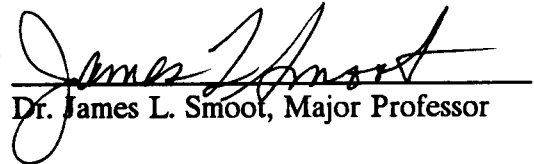
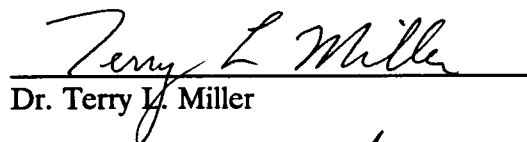


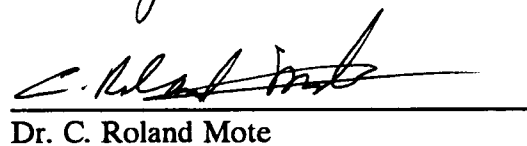
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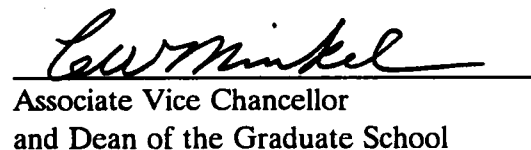

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COMPARATIVE EVALUATION OF KRIGING AS AN INTERPOLATOR
FOR GROUNDWATER CONTAMINANT PLUMES

A Thesis

Presented for the

Master of Science

Degree

The University of Tennessee, Knoxville

Larry S. Blackwelder

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ABSTRACT

This study analyzed the capabilities of three interpolation methods as applied to groundwater contaminant plumes. The three methods selected for evaluation were (1) kriging, (2) inverse distance squared, and (3) regression using a fifth order polynomial. The methods were evaluated over a range of values for four variables: (1) sample density, (2) sample location tolerance, (3) data quality, and (4) network age. Sample values and truth values were determined synthetically using a two-dimensional solute transport equation. The three interpolation methods were also applied to a case study to determine if the properties indicated by the synthetic data were valid for actual sample values.

It was concluded that the kriging method consistently provided the highest quality estimates within the range of variables used in this study, including the case study. The inverse distance squared method provided the second best results and the regression method consistently provided the lowest quality estimates. When variables other than estimate quality were considered, no best method could be determined, with each method demonstrating strengths and weaknesses specific to that method.

TABLE OF CONTENTS

CHAPTER	PAGE
I. INTRODUCTION	1
II. OVERVIEW OF SPATIAL INTERPOLATION METHODS	5
Simple Methods	6
Distance-Weighting Methods	8
Regression Methods	10
Gauss-Markov Methods	13
III. FUNDAMENTALS OF KRIGING	15
Regionalized Variables	15
The Variogram	16
The Intrinsic Hypothesis	21
Geostatistical Interpolation	22
Types of Kriging	24
IV. STUDY METHODOLOGY	32
Sample and Estimate Grids	32
Evaluation Variables	34
Plume Definition	44
Evaluation Metrics	49
Work Flow	50
V. INTERPOLATION METHOD PARAMETERS	52
Distance-Weighting Method	52
Regression Method	54
Kriging	57
VI. RESULTS	60
Inverse Distance Squared Results	60
Regression Method Results	67
Kriging Results	72

VII. METHOD COMPARISON	86
VIII. CASE STUDY	106
IX. CONCLUSIONS	117
BIBLIOGRAPHY	124
VITA	134

LIST OF TABLES

TABLE	PAGE
III-1. Equations for Common Variograms	19
IV-1. Transport Model Input Values	48
VI-1. Variogram Parameters (Sample Density)	84
VI-2. Variogram Parameters (Location Tolerance)	84
VI-3. Variogram Parameters (Data Quality)	85
VI-4. Variogram Parameters (Network Age)	85
VII-1. Summary Statistics (Sample Density)	90
VII-2. Summary Statistics (Location Tolerance)	95
VII-3. Summary Statistics (Data Quality)	100
VII-4. Summary Statistics (Network Age)	105
VIII-1. Measured Nitrate Concentrations	107
VIII-2. Case Study Estimates (Inverse Distance Squared)	113
VIII-3. Case Study Estimates (Regression Method)	114
VIII-4. Case Study Estimates (Kriging)	115
IX-1. Summary of Advantages and Disadvantages	123

LIST OF FIGURES

FIGURE	PAGE
III-1. Examples of Common Variograms	18
IV-1. Relationship of Sampling Grid to Plume Contours	35
IV-2. Estimate Grid	36
IV-3. Example of a Sample Grid (Location Variance = 0)	38
IV-4. Example of a Sample Grid (Location Variance = 0.4 L)	40
IV-5. Plume Migration (15 to 21 years)	42
IV-6. Plume Migration (24 to 30 years)	43
IV-7. Work Flow Schematic	51
V-1. Depiction of Kriging Neighborhood	59
VI-1. Plume Transect at 1600 meters	61
VI-2. Inverse Distance Squared Results (Sample Density)	62
VI-3. Inverse Distance Squared Results (Location Tolerance)	63
VI-4. Inverse Distance Squared Results (Data Quality)	64
VI-5. Inverse Distance Squared Results (Network Age)	65
VI-6. Regression Method Results (Sample Density)	68
VI-7. Regression Method Results (Location Tolerance)	69
VI-8. Regression Method Results (Data Quality)	70
VI-9. Regression Method Results (Network Age)	71
VI-10. Kriging Results (Sample Density)	74

