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**SAMPLE APPLICATION OF SENSITIVITY/UNCERTAINTY ANALYSIS
TECHNIQUES TO A GROUNDWATER TRANSPORT PROBLEM**

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ABSTRACT

The primary objective of this document is to provide sample applications of selected sensitivity and uncertainty analysis techniques within the context of the radiological performance assessment process. These applications were drawn from the companion document *Guidelines for Sensitivity and Uncertainty Analyses of Low-Level Radioactive Waste Performance Assessment Computer Codes* (S. Maheras and M. Kotecki, DOE/LLW-100, 1990). Three techniques are illustrated in this document: one-factor-at-a-time (OFAT) analysis, fractional factorial design, and Latin hypercube sampling. The report also illustrates the differences in sensitivity and uncertainty analysis at the early and latter stages of the performance assessment process, and potential pitfalls that can be encountered when applying the techniques. The emphasis is on application of the techniques as opposed to the actual results, since the results are hypothetical and are not based on site-specific conditions.

EXECUTIVE SUMMARY

Sensitivity and uncertainty analyses are a valuable, but sometimes neglected, part of the performance assessment (PA) process. In some cases, PA is seen only as a method for demonstrating compliance with long-term dose or risk objectives after a facility has been designed. Furthermore, some view PA as a requirement that must be done, without consideration of the other benefits that can be obtained. PA (through the use of sensitivity/uncertainty analysis) can be used as a management tool during all stages of the licensing process. By indicating the relative impact of individual design and site characterization parameters on disposal system performance, sensitivity/uncertainty analysis results can provide justification for specific activities based on quantitative, performance-based measures. Of course, technical judgement and qualitative factors (i.e., reality checks) must also be considered because of the uncertainties involved and complexity of the processes. In any case, improved understanding of the behavior of a system makes it easier for management to defend decisions related to continuing or discontinuing funding for specific activities.

The use of sensitivity/uncertainty analyses in the PA process has two primary benefits:

- Cost savings obtained by focusing site characterization, design, and modeling efforts on the site data, design features, and transport pathways that have the greatest impacts on facility performance
- Quantification of the uncertainty associated with PA predictions used to demonstrate compliance.

Furthermore, the U.S. Nuclear Regulatory Commission (NRC) has emphasized the need for sensitivity/uncertainty analyses by including a requirement in the *Standard Format and Content for a License Application for a Low-Level Radioactive Waste Disposal Facility* (NUREG-1199, Rev. 1; NRC 1988, pp. 6-7 and 6-10).

The primary objective of this document is to provide sample applications of selected sensitivity and uncertainty analysis techniques within the context of the radiological performance assessment process. These applications were drawn from the companion document *Guidelines for Sensitivity and Uncertainty Analyses of Low-Level Radioactive Waste Performance Assessment Computer Codes* (S. Maheras and M. Kotecki, DOE/LLW-100, 1990). Three techniques are illustrated in this document: one-factor-at-a-time (OFAT) analysis, fractional factorial design, and Latin hypercube sampling. The second objective is to illustrate the differences in sensitivity and uncertainty analysis at the early and latter stages of the performance assessment process. The third objective is to identify potential pitfalls that can be encountered when applying the techniques. The emphasis is on application of the techniques as opposed to the actual results, since the results are hypothetical and are not based on site-specific conditions.

Examples are presented for two different sets of circumstances: (a) a poorly defined (wide ranges and no distributions) set of parameters which corresponds to the initial stages of the PA process when minimal data are available, and (b) a relatively well-defined set of parameters with measured distributions representing the latter stages of the performance assessment process after site characterization. By presenting two sets of conditions, a broader illustration of how sensitivity/uncertainty analysis techniques are applied at the early and latter stages of the PA process is provided, as well as sample applications of the different techniques. In general, the emphasis should be on sensitivity analysis early in the process to guide future efforts and shift toward uncertainty analysis as additional data are collected and final calculations are made.

A key purpose of this document is to illustrate that statistical methods must be applied with caution. A potential user must have an understanding of the process being modeled as well as a background in mathematics and statistics. Technical judgement plays a large role in the fractional factorial design and Latin hypercube sampling techniques. There is potential for different conclusions to be drawn based on different interpretations of the process being modeled. Examples of potential pitfalls are provided to demonstrate how different assumptions (e.g., definition of the functional form of a factor) can

lead to different conclusions. Limitations of the techniques are discussed in detail in Section 7.

Transport of contaminants through groundwater was selected for this example because it is probably the most expensive pathway in terms of modeling, design, and site characterization costs, as well as being the most significant transport pathway in many instances. Thus, efforts related to the groundwater pathway would be expected to have the largest potential benefit from the use of sensitivity/uncertainty analysis. Since the emphasis is on the sensitivity/uncertainty analysis process, a simplified transport problem assuming a specified groundwater velocity is considered (see Section 3). An actual application would likely consider the parameters that impact the flow velocity, and thus, would have to model both flow and transport.

Sensitivity of the results to uncertainty in the inventory of waste available for transport is also addressed. The purpose for considering inventory is twofold: to address actual uncertainty in inventory data, and to address source term (release rate) uncertainty, which controls the inventory actually available to the groundwater. Sensitivity to changes in the distance between source and receptor is also assessed to illustrate that sensitivity analysis can be used to demonstrate the impact of political or regulatory considerations.

The variation of OFAT analysis used for this application was found to be relatively easy to apply and interpret (see Section 4). However, it was also limited by the large number of runs required to gain a more complete understanding of the relative importance of the factors, and the potential for interpreting the results to apply to more than the ranges of values considered. OFAT analysis was primarily used to gain an understanding of the functional form of the factors of interest. If the standard OFAT approach would have been used, much of the information that was obtained from the approach used in this document would not have been acquired. Also, if a more limited approach would have been used, the interactions that were discussed would not have been identified. In general, OFAT analysis was found to be useful as a scoping tool and precursor to the more detailed analyses, but would be very limited if applied without follow-up analyses.

Fractional factorial design was found to be more difficult to apply, but this is to be expected since it is a more rigorous technique (see Section 5.1). The difficulty was offset by the fact that only a small number of runs were required to complete the analysis. Fractional factorial design allowed the direct consideration of interactions between factors and provided a quantitative ranking of the factors and interactions by relative impact on the response variable. This information was not directly obtained from the OFAT analysis. Fractional factorial design was found to be very useful in the initial stages of the PA process because the distributions of the factors were not required. Thus, when minimal data are available (such as bounding ranges), fractional factorial design is more applicable. Uncertainty analysis was not conducted with the fractional factorial design; the distributions for the data, and additional Monte Carlo runs using the fitted surface (as opposed to the analytical solution), would have been required. The fitted surface was not deemed adequate to conduct the uncertainty analysis.

Latin hypercube sampling was similar in effort of application to the fractional factorial design (see Section 5.2). Latin hypercube sampling also allowed for direct consideration of interactions between factors and provided a quantitative ranking of the factors and interactions. The primary benefit of Latin hypercube sampling was that the cumulative distribution function for the uncertainty analysis was obtained directly from the analytical groundwater transport model. Because distributions for the parameters were required, Latin hypercube sampling was most appropriate for the latter stages of the PA process when data were available from site characterization. Also, the superiority of Latin hypercube sampling for conducting the uncertainty analysis provided a good basis for use at the latter stages of the PA process.

The most difficult parts of the analysis were determination of the functional forms for the factors and specification of the interactions to be considered. Several iterations were made in order to arrive at the functional forms and interactions used in the final analyses. This is a very subjective process and leaves plenty of room for differing opinions. The authors do not claim to assume that the functional forms and interactions used are the best for this problem. There may be a better combination. The authors did try a number

of combinations and were most comfortable with the combination of factors and functional forms used for the final analyses. Such flexibility emphasizes the need to apply the techniques and interpret results with caution.

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Sample Application of Sensitivity/Uncertainty Analysis Techniques to a Groundwater Transport Problem

1. INTRODUCTION

Sensitivity and uncertainty analyses are a valuable part of the performance assessment (PA) process. The objective of a parameter uncertainty analysis is to determine the effect on output of the uncertainty in the input parameters. The objective of a sensitivity analysis is to rank the input parameters based on their influence on the model output.

The contributions that sensitivity/uncertainty analysis make to the PA process have been recognized for technical and regulatory considerations (Maheras and Kotecki, 1990). The need for sensitivity/uncertainty analysis has also been identified in the Nuclear Regulatory Commission (NRC) standard format and content guide (NRC, 1988). The primary benefits of sensitivity and uncertainty analysis (respectively) are:

- Cost savings obtained by focusing modeling, design, and site characterization efforts on the transport pathways, design features, and site characterization data that have the greatest impact on performance
- Quantification of the uncertainty associated with PA predictions used to demonstrate compliance.

In the initial stages of the PA process, calculations are limited by a lack of data. Thus, initial PA calculations are conducted to (a) determine bounding ranges of the results, and (b) identify the data that are necessary to make the calculations more realistic. To support this approach, sensitivity/ uncertainty analysis is initially used to obtain an estimate of the range of possible results

and to focus future site characterization, design, and modeling efforts on the most essential areas.

In the latter stages of a PA, the emphasis shifts from guiding future efforts to making the final performance prediction for compliance assessment. At the completion of site characterization, data for each parameter are expected in the form of distributions of measured values. If proper data are provided, uncertainty analysis is used to quantify the possible range of performance and the distribution of the results within that range, based on the distribution of input data. At this stage, sensitivity analysis is used to illustrate the impact of specific parameters on the final results.

1.1 Background

A variety of specific approaches for sensitivity and uncertainty analyses are discussed in a companion report by Maheras and Kotecki (1990). Sample applications of selected approaches from the companion report are presented in this report. No implication is intended that the approaches presented in this document are the best for a specific application. Technical judgement should be used to determine the approach that is most appropriate. Transport of contaminants through groundwater was selected for this example because it is probably the most expensive pathway in terms of modeling, design, and site characterization costs, as well as being the most significant transport pathway in many instances. Thus, efforts related to the groundwater pathway would be expected to have the largest potential benefit from the use of sensitivity/uncertainty analysis.

Three sensitivity/uncertainty analysis techniques are demonstrated in this report. The first technique is a variation of a one-factor-at-a-time (OFAT) analysis. The OFAT analysis involves simply varying the value of one parameter while holding the others constant. The second and third techniques are more statistically rigorous. The second technique is response surface fitting using fractional factorial design. The third technique is Latin hypercube sampling. In the second and third techniques, experimental designs are constructed that consider the impacts of individual parameters and interactions between multiple

parameters. For sensitivity analysis, which uses fractional factorial design and Latin hypercube sampling, regression analysis techniques are used to create a model (an equation comprised of each parameter and interaction and corresponding coefficients) that approximates the results predicted by the computer code. A cumulative distribution function (CDF) can also be constructed directly from the results of the computer runs prescribed by the experimental design based on Latin hypercube sampling.

Transport of contaminants in groundwater is the process modeled for this report. Since the emphasis is on the process, a simplified transport problem assuming a specified groundwater velocity is considered. An actual application would likely consider the parameters that impact the flow velocity, and thus, would have to model both flow and transport. Ranges of parameter values selected for the example are intended to represent actual conditions that may be found at a disposal site. However, these results are not intended to be used in support of actual PAs, because the transport parameter ranges should be based on site-specific data.

As applied in this document, all three of the techniques require a detailed understanding of groundwater flow and transport. Application of the OFAT analysis in this document also requires a limited understanding of regression analysis and statistics. OFAT analysis is relatively straightforward to use and the results are generally easy to interpret, but they are limited in applicability. OFAT analysis is limited by the potential for interpreting results to apply to more than the ranges of values and factors considered. Specification of input for the more rigorous statistical techniques requires technical judgement, especially in the functional forms of the factors. As a result, the rigorous methods require a detailed understanding of both groundwater flow and transport and the specific statistical techniques. The limitations of OFAT analysis can be addressed by applying one of the more rigorous techniques. Thus, the best approach is to use the three techniques in conjunction. Such an approach will require a relatively strong technical background and should be conducted by analysts familiar with the processes and techniques being used.

Regression techniques are widely used for scientific experiments when observing a response to different levels of independent variables. In general, the response is subject to variability; that is, a replication of the same trial can result in a different response. Such variability does not exist in a sensitivity analysis of a numerical model. The model is deterministic. Thus, when using regression techniques for sensitivity analysis of computer models, the conclusions that can be drawn from the regression analysis differ from those that one would usually make in a classical experiment. It is also important to understand that the result of a test is dependent upon the other factors included in the model. Furthermore, the significance of a given factor on the response can change depending upon the presence or absence of other factors. In conclusion, the ranking of parameters obtained from a sensitivity analysis are only valid for the factors, functional form of factors, and ranges of factor values used for that analysis.

