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PARAMETER IMPORTANCE OF AN ANALYTICAL MODEL FOR TRANSPORT IN THE VADOSE ZONE

by

Tanner H. Bushnell

A thesis submitted to the faculty of

Brigham Young University

in partial fulfillment of the requirements for the degree of

Master of Science

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BRIGHAM YOUNG UNIVERSITY

GRADUATE COMMITTEE APPROVAL

of a thesis submitted by

Tanner H. Bushnell

This thesis has been read by each member of the following graduate committee and by majority vote has been found to be satisfactory.

Date	Gustavious P. Williams, Chair
Date	Norman L. Jones
Date	E. James Nelson

BRIGHAM YOUNG UNIVERSITY

As chair of the candidate's graduate committee, I have read the thesis of Tanner H. Bushnell in its final form and have found that (1) its format, citations, and bibliographical style are consistent and acceptable and fulfill university and department style requirements; (2) its illustrative materials including figures, tables, and charts are in place; and (3) the final manuscript is satisfactory to the graduate committee and is ready for submission to the university library.

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ABSTRACT

PARAMETER IMPORTANCE OF AN ANALYTICAL MODEL

FOR TRANSPORT IN THE VADOSE ZONE

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Master of Science

The American Society of Testing and Materials (ASTM) has established a three tier risk-based corrective action (RBCA) program for cleaning up petroleum release sites, which is supported by the Environmental Protection Agency. RBCA programs make the cleanup of spill sites more efficient by requiring additional site information only when a more accurate risk assessment is needed. For spill sites that do not pass the first tier general assessment, a Tier 2 evaluation involving site specific information and screening level models to assess the potential risk must be conducted. Screening level models generally require site specific input parameters. To increase efficiency it would be helpful to know which parameters have large affects on model output and which parameters do not affect the model output significantly. There have been many studies focused on model sensitivity to input parameters. For an input parameter to vary there must be uncertainty about the value. This research proposes a method of including

parameter uncertainty with model sensitivity to quantify the importance of a parameter, where the term importance is a combination of parameter uncertainty and sensitivity. Using the method developed in this thesis, an importance assessment was conducted on an analytical model for vadose zone transport. It was found that for sites posing high risk, with large spill volumes and shallow water table depths, the input parameters of water table depth and spill volume were the most important. The input parameters of precipitation and contaminant biodegradation half-life showed high importance in lower risk situations; when the water table was deep. A comparison of sensitivity analysis to importance showed differences in their results. The sensitivity analysis identified those parameters that the model was sensitive to, while the importance assessment identified the parameters that were sensitive and whose range of uncertainty was large enough to affect model output values. This information could be used for resource allocation decisions when acquiring additional site specific information.

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Lastly, I would like to thank my mom, Bobette Bushnell, for instilling in me an interest in education, and my dad, Dwight Bushnell, an interest in engineering. All the support I have received from my family is very much appreciated.

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1 Introduction

Physical and chemical characteristics and site complexity all affect the risk that humans and the environment may be subject to at a petroleum spill location and factor into the priority given to site cleanup (ASTM 1995). Prioritizing cleanup actions based on the risk posed to human health and the environment is often called risk-based corrective action (RBCA) or risk-based decision making. The United States Environmental Protection Agency (USEPA) has encouraged states to implement RBCA into cleaning sites where petroleum products have been released into the environment (EPA 1995). The EPA has stated that RBCA is compatible with CERCLA and RCRA programs and the EPA's own guidelines and initiatives. Using RBCA could help make clean up programs faster and more efficient (EPA 1995). A format supported by the USEPA for establishing a RBCA program was outlined by the American Society for Testing and Materials (ASTM) in their Standard Guide for Risk-Based Corrective Action Applied at Petroleum Release Sites (ASTM 1995).

The ASTM guide establishes a three tier system. Tier 1 requires that conservative general site assessment information be compared against Risk Based Screening Levels (RBSLs). If the RBSLs are exceeded, then a Tier 2 evaluation requiring additional site-specific information should be gathered to make a more accurate assessment. Tier 2 evaluations generally involve using site specific information and screening level models

to assess the potential risk. David Tomasko et al. (2001) developed an analytical model to be used for Tier 2 RBCA evaluations at NAPL-contaminated sites.

The Tomasko model is implemented with easy to use engineering plots to identify maximum NAPL concentrations that may be expected in the groundwater beneath a site, but the model requires fifteen case specific input parameters. Some of the parameters are general contaminant properties while others are specific to the particular site. It can become expensive and time consuming to measure or obtain all fifteen parameters accurately for each application of the model. It is suggested in the literature that some parameters have a considerable effect on the model output, while others may not affect the model output significantly. This is usually referred to as parameter sensitivity (EPA 1997, Frey 2002, Greenland 2001, Hamby 1994, Lenhart et al. 2002, Thornton et al. 2001). In addition to sensitivity, due to uncertainty, some of the input parameters may be more important than others for estimating risk at a site. In performing a Tier 2 assessment it would be more efficient and cost effective to focus on measuring the important parameters accurately.

My research proposes a way to quantify the importance of a parameter using a combination of the parameter sensitivity in the model normalized by the uncertainty in the value. For example, the density of water could be a sensitive parameter but it has low importance because there is little uncertainty in the value for subsurface models.

2 Literature Review

Mathematical models are often used in the fields of engineering, science, physics, sociology, statistics, medicine, and economics to estimate occurring phenomena (Frey and Patil 2002, Hamby 1994). Each model requires some sort of input. The input may be exact, measured, or estimated. The accuracy of the model output, or phenomena estimation, is dependent on the accuracy of the input (Hamed and Bedient 1997, Isukapalli 2000 et al., Saltelli 2002). Increasing accuracy of the input parameters often requires a large expense (Dubus and Brown 2002, EPA 1998, Lenhart et al. 2002). In such cases it would be helpful to know which input parameters have a significant effect on the output and therefore warrant closer examination. Accuracy and validity of output results are important because, in the environmental profession, the results are often used in assessing risk, as in the case studied in this paper. To provide quality assurance to risk assessments, the uncertainty and variability of the model-based risk estimate should be known. This uncertainty and variability in the risk assessment is dependent on the model's sensitivity to variation in the input parameters. The sensitivity of the model to an input parameter and the uncertainty of the parameter for a specific site can be combined to evaluate parameter importance.

My research objective is to develop and present a method to quantify the importance of the input parameters using an analytical model of LNAPL transport in the

vadose zone. This method is presented as a general approach that can be applied to other models and requirements. My research is based on a hypothetical site developed from studies of fuel spills from the Installation Restoration Program (IRP) sites in Hawaii (Tomasko et al. 2001). In this section, to provide a foundation for my research, I review some to the relevant work on uncertainty, sensitivity, and importance analysis. It is not meant to encompass all that was used for my research or that could be used pertaining to the research, but rather provide a general overview.

2.1 Uncertainty

Parameter uncertainty is the range of possible values a parameter can have (Dubus 2003). It can be defined as the lack of knowledge of the scalar value of a parameter (EPA 1997). This uncertainty can come from measurement, sampling, or estimation errors (EPA 1997). The possible range of a parameter can be determined by experimental measurement, standard values, or expert judgment (Dubus et al. 2003). Also important in assessing risk is parameter variability. Variability is defined as the observed differences of the parameter value in space or time, often expressed as a probability density function (PDF). It is the result of heterogeneity or diversity, such as weather conditions or soil types (EPA 1997). Uncertainty and variability can be taken together in defining the overall variance of the parameter (Mon et al. 2004). For this study only uncertainty was used, since all parameters are averages or most likely values, and no distribution data are available. Also, variability cannot be reduced by further measurement or study, so it is not included in the importance analysis, the objective of this research.

The accuracy and uncertainty of model outcomes are influenced by the accuracy and uncertainty of the input parameters (Hamed and Bedient 1997, Isukapalli et al. 2000, Saltelli 2002). Parameter uncertainty has been incorporated into optimal remediation designs, which shows that remediation requirements increase greatly with increasing parameter uncertainty (Wagner and Gorelick 1987).

2.2 Sensitivity

In addition to parameter variability, sensitivity of some models to parameter variation can also influence remediation costs. Sensitivity analysis has become a large topic of study due to the role of science becoming more to establish quality assurance and defend proposals (Saltelli 2002).

Sensitivity is the amount of variation in the model output in response to changes in the parameter inputs. Small changes in some input parameters may make considerable changes to the model results, while larger changes to other parameters may have little or insignificant effects on results. Knowing the sensitivity of a model to each of its inputs can be helpful in many ways (Dubus et al. 2003). Sensitivity analysis can help identify problems with a model's design (Fontaine et al. 1992). It can be used to simplify a model by eliminating the requirement of entering parameters that have no effect on the outcome (Fontaine 1992). It can identify the parameters that have the largest effect on output for model calibration (Lenhart et al. 2002). Sensitivity analysis can give a model more credibility or act as quality assurance (Wauchope 1992). It can also identify the parameters that deserve the most attention, accuracy, or research during data collection (Boesten 1991, Dubus and Brown 2002, Ferreira et al. 1995).

There are many ways to measure and report sensitivity. The literature contains reviews of several of the sensitivity analysis techniques (e.g., Frey and Patil 2002, Hamby 1994, Isukapalli et al. 2000). Different sensitivity analysis techniques have also been compared (Dubus et al. 2003, Hamby 1995, Lenhart et al. 2002, Patil and Frey 2004). While there have been variations in the results from these comparisons, it has been shown that most techniques produce similar results. Although it would provide greater assurance to apply more than one sensitivity technique to a model (Frey and Patil 2002), the actual ranking is not as important as the general knowledge of what is sensitive and not sensitive (Hamby 1995).

Of the sensitivity techniques reviewed, differential analysis was chosen for this research. Differential analysis is the backbone of most other sensitivity techniques (Hamby 1994). The sensitivity calculated using this technique is defined as the ratio of the change in output to the change in input. Often this is normalized by multiplying by a chosen base-case input value divided by its respective output value (Carmichael et al. 1997, Hamby 1994, Patil and Frey 2004). Techniques such as this are referred to as "one-at-a-time" analysis, since only one parameter is allowed to vary at a time. This is one of the major disadvantages of differential analysis, because interactions between parameters are not identified and combinations far from the base-case values are not represented. Although when the model is an explicit algebraic equation, as in this paper, differential analysis is computationally efficient and easy to perform (Hamby 1994), which is consistent with RBCA goals.

2.3 Importance

Importance assessment identifies the input parameters that, with more accurate measurement, will decrease the variance of the model output the most. It is sometimes treated as synonymous to uncertainty analysis (Hamby 1994) and sensitivity analysis (Dubus et al. 2003, Frey and Patil 2002, Pate-Cornell 2002,). It has been suggested that uncertainty and sensitivity be combined in determining a parameter's importance (Saltelli 2002). An important parameter is one with uncertainty and also is sensitive. A parameter that is not sensitive will not cause variance in the output even with large uncertainty, and a parameter that is highly sensitive but known precisely also will not cause variance in the output (Hamby 1994). ,By including both uncertainty and sensitivity, importance assessment identifies the parameters that can best reduce the output variability with better measurements, increasing the effectiveness of sensitivity analysis in all its uses.

With the advanced methods now available, uncertainty and sensitivity analysis can be included when formulating a mathematical model. Knowledge of the uncertainty and sensitivity associated with a model can be an important part of risk assessment (Hamed and Bedient 1997, Saltelli 2002).

3 Methods

To perform a sensitivity analysis, an objective function must be identified as the model output that is tested for variability. The objective function used in this research was the maximum predicted benzene concentration at the water table below a spill at an IRP site in Hawaii. The model used in this study to predict the maximum concentration of benzene at the water table will first be introduced. The method of calculating uncertainty, sensitivity, and importance will be described. The computer code implementing the importance assessment of the LNAPL transport model parameters is then explained, and last the input parameters for the model are presented.

3.1 Model Description

The model analyzed in this research was developed by Tomasko et al. (2001) for evaluating LNAPL-contaminated sites. When an LNAPL spill enters the soil as a slug it moves downward by gravity and capillary forces. Sorption of the LNAPL is assumed to be negligible because the soil is already wet (Reible et al. 1990). The distance the LNAPL penetrates into the soil, *H*, can be estimated by the following equation:

$$H = \frac{V_{Spill}}{\pi R_0^2 \phi_{r0}} \qquad \textbf{(3-1)}$$

where V_{Spill} is the total volume of the spill, R_0 is the spill radius, and ϕ_{r0} is the residual oil fraction of the soil. This estimates a greater distance *H*, than is likely because it assumes no spreading of the spill as it moves into the vadose zone.

