Development of A Screening Method for Prioritizing the Remediation of Groundwater Contamination Sites

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Abstract

Several hazardous waste site ranking methods are available. Most of them are complicated in nature, need numerous input parameters, and therefore call for enormous site investigation efforts. Almost all of them include only a qualitative analysis of site parameters. None of them involve any quantitative analysis to incorporate the fate and transport characteristics of the pollutants in the subsurface. A simple groundwater contamination site ranking methodology was developed based on the probability of impacting receptors. The proposed ranking method includes quantitative analysis of contaminant fate and transport and uncertainties in the flow and transport parameters. It combines them in a probabilistic framework and produces an effective ranking system on the basis of the the risk of impacting an environmental receptor. Hydraulic conductivity was considered as a random variable to represent the heterogeneity of the water aquifer system. Monte Carlo Simulation with a stratified sampling technique was used to calculate the probability of violation of water quality standards at the receptors. The final product is a simple software package which uses easily available site parameters and produces contour plots for probability of violation of water quality standards at any receptor distance. The software can be used to determine the sensitivity of the probability of violation to site parameters.

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1. INTRODUCTION

1.1 Groundwater and Its Contamination

Groundwater constitutes a significant source of water in most areas of the United States and may be defined as the subsurface water that occurs beneath the water table in soils and geologic formations that are fully saturated (Freeze and Cherry, 1979; Pye et al., 1983; Anderson, 1987).

More than 98% of the available fresh water in the world is groundwater, which far exceeds the volume of surface water (Fetter, 1988). The quantity of groundwater which underlies North America is also immense and the amount present is six times greater than the water stored within surface reservoirs (Conservation Foundation, 1985). People depend upon groundwater in every state, and its usage accounts for approximately one-fourth of all water used (Rail, 1989). This consumption includes the following functions and statistics:

1) Thirty-five percent of water withdrawn from municipal water supplies comes from underground sources.

2) Groundwater as a sole source of drinking water is used by more than 50% of the total United States population and 97% of rural residents.

3) Forty percent is agricultural irrigation water usage and 26% is industrial withdrawals (excluding electric power plants).

4) Nourishment and maintenance of ecosystems is valued for fish production, wildlife habitat, and recreational opportunities.
McGuinness (1963) predicted the future U.S. water requirements and suggested that the national water needs will reach $3360 \times 10^6 \text{ m}^3/\text{day}$ by the year 2000. This figure approaches the total water resources potential of the nation, which is estimated to be about $4550 \times 10^6 \text{ m}^3/\text{day}$. If the requirements are to be met, it is widely accepted that groundwater resources will have to provide a greater portion of the total supply. He noted that groundwater usage will increase to $1120 \times 10^6 \text{ m}^3/\text{day}$ in 2000 from the figure of 1980 which was $705 \times 10^6 \text{ m}^3/\text{day}$. He also noted that the desirable properties of groundwater, such as its clarity, bacterial purity, consistent temperature, and chemical quality, may encourage the needed large-scale development (Freeze and Cherry, 1979).

Unfortunately there is growing evidence that this resource, which was once considered free of pollution, is being polluted from different sources. In the U.S. alone, there are over 15,000 potential hazardous waste sites. At about 70% of these sites, contaminants present some degree of threat to groundwater supplies.

The full magnitude of groundwater contamination in the United States is, however, not fully documented and federal, state, and local efforts continue to assess and address the problems (Rail, 1985a). Current estimates by the National Research Council (1984) on the extent of groundwater aquifer contamination in the United States suggest that 0.5 to 2.0 percent may be polluted. Although, the nation is not facing an overall groundwater contamination crisis, in some localities, local contamination has caused significant well closures, public health concerns, and economic losses (Bermaster and Harris, 1982).
Presently in the United States, the national extent of the threat to groundwater is receiving much attention. This is primarily because of the many thousands of publicized well closures and contamination incidents which have occurred throughout the country. In addition, over 200 organic and inorganic chemicals in excessive amounts, including high levels of radioactive isotopes, have been identified in some groundwater supply systems. Attention has been given to these areas because of the direct threat to the health of the individuals that consume the water. Increased costs associated with location of new water supply systems (i.e., if new sources of supply have to be located), pumping water from remote locations or deeper areas, and provision of increased levels of preliminary and final treatment to meet standards related to safe consumption of the water have caused a financial crisis in many areas. Additionally, groundwater contamination and its control are not only technically complex but also involve numerous economic and political demands (Rail, 1989).

The sources of groundwater contamination are many and the contaminants are numerous. The National Research Council (1984) concluded that the largest potential source of contamination of groundwater involves the improper disposal of solid and liquid wastes. This is because during the past several decades, legislation reflecting environmental concerns restricting air and surface water pollution resulted in increased disposal of wastes into subsurface areas. Also, over several decades, human activities have contaminated drinking water supply wells with “traditional” contaminants (Rail, 1989). For example, in sections of the
midwestern United States, the use of agricultural fertilizers raised nitrate concentrations in groundwaters above federal safe drinking water standards. In the snow belt, hundreds of wells were closed because of high concentrations of salt percolating into groundwater from de-icing agents used on highways during the winter months. Suburban areas have groundwater with high levels of nitrate due to the use of lawn fertilizers and septic tank discharges. Common industrial solvents such as trichloroethylene, 1,1,1-trichloroethane, tetrachloroethane, benzene, and carbon tetrachloride have been found in widespread areas. Common organic pollutants such as acetone, toluene, phenols, methyl ethyl ketones, methyl isobutyl ketone, xylene, and several aliphatic and aromatic acids are detected in landfill leachates (Kolega, 1986).

Besides these, there are a number of other sources of potential groundwater contamination. Pollution from sources such as land-treatment systems for municipal wastewater, waste injection wells, cemeteries, mine tailings, acid mine drainage, oil-field brines, and accidental oil, gasoline, and chemical spills have been well documented in the literature. Groundwater contamination can also occur from sea-water intrusion in coastal areas. For example, lateral intrusion of salt-water caused by pumping has contaminated groundwater in New Haven and Bridgeport, Connecticut (Task Committee, 1969).

All solutes introduced into the hydrogeologic environment as a result of human activity are referred to as "contaminants", regardless of whether or not their concentrations reach levels that cause significant degradation of water quality. The term "pollution" is
reserved for situations where contaminant concentrations attain levels that are considered to be objectionable (Freeze and Cherry, 1979).

1.2 Ranking groundwater contamination sites

Over the past several years the public has become increasingly aware of the value and vulnerability of groundwater resources. This awareness has resulted in the identification of many existing groundwater contamination sites. Many of these sites need immediate remediation for the protection of public health. However, government agencies have limited budgets for cleaning up the contamination sites. Therefore, there is an urgent need to prioritize the sites according to their contamination potential in order to invest the limited resources in the most efficient way.

1.3 National Steps Towards Ranking Contamination Sites

In 1980, the Congress enacted the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA), commonly called the Superfund, in response to the dangers posed by uncontrolled releases of hazardous substances, pollutants, or contaminants to the environment. CERCLA section 118, added by SARA (Superfund Amendments and Reauthorization Act), requires that EPA give a high priority to facilities where the release of hazardous substances has resulted in closing of drinking water wells or has contaminated a principal drinking water supply and put such facilities in the National Priorities List (NPL).
The NPL identifies sites that warrant further investigation to
determine if they pose risks to public health or the en-
vironment. Sites on the NPL are eligible for long-term "remedial action" financed
under the CERCLA.

1.4. **Current Site Ranking Methods**

Several site ranking methodologies are available. The most
well known ranking method is the EPA Hazard Ranking System
(HRS). The Washington State Department of Ecology has developed
the Washington Ranking Method (WARM). Other ranking methods
include the New York State Human Exposure Potential Ranking
System, the Air Force Hazard Assessment Rating Methodology II, the
Department of Energy Remedial Action Priority System, etc. All of
these methods are more or less similar in approach and based on
relative risks rather than specific risk values (Olivieri et al.,1984).
All these methods combine groundwater and other contamination
pathways to rank a hazardous waste site. Olivieri et al. (1984)
developed a site ranking methodology on the basis of only
groundwater contamination. In the following sections, HRS, WARM,
and the method of Olivieri will be outlined.

1.4.1 **The EPA Hazard Ranking System (HRS)**

HRS is a scoring system EPA uses to assess the relative threat
associated with actual or potential releases of hazardous substances
from a waste site. The HRS score is the primary criterion used by
EPA to determine whether a site should be placed on the National
Priorities List (NPL).
EPA explained when it adopted the HRS that "the HRS is a means for applying uniform technical judgement regarding the potential hazards presented by a facility relative to other facilities. It does not address the feasibility, desirability, or degree of cleanup required" (Federal Register, 1988). The HRS was designed to assess only relative risks and not designed to be used as a quantitative risk assessment method.

An HRS score is determined for a site by evaluating four migration routes or "pathways": Groundwater (gw), Surface water (sw), Soil Exposure (s), and Air (a). The score for each pathway is obtained by evaluating a set of "factors" that characterize the potential of the site to cause harm to the environment or public health through that pathway. The factors, such as toxicity of the substances at a site, waste quantity, and population served are each assigned a numerical value according to the guidelines established in the procedure. This value is then multiplied by a weighing factor yielding the factor score. The factor scores are then combined within "factor categories". Total scores for the factor categories are multiplied together to develop a score for the relevant pathway. Finally, the scores of the four pathways (gw, sw, s, a) are combined for the site using the following root-mean-square equation to determine the overall HRS site score (Federal Register, 1990).

\[ \text{HRS Migration Score} = \sqrt[4]{\frac{S_{gw}^2 + S_{sw}^2 + S_s^2 + S_a^2}{4}} \]  

where, \( S_{gw} \) = Groundwater migration pathway score,
\( S_{SW} \) = Surface water migration pathway score,
\( S_{S} \) = Soil exposure pathway score, and
\( S_{A} \) = Air migration pathway score.

The HRS score ranges from 0 to 100. Sites scoring 28.50 or above on HRS are eligible for the NPL. The first NPL contained 418 sites. EPA chose 28.50 as the cutoff score as a management tool because it yielded an initial NPL of at least 400 sites as required in CERCLA, not because of any determination that the cutoff score represents a threshold of unacceptable risks present at the site.

1.4.2. The Washington Ranking Method (WARM)

This ranking method was developed for ranking hazardous waste sites to satisfy the requirements of the Model Toxics Control Act. It is also a scoring method and the site scores are generated for the following seven exposure routes.

1) Surface water - Human Health
2) Surface water - Environment
3) Ground water - Human Health
4) Marine sediment - Human Health
5) Marine sediment - Environment
6) Air - Human Health
7) Air - Environment

Within each route, data elements are evaluated in three main subcategories. These are:

1) Substance characteristics
2) Site characteristics or migration potential
3) Exposure targets
For all routes except sediment, an additional subcategory is considered for confirmed releases to the medium under consideration. A multiplicative and additive algorithm combines the scores from the subcategories, resulting in a numerical route score between 1 and 100. The subsequent combination of the four main routes (surface water, groundwater, sediment, and, air) using single scaling method, produces a single "bin" priority value for human health or for the environment. These two priority values are further combined in a matrix to provide a final single bin rank for the site (Washington Ranking Method Scoring Manual, 1990).

1.4.3. Ranking Method developed by Olivieri

Olivieri et al. (1984) presented a risk assessment procedure which was proposed for the numerical rating and ranking of hazardous materials sites in terms of their relative groundwater contamination potential. The method identifies and assigns values to two main groups of factors: 1) Site Sensitivity Factors, which determine the susceptibility of a site to groundwater contamination; and 2) Contamination Severity Factors, which determine the severity and potential to cause groundwater contamination.

Site Sensitivity Factors are the hydrogeologic characteristics of a site which control the behavior of contaminants in the ground. Four factors were considered in this group: 1) distance to water use, 2) intensity of present water use (number of wells, population served), 3) depth to water table, and 4) water table gradient. Contamination Severity Factors include 1) toxicity of the contaminants, 2) physical-chemical properties of the contaminants
and 3) relative magnitude of contaminant release.

Each factor is assigned a numerical value or a range of values depending on the degree of uncertainty associated with that factor. These individual values are summed for both groups. The resulting sub-totals are then added to obtain the contamination potential score which is used to rank the sites.

1.5. The Proposed Ranking Method

Most of the available site ranking methodologies are, in essence, qualitative analysis of site characteristics. None of them contain any quantitative analysis of the fate and transport characteristics of pollutants in the subsurface. The proposed ranking method includes quantitative analysis of contaminant fate and transport and uncertainties in the flow and transport parameters. It combines them in a probabilistic framework and produces an effective ranking system on the basis of the risk of impacting an environmental receptor. As far as the author is concerned, this work is the first of its kind.

The fate of contaminants in the groundwater system is controlled by individual site conditions such as hydrogeologic features of the aquifer system and physico-chemical characteristics of the contaminants. The contamination activity becomes complicated by the fact that the natural aquifer systems are inherently heterogeneous with respect to their hydraulic properties. Our lack of ability to characterize this heterogeneity and inherent uncertainties of the measured aquifer parameters make the groundwater flow analysis and contaminant transport prediction
very uncertain.

A decision concerning the necessity of remediating a groundwater contamination site should be based on the likelihood of the contaminated groundwater impacting the receptors at the site. A receptor was defined to be a specific location in the environment where public health or environmental quality can be affected by groundwater contamination. These will include public supply wells, wetlands, streams, etc. Impacting a receptor means the contaminant concentration at a receptor exceeding some specified maximum allowable levels. This impact will be quantified as probability of violation.

The probability of impacting a receptor will depend on the individual site characteristics, such as hydraulic properties of the underlying aquifer system, amount of contaminant present in the groundwater system, the ability of natural attenuation of the contaminant to play a role in remediation.

Limited financial resources should be utilized to remediate sites where the receptors are at high risk and the contaminant characteristics and specific site conditions do not permit significant natural mitigation of the contaminants. At these sites, if the costimants are allowed to spread without taking any remediation measures, it is observed that they will be much more costly to remediate in the long run. Conversely, if the nature and extent of contamination and site hydrogeologic characteristics are such that the natural degradation of the contaminants will adequately lower the concentrations of the contaminants before they reach the receptors, then there will be no need to design any costly
remediation. Therefore, there is a need for detailed analysis of the site parameters and contaminant characteristics to determine the risk of impacting receptors under different values of the parameters.

