertainties for that method. Methods for which this type of data was used can be identified in Appendix D as having a range listed instead of a single uncertainty value.

e) Exceptions

(1) Hydraulic Gradient

The uncertainty of measuring the hydraulic gradient is not listed as a coefficient of variation. This measurement is typically as simple as reading the depth off a ruler. Therefore, the uncertainty is a factor of the smallest unit of measurement available on the measuring tape. Barcelona et al. (1985) and Standard Method D4750-87 (ASTM, 1996) report that commonly available measuring tapes are accurate to 0.3 centimeter.

(2) Hydraulic Conductivity in General

All studies of hydraulic conductivity assumed lognormal distributions, except those using the Unsaturated Flow Apparatus (UFA™) to estimate the vertical hydraulic conductivity in the vadose zone (Wright et al., 1994; Conca and Wright, 1995). Presumably, these studies did this because spatial variability was not excluded and is often the largest part of the total uncertainty. Additionally, the magnitude of horizontal hydraulic conductivity can vary much more than any other parameter. Due to the extreme range of possible values, researchers may have found a lognormal distribution to fit the experimental data better. Uncertainties for these lognormal distributions were computed as coefficients of variation just as before, except the mean and variance were of the natural log of the data. Estimation methods with lognormal uncertainties have 'lognormal' listed next to the uncertainty in Appendix D.

(3) Excluding Spatial Uncertainty from Studies of Hydraulic Conductivity

Results from studies of hydraulic conductivity at the Borden (Sudicky, 1986), Cape Cod (Wolf et al., 1991; Hess et al., 1992), and Columbus (Rehfeldt et al., 1992) sites did not exclude spatial uncertainty. However, to use data from those studies for determining approximate uncertainties for various parameter estimation methods, spatial uncertainty had to be removed. To accomplish this, the method uncertainty for one method had to be assumed so that the total uncertainty of the other methods could be corrected to remove spatial uncertainty. The original data from these studies are summarized in Table 3.

It is generally agreed that the laboratory permeameter method has the lowest method uncertainty, producing the least variation among replicate analyses (personal communications with: Michael Robinson, Researcher in Department of Civil

Engineering, Virginia Tech; Jeff Farrar, Geotechnical Engineer with Earth Sciences Laboratory, Bureau of Reclamation; Jason Smolensky, Hydrogeologist at SRK-Canada, and Doctors Ed Heyse and Mark Goltz, Department of Engineering and Environmental Management, Air Force Institute of Technology). Considering these discussions, the method uncertainty of the laboratory permeameter was assumed to be +/- 2.0%. This means that in the study by Sudicky (1986), the method uncertainty is +/- 2.0% and the spatial uncertainty is +/- 8.9%.

Table 3: Hydraulic Conductivity Results Used to Exclude Spatial Uncertainty

Site	Method	Geom. Mean K (cm/s)	μ of ln(K) (cm/s)	σ^2 of ln(K)	Total CV (%)	Reference
Borden	Permeameter	7.2E-03	-4.934	0.29	+/- 10.9	Sudicky, 1986
Cape Cod	Permeameter	3.5E-02	-3.352	0.14	+/- 11.2	Hess et al., 1992
Columbus	Permeameter	6.1E-05	-9.700	5.5	+/- 24.2	Rehfeldt et al., 1992
Cape Cod	Flowmeter	1.1E-01	-2.207	0.24	+/- 22.2	Hess et al., 1992
Cape Cod	Flowmeter	1.2E-01	-2.112	0.09	+/- 14.2	Wolf et al., 1991
Columbus	Flowmeter	5.5E-03	-5.200	4.5	+/- 40.8	Rehfeldt et al., 1992
Cape Cod	Grain Size	4.0E-02	-3.219	0.27	+/- 16.1	Wolf et al., 1991
Columbus	Grain Size	4.5E-02	-3.100	3.1	+/- 56.8	Rehfeldt et al., 1992
Columbus	Slug Test	1.7E-02	-4.100	1.8	+/- 32.7	Rehfeldt et al., 1992

For the purposes of this study, the components of the total uncertainty were assumed to be additive. If the components can be considered independent, random variables this assumption is true (Kempthorne and Allmaras, 1986 ; Devore, 1995). Further, Skoog and Leary (1992) suggest that the components are independent meaning that by traditional statistical analysis, the total variance would be equal to the sum of the component variances. Additionally, uncertainty components of lognormally distributed data are additive if the data is transformed to normal data (i.e., the natural log of each data point) (Kempthorne and Allmaras, 1986).

However, not all studies used as data in the current study reported standard deviations or variances; some of them reported coefficients of variation. For this study, it was necessary to convert all data into coefficients of variations to account for large differences in the means of individual studies used as data, and to have a common format for comparison. As a result, it was assumed that the coefficients of variation of the components were additive, so that the spatial uncertainty could be removed from the total uncertainty. As a result of this assumption, the determined method uncertainties may slightly underestimate their true values.

With the assumed lab permeameter method uncertainty of +/- 2.0% and the other statistical assumptions, the spatial uncertainty for the lab permeameter method at each of the three sites was determined (see Table 4). Since spatial uncertainty is due to the spatial variability of the site, it seems reasonable to use this spatial uncertainty determined for each site when removing spatial uncertainty from the total uncertainty for each of the other methods. Since the estimation block volume varies for each method, this may not be entirely correct; however, it seems to be the most logical way of dealing with the spatial uncertainty. The method uncertainties for each of the studies, as well as the average for each method, are shown in Table 4.

Table 4: Hydraulic Conductivity Results Used to Exclude Spatial Uncertainty

Site	Method	Total CV (%)	Spatial CV (%)	Method CV (%)	Average Method CV (%)	Reference
Borden	Permeameter	+/- 10.9	+/- 8.9	+/- 2.0		Sudicky, 1986
Cape Cod	Permeameter	+/- 11.2	+/- 9.2	+/- 2.0		Hess et al., 1992
Columbus	Permeameter	+/- 24.2	+/- 22.2	+/- 2.0	+/- 2.0	Rehfeldt et al., 1992
Cape Cod	Flowmeter	+/- 22.2	+/- 9.2	+/- 13.0		Hess et al., 1992
Cape Cod	Flowmeter	+/- 14.2	+/- 9.2	+/- 5.0		Wolf et al., 1991
Columbus	Flowmeter	+/- 40.8	+/- 22.2	+/- 18.6	+/- 12.2	Rehfeldt et al., 1992
Cape Cod	Grain Size	+/- 16.1	+/- 9.2	+/- 7.0		Wolf et al., 1991
Columbus	Grain Size	+/- 56.8	+/- 22.2	+/- 34.6	+/- 20.8	Rehfeldt et al., 1992
Columbus	Slug Test	+/- 32.7	+/- 22.2	+/- 10.5	+/- 10.5	Rehfeldt et al., 1992

Both the Borden and Cape Cod sites are considered to be highly homogeneous (Mackay et al., 1986b; Sudicky, 1986; Wolf et al., 1991; Hess et al., 1992; Rehfeldt et al., 1992). The low value for spatial uncertainty (approximately +/- 9% for both sites) determined here supports that conclusion. The nearly identical values for total uncertainty determined for the same estimation method (laboratory permeameter) at both sites further supports the belief that both sites have approximately the same degree of homogeneity. Conversely, the Columbus site however, is considered quite heterogeneous

(Rehfeldt et al., 1992). As Table 4 shows, spatial uncertainty accounts for almost three times as much uncertainty at the Columbus site as at the Borden or Cape Cod sites.

The results in Table 4 are not ideal. It would be nice if the results of Wolf et al., (1991) agreed better with those of others. Wolf et al. (1991), discuss their flowmeter results indicating that the determined total uncertainty is probably lower than it should be as a result of well installation technique. Wolf et al., (1991) do not discuss their grain size method results. However, a couple important conclusions can still be drawn from Table 4. First, the rank order of the method uncertainties determined for each of these methods appears to be in the order one would expect. A laboratory method such as the laboratory permeameter is expected to be highly repeatable, while an indirect and somewhat more qualitative method such as grain size analysis is expected to have low repeatability.

Another important conclusion comes from comparing the ratios of spatial to total uncertainty for the methods; as the number of samples increases, the ratio of spatial to total uncertainty decreases. Table 5 contains the ratio of spatial to total uncertainty for each method used at each of the three sites (Borden, Cape Cod, and Columbus).

The ratio for the flowmeter in the study by Hess et al., (1992) is quite a bit smaller than that in the study by Wolf et al., (1991); this is a direct effect of the much larger number of samples used by Hess et al., (1992). Further, the ratio for the permeameter in the study by Sudicky (1986) is smaller than that in the study by Hess et al., (1992); again the result of a larger number of samples. Even though Sudicky (1986) and Hess et al., (1992) performed their studies at different sites, the ratios for these two sites can be compared because the two sites are highly homogenous with very similar spatial uncertainties. When one considers that an estimation block volume equal to the volume of the site would eliminate spatial uncertainty altogether, this result seems very reasonable.

Table 5: Comparing Ratios of Spatial to Total Uncertainty, By Method

Site	Method	Total CV (%)	Spatial CV (%)	Ratio Spatial/ Total	Number of Samples	Reference
Borden	Permeameter	+/- 10.9	+/- 8.9	81.7%	1279	Sudicky, 1986
Cape Cod	Flowmeter	+/- 22.2	+/- 9.2	41.3%	668	Hess et al., 1992
Cape Cod	Flowmeter	+/- 14.2	+/- 9.2	64.5%	33	Wolf et al., 1991
Cape Cod	Grain Size	+/- 16.1	+/- 9.2	56.8%	33	Wolf et al., 1991
Cape Cod	Permeameter	+/- 11.2	+/- 9.2	82.1%	825	Hess et al., 1992
Columbus	Flowmeter	+/- 40.8	+/- 22.2	54.4%	2187	Rehfeldt et al., 1992
Columbus	Grain Size	+/- 56.8	+/- 22.2	39.0%	214	Rehfeldt et al., 1992
Columbus	Permeameter	+/- 24.2	+/- 22.2	91.7%	87	Rehfeldt et al., 1992
Columbus	Slug Test	+/- 32.7	+/- 22.2	67.8%	22	Rehfeldt et al., 1992

Even though the results in Table 4 may not be ideal, they are at least reasonable. Furthermore, the method used to exclude spatial variability from total uncertainty was the best one at hand, and is supported by some reasonable logic. Therefore, the results in Table 4 were used in Appendix D.

(4) Determining Hydraulic Conductivity Based on Soil Type

The study by Tietje and Hennings (1996) determined the uncertainty of hydraulic conductivities calculated based on the soil classification types of the Food and Agriculture Organization (FAO) of the United Nations. Uncertainties were presented for the ratio of predicted to actual hydraulic conductivity. Tietje and Hennings (1996) assumed that the ratios came from lognormal distributions. The results as determined by Tietje and Hennings (1996) are not suitable for converting to a coefficient of variation for this estimation method. As a result, the uncertainty of this method is reported in Appendix D as a specific mean and standard deviation of the natural log of the ratios predicted to actual hydraulic conductivities. Given a predicted value, and a desired confidence interval, one can back out the upper and lower bounds of the actual value.

3. Estimation Block of Estimation Methods

a) General Results

Studies were found that had quantified the estimation block of particular methods. If a study could not be found an attempt was made to calculate a reasonable estimation block. For liquid samples this was done by dividing the volume of the sample over the vertical screen length of the sampling device. Then the radius into the surrounding soil was determined based on the porosity of that soil. For intact solid samples (e.g., soil cores) the estimation block is equal to the volume of the sample actually being measured. Thus if a 1000 cm^3 soil core is obtained from the site and then a five cm^3 sub-sample is removed from the soil core, the estimation block is five cm^3.

However, composite samples (liquid or solid) have an estimation block equal to the volume of material removed from the environment, thoroughly mixed, and then sub-sampled. For example if three 1000 cm^3 soil cores are obtained from the site and mixed, and then a five cm^3 sub-sample is taken from the composite 3000 cm^3 soil core, the estimation block is 3000 cm^3. Results are shown in Appendix E. When an estimation method has (h x r) listed next to the estimation block dimensions, it indicates that the first dimension is the height of the estimation block and the second dimension is the radius.

b) Special Considerations

(1) Liquid samples from Large Screened Intervals

If a screened interval is large, vertical variations in the horizontal hydraulic conductivity due to layering can be important. Several study sites have been extensively characterized, including determination of the vertical correlation scale for hydraulic conductivity (Mackay et al., 1986b; Hess et al., 1992; Rehfeldt et al., 1992). The vertical correlation scale at the Borden site was determined to be the smallest, at 10 centimeters (Mackay et al., 1986b), so it will be used as the length to distinguish between large and small screened intervals.

When calculating the estimation block for a method with a large screened interval, the volume of the liquid sample is not evenly distributed over the screened interval. Distribution of the volume is accomplished based on the ratio of the horizontal hydraulic conductivity within each layer, so that a layer of higher conductivity gets a higher portion of the sample volume attributed to it. The screen length is then divided into equal lengths of approximately 10 centimeters and the radius is computed for each layer based on the sample volume attributed to that layer and the porosity of the soil in that layer.

(2) Slug Test Method of Determining Horizontal Hydraulic Conductivity

Bouwer and Rice (1976) determined functions for computing the radius of influence for a slug test based on well construction details. Bouwer and Rice (1976) found that the uncertainty of their functions is +/- 10-25%; it is probably a direct effect of the fact that this method ignores the hydrogeologic properties. However, it seems like a reasonable amount of uncertainty since the small volume of water displaced (less than a few liters) is only expected to affect the surroundings within a radius of a couple meters or less. For example a difference of 25% would mean that an estimated radius of two meters is really only 1.5 meters. The half meter difference is probably within the horizontal correlation scale. For example, Sudicky (1986) determined the horizontal correlation scale at the Borden site to be approximately 2.8 meters.

The functions determined by Bouwer and Rice (1976) rely on three parameters obtained from a *nomograph* depending on the ratio of screen length to radius of well and gravel pack. A nomograph is simply a chart or graph representing numerical relationships. For this study, numerous data points were taken off the nomograph for each parameter and a non-linear regression performed to determine equations for the three parameters. These equations were incorporated into the functions of Bouwer and Rice (1976) to eliminate the need to rely on a graphical method such as a nomograph. The new functions were verified using data from the study by Bouwer and Rice (1976).

4. Cost of Estimation Methods

Since the purpose of this study was to develop a general tool, approximate costs were calculated for general, generic site conditions using rather general construction details. Well construction costs were determined for only three casing sizes and only two casing materials. However, the cost for each of these six construction types is a function of well depth and screen length, so these factors are adjustable. Most published studies did not include cost data, so the use of unit costing sources for this data was required.

For some estimation methods, the cost of the first sample is much higher than the cost of the second sample. A groundwater sample is a good example. The first sample will include the cost of installing the well, if the well was not previously installed for a different reason. Subsequent samples only include the cost of physically collecting and analyzing the sample.

In this study, costs were determined for the methods by themselves. Costs of installing a sampling point were determined separately. For example, the cost determined for using a bailer to obtain a groundwater sample assumes the well exists, and only includes the acts of obtaining and analyzing the sample. Those methods that require an existing sampling point, have that need indicated in parentheses in the cost matrix of Appendix F. In the bailer example, the cost is indicated as: $750 (well). This entry indicates that an existing well is required, and the cost of obtaining and analyzing a sample by this method is approximately $750. The cost of installing the sampling point (e.g., monitoring well) is computed separately using Equation (37) and Table 8 in Appendix I.

In computing approximate costs for each method, it was assumed that the contaminant is known to be some type of organic compound typically used on an Air Force Base. Analytical costs vary dramatically depending on what laboratory tests are used. If the type of contaminant were completely unknown, analytical costs of a groundwater sample would be two to three times higher.

Additionally, when computing costs for the installation of sampling points, only a small range of construction parameters (e.g., well diameter and casing material) were considered. Furthermore, all drilling costs were computed for a hollow-stem auger. Otherwise, the possible number of combinations of drilling method, well diameter, and casing material would have been too large.

5. Boundary Conditions

A requirement in creating any mathematical model of a site from the conceptual model is to identify boundary conditions. Boundary conditions are mathematical expressions of the state of the real system used to constrain the mathematical model in space or time, depending on the purpose of the model. Standard Guide D5447-93 (ASTM, 1996) points out that every point along the three-dimensional boundary of the modeled site must have an appropriate boundary condition assigned, as must any internal sources or sinks.

In addition, non-steady-state models require the identification of initial conditions. As the name implies, initial conditions provide a starting point for calculations. They usually consist of a specified hydraulic head or contaminant concentration for every node of the model, depending upon what is being modeled. According to Standard Guide D5447-93 (ASTM, 1996), the initial hydraulic head distribution for a transient model often consists of a steady-state solution for the same model.

Ideally, all boundary conditions should be based on natural hydrogeological boundary features within the real site. However, for many models there may be several boundary surfaces of the model that do not align with a natural boundary in the real site, because of the need to limit the size of the modeled site. In these cases, artificial boundaries must be assigned.

Franke et al. (1987) provide a good discussion of the types of boundary conditions and when to apply them, along with good examples. Additionally, Domenico and Schwartz (1990) and Standard Guide D5447-93 (ASTM, 1996) briefly discuss the importance of boundary conditions to transient models as well as the general types of boundary conditions. Only two studies were found that explicitly discussed boundary conditions (Cooley, 1977; Cooley, 1979). See Appendix G for a matrix of available boundary conditions along with a list of references discussing the application of each one.

IV. Results: Simulator Specifications

A. Methodology

Mathematical methods of simulating the uncertainty, estimation block, and cost of each method were determined. The goal of this part of the study was to determine methods of querying a computerized aquifer model database for parameter values at a specific point, selected by the user as a sampling location, in the aquifer.

Object-oriented software design methods were used to formulate a verbal specification of the site characterization simulator software. This entails specifying how the software is going to work and what it is intended to do. The verbal specification is a fairly informal specification method. The ultimate goal will be to take this informal specification and write a set of formal specifications for the software. A computer programmer can then take these formal specifications and write the actual simulation software.