FIGURE	PAGE
VI-11. Kriging Results (Location Tolerance)	75
VI-12. Kriging Results (Data Quality)	76
VI-13. Kriging Results (Network Age)	77
VI-14. Variograms for 10 x 10 Sample Grid (Isotropic)	81
VI-15. Variograms for 10 x 10 Sample Grid (Anisotropic)	82
VII-1. Mean Normalized Absolute Error Comparison (Sample Density)	87
VII-2. Estimate Error Comparison (Sample Density)	88
VII-3. Normalized Absolute Error Comparison (Sample Density)	89
VII-4. Mean Normalized Absolute Error Comparison (Location Tolerance) ..	92
VII-5. Estimate Error Comparison (Location Tolerance)	93
VII-6. Normalized Absolute Error Comparison (Location Tolerance)	94
VII-7. Mean Normalized Absolute Error Comparison (Data Quality)	97
VII-8. Estimate Error Comparison (Data Quality)	98
VII-9. Normalized Absolute Error Comparison (Data Quality)	99
VII-10. Mean Normalized Absolute Error Comparison (Network Age)	102
VII-11. Estimate Error Comparison (Network Age)	103
VII-12. Normalized Absolute Error Comparison (Network Age)	104
VIII-1. Case Study Sample Locations	109
VIII-2. Case Study Estimate Error Comparison	111

FIGURE	PAGE
VIII-3. Case Study Normalized Absolute Error Comparison	112
IX-1. Absolute Error as a Function of Kriging Variance	118
IX-2. Normalized Absolute Error as a Function of Kriging Variance	119

CHAPTER I

INTRODUCTION

Contamination of the nation's groundwater resources has received increased attention over the past decade as both government and industry have realized the importance of the groundwater resource to economic prosperity and the general quality of life. Approximately 50% of the U.S. population draws its water supply from groundwater (Bouwer, 1988). With this in mind, Congress passed the Comprehensive Environmental Response, Liability, and Compensation Act of 1980 (CERCLA) to provide for the restoration of abandoned waste disposal sites which pose a threat to public health or the environment and to provide a response to the release of hazardous chemicals to the environment. The rules promulgated by the Environmental Protection Agency (EPA) under the authority of CERCLA (40 CFR Part 300) include a phased approach to site restoration with success depending on the complete, accurate, and timely completion of site hydrogeologic characterization.

During the planning process, the formulation and evaluation of alternative restoration approaches are based on data gathered during the site investigation phase. During this phase, data are gathered on the source, type, and extent of the suspected contamination and integrated to form an overall assessment of the site. This process includes the determination of the spatial extent and structure of the contaminant plume. Typically, the only source of subsurface contamination data is a network of

sampling wells designed and constructed to provide data on the spatial distribution of the contaminant plume.

The hydrogeologist or environmental engineer is faced with the dilemma of how to characterize the site contamination using this limited information on the subsurface environment. This problem is complicated by limited knowledge of groundwater movement as it is influenced by advection, mechanical dispersion, molecular diffusion, and chemical sorption and transformation. To predict the movement of contaminants in groundwater using traditional modeling, detailed information is needed on the values and spatial relationships of the hydrogeologic and chemical parameters. At most remedial action sites, key decisions must be made well before sufficient details are available to permit accurate modeling. In addition, many of the parameters (such as details of microbiological processes under anaerobic conditions), may not be accurately known even under the best conditions (National Research Council, 1984).

The hydrologic data gathered from the monitoring network is in the form of scattered point values. In addition, the number and location of the sampling wells can be limited and restricted by diverse factors such as site topography and geology, presence of roads and buildings, weather, health and safety considerations, human and technical resources, time constraints, and public reaction. Most of these factors cannot be completely controlled by those responsible for the sampling task. Faced with inadequate information from which to develop an analytical model and an inability to always place wells where data is required, the hydrogeologist or engineer often relies on statistical methods to estimate values where wells are not located. This process is referred to as spatial data interpolation.

Error introduced by this interpolation can significantly impact the evaluation and design of remediation techniques that depend on the spatial characteristics of the contaminant plume, such as the pump-and-treat approach and *in-situ* bioremediation (Nyer, 1992). Interpolation error may mean the difference between a requirement to implement a costly and lengthy remediation effort and a decision that no action is required at the site.

The selection of an interpolation technique, or estimator, is one of many decisions that must be made during the remediation process. The method selected may influence the number of sampling wells required, the geometry of the sampling network, the amount of resources expended during analysis, and the acceptability of the data to technical reviewers and the public. The investigator responsible for this selection needs an understanding of the interaction between the interpolation method and the variables which influence the quality of interpolated data.

In the early 1980's, geostatistics was introduced as a new approach to the analysis of spatially-correlated hydrogeological data. One geostatistical technique which has received much attention for contaminant mapping is the kriging estimator (Delhomme, 1978). Kriging offers increased benefits over traditional interpolation techniques, but at the expense of increased computational complexity and quality of data.

The primary objective of this research was to evaluate kriging as an estimator of the spatial distribution of groundwater contamination against a limited number of other interpolation methods. The evaluation was performed over a range of variables commonly encountered during site investigations. The focus was on understanding and

evaluating the advantages and limitations of kriging that would influence the selection of kriging over an alternative interpolation method.

A secondary objective was to document information useful in designing the sampling network to obtain optimum performance (or to avoid degraded performance) from the chosen estimator. The proper selection and use of an estimator requires an understanding of the function of that estimator and its capabilities. Knowledge of the limitations of an interpolation method can be useful in avoiding circumstances under which the method fails to produce acceptable results.