In this work, a simple procedure for screening contamination sites for their potential of impacting environmental receptors will be presented. The proposed method will combine the analysis of site conditions and contaminant characteristics in a probabilistic framework and estimate probabilities of affecting receptors under different combinations of these parameters. The site conditions will include easily available site information such as: estimates of ground water velocity, approximate location of the source and receptor, average annual infiltration over the site, and other measurable or estimable characteristics of a site. The contaminant characteristics will include the extent of contamination and its physico-chemical properties. The relationship between risk of impacting receptors and these properties will be determined. Importance of remediating a site will be determined by the analyst using graphical displays of the results of this work.
2. OVERVIEW OF THE PROCEDURE

The basis of the proposed ranking method is to determine if the concentration at an environmental receptor resulting from contamination activities will exceed the water quality standard.

2.1. Water Quality Standard

Water quality is a consequence of the natural physical and chemical state of water as well as any alterations that may have occurred as a result of human activity. The usefulness of water for a particular purpose is determined by this water quality. If human activity alters the natural water quality so that it is no longer suitable for the use for which it had previously been suited, the water is said to be polluted or contaminated.

Water quality standards are regulations that serve as a basis for appraisal of the results of chemical analysis of water in terms of suitability of the water for various intended uses. It sets limits on the maximum allowable concentrations of different constituents of groundwater to be allowed for different purposes. In this work, the water quality standard will be expressed in terms of a normalized value so that the procedure can be applied to sites where different standards are enforced.

The constituents, for which maximum permissible concentration limits have been set in drinking water standards, are all considered to have significant potential for harm to human health at concentrations above those specified limits. The specified limits are not to be exceeded in public water supplies. If the limits for one or more of the constituents are exceeded, the water is considered to
be unfit for human consumption. In this study, this exceedence of contaminant concentration from the water quality standard has been termed “violation”.

2.2. General description of the procedure

The proposed method assumes that a site has been contaminated from a contaminant source. The source is somehow stopped or contained and the extent of the plume has been estimated. This plume has been called the “initial plume”. There are some estimates of the contaminant properties. The direction of groundwater flow is known and there is a receptor in the path of the advancing plume. There are also some estimates of hydraulic properties of aquifer systems between the source and receptor. The task is to estimate the probability levels (risks) of violation of the water quality standard at the receptor by using this limited set of available data. Sites with highest risks at the receptors will be ranked highest in remediation needs.

In estimating this violation probability, the first step will be the computation of contaminant concentrations at the receptor and the second step will be the estimation of probability of these concentrations exceeding the specified water quality standard. Therefore, the parameters of this violation study will contain the factors which affect the calculations in these two steps. These parameters will be called the “ranking parameters” or “prioritization parameters”.

The contaminant plume will move downstream with the flowing groundwater and the contaminants themselves will spread in
the subsurface by other mechanisms. Therefore, in order to compute the concentrations of pollutant at a receptor, first the fate and transport of the pollutant must be studied and the factors affecting the transport identified. This will be performed in section three of this work and a numerical model (which has been termed as "MODEL") to compute contaminant concentrations will be developed in that section.

After the calculation of contaminant concentrations, the next step is the calculation of violation probability and the identification of parameters which affect this probability independent of the parameters affecting the transport. It is obvious that if it were possible to determine all the parameters with 100% confidence, the computed concentration would be exact and violation probability would be either 1 or 0 for a certain water quality standard. However, this will never be the case in the real world. There are always uncertainties inherent in the parameters used in the transport equations used to calculate the contaminant concentrations. Therefore, these uncertainties must be taken into account when using any results from those equations.

A key parameter in predicting the contaminant concentration is the hydraulic conductivity (K). Geostatistics defines it as a random variable and expresses it by an expected value, variance, and its probability distribution function. This characteristics of K has been explained in detail in section 4. A single expected value and a variance represents a single distribution. A realization from this distribution represents a flow field which has a uniform hydraulic conductivity equal to the realization value.
The distinct feature of this procedure is this statistical approach in dealing with hydraulic conductivity. If all other parameters in the MODEL are constant, a single hydraulic conductivity will produce a single concentration value. But if a distribution of K is used in the MODEL, a distribution of concentrations will be obtained. From this distribution of concentrations, the probability of concentrations exceeding the water quality standard can be obtained. An approximation to the Monte Carlo Simulation technique was used to transform the uncertainty in the hydraulic conductivity into that in the concentration and eventually to calculate the probability of violation. The violation probability was attributed to the expected value of the distribution of hydraulic conductivity. The measured or estimated value of hydraulic conductivity over a site was assumed as the expected value of the distribution of the hydraulic conductivity for that site.

The expected values of K and the other parameters which affect the probability of violation have their possible ranges of values. To determine their effects on violation probability, a sensitivity analysis was carried out over the range of their values. The probabilities are presented in probability contour plots by taking any two of the prioritization parameters on the two axes and keeping others constant.

To compute the contaminant concentrations at receptor, a unidirectional flow was assumed between the source and the receptor. Transport was assumed two dimensional and the vertically averaged concentrations were obtained from the MODEL simulations.
The initial plume was generated from a point source. The violation studies were based on the ability of this plume to impact the receptor. The MODEL was run by taking the initial plume as the background concentration in the aquifer. Movement of this plume was observed under different values of the prioritization parameters and the probability of violation was estimated.

The water quality standards was taken as fractions of the unit source concentration. This allows the application of the results of this work to any source magnitude and water quality standard.

A graphics package SAS/GRAPH was used to produce the probability contour plots. MODEL was run on the Environmental Research Institute (ERI) Sun System and SAS/GRAPH was run in the University IBM MAINFRAME.
3. DEVELOPMENT OF SIMULATION MODEL

In this section, the fate and transport of contaminants in the groundwater environment will be discussed and factors affecting the phenomena will be identified. A simulation model (MODEL) will be developed, by combining these factors, to compute the contaminant concentrations in the flow field.

The contaminants are often termed as "solute" in the literature. "Solute" are constituents included in the chemical combinations of the elements that are soluble in water. These elements can be ionized, in the form of electrically neutral chemicals, complexes, and in the form of larger aggregates, such as colloids. All these transported substances are called "solute" as long as they do not form a mobile phase distinct from the transporting fluid but integrate themselves with the moving water body and perhaps change its physical and chemical properties (DeMarsily, 1986).

Groundwater contamination is quantified by the term "concentration" of one substance in another, for example concentration of TCE in water. It is general practice to measure contaminant concentration in volumetric units, as mass of solute per unit volume of solution (kg/m³, gm/liter).

There are two principal phenomena affecting the concentration of solutes (contaminants) in the subsurface. One is the "transport of non-reactive solute" and the other is the "interaction between transported substances and the medium". The two phenomena will be discussed separately and then combined to form the standard three-dimensional transport equation. Finally, a vertically averaged
two-dimensional transport equation for an isotropic, homogeneous and unidirectional flow field will be developed.

3.1. The three-dimensional transport equation

3.1.1 Transport of non-reactive solutes

Two basic physical processes affect the transport of non-reactive solutes in the subsurface: Advection and Hydrodynamic Dispersion.

Advection

This is the component of solute movement which is carried along in the subsurface by the flowing groundwater. The rate of transport is equal to the average linear velocity or the pore velocity \(V_p\) of the groundwater flow. This process is also called convection. The bulk of the contaminants are transported by this mechanism.

Hydrodynamic Dispersion

This is the macroscopic outcome of the actual movements of individual fluid particles through the pores and combines two processes. One is Mechanical (or Kinematic) Dispersion and the other is Molecular (or Ionic) Diffusion.

a) Mechanical Dispersion: This is a mixing phenomena mainly due to heterogeneity of the microscopic velocities inside the porous medium. It results in a dilution of contaminants. Mixing that occurs along the streamline of fluid flow is called the longitudinal dispersion and that occurs normal to the streamline is called the transverse dispersion. Generally, longitudinal dispersion is much higher than the transverse dispersion.
b) **Molecular Diffusion**: In this process, both ionic and molecular species dissolved in water move from areas of higher concentration to areas of lower concentration. This phenomena is present even if there is no advection. Flux ($\phi$) due to molecular diffusion is expressed by Fick's Law:

$$\phi = -d_0 \text{grad} C$$  \hspace{1cm} (3.1)

where, $d_0$ is the molecular diffusion coefficient and has units of [L²/T].

A coefficient of hydrodynamic dispersion is defined as the sum of the coefficient of mechanical dispersion and the coefficient of molecular diffusion. In three-dimensions, it is expressed by a three-dimensional tensor $D$ (DeMarsily, 1986).

The basic advective-dispersive equation describes the migration of a nonreactive dissolved constituent due to advection and hydrodynamic dispersion. For a saturated porous media and under steady-state and uniform flow condition, it is given by:

$$\text{div} (D \text{grad} C - C U) = \omega \frac{\partial C}{\partial t}$$  \hspace{1cm} (3.4)

where $U$ is the darcy velocity vector, and $t$ is the time variable.

3.1.2. **Interaction in solute movement**

Certain physical, geochemical, radiological, and biological mechanisms in the subsurface can turn the migration of nonreactive solute in porous media into a reactive phenomena. The whole set of mechanisms is represented by a net "source" or "sink" term $Q$ in the
transport equation. It modifies the transport equation (3.4) as:

\[
\text{div} (D \text{grad} C - C \text{ div} U) = \omega \frac{\partial C}{\partial t} + Q \quad \quad \quad (3.5)
\]

The term Q in equation (3.5) represents the disappearance of contaminants, if it is positive and is called “sink”. It will represent addition of substance, if it is negative and is called a “source”. It is expressed as mass of solutes added or subtracted per unit volume of porous media per unit time. Q is the algebraic sum of the effect of all the individual interaction mechanisms.

DeMarsily (1986) listed and explained in detail all these interaction mechanisms. From those, three commonly occurring phenomena: Adsorption, Decay, and Dilution due to infiltration will be considered in developing the simulation model.

Adsorption

Due to adsorption, contaminant mass partitions from the pore water to the solid part of the porous medium. This results in a net disappearance of solutes from the moving groundwater. The rate of disappearance (Q) is determined as:

\[
Q = \rho_b K_d \frac{\partial C}{\partial t} \quad \quad \quad (3.6)
\]

where, \(\rho_b\) is the bulk dry density of the medium [M/L^3] and \(K_d\) is the distribution coefficient or equilibrium partition coefficient [L^3/M]. \(K_d\) can be expressed as:

\[
K_d = \frac{\text{Mass of solute adsorbed per unit mass of solid phase}}{\text{Concentration of solute in solution}}
\]
Equation (3.6) is based on the following assumptions for adsorption, and fortunately, most constituents of interest in groundwater studies meet these assumptions (Freeze, 1979).

i) Adsorption achieves instantaneous equilibrium,

ii) It is defined by a linear isotherm,

iii) Adsorption is reversible, and

iv) An infinite supply of adsorption sites are available.

Effect of Adsorption is incorporated in the transport equation by a term called the "retardation factor" (R) defined as:

$$ R = 1 + \frac{\rho_s K_d}{\omega} \quad (3.7) $$

The factor R will take a value of 1 if there is no adsorption. For adsorption to take place, a value larger than 1 should be assigned to it. The net effect of adsorption is a retardation of the solute front relative to the bulk mass of water. This retardation of front is described by the following equation:

$$ V_R = \frac{V_p}{R} \quad (3.8) $$

Equation (3.8) is called the retardation equation and $V_R$ is called the retardation velocity.

Decay

Disappearance of solute from the flowing groundwater may also occur due to its radioactive decay, biological decay, hydrolysis, etc. The instantaneous decay for a substance is expressed by the following first-order differential equation:

$$ \frac{\partial C}{\partial t} = - \lambda C \quad (3.9) $$
where $\lambda$ is the decay constant for radioactive decay, or some reaction rate constant for biodegradation or hydrolysis and has a dimension of [1/T]. Decay causes a mass $\lambda C$ per unit volume of the liquid phase to disappear per unit time.

Equation (3.9) can be integrated as:

$$C = C_0 e^{-\lambda t} \quad \text{--------- (3.10)}$$

where $C_0$ is the initial concentration before any decay started. Decay for most solutes is quantified by its half life ($T_{1/2}$). Half life is the period of time during which half of the original amount of a compound will degrade. Therefore, in equation (3.10), at $t = T_{1/2}$, $C = C_0/2$. Using this definition in equation (3.10):

$$e^{-\lambda T_{1/2}} = \frac{1}{2}, \quad \text{or} \quad \lambda = \frac{\ln 2}{T_{1/2}} \quad \text{--------- (3.11)}$$

Dilution

Infiltration from rain water into the groundwater system increases the net volume of water in the aquifer and thereby dilutes the contaminants in subsurface. It is incorporated in the transport equation as a sink term "q" and defined as the volumetric flow rate of water into the aquifer divided by the volume of the aquifer and has a dimension of [1/T].

3.1.3. Complete form of the advective-dispersive equation

Considering all the interaction terms in equation (3.5) and simplifying, the complete three-dimensional solute transport equation can be written as:

$$\text{div} (D \text{grad} C) - U \text{grad} C - qC = \omega \frac{\partial C}{\partial t} + \omega \lambda C - qC_0 \quad \text{--------- (3.12)}$$
where "q" is positive for infiltration. $C_0$ is the concentration of infiltrated water and it was assumed zero. Therefore, equation (3.12) becomes:

$$\text{div}(D\ \text{grad}C) - \nabla \cdot \mathbf{q} = -K \frac{\partial C}{\partial t}$$

(3.13)

3.2 Averaging and two-dimensional equation

In practical application, any modeling effort must incorporate some level of simplification and averaging. Here a vertically averaged two-dimensional transport model was used. The averaging was performed by integrating the conventional three-dimensional equation (equation (3.13)) along the $z$-direction with the following assumptions:

i) Aquifer thickness is constant,

ii) Flow is horizontal,

iii) Coordinates $(x,y)$ are aligned along the principal directions of anisotropy,

iv) Aquifer is homogeneous along vertical axis, and

v) Any well (extraction or injection) is fully penetrating.

The integrated form of equation (3.13) can be written as:

$$\text{bdiv}(D\ \text{grad}C) - b\nabla \cdot (\mathbf{q}) = bK \frac{\partial C}{\partial t}$$

(3.14)

where $b$ is thickness of aquifer, $D$ is the two-dimensional dispersivity tensor, and $C$ is the vertically averaged solute concentration. Here $\text{div}$ and $\text{grad}$ are with respect to $x$ and $y$ only.
The first two terms of equation (3.14) can be written in their expanded forms as:

\[ \text{div}(\nabla \nabla \nabla C) = \frac{\partial}{\partial x} \left( \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left( \frac{\partial C}{\partial y} \right) + \frac{\partial}{\partial z} \left( \frac{\partial C}{\partial z} \right) \]

and

\[ b \nabla \text{grad} C = b \left[ \frac{\partial C}{\partial x} + \frac{\partial C}{\partial y} \right] \ \ \ \ \ \ \ \ \ \ (3.15) \]

Scheidegger (1960) derived a closed form for the dispersivity tensor by treating porous media as a bundle of tubes. For an isotropic medium and a unidirectional flow along x-axis \((U_x \neq 0, U_y = 0)\), he derived the following forms for the dispersivities:

\[ D_{xx} = D_L \alpha_L U_x + \omega d_0; \ \ D_{xy} = D_{yx} = 0; \ \ D_{yy} = D_T = \alpha_T U_x + \omega d_0 \ \ \ \ (3.16) \]

where \(D_L\) is longitudinal dispersion coefficient, \(D_T\) is transverse dispersion coefficient, and \(\omega\) is the total porosity of the medium. \(D_L\) and \(D_T\) have units of \([L^2/T]\). \(\alpha_L\) and \(\alpha_T\) are the longitudinal and transverse dispersivities, respectively, both with units of \([L]\).