B. Simulating Uncertainty, Estimation Block, and Cost

Uncertainties for various parameter estimation methods were reported in several ways, because of the way they were presented in the original studies. As a result there are several methods for incorporating the uncertainties from Appendix D into the simulator.

Many of the methods have a constant estimation block and cost associated with them. For those methods, implementation simply consists of looking up the estimation block and cost when the user selects that method. However, some methods have either an estimation block or cost that is a function of other subsurface parameter properties or the construction of the estimation method. In these cases the simulator must calculate the proper estimation block size or cost.

Finally, horizontal hydraulic conductivity is typically anisotropic; it has a different value in the direction of water flow than it has transverse to the water flow. Some methods calculate a single horizontal hydraulic conductivity (e.g. a slug test) that is a combination of the two values. Other methods determine two conductivities (e.g., a pump test); but, if the method is not aligned with the water flow, the two estimated values are again combinations of the two actual values. The simulator must determine what value or values to report based on the method used, and the degree of anisotropy.

1. Uncertainty

a) Normally Distributed Uncertainties

The uncertainty of most parameter estimation methods is listed in Appendix D as a coefficient of variation. Furthermore, the method uncertainties, represented by these coefficients of variation, are normally distributed random variables unless specified otherwise.

When an estimation method is chosen, the simulator looks up the coefficient of variation for that method. Once a location is specified for application of the method, the simulator obtains the "real" parameter value by going into the computer model database of the "real" site and averaging the parameter's value at every node within the calculated estimation block for that method. This value is considered to be the mean value of a sample size of one. If the estimation block volume is smaller than the "real site" model discretization scale and only one node falls within, an alternate method of incorporating spatial uncertainty must be used. See Chapter IV, Section B.2 for a discussion of this situation.

The mean value is then multiplied by the coefficient of variation, and divided by 100 (because the coefficient of variation is reported as a percentage), to obtain the standard deviation of the population of possible parameter values. The simulator then obtains a random number from a normal distribution having this mean and standard deviation and reports it to the user as the value of the parameter being estimated.

b) Lognormally Distributed Uncertainties

The uncertainties for some methods reported in Appendix D are from lognormally distributed populations. This is particularly true of most of the methods for estimating hydraulic conductivity. These methods are indicated by having (lognormal) next to their coefficients of variation. While the uncertainty of these methods is still reported as a coefficient of variation, it is important to note that it is a coefficient of variation of the natural logs of the parameter values.

When an estimation method with a lognormal uncertainty is chosen, the simulator looks up the coefficient of variation for that method. Once a location is specified for application of the method, the simulator obtains the "real" parameter value by going into the computer model database of the "real" site and averaging the parameter's value at every node within the calculated estimation block for that method. This value is considered to be the geometric mean value of a sample size of one. If the estimation block volume is smaller than the "real site" model discretization scale and only one node falls within, an alternate method of incorporating spatial uncertainty must be used. See Chapter IV, Section B.2 for a discussion of this situation.

Since the coefficient of variation is in terms of the mean and standard deviation of the natural log of the parameter value, the simulator must take the natural log of the geometric mean to obtain the mean of the natural log of the parameter. The mean value (of the natural log) is then multiplied by the coefficient of variation, and divided by 100 (because the coefficient of variation is reported as a percentage), to obtain the standard deviation of the population of possible natural logs of parameter values. The simulator then obtains a random number from a lognormal distribution having this mean and standard deviation. Finally, the simulator takes the exponential of the random number, and reports the result to the user as the value of the parameter being estimated.

c) Uncertainty of Hydraulic Conductivity Using Soil Type Method

This method relies solely on the results of a study by Tietje and Hennings (1986). The uncertainty for this method is lognormally distributed, but it is the uncertainty of the ratio of predicted to actual value of hydraulic conductivity. Tietje and Hennings (1986) reported the geometric mean of the ratio to be 0.8, the natural log of which is -0.22. The coefficient of variation of the ratio is +/- 190.7% (Tietje and Hennings, 1986), which when multiplied by the natural log of the geometric mean corresponds to a standard deviation (lognormal distribution) of 0.42.

Therefore, to determine a value to report to the user, the simulator obtains the "real" value just as for other methods. A random number is then obtained from a lognormal distribution with a mean of -0.22 and a standard deviation of 0.42. The result is the natural log of the ratio of the predicted to the actual value of hydraulic conductivity. The simulator then takes the exponential of the random number and multiplies it by the "real" hydraulic conductivity value to obtain the value to be reported to the user.

d) Absolute Ranges of Uncertainty

Some methods have a range of uncertainty. This range may be a range of measurement units as in the case of using a piezometer to determine hydraulic gradient (+/- 0.3 cm). Alternately, it may be a range of coefficients of variation such as the slug test method for estimating horizontal hydraulic conductivity (+/- 9.8-25%).

When an estimation method with an uncertainty as a range of measurement units is chosen, the simulator will use this range to determine upper and lower bounds for the value to report to the user. Once a location is specified for application of the method, the simulator will obtain the "real" parameter value by going into the computer model database of the "real" site and averaging the parameter's value at every node within the calculated estimation block for that method. The simulator adds and subtracts the uncertainty from the "real" value to obtain the upper and lower bounds of possible values. Then a random number is selected from a uniform distribution within this range and is the parameter value reported to the user. A uniform distribution was chosen for simplicity and because there were an insufficient number of studies pertaining to any estimation method to allow determination of a different distribution.

When an estimation method with an uncertainty as a range of coefficients of variation is chosen, the simulator will select a random number within this range. The random number is treated as the current coefficient of variation for that method and calculation of a value to report to the user is carried out as directed for either a normally or lognormally distributed uncertainty, as appropriate.

2. *Estimation Block*

Each estimation method has an associated estimation block. For some methods the estimation block size varies depending on soil properties or construction methods. If one of these methods is chosen, the simulator must look up the "real" parameter values for the node at the center-point of the method's application. Next, the user must be prompted for the construction details of the method. Considering the "real" parameter values and the construction details, the simulator uses the estimation block equation for that method and calculates the maximum distance from the center-point of application to every boundary of the estimation block. Ideally, the simulator then determines which nodes fall within the estimation block boundary. The parameter values of these nodes are averaged to determine the "real" parameter values as available to the chosen estimation method.

However, this study determined that estimation block volumes of many estimation methods may be smaller than the discretization scale of the "real site" model, as indicated in Figure 2. A typical model discretization scale (distance between nodes of model) of one meter was chosen for comparison. With a model discretization scale of one meter, any estimation block volume less than one cubic meter will be smaller than the model scale and will capture only one model node. The line labeled Model Scale in Figure 2 is located at an estimation block volume of one cubic meter to represent this typical model discretization scale. The assumptions listed for Table 1 in Chapter III, Section B, were used to calculate the estimation block volume for every method for which data was found. After rank ordering the estimation block volumes, they were plotted in Figure 2, and the rank of each volume was used as the Reference number in Table 1.

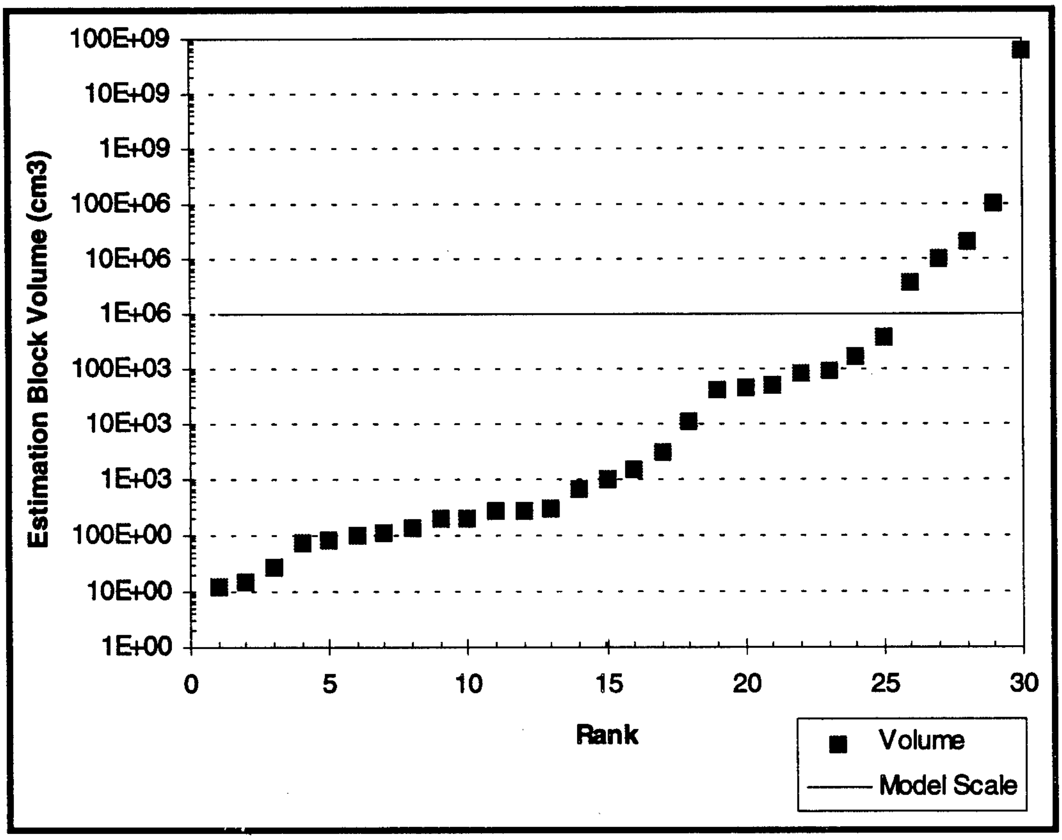

Figure 2: Estimation Block vs. Modeling Scale

Figure 2 clearly shows that 83% of the methods for which data was found have estimation block volumes smaller than the chosen model discretization scale. As a result, an alternate method for the simulator to incorporate spatial uncertainty must be determined for instances when the estimation block of a method is smaller than the discretization scale of the "real site" model. Incorporating this ability will require determining how the parameter being measured varies with space and defining this variation statistically. The simulator will then have to calculate a "real" value for the parameter value based on the statistical definition for that parameter.

3. Cost

Each estimation method has an associated cost. For some methods the cost varies depending on soil properties or construction methods. If one of these methods is chosen, the simulator must look up the "real" parameter values for the node at the center-point of the method's application. Next, the user must be prompted for the construction details of the method. Considering the "real" parameter values and the construction details, the simulator uses the cost equation for that method and calculates the cost of using that method at that location.

4. Incorporating Anisotropy into Reported Hydraulic Conductivity

The horizontal hydraulic conductivity at any particular point is usually different in the longitudinal direction of water flow than in the transverse direction to water flow. When a method that reports a single combined value (radial direction) is used (e.g., a slug test), the simulator needs to average the x-direction (longitudinal with the water flow) and y-direction (transverse to the water flow) values for every node within the estimation block. These average values are then averaged among all the nodes in the estimation block to determine the "real" value for horizontal radial hydraulic conductivity. Uncertainty is then added to this value before reporting it to the user.

If a method is chosen that reports two values (x-direction and y-direction), anisotropy must still be considered. Unless the estimation method is perfectly aligned with the water flow, the estimated values must be adjusted. This adjustment is done by determining the angle between the longitudinal axis of the method and the longitudinal axis of the water flow, then using Equations (1) and (2) to determine the adjusted hydraulic conductivities (Bear, 1979):

$$K_x = \frac{K_{xx} + K_{yy}}{2} + \frac{K_{xx} - K_{yy}}{2} \cdot \cos(2 \cdot \theta) \tag{1}$$

$$K_y = \frac{K_{xx} + K_{yy}}{2} - \frac{K_{xx} - K_{yy}}{2} \cdot \cos(2 \cdot \theta) \tag{2}$$

where,

Kx = adjusted longitudinal hydraulic conductivity (cm/s)

Ky = adjusted transverse hydraulic conductivity (cm/s)

Kxx = "real" longitudinal hydraulic conductivity (cm/s)

Kyy = "real" transverse hydraulic conductivity (cm/s)

θ = angle between longitudinal axis of method and longitudinal axis of water flow (degrees)

The values are adjusted in this way for every node in the estimation block. These adjusted values are then averaged for all the nodes, and uncertainty added before reporting the longitudinal and transverse hydraulic conductivities to the user.

C. Simulator Specifications

1. General Operation

The site characterization simulator (Sim-Site) is an extension of the Groundwater Modeling Software (GMS) developed by Brigham Young University for the U.S. Army Corps of Engineers Waterway Experiment Station. "Reality" in the scenario is defined by a GMS model. The user has reason to believe that a portion of this site is contaminated. The challenge is for the user to use site characterization techniques to build a mathematical model, using GMS, of the "contaminated" portion of the site, including appropriate boundary conditions, while constrained to a fixed budget.

A typical simulation would go through a pre-determined number of sampling seasons (e.g., six months or a year). At the end of each sampling season, the user is provided the results of that season's sampling effort. The user then uses this data to build or modify a model of the site being characterized. After using the season's data to update the model, the simulator will compare the user's model to the "real site," but will not provide any feedback to the user until the end of the simulation. Upon completion of a simulation the simulator will provide the user with each season's results, as well as a graph of the user's score versus season so that the user can easily see if characterization performance improved as the simulation progressed.

The basic operation of the simulator is shown in Figure 3, with each step numbered. The steps are:

1. The user starts the simulator.

2. The simulator provides the user with the opening scenario.

3. The user selects all desired sampling methods and locations for to be sampled during the current sampling season (keeping in mind that the user has a fixed budget). The simulator will not allow selection of a method that costs more than the user's remaining budget. This step can be thought of as developing the sampling plan for the current season.

4. The simulator queries the "real site" database for each sample the user requested for the current sampling season.

5. The simulator adds some random uncertainty to the "real" parameter values and reports them to the user.

6. The user creates or modifies a mathematical computer model of the site, using GMS, from the data provided by the simulator.

7. GMS builds or modifies the model database from the data input by the user.

8. The simulator compares the database of the "real" site to the database of the model to determine how close the model comes to representing "reality," for the current season. The comparison is done on a node by node basis, performing a sum-of-squares difference for each parameter. The result is converted to a score for that season (using a 0-100 scale).

9. Steps 3 through 8 are repeated until the pre-determined number of seasons (set at the simulation start) has passed.

10. The simulator provides the user's results broken out by sampling season, in a graphical format so that trends can be identified in the user's performance.

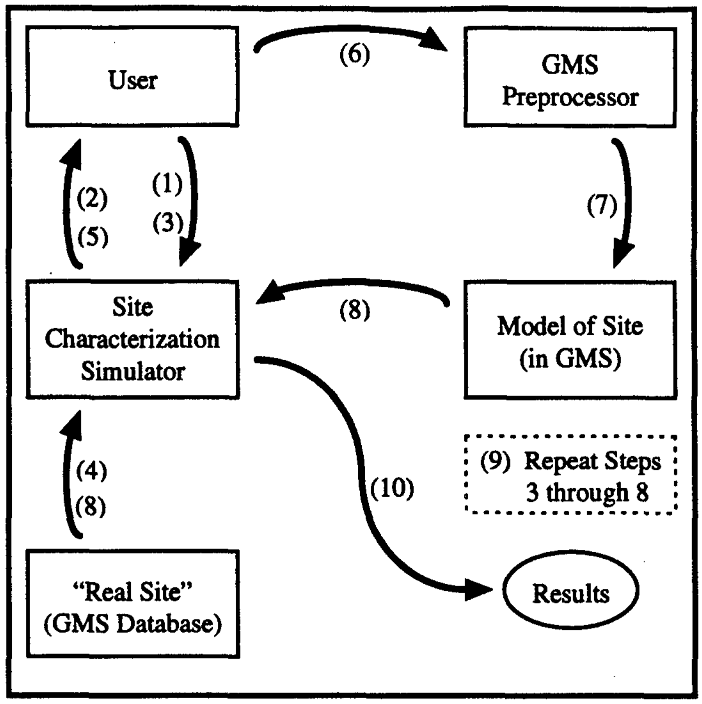

Figure 3: Site Characterization Simulator Operation

2. *Determining Parameter Value to Report to User*

When a tool is selected and applied to the site, the application will look up the uncertainty, estimation block, and cost for each parameter associated with that tool. However, uncertainty and estimation block size are often dependent on the soil properties, so the application will need initial parameter values to use in calculating the method characteristics such as estimation block size. The initial parameter values will be determined by looking up the applicable soil properties at the center-point of tool application. Then the estimation block volume, uncertainty (coefficient of variation in most cases), and cost of obtaining the sample are determined based on the initial parameters. Nothing is reported to the user at this time.

To determine the values to be reported to the user, the application will go into the GMS database of "real" site parameters, at the coordinates of the center-point of the tool's application, and get the values of all parameters associated with that tool that are within the calculated estimation block volume from those coordinates. All values returned will be averaged for each parameter. This average value will then be altered to simulate sampling and analytical uncertainties. A random number generator will be used to select a number from the parameter's population (see discussion in Chapter III, Section B) based on a mean equal to the calculated average, and the coefficient of variation associated with the chosen tool and the particular parameter. This random number will be reported to the user as the data returned by the selected tool for that location in the site, along with the cost of obtaining the sample.

In essence the computer program takes perfect data from the database and adds uncertainty and error to it, just as in the real world. The true value of a parameter exists in the aquifer; however, the act of taking a sample and analyzing it introduces a certain amount of uncertainty and error.

3. Beginning Scenario

At the beginning of the simulation, the user is presented with a scenario and an aerial view map of the site and surrounding area (e.g., aerial view map of an Air Force Base). The scenario details the hypothetical job or position of the user and the event that has transpired to initiate the desire to perform a site characterization. The user's role in the simulation is that of an environmental restoration project manager. For the purpose of this study, the actual details of the opening scenario are not relevant. The scenario will be decided upon when the simulator is developed.

4. User Interaction

After the opening scenario is given to the user, the user takes control and selects estimation methods from a pull-down menu. Once a method has been selected, the user will select where to apply it, and provide any design data necessary (e.g., well depth and diameter). The application will return the kind of data associated with that method. The user will then use this data to build a model of the site, using GMS.