If the depth of the LNAPL penetration is greater than the depth to the water table, then the LNAPL will pool on top of the water table forming a pancake of free product. For pancakes of LNAPL with co-solvents, such as with fuel spills, the aqueous phase concentration of the individual components can be found by using the following relationship (Geller and Hunt 1993):

$$C_i = \gamma_i \chi_i SOL_i \qquad \textbf{(3-2)}$$

where C_i is the concentration of component *i*, γ_i is the activity coefficient of componet *i*, χ_i is the mole fraction of component *i*, and SOL_i is the aqueous solubility of the pure LNAPL.

If the volume of the LNAPL spill is not large enough to reach the water table, an LNAPL smear to a depth *H*, calculated by Equation 3-1, is formed. The concentration of LNAPL in the smear zone is equal to the residual oil-filled porosity of the soil. As precipitation then infiltrates the soil, it will dissolve the soluble components of the LNAPL transporting it down towards the water table. The time required to remove the LNAPL from the contaminated zone, which is the time the zone remains a source of contamination, can be approximated by the following equation:

$$\Delta t = \frac{V_{Spill} \rho X_i}{I_w \pi R_0^2 \phi_{r0} SOL} \qquad \textbf{(3-3)}$$

where I_w = infiltration rate of uncontaminated water,

X_i = mass fraction of constituent *i* in the LNAPL, and

ρ = density of the LNAPL

Δt = time to dissolve LNAPL (source duration)

Infiltration rates are dependent on many different weather, ground cover, and soil conditions (EPA 1998). The Green-Ampt theory (Green and Ampt 1911) assumes that for long-time infiltration events, the rate of infiltration approaches an asymptotic value. For the purpose of this research the asymptotic infiltration rate was simplified and assumed to be equal the recharge rate, or average rainfall. This averages the typical series of infiltration events to a constant velocity and most likely overestimates the downward flux at a site. For shallow water tables less than about 5 feet, this assumption would not be accurate (Tomasko et al. 2001), but in these cases the initial spill would likely reach the shallow water surface and infiltration rates would not be needed to calculate the maximum concentration at the water table. For larger distances I believe this is a reasonable, though conservative, assumption, predicting greater transport rates than actually occur.

The governing one-dimensional partial differential equation for transport of an LNAPL component through a homogeneous, isotropic, porous medium with advection, dispersion, volatilization, and biological degradation is given by the following equation (Jury et al. 1983, 1990):

$$\frac{\partial C}{\partial t} = \frac{D}{R}\frac{\partial^2 C}{\partial z^2} - \frac{V}{R}\frac{\partial C}{\partial z} - \lambda C \qquad \textbf{(3-4)}$$

where C = concentration of the LNAPL component (all phases present),

D = diffusion/dispersion coefficient,

R = effective retardation coefficient,

t = time,

V = volumetric soil water flux,

z = vertical distance, and

λ = first-order rate constant for biological degradation.

The effective diffusion/dispersion coefficient, D, is given as

$$D = D_l + D_g \quad \textbf{(3-5)}$$

where D_g is the gaseous diffusion coefficient. The liquid diffusion/dispersion coefficient, D_l, is assumed to be advection dominated and scale dependent and can be estimated as

$$D_l = \alpha_l V \quad \textbf{(3-6)}$$

where the dispersivity, α_l, is given as (Lallemand-Barres and Peaudecerf 1978)

$$\alpha_l = 0.1L \quad \textbf{(3-7)}$$

and L is the distance from the point of dissolution to the water table.

The effective retardation coefficient, R, can be estimated by the following equation (Jury et al. 1990):

$$R = \rho_b K_d + \phi_w + aK_h \quad \textbf{(3-8)}$$

where ρ_b = bulk density of the porous medium,

K_d = distribution coefficient of the LNAPL component,

ϕ_w = water-filled porosity of the porous medium,

a = air-filled porosity of the porous medium,

K_h = dimensionless value of Henry's constant.

The first-order rate constant, λ, is related to the half-life of the LNAPL component by the equation:

$$\lambda = \ln(2) / \tau_{1/2} \qquad \textbf{(3-9)}$$

where $\tau_{1/2}$ is the LNAPL component effective half-life.

For the scenario of an LNAPL spill in the vadose zone the boundary conditions used to solve Equation 3-4 are: (1) as the depth to the water table becomes very large (z = ∞), the concentration of the LNAPL component goes to zero; and (2) at the bottom of the LNAPL smear (z = 0), the concentration of the LNAPL component behaves as a step function (Hildebrand 1976) with a duration equal to the time required to dissolve all the LNAPL present:

$$\frac{C(z=0,t)}{C(z=0,t=0)} = \begin{cases} 1.0 \ \textit{for} \ 0 \le t \le \Delta t \\ 0.0 \ \textit{for} \ t \ge \Delta t \end{cases} \qquad \textbf{(3-10)}$$

For this model, the initial concentration at the bottom of the LNAPL spill is given by Equation 3-2. The concentration of the LNAPL may be less than this value due to diffusion and heterogeneous field conditions (Mercer and Cohen 1990), but Equation 3-2

provides a conservative estimate of contaminant concentrations which is useful for screening level risk estimates.

The solution to Equation 3-4 for the specified boundary conditions was obtained by Tomasko et al. (2001) using a Laplace transform methodology (Ditkin and Prudikov 1967). In closed form the solution is expressed as:

$$\begin{aligned}\frac{C}{C_0} = {} & \frac{e^{\frac{VZ}{2D}}}{2}\left\{ e^{-\sqrt{\frac{Z^2}{D}\left(\frac{V^2}{4D}+\lambda\right)}}\, erfc\left[\frac{1}{2}\sqrt{\frac{RZ^2}{Dt}} - \sqrt{\left(\frac{V^2}{4DR}+\frac{\lambda}{R}\right)t}\right]\right. \\ & \left. + e^{\sqrt{\frac{Z^2}{D}\left(\frac{V^2}{4D}+\lambda\right)}}\, erfc\left(\frac{1}{2}\sqrt{\frac{RZ^2}{Dt}} + \sqrt{\left(\frac{V^2}{4DR}+\frac{\lambda}{r}\right)t}\right)\right\} \\ & - \frac{e^{\frac{VZ}{2D}}}{2} H(t-\Delta t)\left\{ e^{-\sqrt{\frac{Z^2}{D}\left(\frac{V^2}{4D}+\lambda\right)}}\, erfc\left[\frac{1}{2}\sqrt{\frac{RZ^2}{Dt}} - \sqrt{\left(\frac{V^2}{4DR}+\frac{\lambda}{R}\right)(t-\Delta t)}\right]\right. \\ & \left. + e^{\sqrt{\frac{Z^2}{D}\left(\frac{V^2}{4D}+\lambda\right)}}\, erfc\left(\frac{1}{2}\sqrt{\frac{RZ^2}{Dt}} + \sqrt{\left(\frac{V^2}{4DR}+\frac{\lambda}{r}\right)(t-\Delta t)}\right)\right\}\end{aligned} \quad \textbf{(3-11)}$$

where *H* is the Heaviside function (Hildebrand 1976), with

$$H(t-\Delta t) = 0 \ \textit{for}\ t < \Delta t \quad \textbf{(3-12)}$$

$$H(t-\Delta t) = 1 \ \textit{for}\ t \geq \Delta t$$

Equation 3-11 can be used to estimate the concentration of LNAPL as a function of time and space in the vadose zone beneath the spill site. This solution is valid for the region between the bottom of the spill and the water table. For the purpose of this

research it was used to determine the maximum concentration that would occur at the water table. This value is a good index to the risk posed by a spill (Tomasko et al. 2001).

The complete model used in this research has several steps and two branches (Tomasko et al. 2001). Both branches start with a spill and an estimated depth of infiltration. Then if H is greater than z, the depth to the water table, then the concentration is equal to the solubility multiplied by the mole fraction of the component (Equation 3-2) and is branch one. If the spill does not reach the water table, Equation 3-11 is used to estimate the concentration at the water table and is branch two. These values are then used to determine the maximum concentration.

3.2 Uncertainty

As discussed in Section 2, uncertainty can come from measurement or estimation error and from variations in time and space. For this study, the uncertainty of a parameter was taken to be the range of possible values for the parameter at the site. I assumed that this range is large enough to include the effects of measurement errors.

To compare parameters with widely different magnitudes, I normalized the range of each parameter by dividing by a determined base-case value of the parameter. The base-case value was the best estimate of the parameter value. Calculating relative ranges for parameters cancels out the units leaving dimensionless values. This makes it possible to compare the range of hydraulic conductivity to the range of water depth even though they are expressed in different units. This is useful since with typically used units the entire range of conductivity would not even be measurable at the magnitude of water table depth values.

The relative range was calculated using the following equation:

$$N_i = \frac{R_i}{\xi_{i,b}} \quad \textbf{(3-13)}$$

where N_i = relative range of parameter i (dimensionless),

R_i = expected range of parameter i,

$\xi_{i,b}$ = base-case value of parameter i.

3.3 Sensitivity

Differential analysis was used to determine the sensitivity of the model to a given parameter. Under differential analysis, sensitivity is defined as the derivative of an objective function with respect to the parameter. The objective function used in this research was the maximum concentration of benzene at the groundwater table calculated for all time, not just the estimated benzene concentration at a given time. To normalize sensitivity, the derivative was multiplied by the ratio of the base-case value of the parameter to the value of the objective function taken at the base-case value. The equation for normalized sensitivity is:

$$S_i = \frac{\xi_{i,b}}{F_b}\frac{\partial F}{\partial \xi_i} \quad \textbf{(3-14)}$$

where S_i =normalized sensitivity of parameter i,

F_b = objective function at base-case.

The sign of the normalized sensitivity indicates the effect of the input parameter on the output. Positive sensitivity shows that an increase in the input value will increase the output value, while a negative sensitivity shows that an increase in the input value will decrease the output value.

3.4 Importance

To combine uncertainty and sensitivity into a dimensionless gauge of importance (I_i), the absolute value of the product of the relative range and normalized sensitivity is taken:

$$I_i = \left|N_i S_i\right| = \left|\frac{R_i}{\xi_{i,b}} \frac{\xi_{i,b}}{F_b} \frac{\partial F}{\partial \xi_i}\right| = \left|\frac{R_i}{F_b} \frac{\partial F}{\partial \xi_i}\right| \quad \textbf{(3-15)}$$

Applied to the RBCA method for cleaning up spills as discussed in the introduction, this value could make Tier 2 evaluations more efficient. Larger values of I_i would indicate where efforts to better estimate parameters would have the most effect on providing a more accurate risk assessment and indicate where resources should be focused. It would also indicate parameters that, while sensitive, would not increase model accuracy through additional measurement, since there is little uncertainty in the values.

3.5 Computer Analysis

Matlab version 6.5 by The MathWorks, Inc. was used to implement the LNAPL transport model. The Matlab language was designed for technical computing problems, especially problems with matrix and vector formulations (Matlab 2002). The code used in this research is presented in Appendix B.

Using Equation 3-11, a Matlab function was written to calculate the maximum concentration of benzene at the water table by looping through time steps and calculating the concentration of benzene at the water table at each time step. The maximum concentration was then found using a modified Newton's method to a specified degree of accuracy that could be altered depending on the magnitude of the input parameters varied in the importance assessment.

Matlab functions to calculate the importance of selected input parameters were written using Equations 3-13, 3-14, and 3-15. The partial derivative of the objective function was approximated using numerical differentiation in the following form:

$$\frac{\partial(C/C_0)}{\partial \xi_i} \cong \frac{(C/C_0)_{j+1} - (C/C_0)_j}{\xi_{i,j+1} - \xi_{i,j}} \qquad \textbf{(3-16)}$$

where $\xi_{i,j} < \xi_{i,b} < \xi_{i,j+1}$

Driver programs were written to use the functions described above to determine the maximum concentration of LNAPLs and the importance of the chosen input parameters over their respective ranges. With one-at-a-time analysis only one parameter was allowed to vary at a time. To better show parameter interaction, the importance of a

parameter over the entire parameter range was calculated for three different spill volumes and three different depths to the water table. The driver programs produced plots of the maximum concentration, sensitivity, and importance at the different water table depths and spill volumes, for visual comparison.