1.2 Objectives

The primary objective of this document is to provide sample applications of selected sensitivity and uncertainty analysis techniques from the companion guidelines document to this report (Maheras and Kotecki, 1990) within the context of the PA process. Three techniques are illustrated in this document: OFAT analysis, fractional factorial design, and Latin hypercube sampling. The second objective is to illustrate the differences in sensitivity and uncertainty analysis at the early and latter stages of the PA process. The third objective is to illustrate potential pitfalls that can be encountered when applying the techniques. The emphasis of this document is on the techniques as opposed to the actual results, since the results are hypothetical and are not intended to be used in decision-making for a specific site.

Examples for two different sets of circumstances are presented in this document: (a) a poorly defined (wide ranges and no distributions) set of parameters representing the initial stages of the PA process when minimal data are available, and (b) a relatively well-defined set of parameters with measured distributions representing the latter stages of the performance assessment process after data have been collected. By presenting two sets of conditions, a

broader illustration of how sensitivity and uncertainty analysis are applied at the early and latter stages of the PA process is provided as well as sample applications of the different techniques.

A key purpose of this document is to illustrate that statistical methods must be applied with caution. A potential user must have an understanding of the process being modeled as well as a background in mathematics and statistics. Technical judgment plays a large role in the fractional factorial design and Latin hypercube sampling techniques. Thus, there is potential for analysts to draw different conclusions from a single process being modeled, based on different interpretations. Examples of potential pitfalls are provided to demonstrate how different assumptions (e.g., definition of the functional form of a factor) can lead to different conclusions. Limitations of the techniques are discussed in some detail.

The purpose of the document is not to select the best technique, but to illustrate how different techniques are applied within the context of the PA process. In order to most efficiently meet the objectives of this document, the fractional factorial design and Latin hypercube sampling techniques for sensitivity analysis are applied to different sets of conditions (i.e., early and latter stages of the performance assessment process). Since the two rigorous sensitivity/uncertainty analysis techniques are applied to different sets of data, comparison of the results from the two techniques in the context of this document is inappropriate. Iman and Helton (1985) and Maheras and Kotecki (1990) provide in-depth discussions and evaluations of the relative effectiveness of different sensitivity and uncertainty analysis techniques applied to the same problem.

2. GENERAL APPROACH

A general process for conducting sensitivity/uncertainty analysis is described in the companion document by Maheras and Kotecki (1990). Actual implementation of the general process for the samples in this document is described in this section. Note that the steps are similar to those identified in the companion document; however, in some cases the order may be slightly different. A brief discussion of the actual activities during each step is provided. The steps implemented for this document are:

1. Define the assessment question to be answered by the analysis (Section 1 and Section 3)
2. Choose the tools to be used for the analysis (Section 3, Section 4, and Section 5)
3. Define and reduce the scope of the analysis (Section 4 and briefly in Section 5.2)
4. Evaluate uncertainty in the parameters to be included in the analysis, based on the data (Section 4 and Section 5.2)
5. Perform the calculations and interpret the results (Section 4 and Section 5).

Determination of the parameters with the greatest impact on the response variable (peak concentration was selected for this analysis) for a groundwater transport problem is the question to be answered in this assessment. A simplified groundwater transport problem was used to limit the effort required for the calculations, since the emphasis is on the sensitivity/uncertainty analysis techniques. Two sets of conditions are considered in this analysis: highly uncertain data expected during the initial stages of the PA process and relatively well understood data expected in the latter stages.

Four tools are used for these analyses: an analytic solution to solve the groundwater transport equation and three different techniques to conduct the sensitivity/uncertainty analysis. Since a simplified groundwater transport problem is used, an analytic solution can be used. One aspect that is overlooked with this approach is that all the data required for a detailed groundwater model are not used in the analytic solution (e.g., pore velocity is substituted for a combination of hydraulic gradients, hydraulic conductivities, and porosities). Thus, sensitivity of the more detailed parameters cannot be assessed. However, such a "lumped" parameter approach can be useful as a screening tool and is suitable for the purposes of this document.

The three techniques selected for the sensitivity/uncertainty analysis represent two levels of detail; the OFAT analysis is relatively simple, while the fractional factorial design and Latin hypercube sampling are more complex. Also, the techniques have attributes that fit together nicely for applications related to the PA process [i.e., OFAT analysis provides input to the other two, and fractional factorial design is better suited to the initial stages of the PA process while Latin hypercube sampling is better suited for the latter stages of the PA process (see Section 5.3)].

An OFAT analysis is used to define and reduce the scope of the analysis by providing a preliminary indication of parameters (and the ranges of values for parameters) that can be expected to have the greatest impact on the response variable. Likewise, parameters and ranges of values with minimal impacts can also be identified and removed from further consideration. A limited amount of scope reduction was also conducted prior to the second sample problem based on the results of the first problem (i.e., the list of factors and interactions to be considered was reduced). Screening must be applied with caution, however, because a parameter may have minimal impact for one set of conditions and be critical if the conditions are different (see Section 4.3 and Section 4.5).

Determination of the ranges of values (evaluation of uncertainty) for the factors was loosely based on conditions expected at a waste site (for the first problem, the ranges tended to be overly wide rather than too narrow). Additional reasoning for the ranges included: consideration of several radionuclides by

using a range of half-lives (i.e., if a radionuclide is specified then the half-life would be fixed) and consideration of different well distances (a regulatory uncertainty related to the point of compliance).

The second aspect of Step 3 is the most difficult part of the whole process. Determination of the functional forms for the factors and the interactions tends to be a trial and error process. Iterations between the OFAT analysis and trial runs with the advanced techniques and subsequent regression are required in order to obtain an acceptable set of factors, interactions, and functional forms. This is also a dangerous part of the process, because the results may change as different functional forms are used.

The actual calculations for the advanced techniques are relatively straightforward once the factors, interactions, and functional forms have been defined. A great deal of caution is needed when applying the OFAT analysis to ensure that the necessary ranges of values are considered.

3. PROBLEM DESCRIPTION

The sample problem selected for this document is a relatively simple contaminant transport problem in an aquifer (see Figure 3-1). Since the emphasis is on the sensitivity and uncertainty analysis techniques as opposed to the groundwater modeling, many simplifying assumptions were used. The aquifer is characterized with a constant, uniform groundwater velocity in a homogeneous porous medium of infinite lateral extent and unit thickness. The source region is assumed to be square with sides 24.5 m wide. Predicted concentrations have been vertically averaged in the unit thickness and are only considered along the plume center line. Since a constant, uniform velocity was assumed, no groundwater flow calculations are necessary. This substantially reduces the computational time required for each simulation. Diffusion effects are also assumed to be negligible. Release of contaminants was assumed to be inventory-controlled, where a given quantity of the contaminant is instantaneously introduced into the system. This was implemented in the model by assuming an initial concentration in the source region at time = 0.

By making the simplifying assumptions discussed above, the problem can be solved with an analytic solution. Use of an analytic solution further reduces the time requirements for the transport modeling. The analytic solution used for this problem is presented in Till and Meyer (1983, pp. 4-28 to 4-33) and Codell et al., (1982, pp. 3-1 to 3-74). Given the assumptions described in the previous paragraph, the equation for calculating the concentration (C) at a distance (X) downstream from the center of the source region is:

Figure 3-1. Conceptual model of transport problem.

$$C(X,Y,t) = \frac{QX_2Y_2}{n_e R_d} Z_z$$

$$X_2 = \frac{1}{2l} \left[\operatorname{erf} \frac{\left(X + \frac{l}{2}\right) - \frac{U^* t}{R_d}}{\sqrt{\frac{4D_x t}{R_d}}} - \operatorname{erf} \frac{\left(X - \frac{l}{2}\right) - \frac{U^* t}{R_d}}{\sqrt{\frac{4D_x t}{R_d}}} \right] \exp(-\lambda t)$$

$$Y_2 = \frac{1}{2w} \left[\operatorname{erf} \frac{\left(\frac{w}{2} + y\right)}{\sqrt{\frac{4D_y t}{R_d}}} + \operatorname{erf} \frac{\left(\frac{w}{2} - y\right)}{\sqrt{\frac{4D_y t}{R_d}}} \right]$$

$$Z_z = \frac{1}{b}$$

(3.1)

where

- X = receptor distance downgradient from the center of the source (m)
- Y = receptor distance perpendicular to the plume centerline (m)
(Y = 0 for calculations at the centerline of the plume)
- D_x = dispersion coefficient in the x-direction (m²/s)
- D_y = dispersion coefficient in the y-direction (m²/s)
- R_d = retardation coefficient (unitless)
- l = length of source in the x-direction (m)
- w = width of source in the y-direction (m)
- U* = pore velocity (Darcy velocity/porosity) (m/s)
- n_e = porosity (unitless)
- λ = decay constant (ln(2)/T_{1/2}, s⁻¹)
- t = time (s)
- Q = source inventory of contaminant (mass or activity)
- b = aquifer thickness (m) (assumed to equal 1)

In the absence of diffusion, the dispersion coefficients D_x and D_y are defined as follows:

$$D_x = \alpha_L U^* \text{ and } D_y = \alpha_T U^* \quad (3.2)$$

where

- α_L = longitudinal dispersivity (m)
- α_T = transverse dispersivity (m).

Variations in the source term were simulated by varying the initial inventory (Q) of an individual contaminant. In general, an analysis would have to consider all contaminants. Actual source inventories are subject to a large degree of uncertainty, because many of these inventories are characterized based on the waste generation process and limited measurements. For example, some waste is difficult to characterize due to the physical form (contaminated clothing, tools, etc.) and the nature of the radiation emitted. An additional consideration for uncertainty is the process required to mobilize the contaminants. Release rates will be uncertain, because different mechanisms can move the contaminant from the waste form into the transport medium. In order to maintain a reasonable scope, release rate uncertainties are not directly considered. Only differences in inventory available for transport were considered.

Other parameter values were selected to be representative of conditions that would be found at a disposal site or to address regulatory uncertainties. Well location (point of compliance) was included to illustrate that sensitivity analysis does not have to be limited to site characterization and inventory concerns. The results of the sensitivity analysis will be used to gain a better understanding of the dominant processes and parameters. A ranking of the relative importance of the input parameters will also be obtained. Such a ranking can be used to justify the consideration or lack of consideration of a parameter in a site characterization program, or to demonstrate to regulators the impacts of different locations for a receptor. One must remember that the ranking is only applicable for the parameters, interactions, and ranges of values used for the analysis. If any of these are changed, the rankings may change.

4. SCOPING ANALYSIS

The purpose of this phase of a sensitivity/uncertainty analysis is to define the response variable for the analysis, the factors to be considered, ranges of values for those factors, and the functional form that will be used for each factor in the rigorous analysis. The conclusions from this phase of the analysis are subject to change as the analysis proceeds. In actuality, during the conduct of this sample problem the functional forms for the factors were refined after an initial rigorous analysis was conducted. In this respect, sensitivity/uncertainty analysis is an iterative process. The interim forms are omitted in this document for brevity. However, it is important to note that some iteration (fine tuning) did take place. Also note that as the OFAT analysis progressed, certain factors were screened from consideration to reduce the scope of the analysis.

4.1 Define Response Variable

The endpoint whereby sensitivity of the model to the various factors is measured is termed the response variable. The response variable used in this example was peak (or maximum) concentration. The peak concentration (C_p) was defined as the maximum calculated concentration in the time period from 0 to infinity for a given set of fixed factor values. This response variable was selected for several reasons. First, previous sensitivity analysis showed very little correlation with the transport factors when concentration at a fixed point in time was observed. Second, in performing modeling for regulatory compliance objectives, the most conservative measure of acceptability to legal contamination limits is the peak contaminant concentration which occurs at a receptor point. Third, by only observing variation in the peak concentration, the time factor was essentially removed from the analysis, thus simplifying the interpretation of the data.

4.2 Define Range of Factor Values

Factors are defined as variables which are functionally related to the response variable. For example, a relationship exists such that variables a, b, and c are factors to the response variable C:

$$C = f(a,b,c) \quad . \quad (4.1)$$

Each factor has a specified range of possible values. These values should reflect the actual ranges to be expected or that have been observed. For example, if one of the factors in an analysis was vehicle speed on a rural interstate, a realistic range of speeds would be roughly 40 to 80 mph. It would not be reasonable to let the vehicle speed factor range from 0 to 300 mph, since this range of speed would not be encountered.

The factors considered in the groundwater model examined in this study include dispersivity, contaminant retardation, Darcy velocity, receptor well distance, and radionuclide half-life (Table 4-1). These factors provide a good sample of parameters expected to have a significant impact on the predicted concentrations. The ranges of values selected for these factors are intended to represent a wide range of field conditions, different radionuclides, and different radionuclide source terms. In this respect, the sensitivity analysis is more of a global scoping study to illustrate a wide range of possibilities. Typically, the radionuclide will be specified; thus, the half-life would be fixed and the retardation would likely have less uncertainty. After site characterization has been completed, the ranges of values for uncertain factors will be further refined, and the distributions should also be available.