For methods that essentially consist of historical records reviews, the user will be presented with an image of the document, a summary of the interview, or notification that no information could be found. It is up to the user to draw any conclusions about the validity or usefulness of the information provided by a historical record review or personal interview.

To better simulate real life, some methods will require further choices. For example, selecting "obtain groundwater sample" will require the user to select how that sample will be collected (e.g., bailer, multi-level sampler, pumping, HydroPunch®). Additionally, selection of some methods will require that other actions be performed first. An example would be choosing to obtain a groundwater sample by use of a bailer. The user will then be prompted to identify an existing well from which to obtain the sample. This mirrors reality, where collecting a groundwater sample via a bailer does not include well installation. A well must exist before someone can obtain a sample from it.

V. Conclusions and Recommendations

A. Conclusions

1. General

In any site characterization effort, careful definition of the objectives is the most important step. If the objectives are clearly defined, the data presented in Appendices C through F can be used, along with those objectives, to allocate funds for the best quality samples from the most suitable locations. Additionally, the information shown in Appendices A, B, and G will help the inexperienced environmental manager find answers to the tough questions about site characterization; it may also refresh the memory of the experienced environmental manager.

2. Uncertainty and Estimation Block

By comparing the uncertainty results for various methods of estimating a particular parameter, it can be seen that the methods rank, for the most part, in the order one would qualitatively expect. Some discrepancies occur, but if spatial uncertainty is accounted for most of the discrepancies are resolved. Spatial uncertainty is a function of the estimation block size. However, the relationship is somewhat counter-intuitive; the larger the estimation block, the smaller the spatial uncertainty.

However, it is explained by comparing the average value of many samples obtained by a method with a small uncertainty and a small estimation block to a single sample obtained by a method with a high uncertainty and a large estimation block. The average of the many small samples is likely to be near that of the single large sample because the many samples are effectively taking an average over the same volume as the single sample.. Additionally, the total uncertainty of the small samples (as represented by the standard deviation of the measurements) may now be larger than the total uncertainty of the single large measurement since the total uncertainty of the small samples now includes the effects of spatial variability. The large sample, however, is already an average over the larger volume and no more uncertainty due to spatial variability is added to it.

For example, consider the methods for estimating the horizontal hydraulic conductivity. Without looking at the results of this study, one might rank the total uncertainty of the methods as shown in row 1 of Table 6. It is apparent that this is quite different from the rank order of the uncertainties presented in Appendix D (shown in row 2 of Table 6). However, spatial uncertainty must still be accounted for, so the rank order of the spatial uncertainties, based on estimation block (larger estimation block equals less uncertainty), is shown in row 3 of Table 6.

Estimation block is a qualitative indicator of the spatial uncertainty. To combine the method and spatial uncertainties in a meaningful way for comparison, both must be transformed into scaled ranks; using simple ranks (i.e., 1 to 5) does not account for the magnitude of difference in uncertainty between methods. Therefore, the numbers in parentheses for method uncertainty (row 2 of Table 6) are the method uncertainties from Appendix D.

Table 6: Comparing Total Uncertainty of Methods—Hydraulic Conductivity

	Rank Order of Uncertainty				
	Least (1)	**(2)**	**(3)**	**(4)**	**(5)**
Initial Rank	Slug Test	Flowmeter	Permeameter	History Matching	Grain Size
Method Uncertainty	Permeameter (2)	Slug Test (11)	Flowmeter (12)	Grain Size (21)	History (25)
Spatial Uncertainty	History (4)	Slug Test (7)	Flowmeter (14)	Grain Size (21)	Permeameter (25)
Total Uncertainty	Slug Test (18)	Flowmeter (26)	Permeameter (27)	History (29)	Grain Size (42)
Final Rank	Slug Test	Flowmeter	Permeameter	History Matching	Grain Size

The numbers in parentheses for the spatial uncertainty (row 3) were determined by rounding off the log of the estimation block volume and subtracting it from 9 (since the largest rounded log was 8 and the largest estimation block should have the lowest spatial uncertainty). The results were then multiplied by 3.57 to make the highest scaled rank order value for spatial uncertainty equal to the highest scaled rank order value for method uncertainty; without other data it seems reasonable to make spatial and method uncertainties equally important.

Next, the scaled rank order values for method and spatial uncertainty were added for each method to obtain the numbers in row 4 of Table 6. Finally, it can be seen that the order of these results (row 5 of Table 6) is the same as the initial order, which makes sense. A technique like the lab permeameter gives a very precise estimate of the parameter value within the sample being tested. However, the sample size is very small compared to the size of the site, so the method really gives no idea of what the parameter value is anywhere else in the site. A slug test, on the other hand, samples a significantly larger volume of the site. The reported value is an estimate of the average value throughout that volume so the uncertainty is larger. However, because of the larger estimation block, spatial variability has less effect.

It should be pointed out that the estimation blocks used were those discussed in Section B.2 of Chapter IV. Different assumptions about installation details could change the estimation block volumes.

3. Costs

Overall, the cost estimate results are satisfactory. As expected, methods with a lower total uncertainty are usually more expensive. Depending on the price difference, an environmental manager may discover through experience that taking many low cost, high uncertainty measurements does a better job (for less money) than taking a few high cost, low uncertainty measurements. The results of this study will help the environmental manager make these tradeoffs.

4. Boundary and Initial Conditions

As expected, the references found discussing the use of boundary and initial conditions were in agreement. The practice of modeling has been going on for a long time, and though new processes have been added in recent years, the general application of models has not changed. What were requirements to make a model work twenty years ago are still requirements today.

B. *Recommendations for Further Research*

As can be seen in the estimation method matrices in the appendices, there are many parameters for which estimation technique characteristics have not been identified. Many of these are parameters that have only started to be considered in the last few years. Parameters that have been studied for a long time, such as horizontal hydraulic conductivity in the saturated zone and equilibrium sorption coefficient, have had quite a few studies to determine the characteristics of particular estimation methods. More research is needed to quantify the uncertainty, estimation block, and cost of the methods for estimating those parameters that have only recently become of interest such as dispersion coefficients, storage parameters (except equilibrium sorption), and all fate parameters (e.g., decay rate, irreversible sorption, volatilization).

Additionally, although the literature review for this study has been quite extensive, it has not been exhaustive. There is additional data for some of these methods that was not available for this study. A search concentrating on those methods for which no data is listed in the matrices should be undertaken.

Finally, this study has quantified the characteristics of the various parameter estimation techniques and provided general specifications for a site characterization simulator. Further work must be done to take these results and create such a simulator.

Appendix A: ASTM Standards Related to Site Characterization (ASTM, 1996)

Standard	Title
D 420 - 93	Standard Guide to Site Characterization for Engineering, Design, and Construction Purposes
D 653 - 90	Standard Terminology Relating to Soil, Rock, and Contained Fluids
D 1452 - 80 (90)	Standard Practice for Soil Investigation and Sampling by Auger Borings
D 1586 - 84 (92)	Standard Test Method for Penetration Test and Split-Barrel Sampling of Soils
D 1587 - 94	Standard Practice for Thin-Walled Tube Geotechnical Sampling of Soils
D 2216 - 92	Standard Test Method for Laboratory Determination of Water (Moisture) Content of Soil and Rock
D 2434 - 69 (94)	Standard Test Method for Permeability of Granular Soils (Constant Head)
D 2487 - 93	Standard Classification of Soils for Engineering Purposes (United Soil Classification System)
D 2937 - 94	Standard Test Method for Density of Soil in Place by the Drive-Cylinder Method
D 3385 - 94	Standard Test Method for Infiltration Rate of Soils in Field Using Double-Ring Infiltrometer
D 3404 - 91	Standard Guide for Measuring Matric Potential in the Vadose Zone Using Tensiometers
D 3441 - 94	Standard Test Method for Deep, Quasi-Static, Cone and Friction-Cone Penetration Tests of Soil
D 4043 - 91	Standard Guide for Selection of Aquifer-Test Methods in Determining of Hydraulic Properties by Well Techniques

D 4044 - 91	Standard Test Method for (Field Procedure) for Instantaneous Change in Head (Slug Tests) for Determining Hydraulic Properties of Aquifers
D 4050 - 91	Standard Test Method (Field Procedure) for Withdrawal and Injection Well Tests for Determining Hydraulic Properties of Aquifer Systems
D 4104 - 91	Standard Test Method (Analytical Procedure) for Determining Transmissivity of Nonleaky Confined Aquifers by Overdamped Well Response to Instantaneous Change in Head (Slug Test)
D 4105 - 91	Standard Test Method (Analytical Procedure) for Determining Transmissivity of Nonleaky Confined Aquifers by the Modified Theis Nonequilibrium Method
D 4106 - 91	Standard Test Method (Analytical Procedure) for Determining Transmissivity of Nonleaky Confined Aquifers by the Theis Nonequilibrium Method
D 4448 - 85a (92)	Standard Guide for Sampling Groundwater Monitoring Wells
D 4630 - 86 (91)	Standard Test Method for Determining Transmissivity and Storativity of Low-Permeability Rocks by In Situ Measurements Using the Constant Head Injection Test
D 4631 - 86 (91)	Standard Test Method for Determining Transmissivity and Storativity of Low-Permeability Rocks by In Situ Measurements Using the Pressure Pulse Technique
D 4643 - 93	Standard Test Method for Determination of Water (Moisture) Content of Soil by the Microwave Oven Method
D 4696 - 92	Standard Guide for Pore-Liquid Sampling from the Vadose Zone
D 4700 - 91	Standard Guide for Soil Sampling from the Vadose Zone
D 4750 - 87 (93)	Standard Method for Determining Subsurface Liquid Levels in a Borehole for Monitoring Well (Observation Well)
D 4959 - 89	Standard Test Method for Determination of Water (Moisture) Content of Soil By Direct Heating Method

D 5084 - 90	Standard Test Method for Measurement of Hydraulic Conductivity of Saturated Porous Materials Using a Flexible Wall Permeameter
D 5092 - 90	Standard Practice for Design and Installation of Ground Water Monitoring Wells in Aquifers
D 5093 - 90	Standard Test Method for Field Measurement of Infiltration Rate Using a Double-Ring Infiltrometer with a Sealed-Inner Ring
D 5126 - 90	Standard Guide for Comparison of Field Methods for Determining Hydraulic Conductivity in the Vadose Zone
D 5195 - 91	Standard Test Method for Density of Soil and Rock In-Place at Depths Below the Surface by Nuclear Methods
D 5220 - 92	Standard Test Method for Water Content of Soil and Rock In-Place by the Neutron Depth Probe Method
D 5254 - 92	Standard Practice for Minimum Set of Data Elements to Identify a Ground-Water Site
D 5269 - 92	Standard Test Method for Determining Transmissivity and Storativity of Nonleaky Confined Aquifers by the Theis Recovery Method
D 5270 - 92	Standard Test Method for Determining Transmissivity, Storativity, and Storage Coefficient of Bounded, Nonleaky, Confined Aquifers
D 5314 - 93	Standard Guide for Soil Gas Monitoring in the Vadose Zone
D 5408 - 93	Standard Guide for Set of Data Elements to Describe a Ground-Water Site; Part One--Additional Identification Descriptors
D 5409 - 93	Standard Guide for Set of Data Elements to Describe a Ground-Water Site; Part Two--Physical Descriptors
D 5410 - 93	Standard Guide for Set of Data Elements to Describe a Ground-Water Site; Part Three--Usage Descriptors
D 5447 - 93	Standard Guide for Application of a Ground-Water Flow Model to a Site-Specific Problem

D 5474 - 93	Standard Guide for Selection of Data Elements for Ground-Water Investigations
D 5518 - 94	Standard Guide for Acquisition of File Aerial Photography and Imagery for Establishing Historic Site-Use and Surficial Conditions
D 5609 - 94	Standard Guide for Defining Boundary Conditions in Ground-Water Flow Modeling
D5610 - 94	Standard Guide for Defining Initial Conditions in Ground-Water Flow Modeling
D 5730 - 95a	Standard Guide for Site Characteristics for Environmental Purposes With Emphasis on Soil, Rock, the Vadose Zone and Ground Water
D 5785 - 95	Standard Test Method for (Analytical Procedure) Determining Transmissivity of Confined Nonleaky Aquifers by Underdamped Well Response to Instantaneous Change in Head (Slug Test)
E 1689 - 95	Standard Guide for Developing Conceptual Site Models for Contaminated Sites

Appendix B: Objectives of Site Characterization

A. Defining the Source

(Bedient et al., 1994; ASTM, 1996, D5730-95a)

Has there been some sort of chemical spill?

Has some potentially hazardous chemical entered the soil and/or groundwater?

What chemical is suspected to have spilled?

What is the flux of contaminant to the aquifer, as a function of space and time?

(Domenico and Schwartz, 1990; ASTM, 1996, E1689-95)

When did the spill occur?

How much chemical was spilled (volume, as well as location and area of spill)?

What was the nature of the spill (sudden release versus long-term leak)?

What is the infiltration rate, from the surface to the groundwater, for the area?

What are the properties of the contaminant? (Preslo and Stoner, 1990; Brusseau and Wilson, 1995)

What is the vapor pressure (Henry's law constant)?

What is the solubility?

What is the sorption coefficient?

What is the density and viscosity?

What is the molecular weight?

What chemicals are mixed together in the contaminant?

B. Defining the Exposure Pathways

(Covello and Merkhofer, 1993)

How is the chemical likely to pose a threat?

> Could it contaminate a drinking water aquifer?
>
> Could it contaminate surface water via runoff?

Is there anybody or anything that can possibly be exposed to the contaminant (people drawing water from aquifer, animals drinking from pond, etc.)?

What is the effect of the contamination if it is left alone?

C. Defining the Transport

How will chemical transport occur? (Bedient et al., 1994; ASTM, 1996, D5730-95a)

> Will the contaminant be transported by groundwater flow?
>
> Will the contaminant be transported by vadose zone (gas) transport (i.e., volatilization)?

What is the site hydrogeology that will determine contaminant transport, storage, and fate? (Barcelona et al., 1985)

> What are the dominant processes? (Konikow, 1986; Domenico and Schwartz, 1990; ASTM, 1996, D5447-93)
>
> > What are the important contaminant transport processes (e.g., horizontal and vertical advection, dispersion, diffusion)?

What are the important contaminant storage processes (e.g., equilibrium sorption, rate-limited sorption, volatilization, dissolution, precipitation—if contaminant is re-solubilized)?

What are the important contaminant fate processes (e.g., decay, production, irreversible sorption, precipitation—if contaminant is not re-solubilized, loss of contaminant from the system by transport)?

D. Defining the Boundary and Initial Conditions

(Franke et al., 1987; Domenico and Schwartz, 1990)

What are the system boundary conditions? (ASTM, 1996, D5609-94)

What is the system water budget (i.e., where does water enter and exit system)?

Is the system bounded by any bodies of water or impermeable surfaces?

Are there any constant flux sources or sinks of water or contaminant?

Are there any locations where contaminant concentration is effectively constant?

What initial conditions are to be applied to a model of the system? (ASTM, 1996, D5610–94)

What is the steady-state head distribution (for a non-steady-state model)?

Appendix C: Hydrogeologic Parameter Matrix—General

Hydrogeologic Parameter Matrix—References

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Reference
Process Type			
Process			
Transport			
Vertical Advection			
Water Content in Vadose Zone	θ_v	Gravimetric (tension plate) analysis of soil core	
		Drying soil sample	ASTM, 1996, D2216-92
		Neutron probe	Kramer et al., 1992; ASTM, 1996, D5220-92
		Tensiometry (in-situ)	Green et al., 1986; ASTM, 1996, D3404-91
Darcian Flux (vertical)	q_z	Infiltration rate, from historical data	
		Double-ring Infiltrometer	ASTM, 1996, D3385-94; ASTM, 1996, D5093-90
		Water balance	Todd et al., 1976
Hydraulic Conductivity (z)	K_z	Column test on soil core (steady-state head control)	Khaleel et al., 1995
		Unsaturated flow apparatus (UFA™) test on soil core	Conca and Wright, 1992; Wright et al., 1994; Conca and Wright, 1995; Khaleel et al., 1995
		Estimate from soil parameters and soil/water retention curves	van Genuchten, 1980; Khaleel et al., 1995; Tietje and Hennings, 1996
Soil Type (Classification)		Soil core	ASTM, 1996, D2487-93
Subsurface Lithology		Soil core	ASTM, 1996, D2487-93
		Cone penetrometer (resistivity)	Smolley and Kappmeyer, 1991; Zemo et al., 1994; ASTM, 1996, D3441-94
		Electrical conductivity (direct-push)	McCall, 1996
Average Soil Grain Size		Soil core (sieve analysis)	ASTM, 1996, D1586-84(92)
Depth to Water Table		Monitoring well installation or soil boring	McLaren et al., 1982; Barcelona et al., 1985; Hudak et al., 1993;
		Cone penetrometer (dynamic pore pressure)	
		Advanced geophysical techniques	Pitchford et al., 1989
Depth to Confining Layer		Soil boring	
		Cone penetrometer (resistivity)	Pitchford et al., 1989
		Advanced geophysical techniques	

Hydrogeologic Parameter Matrix—References

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Reference
Process Type			
Process			
Transport			
Horizontal Advection			
Water Content in Saturated Zone	θ_W	Estimate from soil type	
		See above, under Water Content in Vadose Zone	
Effective Porosity (equals Water Content in Saturated Zone, if no separate phase)	n	Soil core (drainable porosity combined with grain size)	
		Tracer experiment (laboratory—soil core)	li, 1995
		Two-well tracer experiment (field)	li, 1995
		Single-well tracer (drift and pumpback)	Hall et al., 1991; Hall, 1996
Darcian Flux (horizontal in x-direction)	q_x	Water balance	
Hydraulic Head	h	Wells (piezometers), via drilled installation	McLaren et al., 1982; Barcelona et al., 1985; Hudak et al., 1993; ASTM, 1996, D4750-87(93)
		Wells, via direct push installation	Casey et al., 1996
		Cone penetrometer (dynamic pore pressure)	
Isotropic 1-D Hydraulic Conductivity (x and y-directions)	K_r	Slug test	Hvorslev, 1951; Bouwer and Rice, 1976; Barcelona et al., 1985; Chirlin, 1989; Melville et al., 1991; Casey et al., 1996; ASTM, 1996, D4044-91; ASTM, 1996, D4104-91; ASTM, 1996, D5785-95
		Single-well pump test with impeller flowmeter in borehole	Molz et al., 1989; Rehfeldt et al., 1992
		Single-well tracer (drift and pumpback)	Hall, 1996
		Lab column permeameter test on soil core (based on K_Z)	Klute and Dirksen, 1986; Sudicky, 1986; Wolf et al., 1991; ASTM, 1996, D2434-68(94); ASTM, 1996, D5084-90
		Cone penetrometer (dynamic pore pressure)	Zemo et al., 1994
		Qualitative based on soil type	Tietje and Hennings, 1996
		Regression on grain size distribution	Tietje and Hennings, 1996