CHAPTER II

OVERVIEW OF SPATIAL INTERPOLATION METHODS

Simply stated, the goal of spatial interpolation is to provide values at locations other than those where samples are collected. The effectiveness of the interpolation is measured by how close the interpolated value is to the actual value and its efficiency is measured by the amount and type of resources required to generate the estimate. The principal motivation behind the use of interpolators is the economics of well construction and sample collection and analysis. If acceptable estimates can be obtained through statistical methods, the cost, and perhaps the schedule, of site characterization can be reduced.

In most situations, hydrogeologic data is collected in the form of point values distributed spatially according to the monitoring network design. A single sample contains two types of data: (1) data associated with the parameter of interest (such as contaminant concentration, hydraulic head, pH, or temperature), and (2) the spatial location of the sample (usually the coordinates of the well and the screen depth). An interpolator may be judged on how efficiently and effectively it uses this data.

Most of the commonly used interpolators are based on a linear combination of the sampling data (Rouhani, 1986). These methods typically take the following general form:

$$Z(X_0) = \sum \lambda_{i0} Z(X_i) \quad (2.1)$$

where

$Z(X_0)$ = the estimated value at X_0

$Z(X_i)$ = the measure value at X_i ($i = 1, \dots, N$)

λ_{i0} = the weighting value of $Z(X_i)$ for estimating $Z(X_0)$

Based on how the weighting function λ_{i0} is determined, interpolators may be classified in one of the following four categories (Rouhani, 1986):

- Simple Methods
- Distance-Weighted Methods
- Regression Methods
- Gauss-Markov Methods

This chapter presents the general characteristics of each of the four categories of interpolators and discusses their strengths and weaknesses. From each category, one method currently used in contaminant mapping was designated as a representative method against which kriging was evaluated.

Simple Methods

The most common of the "simple methods" are (1) arithmetic mean and (2) Thiessen polygons (Rouhani, 1986). Using the arithmetic mean method, the value at the point to be estimated is assumed to be constant over the sampling domain with the

value being the average of the sample values. The values are calculated according to the following:

$$Z(X_0) = \frac{1}{N} \sum Z(X_i) \quad (2.2)$$

where N is number of data points in the sampling domain.

The strengths of the arithmetic mean interpolator are (1) the simplicity of the calculation, (2) the absence of subjective judgements, and (3) the limited amount of data required (no requirements on spatial data or minimum number of samples) (Rouhani, 1986). The major weakness of this method is that it does not allow the use of any sample spatial data, which may be available. This is not a significant concern in those scenarios in which the sample mean is stationary across the sample domain, or for those cases where spatial data is not available. Although not generally applicable to contaminant mapping, the arithmetic mean interpolator demonstrates that any evaluation of the effectiveness of the interpolation method must consider the characteristics of the application, and not just those of the interpolator. Even the most limited methods can produce acceptable results if applied under the right conditions.

The other simple method to be considered is the Thiessen polygon method. This method is also known as "polygons of influence" or the "nearest neighbor" method. Using this technique, the value at the point to be estimated is taken as the value at the nearest data point (Rouhani, 1986). The Thiessen polygon method does make use of the spatial data, but does not make any assumptions about the structure of that data between points. If the areas of influence of a series of data points are

mapped, the result will be a sample domain divided into polygons (hence the name "polygons of influence"). In this method, the value of the weighting function λ_{i0} is unity and just one sample point is used for each point at which a value is to be estimated.

The strengths of the Thiessen polygon method are (1) simplicity of calculation, and (2) the absence of subjective judgements on the part of the investigator. Unfortunately, this method results in discontinuities at the midpoints between samples. For this reason, use of this method is usually limited to applications requiring total mass calculations (such as rainfall over a watershed) where the discontinuities are not a concern (Rouhani, 1986).

The simple methods, although useful in the right application, have severe limitations, or cannot be used at all, when considered for the general tasks required of contaminant interpolators, such as contour mapping and determining locations of maximum concentration. Due to these limitations, no simple methods were evaluated in this study.

Distance-Weighting Methods

In the distance-weighting methods, sample points are assigned weighting factors according to their distance from the point to be estimated. In these methods, the weighting factor λ_{i0} takes the general form:

$$\lambda_{i0} = |X_i - X_0|^{-n} \quad (2.3)$$

where n is a factor to be determined by the user (usually 1 or 2) (Grimm, 1991).

The form of the weighting factor results in samples close to the estimated point having a greater influence on the estimate than far points. This is a significant improvement over the simple methods since this provides an estimate of the structure of spatial variability between points. The selection of " n " allows recognition of the variability of that spatial structure as a function of the parameter being estimated.

As with the simple methods, other than the distances from the estimate location, the relative locations of the sample points do not enter into the calculations. This is a concern if the mean is not stationary. The mean is stationary if the properties of the mean (such as its value or variance) do not change with location (Haan, 1977). Under a non-stationary condition, if the number of samples is greater in any specific region around the estimate location, the estimate will be biased toward those values.

The major weaknesses of the weighted-distance method are the subjectivity in (1) the selection of a value for n , and (2) selection of a search function (if used). The selection of a value for n is usually based on the best judgement of the user and, as such, reflects the skill of that user. Although an inverse-squared function is common for physical processes (Rouhani, 1986), the selection is unbounded and may lead to significant differences in estimates derived from the same data set.

If the investigator does not want to use all of the data points in the sample domain for each estimate, an algorithm is required to select the samples to be used.

For example, although there may be 100 monitoring wells in the network, the samples used in a calculation may be limited to the 4 wells closest to the estimation point.

This algorithm is often referred to as the "search function." As with the selection of n , definition of the search function is subjective and can lead to different estimates from the same data set (Grimm, 1991). Selection of n and the search function for the comparative evaluation are addressed in more detail in Chapter IV on the study methodology.