4.3 OFAT Analysis

Before a rigorous sensitivity analysis was performed using a fractional factorial design, an OFAT analysis was used to gain a better understanding of the

Table 4-1. Range of factor values used in the sensitivity analysis sample problem

<u>Factor</u>	<u>Symbol</u>	<u>Units</u>	<u>Range of Factor Values</u>	
			<u>Minimum Value</u>	<u>Maximum Value</u>
Retardation	R_d	---	1.0E+00	1.0E+02
Longitudinal Dispersivity	α_L	m	1.0E-02	1.0E+01
Transverse Dispersivity	α_T	m	1.0E-03	1.0E+00
Darcy Velocity	U	m/y	1.0E-02	5.0E+00
Half-life	$T_{1/2}$	y	1.0E+01	1.0E+05
Well Distance	X	m	1.0E+02	5.0E+02
Source Inventory*	Q	+	1.0E-01	1.0E+01

+ Source inventory may have units of mass or activity. It was not important to define units in this example, thus units of Q will be omitted.

* The range of values were used for the more rigorous statistical techniques. The range for source inventory was not investigated in the OFAT analysis and was fixed at 1.0 for reasons stated in the text.

Note: Porosity and source area were set at 0.1 and 600 m², respectively.

transport problem and to help define the functional form of the factors. The functional form of a factor can be defined as a mathematical relationship which describes the behavior of the response variable relative to the variation of the factor. OFAT analysis results must be interpreted with caution, because the functional form of a factor may vary depending on the values selected for factors that remain constant. Thus, technical judgment must be applied in the final decisions regarding the factors to be considered and the functional forms of those factors.

In an OFAT analysis, the value of one parameter is varied over its range of values, while the other parameters are held constant. Parameters held constant are usually held at their mean value may be arithmetic or geometric depending on the range of values. In a standard OFAT analysis, parameters varied are first evaluated at their mean value, and then at the mean +/- some multiple of the standard deviation. This technique requires an understanding of groundwater contaminant transport, but minimal statistical analysis is required. Such an analysis is also useful for initial screening and obtaining an understanding of the system and can be applied easily. We suggest that analysts conduct an OFAT analysis prior to using more sophisticated statistical techniques. Since distributions of factor values are typically not available in the initial stages of a PA, the OFAT analysis is limited to varying factors between the expected minimum and maximum values.

All factors considered in this analysis were varied within an assumed range of values. Transverse dispersivity was functionally fixed at a factor of 10 less than the longitudinal dispersivity. Porosity (0.1) and area of the source (600 m²) were fixed throughout the entire analysis. Source inventory was fixed at 1.0. In this sample implementation of an OFAT analysis, factors that were held constant were fixed at approximately the midpoint value between their minimum and maximum value, with the exception of retardation and half-life. Preliminary work suggested that peak concentration was more sensitive to retardation and half-life than the remaining factors. For this reason, the peak concentration response to variation in Darcy velocity, dispersivity, and well distance was observed for several different half-life and/or retardation fixed values, as opposed to just the midpoint.

The effects of varying retardation (R_d) for different half-life contaminants is illustrated in Figure 4-1. Retardation was varied over its range of values used in the analysis (1 to 100) while longitudinal dispersivity and well distance were held at 1.0 m and 300 m, respectively. The results show that the peak concentration appears to be inversely related to retardation for the longer half-life contaminant. The peak concentration decreased by approximately an order of magnitude for an increase in the retardation by an order of magnitude, as is the case of the $1.0E + 05$ -year half-life contaminant. Note that

Figure 4-1. Normalized peak concentration as a function of retardation for contaminants with various half-lives. Peak concentrations were normalized to the peak concentration obtained using a R_d of 1.0 and a half-life of 100,000 years. Factors held constant were longitudinal dispersivity (1.0 m), Darcy velocity (0.224 m/y), and well distance (300 m).

that the concentrations in the graph were normalized to the peak concentration when retardation was equal to 1.0 and half-life was equal to $1.0E + 05$ years.

If decay occurs during contaminant transit, then the peak concentration is further reduced. For a half-life of 100 years, the peak concentration was reduced by almost five orders of magnitude for an increase in the retardation by an order of magnitude. The graph illustrates that peak concentration is more sensitive to changes in retardation when decay is significant during transit.

A measure of the time needed for a contaminant to travel from source to receptor may be approximated by the average contaminant transit time. The average contaminant transit time (T_a) is given by

$$T_a = \frac{X}{U^*} R_d \quad (4.2)$$

where U^* = pore velocity (Darcy velocity/porosity, m/s).

The average contaminant transit time combines the effects of retardation, groundwater velocity, and receptor distance into one term. This parameter approximates the time when the plume centroid is centered over the receptor. For most cases, this approximates the time of peak concentration. For example, the transit time for the contaminants illustrated in Figure 4-1 with a retardation value of 50 is

$$T_a = \frac{300 \text{ m}}{(0.224 \text{ m/y})/(0.1)} \times 50 = 6,696 \text{ years} \quad (4.3)$$

Peak concentration as a function of well distance for various half-life contaminants has been plotted in Figure 4-2. In this example, the longitudinal dispersivity was fixed at 1.0 m, Darcy velocity was fixed at 0.224 m/y, and retardation was fixed at 1.0. The curves for 100,000 and 1,000-year half-life

Figure 4-2. Normalized peak concentration as a function of well distance for contaminants with various half-lives. Peak concentrations were normalized to the peak concentration obtained using a well distance of 100 m and half-life of 100,000 years. Factors held constant were longitudinal dispersivity (1.0 m), Darcy velocity (0.224 m/y), and retardation (1.0).

contaminants are similar; the curve for the 100-year half-life is slightly more sloped, while the curve for the 10-year half-life contaminant has a much steeper slope. A larger well distance allows for more dispersion of the contaminant before reaching the receptor resulting in a lower peak concentration. In addition, the time the contaminant takes to reach the receptor also increases. The contaminant transit time for the well distance of 300 m was 133 years. The fraction of contaminant which remains in the system at the end of this time is given by

$$F_r = e^{-\left[\frac{\ln 2}{T_{1/2}} T_a\right]} \quad (4.4)$$

where F_r = the fraction of contaminant remaining in the system.

The fraction remaining for the 100,000-, 1,000-, and 100-year half-life contaminants was 0.999, 0.912, and 0.398 respectively, while the fraction remaining for the 10-year half-life contaminant was 9.9E-05. The impact well distance has on peak concentration appears to depend on the relative values of the half-life and the transit time of the contaminant being considered. For contaminants with short half-lives relative to the transit time, the impact of well distance is much greater than for contaminants with long half-lives relative to the transit time.

Peak concentration as a function of Darcy velocity for various contaminant half-lives is illustrated in Figure 4-3. In this example, retardation was fixed at 1.0, longitudinal dispersivity was fixed at 1.0, and well distance was fixed at 300 m. Peak concentrations have been normalized to the peak concentration when the Darcy velocity was 1.0 E-02 m/y with a half-life of 100,000 years. Darcy velocity appears to have little impact on peak concentration for the contaminant with the longer half-life (substitution of Equation (4.3) for t in Equation (3.1) will verify this relationship). Darcy velocity appears to have a greater impact on peak concentration for contaminants with shorter half-lives.

Figure 4-3. Normalized peak concentration as a function of Darcy velocity for contaminants with various half-lives. Peak concentrations were normalized to the peak concentration obtained using a Darcy velocity of 0.01 m/y and half-life of 100,000 years. Factors held constant were retardation (1.0), well distance (300 m), and longitudinal dispersivity (1.0).

From the work illustrated so far, three conclusions can be drawn:

1. The half-life of the contaminant appears to be important only when it is close to or less than the contaminant transit time.
2. Well distance appears to have a greater impact on peak concentration Darcy velocity when decay is absent. This difference is primarily due to dispersion.
3. Retardation appears to have the greatest impact on peak concentration.

As stated in Item 1, the effect of decay on peak concentration depends on the relative magnitudes of half-life and T_a . A measure of the amount of decay that occurs during contaminant transit is described by the dimensionless contaminant half-life/transit time ratio (H_r):

$$H_r = \frac{T_{1/2}}{T_a} \quad . \quad (4.5)$$

A large value for H_r indicates that minimal decay occurs during contaminant transit, while a low H_r value indicates significant decay. Based on previous findings regarding the relationship between half-life and transit time, H_r provides information that is useful for identifying contaminants that may be screened from consideration in a PA.

Dispersion also influences the peak concentration, as stated in Item 2. A measure of the amount of dispersion occurring during transit from source to receptor is given by the Peclet number (P_e). The Peclet number is the ratio of advection to dispersion (Huyakorn and Pinder, 1983):

$$P_e = \frac{U^* \Delta L}{D} \quad (4.6)$$

where

$$\begin{aligned} U^* &= \text{pore velocity (L/T)} \\ \Delta L &= \text{characteristic length (L)} \\ D &= \text{dispersion coefficient (L}^2\text{/T)}. \end{aligned}$$

Based on the assumptions necessary for the analytic solution (Equation 3.1), a simplified version of the P_e is applicable. In order to make the simplifications, the P_e must first be written for flow in the x-direction with the dispersion coefficient, D , broken into the components associated with diffusion, D_m , and mechanical dispersion, D_x , as

$$P_e = \frac{U^* X}{D_m + D_x} \quad (4.7)$$

given

$$D_x = \frac{\alpha_L U^2 + \alpha_T V^2}{q' \phi} \quad (4.8)$$

with

$$q' = \sqrt{U^2 + V^2} \quad (4.9)$$

where

$$\begin{aligned} X &= \text{characteristic length in the x-direction (in this case the distance between the source and the receptor) (m)} \\ D_m &= \text{Molecular diffusion coefficient (m}^2\text{/y)} \end{aligned}$$

- D_x = Mechanical component of the dispersion coefficient in the x-direction (m^2/y)
 U, V = Darcy velocity components in the x- and y-directions (m/y)
 q' = Magnitude of the two-dimensional groundwater velocity (m/y)
 ϕ = porosity (-).

Further simplifications can be made based on the assumptions used in this analysis. If it is assumed that diffusion is negligible ($D_m = 0$) and that the model is oriented in the direction of flow (i.e., one-dimensional flow in the x-direction, $V = 0$), P_e simplifies to

$$P_e = \frac{U^* X}{\alpha_L U^2 / (U\phi)} \quad . \quad (4.10)$$

By canceling the velocity terms, a simplified representation of P_e specific to the assumptions of this analysis is obtained

$$P_e = \frac{X}{\alpha_L} \quad . \quad (4.11)$$

A low Peclet number indicates greater contaminant dispersion than a high Peclet number.

The peak concentration has been plotted against the H_r ratio for various Peclet numbers in Figure 4-4. In this graph, the peak concentration for each curve has been normalized to the peak concentration (C_p) obtained when H_r is equal to 100.

Figure 4-4. Normalized peak concentration as a function of contaminant half-life/transit time (H_r) ratio for various P_e . The peak concentrations were normalized to the peak concentration obtained using a H_r ratio of 100. Factors held constant were retardation (1.0), and well distance (300 m).

$$\text{Normalized } C_p(H_r, P_e) = \frac{C_p(H_r, P_e)}{C_p(100, P_e)} \quad (4.12)$$

where $C_p(H_r, P_e)$ = the peak concentration as a function of H_r ratio and Peclet number.

The graph shows that the impact of decay on C_p is greater for H_r ratios less than 1.0. Also, the impact of smaller H_r ratios on the C_p value is much greater for cases which involve high Peclet (low dispersion) numbers. This is evidenced by the shallower slope of the curve generated with a Peclet number of 30 compared to the curves generated with Peclet numbers of 300 and 3000. As the H_r ratio approaches 1.0, all three curves tend to converge at 1.0; as the H_r value approaches zero, the slope of each curve becomes steeper.

In general, high Peclet numbers are characteristic of little contaminant dispersion; thus, the contaminant tends to move like a plug, and if decay is significant, the C_p value is governed more by the decay of the contaminant than dispersion. Low Peclet numbers are characteristic of a large amount of contaminant dispersion; the C_p value is influenced not only by decay, but also by dispersion. The interaction of these factors on the C_p value is not obvious (see Figure 4-5). In Figure 4-5, the normalized C_p value has been plotted against the Peclet number for various H_r ratios. Each C_p value has been normalized to the C_p value for $P_e = 3000$ and $H_r = 750$ (low dispersion, little decay). Normalized C_p values approximate a power curve relationship with respect to Peclet number for high (>7.5) H_r values. In this case the C_p value was controlled by the amount of dispersion that occurred, since decay of the contaminant was relatively insignificant.