Term \(\omega d_0\) in equations (3.16) is the contribution of molecular diffusion in the total dispersion activity. It has a very small value relative to \(\alpha_L U_x\) or \(\alpha_T U_x\) in most aquifer settings. Therefore, it comes into play only when the darcy velocity \(U_x\) is very small. The magnitudes of velocity to be used in this study, are high enough to make the diffusion term insignificant. Therefore, equation (3.16) can be modified as:

\[ D_{xx} = \alpha_L U_x \ \ \text{and} \ \ \ D_{yy} = \alpha_T U_x \ \ \ \ \ \ \ \ \ \ \ (3.17) \]
Substituting equations (3.15) and (3.16) in (3.14), taking $U_x = K_x i$, and simplifying, the following equation can be obtained:

$$\alpha_L \frac{K_x i}{\omega R} \frac{\partial^2 C}{\partial x^2} + \alpha_T \frac{K_x i}{\omega R} \frac{\partial^2 C}{\partial y^2} - \frac{K_x i}{\omega R} \frac{\partial C}{\partial x} \frac{(\omega \alpha + q)}{\omega R} C = \frac{\partial C}{\partial t} \quad (3.18)$$

In equation (3.18), "i" and $K_x$ are hydraulic gradient and hydraulic conductivity, respectively, along x-direction. However, it should be noted that if the equation (3.18) is applied for an isotropic and homogeneous medium, $K_x$ can be simply written as $K$ which is the average conductivity over the domain. Throughout this work, equation (3.18) will be termed as the "MODEL". All the factors which can affect the calculation of contaminant concentration are present in this equation. These factors are discussed in the next section.
4. **PARAMETERS OF THE SIMULATION MODEL**

Parameters of the simulation model, as shown in equation (3.18), are hydraulic conductivity (K), porosity (n), hydraulic gradient (i), dispersivities (\(\alpha_L, \alpha_T\)), retardation factor (R), infiltration rate (q), and the decay coefficient (\(\lambda\)). They will be discussed in this section with respect to their definition, variability, usual range of values found in the literature, and the range of values selected for this study. Some of them have been defined during formulation of the MCDEL. Only the remaining aspects of them will be discussed here. The hydraulic conductivity will be discussed in detail to include its statistical behavior.

4.1. **Hydraulic conductivity**

The definition of hydraulic conductivity goes back to the basic law of flow through porous media, Darcy's Law:

\[
Q = K A i
\]

(4.1)

where, Q is the volumetric fluid flow rate, A is cross-sectional area of the porous media and "i" is the hydraulic gradient. K in the equation is a proportionality constant termed the hydraulic conductivity.

From equation (4.1), the hydraulic conductivity can be redefined as the volumetric flow rate at which a fluid is transmitted through a unit cross-sectional area of an aquifer under a unit hydraulic gradient.
Hydraulic conductivity is a function of both media and the fluid. Experimentally it is established that $K$ can be defined as a function of both fluid and media property as:

$$K = \frac{\kappa \rho g}{\mu}$$  

(4.2)

where, $\rho$ is fluid density, $g$ is gravity, $\mu$ is dynamic viscosity of the fluid, and $\kappa$ is the specific or intrinsic permeability or simply the permeability of the medium and has a dimension $[L^2]$. 

In most groundwater applications, $\rho$, $g$, and $\mu$ are constant. Therefore, $K$ is a function of $\kappa$ [equation (4.2)] and can be considered as a property of the media only.

4.1.1 Uncertainties in hydraulic conductivity

Generally, hydraulic conductivity is estimated from analysis of slug or pump tests data obtained from individual well points. It is also determined by laboratory tests on samples from fields, analysis of grain size and porosity data at a well, etc.

Pump tests generally give the values of in situ hydraulic conductivities, and these values are, in effect, averaged over a large and representative aquifer volume. A slug-test also gives an average value for the media around the bore hole. Conductivities estimated from laboratory tests, grain size and porosity analysis are actually the point estimates of hydraulic conductivity (Freeze, 1979).

In any case, the hydraulic properties estimated by the above methods are the properties that apply at a small area around the
sampling point. All the above methods have their own simplified assumptions of calculating the K-values. At the same time, there can be errors in sampling, measurement, and interpretation of data. These all together introduce some level of uncertainty in the estimated values. However, the measured conductivities are assumed exact ignoring all the probable errors.

The scale of observation in analyzing the hydraulic conductivity data also plays an important role in the meaning and the value of conductivity at a point. For example, on a small scale, e.g., in a single pore, conductivity has no meaning. It will have an infinite or a very large value. Whereas, each soil grain will have a very low or a near zero conductivity. Conductivity values averaged over the thickness of the aquifer will be different from that of the individual strata. Also conductivity measured between two points horizontally separated (e.g., by a pump test) will be different depending on the distance between the two measuring points (Ashfield and Hyder, 1990).

While applying numerical models to contaminant transport equations, the conductivity values are assigned to the nodes of the domain. During solution of these equations, numerical models take these K-values as an average over a certain region around the nodes. This is equivalent to assigning conductivity values at every point on the domain. In reality, conductivity can not be measured at every point in the domain. Even if it is measured, it will be different from point to point. Therefore, the solution process also introduces error in the numerical concentration values.
4.1.2. Statistical Approach to Conductivity Analysis

From the above discussion, it is clear that the hydraulic conductivity cannot be measured with certainty. Some kind of uncertainty must be assigned in its estimated values and any rational analysis must recognize this uncertainty. To place this problem in a probabilistic framework, geostatistics has considered these type of properties as "variables" rather than parameters and more specifically as random variables which may take an infinite number of different values (DeMarsily, 1984).

Under this hypothesis, conductivity at a point is not represented by a single value, but by a probability distribution associated with it. Any particular value of conductivity at a point will be a realization of this distribution. However, it should be kept in mind that the conductivity at a particular point is not a random variable, it is a real value at least on the specified scale of measurement. But it is almost impossible to determine its value at every point with 100% certainty. By treating it as a random variable, it is recognized that although the conductivity at an unmeasured point cannot be estimated with certainty, the likelihood of the actual conductivity possessing certain value can be estimated. This likelihood can be expressed by a functional form of the probability distribution function (pdf) and associated parameters of the distribution. "Therefore, the primary motivation and advantage of conducting the analysis of conductivity from the probabilistic viewpoint is that the uncertainty that is always present can be quantified and the wide variety of analytical methods available from statistics can be utilized" (Ahlfeld and Hyder, 1990).
Greenkorn and Kessler (1969) have provided a definition of heterogeneity, nonuniformity, and anisotropy on the basis of statistical observations. They argue that if all geological formations display spatial variations in $K$, then under the classical definitions, there is no such thing as a homogeneous formation. They redefined a homogeneous formation as one in which the probability density function of hydraulic conductivity is nonmodal. That is, it shows variations in $K$, but maintains a constant mean and variance through space and the variance of the frequency distribution represents the degree of nonuniformity of the formation. They also defined the probability distribution function of $K$ as independent of orientation if the medium is isotropic; if it is dependent on orientation, the medium is anisotropic. They presented examples of frequency distributions (Figure 4.1) of $K$ for the four possible combinations of homogeneity and uniformity in an isotropic media.

Freeze (1975) has accepted these definitions and used them in his study. This study will also use these definitions and be limited to an isotropic, nonuniform, and homogeneous medium (Figure 4.1c). Freeze (1975) termed this type of formations as "stochastically homogeneous" or "statistically homogeneous but geologically heterogeneous". However, in traditional terminology, Figure 4.1a is referred to as being homogeneous and Figure 4.1c as being heterogeneous.
a) uniform, homogeneous  
\[
f(K) \quad K
\]

b) nonuniform, homogeneous  
\[
f(K) \quad K
\]

c) uniform, heterogeneous  
\[
f(K) \quad K
\]

d) nonuniform, heterogeneous  
\[
f(K) \quad K
\]

Figure 4.1. Frequency distributions for hydraulic conductivity \( K \), illustrating Greenkorn and Kessler's (1969) definitions of uniformity and homogeneity.

4.1.3. Review of statistics

In order to conduct statistical analysis of hydraulic conductivity, some of the basic statistical definitions and rules should be reviewed.

**Random Variables**

A random variable is a real-valued function defined on a sample space (Dougherty, 1990). If the set of values a random variable can assume is infinite, the random variable is called a continuous random variable; otherwise it is discrete. Capital letters are used to denote random variables and the corresponding lower case letters represent values of the random variable.
Any function of a random variable is also a random variable. If \( X \) is a random variable then \( Z = g(X) \) is a random variable as well.

**Probability**

If a random event can occur in \( N \) equally likely and mutually exclusive ways, and if \( N_A \) of these ways have an attribute \( A \), then the probability of the occurrence of the event having attribute \( A \) is \( N_A/N \).

It can be written as:

\[
\text{prob}(A) = \frac{N_A}{N} \quad (4.3)
\]

**Probability density function (pdf)**

Probability distributions of continuous random variables are smooth curves. The probability density function of a continuous random variable \( X \) is denoted by \( p_X(x) \). \( p_X(x) \) is not a probability and can have values exceeding one. Any function \( p_X(x) \) defined on the real line can be a probability density function if and only if

1. \( p_X(x) \geq 0 \) for all \( x \)

2. \( \int_{-\infty}^{\infty} p_X(x) \, dx = 1 \)

**Cumulative probability distribution function (cdf)**

The cumulative probability distribution function is denoted by \( P_X(x) \). It represents the probability that \( X \) is less than or equal to \( x \):

\[
P_X(x) = \text{prob}(X \leq x) \quad (4.4)
\]

\( P_X(x) \) is a probability (equation (4.4)) and must have values ranging from 0 to 1.
The probability density function and cumulative probability distribution function of a random variable $X$, evaluated at $X=x$, are related by

$$dP_X(x) = p_X(x) \, dx$$

or

$$P_X(x) = \int_{-\infty}^{x} p_X(t) \, dt \quad (4.5)$$

The probability that $X$ takes on a value between $a$ and $b$ is given by:

$$\text{prob} \left( a \leq X \leq b \right) = \int_{a}^{b} P_X(t) \, dt$$

$$= P_X(b) - P_X(a) \quad (4.6)$$

Therefore, $\text{prob}(a \leq X \leq b)$ is the area under the probability density function between $a$ and $b$. It can be shown that the probability of a random variable taking any particular value from a continuous distribution is zero in the following way.

$$\text{prob} (X=d) = \int_{d}^{d} P_X(t) \, dt$$

$$= P_X(d) - P_X(d) = 0$$

4.1.4. Distribution of hydraulic conductivity

Many hydrogeologists and petroleum geologists have used statistical distributions to provide a quantitative description of the degree of heterogeneity in a geological formation. There is now a large body of direct evidence to support the statement that the
probability density function of hydraulic conductivity is log-normal (Freeze, 1979).

If the variable $K$ is log-normally distributed, its histogram will look similar to the standard left-skewed log-normal curve and that of parameter $Y$, defined as $Y = \ln K$, will look like the standard "bell shaped" normal distribution curve. The log-normal distribution predicts that for a given conductivity field or site, we will tend to measure many values clustered about the mean with a few values much larger than the mean.

This distribution of hydraulic conductivity was first proposed by Law (1944) on the basis of core analysis data from a carbonate oil field reservoir. Bulnes (1946), Warren and Price (1961), and Bennion and Griffiths (1966) also found this to be the case in oil field reservoir rocks. McMillan (1966) analyzed the California Department of water resources transmissivity maps for the Los Angeles basin and found the distribution of hydraulic conductivities to be log-normal. Willardson and Hurst (1965), Brust et. al. (1968), and Davis (1969) supported the conclusion with regard to soils. In a recent study, Ahlfeld and Hyder (1990) conducted an investigation on the statistical behavior of hydraulic conductivity for aquifers of six river basins in Connecticut and concluded that it is log-normally distributed.

There are also a large number of indirect and theoretical evidence to the above conclusion. One of them is that the porosity is normally distributed and hydraulic conductivity can be estimated as an exponential function of porosity which makes hydraulic conductivity log-normally distributed. The grain size distribution is
reported to be log-normally distributed and the hydraulic conductivity can be related in a functional way to some representative grain size diameter \( d_{10} \). Davis (1969) has given a list of authors who have shown that the specific capacities of water wells (which are directly related to formation conductivities) are usually log-normally distributed.

4.1.5. Statistical Analysis of Hydraulic Conductivity

According to the Central Limit Theorem, if a random variable \( K \) is made up of the sum of many small effects, then \( K \) might be expected to be normally distributed (Haan, 1979). Similarly, if \( K \) is equal to the product of many small effects, that is if \( K = K_1 K_2 K_3 \ldots \), \( K_N \), then \( \ln K \) can be expected to be normally distributed. This can be proven by letting \( Y = \ln K \) so that \( Y = \ln (K_1 K_2 K_3 \ldots \ K_N) = \ln K_1 + \ln K_2 + \ldots \ldots + \ln K_N \). Since the \( K \)'s are random variables, the \( \ln K \)'s are also random variables and \( Y = \ln K \) is a random variable made up from the sum of many other random variables.

If \( Y \) is normally distributed with mean \( \mu_Y \) and variance \( \sigma_Y^2 \), its probability distribution function is given by:

\[
p_Y(y) = \frac{1}{\sigma_Y\sqrt{2\pi}} \exp\left(-\frac{1}{2} \left(\frac{y-\mu_Y}{\sigma_Y}\right)^2\right), \quad -\infty < y < \infty \quad (4.7)
\]

The distribution of \( K \) can be found from

\[
p_K(k) = p_Y(y) \left| dy/dk \right| \quad (4.8)
\]
Since \( Y = \ln K \), therefore
\[
\frac{dy}{dk} = \frac{1}{k} \quad k > 0
\]
and
\[
p_K(k) = \frac{1}{k \sigma_y \sqrt{2\pi}} \exp\left[-\frac{1}{2} \left(\frac{\ln k - \mu_y}{\sigma_y}\right)^2\right] \quad k > 0 \quad (4.9)
\]

Equation (4.7) gives the distribution of \( Y \) as a normal distribution with mean \( \mu_y \) and variance \( \sigma_y^2 \) and equation (4.9) gives the distribution of \( K \) as the log-normal distribution with the same parameters \( \mu_y \) and \( \sigma_y^2 \).