Regression Methods

Multiple linear regression is categorized as a linear method that estimates the unknown values through a regression equation. "Linear" indicates that the coefficients appear linearly, regardless of how the independent variables enter the model (Walpole, 1989). The regression equation is expressed by the following (Rouhani, 1986):

$$Z(X_0) = \sum \lambda_p f_p(X_i) \quad (2.4)$$

where

$Z(X_0)$ = the value of the function at the point of estimation

λ_p = the p^{th} regression coefficient (or p^{th} weighting factor)

$f_p(X_i)$ = a function of the location of the i^{th} sample

X_i = the location of the i^{th} sample

For a contaminant plume, the regression fits the measured concentration values and the coordinates of the measurements to a mathematical function. The form of the function most commonly used is a polynomial; however, other functions, such as an exponential or a gaussian may better represent the physical process being estimated. Once established, the regression equation is used to estimate the unknown values. The regression coefficients are often determined by minimizing the "sum of the squares of the errors" (SSE) as shown in the following equation:

$$SSE = [Z(X_i) - \sum \lambda_p f_p(X_i)]^2 \quad (2.5)$$

The regression interpolator provides a potential tool to measure the effectiveness of the interpolator in the form of values relating to the "goodness-of-fit" of the regression equation to the sample values. The goodness-of-fit can be expressed in various forms, including the coefficient of determination, mean square error, standard error of the estimate, and residual values.

This estimate of the error is not available with either the simple methods or the distance-weighting methods. Unfortunately, a goodness-of-fit value provides an overall measure of the fit to the data points rather than an estimate of the accuracy of the individual estimates. This estimate is of little value if the spatial distribution of the contaminant plume does not follow the form of the function being fitted.

An advantage of the regression method is that the results may be used without retention or storage of the original data set since, once the regression coefficients are determined, the original data are no longer needed. Also, the estimates need not be

generated until they are needed. The equation may be incorporated in software programs, allowing calculations that would be overly cumbersome if the original data set had to be included. Among the operations that can be performed with the regression equation, that are not available with other interpolation methods, are calculating the derivatives of the contaminant concentration with respect to location, calculating the total mass of the contaminant through integration, and surface-to-surface operations such as isopaching (subtracting one surface from another) (Davis, 1986).

Although there are numerous ways to calculate the regression coefficients, standard statistics programs are available which takes much of the subjectivity out of the method. However, the user must establish the degree of the polynomial to be used in the regression. For $n+1$ samples, there is an n^{th} -degree polynomial which provides a perfect fit (Lancaster, 1986). For any other polynomial, a decision must be made between goodness-of-fit and the complexity of the equation.

If a perfect fit is not obtained, the regression equation will not return the original sample values when the sample coordinates are used (Lancaster, 1986). Key people in the decision process and the general public, who may not be familiar with multiple regression techniques, may view this inability to reproduce known values as an indication that the process is flawed and may not accept the estimates as accurate and unbiased. Although not a technical limitation, this potential for rejection of the results is an issue that must be considered if the overall site characterization task is to be successful.

Gauss-Markov Methods

A Gauss-Markov estimator is a stochastic, probabilistic model having parameters that must be obtained from an analysis of the observed data. The initial assumptions about the spatial distribution of the function are limited to an assumption that the function $Z(X)$ is a spatial random function that satisfies the following general equation (Zirschky, 1985):

$$Z(X) = M(X) + R(X) \quad (2.6)$$

where

$Z(X)$ = a variable at the point X

$M(X)$ = the deterministic component of $Z(X)$

$R(X)$ = the stochastic component of $Z(X)$

There are numerous variations within the Gauss-Markov family of estimators. However, in general, the estimated values are obtained by satisfying the following two conditions:

- (1) The estimator must be unbiased. This means that the expected value of the difference between actual and estimated values must be zero.
- (2) The estimator must be optimum. This means that the variance of the difference between the actual and the estimated values must be a minimum.

The Gauss-Markov methods are essentially linear regression models with autocorrelated residues. When the Gauss-Markov method is applied to time series that exhibits significant serial correlation, it is known as a Markov or autoregressive process (Hann, 1977). If the method is applied to a distribution that can be assumed to be normally or lognormally distributed, it may be referred to as a gaussian stochastic model. When applied to the spatial distribution of geological data, this special form of the Gauss-Markov process is known as kriging (Rouhani, 1986).

Since the purpose of this thesis research was to compare kriging against the alternative methods already mentioned, kriging was the only Gauss-Markov method considered for evaluation. In contrast to the simple, intuitive processes described under the other methods, an understanding of kriging requires a detailed description of the basic theory and implementing procedures. Therefore, Chapter III (Fundamentals of Kriging) provides a more in-depth discussion of this special form of the Gauss-Markov method.

CHAPTER III

FUNDAMENTALS OF KRIGING

Kriging, a specific estimation method, is often used interchangeably with the more general term, geostatistics. Geostatistics is a field of statistics developed to solve spatial estimation problems in the mining industry. The fundamentals of geostatistics were developed by Krige, Sichel, and de Wijs in the 1950's to estimate ore reserves in the gold fields of South Africa (Cooper, 1988). In the 1970's, Delhomme introduced the concept of kriging as a new tool for the solution of interpolation and spatial averaging in the hydrosiences (Delhomme, 1978). Recently, geostatistical techniques have also been successfully applied to the other environmental sciences such as acid rain deposition and surface biomass estimation (Dancy, 1986; Grimm, 1991).