3.6 Input Parameters

To use Equation 3-11 for estimating LNAPL transport, several input parameters describing the properties of the contaminants, infiltration, the spill, and the soil are required. For the contaminant the aqueous solubility, distribution coefficient (K_d), biodegradation half-life ($\tau_{1/2}$) or first-order rate constant (λ), Henry's dimensionless constant, gaseous diffusion coefficient, mole fraction or mass fraction of LNAPL components, and overall contaminant density were required. Since this study was based on the transport of benzene, the above properties were needed for benzene only. Most of the benzene properties were found in a review of the literature (Howard et al. 1991, Lyman et al. 1992).

The infiltration, spill, and soil data used for input were obtained from Tomasko et al. (2001) who used an IRP database established from field data from more than 100 Air Force sites in Hawaii (Tomasko et al. 1997). Data for average precipitation, residual oil fraction, bulk density, water-filled porosity, air-filled porosity, the depth to the water table, spill volume, and spill radius were needed and also obtained from the Tomasko et al. (2001) paper.

While all of the input parameters have a possible range that could contribute to uncertainty, some parameter ranges were considered insignificant for the importance

assessment. These parameter ranges were either too small or limited by other parameters to have an effect on the model output when compared to the large variability of the other parameters. The benzene density, solubility, Henry's constant, gaseous diffusion, and mole/mass fraction were considered to have a small enough range to be insignificant and thus were not varied for this study. Soil air, water, and residual oil fractions and the soil bulk density are all limited by porosity with ranges considered insignificant. The half-life and distribution coefficient of benzene showed large ranges in the literature. Tomasko et al. (2001) reported that the IRP database showed large ranges in precipitation, depth to water table, and spill volume.

Therefore, this study considers the range of the following parameters: benzene biodegradation half-life, the benzene distribution coefficient, precipitation, depth to water table, and spill volumes in the assessment of importance. To show parameter interaction, importance was calculated at three different depths to the water table and three different spill volumes. The depths to the water table were the base-case value (7.5 m) and two other depths representative of the range (15 m and 30 m). The spill volumes represented a small spill (28 m^3), the median spill volume for the IRP sites (75 m^3), and a large spill (115 m^3) that is big but small enough to not reach the water table initially when the other parameters are set at their base-case values. All of the parameter base-case values and ranges used in the analysis of the Tomasko model are presented in Appendix A.

4 Results

Five input parameters were involved in the importance assessment including the distribution coefficient, the half-life of benzene, precipitation, the depth to the water table, and the spill volume. The importance assessment was conducted by the one-at-a-time method, so first the importance of each individual parameter will be discussed. By linking uncertainty and sensitivity to importance, identification of the parameters having the most influence on model output is more efficient. Traditionally sensitivity analysis is used in risk assessments, so the parameter importance will be compared to parameter sensitivity to illustrate the increased accuracy of importance analysis. The model is sensitive to variation in each parameter and also to interaction between the parameters. Therefore the interaction of the parameters will also be discussed.

4.1 Distribution Coefficient Importance

Figure 4-1shows the change in maximum concentration of benzene at the water table as a function of the distribution coefficient (K_d). All other parameters are held constant at their respective base-case values. Plotted with the maximum concentration is the derivative of the maximum concentration with respect to K_d, which is the non-normalized sensitivity of the model to K_d. Figure 4-1 shows that the steepest change in maximum concentration for the base-case values occurs for large K_d values, indicating

that the transport model is most sensitive to changes in K_d at the upper end of its range and all other parameters are at their base-case values.

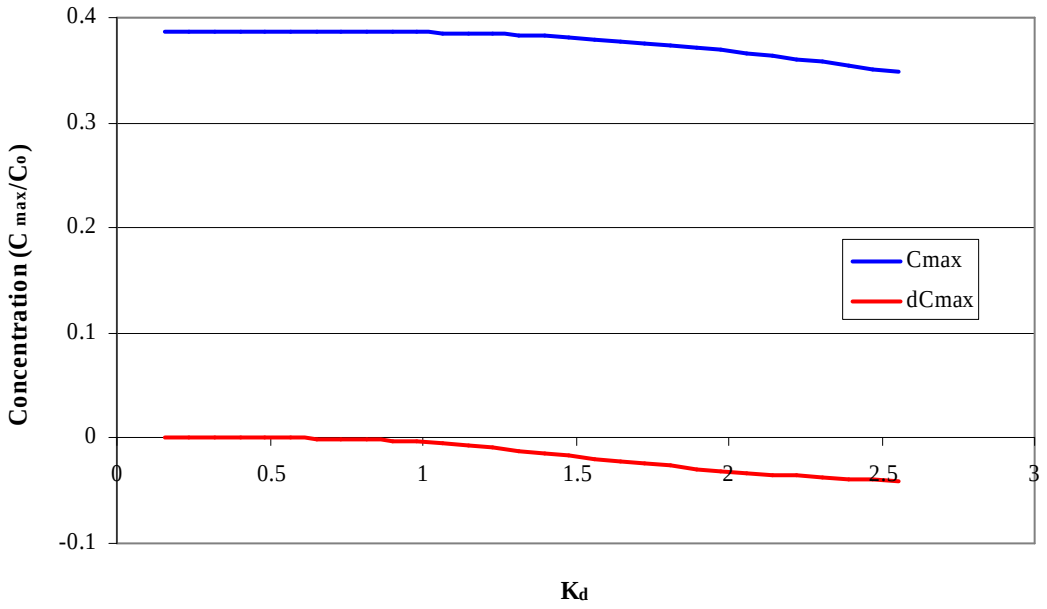

Figure 4-1: Maximum Benzene Concentration Based on K_d

Figure 4-2 shows the importance of K_d for three different spill volumes. The plots show that as spill volumes become small, small K_d values become more important to model outcome. Meaning that if the spill volume is small and the benzene does not partition well to the soil, then inaccuracies in measuring partitioning will significantly affect the model results.

Figure 4-3 shows the importance of K_d for three different depths to the water table. As the depth to the water table increases, again, small values of K_d become more important. These trends suggest that as the distance contaminants must travel through the vadose zone increases, small K_d values become more important.

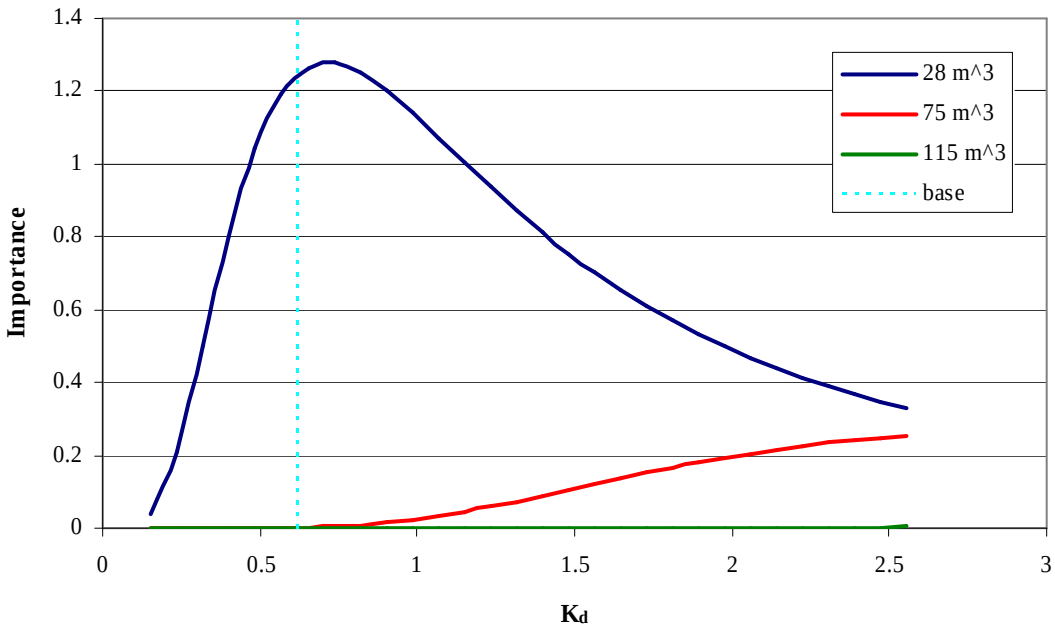

Figure 4-2: K_d Importance for Spill Volumes

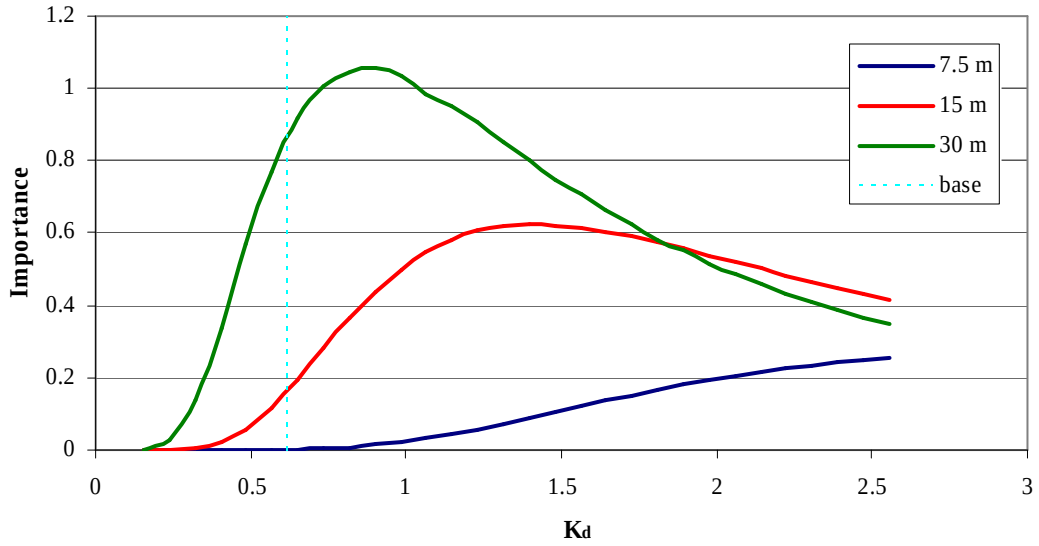

Figure 4-3: K_d Importance at Water Table Depths

At the input parameter values tested, the greatest importance of K_d was a value of 1.28. With the input parameters at their base-case values, the greatest importance K_d reached was 0.25. With all input parameters, including K_d, at their base-case values K_d importance was 0.0015. The graphs clearly show that the importance of Kd changes significantly over the parameter space presented.

4.2 Half-Life Importance

Figure 4-4 shows the importance of half-life on model output for three different spill volumes. For longer half-life values, small spill volumes create more half-life importance, while half-life is most important for large spills and a short half-life.

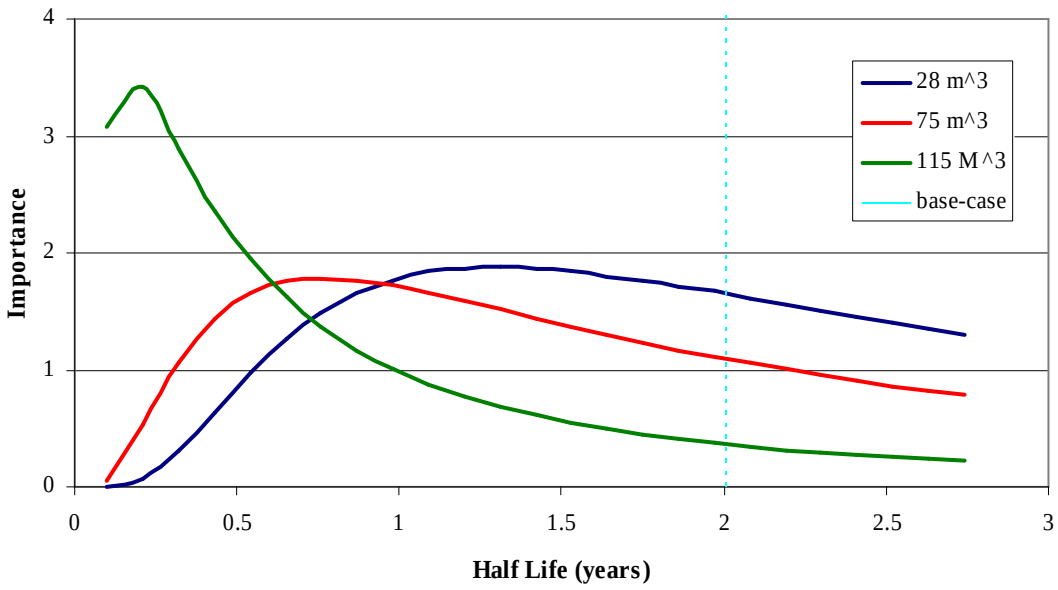

Figure 4-4: Half-Life Importance for Spill Volumes

Figure 4-5 shows the importance of half-life at three different depths to the water table. At shallow depths short half-lives are more important. Half-life becomes most important when it reaches its maximum length of time and the water table is deep. These plots suggest that short half-lives are important when the contaminant travel distance is small, and long half-lives are important when the contaminant travel distance is large.