Hydrogeologic Parameter Matrix—References

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Reference
Process Type			
Process			
Transport			
Horizontal Advection			
Anisotropic 1-D Hydraulic Conductivity (x-direction)	K_x	Pump test with observation wells aligned in x-direction	Barcelona et al., 1985; Capuano and Jan, 1996; ASTM, 1996, D4105-91; ASTM, 1996, D4106-91; ASTM, 1996, D5269-92; ASTM, 1996, D5270-92
		Field tracer test with observation wells aligned in x-direction	Molz et al., 1985; Molz et al., 1986; Molz et al., 1988; Capuano and Jan, 1996
		History matching (parameter estimation model, based on hydraulic heads)	Cooley and Sinclair, 1976; Yeh, 1986
Anisotropic 1-D Hydraulic Conductivity (y-direction)	K_y	Pump test with observation wells aligned in y-direction	Barcelona et al., 1985; Capuano and Jan, 1996; ASTM, 1996, D4105-91; ASTM, 1996, D4106-91; ASTM, 1996, D5269-92; ASTM, 1996, D5270-92
		Field tracer test with observation wells aligned in y-direction	Molz et al., 1985; Molz et al., 1986; Molz et al., 1988; Capuano and Jan, 1996
		History matching (parameter estimation model, based on hydraulic heads)	Cooley and Sinclair, 1976; Yeh, 1986
Dispersion			
Horizontal Longitudinal Dispersion Coefficient	D_L	Laboratory column experiment (electrical conductivity)	Piquemal et al., 1992
		Tracer experiment (laboratory—soil core)	li, 1995
		Tracer experiment (field)	Sudicky et al., 1983; Güven et al., 1985; Güven et al., 1986; Zou and Parr, 1994; Welty and Gelhar, 1994; li, 1995
		Moment analysis of plume data (if plume is well known)	Freyberg, 1986; Zou and Parr, 1994
		Estimate from textbook using grainsize and v_X	
Horizontal Transverse Dispersion Coefficient	D_T	Laboratory column experiment (electrical conductivity)	Piquemal et al., 1992
		Tracer experiment (laboratory—soil core)	Pisani and Tosi, 1994
		Tracer experiment (field)	Sudicky et al., 1983; Zou and Parr, 1994
		Moment analysis of plume data (if plume is well known)	Freyberg, 1986; Zou and Parr, 1994
		Estimate from textbook using grainsize and v_Y	

Hydrogeologic Parameter Matrix—References

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Reference
Process Type			
Process			
Transport			
Dispersion			
Vertical Transverse Dispersion Coefficient	D_z	Laboratory column experiment (electrical conductivity)	Piquemal et al., 1992
		Tracer experiment (field)	Sudicky et al., 1983
		Moment analysis of plume data (if plume is well known)	Freyberg, 1986
		Textbook value based on grain size	
Water Velocity in x-direction (q/n)	v_x	Tracer experiment	Hall et al., 1991; Hall, 1996
		Heat sensor groundwater velocity detector (in-situ Permeable Flow Sensor)	Ballard, 1996; Ballard et al., 1996
Water Velocity in z-direction (q/n)	v_z	Heat sensor groundwater velocity detector (in-situ Permeable Flow Sensor)	Ballard, 1996; Ballard et al., 1996
Tortuosity	τ	Look up in table based on soil type and grain size	
Diffusion			
Diffusion Coefficient	D	Look up for free liquid and adjust by tortuosity	
		Tracer experiment	
		UFA™ analysis of soil core (for vadose zone D)	Conca and Wright, 1990; Conca and Wright, 1992; Wright et al., 1994

Hydrogeologic Parameter Matrix—References

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Reference
Process Type			
Process			
Storage			
Equilibrium Sorption			
Retardation Factor	R	Partitioning tracer experiment	Roberts et al., 1986; van Genuchten and Wierenga, 1986
		Moment analysis of plume data	Roberts et al., 1986
		<<< or calculate using parameters for each process below >>>	
Soil Bulk Density	ρ_B	Laboratory analysis of soil core	Mackay et al., 1986b; ASTM, 1996, D2216-92
Sorption Coefficient	K_d	Laboratory batch experiment (isotherm)	Anderson and Pankow, 1986; Curtis et al., 1986; Mackay et al., 1986a; MacIntyre et al., 1991; Grathwohl and Reinhard, 1993; Hegeman et al., 1995
		Laboratory batch experiment (one-point)	Mackay et al., 1986a; MacIntyre et al., 1991
		Column experiment or box model	MacIntyre et al., 1991
Fraction Organic Content	f_{OC}	Laboratory analysis of soil core	Curtis et al., 1986
		Literature value based on soil type	
Concentration in Water	C_W	Cone penetrometer (membrane sensor)	Christy, 1996
		HydroPunch® sample	Smolley and Kappmeyer, 1991; Zemo et al., 1994; Zemo et al., 1995
		BAT® sampler	Mines et al., 1993; ASTM, 1996, D4696-92
		Monitoring well, via pumping	McLaren et al., 1982; Schmidt, 1982; Zemo et al., 1994; Casey et al., 1996
		Monitoring well, via bailer	McLaren et al., 1982; Schmidt, 1982; Casey et al., 1996
		Monitoring well, via thief sampler	McLaren et al., 1982; Schmidt, 1982; Casey et al., 1996; Kabis, 1996
		Multi-level sampler	Gibs et al., 1993; Reilly and Gibs, 1993

Hydrogeologic Parameter Matrix—References

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Reference
Process Type			
Process			
Storage			
Equilibrium Sorption			
Concentration in Air	C_A	Soil gas	Pitchford et al., 1989; Durant et al., 1993; Casey et al., 1996; ASTM, 1996, D5314-93
		Cone penetrometer	Christy, 1996
		Fixed gas sampling well	Durant et al., 1993; Lindquist et al., 1996
Concentration in Soil	C_S	Soil core, via drilling	Anderson and Pankow, 1986
		Soil core, via direct push	Casey et al., 1996
		Estimate from historical data	
Concentration in NAPL	C_N	Estimate from historical data and contaminant properties	
Rate-Limited Sorption Using Effective Dispersion			
Effective Dispersion Coefficient	D_{eff}	Moment analysis of plume data (see D_T, D_L, and D_Z)	Freyberg, 1986
		Literature value	
Rate-Limited Sorption Using 1st Order, 2-Site Model			
Desorption Rate Coefficient	k_2	Laboratory column experiment	Grathwohl and Reinhard, 1993
		Regression equation	Brusseau and Rao, 1989
Fraction of Fast Sorption Sites	F	Laboratory column experiment	
Rate-Limited Sorption Using Spherical Diffusion			
Effective Diffusion Coefficient	D_S	Laboratory batch experiment	Grathwohl and Reinhard, 1993
		Literature data based on diffusion coefficient (D), tortuosity, and average grain size	

Hydrogeologic Parameter Matrix—References

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Reference
Process Type			
Process			
Storage			
Volatilization			
Air Content	θ_A		
Henry's Constant	H	Look up in table	
Dissolution			
NAPL Content	θ_N	Partitioning tracer experiment	
		Neutron probe	Endres and Greenhouse, 1996
		Advanced geophysical techniques	
		Estimate from historical records	
Water/NAPL Partition Coefficient	$K_{N/W}$	Laboratory batch experiment	
		Calculate from $\underline{v}_N$ and S_{SCL}	
Avg Molar Volume of NAPL	$\underline{v}_N$	Estimate from chemical make-up of NAPL, if known	
Hypothetical Super-Cooled Liquid Solubility	S_{SCL}	Look up in table	

Hydrogeologic Parameter Matrix—References

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Reference
Process Type			
Process			
Fate			
Decay (1st Order, Equilibrium Sorption)			
Decay Rate in Aqueous Phase	k	Experimentally derived (batch studies)	Li et al., 1993; Li et al., 1994; Young, 1994; Chapelle et al., 1996; Nyholm et al., 1996
		Zero moment analysis of field data	Wiedemeier et al., 1993; Chapelle et al., 1996
		Conservative tracer experiment	Wiedemeier et al., 1993
		Microbial counts	
Decay (Michalis-Menton)			
Correction Factor	b	Non-linear regression on field or experimental data	
Decay (Mass-Balance Approximation) [Model O_2 or Alternate Electron Acceptor]			
O_2 (e- acceptor) Solubility		Look up in table	
O_2 (e- acceptor) Flux Into System		Estimate	
O_2 (e- acceptor) Concentration		Water sample	
		Estimate	
Decay (1st Order, Rate-Limited Sorption)			
Production (1st Order, Equilibrium Sorption)			
Production (Michalis-Menton)			
Irreversible Sorption			
		Experimentally derived isotherms	
Precipitation			
Oxidation State of Metal	Z	Look up in table	
		Estimate	
Solubility Product	K_{SP}	Look up in table	
		Estimate	
Loss from System by Transport (Flux In/Out of System)			
Water Flow to/from System		Estimate flow from surface water and to lower aquifer	
Volatilization		Measure concentration profile in vadose zone	
		Measure flux at ground surface directly	
		Look up in literature	

Appendix D: Hydrogeologic Parameter Matrix—Uncertainty

Hydrogeologic Parameter Matrix—Uncertainty

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Uncertainty	Reference
Process Type				
Process				
Transport				
Vertical Advection				
Water Content in Vadose Zone	θ_v	Gravimetric (tension plate) analysis of soil core		
		Drying soil sample	+/- 5%	ASTM, 1996, D2216-92
		Neutron probe	+/- 3.8%	Kramer et al., 1992; ASTM, 1996, D5220-92
		Tensiometry (in-situ)	+/- 20 - 30%	Green et al., 1986
Darcian Flux (vertical)	q_z	Infiltration rate, from historical data		
		Double-ring Infiltrometer		
		Water balance		
Hydraulic Conductivity (z)	K_z	Column test on soil core (steady-state head control)	+/- 13.2% (lognormal)	Wolf et al., 1991
		Unsaturated flow apparatus (UFA™) test on soil core	+/- 7.5 - 15%	Wright et al., 1994; Conca and Wright, 1995
		Estimate from soil parameters and soil/water retention curves	+/- 28.8% (lognormal)	Khaleel et al., 1995
Soil Type (Classification)		Soil core		
Subsurface Lithology		Soil core		
		Cone penetrometer (resistivity)	+/- 15%	ASTM, 1996, D3441-94
		Electrical conductivity (direct-push)		
Average Soil Grain Size		Soil core (sieve analysis)		
Depth to Water Table		Monitoring well installation or soil boring		
		Cone penetrometer (dynamic pore pressure)		
		Advanced geophysical techniques		
Depth to Confining Layer		Soil boring		
		Cone penetrometer (resistivity)		
		Advanced geophysical techniques		

Hydrogeologic Parameter Matrix—Uncertainty

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Uncertainty	Reference
Process Type				
Process				
Transport				
Horizontal Advection				
Water Content in Saturated Zone	θ_W	Estimate from soil type		
		See above, under Water Content in Vadose Zone		
Effective Porosity (equals Water Content in Saturated Zone, if no separate phase)	*n*	Soil core (drainable porosity combined with grain size)	+/- 1.4 - 22.2%	Mackay et al., 1986b; Boggs et al., 1992; Endres and Greenhouse, 1996
		Tracer experiment (laboratory—soil core)		
		Two-well tracer experiment (field)		
		Single-well tracer (drift and pumpback)		
Darcian Flux (horizontal in x-direction)	q_x	Water balance		
Hydraulic Head	h	Wells (piezometers), via drilled installation	+/- 0.3 cm	Barcelona et al., 1985; ASTM, 1996, D4750-87
		Wells, via direct push installation		
		Cone penetrometer (dynamic pore pressure)		
Isotropic 1-D Hydraulic Conductivity (x and y-directions)	K_r	Slug test	+/- 10.3 - 25% (lognormal)	Bouwer and Rice, 1976; Rehfeldt et al., 1992
		Single-well pump test with impeller flowmeter in borehole	+/- 12.2% (lognormal)	Wolf, 1991; Hess et al., 1992; Rehfeldt et al., 1992
		Single-well tracer (drift and pumpback)		
		Lab column permeameter test on soil core (based on K_Z)	+/- 2.0% (lognormal)	Sudicky, 1986; Hess et al., 1992; Rehfeldt et al., 1992
		Cone penetrometer (dynamic pore pressure)		
		Qualitative based on soil type	uncertainty for ratio of predicted/actual K_r (lognormal) μ=0.22, σ=0.42	Tietje and Hennings, 1996
		Regression on grain size distribution	+/- 20.8% (lognormal)	Wolf, 1991; Rehfeldt et al., 1992

Hydrogeologic Parameter Matrix—Uncertainty

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Uncertainty	Reference
Process Type				
Process				
Transport				
Horizontal Advection				
Anisotropic 1-D Hydraulic Conductivity (x-direction)	K_x	Pump test with observation wells aligned in x-direction	+/- 54.6% (lognormal)	Keely and Wolf, 1983; Goltz, personal communication, 1996
		Field tracer test with observation wells aligned in x-direction		
		History matching (parameter estimation model, based on hydraulic heads)	+/- 25% (lognormal)	Cooley and Sinclair, 1976
Anisotropic 1-D Hydraulic Conductivity (y-direction)	K_y	Pump test with observation wells aligned in y-direction	+/- 54.6% (lognormal)	Keely and Wolf, 1983; Goltz, personal communication, 1996
		Field tracer test with observation wells aligned in y-direction		
		History matching (parameter estimation model, based on hydraulic heads)	+/- 25% (lognormal)	Cooley and Sinclair, 1976
Dispersion				
Horizontal Longitudinal Dispersion Coefficient	D_L	Laboratory column experiment (electrical conductivity)		
		Tracer experiment (laboratory—soil core)		
		Tracer experiment (field)		
		Moment analysis of plume data (if plume is well known)		
		Estimate from textbook using grainsize and v_X		
Horizontal Transverse Dispersion Coefficient	D_T	Laboratory column experiment (electrical conductivity)		
		Tracer experiment (laboratory—soil core)		
		Tracer experiment (field)		
		Moment analysis of plume data (if plume is well known)		
		Estimate from textbook using grainsize and v_Y		

Hydrogeologic Parameter Matrix—Uncertainty

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Uncertainty	Reference
Process Type				
Process				
Transport				
Dispersion				
Vertical Transverse Dispersion Coefficient	D_z	Laboratory column experiment (electrical conductivity)		
		Tracer experiment (field)		
		Moment analysis of plume data (if plume is well known)		
		Textbook value based on grain size		
Water Velocity in x-direction (q/n)	v_x	Tracer experiment	+/- 5%	Hall et al., 1991
		Heat sensor groundwater velocity detector (in-situ Permeable Flow Sensor)	+/- 13.6%	Ballard, 1996; Ballard et al., 1996
Water Velocity in z-direction (q/n)	v_z	Heat sensor groundwater velocity detector (in-situ Permeable Flow Sensor)	+/- 13.6%	Ballard, 1996; Ballard et al., 1996
Tortuosity	τ	Look up in table based on soil type and grain size		
Diffusion				
Diffusion Coefficient	D	Look up for free liquid and adjust by tortuosity		
		Tracer experiment		
		UFA™ analysis of soil core (for vadose zone D)	+/- 0.1%	Conca and Wright, 1992

Hydrogeologic Parameter Matrix—Uncertainty

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Uncertainty	Reference
Process Type				
Process				
Storage				
Equilibrium Sorption				
Retardation Factor	R	Partitioning tracer experiment	+/- 15.3%	Roberts et al., 1986
		Moment analysis of plume data	+/- 15.2%	Roberts et al., 1986
		<<< or calculate using parameters for each process below >>>	+/- 8.6%	Curtis et al., 1986
Soil Bulk Density	ρ_B	Laboratory analysis of soil core	+/- 4.6%	Mackay et al., 1986b; Boggs et al., 1992; ASTM, 1996, D2216-92
Sorption Coefficient	K_d	Laboratory batch experiment (isotherm)	+/- 8.7%	Anderson and Pankow, 1986; Mackay et al., 1986a; MacIntyre et al., 1991
		Laboratory batch experiment (one-point)	+/- 7.3%	Mackay et al., 1986a; MacIntyre et al., 1991
		Column experiment or box model		
Fraction Organic Content	f_{OC}	Laboratory analysis of soil core	+/- 11.2 - 23%	Anderson and Pankow, 1986; Mackay et al., 1986a; MacIntyre et al., 1991; Grathwohl and Reinhard, 1993
		Literature value based on soil type		
Concentration in Water	C_W	Cone penetrometer (membrane sensor)	+/- 3.6%	Christy, 1996
		HydroPunch® sample	+/- 8.8%	Chiang et al., 1992; Zemo et al., 1995
		BAT® sampler	+/- 19.0%	Mines et al., 1993; Zemo et al., 1995
		Monitoring well, via pumping	+/- 7.9 - 26.1%	Sgambat and Stedinger, 1981; McLaren et al., 1982; Reilly and Gibs, 1993; Graham and Goodlin, 1996
		Monitoring well, via bailer	+/- 16.9 - 108.4%	Mines et al., 1993; Graham and Goodlin, 1996
		Monitoring well, via thief sampler	+/- 10.8%	Patterson et al., 1993
		Multi-level sampler	+/- 5.1%	Boggs et al., 1992; Gibs et al., 1993; Patterson et al., 1993