Low H_r values result in a more complex relationship between normalized C_p and Peclet number. The normalized C_p for the curve representing an H_r value of 0.075, decreases with increasing Peclet number for Peclet numbers in the 10 to 100 range; the normalized C_p then increases with increasing Peclet number. The other curves on the graph represent gradations between the two extremes.

Figure 4-5. Normalized peak concentration as a function of Peclet number for various H_r ratios. The peak concentrations were normalized to the peak concentration obtained using a H_r ratio of 750 and P_e of 3000. Factors held constant were retardation (1.0), well distance (300 m), and Darcy velocity (0.224 m/y).

The reason for this observed opposite relationship of dispersivity effects on C_p values for short and long half-life contaminants is that greater dispersivity results in greater plume spreading; thus, a shorter amount of time is needed for the plume front (leading edge of the plume) to arrive at the receptor, and less of the contaminant is allowed to decay before reaching the receptor. Figure 4-6 shows the distribution of normalized concentrations along the plume centerline at the time of peak concentration at the receptor (300 m downgradient) for two different Peclet numbers and two contaminants with different half lives. The C_p values have been normalized to the maximum C_p for a given half-life. For example, the maximum C_p value for the 10-year half-life contaminant occurred using a P_e value of 30 ($3.27E-6$); therefore, all 10-year half-life results were normalized to this value. Since the receptor distance was fixed at 300 m, then the P_e numbers represent α_L values of 1.5 m and 10 m.

Greater dispersion of a limited contaminant mass results in lower concentrations at the receptor location; however, the contaminant plume front reaches the receptor in a shorter amount of time. For short-lived contaminants in conditions of high dispersion (low P_e number), the peak concentration at the receptor location is achieved while the plume front is advancing to the receptor.

By the time the plume centroid reaches the receptor (Equation 4.2), decay has significantly reduced the centroid concentration to less than the value when the plume front was at the receptor. For long-lived contaminants in conditions of low dispersion (high P_e number), the peak concentration is reached when the plume centroid is centered over the receptor. The time of peak concentration for short-lived contaminants with high dispersion occurs before the plume centroid is centered over the receptor, and thus is smaller than what is predicted by Equation (4.2).

One of the more severe limitations with an OFAT analysis is that interactions between the factors are not observed. In addition, the effect of a single factor on the response variable may be dependent on the values chosen for the other factors in the response function. This was observed in the different results generated when using different half-lives. In performing a sensitivity

Figure 4-6. Normalized concentration as a function of distance along the plume centerline at the time of peak concentration at the receptor (300 m downgradient) for contaminants with a 10-year and 100,000-year half-life and different Peclet numbers. Concentrations were normalized to the maximum peak concentration for a given half-life.

analysis, one should always consider the range of expected factor values. The sensitivity of some factors in a model may depend on the values of the fixed factors. This sample OFAT analysis used some variations of the general OFAT approach to address these concerns.

4.4 Determination of Functional Form

The final purpose of the OFAT analysis is to identify data transformations to be used in the regression model. In this example, selection of the data transformations were made by a qualitative assessment of observations made during the OFAT analysis (Table 4-2). Selection of the functional form to be used in a regression analysis is an iterative process. A form which may initially seem appropriate may in fact not represent the response surface adequately. Some trial and error can be expected as part of this process.

Retardation was given an inverse relationship to C_p (Table 4-2). The decision to use an inverse relationship was based on Figure 4-1 and the functional form of R_d in Equation (3.1). Retardation's true relationship to C_p was more complex when significant decay occurred during transit, as evidenced by Figure 4-1. It was felt however, that the inverse functional form was the simplest, most effective representation of R_d .

As shown in Figure 4-4 and Figure 4-5, the impact of the contaminant's half-life on peak concentration was related to the contaminant transit time. In turn, the contaminant transit time was also related to the pore velocity, distance to receptor, and R_d . Half-life was represented in Equation (3.1) as a first-order rate constant that was used to account for radioactive decay. The radioactive decay rate constant (λ) is given by

$$\lambda = \frac{\ln 2}{T_{1/2}} \quad . \quad (4.13)$$

Table 4-2. Functional form of the factors used in the fractional factorial analysis as derived by the OFAT analysis

<u>Factor</u>	<u>Functional Form</u>
Retardation (R_d)	$1/R_d$
Half-Life (T_h)	$\ln(2)/T_h$
Darcy Velocity	U
Dispersivity	$1/\alpha_L$
Well Distance	X
Source Inventory	Q
<u>Interactions</u>	
Dispersivity, Pore Velocity	$\alpha_L \cdot U^*$
Retardation, Half-life Contaminant Transit Time, and Well Distance	$\exp[- \ln(2)/T_h \cdot T_a]$
<hr/> Note: $T_a = \frac{X}{U^*} \cdot R_d$ <hr/>	

Due to the complex relationship half-life has to peak concentration, it was decided to present half-life as a linear rate constant in the regression models as given in Equation (4.13).

Darcy velocity was given a simple linear form based on observations in Figure 4-3. For most cases Darcy velocity had minimal impact on peak concentration except where the half-life was small relative to the contaminant transit time.

Dispersivity was given an inverse relationship ($1/\alpha_L$) based on the data in Figure 4-5. The curve for long half-life contaminants approximates a $1/\alpha_L$ relationship when the Peclet number is converted to longitudinal dispersivity in Figure 4-5. Again, the functional relationship was not clear for the shorter half-life contaminants.

Well distance was given a negative exponential relationship with respect to peak concentration. This relationship was based on the data presented in Figure 4-2 (a straight line on a log-linear plot indicates an $\text{EXP}[-ax]$ functional form).

Functional relationships of other factors may be deduced from observation of the governing equation. For example, it is apparent from Equation (3.1) that Q (source inventory) is linearly related to the concentration at any point in time. This is why it was omitted from the OFAT analysis. If analytical solutions do exist, then it is important to examine them before performing a rigorous sensitivity analysis so that simple functional relationships may be established early in the process.

Two factor interactions were also derived from this analysis. These interactions were used later in the fractional factorial regression model (see Section 5.1). The first interaction was the product of pore velocity and dispersivity and is referred collectively as the dispersion coefficient. This interaction was chosen because dispersivity is always multiplied by the pore velocity in Equation (3.1). The second interaction was an attempt to combine the contaminant transit time, half-life, and retardation into one term. The value of the interaction term represented the fraction of contaminant which was remaining at the time the plume centroid reached the receptor. Overall, the selected functional relationships were weak for short half-lives.

4.5 Discussion

Results of the OFAT analysis indicated that peak concentration was the most sensitive to retardation. This sensitivity was greatly enhanced for contaminants with short half-lives. Furthermore, the results indicated that peak concentration was also the most sensitive to changes in the other parameters when the half-life was relatively short.

Functional forms to be used for the rigorous methods were qualitatively derived from observations made in the OFAT analysis. The functional forms are intended to provide a better representation of the response surface than one derived by simple linear forms. The selected functional forms appeared to be

best for longer half-lives. In the case of groundwater transport, it was clear from the results of the analysis that nonlinear terms were needed.

The results presented in Section 4 are more than would be obtained with a typical OFAT analysis, since some of the results are based on two or more factors. The simplicity of the model used in this example allowed a large number of computer runs to be made in a relatively short time. A total of 309 individual runs were made to produce the smooth curves presented in this section. With a more complex model it would not be practical to perform a large number of runs; thus, the user would have to follow the more common OFAT methodology presented in Section 4.3. In this respect, the interactions would not have been as clearly identified, and only a limited understanding of the functional form of the factors would have been obtained.

Because the data set considered a wide range of possible values for the parameters, results were obtained that illustrate some general concepts that may aid in determining what conditions would allow a contaminant to be screened from further consideration. For example, the results suggest that the contaminant half-life/transit time ratio (H_r) is a good indicator of the potential impact to a downgradient receptor. If H_r is significantly less than 1, then sufficient justification may be available to screen the contaminant from further consideration.

OFAT analysis is attractive because of the ease of application and subsequent interpretation of results. However, the analyst must remember that OFAT results are only applicable for the values at which the factors were evaluated. If the OFAT analysis is limited to a small number of runs, broad conclusions typically cannot be made based on the results. OFAT analysis is most effective as a scoping tool.

5. SENSITIVITY/UNCERTAINTY ANALYSIS

Rigorous statistical analysis techniques can use the results of an OFAT analysis to provide a more complete sensitivity analysis. Although the OFAT approach is appealing because of easy application and interpretation, there are limitations to the technique. The results are useful for scoping and understanding the problem. However, the analyst must recognize the following limitations:

1. Lack of ability to simultaneously compare a large number of factors
2. Lack of ability to quantitatively rank the impact of factors on the response
3. Inefficient method of comprehensively assessing factor effects.

In the OFAT approach, the response is observed for different values of one factor while the remaining factors are held constant, typically at a midpoint value. However, it is common that the effect of a factor on the response depends upon the level of the other factors. When this occurs, the factors are said to interact. Examples of interactions with respect to the groundwater transport results are shown in Section 4. These were only identified because of the modified approach used for the OFAT analysis in this report. In a strict OFAT approach such interactions would be difficult to detect. Indeed, in the presence of interaction, the OFAT approach can lead to incorrect conclusions.

For example, consider the hypothetical contour plot in Figure 5-1. In this figure, the contours represent concentrations across the levels of Factors A and B. If the OFAT approach is applied to this process, then the researcher might first vary Factor A with Factor B held at 0. The result would be a constant concentration for all levels of Factor A. Thus the researcher would conclude that Factor A has no effect on concentration. Next the researcher would vary the levels of Factor B while holding Factor A at 0. Again, a constant concentration would occur across the levels of Factor B and the researcher would conclude that

Figure 5-1. Hypothetical concentration contours as a function of two factors.

Factor B has no effect. Thus the researcher might, based on the OFAT results, conclude that neither Factor A nor Factor B affect the concentration.

In contrast, consider what happens in the situation depicted in Figure 5-1 when the simplest factorial design is implemented. In the simplest case, the researcher would use a 2^2 design. This is a design with two factors each observed at two levels. The researcher may select the two levels for Factor A as -1 and 1, and use the same levels for Factor B (it is common to use "endpoints" as the levels in 2^k designs). Thus the design points are (-1,-1), (-1,1), (1,-1), and (1,1), where the first number corresponds to the level of Factor A and the second to Factor B. The responses for the design points in the same order would be 1, 0, 0, 1. It is immediately obvious from these results that the factors do affect the response. A closer look at the results reveals that when Factor B is held to -1, the effect of Factor A going from -1 to 1 reduces the concentration by 1. When Factor B is held to 1, the effect of Factor A going from -1 to 1 increases the concentration by 1. Thus, since the effect of Factor A depends upon the level of Factor B, the researcher concludes that the factors interact.

Results from Section 4 suggest that the concentration depends upon a number of factors. However, these results do not suggest which of the factors are the most important. In order to assess the importance of the factors, they need to be considered simultaneously. The experimental design approach lends its results to analyzing the data through response surfaces. These analyses have objective methods for assessing the relative importance of the factors. The problem with implementing the technique is to determine the form of the response surface. It is in determining the form of the surface that the OFAT results can be put to good use.

Furthermore, the OFAT method may be inefficient compared to the use of experimental design. The general OFAT method requires a moderate number of runs per factor varied. Experimental design allows factors to be varied simultaneously, thus reducing the number of required runs over the OFAT method. A large number of runs (i.e., 309) were conducted for the analyses in Section 4.

This section includes sample applications of two rigorous techniques: fractional factorial design and Latin hypercube sampling. Fractional factorial design is applied to a problem at the initial stages of the PA process (Section 5.1), and Latin hypercube sampling is applied to a problem at the latter stages of the PA process (Section 5.2). Regression analysis is used to complete the sensitivity analysis in both cases. A detailed discussion regarding regression analysis as applied to sensitivity analysis is provided separately in Appendix A. A brief discussion of uncertainty is included below for the fractional factorial design, along with results of an uncertainty analysis for Latin hypercube sampling.

5.1 Implementation for the Initial Stages of the PA Process

The initial stages of the PA process are typically characterized by a lack of site-specific data. The objectives are to determine the level of effort that will be required and to specify necessary activities. Likewise, the priorities are focused on the following:

- Obtaining a rough estimate of performance
- Identifying critical pathways
- Identifying critical data needs related to those pathways
- Identifying critical design features that may be required.

Sensitivity analyses are the primary source for addressing these concerns. Uncertainty analysis should only be used to establish bounds. The sample problem for this section will provide a rough estimate of performance and information regarding critical data needs for the groundwater pathway.

Site-specific groundwater flow and transport data would typically be sparse at this stage in the analysis. Thus, large uncertainty would be associated with the data values used to conduct the analysis. The ranges of values selected for the sample problem are intended to represent this uncertainty. Fractional

factorial design is used for the sample problem at this stage of the process. This was deemed appropriate because distributions for the data do not need to be specified, and fractional factorial design provides a large amount of information from a sensitivity analysis with a small number of runs.