Regionalized Variables

The statistical techniques which comprise kriging are based on the theory of regionalized variables. The term "regionalized variable" (ReV) describes a phenomenon that is distributed in space (and/or time) and that shows a certain structure. All of the variables describing the surface, subsurface, or the atmospheric environment may be considered as regionalized variables (Delhomme, 1978). Samples taken closely together show more correlation in their values than samples taken farther apart.

A regionalized variable may be interpreted as the realization of a random function representing the parameter of interest, such as contaminant concentration. The regionalized variable is composed of a deterministic component called the "drift" and a stochastic component called the "fluctuation." The stochastic component may be spatially independent or it may be correlated to the location of the point of interest. As discussed in the previous chapter, a regionalized variable may be expressed as the following (Zirschky, 1985):

$$Z(X) = M(X) + R(X) \quad (3.1)$$

where

$Z(X)$ = the regionalized variable

$M(X)$ = the deterministic component or drift

$R(X)$ = the stochastic component or fluctuation

The Variogram

In order to account for the spatial structure of the regionalized variable, a correlation function is constructed based on an analysis of the sample values. This function is called the "variogram" and is closely related to the autocorrelation function used in statistics (Zirschky, 1985). The variogram describes how the variability of the regionalized variable changes with distance between points. Mathematically, the variogram is represented by the following:

$$2\gamma(h) = E [Z(X + h) - Z(X)]^2 \quad (3.2)$$

where

$2\gamma(h)$ = the variogram function

E = the "expected value" operator

$Z(X + h)$ = the value of the ReV at a point located a distance of h from X

The variogram function is usually expressed as a "semi-variogram" or $\gamma(h)$. Often in literature, the term "variogram" actually refers to the semi-variogram (Zirsky, 1985). Since the semi-variogram is the form of the variogram most commonly used, unless otherwise specified, the term "variogram" as used in this thesis refers to the semi-variogram form of the variogram. Also, since it is not possible to determine the "true" variogram from samples, and since the value of the regionalized variable is known only at a finite number of points, the variogram function shown above is replaced by an expression for the experimental variogram (Zirsky, 1985):

$$\gamma^*(h) = \frac{1}{2N(h)} \sum [Z(X_i + h) - Z(X_i)]^2 \quad (3.3)$$

where

$\gamma^*(h)$ = the experimental variogram

$N(h)$ = the number of pairs of points separated by a distance h

To facilitate calculations, the experimental variogram is modeled by a mathematical function. Commonly used types of models are shown in Figure III-1 and their mathematical functions are given in Table III-1. These models can generally be