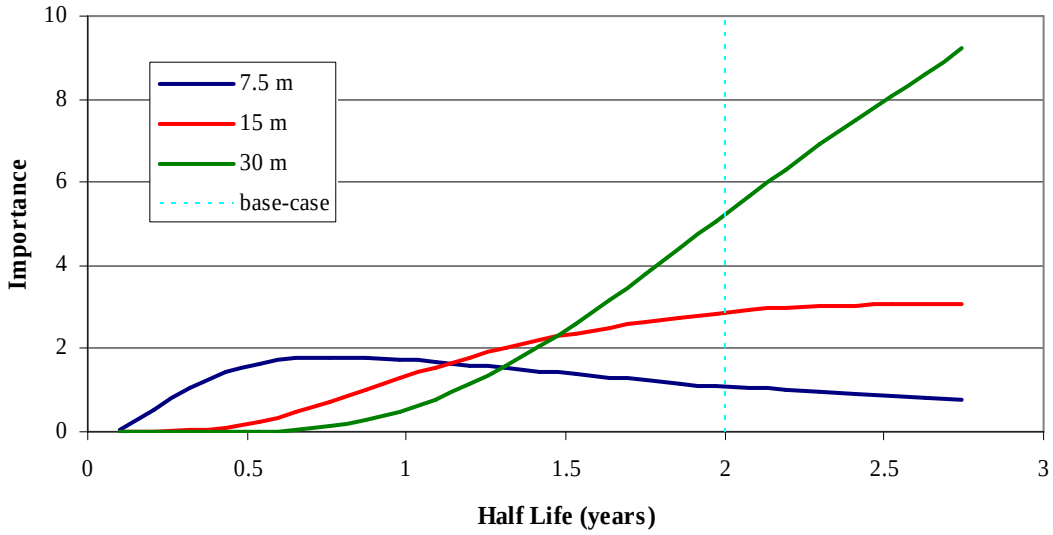

Figure 4-5: Half-Life Importance at Water Table Depths

The largest half-life importance measured was 9.2. The largest importance with the other parameters at their base-case values was 1.79. Half-life importance at its base-case value was 1.10.

4.3 Precipitation Importance

Figure 4-6 shows the importance of precipitation on model output for three different spill volumes. Over the full range of precipitation it is shown that precipitation importance increases with decreasing spill volume.

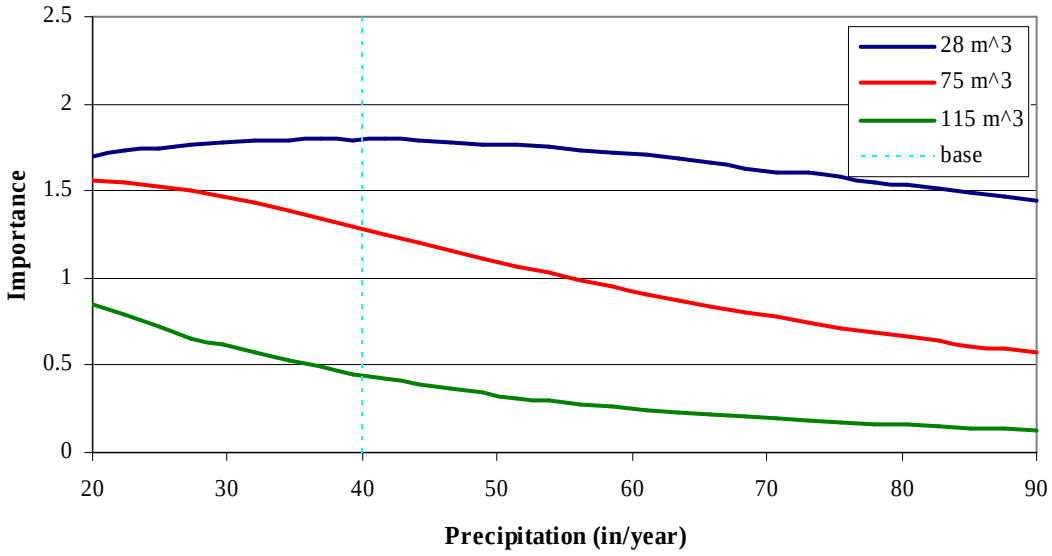

Figure 4-6: Precipitation Importance for Spill Volumes

Figure 4-7 shows the importance of precipitation at three different depths to the water table. For small amounts of precipitation the depth to the water table has little effect on importance. As precipitation increases, increasing the depth to water makes precipitation much more important. These plots suggest that precipitation is more important when contaminants must travel further, particularly when there is a lot of precipitation.

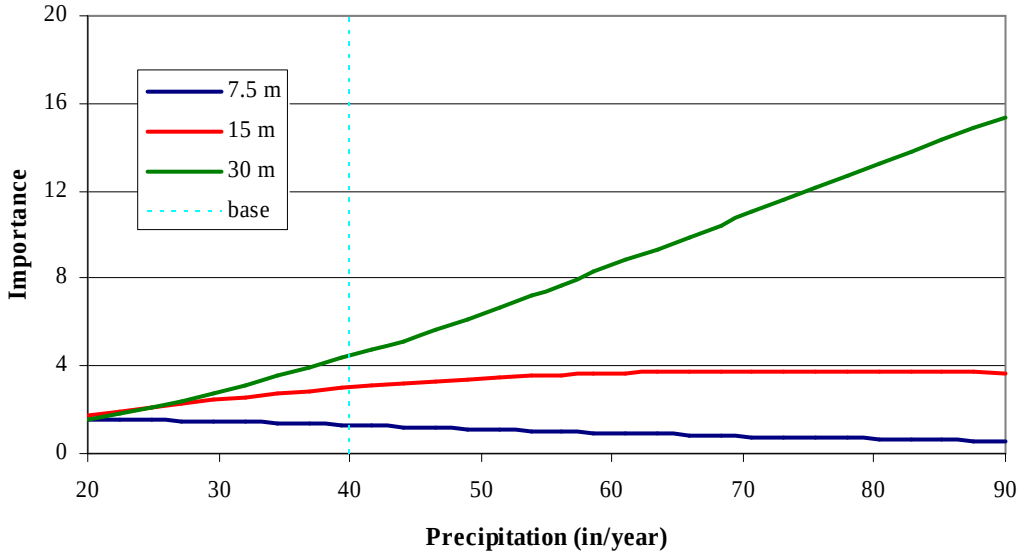

Figure 4-7: Precipitation Importance at Water Table Depths

The largest precipitation importance measured was 15.3. The largest precipitation importance with the other parameters at their base-case values was 1.56. Precipitation importance at its base-case value was 1.28.

4.4 Water Table Depth Importance

Figure 4-8 shows the importance of water table depth for three different spill volumes. No matter what the spill volume, the water depth becomes relatively unimportant at about 20 meters deep. This could significantly affect data measurements for Tier 2 risk assessments at these specific sites. The water depth importance peaks at the transition from the advection/dispersion model to the slug model (LNAPL pancake on the water table). As spill volumes decease, the importance at the transition peaks dramatically. It is so dramatic that an importance of 77.3 was measured. At base-case

inputs, the water depth importance peaked at 40.2 and the water depth importance at its base-case value was 14.8.

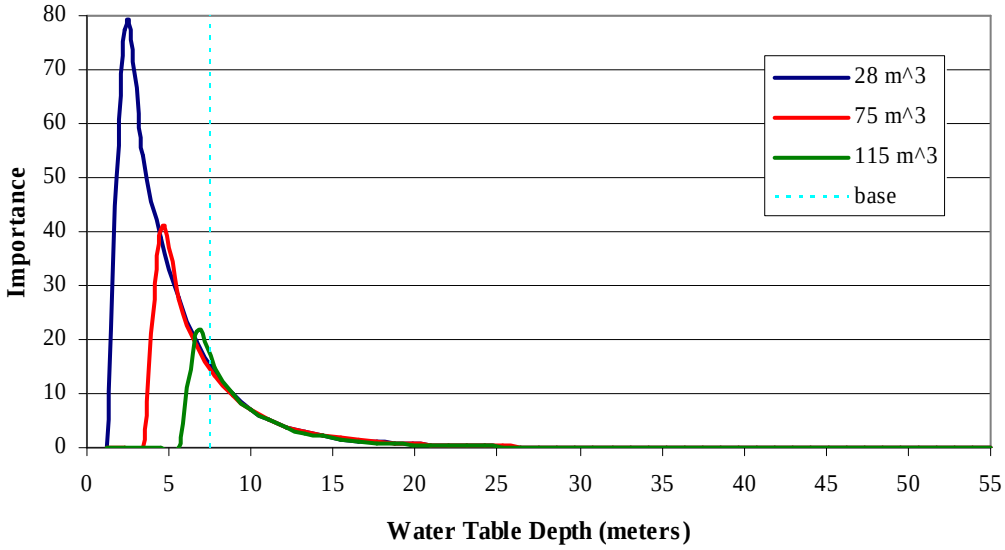

Figure 4-8: Water Table Depth Importance for Spill Volumes

4.5 Volume Importance

Figure 4-9 shows the importance of the spill volume at three different water table depths. Similar to the water depth importance, the spill volume importance peaks at the transition from the advection/dispersion model to the contaminant slug model. But opposite to water depth importance, as the water depth increases the spill volume importance peaks dramatically, although the two larger peaks at transition are off the plot in Figure 4-9. At base-case values the spill volume importance peaked at 11.7. At its own base-case value spill volume importance was 3.93. For the cases tested, spill volume maintained an importance greater than 2.6.

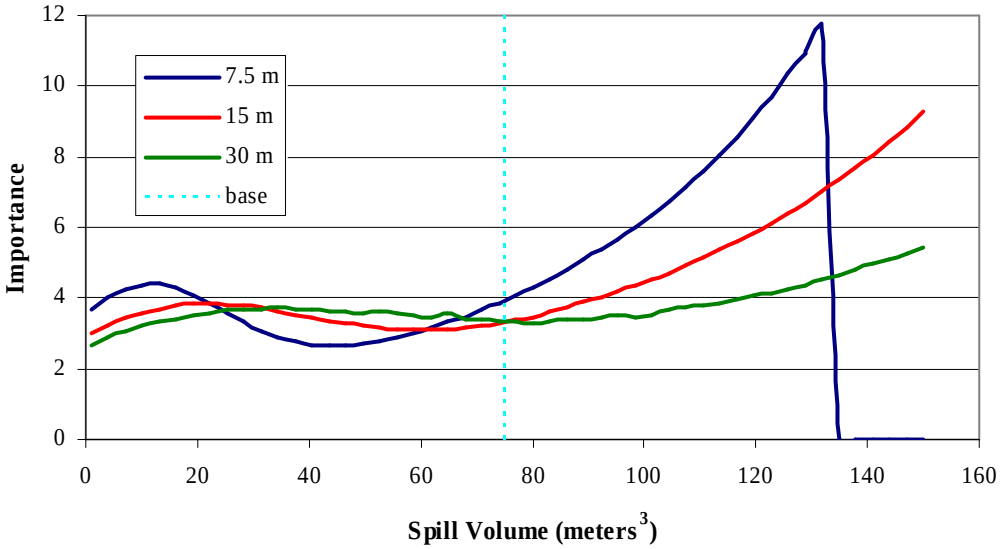

Figure 4-9: Spill Volume Importance at Water Table Depths

4.6 Parameter Importance and Sensitivity

Sensitivity analysis identifies the input parameters that, when varied, affect the model output the most. This does not account for the amount an input parameter could vary due to its uncertainty. Importance analysis includes the range of the input parameters in the analysis. Figure 4-10 shows the importance of each parameter at varying water table depths compared to the sensitivity of each parameter at the same water table depths. All parameters, except water table depth, are held at their base-case values. Figure 4-10 shows that the highest importance value is obtained by water table depth. The most sensitive parameter in Figure 4-10 is half-life. The small range of possible half-life values keeps it from varying the output as much as water table depth with its large range.