5.1.1 Fractional Factorial Design Approach

Assessing the sensitivity of a model by looking at each factor in an OFAT approach does not allow for the possibility that the effect of a factor depends upon the levels of the other factors at which it is observed. To consider the factors simultaneously, and hence to be able to detect interactions, the levels of each factor must be crossed with different levels of each of the other factors. Designs that have factor levels crossed with one another are called factorial designs (Montgomery, 1984). An example of a factorial design was provided in the first several pages of this section.

The effectiveness of factorial designs are often limited by a practical problem. As the number of factors and levels becomes even moderately large, the number of combinations that must be considered becomes prohibitive. For example, for five factors each at three levels, the factorial design would require 243 (3^5) observations. This full factorial design would allow estimation of all interactions, including the interaction of all five factors simultaneously. In many practical situations, the higher order interactions (typically three-way and higher) are assumed to be negligible due to the nature of the system being studied. Even if there is some significance to the higher order interactions, it would be difficult--if not impossible--to interpret. By assuming that higher order interactions are negligible, the design no longer needs so many runs to estimate all the effects of interest. The best way to reduce the number of runs in the factorial design is to look at fractions of the full design. This is the motivation for fractional factorial designs.

To develop the fractional factorial design, consider first the full factorial design. In Section 4 it was determined that there are six factors of interest: R_d , half-life, velocity, distance from source, dispersion, and source inventory. The number of levels for each factor needs to be determined. If

there are only two levels for a factor, then that factor must be modeled as a straight line, since only two points will be observed. If three levels are used, then the factor can be modeled as a curved line. The effects and interactions of interest are listed in Table 5-1. (Note: At the conclusion of the analysis, it was discovered that dispersion should have been considered at three levels. Given the purposes of this document, it was determined that the analyses would not be rerun to correct this oversight.)

As in the OFAT analysis, the lowest and highest levels should bracket the range at which the factor is expected to affect the response. This range needs to be realistic. The middle level for those factors with three levels is typically set to the midpoint of the other two levels. However, if the effect of the factor is expected to be nonlinear, it may be more informative to use another point, such as the geometric mean of the two extreme levels. The factor levels chosen for the sample problem are shown in Table 5-2. Note that the midpoint for ranges varying over orders of magnitude was the geometric mean (i.e., retardation, velocity, and half-life), and for factors varying over a range less than an order of magnitude the arithmetic mean was used (i.e., well location).

In the case of full factorial design, four factors at three levels each and two factors at two levels would require 324 runs ($3^4 \cdot 2^2$). However, many of the higher order interactions are expected to be negligible. Furthermore, many of the lower order interactions can be screened based on an understanding of the problem. For example, in Equation 3.1 Q is simply multiplied by the other terms. Thus, changes in Q will have the same effect on the final solution regardless of the values of the other parameters. Therefore, Q does not interact with any other parameters. Many interactions (or non-interactions) will not be as easy to identify as this one. In that respect, selection of interactions to be considered is one of the most difficult aspects of the rigorous statistical techniques.

The effects and interactions of interest are displayed in Table 5-2. The fractional factorial design selected will be the portion of the full factorial design that allows estimation of the main effects and interactions of interest.

Table 5-1. Effects estimated by the fractional factorial design

<u>Main Effects</u>	<u>Levels</u>
Retardation	3
Half-Life	3
Darcy Velocity	3
Dispersivity	2
Well Distance	3
Source	2
<u>Interactions</u>	
Dispersivity, Velocity	
Retardation, Half-life, Contaminant Transit Time, and Well Distance	

Table 5-2. Factor levels considered in the fractional factorial design

<u>Factor</u>	<u>Units</u>	<u>Factor Levels</u>		
		<u>Low Value</u>	<u>Mid Value</u>	<u>High Value</u>
Retardation	(-)	1.0	10.0	100.0
Half-Life	(y)	10.0	1000.0	100,000.0
Darcy Velocity ^a	(m/y)	0.01	0.224	5.0
Longitudinal Dispersivity ^b	(m)	0.01	----	10.0
Well Distance	(m)	100.0	300.0	500.0
Source	(activity or mass)	0.1	---	10.0

a. Pore Velocity = Darcy Velocity/Porosity (Porosity assumed to be 0.1)

b. Transverse Dispersivity is assumed to be 0.1 x Longitudinal Dispersivity

5.1.2 Determination of Necessary Computer Runs

Based on the specified factors, factor levels, and effects to be estimated, a fractional factorial design can be developed. The design consists of a set of computer runs with the factors set a specified levels in each run. With fractional factorial designs, this is a tedious task that is best done using a computer program or one of the available table of designs. For a rigorous discussion of the development of the fractional factorial design, see Montgomery (1984) or Cochran and Cox (1957). Cochran and Cox include some tables of fractional factorial designs in their book.

SAS/QC software (SAS Institute, 1989) was used to determine the necessary runs. In this program, the user inputs the number of factors, levels, and effects to be estimated, and the program develops a design that uses the minimum number of runs. However, SAS/QC expects all factors to have the same number of levels. In the sample problem there are two different numbers of levels. The resulting design is shown in Table 5-3. Fractional factorial design reduced the number of runs from 324 to 36. The design allows for the estimation of the effects in Table 5-1. Some customizing was necessary to develop the final design, the details of which are beyond the scope of this document. Such customizing can be completed using existing options in the SAS/QC program. The main point is to ensure that all of the effects being considered are estimable with the existing design. SAS/QC has options to ensure that this is accomplished. In cases where customizing is necessary, these programs (and tables of designs) should only be used by an analyst technically competent in the statistical design of experiments.

5.1.3 Sensitivity Analysis Results

A computer program (Rood et al., 1989) was used to solve the analytic solution for each set of factor values identified in Table 5-3. The program

Table 5-3. Combinations of factor values for the 36 runs identified by the fractional factorial design

Case	Darcy Velocity (m/y)	R _d (-)	Half-Life (y)	Source (Ci)	a _L (m)	a _T (m)	Well Dist. (m)
1	0.010	1	1.000E+01	1.00E-01	0.01	0.001	100
2	0.010	1	1.000E+03	1.00E-01	10.00	1.000	500
3	0.010	1	1.000E+03	1.00E+01	0.01	0.001	100
4	0.010	1	1.000E+05	1.00E+01	10.00	1.000	500
5	0.010	10	1.000E+01	1.00E-01	10.00	1.000	300
6	0.010	10	1.000E+01	1.00E+01	0.01	0.001	500
7	0.010	10	1.000E+03	1.00E+01	10.00	1.000	300
8	0.010	10	1.000E+05	1.00E-01	0.01	0.001	500
9	0.010	100	1.000E+01	1.00E+01	10.00	1.000	100
10	0.010	100	1.000E+03	1.00E-01	0.01	0.001	300
11	0.010	100	1.000E+05	1.00E-01	10.00	1.000	100
12	0.010	100	1.000E+05	1.00E+01	0.01	0.001	300
13	0.224	1	1.000E+01	1.00E-01	0.01	0.001	500
14	0.224	1	1.000E+03	1.00E-01	10.00	1.000	300
15	0.224	1	1.000E+03	1.00E+01	0.01	0.001	500
16	0.224	1	1.000E+05	1.00E+01	10.00	1.000	300
17	0.224	10	1.000E+01	1.00E-01	10.00	1.000	100
18	0.224	10	1.000E+01	1.00E+01	0.01	0.001	300
19	0.224	10	1.000E+03	1.00E+01	10.00	1.000	100
20	0.224	10	1.000E+05	1.00E-01	0.01	0.001	300
21	0.224	100	1.000E+01	1.00E+01	10.00	1.000	500
22	0.224	100	1.000E+03	1.00E-01	0.01	0.001	100
23	0.224	100	1.000E+05	1.00E-01	10.00	1.000	500
24	0.224	100	1.000E+05	1.00E+01	0.01	0.001	100
25	5.000	1	1.000E+01	1.00E-01	0.01	0.001	300
26	5.000	1	1.000E+03	1.00E-01	10.00	1.000	100
27	5.000	1	1.000E+03	1.00E+01	0.01	0.001	300
28	5.000	1	1.000E+05	1.00E+01	10.00	1.000	100
29	5.000	10	1.000E+01	1.00E-01	10.00	1.000	500
30	5.000	10	1.000E+01	1.00E+01	0.01	0.001	100
31	5.000	10	1.000E+03	1.00E+01	10.00	1.000	500
32	5.000	10	1.000E+05	1.00E-01	0.01	0.001	100
33	5.000	100	1.000E+01	1.00E+01	10.00	1.000	300
34	5.000	100	1.000E+03	1.00E-01	0.01	0.001	500
35	5.000	100	1.000E+05	1.00E-01	10.00	1.000	300
36	5.000	100	1.000E+05	1.00E+01	0.01	0.001	500

required 5 to 10 seconds on a personal computer to solve each case. Peak concentrations, and times of peak concentration calculated with the analytic solution, are listed in Table 5-4. Peak concentration is the response variable considered in the statistical analysis. Time of peak is included to illustrate travel times for the different sets of conditions. Peak concentrations predicted by the analytic solution are then used as inputs for the regression analysis.

Regression techniques are used to assess the influence of the factors on peak concentration. Appendix A provides an overview of the regression calculations and their interpretations. The regression analysis was accomplished using SAS software (SAS Institute, 1989). Two different models were constructed: a simple linear model and a model using functional forms obtained from the OFAT analysis (Table 4-2). The simple linear model is included to illustrate the results that would be obtained if no fine tuning of the functional form occurred. The linear model is not intended to be a correct representation. It also should be noted that a few other combinations of functional forms were tested during the course of the analysis prior to deciding on the final form. Such iterations are not uncommon in this form of analysis.

5.1.3.1. Simple Model. The first model to be fit to the results was a simple model assuming that each factor responded linearly as defined by the following:

$$C = \beta_0 + \beta_1 R_d + \beta_2 T_{1/2} + \beta_3 U + \beta_4 \alpha_L + \beta_5 X + \beta_6 Q \quad (5.1)$$

where

C	=	peak concentration
β_*	=	intercept and coefficients calculated by regression analysis
R_d	=	retardation
$T_{1/2}$	=	half-life
U	=	Darcy velocity

Table 5-4. Peak concentration and time of peak concentration calculated for the 36 test cases

<u>Case</u>	<u>Peak Concentration</u>	<u>Peak Time (years)</u>
1	3.160E-30	8.750E+02
2	2.170E-06	4.280E+03
3	8.810E-02	9.150E+02
4	4.283E-03	4.800E+03
5	<1.000E-99 ^a	4.280E+03
6	<1.000E-99	0.000E+00
7	1.190E-09	1.484E+04
8	1.180E-04	4.970E+04
9	<1.000E-99	4.900E+03
10	4.270E-92	2.850E+05
11	1.370E-06	7.560E+04
12	2.166E-04	2.938E+05
13	3.760E-10	2.200E+02
14	7.580E-05	1.250E+02
15	1.430E-01	2.230E+02
16	8.258E-03	1.260E+02
17	3.900E-10	1.000E+02
18	1.960E-10	1.253E+03
19	1.850E-03	3.570E+02
20	1.650E-04	1.330E+03
21	<1.000E-99	4.700E+03
22	9.920E-07	4.050E+03
23	4.360E-07	2.136E+04
24	1.620E-03	4.150E+03
25	1.120E-03	5.760E+00
26	2.240E-04	1.650E+00
27	1.660E-01	6.000E+00
28	2.380E-02	1.700E+00
29	1.290E-08	7.800E+01
30	4.670E-03	1.820E+01
31	4.670E-04	9.600E+01
32	1.660E-04	1.890E+01
33	1.610E-14	2.260E+02
34	8.340E-06	1.000E+03
35	8.230E-07	5.650E+02
36	1.650E-03	1.000E+03

a. Values less than 1.0e-99 were represented as 1.0e-99 in the regression analysis.

α_L = longitudinal dispersion
 X = well distance
 Q = source inventory.

The results of the regression analysis for the simple model are presented in Table 5-5. Two measures of sensitivity are listed: ΔR^2 and the standardized coefficient (see Appendix A for definitions). The rankings of significance are also provided. The coefficient of determination (R^2) for this model was 0.2654, which indicates that the model is a poor predictor of the results that would be obtained with the analytical solution. A value of 0.2654 indicates that the simple model only accounts for 26.5% of the variation in peak concentration that would be predicted by the analytical solution.

Results for the first model suggest that the source, dispersivity, and retardation are the most important factors in determining peak concentration. This ranking is determined by the magnitude of the ΔR^2 and standardized estimates (Table 5-5). Note that the values for the other factors are significantly less. The rankings were the same for both measures of sensitivity.