**Estimation of parameters:**

In field estimation of the distribution parameters, conductivity values are measured at different points. Suppose, there are \( N \) observations of the variable \( K \) and the parameters for their distribution has to be determined. As shown above, the probability distribution functions of both \( K \) and \( Y \) are defined by the two parameters \( \mu_y \) and \( \sigma_y^2 \). These two parameters can be estimated from sample mean \( \bar{Y} \) and variance \( s_y^2 \), respectively, by following the procedure described below.

Under the assumption that the probability distribution function of variable \( K \) is log-normal and the \( K \)-field has a stationary correlation structure, \( \overline{K} \) is given by the geometric mean (Gelhar, 1976, Bakr et. al., 1978, Gutiahr et. al., 1978, DeMarsily, 1986). The geometric mean is defined as the \( n \)th root of the product of \( n \) observations:

\[
\overline{K} = (K_1K_2K_3\ldots\ldots K_N)^{1/N} \quad (4.10)
\]
Taking logarithms of both sides of (4.10) yields

$$\ln(\overline{K}) = \frac{1}{N} \sum_{i=1}^{N} \ln(K_i)$$  \hspace{1cm} (4.11)

Equation (4.11) is equivalent to the arithmetic average of \(\ln(K)\).
The quantity \(\ln(\overline{K})\) is taken as the mean of the variable \(Y\) and denoted as \(\overline{Y}\).

\(S_Y^2\) is the variance of \(\ln(K)\) and is defined as:

$$S_Y^2 = \frac{1}{N-1} \sum_{i=1}^{N} (Y_i - \overline{Y})^2$$  \hspace{1cm} (4.12)

where \(Y_i = \ln(K_i)\).

In this study, a slightly different approach of estimation of distribution parameters was used. In most of the field study, the variance of conductivity field is expressed by \(S_Y^2\). Therefore, its value can be obtained directly from the literature. Next is the estimation of the mean value \(\mu_Y\). But in field measurements, only the expected values of \(K\) \([\overline{K} \text{ or } E(K)]\) is reported. This leads to the following calculation of expected value of \(K\) from the distribution of \(Y\).

\(Y = \ln K\). So, \(K = e^Y\). Therefore,

$$\overline{K} = E(K) = E(e^Y)$$

$$= \int_{-\infty}^{\infty} e^y p_Y(y) \, dy$$

$$= \exp(\mu_Y + \frac{1}{2} \sigma_Y^2)$$ \hspace{1cm} [Ang, 1975]
By arranging,
\[ \mu_y = \ln(\bar{K}) - \frac{1}{2} \sigma_y^2 \]  (4.13)

Reported \( S_y^2 \) values from the literature can be taken as an estimate of \( \sigma_y^2 \) and it can be used in equation (4.13) to determine the mean of the distribution. Finally, equation (4.9) can be used to obtain the probability distribution function of \( K \).

Calculating probabilities for realizations from the pdf

As the variable \( K \) is expressed in terms of its pdf and realizations have to be drawn from it to calculate probability of violation, there will be a need to calculate the probabilities associated with the selected realizations.

These probabilities can be related to the corresponding relative frequencies of the realization values by considering an experiment whose outcome is the random variable \( K \). Let \( p_K(k) \) be the probability density function of the variable \( K \). The probability that a single trial of the experiment will result in an outcome between \( K=k_1 \) and \( K=k_2 \) is given by \( \text{prob}(k_1 \leq K \leq k_2) \). From equation (4.6),

\[ \text{prob}(k_1 \leq K \leq k_2) = \int_{k_1}^{k_2} p_K(k) \, dk = P_K(k_2) - P_K(k_1) \]  (4.14)

In \( N \) independent trials of the experiment, the expected number of outcomes \( (n_e) \) in the interval \( k_1 \) and \( k_2 \) would be:

\[ n_e = N \left[ P_K(k_1) - P_K(k_2) \right] \]  (4.15)
The expected relative frequency \( f_e \) of outcomes in the interval \( k_1 \) and \( k_2 \) is:
\[
f_e = \frac{n_e}{N} = \left[ P_K(k_1) - P_K(k_2) \right] \quad (4.16)
\]

If \( k_i \) represents the midpoint of an interval of \( K \) bounded by \( K_j + \Delta K_j/2 \) to \( K_j - \Delta K_j/2 \), then from equation (4.16), the expected relative frequency of outcomes of repeated and independent trials of the experiment in this interval will be given by:
\[
f_{k_i} = P_K(k_i + \Delta k_i/2) - P_K(k_i - \Delta k_i/2) \quad (4.17)
\]

\( f_K \) in equation (4.17) is taken as the relative frequency or the probability associated with the realization \( k_i \) when it is drawn from the distribution \( p_K(k) \). Equation (4.17) in fact calculates the area under \( p_K(k) \) between \( K_j + \Delta K_j/2 \) and \( K_j - \Delta K_j/2 \).

4.2. Porosity

If the total unit volume (\( V_T \)) of a soil is divided into the volume of the solid portion \( V_s \) and the volume of the voids \( V_v \), the porosity \( \omega \) is defined as \( \omega = V_v/V_T \). It is usually expressed as a decimal fraction or a percent.

Porosity can range from zero or near zero to more than 0.6 (Domenico, 1990). Generally, rocks have lower porosities than soils; gravels, sands, and silts have lower porosity values than soils rich in clay minerals; and poorly sorted media have lower porosity than well-sorted media.

Davis (1969) reported porosity values of 0.25 for gravel and 0.5 for silt. DeMarsily (1979) gives a range of 0.15-0.48 for sand. For unconsolidated granular deposits, Freeze (1979) reports a range
of 0.2-0.4 for their porosity. Porosity values are normally distributed (Freeze, 1975).

In this study, an average porosity value of 0.3 was chosen.

4.3. Hydraulic gradient

It is the slope of water table or peizometric surface. A uniform hydraulic gradient of 0.005 ft/ft was chosen for this study. This value is typical of Connecticut’s stratified drift aquifers (Ahfeld and Hyde, 1990).

4.4. Dispersivity

Dispersivity values are scale dependent. The greater the area over which it is measured, the larger the value seems to be. At laboratory scale, it is of the order of mm to cm. At a small field scale, it is of the order of cm to dm. At large field scale, it takes values of the order of meters and even tens of meters.

Very little work has been done to determine field values of dispersivities. Values of $\alpha_1$ as large as 100m and those of $\alpha_1$ as large as 50m have been used in mathematical simulation studies of the migration of large contaminant plumes in sandy aquifers (Pinder, 1973; Konikow and Bredehoef, 1974). Freeze (1979) reported a range of 39-200 ft for longitudinal dispersivity of alluvial sediments and a range of 13-98 ft for transverse dispersivity of the same type of rock. For a glacial deposit, $\alpha_1$ was found to be 69 ft and $\alpha_1$ was found to be 13 ft (Freeze, 1979). Larger values are found for fractured salt which has more heterogeneities (Fetter, 1987).
Values of $\alpha_t$ are found to be dependent on grain-size and grain-size distribution and are independent of grain shape, roughness, and angularity (Freeze, 1979). Generally, $\alpha_t$ has values between 1/5 and 1/100 of $\alpha_L$. In this study $\alpha_t$ was set at 100 ft and $\alpha_t$ was taken as $\alpha_t/10$.

4.5. Retardation Factor (R)

Priddle and Jackson (1991) determined retardation factors for several VOCs from laboratory column tests and from field test data. They reported a range of 1-14 for R values. Most of the values were between 1 and 5. In this study, a range of 1-5 was chosen.

4.6. Infiltration

A range of 6-24 inches of infiltration per year was selected.

4.7. Decay Coefficient

Decay coefficients are calculated from half lives. A range of 1-100 years for half life was chosen in this study.
5. PARAMETERS OF THE PRIORITIZATION MODEL

Prioritization parameters are the factors which can determine the priority of a site for its remediation needs. Mathematically, they are the parameters which can affect the probability of violation of water quality standards at a receptor. They can be of two kinds. One include parameters affecting the concentrations directly. These can be obtained from the formulation of the MODEL. Others can be factors which indirectly affect the concentration or the violation probability.

5.1. Parameters from MODEL

In section 4, all of the individual factors involved in calculation of concentrations were discussed. Some of the factors have independent effects on concentrations while the others have combined effects. This can be observed by taking the parameters of equation (3.18) in their most concise form. They can be combined into lumped parameters by defining:

\[ \alpha_T = \beta \alpha_L; \quad U' = \frac{U_L}{\alpha R}; \quad \Lambda' = \frac{\alpha_L + q}{\alpha R} \]

Considering these new factors, equation (3.18) becomes:

\[ \alpha_L U' \left[ \frac{\partial^2 C}{\partial x^2} + \beta \frac{\partial^2 C}{\partial y^2} \right] - U' \frac{\partial C}{\partial x} - \Lambda' C = \frac{\partial C}{\partial t} \quad \text{(5.1)} \]

The MODEL, while solving the transport equation (3.18), does not consider all the components of \( \Lambda' \) or \( U' \) separately, rather it takes
them as a single parameter of the differential equation as shown in equation (5.1) or in other words the MODEL actually solves equation (5.1) to produce the concentration values. As long as the value of $A'$ or $U$ is constant, regardless of the values of their individual components, the MODEL will give the same results of contaminant concentrations under a particular contamination scenario. Therefore, parameters $\alpha$, $U$, and $A'$ were chosen as the prioritization parameters for the violation study. $\alpha$ is the longitudinal dispersivity, $U$ is the retardation velocity, and $A'$ is the attenuation factor. The factor $\beta$ was chosen as 0.1 in the previous section. The range of values of these new factors can be obtained from that of their constituents.

5.1.1. Attenuation Factor ($A'$)

The attenuation factor represents the rate of disappearance of the solute concentration ($C$) with time and has a dimension of [1/T]. It contains all the interaction terms of the MODEL.

The infiltration rate ($q$) in equation (3.19) was in units of [L/T] but in the selected MODEL it ($q'$) was in units of [L/T]. This $q$ should be distributed over the entire aquifer thickness ($b$) to match with $q$. Therefore, the following form of equation was used to calculate $A'$:

$$A' = \frac{\alpha \lambda + q'b}{\alpha R} \quad (5.2)$$

A constant aquifer thickness of 40 ft was chosen for this study. Therefore, $A'$ is a function of three variables with $R$ as a multiplication factor. The range of $A'$ can be calculated from that of its constituents. To show its variation, contours of $A'$ were plotted
against the half life ($T_{1/2}$) and the infiltration rate ($q'$). The contours are shown in Figures 5.1, 5.2, and 5.3. A range of 0.01-0.2 was chosen for $\lambda'$ from these Figures because it encompasses most of the parts of its values.

5.1.2. Retardation Velocity ($u'$)

Its formulation was discussed in adsorption section during MODEL formulation. All of its components except $K$ have deterministic values.

Therefore,

$$E(u') = E\left(\frac{Ki}{\omega R}\right) = \frac{i}{\omega R} E(K) \quad \text{(5.3)}$$

which shows that $E(K)$ will behave in the same way as $E(u')$. For a given site, it is more likely to have estimates of $E(K)$ than that of $E(u')$. Therefore, the probability plots are presented in terms of $E(K)$. However, the plots are equally applicable for $E(u')$. The corresponding value of $E(u')$ can be obtained by multiplying $E(K)$ with $i/\omega R$. $E(K)$ has a range of 50-150 ft/day. This produces a range of 0.28-0.84 ft/day for $E(u')$. Therefore, the results are applicable for any values of $E(u')$ within this range.

5.1.3. Longitudinal Dispersivity ($\alpha_L$)

It is an independent parameter and it was discussed among the MODEL parameters. The entire study was conducted for a single $\alpha_L$ of 100 ft.
Figure 5.1. Contours of attenuation factors (1/yr) for R=1.
(q=infiltration, in/yr)
Figure 5.2. Contours of attenuation factors (1/yr) for R=3.
(q'=infiltration, in/yr)
5.2. Other Parameters

Some other factors, which are not included in MODEL parameters, can also affect the violation probability independently. Those will now be identified and their variability will be discussed.

5.2.1. Initial Plume Length (L)

The first among them is the length of the initial plume (L), because it defines the initial conditions for all subsequent simulations and therefore affects the probability of violation.

The initial plumes were obtained by introducing a continuing point source of concentration of 1 unit in the simulation domain. The domain was assumed initially free from contamination by setting the background concentration level to zero. The MODEL was run with this source for two different time lengths to produce the two initial plumes. The source point of the plumes has a concentration level of 1 unit. Length of the plumes was defined as the distance between this source point and a point axially downstream of the source point with a concentration level of .001 unit.

5.2.2. Receptor Distance (D)

Another independent parameter is the distance of receptor from source. It can affect the probabilities of violation independent of other parameters. The closer the receptors are the more will be the probability of the contaminants reaching it at higher concentrations.

In this work, the flow field between source and receptor was assumed unidirectional. This requires a single aquifer formation
throughout the entire domain. In practice, this can be valid for relatively small flow fields. Hydrogeologic barriers were assumed to be within 5500 ft of the source and a range of 1700-5500 ft was chosen for receptor distance. Receptor distance was defined as the distance between the source point of the initial plume and the receptor.

5.2.3. Water quality standard (C*)

Water quality standard should also be taken as a prioritization parameter due to its own independent effect on probability calculations. If the standard is set to a low value, for a given contamination activity, the probability of violation will be higher.

Values of water quality standard depend on the purpose for which the water is being used. In many regions, the most important uses of groundwater are for agriculture. In these areas, standards are set relative to criteria or guidelines established for livestock or irrigation. The list of constituents and the concentration limits are not as stringent as for drinking waters. Also it can be different for different constituents of interest. Considering these factors, a range of .001-.00001 unit, relative to source concentration of 1 unit, was chosen as the standard.

5.2.4. Variance of hydraulic conductivity (σ_y)

Hydraulic conductivity is defined with probability distribution function. The expected value of the distribution is an independent parameter. In order to describe the distribution completely, the variance of the distribution also has to be specified. Variance
expresses the degree of variability or the spread of the distribution of $K$ in an aquifer system. Because of the log-normal distribution of $K$, variance is generally reported on its log-transformed values, i.e., on variable $Y = \ln K$.