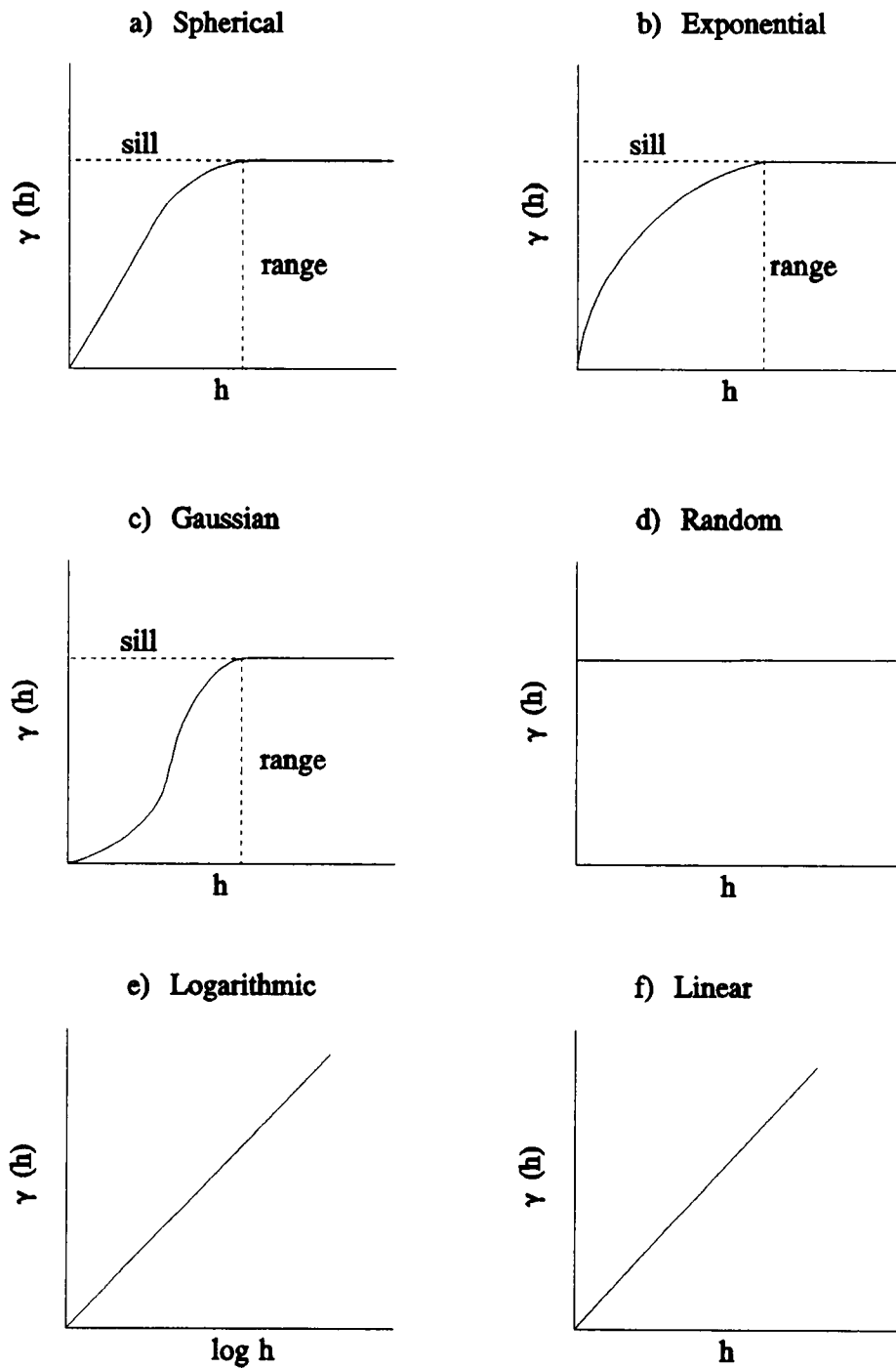


Figure III-1. Examples of Common Variograms (Zirschky, 1985)

Table III-1. Equations for Common Variograms (Zirschky, 1985)

Transitional Models		
Spherical	$\gamma(h) = C [1.5(h/a) - 0.5(h/a)^3]$	for $h \leq a$
	$\gamma(h) = C$	for $h \geq a$
Exponential	$\gamma(h) = C [1 - \exp(-h/a)]$	for all h
Gaussian	$\gamma(h) = C [1 - \exp(-h/a)^2]$	for all h
Random (Pure Nugget)	$\gamma(h) = C$	$h > E$
Non-Transitional Models		
Linear	$\gamma(h) = p \times h$	for all h
Logarithmic	$\gamma(h) = p \log(h)$	for all h
where - a = the range - C = the sill (in the absence of a nugget effect) - h = the lag - E = a distance smaller than the scale of observation - p = the slope		

For all models, $\gamma(0) = 0$. To all of these models, an additional component of variance, the nugget effect (C_0) may be added, [e.g. for the linear model, $\gamma(h) = (p \times h) + C_0$].

divided into two classes: (1) transition models, and (2) non-transition models.

Transition models are used when there is some distance beyond which the samples are independent. This distance is called the "range" and the value at and beyond the range is called the "sill." The value of the sill is equal to the variance of the observations beyond the range. For non-transition models, the variance between samples increases infinitely as the distance between samples increases with no range or sill. (Zirschky, 1985)

In many cases, the variogram does not approach the origin as the distance between points approaches zero, even though, by definition, $\gamma(0) = 0$. The discontinuity at the origin is called the "nugget effect" and the value at $h = 0$ is called the "nugget." The nugget represents the random component of the variance at a given scale of observation (Zirschky, 1985). The nugget effect can result from variabilities that occur at distances smaller than the scale of observation and from sampling and measurement errors.

Validation of the variogram presents a problem since there is no standard or "true" variogram available against which to compare the selected model. This problem is solved through cross-validation. The cross-validation is performed by kriging each sampled location with all of the other samples (minus the location being kriged). The resulting estimates are then compared with the measured, or true, values (USEPA, 1991). This provides a measure against which alternative variogram models can be compared.

From an analysis of the variogram, a significant amount of information can be gained about the regionalized variable even if the kriging calculations are not

performed. If sufficient data are available, variograms can be constructed for several directions and compared. Differences in the directional variograms indicate anisotropy in the regionalized variable. In addition, the value of the range indicates a maximum spacing for sample locations. Samples separated by distances greater than the range are independent and have a constant difference defined by the sill. These sample pairs will provide insufficient correlation data for interpolation.

The Intrinsic Hypothesis

To produce estimates for an unsampled location using the variogram, a restriction is introduced that the regionalized variable must be statistically stationary, which permits the use of statistical inference (Vieira, 1983). A random function is said to be stationary if its joint probability density function (pdf) at k arbitrary points is invariant under simultaneous translation of all these points. For kriging purposes, a regionalized variable satisfies this restriction if it is "weak stationary" or "stationary in the second order." To be weak stationary, the regionalized variable must satisfy two conditions: (1) the mean is a constant, and (2) the variance is independent of location.

The assumption of weak stationarity may not be satisfied for some physical phenomena having an infinite capacity for dispersion. In this situation, the requirement that the regionalized variable be weak stationary is more restrictive than what is required for the kriging process. Fortunately, the derivation of the kriging equations requires weak stationarity not for $Z(X)$ itself, but for its increments. Therefore, the requirement is that, for any vector h , the increment $Z(X+h) - Z(X)$

have a constant mean and a variance that is independent of location. This requirement is known as the "intrinsic hypothesis" (Delhomme, 1978). A random function that satisfies this hypothesis is called an "intrinsic random function." Mathematically, the intrinsic hypothesis is expressed as the following:

$$E [Z(X + h) - Z(X)] = 0 \quad (3.4)$$

$$Var [Z(X + h) - Z(X)] = 2\gamma(h) \quad (3.5)$$

Geostatistical Interpolation

Having selected and fitted an appropriate variogram model to the sample data, the actual interpolation process can now proceed. Linear geostatistics estimates the expected value of Z at some point X_0 by calculating the weighted sum of measured data $Z(X_1), Z(X_2), \dots, Z(X_n)$, which are the sample measurements at $X_1, X_2, \dots, X_n$, such that

$$Z^*(X_0) = \sum \lambda_i Z(X_i) \quad i = 1, 2, \dots, n \quad (3.6)$$

where

$Z^*(X_0)$ = the estimated value of Z at X_0

λ_i = the weighting value selected for point X_i

n = the number of samples used in the estimate (known as the neighborhood)

There are two sets of conditions that must be satisfied by the estimated value. The first condition is that the estimator must be unbiased (having no systematic over- or under-estimation). This condition is satisfied if the following two equations hold:

$$E [Z^*(X_0) - Z(X_0)] = 0 \quad (3.7)$$

$$\sum \lambda_i = 1 \quad (3.8)$$

The second condition is that the estimator $Z^*(X_0)$ must have a minimum variance of estimation. The second condition is satisfied when the following equation is minimized:

$$Var [Z^*(X_0) - Z(X_0)] = 2 \sum \lambda_i \gamma_{i0} - \sum \sum \lambda_i \lambda_j \gamma_{ij} \quad (3.9)$$

where $\gamma_{ij} = \gamma(|X_i - X_j|)$.