Table 5-5. Simple model--fractional factorial design

Factor	ΔR^2		Standardized Coefficient	
	Value	Rank	Value	Rank
R_d	0.0504	3	-0.2317	3
$T_{1/2}$	0.0110	4	-0.1084	4
Darcy Vel.	0.0063	5	0.0794	5
Disp	0.0736	2	-0.2713	2
Well Dist.	0.0007	6	0.0268	6
Source	0.1069	1	0.3269	1

Note: R^2 for the simple model was 0.2654.

5.1.3.2 Final Model. The final model to be fit used the functional forms for the factors and interactions determined in the OFAT analysis is governed by the following:

$$C = \beta_0 + \beta_1 \left(\frac{1}{R_d} \right) + \beta_2 \left(\frac{\ln 2}{T_{1/2}} \right) + \beta_3 U + \beta_4 \left(\frac{1}{\alpha_L} \right) + \beta_5 e^{-X} + \beta_6 Q + \beta_7 U^* \alpha_L + \beta_8 e^{-\left(\frac{\ln 2}{T_{1/2}} T_a \right)} \quad (5.2)$$

where

C	=	peak concentration
β_*	=	intercept and coefficients calculated by regression analysis
R_d	=	retardation
$T_{1/2}$	=	half-life
U	=	Darcy velocity
α_L	=	longitudinal dispersion
X	=	well distance
Q	=	source inventory
U^*	=	pore velocity
T_a	=	Average contaminant transit time $((X/U^*) * R_d)$.

The results from this model are summarized in Table 5-6. The coefficient of determination for this model was 0.4225 (other fits were attempted, but failed to produce a significant increase in R^2). This is a substantial improvement over the simple linear model, but still should be considered a poor predictor of the results from the analytic solution. This model indicates that retardation, source term, and dispersivity are the most important factors in determining peak concentration. These are the same three factors as the simple model, but in a different order. The indication that retardation is the most important factor agrees with the conclusion of the OFAT analysis in which retardation was deemed most significant.

Table 5-6. Final Model--fractional factorial design

<u>Factor</u>	<u>ΔR^2</u>		<u>Standardized Coefficient</u>	
	<u>Value</u>	<u>Rank</u>	<u>Value</u>	<u>Rank</u>
$1/R_d$	0.1696	1	0.438	1
$\ln 2/T_{1/2}$	0.0191	4	-0.203	4
Darcy Vel.	0.0079	5	0.141	5
$1/\alpha_L$	0.0347	3	0.235	3
Well Distance	0.0019	7	-0.043	7
Source	0.1073	2	0.330	2
<u>Interactions</u>				
Pore Vel. and Dispersivity	0.0021	6	0.075	6
Decay-Transit Time ^a	0.0006	8	0.041	8

a. Decay-Transit Time = $\exp[-(\ln 2/T_{1/2}) \cdot T_a]$

Note: R^2 for the final model was 0.4225.

5.1.4 Uncertainty Analysis

When the input distribution is known or assumed known, one can implement techniques such as Monte Carlo methods to assess the uncertainty in the response. However, without any information on an input distribution, there is little that can be done with respect to uncertainty analysis. In the sample problem, the input distribution is not known (lack of data is a typical problem in the initial stages of a PA). However, the range of values that the input parameters can take is well understood. This will allow an assessment of the possible range of the response. While this may not at first seem very informative, it may preclude the need for further study of a problem if, for example, the range of possible response values is substantially less than a regulatory action limit. Thus, in the initial stages of the PA process, uncertainty analysis is best used as a bounding tool.

The final model was used for the uncertainty analysis (Equation 5.2). From the results of Table 5-4, we can get a general feel for the distribution of the results. The maximum value for peak concentration, $1.66\text{E-}1$, was obtained in Case 27. The minimum value for peak concentration was essentially 0.0 for a number of cases (shown as $1.0\text{E-}99$). Approximately 50% of the results are on the order $1.0\text{E-}1$ to $1.0\text{E-}5$; the remaining 50% range between $1.0\text{E-}5$ and 0.0. For this sample problem the bounding range is very large. This is as expected, because each of the parameters was allowed to vary over a large range. In a typical PA, the ranges of values may be smaller than those assumed for this sample problem.

A true uncertainty analysis for a factorial design is conducted using a Monte Carlo approach. A set of computer input files with different factor levels (as specified by the Monte Carlo analysis) for the parameters is generated. The computer runs are then conducted using the regression model obtained from the regression analysis (Equations 5.1 and 5.2). In this respect, the accuracy of the uncertainty analysis is dependent on the accuracy of the regression model. In Section 5.1.3, regression analysis was used to generate two regression models for predicting the results of the analytical solution. The coefficients of determination for these models were very low (0.2654 and 0.4225). The results of an uncertainty analysis based on Monte Carlo runs using either of these models would be questionable.

A lack of well defined distributions for the data also limits the effectiveness of the uncertainty analysis. Such a lack of data is typical during the initial stages of the PA process. In general, Latin hypercube sampling is recommended for uncertainty analyses (Iman and Helton, 1985), because the results are based on the actual output from the computer code that is being used (as opposed to the regression model). Based on the reasoning presented in these two paragraphs, a detailed uncertainty analysis is only provided for the Latin hypercube sampling problem.

5.2 Implementation for the Latter Stages of the PA Process

The latter stages of the PA process should be consistent with the latter stages of characterization and design activities. Thus, the design should be relatively well defined, and site characterization data should have been collected. Likewise, the priorities are focused on the following:

- Demonstrating compliance
- Discussing the uncertainty associated with the prediction.

Uncertainty analysis has a greater emphasis at this stage. Sensitivity analysis results can document the parameters with the greatest influence on the results.

At the end of characterization, groundwater flow and transport data would have been collected. Thus, relatively well-defined ranges of values and associated distributions should be available for the parameters of concern. The ranges of values for the sample problem have been refined to simulate the improved understanding. Distributions for the parameters are also assumed to be available.

5.2.1 Latin Hypercube Random Sampling Approach

Latin hypercube sampling (LHS) is a method that allows a random sample to be drawn from the input factors of the model, assuming that the distributions on the input factors are known. The random sample allows one to make inferences about the distribution of the response that one could not make based on the factorial design. That is, the LHS method allows one to directly implement an uncertainty analysis. Sensitivity analysis can also be conducted with LHS, but it also requires that the distributions be specified--as opposed to fractional factorial design, which does not require input distributions for the sensitivity analysis.

The fractional factorial design does not lend itself well to an uncertainty analysis. Because it only looks at a small number of values of a

factor over a wide range, it cannot model what occurs between the observed levels. Yet an uncertainty analysis needs to be able to assess what is occurring at these intermediate values, since these values typically are more likely to occur than the extreme values. Thus, the fractional factorial design requires gross interpolation when using it for an uncertainty analysis. Such interpolation is valid only if a simple response surface (e.g., linear) fits the model well.

The LHS method uses more intermediate values; those values are selected based on their assumed (or known) probability of occurrence. By observing the response at a larger number of intermediate values of each factor, the relationship between the response and the factor can be more adequately modeled. This improves the estimate of the cumulative distribution function of the response over that produced by doing Monte Carlo simulations of the response surface built from a fractional factorial.

To select a sample of size n from p factors ($X_1, X_2, \dots, X_p$) under the LHS method, first determine the probability density function (PDF) of each of the input factors. Each factor's PDF is then broken into n segments, with each segment containing an area of $1/n$ under the PDF. Within each segment a value is selected, with probability of selecting the point based on the PDF. (Alternatively, the cumulative distribution function, CDF, can be used in place of the PDF.) Thus, for each factor, n values are chosen based on stratifying the PDF into n equally likely segments and then probabilistically selecting a point from each segment. Iman and Helton (1985) suggest a minimum sample size of $(4/3)p$. The actual sampling points are generated by first pairing the n values from X_1 with the n values from X_2 . Then the n values from X_3 are randomly paired with the X_1 and X_2 pairs. The process continues until n p -tuples have been generated.

As an example, consider the case when there are two factors ($p = 2$) and five samples are to be collected ($n = 5$). If the first factor, X_1 , is normally distributed, then the PDF is divided into five sections, each with an area of 0.2 as shown in Figure 5-2. Because of the shape of the normal

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Figure 5-2. Intervals used with a LHS of size $n = 5$ in terms of the density function and cumulative distribution function for a normal random variable. (Iman and Shortencarier, 1984).

distribution, the actual lengths of the intervals are larger for the intervals near the tails of the distribution. A single value is then selected from each interval. If the second factor, X_2 , is uniformly distributed between G and H (all values between G and H have equal probability of occurrence), then the five equally probable intervals also have equal length. One possible realization of the random pairing of the X_1 and X_2 values is shown in Figure 5-3.

The above algorithm for obtaining n samples can be constrained so that there is little or no correlation between the factors' values (e.g., changes in the value of one factor are independent of changes to another factor). Figure 5-4 shows the possible interval combinations for two factors each at three levels. Figure 5-4 (a) and (b) show cases where the rank correlation between the two factors is 1 and -1, respectively. This high correlation is undesirable because it will lead to highly unstable estimates. However, if there is a true correlation between factors it may be desirable to maintain this structure in the sample; the sample selection can be restricted to mimic this correlation. See Iman and Helton (1985) for further information and references.

For the sample problem, four factors are considered in the uncertainty analysis. They are velocity, R_d , dispersion, and source concentration. An interaction was also assumed between pore velocity and dispersivity. This was assumed for the fractional factorial design and is used to illustrate that interactions can be considered in LHS. (Note that interactions do not have to be specified prior to formulating the LHS design. This was not true for fractional factorial). The complex interaction assumed for the fractional factorial design was not significant; thus, it was not included in this analysis. Note that well distance and half-life are not considered. The well distance was assumed to be 100 m, and the radionuclide was assumed to be Cs-137 (half-life = 30.17 y). A short half-life was selected because the OFAT analysis showed that peak concentration was most sensitive to changes in

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Figure 5-3. A two-dimensional representation of one possible LHS of size 5 utilizing X_1 and X_2 (Iman and Shortencarier, 1984).

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Figure 5-4. Examples of correlation in LHS design (Iman and Helton, 1985).

factors for short half-lives. These assumptions are realistic and could have been made for the sample problem at the initial stages of the PA process. They were left flexible in the first sample to provide a more global sensitivity analysis.

It was assumed that site characterization data had been collected and that distributions had been defined for the factors. Velocity, R_d , diffusion, and source concentration are considered to have lognormal distributions. Dispersion is considered to have a uniform distribution. It was decided to use a sample of size 25 (this is larger than the recommended minimum of 4/3 times the number of factors) for the uncertainty analysis. The additional runs were used to obtain more data points for the cumulative distribution function. A summary of the input factors and distributions is provided in Table 5-7.

Table 5-7. Factors and distributions considered in the Latin hypercube sampling

<u>Factor</u>	<u>Units</u>	<u>Distribution</u>	<u>Low Endpoint</u>	<u>High Endpoint</u>
$1/R_d$	(-)	Lognormal	1.0	100.0
Darcy Velocity ^a	(m/y)	Lognormal	0.5	5.0
$1/\alpha_L^b$	(m)	Uniform	0.1	10.0
Source	(Ci)	Lognormal	0.316	3.16

a. Pore Velocity = Darcy Velocity/Porosity (porosity assumed to be 0.1)

b. Transverse Dispersivity is assumed to be 0.1 x Longitudinal Dispersivity.

Ranges of values were also defined for each of the factors to be considered. Dispersivity has a uniform distribution between 0.1 and 10 m. The range the user must specify for the lognormal distributions cuts off the 0.1 and 99.9 percentiles of the distribution. For velocity, these endpoints were assumed to be 0.5 to 5 m/y. Likewise, the endpoints for R_d are 1 and 100

and for source concentration are 0.316 and 3.16 Ci. The distributions are assumed to be independent (i.e., knowledge of one parameter gives no information about the others).

5.2.2 Determination of Necessary Computer Runs

The program used to generate the sample is from Iman and Shortencarier (1984) and is called LHS Program. Based on the input distribution and range of values for each factor, the program generates a set of computer runs. The sample developed by the program is shown in Table 5-8. Note that the factor levels are distributed throughout the range as opposed to simply at two or three levels, as was the case for fractional factorial design. The rank correlations between the factors were low (near zero); thus, colinearity between the factors should not be a problem (i.e., distributions are independent). Sample means and variances for each factor closely match the underlying population mean and variance. This means that the sample is representative of the conditions that are expected to be encountered, and that the uncertainty analysis results for the response are also representative of what will be encountered.

5.2.3 Sensitivity Analysis Results

The same computer program that was used for Section 5.1.3 was used for the Latin hypercube sampling runs. Peak concentrations calculated with the analytic solution have been tabulated in Table 5-9. Peak concentration is the response variable considered in the statistical analysis. Thus, peak concentrations predicted by the analytic solution are subsequently used as inputs for the regression analysis. A similar approach to the one used for the regression analysis in Section 5.1.3 was used for this problem. Only one sensitivity analysis was run using the same functional forms as were used for the final model in the first sample problem.