Figure 4-11 is a close up view of the plots in Figure 4-10 showing the range from a water table depth of five to twenty meters. It can be seen that water table depth is the

most important to a depth of 13 meters, while it is the most sensitive only to a depth of 9 meters. Spill volume is the most important from 13 to 16 meters, while it is never the most sensitive. Half-life is the most sensitive parameter over a water table depth of 9 meters, while it is not the most important until water table depths greater than 19 meters.

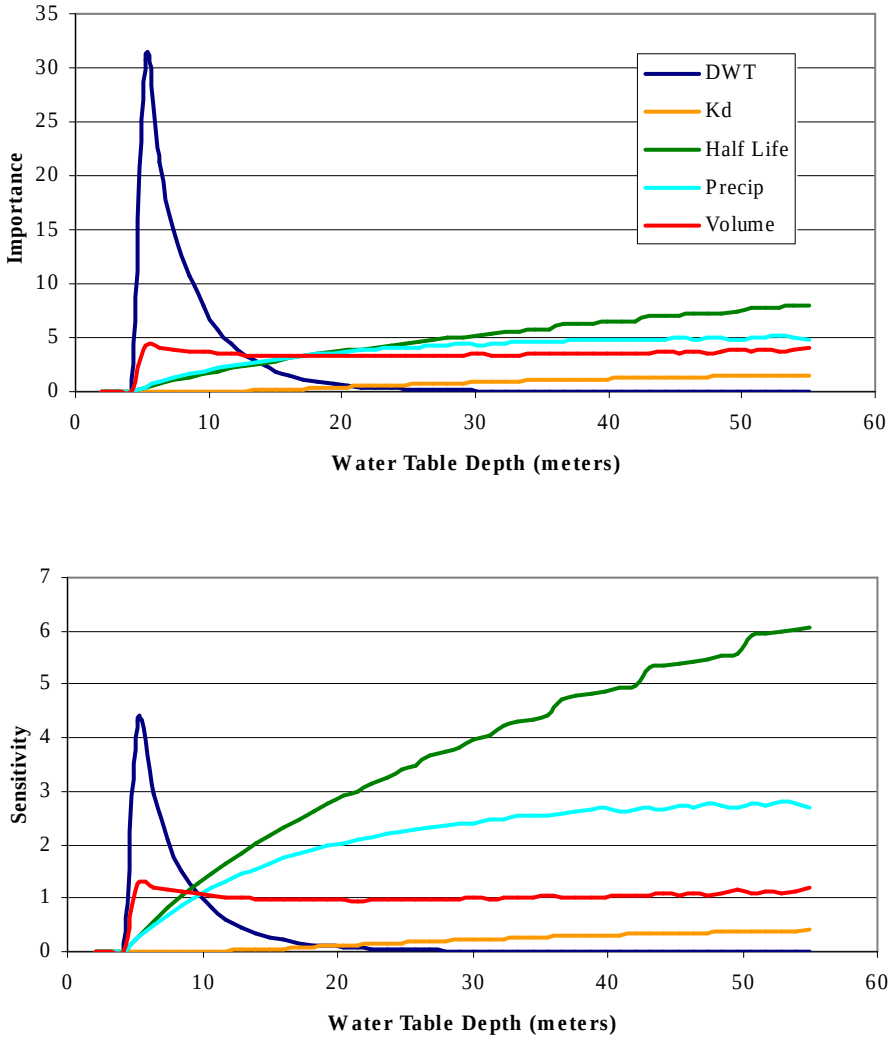

Figure 4-10: Parameter Importance and Sensitivity With Respect to Water Table Depth

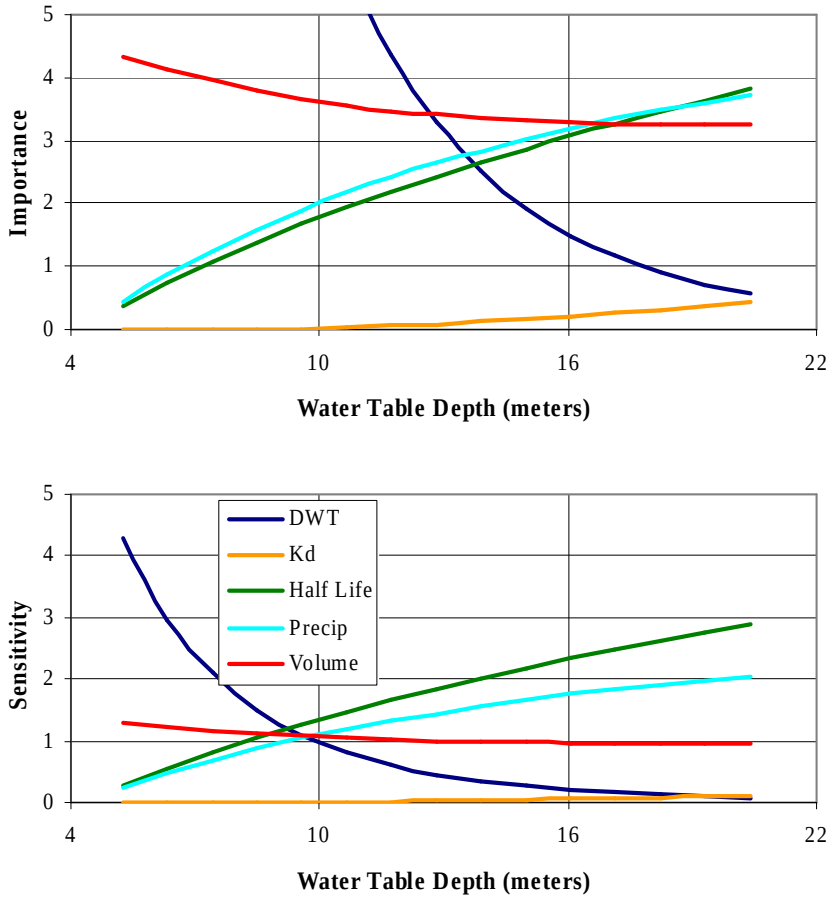

Figure 4-11: Small Scale View of Figure 10

Figure 4-12 shows the importance compared to the sensitivity of each parameter at varying spill volumes. The sensitivity of the parameters at each spill volume are all similar to each other. However, the importance of the parameters shows distinct differences, identifying water table depth as the most important and then spill volume the next most important with the parameters at their base-case values.

There are no points over the range of spill volumes in which the order of parameter importance matches parameter sensitivity. Only for spill volumes from 65 cubic meters to 110 cubic meters are the parameter importance and sensitivity orders

similar, when half-life and precipitation are near equal for both importance and sensitivity.

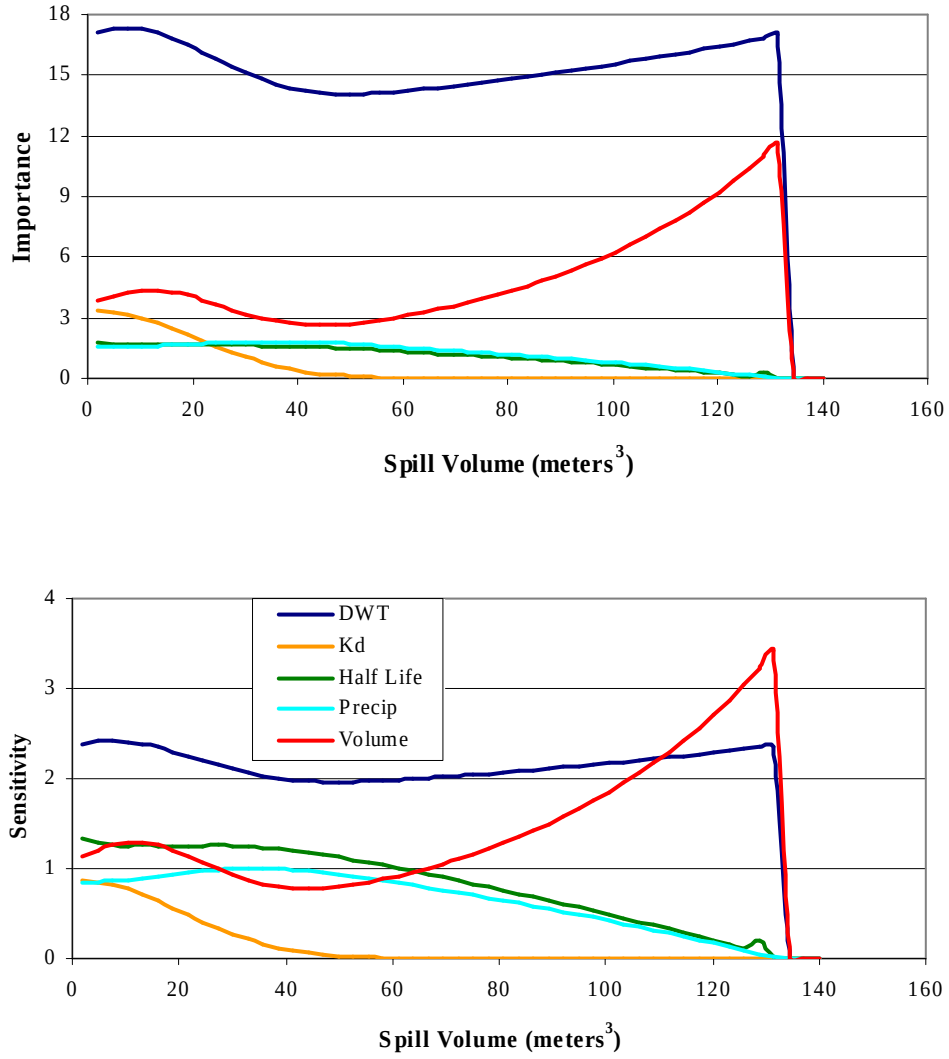

Figure 4-12: Parameter Importance and Sensitivity With Respect to Spill Volume

4.7 Parameter Interaction

Figure 4-13 contains the importance plots of all the varied input parameters (water table depth, partitioning coefficient, half-life, precipitation, and spill volume) over the range of water table depth. All of the parameters are held at their base-case value except the parameter on the abscissa, water table depth. The plot shows that the water table depth becomes insignificant at about 20 meters as in Figure 4-8. Water depth importance is approximately equal to the other parameters at about 13 meters.

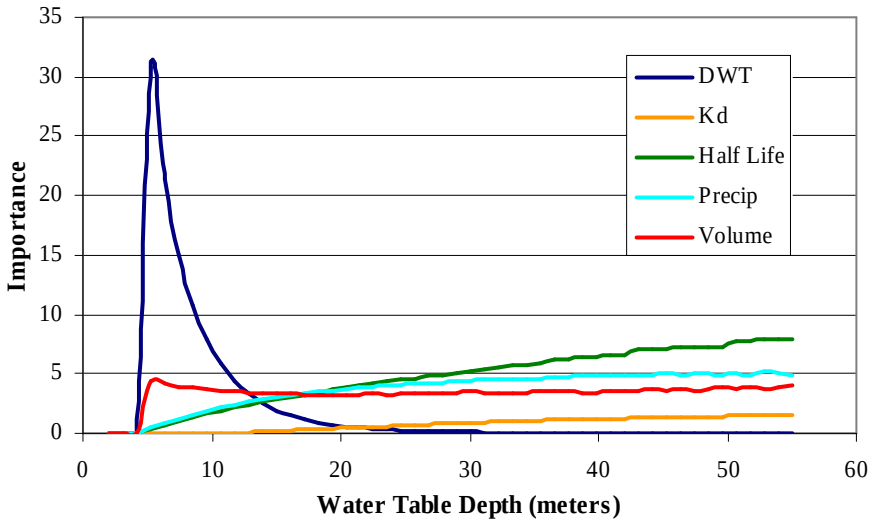

Figure 4-13: Parameter Importance With Respect to Water Table Depth

Like Figure 4-13, Figure 4-14 shows the importance of each parameter, but over the range of spill volumes. The plot on the left is with all the parameters at their base-case values. The plot on the right has water table depth set at 13 meters, the approximate intersection of water table depth importance to the importance of the other parameters in Figure 4-13. By increasing the water table depth to 13 meters, water table depth has very

similar importance to precipitation and half-life. At 13 meters, water table depth maintains an importance of about three, while at the base-case depth of 7.5 meters, its importance ranges from 14 to 17.