Hydrogeologic Parameter Matrix—Uncertainty

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Uncertainty	Reference
Process Type				
Process				
Storage				
Equilibrium Sorption				
Concentration in Air	C_A	Soil gas		
		Cone penetrometer	+/- 3.6%	Christy, 1996
		Fixed gas sampling well		
Concentration in Soil	C_S	Soil core, via drilling		
		Soil core, via direct push		
		Estimate from historical data		
Concentration in NAPL	C_N	Estimate from historical data and contaminant properties		
Rate-Limited Sorption Using Effective Dispersion				
Effective Dispersion Coefficient	D_{eff}	Moment analysis of plume data (see D_T, D_L, and D_Z)		
		Literature value		
Rate-Limited Sorption Using 1st Order, 2-Site Model				
Desorption Rate Coefficient	k_2	Laboratory column experiment		
		Regression equation		
Fraction of Fast Sorption Sites	F	Laboratory column experiment		
Rate-Limited Sorption Using Spherical Diffusion				
Effective Diffusion Coefficient	D_S	Laboratory batch experiment		
		Literature data based on diffusion coefficient (D), tortuosity, and average grain size		

Hydrogeologic Parameter Matrix—Uncertainty

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Uncertainty	Reference
Process Type				
Process				
Storage				
Volatilization				
Air Content	θ_A			
Henry's Constant	H	Look up in table		
Dissolution				
NAPL Content	θ_N	Partitioning tracer experiment		
		Neutron probe	+/- 15%	Endres and Greenhouse, 1996
		Advanced geophysical techniques		
		Estimate from historical records		
Water/NAPL Partition Coefficient	$K_{N/W}$	Laboratory batch experiment		
		Calculate from $\underline{v}_N$ and S_{SCL}		
Avg Molar Volume of NAPL	$\underline{v}_N$	Estimate from chemical make-up of NAPL, if known		
Hypothetical Super-Cooled Liquid Solubility	S_{SCL}	Look up in table		

Hydrogeologic Parameter Matrix—Uncertainty

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Uncertainty	Reference
Process Type				
Process				
Fate				
Decay (1st Order, Equilibrium Sorption)				
Decay Rate in Aqueous Phase	k	Experimentally derived (batch studies)	+/- 11%	Li et al., 1993; Nyholm et al., 1996
		Zero moment analysis of field data		
		Conservative tracer experiment		
		Microbial counts		
Decay (Michalis-Menton)				
Correction Factor	b	Non-linear regression on field or experimental data		
Decay (Mass-Balance Approximation) [Model O_2 or Alternate Electron Acceptor]				
O_2 (e- acceptor) Solubility		Look up in table		
O_2 (e- acceptor) Flux Into System		Estimate		
O_2 (e- acceptor) Concentration		Water sample		
		Estimate		
Decay (1st Order, Rate-Limited Sorption)				
Production (1st Order, Equilibrium Sorption)				
Production (Michalis-Menton)				
Irreversible Sorption				
		Experimentally derived isotherms		
Precipitation				
Oxidation State of Metal	Z	Look up in table		
		Estimate		
Solubility Product	K_{SP}	Look up in table		
		Estimate		
Loss from System by Transport (Flux In/Out of System)				
Water Flow to/from System		Estimate flow from surface water and to lower aquifer		
Volatilization		Measure concentration profile in vadose zone		
		Measure flux at ground surface directly		
		Look up in literature		

Appendix E: Hydrogeologic Parameter Matrix—Estimation Block

Hydrogeologic Parameter Matrix—Estimation Block

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Estimation Block	Reference
Process Type				
Process				
Transport				
Vertical Advection				
Water Content in Vadose Zone	θ_v	Gravimetric (tension plate) analysis of soil core	15.7 cm x 2.5 cm (h x r)	Khaleel et al., 1995
		Drying soil sample	61.0 cm x 1.9 cm (h x r)	ASTM, 1996, D1586-84(92)
		Neutron probe	30.5 cm x 30.5 cm (h x r)	Kramer et al., 1992; ASTM, 1996, D5220-92
		Tensiometry (in-situ)	3.8 cm x 1.1 cm (h x r)	ASTM, 1996, D3404-91
Darcian Flux (vertical)	q_z	Infiltration rate, from historical data		
		Double-ring Infiltrometer	15.2 cm x 30.5 cm (h x r)	ASTM, 1996, D3385-94
		Water balance		
Hydraulic Conductivity (z)	K_z	Column test on soil core (steady-state head control)	15.7 cm x 2.5 cm (h x r)	Khaleel et al., 1995
		Unsaturated flow apparatus (UFA™) test on soil core	6.9 cm x 0.75 cm (h x r)	Conca and Wright, 1995
		Estimate from soil parameters and soil/water retention curves		
Soil Type (Classification)		Soil core	61.0 cm x 1.9 cm (h x r)	ASTM, 1996, D1586-84(92)
Subsurface Lithology		Soil core	91.4 cm x 1.9 cm (h x r)	Casey et al., 1996
		Cone penetrometer (resistivity)	22.9 cm x 1.9 cm (h x r)	Smolley and Kappmeyer, 1991; ASTM, 1996, D3441-94
		Electrical conductivity (direct-push)	20.3 cm x 1.3 cm (h x r)	McCall, 1996
Average Soil Grain Size		Soil core (sieve analysis)	61.0 cm x 1.9 cm (h x r)	ASTM, 1996, D1586-84(92)
Depth to Water Table		Monitoring well installation or soil boring	Depth x radius of well (h x r)	
		Cone penetrometer (dynamic pore pressure)	2.5 cm x 1.9 cm (h x r)	Smolley and Kappmeyer, 1991
		Advanced geophysical techniques		
Depth to Confining Layer		Soil boring	Depth x radius of well (h x r)	
		Cone penetrometer (resistivity)	22.9 cm x 1.9 cm (h x r)	Smolley and Kappmeyer, 1991; ASTM, 1996, D3441-94
		Advanced geophysical techniques		

Hydrogeologic Parameter Matrix—Estimation Block

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Estimation Block	Reference
Process Type				
Process				
Transport				
Horizontal Advection				
Water Content in Saturated Zone	θ_W	Estimate from soil type	61.0 cm x 1.9 cm (h x r)	ASTM, 1996, D1586-84(92)
		See above, under Water Content in Vadose Zone		
Effective Porosity (equals Water Content in Saturated Zone, if no separate phase)	n	Soil core (drainable porosity combined with grain size)	61.0 cm x 1.9 cm (h x r)	ASTM, 1996, D1586-84(92)
		Tracer experiment (laboratory—soil core)	3.6 cm x 2.5 cm (h x r)	li, 1995
		Two-well tracer experiment (field)	Appendix H, Equation (29)	
		Single-well tracer (drift and pumpback)	Appendix H, Equation (33)	
Darcian Flux (horizontal in x-direction)	q_x	Water balance		
Hydraulic Head	h	Wells (piezometers), via drilled installation	Depth x radius of well (h x r)	
		Wells, via direct push installation	Depth x 2.5 cm (h x r)	
		Cone penetrometer (dynamic pore pressure)	2.5 cm x 1.9 cm (h x r)	Smolley and Kappmeyer, 1991
Isotropic 1-D Hydraulic Conductivity (x and y-directions)	K_r	Slug test	Appendix H, Equation (23)	Taylor et al., 1990
		Single-well pump test with impeller flowmeter in borehole	Appendix H, Equation (3)	Molz et al., 1989
		Single-well tracer (drift and pumpback)	Appendix H, Equation (33)	
		Lab column permeameter test on soil core (based on K_Z)	10.2 cm x 2.5 cm (h x r)	Wolf et al., 1991
		Cone penetrometer (dynamic pore pressure)	2.5 cm x 1.9 cm (h x r)	Smolley and Kappmeyer, 1991
		Qualitative based on soil type	Total volume of all soil cores used	
		Regression on grain size distribution	61.0 cm x 1.9 cm (h x r)	ASTM, 1996, D1586-84(92)

Hydrogeologic Parameter Matrix—Estimation Block

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Estimation Block	Reference
Process Type				
Process				
Transport				
Horizontal Advection				
Anisotropic 1-D Hydraulic Conductivity (x-direction)	K_x	Pump test with observation wells aligned in x-direction	Appendix H, Equation (18)	
		Field tracer test with observation wells aligned in x-direction	Appendix H, Equation (29)	
		History matching (parameter estimation model, based on hydraulic heads)	Area between observation points times screen length	
Anisotropic 1-D Hydraulic Conductivity (y-direction)	K_y	Pump test with observation wells aligned in y-direction	Appendix H, Equation (19)	
		Field tracer test with observation wells aligned in y-direction	Appendix H, Equation (29)	
		History matching (parameter estimation model, based on hydraulic heads)	Area between observation points times screen length	
Dispersion				
Horizontal Longitudinal Dispersion Coefficient	D_L	Laboratory column experiment (electrical conductivity)	5.1 cm x 2.5 cm (h x r)	Piquemal et al., 1992
		Tracer experiment (laboratory—soil core)	3.6 cm x 2.5 cm (h x r)	li, 1995
		Tracer experiment (field)	Appendix H, Equation (29)	
		Moment analysis of plume data (if plume is well known)	Area between observation points times screen length	
		Estimate from textbook using grainsize and v_X		
Horizontal Transverse Dispersion Coefficient	D_T	Laboratory column experiment (electrical conductivity)	5.1 cm x 2.5 cm (h x r)	Piquemal et al., 1992
		Tracer experiment (laboratory—soil core)	3.6 cm x 2.5 cm (h x r)	li, 1995
		Tracer experiment (field)	Appendix H, Equation (29)	
		Moment analysis of plume data (if plume is well known)	Area between observation points times screen length	
		Estimate from textbook using grainsize and v_Y		

Hydrogeologic Parameter Matrix—Estimation Block

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Estimation Block	Reference
Process Type				
Process				
Transport				
Dispersion				
Vertical Transverse Dispersion Coefficient	D_z	Laboratory column experiment (electrical conductivity)	5.1 cm x 2.5 cm (h x r)	Piquemal et al., 1992
		Tracer experiment (field)	Appendix H, Equation (29)	
		Moment analysis of plume data (if plume is well known)	Area between observation points times screen length	
		Textbook value based on grain size		
Water Velocity in x-direction (q/n)	v_x	Tracer experiment	Appendix H, Equation (29)	
		Heat sensor groundwater velocity detector (in-situ Permeable Flow Sensor)	75.0 cm x 2.5 cm (h x r)	Ballard, 1996
Water Velocity in z-direction (q/n)	v_z	Heat sensor groundwater velocity detector (in-situ Permeable Flow Sensor)	75.0 cm x 2.5 cm (h x r)	Ballard, 1996
Tortuosity	τ	Look up in table based on soil type and grain size		
Diffusion				
Diffusion Coefficient	D	Look up for free liquid and adjust by tortuosity		
		Tracer experiment	Appendix H, Equation (29)	
		UFA™ analysis of soil core (for vadose zone D)	17.5 cm x 1.9 cm (h x r)	Conca and Wright, 1995

Hydrogeologic Parameter Matrix—Estimation Block

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Estimation Block	Reference
Process Type				
Process				
Storage				
Equilibrium Sorption				
Retardation Factor	R	Partitioning tracer experiment	Appendix H, Equation (29)	
		Moment analysis of plume data	Area between observation points times screen length	
		<<< or calculate using parameters for each process below >>>		
Soil Bulk Density	ρ_B	Laboratory analysis of soil core	61.0 cm x 1.9 cm (h x r)	ASTM, 1996, D1586-84(92)
Sorption Coefficient	K_d	Laboratory batch experiment (isotherm)	61.0 cm x 1.9 cm (h x r)	ASTM, 1996, D1586-84(92)
		Laboratory batch experiment (one-point)	61.0 cm x 1.9 cm (h x r)	ASTM, 1996, D1586-84(92)
		Column experiment or box model	24.9 cm x 1.0 cm (h x r)	MacIntyre et al., 1991
Fraction Organic Content	f_{OC}	Laboratory analysis of soil core	61.0 cm x 1.9 cm (h x r)	ASTM, 1996, D1586-84(92)
		Literature value based on soil type		
Concentration in Water	C_W	Cone penetrometer (membrane sensor)	2.5 cm x 1.9 cm (h x r)	Christy, 1996
		HydroPunch® sample	Appendix H, Equation (3)	Smolley and Kappmeyer, 1991; Zemo et al., 1995
		BAT® sampler	Appendix H, Equation (3)	Zemo et al., 1994
		Monitoring well, via pumping	Appendix H, Equation (3) or (7)	
		Monitoring well, via bailer	Appendix H, Equation (3) or (7)	
		Monitoring well, via thief sampler	Appendix H, Equation (3)	Kabis, 1996
		Multi-level sampler	Appendix H, Equation (3)	Gibs et al., 1993

Hydrogeologic Parameter Matrix—Estimation Block

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Estimation Block	Reference
Process Type				
Process				
Storage				
Equilibrium Sorption				
Concentration in Air	C_A	Soil gas	Appendix H, Equation (15)	Pitchford et al , 1989
		Cone penetrometer	Appendix H, Equation (15)	Casey et al., 1996
		Fixed gas sampling well	Appendix H, Equation (15)	
Concentration in Soil	C_S	Soil core, via drilling	61.0 cm x 1.9 cm (h x r)	ASTM, 1996, D1586-84(92)
		Soil core, via direct push	91.4 cm x 1.9 cm (h x r)	Casey et al., 1996
		Estimate from historical data		
Concentration in NAPL	C_N	Estimate from historical data and contaminant properties		
Rate-Limited Sorption Using Effective Dispersion				
Effective Dispersion Coefficient	D_{eff}	Moment analysis of plume data (see D_T, D_L, and D_Z)	Area between obseration points times screen length	
		Literature value		
Rate-Limited Sorption Using 1st Order, 2-Site Model				
Desorption Rate Coefficient	k_2	Laboratory column experiment		
		Regression equation		
Fraction of Fast Sorption Sites	F	Laboratory column experiment		
Rate-Limited Sorption Using Spherical Diffusion				
Effective Diffusion Coefficient	D_S	Laboratory batch experiment	61.0 cm x 1.9 cm (h x r)	ASTM, 1996, D1586-84(92)
		Literature data based on diffusion coefficient (D), tortuosity, and average grain size		

Hydrogeologic Parameter Matrix—Estimation Block

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Estimation Block	Reference
Process Type				
Process				
Storage				
Volatilization				
Air Content	θ_A			
Henry's Constant	H	Look up in table		
Dissolution				
NAPL Content	θ_N	Partitioning tracer experiment	Appendix H, Equation (29)	
		Neutron probe	30.5 cm x 30.5 cm (h x r)	Kramer et al., 1992; ASTM, 1996, D5220-92
		Advanced geophysical techniques		
		Estimate from historical records		
Water/NAPL Partition Coefficient	$K_{N/W}$	Laboratory batch experiment	61.0 cm x 1.9 cm (h x r)	ASTM, 1996, D1586-84(92)
		Calculate from $\underline{v}_N$ and S_{SCL}		
Avg Molar Volume of NAPL	$\underline{v}_N$	Estimate from chemical make-up of NAPL, if known		
Hypothetical Super-Cooled Liquid Solubility	S_{SCL}	Look up in table		

Hydrogeologic Parameter Matrix—Estimation Block

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Estimation Block	Reference
Process Type				
Process				
Fate				
Decay (1st Order, Equilibrium Sorption)				
Decay Rate in Aqueous Phase	k	Experimentally derived (batch studies)		
		Zero moment analysis of field data		
		Conservative tracer experiment		
		Microbial counts		
Decay (Michalis-Menton)				
Correction Factor	b	Non-linear regression on field or experimental data		
Decay (Mass-Balance Approximation) [Model O_2 or Alternate Electron Acceptor]				
O_2 (e- acceptor) Solubility		Look up in table		
O_2 (e- acceptor) Flux Into System		Estimate		
O_2 (e- acceptor) Concentration		Water sample		
		Estimate		
Decay (1st Order, Rate-Limited Sorption)				
Production (1st Order, Equilibrium Sorption)				
Production (Michalis-Menton)				
Irreversible Sorption				
		Experimentally derived isotherms		
Precipitation				
Oxidation State of Metal	Z	Look up in table		
		Estimate		
Solubility Product	K_{SP}	Look up in table		
		Estimate		
Loss from System by Transport (Flux In/Out of System)				
Water Flow to/from System		Estimate flow from surface water and to lower aquifer		
Volatilization		Measure concentration profile in vadose zone		
		Measure flux at ground surface directly		
		Look up in literature		

Appendix F: Hydrogeologic Parameter Matrix—Cost

Hydrogeologic Parameter Matrix—Cost

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Estimated Cost ($)	Reference
Process Type				
Process				
Transport				
Vertical Advection				
Water Content in Vadose Zone	θ_v	Gravimetric (tension plate) analysis of soil core		
		Drying soil sample	18 (core)	Everett, 1987; RACER, 1995
		Neutron probe	663 (well)	Everett, 1987
		Tensiometry (in-situ)	84	ECHOS, 1995
Darcian Flux (vertical)	q_z	Infiltration rate, from historical data		
		Double-ring Infiltrometer	654	ECHOS, 1995
		Water balance		
Hydraulic Conductivity (z)	K_z	Column test on soil core (steady-state head control)	578 (core)	Everett, 1987; ECHOS, 1995
		Unsaturated flow apparatus (UFA™) test on soil core		
		Estimate from soil parameters and soil/water retention curves		
Soil Type (Classification)		Soil core	69 (core)	Everett, 1987, ECHOS, 1995
Subsurface Lithology		Soil core	69 (core)	Everett, 1987, ECHOS, 1995
		Cone penetrometer (resistivity)	224 + [81 * depth (m)]	ECHOS, 1995
		Electrical conductivity (direct-push)	224 + [81 * depth (m)]	ECHOS, 1995
Average Soil Grain Size		Soil core (sieve analysis)	69 (core)	Everett, 1987, ECHOS, 1995
Depth to Water Table		Monitoring well installation or soil boring	69 (core)	Everett, 1987, ECHOS, 1995
		Cone penetrometer (dynamic pore pressure)	224 + [81 * depth (m)]	ECHOS, 1995
		Advanced geophysical techniques	2030 / day	ECHOS, 1995
Depth to Confining Layer		Soil boring	69 (core)	Everett, 1987, ECHOS, 1995
		Cone penetrometer (resistivity)	224 + [81 * depth (m)]	ECHOS, 1995
		Advanced geophysical techniques	2030 / day	ECHOS, 1995