Table 5-8. Combinations of factor values for the 25 runs identified by the Latin hypercube sampling

<u>Case</u>	<u>R_d (-)</u>	<u>Darcy Velocity (m/y)</u>	<u>a_L (m)</u>	<u>Source (Ci)</u>
1	16.6	1.30	8.58	0.83
2	39.0	1.99	2.85	1.51
3	7.7	1.42	1.77	1.56
4	13.2	1.83	2.73	0.61
5	3.7	3.43	3.34	1.35
6	14.7	1.63	1.52	0.89
7	6.0	1.53	5.21	1.72
8	8.3	1.90	4.39	0.59
9	11.5	0.86	6.01	1.07
10	10.9	2.31	3.80	0.49
11	5.1	1.75	7.29	0.72
12	12.6	1.49	2.20	0.86
13	10.3	1.19	6.79	0.77
14	9.1	0.81	1.03	1.02
15	31.7	1.15	9.30	0.94
16	21.1	1.36	9.06	1.14
17	5.6	1.07	5.13	1.39
18	7.3	1.25	5.71	1.22
19	18.1	2.15	4.76	3.16
20	2.6	1.00	8.11	0.66
21	24.8	2.61	9.88	1.01
22	19.8	1.68	0.34	0.76
23	6.7	1.59	0.47	0.97
24	4.6	2.72	6.90	1.15
25	2.9	2.25	7.66	1.27

Table 5-9. Peak concentration calculated for the 25 LHS test cases

<u>CASE</u>	<u>Peak Concentration</u>
1	1.585E-05
2	4.914E-06
3	4.808E-04
4	6.120E-05
5	1.544E-03
6	7.159E-05
7	5.076E-04
8	1.280E-04
9	2.920E-05
10	8.236E-05
11	2.406E-05
12	2.846E-07
13	4.865E-05
14	9.526E-05
15	1.448E-06
16	1.158E-05
17	3.446E-04
18	1.948E-04
19	1.394E-04
20	4.321E-04
21	2.001E-05
22	3.918E-05
23	7.360E-04
24	5.660E-04
25	9.770E-04

Note: These results are directly used for the CDF in Figure 5-5.

The model to be fit to the results is defined by the following equation (the variables are the same as Equation 5.2):

$$C = \beta_0 + \beta_1 \left(\frac{1}{R_d} \right) + \beta_2 U + \beta_3 \left(\frac{1}{\alpha_L} \right) + \beta_4 Q + \beta_5 U \cdot \alpha_L \quad (5.3)$$

The sensitivity analysis results from this model are presented in Table 5-10. The coefficient of determination for this model was 0.7961. This is a relatively good value, significantly better than the results using the wide data ranges. This model could be considered a relatively good predictor of the results that would be calculated with the analytic solution. By a relatively large margin retardation was the most important factor in determining the peak concentration. Darcy velocity showed somewhat less impact on the predicted concentrations, but was still much more important than the other three factors. These results cannot be compared to the results of the OFAT analysis and fractional factorial design because different factors and ranges of values were used.

Table 5-10. Final Model--Latin hypercube sampling

<u>Factor</u>	<u>ΔR^2</u>		<u>Standardized Coefficient</u>	
	<u>Value</u>	<u>Rank</u>	<u>Value</u>	<u>Rank</u>
Darcy Vel.	0.1468	2	0.497	2
1/R _d	0.4860	1	0.721	1
Source	0.0272	3	0.171	4
1/ α_L	0.0042	5	0.084	5
Pore Vel. x α_L	0.0194	4	0.210	3

Note: R^2 for this model was 0.7961.

5.2.4 Uncertainty Analysis Results

The primary benefit of LHS is that the results of the computer runs presented in Table 5-9 can be directly used to generate a cumulative distribution function. In the fractional factorial design, an additional set of runs would be necessary to generate a CDF. Furthermore, the additional runs would be based on the fitted surface as opposed to output from the analytic solution. The CDF for the results of the LHS analysis is plotted in Figure 5-5. A CDF can be used to demonstrate the probability that the peak concentration predicted for a given set of conditions will be below a specified value. For example, Figure 5-5 illustrates that 90% of the predicted peak concentrations will be below $\sim 6.5\text{E-}4 \text{ Ci/m}^3$. Likewise, it can be seen that 50% of the predicted peak concentrations will be below $\sim 8.0\text{E-}5 \text{ Ci/m}^3$. From a broader perspective, the plot shows that predictions based on the relatively tight ranges of values still provide a rather wide range of results (roughly four orders of magnitude). However, this range of predictions is significantly less than the range predicted using the initial data. This illustrates that as more data are collected, the factors will be better known; therefore, the uncertainty in predictions will generally be reduced.

5.3 Discussion

Two different techniques for sensitivity/uncertainty analysis were demonstrated in Section 5: fractional factorial design and Latin hypercube sampling. Fractional factorial design requires less information regarding the distributions of the factors of interest. Thus, it was applied to a sample problem representing the initial stages of the PA process when limited data are available. Latin hypercube sampling requires knowledge of the ranges and distribution of the factor values in that range. It was applied to a problem representing the latter stages of the PA process when more detailed data will be available. Latin hypercube sampling was also much easier to apply for uncertainty analysis, which is most important in the latter stages of the PA process.

Figure 5-5. Cumulative distribution function for Latin hypercube sampling results.

Each of the techniques was appropriate for the objectives of sensitivity/ uncertainty analysis at the corresponding stage of the PA process. The requirements of the two techniques corresponded well with the information expected to be available when the analysis would be conducted. If the order of application was reversed, it appeared that it would be easier to apply the Latin hypercube sampling approach in the early stages (if proper information was available) than it would be to use the fractional factorial design in the latter stages of the process. This is primarily due to the extra effort required to conduct the uncertainty analysis.

The greatest difficulty in applying the two techniques was determination of the functional form of the factors used in the regression analysis to determine sensitivity. Several tests were necessary to find a reasonable form for the different parameters. Another difficulty had to do with specifying interactions to be considered. This also required some trial and error. The results for the first sample were different when a linear model was used, as opposed to the functional forms based on the results of the OFAT analysis (Section 4). This shows the potential for problems if the functional forms are oversimplified.

6. SUMMARY

Sample applications were provided for three sensitivity/uncertainty analysis techniques: OFAT analysis, fractional factorial design, and Latin hypercube sampling. The techniques were applied to a groundwater transport problem in the context of the initial and latter stages of the PA process. The advantages and disadvantages of the techniques were discussed and illustrated with respect to the goals of sensitivity/uncertainty analysis in the PA process. Potential pitfalls and limitations of the techniques were also discussed and illustrated.

A variation of OFAT analysis was found to be relatively easy to apply and interpret. However, it was also limited by the large number of runs required to gain a more complete understanding of the relative importance of the factors. OFAT analysis was primarily used to gain an understanding of the functional form of the factors of interest. If the standard OFAT approach had been used, much of the information that was obtained from the approach used in this document would not have been acquired. Also, if a more limited approach had been used, the interactions that were discussed would not have been assessed. A side benefit of the OFAT analysis was identification of a dimensionless number (contaminant half-life/transit time ratio) that may be useful as a general screening tool for site-specific PAs. In general, OFAT analysis was found to be useful as a scoping tool and precursor to the more detailed analyses, but would be very limited if applied without followup analyses.

Fractional factorial design was found to be more difficult to apply, but this is to be expected since it is a more rigorous technique. The difficulty was offset by the fact that only a small number of runs were required to complete the analysis. Fractional factorial design allowed the direct consideration of interactions between factors, and provided a quantitative ranking of the factors and interactions by relative impact on the response variable. This information was not directly obtained from the OFAT analysis. Fractional factorial design was found to be very useful in the initial stages of the PA process because the distributions of the factors were not required.

Thus, when minimal data are available (such as bounding ranges), fractional factorial design can be a useful tool. Uncertainty analysis was not conducted with the fractional factorial design because distributions for the data and additional runs using the fitted surface would have been required. Furthermore, the fitted surface was not deemed adequate to conduct the uncertainty analysis.

Latin hypercube sampling was similar in effort of application to the fractional factorial design. Latin hypercube sampling also allowed for direct consideration of interactions between factors and provided a quantitative ranking of the factors and interactions. The primary benefit of Latin hypercube sampling was that the CDF for the uncertainty analysis was obtained directly from the groundwater transport model. Because distributions for the parameters were required, Latin hypercube sampling was appropriate for the latter stages of the PA process when data are available from site characterization. Also, the ease of conducting the uncertainty analysis provided a good basis for use at the latter stages of the PA process.

The most difficult parts of the sensitivity analyses were determining the functional forms for the factors and specifying the interactions to be considered. Several iterations were made in order to arrive at the functional forms and interactions used in the final analysis. This is a very subjective process and leaves plenty of room for differing opinions. The authors do not claim to assume that the functional forms and interactions used are the best for this problem. There may be a better combination. The authors did try a number of combinations and were most comfortable with the combination of factors and functional forms used for the final analysis.

7. LIMITATIONS

When using regression analysis as part of a sensitivity analysis, the analyst must understand that the technique does have limitations. The user must guard against using the technique beyond its capabilities, since doing so may lead to misleading results and invalid conclusions. The limitations most likely violated are its application to uncertainty analysis and the use of significance tests. Other limitations that the user should be aware of before choosing this sensitivity technique include the often large number of trials required and the lack of ability to detect nonlinear effects.

Classical tests of significance assume that the residuals are normally distributed, and that the model is fully and correctly specified. However, in the application of regression techniques as part of a sensitivity analysis on an analytical model, these requirements are not met. The residuals are not due to measurement error, and the correct model is the complete analytical model. Thus, the assumptions underlying the tests of significance are not met. While these justifications are not valid, some of the tests can be reformulated. The most important test for sensitivity analysis is the change in the amount of variation accounted for by the addition or deletion of a factor to the model.

When using a complete factorial design, the number of trials required to assess all factors and their interactions can become excessively large. In this case, the researcher often assumes that higher order interactions are negligible. The researcher may also eliminate lower order interactions based on knowledge of the problem. When the researcher does assume that some interactions are negligible, fractional factorial designs can be used to reduce the size of the experiment to a more manageable size. It should be noted that, theoretically, the use of statistical experimental design, including fractional factorials and Latin hypercube, is the most efficient method of experimentation.

If the factors have a significant nonlinear effect on the response, the effect of the factor on the response may be missed by simple linear

regression. The researcher must guard against this by first establishing the relationship between the factor and the response by looking at the response (or a simple approximation of the response) across all levels of the factor, with other factors held constant. Once this relationship has been established the factor may be transformed to make the response a linear function of the transformed factor, or more advanced nonlinear regression techniques can be implemented. In the analytical groundwater model, for example, the researchers knew that the retardation (R_d) was inversely related to the peak concentration. Thus, the effect of R_d was estimated in the model through the transformation $1/R_d$.

Specification of factor levels to be considered in the sensitivity analysis is also a crucial concern. Factor levels should be defined based on a combined consideration of expected values from field or laboratory data (e.g., retardation factors) and regulatory concerns (well location). Factor levels considered in the sensitivity analysis should bound the range of values expected for a given PA application, with emphasis on those levels where effects would be expected to be largest. In this case, if factor levels are not selected wisely, the effect of the factor may be underestimated and lead to incorrect conclusions.

It should be emphasized that sensitivity analysis is used to determine the most important factors with respect to the response of interest. It is not used to determine a simpler form of the model. Thus, an initial assessment of the relationship between the factors and the response is necessary to assure that nonlinear effects are not missed. While this assessment may lead the researcher to conclude that since the response varies for each factor (and hence is sensitive to each factor), it is the role of sensitivity analysis to determine which factors override the effects of the other factors.

A problem can also occur when the researcher uses the nonstandardized coefficient as a measure of the importance of the factor. This is totally unjustified. The magnitude of the nonstandardized coefficient is purely a function of the units of the factor and the response. For example, a

nonstandardized coefficient that looks large when the factor is measured in miles will be very small when the factor is measured in inches, yet still be just as significant when determining the response's sensitivity to that factor. Nonstandardized coefficients were not reported in this analysis to avoid such confusion.

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Appendix A

Regression Analysis

APPENDIX A

REGRESSION ANALYSIS

Regression analysis (least squares fitting) is one of the most widely used modeling techniques. The calculations involved in linear regression analysis are discussed in this section. This appendix covers some of the aspects of regression that are important for this report; however, it is certainly not a comprehensive coverage of the subject. The reader is strongly advised to consult a text on regression analysis when implementing the procedures presented in this report. Two comprehensive and well written texts are by Weisberg (1980) and Neter and Wasserman (1974). The first part of the discussion below presents the classical interpretation of regression. A more rigorous theoretical development of regression can be found in Graybill (1976). The application of regression analysis is further developed in Weisberg (1980). The latter part of this appendix discusses regression in the context of sensitivity analysis. It is assumed that the reader has a background in linear algebra.