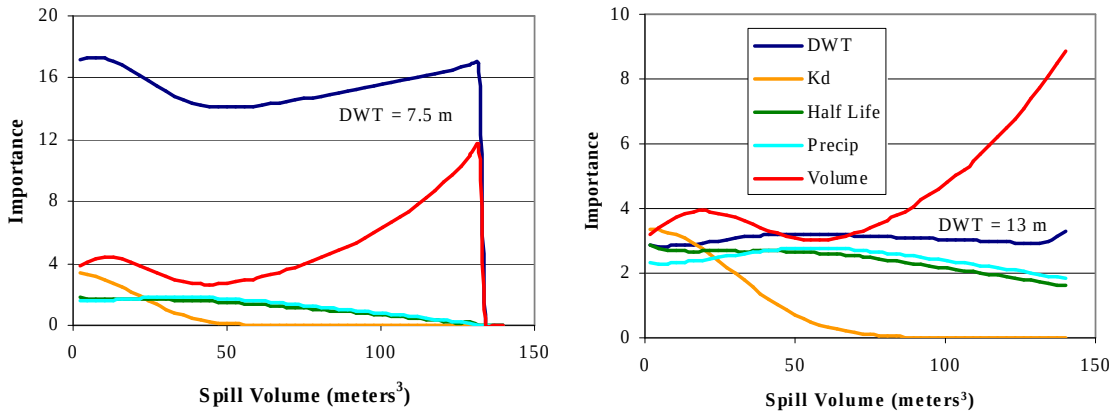

Figure 4-14: Parameter Importance With Respect to Spill Volume

Figure 4-15 is a plot of each parameter's importance over the range of precipitation. The plot on the left is at base-case values, while the plot on the right has water table depth set to 13 meters. At 13 meters, again, water table depth has importance similar to precipitation, with values ranging from 2.5 to 3.5. At 7.5 meters, water table depth importance ranges from 8 to 21.

Figure 4-16 shows parameter importance over the range of the distribution coefficient at base-case values and with water table depth set to 13 meters. By increasing the water table depth from 7.5 to 13 meters, water table depth importance changes from an increasing trend from 15 to 18, to a relatively flat trend at about 3, again very similar to precipitation and half-life.

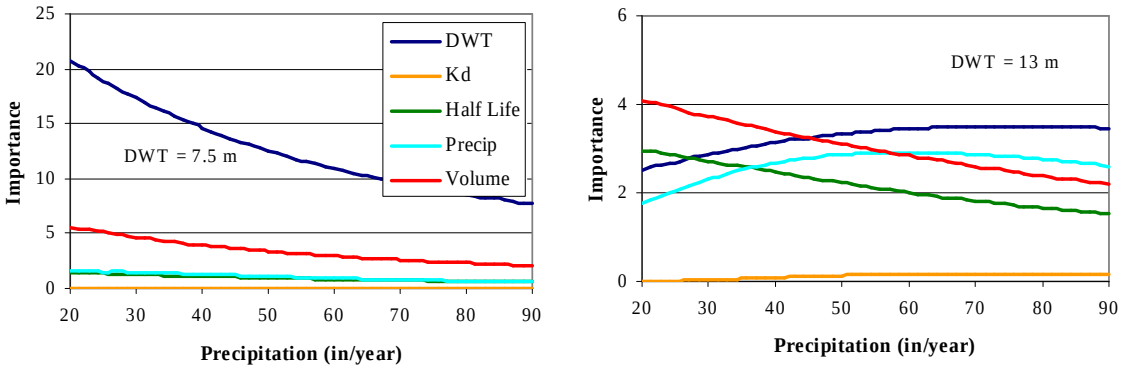

Figure 4-15: Parameter Importance With Respect to Precipitation

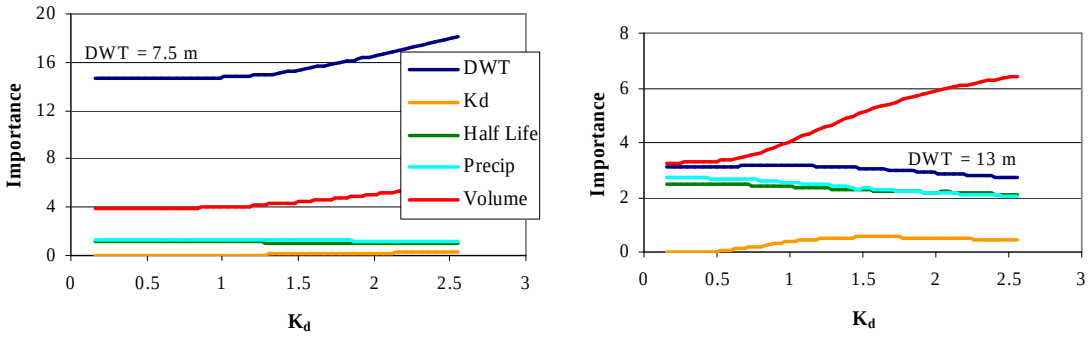

Figure 4-16: Parameter Importance With Respect to the Distribution Coefficient

Figure 4-17 shows parameter importance over the range of half-lives at base-case values and with water table depth set to 13 meters. Changing the water table depth completely alters its trend of extremely high importance at short half-lives to no importance at short half-lives. Again, water table depth importance changes from having a significant range of variation up to a high importance, to having similarly low importance to half-life.

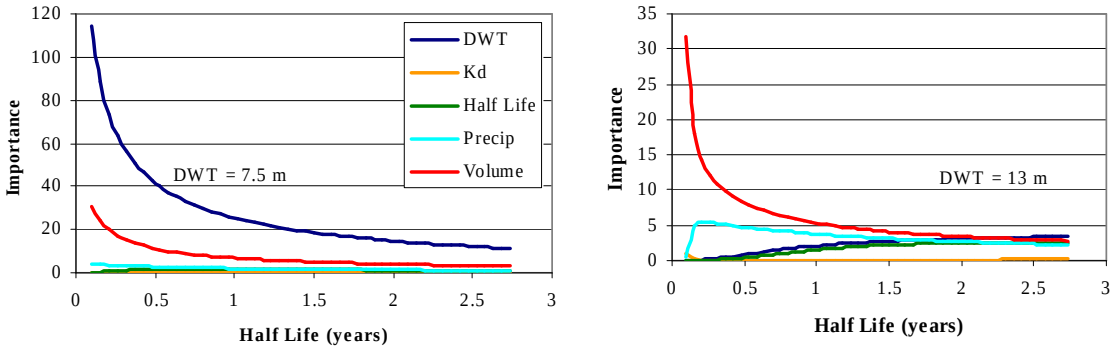

Figure 4-17: Parameter Importance With Respect to Half-Life

In Figure 4-14 through Figure 4-17 it can be seen that at base-case values, water table depth is most important over the range of all the other parameters. By setting water table depth to 13 meters, which is approximately when water table depth has equal importance to the other parameters in Figure 4-13, its importance is now very near that of the other parameters.

5 Discussion of Results

Based on the numbers obtained through the one-at-a-time analysis, the depth to the water table was identified as the most important parameter for estimating the maximum concentration of benzene at the water table. Near the parameter's base-case values, water depth is the most important and will likely be one of the most important parameters whenever the water table is less than 13 meters deep.

There are circumstances in which other parameters will become more important. If the water table is deep and the half life is expected to be long, it would likely be important to know the half-life accurately. Also if the water table is deep, and the precipitation is large, precipitation will likely have a considerable effect on results. Although, for a risk assessment, if the water table is very deep the maximum concentration at the water table could be small – below the risk assessment standards or at least low enough to result in a lower priority than other sites.

Over the ranges studied, the partitioning coefficient importance was always low compared to the other parameters. No circumstances were identified in which the partitioning coefficient would have a high importance. The small range for the partitioning coefficient does not allow this input to make large changes in the model output, even though the model is sensitive to these values.

It was shown that when the spill volume is high and when the depth to the water table is small, both are significantly important when the advection/dispersion model is still valid. These circumstances would create conditions that could have considerable risk, allowing high concentrations of contaminants to reach the ground water. This is a positive result since the water table depth can be measured accurately, directly from observation wells, while precipitation is a conservative estimate of infiltration, half-life depends on exposure to oxygen and microbes and must be estimated, and the partitioning coefficient can change with varying soil conditions.

It has been shown that sensitivity analysis results can be dependent on the base-case values used (Ferreira et al. 1995). This study is a good example of that. By determining the base-case water table depth to be 7.5 meters, water table depth was calculated to clearly be the most important. If the base case for water table depth was chosen at just 20 meters, very much within the potential range, it would have minimal importance. Graphing the importance of each parameter over its range is useful in identifying if altering its base case value would have an effect on its importance.

As stated in Section 2.3, an input parameter that is important to model outcome is one with uncertainty and also is sensitive. The importance analysis presented in this paper made it clear which parameters were sensitive enough, and also could vary enough, to make significant changes in the model output values. Analyzing parameters by their importance gave different results than analysis based only on sensitivity.

At water table depths less than about five meters, when the advection/dispersion model is still valid, the Tomasko model is so sensitive to water table depth input that it is unrealistic to believe that the model precision matches the precision at which the depth

should be measured. Under five meters, a conservative value for depth or the slug model for contaminant transport should be used in risk assessments. The Green-Ampt theory of infiltration approaching an asymptotic value is used in the Tomasko model. As stated earlier, this assumption is not accurate for water tables at less than about 1.5 meters, at which depth the slug model should be used.

This study was specific to Air Force spill sites in Hawaii presented by Tomasko et al. (2001). All of the soil and spill data for input are obtained from this paper which cited a database about these sites. The conditions in Hawaii do not represent typical LNAPL spill sites. Therefore the results from this study are only valid for the analysis of spills at this IRP site. Model users have been cautioned not to use sensitivity results that were conducted under conditions other than those being simulated (Ferreira et al. 1995). However, the method developed in this study should be used at other spill sites, using site specific values and parameters from those sites.

The objective of my research was to develop a method to quantify the importance of an analytical model for vadose zone transport. The Matlab computer code was developed so that the input parameters needed for the model could be input from any spill site. Site specific data input to the code would give the importance of the partitioning coefficient, contaminant half-life, precipitation, water table depth, and spill volume based off the current knowledge of that site.

6 Conclusion

A general method for determining parameter importance has been presented in this thesis. It has been developed so it can benefit any mathematical model, even outside the discipline of engineering. To illustrate the use of importance analysis, it has been applied to the Tomasko vadose zone transport model with data from IRP sites in Hawaii.

The USEPA has encouraged using RBCA programs to clean up petroleum spills to make the process more efficient. For IRP sites in Hawaii that do not pass the first tier of the ASTM procedure, the Tomasko vadose zone transport model could be used in the second tier assessment. In gathering data to be used in the model, the most important parameters to accurately measure have been identified.

The importance analysis of the input parameters to the Tomasko vadose zone transport model was specifically performed for the partitioning coefficient, benzene half-life, precipitation, water table depth, and spill volume. At the base case values it was determined that the water table depth was significantly more important than the other parameters analyzed. Although at water table depths greater than 13 meters its accuracy becomes no more important than the other parameters. The spill volume was found to have the second most importance, but could be attributed to the large range of spill volumes found in the input data. In specific cases precipitation and half-life could be the

most important parameters. In the view of risk analysis, the water table depth and spill volume were most important in conditions that allow high risk.

While the results from this study are useful in determining where to focus efforts at IRP sites in Hawaii, they cannot be counted on for other LNAPL spill sites. If the Tomasko model is used as part of the risk assessment at other spill sites, the code developed in this study can be used with the input parameters updated.

The method used in this research to determine the importance of each parameter is relatively simple and could easily be applied to other mathematical models involving results that are numerically differentiable. The differentiable results would be input as the objective function, and model parameters to be included in the importance analysis would need to be chosen, with their expected range and base-case values. With the technology and computing power now available, there is no reason to not to include importance analysis in risk assessments. Many regulatory agencies are requiring that uncertainty analysis be included as part of risk assessment (Linkov and Burmistrov 2003). The method presented in this study includes uncertainty analysis with all the benefits of identifying the important parameters.

As shown by Figures 4-11 and 4-12, importance analysis is different than sensitivity analysis. Sensitivity analysis was developed to make mathematical modeling more efficient. It has helped to identify where efforts should be focused to increase the accuracy of models. Importance analysis links sensitivity to parameter uncertainty, identifying which sensitive parameters could realistically cause uncertainty in model output values, and identifies where additional resources should be used to provide better estimates of input parameters. As shown by Figure 4-12, the method of importance

analysis presented in this paper narrowed the number of sensitive parameters down to those that are most important to the model.