Freeze (1975) has provided a table that shows the range for standard deviation on $Y \{\sigma_Y\}$. These values, which are independent of the units of measurement, were usually in the range of 0.5-1.5. Delhomme (1979) provided a range of 0.8-2.3 for $\sigma_Y$. In the study by Ahlfeld and Hydor (1990), the range of $\sigma_Y$ was found to be 0.42-0.97 for the Connecticut Stratified Drift Aquifer. For this study, a variance of 0.5 was selected.
6. DEVELOPMENT OF THE PRIORITIZATION MODEL

The main body of this work is the development of the prioritization model. The underlying idea is to transform the uncertainty in hydraulic conductivity into that of contaminant concentration and eventually produce the probability of exceedence.

So far a set of seven independent parameters have been identified. The probability of violation will be affected by each of them independently. However, in the scope of this study, the work was conducted for two plume lengths (L), a single dispersivity ($\alpha_L$), and a single variance ($\sigma_Y^2$). Four parameters $A', E(K), D,$ and $C^*$ were studied and the contour plots were produced by taking any two of them on the two axes and keeping the other two parameters constant. The following Table lists a description of the parameters and their values used in this study.

<table>
<thead>
<tr>
<th>Variable</th>
<th>Explanation</th>
<th>Number of values used</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E(K)$</td>
<td>Expected value of the Hydraulic Conductivity</td>
<td>25</td>
<td>30-150 (ft/day)</td>
</tr>
<tr>
<td>$\sigma_Y^2$</td>
<td>Variance of conductivity field</td>
<td>1</td>
<td>0.5</td>
</tr>
<tr>
<td>$L$</td>
<td>Length of the initial plume</td>
<td>2</td>
<td>500, 1000 ft</td>
</tr>
<tr>
<td>$D$</td>
<td>Receptor distance</td>
<td>20</td>
<td>1700-5500 ft</td>
</tr>
<tr>
<td>$C^*$</td>
<td>Water quality standard</td>
<td>1</td>
<td>1e-6 -1e-2</td>
</tr>
<tr>
<td>$A'$</td>
<td>Attenuation factor</td>
<td>20</td>
<td>0.01 - 0.2/yr</td>
</tr>
<tr>
<td>$\alpha_L$</td>
<td>Longitudinal Dispersivity</td>
<td>1</td>
<td>100 ft</td>
</tr>
</tbody>
</table>
The first step in the procedure is the calculation of contaminant concentrations at receptors using different values of the study parameters in the MODEL. A simulation domain is necessary for this purpose. In section 6.1, this simulation domain will be described.

After obtaining the concentrations, the next step is the calculations of probabilities of violations. In section 6.2, the procedure of calculating the probability of violation, at a particular receptor distance, for a single probability distribution of K will be discussed. In section 6.3, the procedure will be extended to calculation of probabilities for many distributions. Finally, the procedure to calculate probability points to construct the contour plots (like Figures A.1 - A.37) will be discussed.

6.1. Simulation Domain and Boundary Conditions

A 25X60 grid of 100 ft square was chosen as the simulation domain (Figure 6.1).

\[ \text{AB} = \text{CD} = 6000 \text{ ft} \]
\[ \text{AD} = \text{BC} = 2500 \text{ ft} \]

Figure 6.1. Simulation domain.
Sides AB and CD of Figure 6.1 were taken as no flow boundaries. Sides AD and BC were taken as constant head boundaries to produce a uniform hydraulic gradient along x-direction from AD towards BC. Dispersive flux (\( \partial C/\partial n \)) was set to zero along all sides for all time.

6.2. **Probability of violation for a single pdf of K**

A single pdf of K is defined by a single E(K) and a single variance. The pdf \([p_k(k)]\) can be obtained from equation (4.9).

6.2.1. **Defining Probability of Violation**

From the transport equation, keeping all other transport parameters constant, the following relationship between variables C and K can be written:

\[
C = \text{MODEL}(K) \quad \text{----------------------- (6.1)}
\]

The result of equation (6.1) is a time-history of concentration. The time-history can be recorded at various points along the domain located at different receptor distances from the source. At any point downgradient of the source, if the initial concentration is lower than the source concentration, there will be a gradual increase in concentration as the contaminant plume starts moving downgradient. The concentration will reach a maximum value \((C_{\text{max}})\) when the center of mass of the plume is just over the recording point. Concentration will start dropping as the plume center of mass crosses the point. The magnitude of the maximum concentration \((C_{\text{max}})\) can be identified for each of the recorded time-histories obtained from the MODEL simulations.
The event that $C_{\text{max}}$ equals or exceeds the water quality standard ($C^*$) was called the "violation" or "exceedence". The probability of such an exceedence is the target parameter to estimate.

The MODEL was run for sufficient time-length to ensure that the center of mass of the source passed the points where the concentrations were recorded. Therefore, the recorded concentration-time history contains the maximum concentration value ($C_{\text{max}}$) that can ever be achieved at the receptor. The probability of violation calculated from this $C_{\text{max}}$ is the maximum possible probability at a receptor.

The magnitude of $C_{\text{max}}$ depends on the value of hydraulic conductivity. For higher conductivity values, the groundwater will flow faster. The source center of mass will reach a receptor in a shorter time. As the attenuation is time dependent, degradation of the contaminant will be less. Therefore, the concentrations downgradient will be higher and will result in a higher chance of violation. Conversely, for lower conductivity values, travel time of the plume to receptor will be higher, natural attenuation will be more significant and the concentrations will be lower and in turn, the chance of violation will be less.

The conductivity value over the domain is expressed by a probability distribution function $p_K(k)$ and the probability of exceedence will be dependent on this distribution. Therefore, the violation probability can be written as:

\[
\text{Probability of violation} = \text{prob}(C_{\text{max}} \geq C^* | p_K(k), \text{all other parameters}) \quad (6.2)
\]
6.2.2. Monte Carlo Simulation

Calculation of $\text{prob}(C_{max} \geq C^*)$ requires a distribution of $C_{max}$. To obtain this distribution, the traditional Monte Carlo Simulation method can be applied. It is a common technique to derive the distribution of a dependent random variable (in this case $C_{max}$) when the distribution of the independent random variable (in this case $K$) is known.

In Monte Carlo Simulation, numerous realizations of the dependent random variable are produced and the distribution of these realizations is examined. If sufficient realizations are generated, the approximate distribution will approach the actual distribution of the dependent variable. Each realization of the dependent variable will require a realization of the hydraulic conductivity field and a corresponding simulation of that conductivity field by using the MODEL.

Choosing Realizations For Monte Carlo Simulation

Choosing realizations for the Monte Carlo Simulation technique is an important factor which affects the cost and effectiveness of the Method. The conventional way of choosing realizations of independent variable is the Random Sampling Technique. In this method, the realizations are drawn randomly from the selected distribution. However, this method requires too many realizations and at the same time there are uncertainties as to whether or not all portions of the pdf are sampled. Mackay (1979) concluded that the Stratified Sampling Technique improves the estimators over the
Random Sampling Method. In the Stratified Sampling Technique, all parts of the sample space are represented by input values.

For this method, a particular probability value is assigned to each of the realizations drawn from the pdf of the input variable (Mackay, 1979). The sample space of \( K \) (the input variable) is partitioned into \( N \) equal disjoint strata as \( S_j \) (\( j = 1, \ldots, N \)). Let

\[ p_j = \text{prob}(K \in S_j) \]

represent the size of \( S_j \). The midpoint of \( S_j \) is taken as the representative sample value for strata \( S_j \) and is called \( K_j \). The probability \( p_j \) is assigned to this \( K_j \)-value. These \( p_j \)-values can be calculated from equation (4.17). The technique proceeds by producing \( N \) realization of \( K \)-values \( (K_j) \) and the probabilities \( (p_j) \) associated with them.

These \( N \) realizations of \( K \) \( (K_j) \) were used in the MODEL to produce corresponding \( N \) realizations of the dependent variable \( C_{\text{max}} \). The histogram of variable \( C_{\text{max}} \) can be constructed to calculate

\[ \text{prob}(C_{\text{max}} \geq C^*) \]

The ultimate product of this work are probability contour plots. Each contour plots require many probability points each of which has to be calculated from independent histograms of the variable \( C_{\text{max}} \). While conducting the sensitivity analysis of the probability of violations over the range of the prioritization parameters, an enormous number of histogram constructions would be involved making the proposed ranking procedure essentially impractical. Alternately, procedures for large numbers of similar calculations (construction of histograms and calculation of probabilities) can be automated for economic use of computer time. Therefore, an
alternative procedure was used which efficiently calculates these probabilities and yet does not lose the accuracy in calculations. For these reasons, an approximation to the traditional Monte Carlo Simulation technique, described in the sections to follow, was used in this study to calculate these numerous probability values.

6.2.3. Approximation of Monte Carlo Simulation

A typical pdf of the variable $C_{\text{max}}$ may be similar to Figure 6.2.

$$f(C_{\text{max}})$$

$C_{\text{max}}$  $C^*$

Figure 6.2. Typical pdf of variable $C_{\text{max}}$

The prob($C_{\text{max}} \geq C^*$) is the shaded area under the pdf at right side of $C^*$ (Figure 6.2). Therefore, the probability calculations can be limited to only this portion of the pdf.

As the probability of violation is a measure of the number of $C_{\text{max}}$'s equal to or greater than $C^*$ among the total number of $C_{\text{max}}$'s, an additional variable "$g$" can be introduced to identify these high magnitudes. These $C_{\text{max}}$'s will be in the shaded region of Figure 6.2.
The variable "g" can be defined such that it will take a value of 1 if $C_{\text{max}}$ exceeds or equals the standard $C^*$; otherwise it will take a value of zero. Mathematically,
\[ g = 1, \text{ if } C_{\text{max}} \geq C^* \]
and
\[ g = 0, \text{ if } C_{\text{max}} < C^* \]  
(6.3)

Variable "g" will be called the "violation variable". From equation (6.3), $\text{prob}(C_{\text{max}} \geq C^* \mid p_k)$ can be taken as the probability of variable "g" taking value of 1 when the corresponding $K$-values are drawn from a probability distribution function $p_K(k)$. In other words, $\text{prob}(C_{\text{max}} \geq C^* \mid p_k) = \text{prob}(g=1 \mid p_k)$.

There are $N$-values of the "g" variable. Variable "g" can be considered as an array $g_j$, $j = 1, \ldots, N$. Some of the "g"-values will be 1 in case of violation and the rest will be 0 for no violation. Therefore, for a particular realization of $K$, $\text{prob}(g=1)$ has two values; either one or zero. In other words, for a given $K$, the outcome "g" is deterministic. The realizations have their own probability of occurrence and all of these probabilities will add up to 1. The calculation of probabilities of these types of quantities, whose occurrence is accompanied by the occurrence of another variable, can be performed by the Total Probability Theory.

**Total Probability Theory**

If $K_1, K_2, \ldots, K_N$ represent a set of mutually exclusive and collectively exhaustive events, the probability of another event A, whose occurrence is accompanied by the occurrence of these events,
can be defined by the total probability through equation (6.4) 
(Daugherty, 1990).

\[ \text{prob}(A) = \sum_{j=1}^{N} \text{prob}(A \mid K_j) \text{prob}(K_j) \]  \hspace{1cm} (6.4)

Event A can be taken as the event \( g=1 \). The \( \text{prob}(K_j) \) values can be determined from equation (4.19). \( \text{Prob}(A \mid K_j) \) is probability of the event \( g=1 \) given that the event \( K=K_j \) has occurred. Therefore, equation (6.4) can be modified as:

\[ \text{prob}(g=1) = \sum_{j=1}^{N} \text{prob}(g=1 \mid K_j) \text{prob}(K_j) \]

\[ = \text{prob}(C_{\text{max}} \geq C^*) \] \hspace{1cm} (6.5)

\( \text{Prob}(g=1 \mid K_j) \) in the above equation is a one-dimensional array with values starting from 0's for lower realizations of \( K \) and ending with 1's for higher realizations. Therefore, it can be denoted as \( g(j) \), to represent \( \text{prob}(g=1) \) for realization \( K_j \) and the equation (6.5) can be modified accordingly:

\[ \text{prob}(C_{\text{max}} \geq C^*) = \sum_{j=1}^{N} g(j) \text{prob}(K_j) \] \hspace{1cm} (6.6)

Equation (6.6) requires that the \( N \)-realizations be drawn from the entire sample space of \( p_K(k) \), probability values be assigned to all of them, and MODEL be run \( N \) times. This is a very tedious job because the range of \( K \)-values in \( p_K(k) \) are from 0 to \( \infty \) and an infinite number or at least a very large number of realizations have to be drawn and the MODEL has to be run as many times as the number of realizations.
However, the number of simulations can be narrowed down by keeping in mind the characteristics of the violation variable \( g \) and equation (6.6). A typical plot of \( g(j) \) vs. \( K_j \) can be shown by Figure 6.3.

![Plot of \( g(j) \) or \( \text{prob}(g(j)=1) \) vs. \( K_j \)](image)

**Figure 6.3.** Plot of \( g(j) \) or \( \text{prob}(g(j)=1) \) vs. \( K_j \)

For very low values of \( K_j \), concentrations will be very low at a receptor. For most of the cases, they may not exceed the standard and therefore variable \( g \) will be zero. For any \( K_j \) (say \( K_L \)), if \( g \) takes a value of zero, it will be zero for all the \( K_j \) values lower than \( K_L \). This will make \( g(j) \) of equation (6.6) zero. Therefore, for these realizations, equation (6.6) will become zero which means they are contributing nothing in calculating the probability of violation. This indicates that there is no need to run the MODEL or use equation (6.6) for realizations lower than some chosen minimum value \( K_{j\min} \).