The optimum linear unbiased estimate of $Z(X_0)$ can be obtained by using Lagrangian techniques to minimize the estimation variance equation. The kriging system of equations consists of $n+1$ linear equations in n unknowns and is obtained by setting equal to zero each of the partial derivatives of the estimation variance equation (Hohn, 1988). The solution yields the n weights plus the Lagrange multiplier. This particular derivation is sometimes called "point" or "punctual kriging" because it gives estimates in the form of point values. "Block kriging" provides estimates in the form of area estimates and is not covered in this thesis.

An advantage of using geostatistics is that the variance of estimation can be calculated. The estimation variance (a measure of the uncertainty in the estimated value) can be obtained by substituting the values calculated into the estimation variance equation. In addition, the variance depends only on the geometry of the sampling network and the variogram. Therefore, if the variogram is known, the precision of the sampling network can be determined before the samples are obtained and this knowledge can be used to design an optimum network design (Dunlap, 1984).

The kriging variance should not be confused with quantification of the estimate error. A low kriging variance does not always result in a low estimate error. A low variance indicates stability in the spatial correlation of the measured values rather than accurate estimates at unsampled locations. The kriging variance is most useful in determining the quality of the variogram and in determining additional well locations to reduce network uncertainty.

Types of Kriging

Various types of kriging have been developed to handle the different forms of data encountered by the interpolation process. Of these, four have particular significance to groundwater contaminants (ASCE Task Committee, 1990):

- Simple or ordinary kriging
- Universal kriging
- Cokriging
- Disjunctive kriging

Simple or Ordinary Kriging

If the mean value of the regionalized variable is constant, simple or ordinary kriging is applicable. Some references distinguish between simple and ordinary kriging by using the term simple kriging when the true mean is known and ordinary kriging when the true mean is unknown (ASCE Task Committee, 1990). In several references, the two terms are used interchangeably. For most hydrogeological applications, this distinction is academic since the true mean is rarely known.

If the true mean is unknown and ordinary kriging is used, the kriging equations given in the previous section [(3.6) through (3.9)] are used to determine the kriging weighting factors. For ordinary kriging, the minimum estimation variance is given by the following:

$$\sigma_{OK}^2 = \sum \lambda_i \gamma_{0i} + \mu - \gamma_{00} \quad (3.10)$$

where

σ_{OK}^2 = the ordinary kriging minimum estimation variance

λ_i = the kriging factor for the measured value at X_i

γ_{0i} = the variogram value for X_i

μ = a Lagrangian multiplier

γ_{00} = the nugget value

If the mean is known and simple kriging is used, the estimator function and the minimum estimation variance equation, previously given by (3.6) and (3.9), can be written to include the value of the mean as follows:

$$Z^*(X_0) = m + \sum \lambda_i [Z(X_i) - m] \quad (3.11)$$

$$\sigma_{SK}^2 = \sum \lambda_i \gamma_{0i} - \gamma_{00} \quad (3.12)$$

where

σ_{SK}^2 = the simple kriging minimum estimation variance

$Z(X_i)$ = the measurement at X_i

m = the mean of the regionalized variable

Universal Kriging

In many applications, the requirement for stationarity of the mean is difficult to satisfy and the simple or ordinary kriging equations cannot be used. One method for handling this problem is to define a smaller sampling domain or "neighborhood" within which the mean can be considered constant. Since the location of smaller sampling domain moves depending on the location of the estimate, it is often referred to as a "moving neighborhood." The simple or ordinary kriging equations may then be applied as previously stated.

If a moving neighborhood concept cannot be used (perhaps due to insufficient sample locations), the changing mean must be accounted for in the kriging equations. This method is called "universal" or "nonstationary" kriging. In universal kriging, the estimates are obtained in the same manner as with simple or ordinary kriging, except that the deterministic component of the regionalized variable is replaced by a summation of monomials (Zirschky, 1985). The deterministic component in universal kriging can be expressed as the following:

$$M(X) = \sum b_i F_i(X) \quad i = 1, 2, \dots, k \quad (3.13)$$

where

b_i = drift coefficients

$F_i(x)$ = monomial functions

k = number of monomials required to account for the drift

The number and form of the monomials required to determine $M(X)$ must be estimated from the data, but since the drift influences the data, the variogram cannot be constructed directly from the data. Instead, the differences, or residuals, between the data values and the drift are used to construct what is called a "variogram of residuals." This is not an easy task since to determine the residuals, the coefficients of the drift must be known; however, if the variogram is not known, the optimum drift coefficients cannot be determined.

The process of determining a variogram of residuals is usually an iterative process of (1) assuming a model for the variogram of residuals, (2) calculating the drift coefficients, (3) calculating the residuals, and (4) constructing a new variogram of residuals. If the calculated variogram agrees with the assumed model, the process is complete. If not, a new variogram model is assumed and the process repeated until agreement is reached.