RBCA programs are designed to make clean-up processes more efficient. There are other ways to perform sensitivity analyses that have been proven to be more conclusive or accurate than the one-at-a-time differential analysis used in this research. These methods are more computationally intensive. The method of importance analysis described in this study is simple and efficient, meeting the goals of RBCA programs.

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Appendix A. Input Parameters

Table A-1: Base-Case Values and Ranges of the Parameters in the Importance Analysis

Analyzed Parameters	Base-Case Value	Range
Distribution Coefficient (K_d)	0.62 mL/g	0.155 to 2.555 mL/g
Half-Life ($\tau_{1/2}$)	2 years	0.1 to 2.74 years
Precipitation (I_w)	40 in/year	20 to 90 in/year
Spill Volume (VOL)	75 m^3	0 to 255 m^3
Water Table Depth (Z)	7.5 m	1.2 to 55 meters

Table A-2: Constant Input Parameter Values for the Vadose Zone Transport Model

Constant Parameters	Value
Spill Radius (R_0)	7.5 m
Porosity (n)	0.3
Water Filled Porosity (Φ_w)	0.15
Residual Oil Fraction (Φ_{r0})	0.1
Air Void Fraction (a)	0.05
Henry's Constant (K_h)	0.2199
Soil Bulk Density (ρ_b)	1.75 g/cm^3
Gaseous Diffusion Coefficient (D_g)	0.00744 ft^2/day
LNAPL Density (ρ)	0.7457 g/cm^3
Mass Fraction (X_i)	0.03
Mole Fraction (χ_i)	0.0359
Solubility (SOL)	0.001789 g/mL

Appendix B. Matlab Code

B.1 Parameter Setup

```
% Base-case parameter input for importance analysis
%
%
%
% vol = volume of spill, m^3
% dia = dia of spill area/column, m
% n = porosity
% resid = residual NAPL saturation, % (typically about 20%)
% H = depth of NAPL infiltration, m
% K = saturated hydraulic conductivity, meters/year
% Ks = saturated hydraulic conductivity, meters/sec
% n = porosity
% Z = depth to water table, m
% z = vertical coordinate, m
% rho = density of LNAPL
% X = mass fraction of LNAPL
% rain = average annual rainfall, inches/year
% v = velocity/infiltration rate of water
% SOL = solubility of LNAPL
% Dg = gaseous diffusion coefficient, meters^2/year
% Dgf = gaseous diffusion coefficient, ft^2/day
% pb = bulk density of medium
% Kd = distribution coeff. of LNAPL
% phiW = water filled porosity
% a = air filled porosity
% Kh = Henry's constant (dimensionless)
% DWT = depth to water table, meters

global n resid K pb phiW a rain DWT vol dia SOL X rho Dgf Kd Kh thalf

% SOIL
n = .3;     % percent
resid = .333; % percent
Ks=1e-7;     % in m/s
K=Ks*31536000;     % in m/year
pb = 1.75;   % g/cm^3
phiW = .15;
a = .05;
rain = 40;   % rainfall, inches per year
v = rain*0.0254;, if rain*0.0254<=K, else v=K;, end % velocity, m/year
DWT = 7.5;   % meters

% SPILL
```

```
vol = 75;   % meters^3
dia = 15;    % meters
SOL = 0.00178;   % g/mL
X = 0.03;
rho = 0.7457;    % g/cm^3
Dgf = 0.00744;   % ft^2/d
Dg = Dgf*365/(3.28^2);  %meters^2/yr
Kd = 0.62;   %mL/g
Kh = 0.2199;
thalf = 2;    % half-life, year^-1
lamda = log(2)/thalf; % decay coeff
R = ret(pb,Kd,phiW,a,Kh);       % retardation
delTsrc = delT(vol,rho,X,v,dia,resid,SOL);% length of source term, years

H=Spill(vol,dia,n,resid);   % meters
Z=DWT-H;       % depth to water table, meters
D = (0.1*Z)+Dg;   % Dispersivity, 0.1 times transport length
```

B.2 Distribution Coefficient

B.2.1 Driver

```
% Driver to plot the distribution coefficient importance over the range
% of the distribution coefficient at selected spill volume sizes and
% water table depths.  Determines the relative range, normalized
% sensitivity, and importance at base-case values.

clear
Parameters;
num=30;     % number of steps in depth to water table range
maxD=2.555;    % maximum range for depth to water table
minD=0.155;   % minimum range for depth to water table
d=0.00000001;  % difference for numerical differentiation
BCi=.62;    % base case value
Ri=2.4;    % range of values

vol=28;
[Cmax,dCmax,S,I,Kd]=ikd(vol,DWT,num,maxD,minD,d,BCi,Ri);
I1=I;


vol=75;
[Cmax,dCmax,S,I,Kd]=ikd(vol,DWT,num,maxD,minD,d,BCi,Ri);
I2=I;
subplot(4,1,1)
plot(Kd, dCmax, Kd, Cmax)
subplot(4,1,2)
plot(Kd, S, Kd, I)

DWT=15;
[Cmax,dCmax,S,I,Kd]=ikd(vol,DWT,num,maxD,minD,d,BCi,Ri);
I4=I;

DWT=30;
[Cmax,dCmax,S,I,Kd]=ikd(vol,DWT,num,maxD,minD,d,BCi,Ri);
I5=I;
subplot(4,1,4)
plot(Kd, I2, Kd, I4,Kd,I5)
```

```
vol=115;
DWT=7.5;
[Cmax,dCmax,S,I,Kd]=ikd(vol,DWT,num,maxD,minD,d,BCi,Ri);
I3=I;

subplot(4,1,3)
plot(Kd, I1, Kd, I2, Kd, I3)


Parameters;
Ni=Ri/BCi
Si=(BCi/mkd(BCi))*((mkd(BCi+d)-mkd(BCi-d))/(2*d))
Ii=abs(Ni*Si)
```

B.2.2 Distribution Coefficient Importance Function

```
function [Cmax,dCmax,S,I,Kd]=ikd(vol,DWT,num,maxD,minD,d,BCi,Ri)
% Calculates the maximum concentration, the derivative of the maximum
% concentration with respect to the distribution coefficient, the
% normalized sensitivity and importance with respect to the distribution
% coefficient, over the range of the distribution coefficient.

Kd=linspace(minD,maxD,num);

for i=1:1:num

    Cmax(i)=mkd(Kd(i));
    m=Kd(i)-d;
    p=Kd(i)+d;
    Cmm=mkd(m);
    Cmp=mkd(p);
    dCmax(i)=(Cmp-Cmm)/(2*d);
    N=Ri/BCi;
    S(i)=(BCi/mkd(BCi))*(dCmax(i));
    I(i)=abs(N*S(i));

End
```

B.2.3 Maximum Concentration Function

```
function Cmkd = mkd(Kd)
% Calculates maximum concentration as a function of distribution
% coefficient.
%
global n resid K pb phiW a rain DWT vol dia SOL X rho Dgf Kh thalf

v = rain*0.0254; % velocity, m/year
Dg = Dgf*365/(3.28^2);
lamda = log(2)/thalf; % decay coeff
R = ret(pb,Kd,phiW,a,Kh);       % retardation
delTsrc = delT(vol,rho,X,v,dia,resid,SOL);% length of source term, years

H=Spill(vol,dia,n,resid);
Z=DWT-H;       % depth to water table, meters
D = (0.1*Z)+Dg;   % Dispersivity, 0.1 times transport length


if H<DWT
Cold=0;
done=1;
```

```
t=1;
ts=2;
while done;
    Conc=Tomask2(v,Z,D,t,delTsrc,lamda,R);
    if Conc>=Cold;
            t=t+ts;
            done=1;
            Cold=Conc;
        else if Conc<Cold;
            t=t-2*ts;
            ts=ts/2;, end
        if abs(Conc-Cold)<0.00000001;
            done =0;
        end
        Cold=0;
end, end

else
    Conc=1;
end
Cmkd=Conc;
```

B.3 Half-Life

B.3.1 Driver

```
% Driver to plot the half-life importance over the range of the half-life
% at selected spill volume sizes and water table depths.  Determines
% the relative range, normalized sensitivity, and importance at base-case
% values.

clear
Parameters;
num=25;     % number of steps in depth to water table range
maxD=2.74;    % maximum range for depth to water table
minD=0.1;   % minimum range for depth to water table
d=0.0001;  % difference for numerical differentiation
BCi=2;    % base case value
Ri=2.63;    % range of values

vol=28;
[Cmax,dCmax,S,I,thalf]=ithf(vol,DWT,num,maxD,minD,d,BCi,Ri);
I1=I;


vol=75;
[Cmax,dCmax,S,I,thalf]=ithf(vol,DWT,num,maxD,minD,d,BCi,Ri);
I2=I;
subplot(4,1,1)
plot(thalf, dCmax,thalf, Cmax)
subplot(4,1,2)
plot(thalf, S, thalf, I)

DWT=15;
[Cmax,dCmax,S,I,thalf]=ithf(vol,DWT,num,maxD,minD,d,BCi,Ri);
I4=I;

DWT=30;
[Cmax,dCmax,S,I,thalf]=ithf(vol,DWT,num,maxD,minD,d,BCi,Ri);
I5=I;
```

```
subplot(4,1,4)
plot(thalf,I2,thalf,I4,thalf,I5)


vol=115;
DWT=7.5;
[Cmax,dCmax,S,I,thalf]=ithf(vol,DWT,num,maxD,minD,d,BCi,Ri);
I3=I;

subplot(4,1,3)
plot(thalf, I1, thalf, I2, thalf, I3)


Parameters;
Ni=Ri/BCi
Si=(BCi/mthf(BCi))*((mthf(BCi+d)-mthf(BCi-d))/(2*d))
Ii=abs(Ni*Si)
```

B.3.2 Half-life Importance Function

```
function [Cmax,dCmax,S,I,thalf]=ithf(vol,DWT,num,maxD,minD,d,BCi,Ri)
% Calculates the maximum concentration, the derivative of the maximum
% concentration with respect to the half-life, the normalized
% sensitivity and importance with respect to the half-life, over
% the range of the half-life.

thalf=linspace(minD,maxD,num);

for i=1:1:num

    Cmax(i)=mthf(thalf(i));
    m=thalf(i)-d;
    p=thalf(i)+d;
    Cmm=mthf(m);
    Cmp=mthf(p);
    dCmax(i)=(Cmp-Cmm)/(2*d);
    N=Ri/BCi;
    S(i)=(BCi/mthf(BCi))*(dCmax(i));
    I(i)=abs(N*S(i));

End
```

B.3.3 Maximum Concentration Function

```
function Cmt = mthf(thalf)
% Calculates maximum concentration as a function of contaminant half-
% life.
%
global n resid K pb phiW a rain DWT vol dia SOL X rho Dgf Kd Kh

v = rain*0.0254; % velocity, m/year
Dg = Dgf*365/(3.28^2);
lamda = log(2)/thalf; % decay coeff
R = ret(pb,Kd,phiW,a,Kh);       % retardation
delTsrc = delT(vol,rho,X,v,dia,resid,SOL);% length of source term, years

H=Spill(vol,dia,n,resid);
Z=DWT-H;       % depth to water table, meters
D = (0.1*Z)+Dg;   % Dispersivity, 0.1 times transport length
```

```
if H<DWT
Cold=0;
done=1;
t=1;
ts=2;
while done;
    Conc=Tomask2(v,Z,D,t,delTsrc,lamda,R);
    if Conc>=Cold;
            t=t+ts;
            done=1;
            Cold=Conc;
        else if Conc<Cold;
            t=t-2*ts;
            ts=ts/2;, end
        if abs(Conc-Cold)<0.0001;
            done =0;
        end
        Cold=0;
end, end

else
    Conc=1;
end
Cmt=Conc;
```