Therefore, equation (6.6) can be modified as:

\[
\text{prob}(C_{\text{max}} > C^*) = \sum_{j = j_{\min}}^{N} g(j) \text{prob}(K_j) \quad (6.7)
\]
As $K_{jmin}$ is the first realization, $jmin$ can be set equal to 1. Equation (6.7) can be written as:

$$\text{prob}(C_{max} \geq C^*) = \sum_{j=1}^{N} g(j) \text{prob}(K_j)$$  \hspace{1cm} (6.8)

However, if the water quality standard does exceed the concentration corresponding to this $K_{jmin}$, it will also exceed the concentration values for all other $K_j$'s. This will make $g(j)$ equal to 1 for all $j$'s. Therefore, equation (6.8) will become:

$$\sum_{j=1}^{N} g(j) \text{prob}(K_j) = \sum_{j=1}^{N} 1 \cdot \text{prob}(K_j) = \sum_{j=1}^{N} \text{prob}(K_j)$$

$$= \int_{0}^{\infty} p_K(\xi) \, d\xi = 1$$  \hspace{1cm} (6.9)

A similar simplification can be made by keeping the largest value of realizations at a fixed magnitude. The $g(j)$'s will be 1 for higher $K_j$'s. Once for some $K_j$ (say $K_M$), if it takes a value of 1, it will keep doing so for all $K_j$ values higher than $K_M$. A maximum $K_j$ value ($K_{jmax}$) can be chosen such that, when it is used in the MGDEL, $g(jmax)$ will be 1 for most of the combinations of the study parameters. This will ensure that $g(j)$ will be 1 for all the realizations with values higher than $K_{jmax}$. For these realizations, the quantity $\text{prob}(K_j)$ of equation (6.8) is being multiplied by 1's and then added together; this can be expressed as:

$$\sum_{j=j_{max}+1}^{N} g(j) \text{prob}(K_j) = \sum_{j=j_{max}+1}^{N} 1 \cdot \text{prob}(K_j)$$
\[
= \sum_{j = j_{\text{max}} + 1}^{N} \text{prob}(K_j) = \int_{K_{j_{\text{max}} + 1}}^{x} p_K(\xi) \ d\xi \tag{6.10}
\]

Using equation (6.10) in equation (6.8):

\[
\text{prob}(C_{\text{max}} \geq C^*) = \sum_{j = 1}^{j_{\text{max}}} g(j) \text{prob}(K_j) + \int_{K_{j_{\text{max}} + 1}}^{x} p_K(\xi) \ d\xi \tag{6.11}
\]

The last term of equation (6.11) can be calculated by:

\[
\int_{K_{j_{\text{max}} + 1}}^{x} p_K(\xi) \ d\xi = 1 - \int_{0}^{K_{j_{\text{max}}}} p_K(\xi) \ d\xi = 1 - \sum_{j = 1}^{j_{\text{max}}} \text{prob}(K_j) \tag{6.12}
\]

\(K_{j_{\text{min}}}\) was chosen 10 ft/day. To calculate \(\text{prob}(K_j)\)'s using equation (4.19), an interval of integration (\(\Delta K_j\)) is required. This was also chosen to be 10 ft/day. Therefore, from equation (4.9)

\[
\begin{align*}
\text{prob}(K_j) &= \int_{K_j - 5}^{K_j + 5} p_K(\xi) \ d\xi \tag{6.13} \\
\text{prob}(K_{j_{\text{min}}}) &= \text{prob}(K_j = 10) = \int_{0}^{15} p_K(\xi) \ d\xi \tag{6.14}
\end{align*}
\]

\(C_{\text{max}}\) may not exceed some higher values of \(C^*\) at \(K_{j_{\text{max}}}\). This will make the first part of equation (6.11) zero. However, it will exceed the \(C^*\) for some \(K_j\)'s greater than \(K_{j_{\text{max}}}\). This higher \(K_j\) is not
known because the MODEL was run only for realizations up to $K_{j_{\text{max}}}$. If this unknown realization is denoted by $K_{j_{\text{u}}}$, the equation (6.11) becomes:

$$\text{prob}(C_{\text{max}} > C^*) = \int_{K_{j_{\text{u}}}}^{\infty} p_K(\xi) d\xi = S \text{ (suppose) \quad (6.15)}$$

The quantity $S$ will be different for different values of $K_{j_{\text{u}}}$. It will be maximum for the lowest $K_{j_{\text{u}}}$ ($K_{j_{\text{max}}+1}$). For $E(K) = 150$ ft/day and $\sigma^2_K = 0.5$, $S$ is 0.011. For any $E(K) < 150$ ft/day and $K_{j_{\text{u}}} > K_{j_{\text{max}}+1}$, the quantity $S$ is less than 0.011. However, for all cases, whenever $g(j_{\text{max}})$ becomes zero, quantity $S$ was taken as 0.011. Due to this simplification, the obtained violation probabilities were overestimated. In the contour plots, probability levels were started from 0.1. Therefore, the above simplification does not affect the results of this study.

Combining equations (6.11) and (6.12), the final form of the probability of violations becomes:

$$\text{prob}(C_{\text{max}} > C^*) = \sum_{j=1}^{j_{\text{max}}} g(j) \text{ prob}(K_j) + \sum_{j=1}^{j_{\text{max}}} \text{prob}(K_j) \quad (6.16)$$

Introduction of equation (6.16) has significantly reduced the computation effort to only running the MODEL for $K_j$ values between $K_{j_{\text{min}}}$ and $K_{j_{\text{max}}}$. If there are $M$ realizations between this range, then the MODEL run number will be equal to $M$.

The procedure up to equation (6.16) gives the probability of violation for a single distribution of hydraulic conductivity (defined by a single expected value of $K$ and a variance), keeping all other parameters constant, and produces one probability value.
6.3. Calculating Probabilities for Many Distributions

If there are \( P \) expected values of \( K \) and \( Q \) chosen variances, a total of \( P \times Q \) distributions will be obtained. If \( M \) realizations are to be drawn from each of them, to calculate the violation probabilities for all of these distributions, \( M \times P \times Q \) realizations have to be drawn and MODEL should be run \( M \times P \times Q \) times to use the equation (6.16).

This enormous computational effort can be reduced by making a simplification to the process of choosing realizations for the selected distributions of \( K \). Values of \( K_{\text{min}} \) and \( K_{\text{max}} \) can be kept the same for all the distributions and the range between \( K_{\text{min}} \) and \( K_{\text{max}} \) can be divided into equal portions. This will result in the same number (suppose \( R \)) of realizations of the same magnitudes for all the distributions of \( K \).

In this study, \( K_{\text{min}} \) and \( K_{\text{max}} \) were taken as 10 ft/day and 600 ft/day, respectively, with an interval of 10 ft/day. This implies 60 realizations. Therefore, all the distributions now have these 60 realizations with \( K_j = 10, 20, 30, \ldots, 600 \) for \( j = 1, 2, 3, \ldots, 60 \), respectively. If an index "i" is chosen to denote distributions, then in equation (6.16), the quantity \( g(i, j) \), \( j = 1, \ldots, 60 \) will be the same for all "i" s but different for different "j" s. Therefore, MODEL needs to be run only 60 times with these 60 realizations. The quantity \( \text{prob}(K_j) \) of equation (6.16) will be different for different distributions because the same \( K_j \) is being used for each of the "i" different distributions.
Therefore, the calculations can be performed according to:
\[
\text{prob}(C_{\text{max}} \geq \sum_{i=1}^{\mathcal{Q}} p_{K_i}(k)) = \sum_{j=1}^{60} g(j) \text{prob}(K_{ij}) + 1 - \sum_{j=1}^{60} \text{prob}(K_j), \text{for all } i's \rightarrow \cdots (6.17)
\]

The principal advantage of the above method of selecting realizations is that any number of distributions (or expected values) of \(K\) can be chosen for study but the MODEL has to be run only 60 times. However, these same \(M\) MODEL runs have to be performed even for a single distribution of \(K\).

6.4. Calculating Probability Points for Contour Plots

Equation (6.17) produces violation probabilities for \(P\times\mathcal{Q}\) distributions of \(K\) for fixed values of other parameters. Therefore, for a constant variance, it produces the probability points on the \(E(K)\)-axis of the probability contour plots. To complete the contour plots, these probability values have to be computed for each of the selected values of the variable on the other axis. If the variable on the other axis is "D" and "nd" (id=1,nd) number of its values are chosen for study, then the MODEL has to be run 60*nd times. This will produce 60*nd \(C_{\text{max}}\)’s, and same number of \(g(j)\) variables. Now variable "g" is a two-dimensional array varying with both \(K_j\) and "id".

Therefore, equation (6.17) will be modified as:
\[
\text{prob}(C_{\text{max}} \geq \sum_{i=1}^{\mathcal{Q}} p_{K_i}(k), d_{id}) = \sum_{j=1}^{60} g(id,j) \text{prob}(K_{ij}) + 1 - \sum_{j=1}^{60} \text{prob}(K_j), \text{for all } i's \text{ and all } id's \rightarrow \cdots (6.18)
\]
The selected range of E(K) is 30-150 ft/day with an interval of
5 ft/day and the variance is 0.5. This produces 41 distributions.
Therefore, equation (6.18) gives 41 * nd probability points for
contouring. This procedure was be followed in making probability
plots which have E(K) in one of their axis. These are: C* .vs. E(K),
A'. vs. E(K), and D .vs. E(K) plots.

For the plots which do not have E(K) on either of their axes, the
above procedure needs to be further modified. These are: A' .vs. D,
A' .vs. C*, and C*.vs. D plots. For example, A' .vs. D plots have to be
constructed for a particular C* and E(K). The distribution defined by
E(K) [say p_{K1(k)}] has N-realizations, A' has na(ia=1,na) values, and d
has nd(id=1,nd) values. Variable "g" is now a three-dimensional
matrix g(ia,id,j) because it varies with each realization Kj, each
distance (id), and each attenuation factor (ia). Therefore, equation
(6.18) has to be used "na" times for different ia's. This produces the
following form of the equation for probability calculation:

\[
\text{prob}(C_{\text{max}} \geq C* | p_{K1(k)}, d_{id}, A'_{ia}) = \\
\left[ \left\{ \left( \sum_{j=1}^{nd} g(ia,id,j) \right) \text{prob}(K_{j1}) \right\}, \text{id=1,nd}, \text{ia=1,na} \right] \\
+ 1 - \sum_{j=1}^{nd} \text{prob}(K_{j1}) \quad \quad \quad \quad \quad \quad \quad (6.19)
\]

Similar procedure will be followed to produce probability

Any plot not involving A' need only 60 MODEL runs. Because
concentrations at all "id" are automatically computed during a MODEL
run and concentrations calculated at a particular "id" are compared
with different $C^*$'s. However, plots involving $A$ need "na" sets of 60
MODEL runs by using different values of $A$ for each set of 60 MODEL
runs.

The procedure up to equation (6.19) is for a single initial
condition, i. e., a single initial plume length ($L$). As "na" is 20, 1200
($60 \times \text{na}$) MODEL runs had to be performed for a single $L$. Two initial
plume lengths were selected for this study which resulted in a total
of 2400 MODEL runs. Each of the MODEL runs took about 3 minutes
on the ERI Sparc Stations.
7. RESULTS AND DISCUSSION

7.1. Results

Appendix A and B present results for initial plume lengths of 500 ft and 1000 ft, respectively. Results in both Appendix A and B are for a longitudinal dispersivity ($\alpha_L$) of 100 ft and a variance ($\sigma^2$) of 0.5. Contour plots constructed from the same parameter values have been presented with the same Figure numbers except for the indices A or B which refer to the two different initial conditions. For example, Figures A.17 and B.17 are both Attenuation factor $\cdot$ vs. E(K) plots constructed for $C^*=0.003$ and $D=4500$ ft; the only difference between them is that Figure A.17 is for the initial condition 1 (plume length=500 ft) and Figure B.17 is for the initial condition 2 (plume length=1000 ft).

For a particular distance and attenuation factor, $C_{max}$ will be lowest for the lowest $K_j$ ($j=1, K_j=10$ ft/day) and highest for the highest $K_j$ ($j=60, K_j=600$ ft/day). For a particular $C^*$ (say $C_1^*$), if $g(j=1)$ is 1, the probability of violation will be 1 for all $C^*$ lower than $C_1^*$ (equation (6.9)). Similarly, for a particular $C^*$ (say $C_2^*$), if $g(j=60)$ is zero, the probability of violation will be less than or equal to 0.011 for all $C^*$ higher than $C_2^*$ (equation (6.15)). Therefore, $C_1^*$ and $C_2^*$ constitute a range of $C^*$ values for a particular set of $A$ and $d$, where probability of violation is 1 for $C^*$ less than or equal to $C_1^*$ and probability of violation is less than or equal to 0.011 for $C^*$ greater than $C_2^*$. Probability of violation will vary from 1 to 0.011 between
C_1^* and C_2^*. These ranges of C^* are presented in Table A.1 and Table B.1 for different combinations of A' and D.

In Tables A.1 and B.1, the range of C^* is of lower orders of magnitude for lower A' and shorter receptor distances. It increases with increasing A's and increasing d's.

The probability plots are presented in Figures A.1 through A.37 and Figures B.1 through B.37. The lines on the plots represent equal probability contours of the probability surface for different values of the prioritization parameters. Equivalent lines can be obtained by plotting the probability values along z-axis and any of the two prioritization parameters along x- and y- axis and joining the equal probability lines on the three-dimensional plot.

In referring to any plot, for example, the C^* .vs. E(K) plot, C^* is not plotted against E(K). Probability of exceedence corresponding to the different values of C^* and E(K) are plotted and the equal probability lines are drawn on the plot. However, to keep terminologies simple, although they are equivalent to three-dimensional plots, only variables in the x- and y- axis were used to identify them.

Presented in the following sections are descriptions of different types of generated plots. First the plots of Appendix A will be discussed in detail and then they will be compared with those of Appendix B.

7.1.1. C^* vs. E(K) Plots

These plots were constructed for constant values of receptor distance and attenuation factor. Plots for A' = .01/yr are presented
for three different distances (3500, 4500, and 5500 ft) in Figures A.1 through A.3. Contours at receptor distance 5500 ft are presented in Figures A.4 through A.7 for $A = .05, 0.1, 0.15$, and $0.20/yr$.

For lower $A$, the variation of $C^*$ was of one order of magnitude and therefore it was plotted on a plain scale (Figures A.1-A.3). For higher $A$'s, $C^*$ varied over more than 3 orders of magnitude. To show its behavior more precisely, it was plotted on logarithmic scale (Figures A.4-A.7).

All contour plots show a common behavior for probability of violation. After some $E(K)$, the contour lines tend to be parallel to $E(K)$-axis and this tendency increases with increasing receptor distance an decreasing $A$. This implies that after some $E(K)$, probability does not change significantly with increasing $E(K)$ values. However, probability increases much more significantly with $E(K)$ for lower values of $E(K)$.

Probability of violations are highly sensitive to $C^*$ for lower values of $E(K)$. This sensitivity decreases with increasing $E(K)$ and increasing $A$. For example, in Figure A.4, at $E(K)=30\text{ ft/day}$, for a change of probability from 0.72 to 0.1, the corresponding change of $C^*$ was about three orders of magnitude ($1e-6$ to $8e-4$). For the same change in probability level at $E(K)=150\text{ ft/day}$, change in $C^*$ was only of one order ($0.0015$ to $0.0045$).

Figures A.1 through A.3 show sensitivity of $C^*$ vs. $E(K)$ plots for different receptor distances. They indicate that the probability of violations and the maximum $C^*$ value on $C^*$-axis ($C_2^*$) decreases with increasing receptor distance. This characteristic can be explained by
the fact that as receptor distance increases, the concentration values will decrease and therefore, probability values will be lower.

Figures A.3 through A.7 show sensitivity of C* vs. E(K) plots for different attenuation factors. As attenuation factor increases, the C2* and the probability levels decreases. This can be explained as when attenuation factor increases, more contaminants disappear (get attenuated) on their way before reaching the receptors. Therefore, the concentration at the receptor becomes less which makes the probability of violation lower.