Hydrogeologic Parameter Matrix—Cost

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Estimated Cost ($)	Reference
Process Type				
Process				
Transport				
Horizontal Advection				
Water Content in Saturated Zone	θ_w	Estimate from soil type	93 (core)	ECHOS, 1995
		See above, under Water Content in Vadose Zone		
Effective Porosity (equals Water Content in Saturated Zone, if no separate phase)	n	Soil core (drainable porosity combined with grain size)	32 (core)	Everett, 1987
		Tracer experiment (laboratory—soil core)		
		Two-well tracer experiment (field)	5300 (2 wells)	
		Single-well tracer (drift and pumpback)	2050 (well)	
Darcian Flux (horizontal in x-direction)	q_x	Water balance		
Hydraulic Gradient (x-direction)	dh/dx	Wells (piezometers), via drilled installation	$25 (well)	ECHOS, 1995
		Wells, via direct push installation	$25 (well)	ECHOS, 1995
		Cone penetrometer (dynamic pore pressure)	224 + [81 * depth (m)]	ECHOS, 1995
Isotropic 1-D Hydraulic Conductivity (x and y-directions)	K_r	Slug test	$550 (well)	RACER, 1995
		Single-well pump test with impeller flowmeter in borehole		
		Single-well tracer (drift and pumpback)	2050 (well)	
		Lab column permeameter test on soil core (based on K_z)	289 (core)	ECHOS, 1995
		Cone penetrometer (dynamic pore pressure)	224 + [81 * depth (m)]	ECHOS, 1995
		Qualitative based on soil type	117 / core (core)	ECHOS, 1995
		Regression on grain size distribution	117 / core (core)	ECHOS, 1995

Hydrogeologic Parameter Matrix—Cost

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Estimated Cost ($)	Reference
Process Type				
Process				
Transport				
Horizontal Advection				
Anisotropic 1-D Hydraulic Conductivity (x-direction)	K_x	Pump test with observation wells aligned in x-direction	1200 (2 wells)	
		Field tracer test with observation wells aligned in x-direction	2500 (2 wells)	
		History matching (parameter estimation model, based on hydraulic heads)		
Anisotropic 1-D Hydraulic Conductivity (y-direction)	K_y	Pump test with observation wells aligned in y-direction	1200 (2 wells)	
		Field tracer test with observation wells aligned in y-direction	2500 (2 wells)	
		History matching (parameter estimation model, based on hydraulic heads)		
Dispersion				
Horizontal Longitudinal Dispersion Coefficient	D_L	Laboratory column experiment (electrical conductivity)	16 (core)	Everett, 1987
		Tracer experiment (laboratory—soil core)		
		Tracer experiment (field)	2500 (2 wells)	
		Moment analysis of plume data (if plume is well known)		
		Estimate from textbook using grainsize and v_X		
Horizontal Transverse Dispersion Coefficient	D_T	Laboratory column experiment (electrical conductivity)	16 (core)	Everett, 1987
		Tracer experiment (laboratory—soil core)		
		Tracer experiment (field)	2500 (2 wells)	
		Moment analysis of plume data (if plume is well known)		
		Estimate from textbook using grainsize and v_Y		

Hydrogeologic Parameter Matrix—Cost

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Estimated Cost ($)	Reference
Process Type				
Process				
Transport				
Dispersion				
Vertical Transverse Dispersion Coefficient	D_Z	Laboratory column experiment (electrical conductivity)	16 (core)	Everett, 1987
		Tracer experiment (field)	2500 (2 wells)	
		Moment analysis of plume data (if plume is well known)		
		Textbook value based on grain size		
Water Velocity in x-direction (*q*/*n*)	v_X	Tracer experiment	2500 (2 wells)	
		Heat sensor groundwater velocity detector (in-situ Permeable Flow Sensor)	3900 + [66 * depth (m)]	ECHOS, 1995; Ballard, 1996
Water Velocity in z-direction (*q*/*n*)	v_Z	Heat sensor groundwater velocity detector (in-situ Permeable Flow Sensor)	3900 + [66 * depth (m)]	ECHOS, 1995; Ballard, 1996
Tortuosity	τ	Look up in table based on soil type and grain size		
Diffusion				
Diffusion Coefficient	D	Look up for free liquid and adjust by tortuosity		
		Tracer experiment	2500 (2 wells)	
		UFA™ analysis of soil core (for vadose zone D)		

Hydrogeologic Parameter Matrix—Cost

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Process Type

Process

Parameter	Symbol	Determined By	Estimated Cost ($)	Reference
Storage				
Equilibrium Sorption				
Retardation Factor	R	Partitioning tracer experiment	5300 (2 wells)	
		Moment analysis of plume data		
		<<< or calculate using parameters for each process below >>>		
Soil Bulk Density	ρ_B	Laboratory analysis of soil core	27 (core)	Everett, 1987
Sorption Coefficient	K_d	Laboratory batch experiment (isotherm)		
		Laboratory batch experiment (one-point)		
		Column experiment or box model		
Fraction Organic Content	f_{OC}	Laboratory analysis of soil core		
		Literature value based on soil type		
Concentration in Water	C_W	Cone penetrometer (membrane sensor)	1250 + [81 * depth (m)]	ECHOS, 1995
		HydroPunch® sample	1250 + [81 * depth (m)]	ECHOS, 1995
		BAT® sampler	1250 + [81 * depth (m)]	ECHOS, 1995
		Monitoring well, via pumping	673 + [6 * depth (m)]	ECHOS, 1995
		Monitoring well, via bailer	680 + [4 * depth (m)]	Zemo et al., 1994; ECHOS, 1995
		Monitoring well, via thief sampler	673 + [4 * depth (m)]	ECHOS, 1995
		Multi-level sampler	$18 + \Sigma$ {655 + [6 * $depth_i$ (m)]} $depth_i$ is depth of each level	ECHOS, 1995

Hydrogeologic Parameter Matrix—Cost

Note: X-direction is longitudinal in direction of groundwater flow. Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Estimated Cost ($)	Reference
Process Type				
Process				
Storage				
Equilibrium Sorption				
Concentration in Air	C_A	Soil gas	$150	Pitchford et al., 1989
		Cone penetrometer	1066 + [81 * depth (m)]	ECHOS, 1995
		Fixed gas sampling well	489 + [6 * depth (m)] (well)	ECHOS, 1995
Concentration in Soil	C_S	Soil core, via drilling	798 (core)	ECHOS, 1995
		Soil core, via direct push	798 (core)	ECHOS, 1995
		Estimate from historical data		
Concentration in NAPL	C_N	Estimate from historical data and contaminant properties		
Rate-Limited Sorption Using Effective Dispersion				
Effective Dispersion Coefficient	D_{eff}	Moment analysis of plume data (see D_T, D_L, and D_Z)		
		Literature value		
Rate-Limited Sorption Using 1st Order, 2-Site Model				
Desorption Rate Coefficient	k_2	Laboratory column experiment		
		Regression equation		
Fraction of Fast Sorption Sites	F	Laboratory column experiment		
Rate-Limited Sorption Using Spherical Diffusion				
Effective Diffusion Coefficient	D_S	Laboratory batch experiment		
		Literature data based on diffusion coefficient (D), tortuosity, and average grain size		

Hydrogeologic Parameter Matrix—Cost

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Estimated Cost ($)	Reference
Process Type				
Process				
Storage				
Volatilization				
Air Content	θ_A			
Henry's Constant	H	Look up in table		
Dissolution				
NAPL Content	θ_N	Partitioning tracer experiment		
		Neutron probe	663 (well)	Everett, 1987
		Advanced geophysical techniques	2030 / day	ECHOS, 1995
		Estimate from historical records		
Water/NAPL Partition Coefficient	$K_{N/W}$	Laboratory batch experiment		
		Calculate from $\underline{v}_N$ and S_{SCL}		
Avg Molar Volume of NAPL	$\underline{v}_N$	Estimate from chemical make-up of NAPL, if known		
Hypothetical Super-Cooled Liquid Solubility	S_{SCL}	Look up in table		

Hydrogeologic Parameter Matrix—Cost

Note: X-direction is longitudinal in direction of groundwater flow.
Y-direction is transverse to direction of groundwater flow.

Parameter	Symbol	Determined By	Estimated Cost ($)	Reference
Process Type				
Process				
Fate				
Decay (1st Order, Equilibrium Sorption)				
Decay Rate in Aqueous Phase	k	Experimentally derived (batch studies)		
		Zero moment analysis of field data		
		Conservative tracer experiment	5300 (2 wells)	
		Microbial counts		
Decay (Michalis-Menton)				
Correction Factor	b	Non-linear regression on field or experimental data		
Decay (Mass-Balance Approximation) [Model O_2 or Alternate Electron Acceptor]				
O_2 (e- acceptor) Solubility		Look up in table		
O_2 (e- acceptor) Flux Into System		Estimate		
O_2 (e- acceptor) Concentration		Water sample	40 + [6 * depth (m)]	ECHOS, 1995
		Estimate		
Decay (1st Order, Rate-Limited Sorption)				
Production (1st Order, Equilibrium Sorption)				
Production (Michalis-Menton)				
Irreversible Sorption				
		Experimentally derived isotherms		
Precipitation				
Oxidation State of Metal	Z	Look up in table		
		Estimate		
Solubility Product	K_{SP}	Look up in table		
		Estimate		
Loss from System by Transport (Flux In/Out of System)				
Water Flow to/from System		Estimate flow from surface water and to lower aquifer		
Volatilization		Measure concentration profile in vadose zone		
		Measure flux at ground surface directly		
		Look up in literature		

Appendix G: Hydrogeologic Boundary Condition Matrix

Boundary Condition Matrix

Boundary Condition Type		
Boundary Condition		
Formal Name	**Determined From**	**Reference**
Hydraulic		
Recharge Area		
Specified flux (Neumann)	Geological data	Franke et al., 1987
	Maps/satellite	ASTM, 1996, D5518-94
	History matching (parameter estimation model based on heads)	Cooley, 1977;Cooley, 1979
Discharge Area		
Constant flux (Neumann)	Geological data	Franke et al., 1987
	Maps/satellite	ASTM, 1996, D5518-94
	History matching (parameter estimation model based on heads)	Cooley, 1977;Cooley, 1979
Body of Water		
Specified head (Dirichlet)	Site visit (visual investigation)	Franke et al., 1987; ASTM, 1996, D5609-94
	Maps/satellite	ASTM, 1996, D5518-94
Containment Wall (object)		
Streamline (no-flow)	Borehole data	Franke et al., 1987; ASTM, 1996, D5609-94
Precipitation Rate		
Specified flux (Neumann)	Historical weather data	Franke et al., 1987; ASTM, 1996, D5609-94
	Collect and measure precipitation	
Infiltration Rate		
Constant flux (Neumann)	Determine from precipitation rate, soil type, and site geology	Todd et al., 1976; Franke et al., 1987
Evapo-Transpiration Rate		
Seepage surface	Measure	Todd et al., 1976; Franke et al., 1987; ASTM, 1996, D5609-94
	Look up in literature	
Run-Off		
Seepage surface	Surface water data	Franke et al., 1987
Water Table		
Free-surface	Piezometers	Franke et al., 1987; ASTM, 1996, D5609-94

Boundary Condition Matrix

Boundary Condition Type		
Boundary Condition		
Formal Name	**Determined From**	**Reference**
Hydraulic		
Leakage between Aquifers		
Head-dependent flux (Cauchy)	Piezometers	Franke et al., 1987; ASTM, 1996, D5609-94
	Borehole data (continuous soil core)	
	History matching (parameter estimation model based on heads)	Cooley, 1977;Cooley, 1979
Contaminant Transport (Source)		
Constant Concentration		
	Water/soil samples	Franke et al., 1987
	Source data	
	Fate data	
Variation of Source w/Time		
	Records review	
	Employee interviews	
	Analyze plume data	
	Link to precipitation data (specifically infiltration rate)	
Mass/Volume of Source		
	Records review	
	Employee interviews	
	Soil sample	ASTM, 1996, D4700-91
	Groundwater sample	
Location/Area of Source		
	Aerial/satellite photos	ASTM, 1996, D5518-94
	Records review	
	Employee interviews	
	Soil sample	ASTM, 1996, D4700-91
	Groundwater sample	
	Advanced geophysical techniques (e.g., GPR, sounding, electro-magnetic)	Pitchford et al., 1989

Appendix H: Estimation Block Equations

A. Groundwater Samples—Short Screen Length (less than 10 cm).

Equations for determining estimation block size for a method that obtains a liquid sample, utilizing a short screen length (less than 10 cm):

$$EB = S \cdot \pi \cdot r_e^{2} \tag{3}$$

$$r_e = r_w + \left(\frac{V}{\pi \cdot n \cdot S} - r_w^{2} \right)^{\frac{1}{2}} \tag{4}$$

where,

EB = estimation block volume (cm^3)
S = screen length (cm)
r_e = radius of estimation block (cm)
r_w = radius of well casing (cm)
V = volume of liquid purged/removed (cm^3)
n = porosity of soil adjacent to screen

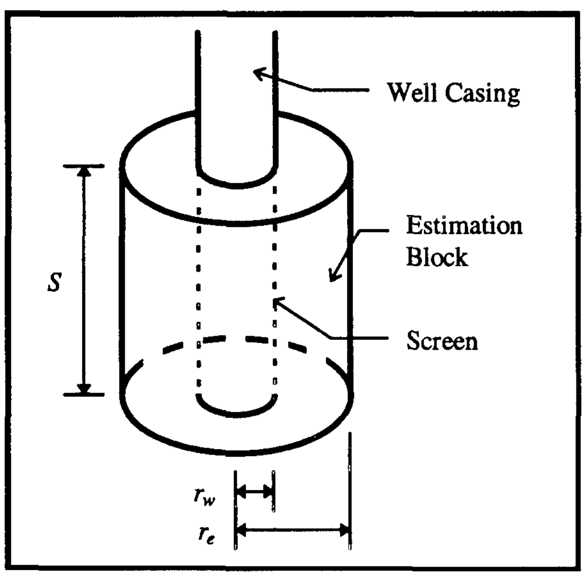

Figure 4: Monitoring Well Detail, for Short Screen Groundwater Samples

Via Pump or Bailer:

Assumes that the well is purged (3 well volumes) before obtaining the sample, so that the water flowing back into the casing is considered a composite sample if sampled soon after purging.

Use Equation (3), with

S and r_w are dimensions of the monitoring well, and

$$V = 3 \cdot S \cdot \pi \cdot r_w^2 \qquad (5)$$

where,

V = volume of liquid within the screened interval of the well casing (cm^3)

Via BAT® Sampler (Zemo et al., 1994):

Use Equation (3), with

$S = 10.2$ cm
$r_w = 1.9$ cm
$V = 35\ cm^3$ (volume of sampler, no purge)

Via HydroPunch® Sampler (Smolley and Kappmeyer, 1991; Zemo et al., 1995):

Use Equation (3), with

$S = 25.4$ cm
$r_w = 1.9$ cm
$V = 500\ cm^3$ (volume of sampler, no purge)

Via Thief Sampler (Kabis, 1996):

Use Equation (3), with

$S = 2$ cm
$V = 40$ cm^3 (volume of sampler, no purge)

Via Multi-Level Sampler (Gibs et al., 1993):

Use Equation (3) for each individual sampling section, with

$$V = Q_w \cdot t \qquad (6)$$

where,

V = volume of liquid obtained in sample (cm^3)
Q_W = rate at which liquid is pumped (cm^3/s)
t = length of time taken to obtain sample (s)