Classical Regression

The classical justification of regression assumes that there are n observations of a fundamental process, and that each observation is subject to some random error. The basic problem is to relate a set of p independent variables (factors) to a dependent (response) variable. A solution is to fit a linear model to the response variable based on the factors. The solution is determined by finding the model that minimizes the sum of squared distances between the observed responses and the line specified by the model (hence the name "least squares regression").

Development of the Regression Model and Solution

Consider the model

$$y = \beta_0 + \beta_1 x_1 + \dots + \beta_p x_p + \epsilon \quad (\text{A.1})$$

where y is the response variable, $x_1, \dots, x_p$ are the predictor variables, ϵ is the random error term (residual), and $\beta_0, \beta_1, \dots, \beta_p$ are the model coefficients. It is assumed that the expected value of ϵ is 0 and the variance is σ^2 .

If n independent observations of the response are taken for n realizations of the set of x 's, then for each observation the model is

$$y_i = \beta_0 + \beta_1 x_{1i} + \dots + \beta_p x_{pi} + \epsilon_i, \quad i = 1(1)n. \quad (\text{A.2})$$

In this model, the y_i 's and x_{ji} 's, $j = 0(1)p$, are known, while the β_j 's and ϵ_i 's are unknown and must be estimated. The model (A-2) with n observations can be rewritten in matrix form as

$$y = X\beta + \epsilon \quad (\text{A.3})$$

where y , the vector of response values, and ϵ , the vector of residuals, are $n \times 1$ vectors; X is an $n \times (p+1)$ matrix with column $j+1$ corresponding to the predictor variable x_j and the first column being a column of 1's; and $\beta = (\beta_0, \dots, \beta_p)^T$, the vector of coefficients. The expected value of ϵ is 0 with dispersion matrix $\sigma^2 I$.

The vector y and matrix X in Equation (A-3) are known from the n observations. It remains to determine estimates of β , ϵ , and σ^2 . Substituting the estimates, $\hat{\beta}$ and $\hat{\epsilon}$, into Equation (A-3) gives

$$y = X\hat{\beta} + \hat{\epsilon} . \quad (A.4)$$

The estimates of β and ϵ are found by minimizing the sum of squared residuals; that is, minimize the value of $\hat{\epsilon}^T \hat{\epsilon}$ with respect to $\hat{\beta}$ (with y and X constant).

From Equation (A-4), $\hat{\epsilon} = y - X\hat{\beta}$ and

$$\hat{\epsilon}^T \hat{\epsilon} = (y - X\hat{\beta})^T (y - X\hat{\beta}) = y^T y - 2\hat{\beta}^T X^T y + \hat{\beta}^T X^T X \hat{\beta} . \quad (A.5)$$

A minimum for $\hat{\epsilon}^T \hat{\epsilon}$ is found by setting the derivative of $\hat{\epsilon}^T \hat{\epsilon}$ with respect to $\hat{\beta}$ to zero. Hence,

$$\frac{\partial \hat{\epsilon}^T \hat{\epsilon}}{\partial \hat{\beta}} = \frac{\partial (y^T y - 2\hat{\beta}^T X^T y + \hat{\beta}^T X^T X \hat{\beta})}{\partial \hat{\beta}} = 0 . \quad (A.6)$$

Taking the derivative gives

$$-2X^T y + 2X^T X \hat{\beta} = 0 , \quad (A.7)$$

or

$$X^T X \hat{\beta} = X^T y . \quad (A.8)$$

Equation (A-5) is called the "normal equation." The solution for $\hat{\beta}$ depends upon the rank of the $n \times (p + 1)$ matrix X . When the columns of X are linearly independent, then the rank of X is $p + 1$ and X is said to be of full column rank. In the typical regression setting, X will have full column rank. Only this case will be considered here.

When X has full column rank, the inverse of $X^T X$ exists. Thus, by premultiplying both sides of Equation (A-8) by $(X^T X)^{-1}$, we find the solution to $\hat{\beta}$ is

$$\hat{\beta} = (X^T X)^{-1} X^T y \quad . \quad (A.9)$$

Then from Equation (A-4), $\hat{\epsilon}$ is

$$\hat{\epsilon} = y - X\hat{\beta} \quad , \quad (A.10)$$

and the variance of the residuals, σ^2 , is estimated as

$$\hat{\sigma}^2 = \frac{\hat{\epsilon}^T \hat{\epsilon}}{n - p - 1} \quad . \quad (A.11)$$

The fitted values of the model are

$$\hat{y} = X\hat{\beta} \quad . \quad (A.12)$$

This same formula can be used to determine predicted values by substituting the factors and levels of interest into the rows of X . Finally, an important property of the estimate $\hat{\beta}$ is the variation in the estimation. This is contained in the estimated dispersion matrix, $\text{var}(\hat{\beta})$, which is calculated as

$$\text{var}(\hat{\beta}) = \hat{\sigma}^2 (X^T X)^{-1} \quad . \quad (A.13)$$

The structure of $\text{var}(\hat{\beta})$ is

$$\text{var}(\hat{\beta}) = \begin{bmatrix} \text{var}(\hat{\beta}_0) & \text{cov}(\hat{\beta}_0, \hat{\beta}_1) & \dots & \text{cov}(\hat{\beta}_0, \hat{\beta}_p) \\ \text{cov}(\hat{\beta}_0, \hat{\beta}_1) & \text{var}(\hat{\beta}_1) & \dots & \text{cov}(\hat{\beta}_1, \hat{\beta}_p) \\ \vdots & \vdots & \ddots & \vdots \\ \text{cov}(\hat{\beta}_0, \hat{\beta}_p) & \text{cov}(\hat{\beta}_1, \hat{\beta}_p) & \dots & \text{var}(\hat{\beta}_p) \end{bmatrix} \quad . \quad (A.14)$$

The covariance between two coefficients, $\text{cov}(\hat{\beta}_i, \hat{\beta}_j)$, is generally nonzero, and therefore the estimators of the coefficients are correlated.

Coefficient of Determination

A simple measure of the model's fit to the data is the coefficient of determination, R^2 , which is computed as

$$R^2 = \frac{TSS - RSS}{TSS}, \quad (A.15)$$

where

$$TSS = \sum_{i=1}^n (y_i - \bar{y})^2, \quad (A.16)$$

and

$$RSS = \sum_{i=1}^n \hat{\epsilon}_i^2. \quad (A.17)$$

The $\hat{\epsilon}_i$ are defined in Equation (A-10) and $\bar{y}$ is the mean of the response values. R^2 measures the proportion of variability in the response explained by regression on the factors. The value can range from 0 to 1, with values near 1 indicating that the model fits the data well. However, this measure should be interpreted with caution. The R^2 value increases with the addition of more factors to the model, whether those factors are relevant to the response or not. Indeed if there are n linearly independent columns in X , then the R^2 value will be 1 no matter what the columns of X represent. R^2 also depends on the spacing of the levels of the factors. If the factor levels are randomly drawn, then the interpretation of R^2 given above is valid. However, if factor levels are selectively determined (as in a controlled experiment), then the R^2 value can be influenced by the spacing of the levels and the interpretation of R^2 is less clear.

Sensitivity Analysis

The methods discussed in section A.1 can still be applied to a sensitivity analysis (SA) of a computer model. However, the standard hypothesis tests used in regression analysis do not directly apply to the sensitivity analysis of a computer model. The reason for this change is that the response variables are no longer subject to random error. That is, the response is determined exactly by the computer model.

In the case where the response is subject to random error, the residuals (the difference between the observed values and the fitted values) are composed of both random error and the regression model's lack of fit error. When fitting a simple model to a more complex model such as a computer model, the residuals are entirely due to lack of fit error.

The fundamental idea of the sensitivity analysis discussed in this report is to assess which factors are the most important in determining the response. That is, the SA allows one to rank the factors from most to least important. The factors found to be most important are the factors that should be concentrated on in further studies. There are a number of ways of performing sensitivity analyses (see Iman and Helton, 1985, and Maheras and Kotecki, 1990, for overviews).

The use of a fractional factorial design for sampling restricts the possible sensitivity analysis methods to those based on the coefficients of a response surface model. In this case, the response surface model replaces the more elaborate computer model. The difficulty is in trying to get the response surface model to adequately represent the computer model. Thus, it is useful to spend time on the one-factor-at-a-time (OFAT) approach to determine relationships between the factors and the response.

In the environmental model considered, there are many factors that simultaneously influence the response (ground water concentration). As such, it is important that the SA consider these same factors simultaneously rather than one at a time. The use of response surface analysis techniques along with

sensitivity analyses based on the computed coefficients allows the factors to be considered simultaneously.

Two coefficient based methods of sensitivity analysis are used in this report, each with a slightly different interpretation. The first interpretation is that the most important factor causes the largest change in concentration (per some unit change in the factor). This interpretation is handled by the use of standardized coefficients. The second interpretation is that the most important factor is the best predictor of the concentration. This interpretation is handled by the use of the change in the coefficient of determination. Actually, the two methods are essentially the same. They will produce the same factor rankings when the input factors are orthogonal (Iman and Helton, 1985).

Change in R^2

If a factor is removed from the equation and the remaining factors are regressed on the response, the resulting R^2 value will be less than or equal to the R^2 value for the fit including all factors. The larger the difference between the two R^2 values, the more important the removed factor is in determining the response. The difference between R^2 values can be calculated for each factor and ranked. The ranks can allow one to assess the importance of each of the factors on the response.

Computing the difference in R^2 values for the i 'th factor requires computing two least square fits: the first with all factors and the second without the i 'th factor. The difference, ΔR_i^2 , is computed as

$$\Delta R_i^2 = \frac{RSS_{ri} - RSS_f}{TSS}, \quad (A.18)$$

where

RSS_{ri} = the RSS for the reduced model with the i 'th factor removed, and
 RSS_f = the RSS for the full model.

If there are p factors, then $p + 1$ regression calculations are required to get all the RSS values needed to compute and rank the ΔR_i^2 . However, the output from many regression programs include a t-statistic for the test of whether a factor coefficient is zero or not. These t-statistics are directly related to the ΔR_i^2 . Ranking the absolute values of the t-statistics is equivalent to ranking the ΔR_i^2 . The exact relationship between the ΔR_i^2 and the t-value is

$$\Delta R_i^2 = \frac{t^2 RSS_f / (df_{rss})}{TSS} \quad (A.19)$$

where

df_{rss} = the degrees of freedom associated with the residual sum of squares for the full model.

Therefore, only the full model needs to be fitted, if the output shows the t-statistics for each factor.

Standardized Coefficients

The magnitude of the coefficients calculated in Equation (A-9) depends upon the magnitude (units) of the factor levels. Thus, one cannot directly compare the coefficients of the various factors to determine which factor is most important. For example, if one of the factors was distance, the coefficient would be relatively large if the distance was measured in miles and relatively small if measured in inches. Thus, if one were to directly compare the distance coefficient to the remaining factor coefficients, one might conclude that distance is important when the measurement is in miles and not important when the measurement is in inches. Of course, this is contradictory since the effect is the same.

However, by standardizing the factors and response so that they all have mean 0 and variance 1, the coefficients resulting from the standardized data can be compared. These coefficients are called standardized coefficients. To

compute the standardized coefficients, begin by computing the sample mean and sample standard deviation of each factor and the response. Then replace the response values, y_i , with the standardized response values, y_i^* , where

$$y_i^* = \frac{y_i - \bar{y}}{s_y} . \quad (\text{A.20})$$

Here $\bar{y}$ is the sample arithmetic mean and $s_y = \sqrt{\text{TSS}/(n-1)}$ is the standard deviation in y . Likewise, compute the standardized response values for each factor, x_{ji}^* , $j = 1(1)p$, as

$$x_{ji}^* = \frac{x_{ji} - \bar{x}_j}{s_{x_j}} , \quad (\text{A.21})$$

where $\bar{x}_j$ and s_{x_j} are the mean and standard deviation of the j 'th factor, respectively.

Now implement the same calculations described in the first section, except use the values of y_i^* and x_{ji}^* in place of the y_i and x_{ji} , respectively. The resulting coefficients (which will be symbolized by β_j^* rather than β_j) can now be compared to one another since they are all in the same units. The larger the value of the β_j^* , the more effect it has on the response. The exact interpretation of the standardized coefficient is that a single standard deviation change in the i 'th factor level will change the response by β_j^* standard deviation units, holding the remaining factors constant.

With a designed experiment, we must keep in mind that the standard

deviation of x_j depends on the levels selected for the j 'th factor. An unrealistic choice of levels will yield a misleading measure of importance.

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