7.1.2. D vs. E(K) Plots

These plots were constructed by keeping C* and the attenuation factor constant. Figures A.8 through A.11 present contours for C*=0.005 and A' = 0.05, 0.1, 0.15, and 0.2. Figures A.12 through A.15 present contours for C*=0.004, 0.003, 0.002, 0.001 and A' = 0.20.

Probability contours were almost straight lines. This straight line behavior implies that if three points A, B, and C (Figures A.9 and A.10) are chosen in such a way that D_B-D_A=D_C-D_B, then for the corresponding E(K)'s, the relationship E(K)_B-E(K)_A=E(K)_C-E(K)_B will hold.

The jumps in the contour line in Figure A.8 reflect that probabilities for receptor distance 1900 and 2100 ft have the same values. This implies that at these two distances, although the concentration values are different, they have the same number of Cmax's exceeding C* and thereby producing equal "g" vectors.
However, the jumps can be eliminated by choosing a smaller interval in the $K_j$ values.

Figures A.8-A.11 show sensitivity of $D$ vs. $E(K)$ plots with different values of $A$. As the attenuation factor increases, the probability lines move downward, i.e., probabilities decrease.

Figures A.11-A.15 show sensitivity of the plots for different values of $C^*$. With decreasing $C^*$, the probability lines moved upward as a result of increase in probabilities.

7.13. $A$ vs. $E(K)$ Plots

These contours are presented in Figures A.16 through A.20. Figures A.16 through A.18 are for $C^*=0.002$, $0.003$, and $0.004$ and $d=4500$ ft. Figures A.19 and A.20 are for $C^*=0.004$ and $d=3500$ ft, and $2500$ ft, respectively.

Probability contours show similar linear behavior as that of the $D$ vs. $E(K)$ plots. The jumps in contour line in Figure A.20 reflect equal probability levels for two values of attenuation factor. These can also be explained the same way as the jumps in Figure A.8.

Figures A.16-A.18 present sensitivity of the contour plots with different values of $C^*$. As $C^*$ increases, the probabilities decrease. Figures A.18-A.20 show sensitivity of the probability for different receptor distances. With decreasing distances, the probabilities increase.
7.1.4. $A'$ vs. D Plots

These plots were constructed for constant values of $E(K)$ and $C^*$. Figures A.21 through A.23 are for $E(K)=50$ ft/day and $C^*=0.004$, 0.005, and 0.006. They show the sensitivity of the probability for different $C^*$. With increasing $C^*$, probability contours move downwards, i.e., probabilities are decreasing.

Figures A.24 and A.25 are for $C^*=0.004$ and $E(K)=100$ ft/day and 150 ft/day, respectively. They represent sensitivity of the contours for different values of $E(K)$. With increasing $E(K)$, probabilities are increasing. Overall variations in probability were non-linear with $A'$ and D.

7.1.5. $C^*$ vs. D Plots

Figures A.26 through A.28 show $C^*$ vs. D plots for $A'=0.01/yr$ and $E(K)=50$, 100, and 150 ft/day. As $E(K)$ increases, probability values are increasing and an upward shifting of the contours are observed.

Figures A.29-A.32 show plots for $A'=0.05$, .10,.15, and .20/yr and $E(K)=150$ ft/day. They represent sensitivity of $C^*$ vs. D plots with attenuation factor. As $A'$ increases, the probabilities are decreasing and contours are moving downward.

The overall relationship of probability contours with $C^*$ and D is non-linear. One interesting behavior of these plots is the gradual smoothing of higher probability contours with increasing $E(K)$'s (Figures A.26-A.28). As all other factors have the same values, the "g" vector is the same for all these plots. The only difference has
occurred due to the difference in E(K) or in the distribution from which the realizations are drawn.

Another important behavior is the increasing slope of the probability surface with increasing E(K) (Figures A.26-A.28) and decreasing slope with increasing attenuation factor (Figures A.29-A.32).

7.1.6. C* vs. A' Plots

These plots are presented in Figures A.33 through A.37. The overall relationship of probability contours with C* and A' is non-linear. Probabilities are decreasing with increasing C* and increasing attenuation factor.

Figures A.33-A.35 show a decrease of probabilities with increasing receptor distance which resulted in a downward movement of the contour lines. Similarly, Figures A.35-A.37 show a decrease of probabilities with decreasing E(K)'s and a downward movement of the contour lines are observed.

The slope of the probability surface decreases with increasing receptor distance (Figures A.33-A.35) and decreasing E(K)'s (Figures A.35-A.37).

Comparison between results of Appendix A and B

Results of Appendix B show similar behavior as those of Appendix A. The primary difference is that for the same parameter values, the probability levels are higher for the plots in Appendix B than those in Appendix A. This is because of the larger plume lengths for the later case. Larger plume has more mass and for the
same attenuation rate as the shorter plume, the net concentration reaching at the receptor will be higher. Following Tables show the variation of probabilities for the two initial plume lengths.

### C* vs. E(K) Plots

<table>
<thead>
<tr>
<th>No.</th>
<th>C*</th>
<th>D</th>
<th>E(K)</th>
<th>A</th>
<th>Probabilities of violations from Appendix A</th>
<th>Appendix B</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>.0055</td>
<td>3500 ft</td>
<td>60</td>
<td>.01</td>
<td>0.72</td>
<td>0.90</td>
</tr>
<tr>
<td>2</td>
<td>.0055</td>
<td>4500 ft</td>
<td>60</td>
<td>.01</td>
<td>0.30</td>
<td>0.75</td>
</tr>
<tr>
<td>3</td>
<td>.0055</td>
<td>5500 ft</td>
<td>60</td>
<td>.01</td>
<td>&lt; 0.1</td>
<td>0.52</td>
</tr>
</tbody>
</table>

### D vs. E(K) Plots

<table>
<thead>
<tr>
<th>No.</th>
<th>C*</th>
<th>D</th>
<th>E(K)</th>
<th>A</th>
<th>Probabilities of violations from Appendix A</th>
<th>Appendix B</th>
</tr>
</thead>
<tbody>
<tr>
<td>13</td>
<td>.003</td>
<td>2650 ft</td>
<td>90</td>
<td>.20</td>
<td>0.15</td>
<td>0.25</td>
</tr>
<tr>
<td>14</td>
<td>.002</td>
<td>2650 ft</td>
<td>90</td>
<td>.20</td>
<td>0.25</td>
<td>0.37</td>
</tr>
<tr>
<td>15</td>
<td>.001</td>
<td>2650 ft</td>
<td>90</td>
<td>.20</td>
<td>0.40</td>
<td>0.55</td>
</tr>
</tbody>
</table>

### A vs. E(K) Plots

<table>
<thead>
<tr>
<th>No.</th>
<th>C*</th>
<th>D</th>
<th>E(K)</th>
<th>A</th>
<th>Probabilities of violations from Appendix A</th>
<th>Appendix B</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>.002</td>
<td>4500 ft</td>
<td>90</td>
<td>.058</td>
<td>0.37</td>
<td>0.55</td>
</tr>
<tr>
<td>17</td>
<td>.003</td>
<td>4500 ft</td>
<td>90</td>
<td>.058</td>
<td>0.20</td>
<td>0.40</td>
</tr>
<tr>
<td>18</td>
<td>.004</td>
<td>4500 ft</td>
<td>90</td>
<td>.058</td>
<td>&lt; 0.1</td>
<td>0.24</td>
</tr>
</tbody>
</table>
### A vs. D Plots

**Figure**

<table>
<thead>
<tr>
<th>No.</th>
<th>C*</th>
<th>D</th>
<th>E(K)</th>
<th>( \ell )</th>
<th>Probabilities of violations from Appendix A</th>
<th>Probabilities of violations from Appendix B</th>
</tr>
</thead>
<tbody>
<tr>
<td>23</td>
<td>.006</td>
<td>2650 ft</td>
<td>50</td>
<td>.105</td>
<td>&lt; 0.1</td>
<td>&lt; 0.1</td>
</tr>
<tr>
<td>24</td>
<td>.006</td>
<td>2650 ft</td>
<td>100</td>
<td>.105</td>
<td>0.15</td>
<td>0.38</td>
</tr>
<tr>
<td>25</td>
<td>.006</td>
<td>2650 ft</td>
<td>150</td>
<td>.105</td>
<td>0.30</td>
<td>0.55</td>
</tr>
</tbody>
</table>

### C* vs. D Plots

**Figure**

<table>
<thead>
<tr>
<th>No.</th>
<th>C*</th>
<th>D</th>
<th>E(K)</th>
<th>( \ell )</th>
<th>Probabilities of violations from Appendix A</th>
<th>Probabilities of violations from Appendix B</th>
</tr>
</thead>
<tbody>
<tr>
<td>29</td>
<td>.001</td>
<td>2650 ft</td>
<td>150</td>
<td>.05</td>
<td>&gt; 0.9</td>
<td>&gt; 0.9</td>
</tr>
<tr>
<td>30</td>
<td>.001</td>
<td>2650 ft</td>
<td>150</td>
<td>.10</td>
<td>0.75</td>
<td>0.82</td>
</tr>
<tr>
<td>31</td>
<td>.001</td>
<td>2650 ft</td>
<td>150</td>
<td>.15</td>
<td>0.55</td>
<td>0.62</td>
</tr>
</tbody>
</table>

### C* vs. A Plots

**Figure**

<table>
<thead>
<tr>
<th>No.</th>
<th>C*</th>
<th>D</th>
<th>E(K)</th>
<th>( \ell )</th>
<th>Probabilities of violations from Appendix A</th>
<th>Probabilities of violations from Appendix B</th>
</tr>
</thead>
<tbody>
<tr>
<td>33</td>
<td>.001</td>
<td>3500 ft</td>
<td>150</td>
<td>.105</td>
<td>0.75</td>
<td>0.85</td>
</tr>
<tr>
<td>34</td>
<td>.001</td>
<td>4500 ft</td>
<td>150</td>
<td>.105</td>
<td>0.58</td>
<td>0.60</td>
</tr>
<tr>
<td>35</td>
<td>.001</td>
<td>5500 ft</td>
<td>150</td>
<td>.105</td>
<td>0.49</td>
<td>0.50</td>
</tr>
</tbody>
</table>
7.2. Discussion

A point source was used to generate the initial plumes. As the grid dimensions were 100 ft X 100 ft, MODEL took the source as a unit concentration over an area of 10,000 square feet. This is comparable with typical sources of contaminants.

All the simulations were carried out for a single aquifer thickness, porosity, and retardation factor. These parameters were used for calculating attenuation factors. However, the model results are applicable over the entire range of values of the attenuation factor irrespective of the individual values of its constituents.

In this study, a minimum realization value of 10 ft/day was selected and it was assumed that if the water quality standard is exceeded at $K_j=10$ ft/day, then the probability is 1. Although this is true for many aquifer settings, a more rigorous analysis can be made by choosing a lower value for the minimum realization.

The procedure does not produce interesting results for zero attenuation factor. For zero attenuation, with all other parameters fixed at constant values, MODEL runs produced same concentration-time histories for all the realizations of $K$. For example, for plots of $d$ vs. $E(K)$, if $g(i,d_1,jk=1)=0$, it will be zero for all $g(i,d_1,jk=2,\ldots,60)$. Similarly, if $g(i,d_2,jk=1)=1$, it will also be 1 for all $g(i,d_2,jk=2,\ldots,60)$. This makes the whole method deterministic in nature and the probability values become either zero or one.

The water quality standard ($C^*$) used in this study can also be used as the percent reduction of source concentration. If $p_1$ is taken as the probability of exceedence, then
1 - p1 = 1 - \text{prob}(C_{\text{max}} \geq C^*) = \text{prob}(C_{\text{max}} < C^*) = p2 \ (\text{say}).

Here \( p2 \) is the probability that \( C_{\text{max}} \) becomes less than \( C^* \). Quantity \( C_{\text{max}} \) was 1 unit for the initial plume and \( C^* \) is a fraction of it.

Therefore, 1 - p1 is the probability that the source maximum concentration is reduced to less than \( C^* \). In that case, the presented probability values have to be subtracted from 1.3 to obtain \( p2 \).

For sites where very few data are in hand, probability plots for D vs. E(K) can be most useful for decision making. It is likely that more estimates are available for \( K \) [E(K)] and receptor distance (D) than any other parameters. If nothing is known about the contaminant characteristics, D vs. E(K) plots with a very low value for the attenuation factor (0.01) can be used for a conservative estimate.

Plots for A vs. D can be useful when E(K) is known more precisely. Then ideas about sensitivity of probability with respect to \( A \) and D can be obtained from these plots. It can indicate which of them (\( A \) or D) are more crucial in making decision. This way, the plots can indicate the parameter for which data should be collected with more priority.

Described below is a demonstration of how to use the results of this work.

\textbf{Problem Statement:}

A particular site was contaminated by a suite of chemicals. The aquifer material is gravelly coarse to fine sand. The formation has an average thickness of 40 ft. The average hydraulic conductivity over the site is 100 ft/day. The hydraulic gradient is about .005 ft/ft.
A plume of Toluene has travelled about 1000 ft from the source. The average concentration of Toluene over the source area (100 ft X 100 ft) is 1000 ppb. The water quality standard for Toluene is 5 ppb. What is the probability of violation of water quality standard at a receptor distance of 5500 ft.

**Solution:**

Parameters needed:

1) Initial Plume length \((L) = 1000\) ft (given)

2) Variance of the K-field \((\sigma^2_k)\): For the gravelly coarse to fine sand, variance= 0.5 (Freeze, 1975).

3) Longitudinal dispersivity \((\alpha_L) = 100\) ft (assume)

4) \(E(K) = \) The average conductivity = 100 ft/day (given)

5) Receptor distance \((D) = 5500\) ft (given)

6) Attenuation factor \((A) = 0.01\) (assume for a conservative estimate).

7) Water quality standard \((C)\): In this work, \(C\) is the ratio of the permissible contaminant concentration divided by the maximum concentration at the source area. Therefore, \(C = 5\) ppb/1000 ppb = .005.

To match the requirements of the problem, Figure B.3 for \(C\) vs. \(E(K)\) can be used. From the Figure B.3, Probability of violation is 82.5% for the site. To obtain an idea about how this probability value can change as the attenuation factor \((A)\) changes from .01 to .05, Figure B.36 for \(C\) vs. \(A\) can be used. It shows a change of probability from 82.5% to 10% for this variation. Therefore, this factor should be determined more precisely.
8. CONCLUSION AND EXTENSIONS

A groundwater contamination site ranking methodology was developed on the basis of the probability of violation of water quality standards at a receptor. Seven independent parameters were identified which can affect the violation probability. Those were, the initial plume length (L), water quality standard (C*), the retardation velocity (u) [expressed by E(K)], attenuation factor (A), longitudinal dispersivity (σL), distance to the receptor (D), and the variance of the hydraulic conductivity distribution (σH^2). The whole analysis was done for plume lengths of 500 ft and 1000 ft, a longitudinal dispersivity of 100 ft, and a variance of 0.5. Sensitivity analysis was performed over four of the parameters: A, E(K), d, and C*.