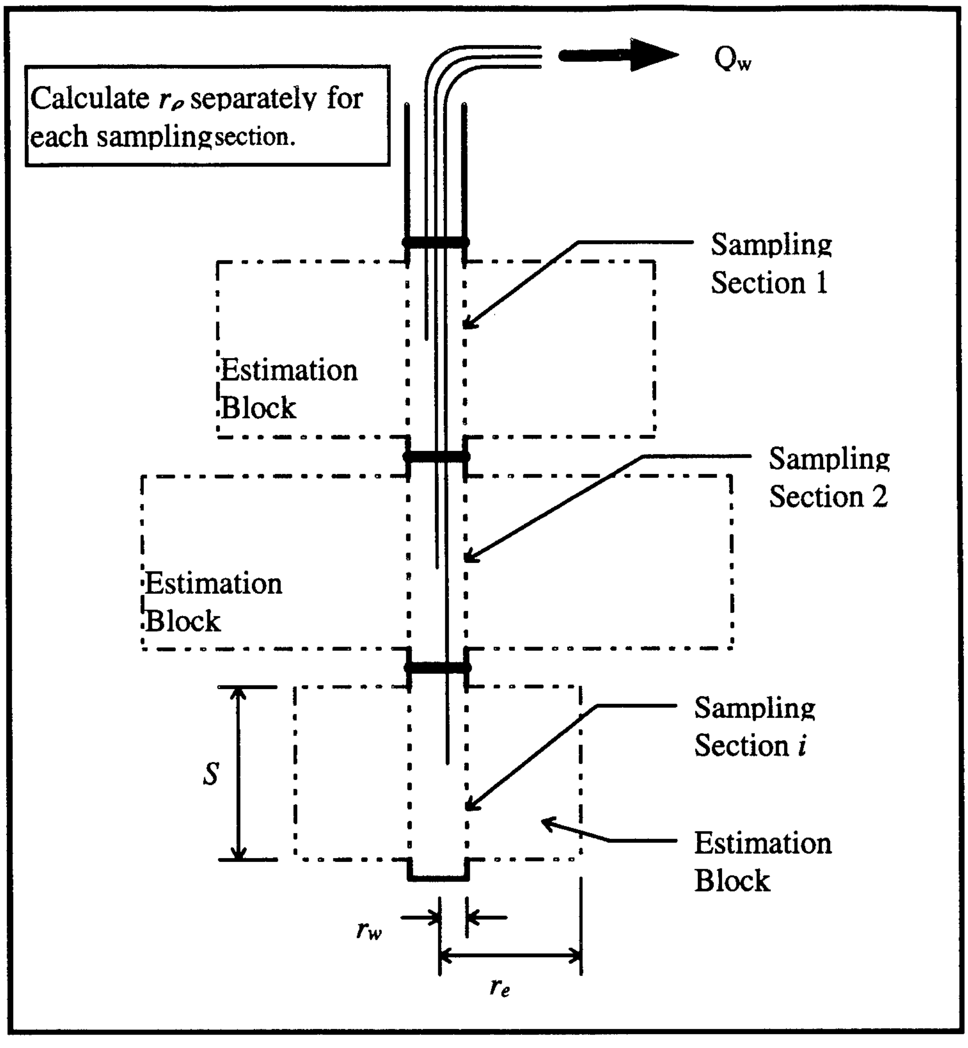

Figure 5: Multi-Level Sampler

B. Groundwater Samples—Long Screen Length (greater than 10 cm)

Equations for determining estimation block size for a method that obtains a liquid sample, utilizing a long screen length (greater than 10 cm):

$$EB_{tot} = \sum_{i=1}^{N} EB_i \tag{7}$$

$$EB_i = S_i \cdot \pi \cdot \left(r_{e_i}\right)^2 \tag{8}$$

$$r_{e_i} = r_w + \left(\frac{V_i}{\pi \cdot n \cdot S_i} - r_w^{\,2}\right)^{\frac{1}{2}} \tag{9}$$

$$V_i = S_i \cdot \pi \cdot r_w^{\,2} \cdot \left(\frac{R_i}{R_{tot}}\right) \tag{10}$$

$$S_i = \frac{S_{tot}}{N} \tag{11}$$

$$R_i = \frac{K_i}{K_{min}} \tag{12}$$

$$R_{tot} = \sum_{i=1}^{N} R_i \tag{13}$$

$$N = \mathrm{round}\left(\frac{S_{tot}}{60}\right) \tag{14}$$

where,

EB_{tot} = total estimation block volume (cm^3)

EB_i = estimation block volume of layer i (cm^3)

N = number of layers that screened interval is divided into

S_i = screen length (thickness) of layer i (cm)

S_{tot} = total screen length of monitoring well (cm)

r_{ei} = radius of estimation block for layer i (cm)

r_w = radius of well casing (cm)

V_i = portion of total volume purged/removed, that is attributed to entering well from layer i (cm^3)

R_i = ratio of horizontal hydraulic conductivity (K_i) of layer i to K_i of the layer with the lowest K_i

R_{tot} = sum of the hydraulic conductivity ratios for all layers

K_i = horizontal hydraulic conductivity of layer i (cm/s)

K_{min} = horizontal hydraulic conductivity of the layer with the lowest horizontal hydraulic conductivity

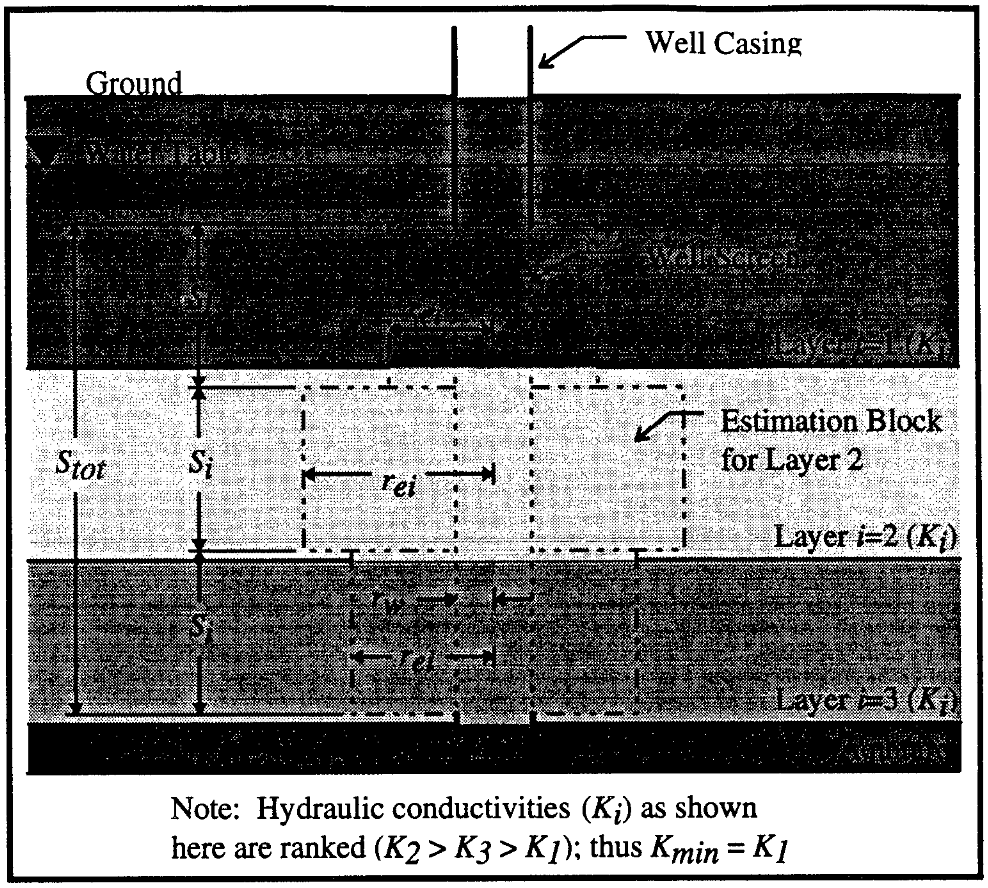

Figure 6: Estimation Block for Long Screen Length Installation

Procedure:

1. Determine number of layers (N).
2. Obtain "real" value of horizontal hydraulic conductivity (isotropic) for the vertical center-point of each layer (K_i).
3. Determine the value of the minimum horizontal hydraulic conductivity (K_{min}).
4. Calculate the horizontal hydraulic conductivity ratio for each layer (R_i).
5. Calculate the sample volume for each layer (V_i).
6. Calculate the estimation block radius for each layer (r_{ei}).
7. The total estimation block volume can now be calculated.

C. Soil Gas Samples

Equations for determining estimation block size for soil gas sampling methods:

$$EB = \frac{4}{3}\cdot\pi\cdot r_e^{3} \tag{15}$$

$$r_e = \left(\frac{3\cdot V}{\theta_A\cdot 4\cdot\pi}\right)^{\frac{1}{3}} \tag{16}$$

$$\theta_A = n - \theta_v$$ (if no separate phase contaminant is present) (17)

where,

EB = estimation block volume (cm^3)
r_e = radius of estimation block (cm)
V = volume of gas purged/removed (cm^3)
θ_A = air content of soil at location of sample
n = porosity of soil at location of sample
θ_v = water content of soil at location of sample

Via Fixed Gas Sampling Well:

Use Equation (15), with

$$V = Q_g\cdot t \tag{6}$$

where,

V = volume of gas purged/removed (cm^3)
Q_g = rate at which gas is pumped (cm^3/s)
t = length of time taken to purge and obtain sample (s)

Via Soil Gas (Pitchford et al., 1989):

This assumes that the that several liters of gas are purged before obtaining the sample, so that the gas flowing into the casing is representative of that in the surrounding subsurface. Additionally, it is assumed that the sample is obtained by using a syringe to extract gas from the sampling hose while a pump is drawing gas out of the installation. The syringe actually obtains a small sub-sample of approximately a liter of gas withdrawn by the pump.

Use Equation (15), with

$$V = 5000 \text{ cm}^3$$

Via Cone Penetrometer (Casey et al., 1996):

This assumes that the that several liters of gas are purged before obtaining the sample, so that the gas flowing into the casing is representative of that in the surrounding subsurface. Additionally, it is assumed that the sample is obtained by using a syringe to extract gas from the sampling hose while a pump is drawing gas out of the installation. The syringe actually obtains a small sub-sample of approximately a liter of gas withdrawn by the pump.

Use Equation (15), with

$$V = 5000 \text{ cm}^3$$

D. Pump Test

Equations for determining estimation block size for a pump test:

$$EB_x = \frac{1}{4} \cdot \pi \cdot RI^2 \cdot (S_1 + S_2) \tag{18}$$

$$EB_y = \frac{1}{4} \cdot \pi \cdot RI^2 \cdot (S_1 + S_3) \tag{19}$$

$$EB_R = S_1 \cdot \pi \cdot RI^2 \tag{20}$$

$$RI = 3000 \cdot s_w \cdot K^{\frac{1}{2}} \quad \text{(Bear, 1979)} \tag{21}$$

$$s_w = \left(\frac{Q_w}{2 \cdot \pi \cdot K \cdot B} \right) \cdot \ln\left(\frac{RI}{r_w} \right) \quad \text{(Bear, 1979)} \tag{22}$$

where,

EB_x = estimation block volume for determining horizontal hydraulic conductivity in x-direction (longitudinal with water flow) (m^3)—see Figures 7b and 7c

EB_y = estimation block volume for determining horizontal hydraulic conductivity in y-direction (transverse to water flow) (m^3)—see Figures 7b and 7c

EB_R = estimation block volume for determining a single isotropic horizontal hydraulic conductivity based on an average of the values in the x and y-directions (m^3)—see Figure 7a

RI = radius of influence of pumping well (m)

d_x = distance between pumping well and observation well in the x-direction (m)

d_y = distance between pumping well and observation well in the y-direction (m)

S_1 = screen length of pumping well (m)

S_2 = screen length of observation well, located in x-direction (m)

S_3 = screen length of observation well, located in y-direction (m)

s_w = drawdown in pumping well (m)

K = horizontal hydraulic conductivity (isotropic) next to pumping well (m/s)

Q_w = rate at which water is pumped from pumping well (m^3/s)

B = thickness of aquifer (m)

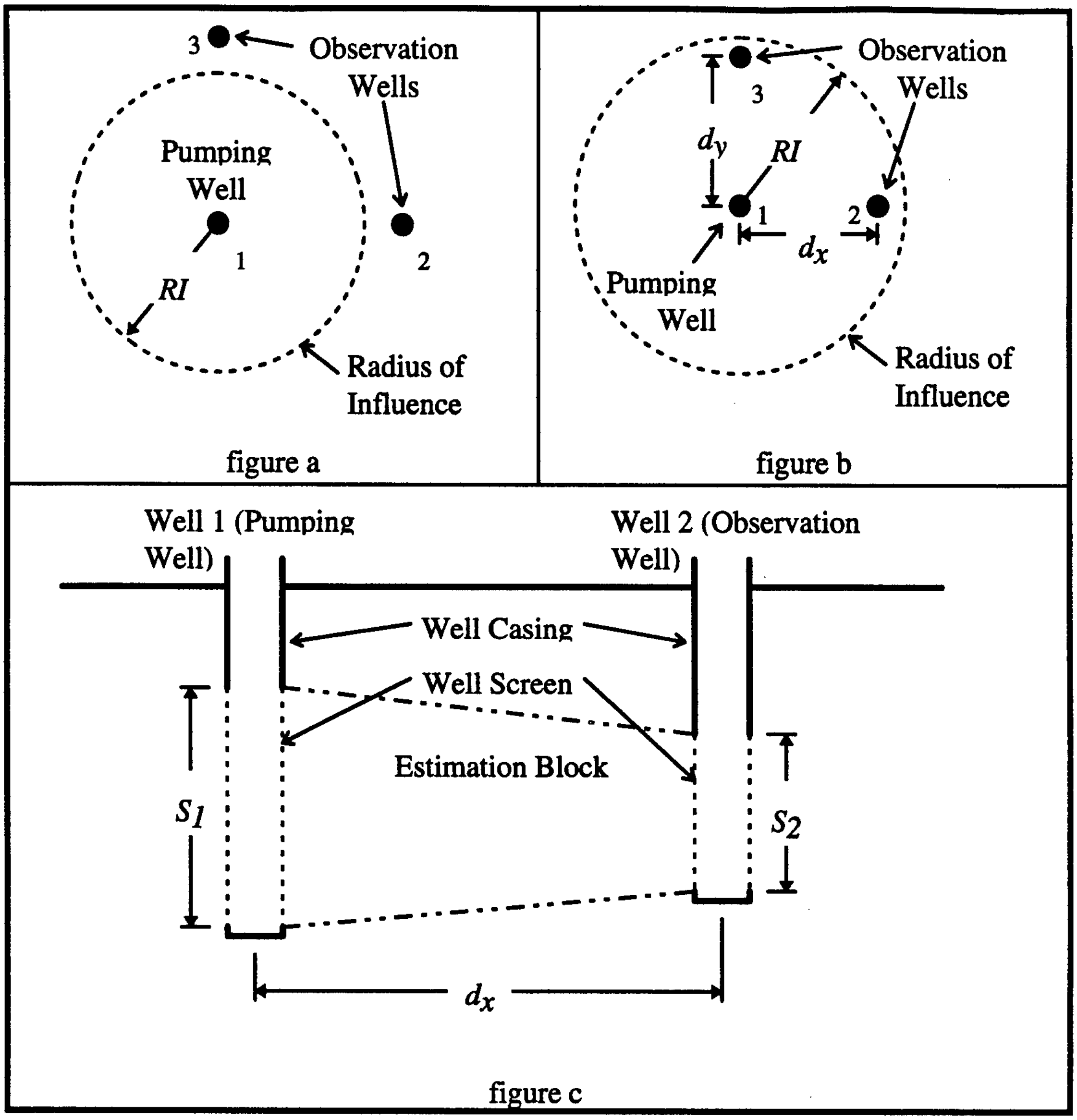

Figure 7: Estimation Block for Pump Test

Procedure:

1. Assume a radius of influence (*RI*)–a good starting value is $\frac{Q_w}{2 \cdot B \cdot K \cdot I}$ where I is the hydraulic gradient at the location of the pumping well).
2. Calculate the drawdown based on the radius of influence (s_w).
3. Use the calculated drawdown to determine the radius of influence (*RI*).
4. Compare the new radius of influence to the previous one.
5. If the new radius of influence is more then 10% different from the previous one, repeat from step 2.
6. Use the computed radius of influence to determine the estimation block as follows:
    a) If $d_x < RI$ and $d_y < RI$, use Equations (18) and (19) to determine the estimation blocks for computing the horizontal hydraulic conductivities in the x and y-directions, respectively.
    b) If $d_x > RI$ or $d_y > RI$, use Equation (20) to determine the estimation block for computing a single combined horizontal hydraulic conductivity (isotropic) based on the x and y-direction values.

*E. **Slug Test***
(Taylor et al., 1990):

Equations for determining estimation block size for a slug test. Choice of Equation (24) or (25) depends whether the well fully penetrates the aquifer, or not:

$$EB = 1.4 \cdot \left(S \cdot \pi \cdot r_e^{\,2} \right) \tag{23}$$

For a fully penetrating well:

$$r_e = r_w \cdot \exp\left[\frac{1.1}{\ln\left(\frac{D}{r_w}\right)} + \frac{y_c}{\left(\frac{S}{r_w}\right)} \right]^{(-1)} \tag{24}$$

For a fully penetrating well:

$$r_e = r_w \cdot \exp\left[\frac{1.1}{\ln\left(\frac{D}{r_w}\right)} + \frac{y_a + y_b \cdot \left(\frac{B - D}{r_w}\right)}{\left(\frac{S}{r_w}\right)} \right]^{(-1)} \tag{25}$$

$$y_a = 1.516 + 3.568 \cdot 10^{-2} \cdot \left(\frac{S}{r_w}\right) - 7.777 \cdot 10^{-5} \cdot \left(\frac{S}{r_w}\right)^2 + 8.064 \cdot 10^{-8} \cdot \left(\frac{S}{r_w}\right)^3 - 3.096 \cdot 10^{-11} \cdot \left(\frac{S}{r_w}\right)^4 \tag{26}$$

$$y_b = 2.294 \cdot 10^{-1} + 5.325 \cdot 10^{-3} \cdot \left(\frac{S}{r_w}\right) - 3.990 \cdot 10^{-6} \cdot \left(\frac{S}{r_w}\right)^2 + 1.948 \cdot 10^{-9} \cdot \left(\frac{S}{r_w}\right)^3 - 6.845 \cdot 10^{-13} \cdot \left(\frac{S}{r_w}\right)^4 \tag{27}$$

$$y_c = 7.512 \cdot 10^{-1} + 54.266 \cdot 10^{-2} \cdot \left(\frac{S}{r_w}\right) - 7.098 \cdot 10^{-5} \cdot \left(\frac{S}{r_w}\right)^2 + 5.913 \cdot 10^{-8} \cdot \left(\frac{S}{r_w}\right)^3 - 1.926 \cdot 10^{-11} \cdot \left(\frac{S}{r_w}\right)^4 \tag{28}$$

Special cases:

If the term $\frac{S}{rw} > 1000$; then use 1000 for this term.