B.4 Precipitation

B.4.1 Driver

```
% Driver to plot the precipitation importance over the range of the
% precipitation at selected spill volume sizes and water table depths.
% Determines the relative range, normalized sensitivity, and importance
% at base-case values.

clear
Parameters;
num=30;     % number of steps in rainfall range
maxD=90;    % maximum range for rainfall
minD=20;   % minimum range for rainfall
d=0.0001;  % difference for numerical differentiation
BCi=38.39;    % base case value
Ri=70;    % range of values

vol=28;
[Cmax,dCmax,S,I,rain]=irain(vol,DWT,num,maxD,minD,d,BCi,Ri);
I1=I;


vol=75;
[Cmax,dCmax,S,I,rain]=irain(vol,DWT,num,maxD,minD,d,BCi,Ri);
I2=I;

subplot(4,1,1)
plot(rain, dCmax,rain, Cmax)
subplot(4,1,2)
plot(rain, S, rain, I)

DWT=15;
[Cmax,dCmax,S,I,rain]=irain(vol,DWT,num,maxD,minD,d,BCi,Ri);
```

```
I4=I;

DWT=30;
[Cmax,dCmax,S,I,rain]=irain(vol,DWT,num,maxD,minD,d,BCi,Ri);
I5=I;
subplot(4,1,4)
plot(rain, I2, rain, I4,rain,I5)


vol=115;
DWT=7.5;
[Cmax,dCmax,S,I,rain]=irain(vol,DWT,num,maxD,minD,d,BCi,Ri);
I3=I;

subplot(4,1,3)
plot(rain, I1, rain, I2, rain, I3)


Parameters;
Ni=Ri/BCi
Si=(BCi/mrain(BCi))*((mrain(BCi+d)-mrain(BCi-d))/(2*d))
Ii=abs(Ni*Si)
```

B.4.2 Precipitation Importance Function

```
function [Cmax,dCmax,S,I,rain]=irain(vol,DWT,num,maxD,minD,d,BCi,Ri)
% Calculates the maximum concentration, the derivative of the maximum
% concentration with respect to precipitation, the normalized
% sensitivity and importance with respect to precipitation, over
% the range of precipitation.

rain=linspace(minD,maxD,num);

for i=1:1:num

    Cmax(i)=mrain(rain(i));
    m=rain(i)-d;
    p=rain(i)+d;
    Cmm=mrain(m);
    Cmp=mrain(p);
    dCmax(i)=(Cmp-Cmm)/(2*d);
    N=Ri/BCi;
    S(i)=(BCi/mrain(BCi))*(dCmax(i));
    I(i)=abs(N*S(i));

End
```

B.4.3 Maximum Concentration Function

```
function Cmr = mrain(rain)
% Calculates maximum concentration at water table as a function of
% precipitation
%
%
global n resid K pb phiW a DWT vol dia SOL X rho Dgf Kd Kh thalf
v = rain*0.0254; % velocity, m/year
Dg = Dgf*365/(3.28^2);  % gaseous diffusion coefficient
lamda = log(2)/thalf; % decay coeff
```

```
R = ret(pb,Kd,phiW,a,Kh);       % retardation
delTsrc = delT(vol,rho,X,v,dia,resid,SOL);% length of source term, years

H=Spill(vol,dia,n,resid);   % depth of spill, meters
Z=DWT-H;       % depth to water table, meters
D = (0.1*Z)+Dg;   % Dispersivity, 0.1 times transport length


if H<DWT
Cold=0;
done=1;
t=1;
ts=2;
while done;
    Conc=Tomask2(v,Z,D,t,delTsrc,lamda,R);
    if Conc>=Cold;
            t=t+ts;
            done=1;
            Cold=Conc;
        else if Conc<Cold;
            t=t-2*ts;
            ts=ts/2;, end
        if abs(Conc-Cold)<0.000001;
            done =0;
        end
        Cold=0;
end, end

else
    Conc=1;
end
Cmr=Conc;
```

B.5 Water Table Depth

B.5.1 Driver

```
% Driver to plot the water table depth importance over the range of water
% table depth at selected spill volume sizes.  Determines the relative
% range, normalized sensitivity, and importance at base-case values.

clear
Parameters;
num=50;     % number of steps in depth to water table range
maxD=55;    % maximum range for depth to water table
minD=1.2;   % minimum range for depth to water table
d=0.0001;   % difference for numerical differentiation
BCi=7.5;    % base case value
Ri=53.8;    % range of values

vol=28;
[Cmax,dCmax,S,I,DWT]=idwt(vol,num,maxD,minD,d,BCi,Ri);
I1=I;

vol=75;
[Cmax,dCmax,S,I,DWT]=idwt(vol,num,maxD,minD,d,BCi,Ri);
I2=I;
subplot(3,1,1)
plot(DWT, dCmax, DWT, Cmax)
subplot(3,1,2)
```

```
plot(DWT, S, DWT, I)

vol=115;
[Cmax,dCmax,S,I,DWT]=idwt(vol,num,maxD,minD,d,BCi,Ri);
I3=I;

subplot(3,1,3)
plot(DWT, I1, DWT, I2, DWT, I3)

Parameters;
Ni=Ri/BCi
Si=(BCi/mdwt(BCi))*((mdwt(BCi+d)-mdwt(BCi-d))/(2*d))
Ii=abs(Ni*Si)
```

B.5.2 Water Table Depth Importance Function

```
function [Cmax,dCmax,S,I,DWT]=idwt(vol,num,maxD,minD,d,BCi,Ri)
% Calculates the maximum concentration, the derivative of the maximum
% concentration with respect to the water table depth, the normalized
% sensitivity and importance with respect to the water table depth, over
% the range of the water table depth.

DWT=linspace(minD,maxD,num);

for i=1:1:num

    Cmax(i)=mdwt(DWT(i));
    m=DWT(i)-d;
    p=DWT(i)+d;
    Cmm=mdwt(m);
    Cmp=mdwt(p);
    dCmax(i)=(Cmp-Cmm)/(2*d);
    N=Ri/BCi;
    S(i)=(BCi/mdwt(BCi))*(dCmax(i));
    I(i)=abs(N*S(i));

End
```

B.5.3 Maximum Concentration Function

```
function Cmd = mdwt(DWT)
% Calculates maximum concentration as a function of depth to water table
%
%
%
global n resid K pb phiW a rain vol dia SOL X rho Dgf Kd Kh thalf

v = rain*0.0254;    % velocity, m/year
Dg = Dgf*365/(3.28^2);  %meters^2/yr
lamda = log(2)/thalf;   % decay coeff
R = ret(pb,Kd,phiW,a,Kh);   % retardation
delTsrc = delT(vol,rho,X,v,dia,resid,SOL); % length of source term, years

H=Spill(vol,dia,n,resid);
Z=DWT-H;    % depth to water table, meters
D = (0.1*Z)+Dg; % Dispersivity, 0.1 times transport length


if H<DWT
Cold=0;
```

```
done=1;
t=1;
ts=0.5;
while done;
    Conc=Tomask2(v,Z,D,t,delTsrc,lamda,R);
    if Conc>=Cold;
            t=t+ts;
            done=1;
            Cold=Conc;
        else if Conc<Cold;
            t=t-2*ts;
            ts=ts/2;, end
        if abs(Conc-Cold)<0.000001;
            done =0;
        end
        Cold=0;
end, end

else
    Conc=1;
end
Cmd=Conc;
```

B.6 Spill Volume

B.6.1 Driver

```
% Driver to plot the spill volume importance over the range of spill
% volumes at selected water table depths.  Determines the relative range,
% normalized sensitivity, and importance at base-case values.

clear
Parameters;
num=50;     % number of steps in volume range
maxD=150;    % maximum range for volume
minD=1;   % minimum range for volume
d=0.0001;  % difference for numerical differentiation
BCi=75;    % base case value
Ri=255;    % range of values

DWT=7.5;
[Cmax,dCmax,S,I,vol]=ivol(DWT,num,maxD,minD,d,BCi,Ri);
I1=I;
subplot(3,1,1)
plot(vol, dCmax,vol, Cmax)
subplot(3,1,2)
plot(vol, S, vol, I)

DWT=15;
[Cmax,dCmax,S,I,vol]=ivol(DWT,num,maxD,minD,d,BCi,Ri);
I2=I;

DWT=30;
[Cmax,dCmax,S,I,vol]=ivol(DWT,num,maxD,minD,d,BCi,Ri);
I3=I;

subplot(3,1,3)
plot(vol, I1, vol, I2, vol, I3)

Parameters;
```

```
Ni=Ri/BCi
Si=(BCi/mvol(BCi))*((mvol(BCi+d)-mvol(BCi-d))/(2*d))
Ii=abs(Ni*Si)
```

B.6.2 Spill Volume Importance Function

```
function [Cmax,dCmax,S,I,vol]=ivol(DWT,num,maxD,minD,d,BCi,Ri)
% Calculates the maximum concentration, the derivative of the maximum
% concentration with respect to spill volume, the normalized
% sensitivity and importance with respect to spill volume, over
% the range of spill volumes.

vol=linspace(minD,maxD,num);

for i=1:1:num

    Cmax(i)=mvol(vol(i));
    volm=vol(i)-d;
    volp=vol(i)+d;
    Cmm=mvol(volm);
    Cmp=mvol(volp);
    dCmax(i)=(Cmp-Cmm)/(2*d);
    N=Ri/BCi;
    S(i)=(BCi/mvol(BCi))*(dCmax(i));
    I(i)=abs(N*S(i));

End
```

B.6.3 Maximum Concentration Function

```
function Cmv = mvol(vol)
% Calculates maximum concentration as a function of spill volume.
%
%
global n resid K pb phiW a rain DWT dia SOL X rho Dgf Kd Kh thalf

v = rain*0.0254; % velocity, m/year
Dg = Dgf*365/(3.28^2);  %meters^2/yr
lamda = log(2)/thalf; % decay coeff
R = ret(pb,Kd,phiW,a,Kh);       % retardation
delTsrc = delT(vol,rho,X,v,dia,resid,SOL);% length of source term, years

H=Spill(vol,dia,n,resid);
Z=DWT-H;       % depth to water table, meters
D = (0.1*Z)+Dg;   % Dispersivity, 0.1 times transport length


if H<DWT
Cold=0;
done=1;
t=1;
ts=2;
while done;
    Conc=Tomask2(v,Z,D,t,delTsrc,lamda,R);
    if Conc>=Cold;
            t=t+ts;
            done=1;
            Cold=Conc;
        else if Conc<Cold;
            t=t-2*ts;
```

```
            ts=ts/2;, end
        if abs(Conc-Cold)<0.000001;
            done =0;
        end
        Cold=0;
end, end

else
    Conc=1;
end
Cmv=Conc;
```

B.7 Tomasko Function

```
% Function to calculate the concentration at a location z
% Calculates C/C0 - percent of initial concentration
%
function Cco=Tomask2(v,z,D,t,delTsrc,lamda,R)
%
% v = velocity, m/s
% z = location, m
% D = Dispersion, m
% t = time, years
% delTsrc = length of source term, years
% lamda = decay coeff for contaminant
% R = retardation coeff for contam

% a=(exp(v.*z./(2.*D)))./2;
b=(((z.^2)./D).*((v.^2./(4.*D))+lamda)).^0.5;
c=(((v.^2)./(4.*D.*R))+(lamda./R));
d=R.*(z.^2)./D;

a1=(exp(((v.*z)./(2.*D))-b)).*(erfc((0.5).*((d./t).^0.5)-
       (((c).*t).^0.5)));
b1=(exp(((v.*z)./(2.*D))+b)).*(erfc((0.5).*((d./t).^0.5)+(((c).*t).^0.5))
       );

if t<=delTsrc
    c1=0;
    d1=0;
else
    c1=(exp(((v.*z)./(2.*D))-b)).*(erfc((0.5).*((d./(t-delTsrc)).^0.5)-
       (((c).*(t-delTsrc)).^0.5)));
    d1=(exp(((v.*z)./(2.*D))+b)).*(erfc((0.5).*((d./(t-
       delTsrc)).^0.5)+(((c).*(t-delTsrc)).^0.5)));

end
Cco= ((0.5).*(a1+b1))-((0.5).*(c1+d1));
```

Source Time Function

```
% Calculates the time in which the spill is a source of contamination.
function dt=delT(vol,rho,X,v,dia,resid,SOL)

dt=vol*rho*X/(v*pi*dia^2/4*resid*SOL);
```

Retardation Function

```
% Calculates the effective retardation
function R1=ret(pb,Kd,phiW,a,Kh)

R1=pb*Kd+phiW+a*Kh;
```

Spill Saturation Depth Function

```
% Function to calculate depth of residual saturation after a spill
function H=Spill(vol, dia, n, resid)
% vol = volume of spill, m^3
% dia = dia of spill area/column, m
% n = porosity
% resid = residual NAPL saturation, % (typically about 20%)
% H = depth of NAPL infiltration, m
r=dia/2;

 H = vol/(pi*(r^2)*n*resid);
```