Probability contours were linear for A vs. E(K) and D vs. E(K) plots and non-linear for C* vs. E(K), C* vs. A, C* vs. D, and A vs. D plots.

While ranking different sites, available site parameters can be used in the produced contours to determine the levels of probability. The site which has the highest probability of violation will be ranked the highest in remediation needs.

The results presented here can be used for E(K) up to 150 ft/day and variance of 0.5, with an error in probability of less than 0.011. This is because of the relatively small number of realizations chosen. However, this applicability can be widened by taking more realizations.
The procedure computes the highest probability level that can ever occur at a receptor. However, if it is intended to determine the violation probability over a certain period, all the MODEL runs should be performed for that time period.

Longitudinal dispersivity was assumed to be 100 ft. To analyze sensitivity of probabilities for its variation, similar probability plots can be produced by running the MODEL with different longitudinal dispersivities. Similar analysis can also be carried out for different variances of the conductivity field.

Pumping or injection wells can be introduced to make the procedure more general. For a particular site, the calibrated model for the site should be used in place of the MODEL of this work to calculate the contaminant concentrations.
BIBLIOGRAPHY


APPENDIX A

Results for the Initial Plume Length of 500 ft
<table>
<thead>
<tr>
<th>Attenuation Factor</th>
<th>Receptor distances (D)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1700 ft</td>
</tr>
<tr>
<td>.01/yr</td>
<td>.01 - .0192</td>
</tr>
<tr>
<td>.05/yr</td>
<td>.003 - .018</td>
</tr>
<tr>
<td>.10/yr</td>
<td>.001 - .017</td>
</tr>
<tr>
<td>.15/yr</td>
<td>1e-4 - .016</td>
</tr>
<tr>
<td>.20/yr</td>
<td>1e-4 - .015</td>
</tr>
</tbody>
</table>
PROBABILITY CONTOURS

(ATTN. = .01/yr, DIST = 4500 FT)

**Figure A.7.** CSTAR vs. E(x) Plot
PROBABILITY CONTOURS
(ATTL = 0.01/YR, DIST = 5500 FT)

FIGURE A.3. CSTAR VS. E(X) PLOT
PROBABILITY CONTOURS
(ATTN. = .10/yr, DIST = 5500 ft)

FIGURE A.5. CSTAR .VS. E(K) PLOT
PROBABILITY CONTOURS
(COSTAR = 0.005, ATTN. = 0.05/YR)

FIGURE A.8. RECEPTOR DISTANCE VS. E(X) PLOT
FIGURE A.9. RECEPTOR DISTANCE VS. Z(X) PLOT
PROBABILITY CONTOURS
(CSTAR= .005, ATTN= .15/YR)

FIGURE A.10. RECEPTOR DISTANCE VS. E(X) PLOT
PROBABILITY CONTOURS
(CSTAR=.004, ATTN=.20/yr)

Figure A.12. Receptor Distance vs. E(x) Plot
FIGURE A.14. RECEPTOR DISTANCE VS. E(K) PLOT
PROBABILITY CONTOURS
(CSTAR=.002, DIST=4500 FT)

ATTN. E/K

.100

.152

.105

.058

.010

(E/K), FT/Day

2 0.10 0.25 0.50 0.75 0.90

FIGURE A.18. ATTN. FACTOR VS. E(K) PLOT
PROBABILITY CONTOURS
(CSIN=0.004, DIST=2500 FT)

ATTN. (1/ft²)

-1.0
-1.25
-0.75
-0.5
-0.05
0.01
0.1
0.152
0.185
0.269

E(X), FT/DAY
30 60 90 120 150

2 0.1 0.25 0.5 0.75 0.9

FIGURE A.20. ATTN. FACTOR VS. E(X) PLOT
PROBABILITY CONTOURS

(CSTAR=0.004, E(K)=50 FT/DAY)

ATTN. [1/FT]

0.150

0.152

0.100

0.105

0.058

0.010

RECEPOT DISTANCE (FT)

1700

2650

3600

4550

5500

Z

0.10

0.25

0.50

0.75

0.90

FIGURE A.21. ATTN. FACTOR VS. RECEPTOR DISTANCE PLOT
PROBABILITY CONTOURS
(CSIA=0.005, EQ=50 FT/DAY)

FIGURE A.22. ATTN. FACTOR VS. RECEPTOR DISTANCE PLOT
PROBABILITY CONTOURS
(CSIAR=.006, E(x)=50 FT/DAY)

ATTN. [1/FT]
0.150

0.152 10

0.105 25

0.058 75

0.010 50

0.010 90

1700 2550 3500 4550 5500
RECEPTOR DISTANCE (FT)

Z 0.10 0.25 0.50 0.75 0.90

FIGURE A.23. ATTN. FACTOR VS. RECEPTOR DISTANCE PLOT
PROBABILITY CONTOURS
(CSTAN = 0.006, E(k) = 150 FT/DAY)

ATTN. (1/FE)

0.200

0.152

0.105

0.058

0.010

1700

2500

3600

4500

5500

RECEPTOR DISTANCE (FT)

Z

0.10

0.25

0.50

0.75

0.90

FIGURE A.25. ATTN. FACTOR VS. RECEPTOR DISTANCE PLOT
FIGURE A.29. CSTAR VS. RECEPTOR DISTANCE PLOT
Figure A.31. CSTAB. vs. receptor distance plot.
PROBABILITY CONTOURS
(E(K)=150 FT/DAY, DIST=5500 FT)

FIGURE A.35. CSTAR VS. ATTENUATION FACTOR PLOT
PROBABILITY CONTOURS
(E(k)=100 ft/day, DIST=5500 ft)

FIGURE A.36. CSTAR VS. ATTENUATION FACTOR PLOT
APPENDIX  B

Results for the Initial Plume Length of 1000 ft
<table>
<thead>
<tr>
<th>Attenuation Factor (A)</th>
<th>1700 ft</th>
<th>2500 ft</th>
<th>3500 ft</th>
<th>4500 ft</th>
<th>5500 ft</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01/yr</td>
<td>.016 - .029</td>
<td>.008 - .0193</td>
<td>.005 - .0136</td>
<td>.002 - .0105</td>
<td>.001 - .0089</td>
</tr>
<tr>
<td>0.05/yr</td>
<td>.005 - .028</td>
<td>5e-4 - .0180</td>
<td>5e-5 - .0125</td>
<td>5e-6 - .0092</td>
<td>1e-6 - .0075</td>
</tr>
<tr>
<td>0.10/yr</td>
<td>.001 - .026</td>
<td>1e-4 - .0164</td>
<td>1e-5 - .0100</td>
<td>1e-6 - .0077</td>
<td>1e-9 - .0061</td>
</tr>
<tr>
<td>0.15/yr</td>
<td>1e-4 - .025</td>
<td>1e-5 - .0150</td>
<td>1e-6 - .0094</td>
<td>1e-9 - .0065</td>
<td>1e-10 - .0050</td>
</tr>
<tr>
<td>0.20/yr</td>
<td>1e-4 - .024</td>
<td>1e-5 - .0138</td>
<td>1e-7 - .0083</td>
<td>1e-9 - .0055</td>
<td>1e-10 - .0040</td>
</tr>
</tbody>
</table>
PROBABILITY CONTOURS

$\text{ATN} = 0.01/\text{yr}$, $\text{DIST} = 3500 \text{ ft}$

![Graph showing probability contours with labels and values](image)

**Figure H.1:** CTSTAR, JR. E(x) Plot
PROBABILITY CONTOURS

\( \text{ATTN} = 0.01/\text{yr}, \text{DIST} = 4500 \text{ FT} \)

\( \text{CSTAR} \)

\( 0.0100 \)

\( 0.0075 \)

\( 0.0050 \)

\( 0.0025 \)

\( 0.0010 \)

\( \begin{aligned} &30 & & & & & & & \end{aligned} \)

\( 60 \)

\( 90 \)

\( 120 \)

\( 150 \)

\( \text{FIGURE R.3. CSTAR VS. Z(E) PLOT} \)
PROBABILITY CONTOURS
(ATTN=.01/YR, DIST=5500 FT)

FIGURE B.3. CSTAR VS. E(X) PLOT
PROBABILITY CONTOURS
(ATTN.=.05/YR, DIST=5500 FT)

FIGURE B.4. CSTAR VS. E(K) PLOT
PROBABILITY CONTOURS
(ATTN.=.20/YR, DIST=5500 FT)

FIGURE B.7. CSTAR VS. E(K) PLOT
PROBABILITY CONTOURS
(CSTAR=0.005, ATTN=10/yr)

DIST. [Ft] vs. [E(x), FT/DAY]

-10
-25
-50
-75
-90

FIGURE B.1. RECEPTOR DISTANCE VS. E(X) PLOT
PROBABILITY CONTOURS

\[ \text{DIST. [FT]} \]

\[ 5500 \]

\[ 4500 \]

\[ 3500 \]

\[ 2500 \]

\[ 1500 \]

\[ 30 \]

\[ 60 \]

\[ 90 \]

\[ 120 \]

\[ 150 \]

\[ f(x), \text{FT/DAY} \]

\[ 0.10 \]

\[ 0.25 \]

\[ 0.50 \]

\[ 0.75 \]

\[ 0.90 \]

\[ Z \]

\[ \text{FIGURE B.11. RECEPTOR DISTANCE VS. } f(x) \text{ PLOT} \]
PROBABILITY CONTOURS

(CSTAR=.003, ATTN=.20/YR)

DIST. [FT]

3000
4500
6000

4000
3500
3000
2500
1700

0
20
50
90
120
150

E(X), FT/DAY

0.10
0.25
0.50
0.75
0.90

FIGURE B.13. RECEPTOR DISTANCE VS. E(X) PLOT
PROBABILITY CONTOURS
(CSTAR=.002, ATIN=.20/yr)

Figure B.14. Receptor Distance vs. E(k) Plot
PROBABILITY CONTOURS
(CSR=0.052, DIST=4500 FT)

FIGURE B.16. ATTIN. FACTOR VS. E(K) PLOT
FIGURE B.17. ATTIN. FACTOR VS. E(X) PLOT
PROBABILITY CONTOURS
(CSTAR=.004, DIST=3500 FT)

ATTN., 1/FEET
0.25
0.152
0.105
0.058
0.010

E(K), FT/SEC
30
60
90
120
150

2 — — 0.10 — — 0.25 — — 0.50 — — 0.75 — — 0.90

FIGURE R.10. ATTN. FACTOR VS. E(K) PLOT
PROBABILITY CONTOURS

(CTAR=.004, E(X)=50 FT/DAY)

1.0
2.5
5.0
10

ATTN. (1/yr)

0.010
0.015
0.020

RECEPTOR DISTANCE (FT)

1700
2500
3500
4500
5500

FIGURE B.21. ATTN. FACTOR VS. RECEPTOR DISTANCE PLOT
Figure B.22: Attn. Factor vs. Receptor Distance Plot
PROBABILITY CONTOURS
(CSTAN=.006, Z(X)=50 FT/DAY)

ATTN. (1/yr)

0.200

0.150

0.105

0.050

0.010

1700

2600

3600

4500

5500

RECEIPTOR DISTANCE (FT)

Z

0.10

0.25

0.50

0.75

1.00

FIGURE B.23. ATTN. FACTOR VS. RECEPTOR DISTANCE PLOT
PROBABILITY CONTOURS
(CSTAR=.008, E(K)=100 FT/DAY)

ATTN. (1/FT)

0.200

0.152

0.105

0.058

0.010

1700 2950 2000 4500 5500
RECEPTOR DISTANCE (FT)

110 25 50 90 10

Z 0.10 0.25 0.50 0.75 0.90

FIGURE B.24. ATTN. FACTOR VS. RECEPTOR DISTANCE PLOT
Figure B.25. Attn. Factor vs. Receptor Distance Plot
PROBABILITY CONTOURS
(ATTN=0.01/yr, E(x)=50 ft/day)

Figure B.26. CStar vs. Receptor Distance Plot
PROBABILITY CONTOURS

\( \text{APTIN}=0.01/\text{YR}, \ E(K)=150 \text{ FT/DAY} \)

\[
\begin{array}{c}
\text{CSTAR} \\
0.01000 \\
0.00750 \\
0.00550 \\
0.00350 \\
0.00100 \\
\end{array}
\]

\[
\begin{array}{c}
1700 \\
2500 \\
2000 \quad 4500 \\
5500 \\
\end{array}
\]

\[ Z \quad 0.10 \quad 0.25 \quad 0.50 \quad 0.75 \quad 0.90 \]

FIGURE B.26. CSTAR VS. RECEPTOR DISTANCE PLOT
PROBABILITY CONTOURS
(ATTN. = .10/YR, E(K) = 150 FT/DAY)

FIGURE B.30. CSTAR VS. RECEPTOR DISTANCE PLOT
PROBABILITY CONTOURS
(ATN.=.15/yr, E(k)=150 FT/DAY)

FIGURE B.31. CSTAR VS. RECEPTOR DISTANCE PLOT
PROBABILITY CONTOURS
(ATTN. = .20/yr, E(k) = 150 ft/day)

FIGURE B.32. CSTAR VS. RECEPTOR DISTANCE PLOT
PROBABILITY CONTOURS
(E(K)=150 FT/DAY, DIST=3500 FT)

FIGURE B.33. CSTAR VS. ATTENUATION FACTOR PLOT
PROBABILITY CONTOURS

\( E(K) = 150 \text{ FT/DAY, DIST}=4500 \text{ FT} \)

\[ \begin{array}{c}
\text{ATTENUATION FACTOR (1/yr)} \\
0.01000 \\
0.00100 \\
0.00010 \\
0.00001
\end{array} \]

\[ \begin{array}{c}
0.010 \\
0.058 \\
0.105 \\
0.152 \\
0.200
\end{array} \]

\[ \begin{array}{c}
0.10 \\
0.50 \\
0.75 \\
0.90
\end{array} \]

\[ z \quad 0.10 \quad 0.25 \quad 0.50 \quad 0.75 \quad 1.90 \]

FIGURE B.34. CSTAR VS. ATTENUATION FACTOR PLOT
PROBABILITY CONTOURS
(E(H)=150 FT/DAY, DIST=5500 FT)

FIGURE B.35. CSTAR VS. ATTENUATION FACTOR PLOT
PROBABILITY CONTOURS
(E(K)=50 FT/DAY, DIST=5500 FT)

FIGURE B.37. CSTAR VS. ATTENUATION FACTOR PLOT