If the term $\ln\left(\frac{B - D}{r_w}\right) > 6$; then use 6 for this term.

where,

EB = estimation block volume (cm^3)
S = screen length (cm)
r_e = radius of estimation block (cm)
r_w = radius of well casing + gravel pack (cm)
D = depth well penetrates aquifer (cm)
B = thickness of aquifer (cm)

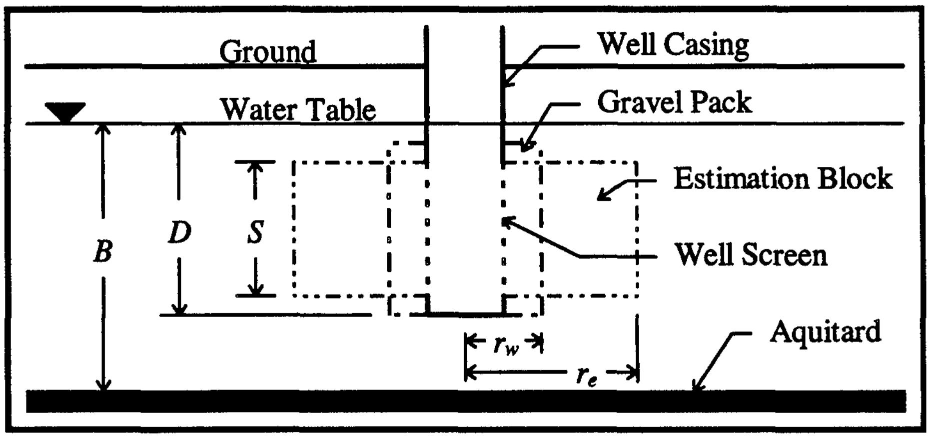

Figure 8: Monitoring Well Detail for Slug Test

Determine r_w from Table 7, based on the diameter of the well casing:

Table 7: Determination of r_w for Slug Test

Well Casing Diameter (cm)	Construction Method	r_w (cm)
5.1	Drilled	10.2
5.1	Direct Push	2.5
10.2	Drilled	14.0
10.2	Direct Push	5.1
15.2	Drilled	17.8
15.2	Direct Push	7.6

F. Single Well Pump Test with Impeller Flowmeter in Borehole
(Molz et al., 1989)

Equations for determining estimation block size for impeller flowmeter method:

$$EB = S \cdot \pi \cdot r_e^2 \qquad (3)$$

$$r_e = r_w + \left(\frac{V}{\pi \cdot n \cdot S} - r_w^2 \right)^{\frac{1}{2}} \qquad (4)$$

$$V = Q_w \cdot t \qquad (6)$$

where,

B = estimation block volume (cm^3)
S = vertical distance between two consecutive flowmeter readings (cm)
r_e = radius of estimation block (cm)
r_w = radius of well casing (cm)
V = volume of liquid removed during sampling (cm^3)
n = porosity of soil adjacent to screen
Q_w = rate at which liquid is pumped from well (cm^3/s)
t = length of time from beginning of first flowmeter reading to end of second flowmeter reading (s)

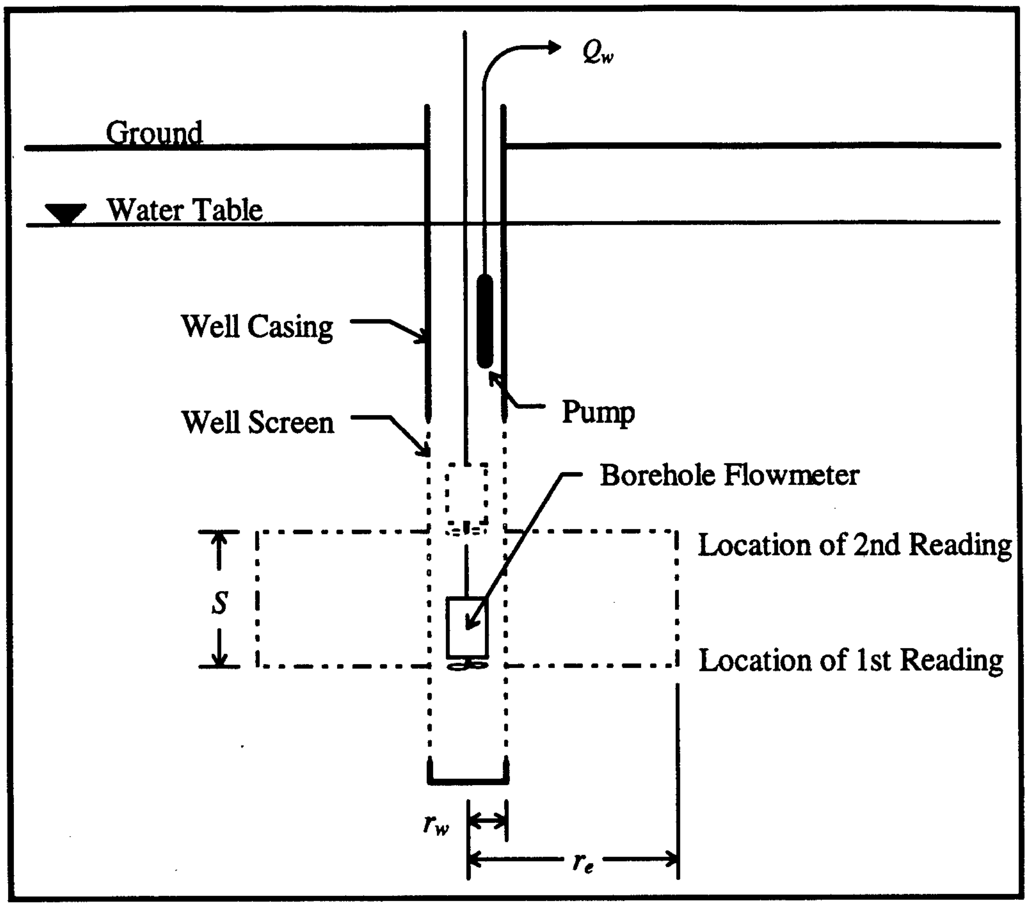

Figure 9: Monitoring Well Detail for Borehole Flowmeter

G. Two-Well Tracer Test

Equations for determining estimation block size for a two-well tracer test:

$$EB = 2 \cdot d_y \cdot d_x \cdot \frac{1}{2} \cdot \left(S_1 + S_2\right) \tag{29}$$

$$y = \frac{Q_w}{2 \cdot B \cdot K \cdot I} \cdot \left(1 - \frac{\phi}{\pi}\right) \qquad \text{(Masters, 1991)} \tag{30}$$

$$\phi = \arctan\left(\frac{y}{d_x}\right) \qquad \text{(Masters, 1991)} \tag{31}$$

$$RT = \left(\frac{V}{n \cdot \pi \cdot S_1}\right)^{\frac{1}{2}} \tag{32}$$

where,

EB = estimation block volume (cm^3)
d_x = distance between injection well and pumping well in the x-direction (cm)
d_y = width of estimation block. It is the <u>smaller</u> of: RT and y (cm)
S_1 = screen length of injection well (cm)
S_2 = screen length of pumping well (cm)
Q_w = rate at which tracer is injected into injection well (cm^3/s)
B = thickness of aquifer (cm)
K = horizontal hydraulic conductivity (isotropic) adjacent to pumping well (cm/s)
I = hydraulic gradient at the location of the pumping well
ϕ = angle between the pumping well and the maximum width of plume it can intercept (radians)
y = maximum width of plume (centered on injection well) that the pumping well can intercept (cm)
RT = radius of injected tracer plume (cm)
V = volume of tracer injected (cm^3)
n = porosity of soil adjacent to injection well

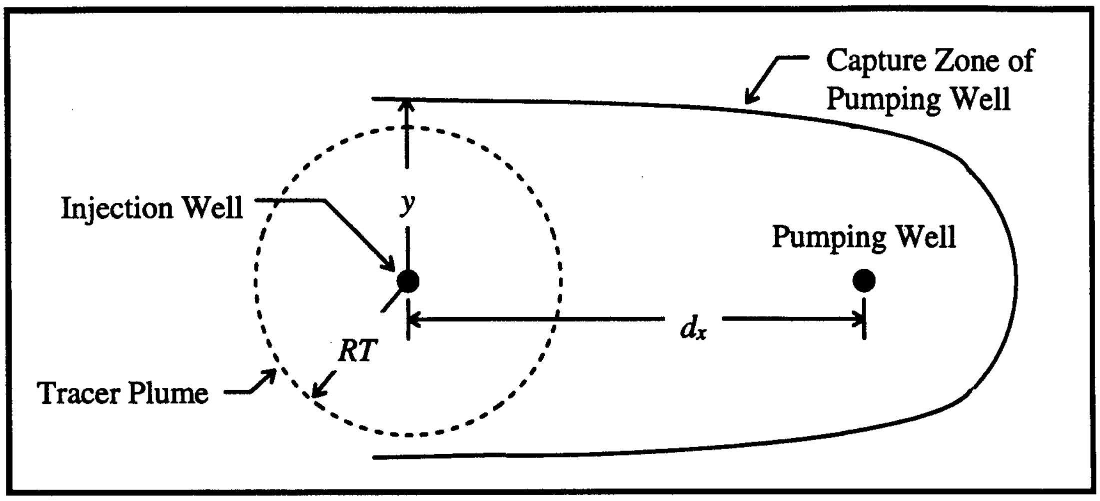

Figure 10: Two-Well Tracer Test

Procedure:

1. Assume value for *y*. A good initial guess is to use *RT*.
2. Calculate ϕ based on *y*.
3. Use ϕ to determine *y*.
4. Compare new value of *y* to previous value of *y*.
5. If new value of *y* is more than 10% different from previous value, repeat from step 2.
6. Determine estimation block volume based on the following:
   a) If $RT > y$, then $d_y = y$.
   b) If $RT < y$, then $d_y = RT$.

H. Single-Well Tracer Test

Equations for determining estimation block size for a single-well (drift and pumpback) tracer test:

$$EB = 2 \cdot RT \cdot d_x \cdot S \tag{33}$$

$$RT = \left(\frac{V}{n \cdot \pi \cdot S} \right)^{\frac{1}{2}} \tag{34}$$

$$x_t = RT + K \cdot I \cdot t \tag{35}$$

$$x_{sp} = \frac{Q_w}{2 \cdot \pi \cdot B \cdot K \cdot I} \tag{36}$$

where,

EB = estimation block volume (cm^3)
RT = radius of injected tracer plume (cm)
d_x = length of estimation block. It is the <u>smaller</u> of: x_t and x_{sp} (cm)
S = screen length of well (cm)
V = volume of tracer injected (cm^3)
n = porosity of soil adjacent to injection well
B = thickness of aquifer (cm)
x_t = distance leading edge of tracer plume will travel (from injection point) in time t (cm)
x_{sp} = stagnation point—farthest leading edge of plume can travel before it can not be recovered by pumping (cm)
K = horizontal hydraulic conductivity (isotropic) next to pumping well (cm/s)
I = hydraulic gradient at the location of the pumping well
t = length of time before beginning to recover tracer (s)
Q_w = rate at which well is pumped to recover tracer (cm^3/s)

Note:

If $x_t < x_{sp}$, then $d_x = x_t$.
If $x_t > x_{sp}$, then $d_x = x_{sp}$.

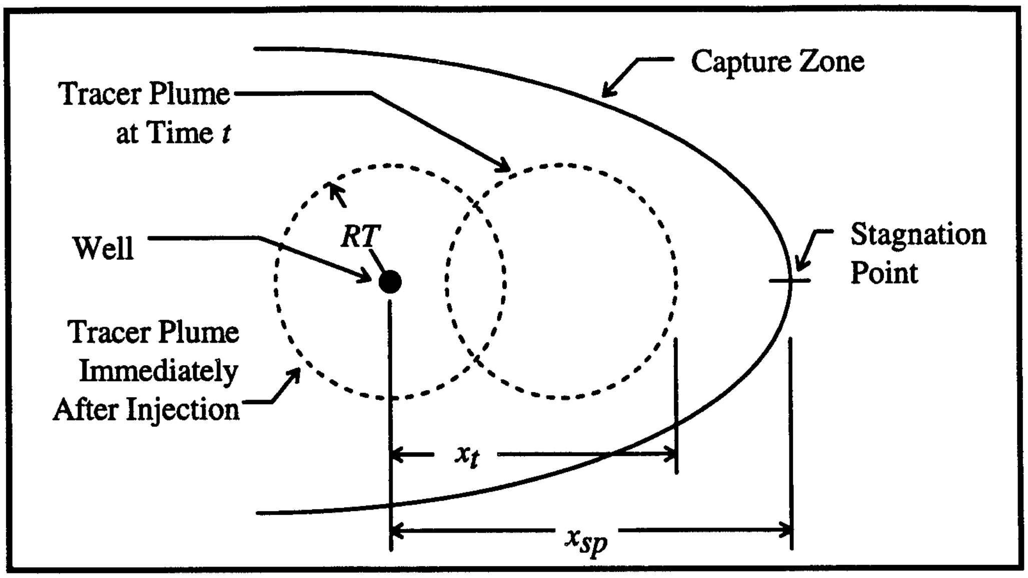

Figure 11: Single-Well Tracer Test

Appendix I: Cost Equations

A. Well Construction Costs

Equation for determining the cost of installing a well (ECHOS, 1995; RACER, 1995):

$$Cost = FC + P + B*(D) + A*(D-S-1) + G*(S+1) + C*(D-S) + W*(S) \quad (37)$$

where,

$Cost$ = total cost of installing well
FC = fixed costs ($)
P = cost of well plug
B = cost of drilling ($/m)
D = depth from ground surface to bottom of well (m)
A = cost of portland cement annular seal to ground surface ($/m)
G = cost of gravel pack ($/m)
S = length of screen (m)
C = cost of well casing ($/m)
W = cost of well screen ($/m)

via Direct Push:

Use Equation (37) with

$FC = \$224$
$P = \$36$
$B = \$55$
$A = \$0$
$G = \$0$
$C = \$66$
$W = \$144$

via Drilling:

Use Equation (37) with

$FC = \$1400$

Select *P*, *B*, *A*, *G*, *C*, and *W* from Table 8.

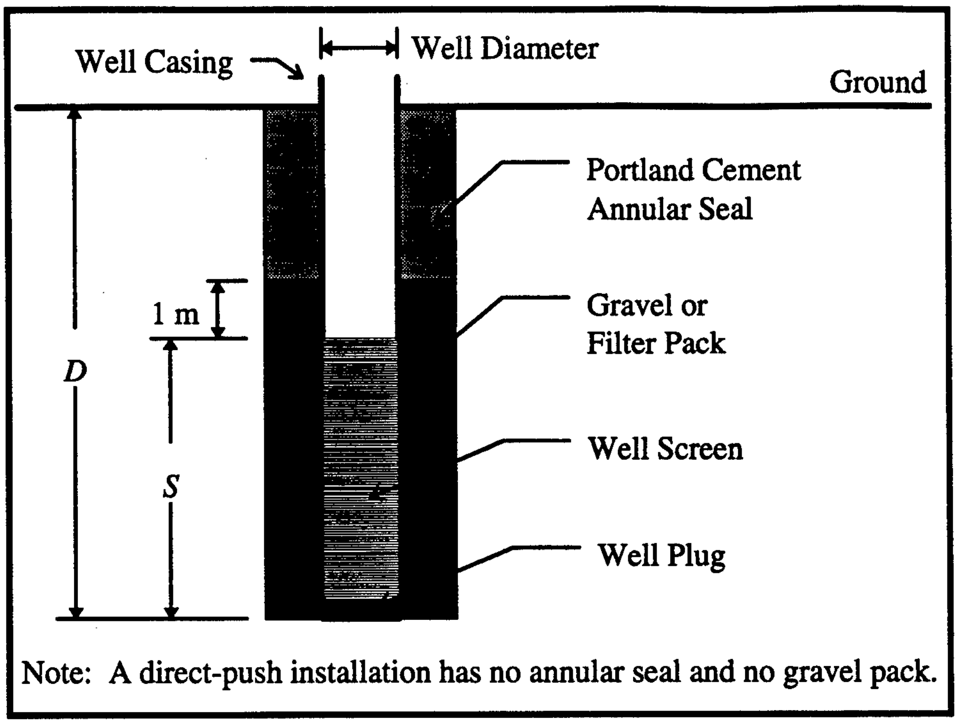

Figure 12: Well Construction Detail

Table 8: Well Construction Costs

Well Diameter (cm)	Casing Material	P: Well Plug Cost ($)	B: Boring Cost ($/m)	A: Annular Seal Cost ($/m)	G: Gravel Pack Cost ($/m)	C: Casing Cost ($/m)	W: Screen Cost ($/m)
5.1	PVC	13	66	4	30	16	30
5.1	Stainless Steel	36	66	4	30	66	144
10.2	PVC	34	92	6	55	45	52
10.2	Stainless Steel	67	92	6	55	151	181
15.2	PVC	85	118	31	79	82	98
15.2	Stainless Steel	225	118	31	79	338	440

B. Soil Core Extraction Costs

Equation for determining the cost of obtaining a soil core (ECHOS, 1995; RACER, 1995):

$$Cost = FC + B*(D) \tag{38}$$

where,

$Cost$ = total cost of installing well
FC = fixed costs ($)
B = cost of boring ($/m)
D = depth from ground surface to point where core is obtained (m)

Select method of obtaining soil core. Then use Table 9 to determine the cost factors. Note that the two methods that involve obtaining a soil core during well installation have no boring cost directly associated with them. The boring costs for these two methods are associated with the well that is being constructed simultaneously. These two methods have (well) in the boring cost column as a reminder to figure in the well construction costs.

Table 9: Soil Core Extraction Costs

Method	FC: Fixed Cost ($)	B: Boring Cost ($/m)
Drilling	1000	32
Drilling (during drilled well installation)	31	0 (well)
Direct-push	410	55
Direct-push (during direct-push well installation)	186	0 (well)

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13. ABSTRACT *(Maximum 200 words)*

The purpose of this study was to develop a tool for evaluating data quality when characterizing a potentially contaminated groundwater aquifer, and to provide a basis for developing a simulator to allow environmental managers and engineers to practice and learn about the site characterization process. This study characterized the uncertainty, estimation block size, and cost for the various methods of determining the value of each geological, hydrological, and contaminant parameter necessary to characterize a site. Site characterization objectives and parameters necessary to obtain those objectives were identified. Methods of estimating each parameter were identified, and research performed to characterize each method. This research resulted in a list of site characterization objectives and matrices of process parameters, parameter estimation methods, method uncertainties, volumes, costs, applicable model boundary conditions, and references. Fifty transport, storage, and fate parameters were identified along with 85 different estimation methods. Of these methods, 61 were partially characterized and 24 were completely characterized (primarily pertaining to transport). Results were used to define the initial specifications for a site characterization simulator. Considering this research, more study is needed to characterize methods pertaining to storage (except equilibrium sorption) and all fate parameters.

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