For universal kriging, the estimation variance can be calculated from the following equation:

$$\sigma_{UK}^2 = \sum \lambda_i \gamma_{0i} + \sum \mu_i F_i(X) - \gamma_{00} \quad (3.14)$$

where

σ_{UK}^2 = the universal kriging minimum estimation variance

μ_i = the Lagrangian multiplier for $F_i(X_0)$

Cokriging

If more than one variable is sampled at a location, there may exist a relationship between the variables. In this situation, estimation of one variable using information gained from sampling of both variables is called "cokriging." Information enters the kriging equations through a cross-variance function (or cross-variogram), which gives the correlation between the two variables as a function of their separation distance (ASCE Task Committee, 1989).

The cokriging estimator for two random variables is defined as the linear combination of the sample values of both functions. This relationship is defined by the following equation:

$$Z^*(X_0) = \sum \lambda_i Z(X_i) + \sum v_j Y(X_j) \quad (3.15)$$

where

$Z(X_i)$ = the sample values for variable Z

$Y(X_j)$ = the sample values for variable Y

λ_i = weighting factors for Z(X)

v_j = weighting factors for Y(X)

Similar to ordinary kriging, the cokriging estimator is required to be unbiased and have a minimum variance of estimation. For the estimator to be unbiased, the following conditions must be satisfied:

$$\sum \lambda_i = 1 \quad (3.16)$$

$$\sum v_j = 0 \quad (3.17)$$

The cokriging estimation variance incorporates the cross-variance of the two variables and, for the case of two correlated variables, is given by the following (Vieira, 1983):

$$\sigma_{CK}^2 = C_{YY}(0) + \mu_2 - \sum \lambda_i C_{ZY}(X_i, X_0) - \sum v_j C_{YX}(X_j, X_0) \quad (3.18)$$

where

σ_{CK}^2 = the cokriging minimum estimation variance

C_{YY} = the covariance of $Y(X)$

C_{ZY} = the cross-variance between $Z(X)$ and $Y(X)$

μ_2 = a Lagrangian multiplier

Cokriging is typically applied to increase the quality of an undersampled variable. The variable may be undersampled because of physical difficulty or high cost in obtaining samples. Therefore, samples for a second variable may be obtained, at relatively less difficulty or lower cost, and used to improve the knowledge of the first variable. This may allow a more efficient sampling program by increasing the ratio of

samples from the related variable to samples from the variable of interest. In theory, there is no limit to the number of variables used in a cokriging estimate; however, in practice, three or four is the most that can be handled efficiently (ASCE Task Committee, 1990).

Disjunctive or Non-Linear Kriging

Statistical inference, as used with kriging, requires the use of gaussian distributions. Since many hydrological distributions are lognormally distributed, this requirement can be satisfied through a logarithmic transformation of the data, allowing the use of linear kriging. However, some data exhibit non-gaussian characteristics whose log-transforms are also non-gaussian, limiting the use of linear kriging. If the original non-gaussian variable can be transformed into a bivariate normal variable, disjunctive kriging can be used. Ordinary kriging can be considered a linear form of disjunctive kriging.

As the more general form of kriging, the disjunctive kriging estimator is composed of a series of nonlinear functions such that

$$Z^*(X_0) = \sum f_i(X_0) \quad (3.19)$$

where $f_i(X_0)$ are functions to be determined.

The solution of the disjunctive kriging equations requires more steps and is more complex than linear kriging. Since it uses more information contained in the sampling data (not having to force the data to conform to a linear relationship), disjunctive kriging can provide better estimates than linear kriging. However, this

advantage alone is usually not sufficient to justify the additional computational expense.

The major advantage of disjunctive kriging is the ability to calculate the conditional probability that an indicator variable exceeds some prescribed tolerance level. In linear kriging, this is not possible since only the coefficients are required for the solution, the actual functions are not determined. With disjunctive kriging, the functions $f_i(X_i)$ are available to construct joint probability density functions. Given the joint pdf's, the conditional probabilities can be calculated.

Disjunctive kriging should be considered if the probability of the variable exceeding a specified value at an unsampled location is desired. This is of particular interest in the areas of groundwater contamination and site characterization, where the probability of contaminant concentration reaching above a regulatory limit may be a key factor in the decision process. Although the computational complexities are intimidating, software packages, such as GEOPACK (USEPA, 1990), are available that make much of the complexity transparent to the user.

CHAPTER IV

STUDY METHODOLOGY

The stated objective of this study was to evaluate kriging against selected alternative methods described in Chapter II. To accomplish this objective, each interpolation method was used to generate a specified number of estimates over a range of conditions. The calculated values were then compared with the "true" values to determine which interpolator provided the estimate with the least overall estimation error.

Before calculations could be performed, the conditions under which the estimates are to be calculated needed to be determined. This chapter discusses the following decisions:

- Definition of sampling grid and estimate grid
- Selection of the evaluation variables and their ranges
- Definition of plume structure or "true" values of contaminant concentration
- Establishment of evaluation metrics
- Organization of work flow

Sample and Estimate Grids

Typically, the first decision made in the design of a sampling network is the network geometry. This decision is based on the desired spatial resolution of the

measurement program and determines the number and location of the sampling wells. Studies have shown that a systematic grid provides the best compromise between minimizing the sampling variance and minimizing cost (Flatman, 1984). For this study, two systematic grid configurations were considered: (1) equilateral triangular, and (2) square. Within the family of regular patterns, the equilateral triangular grid is slightly more optimum for an isotropic plane stochastic process (Trujillo-Ventura, 1991). For a range of estimate locations, the triangular grid produces the minimum average spacing between the estimate location and the nearest sample point (McBratney, 1981).

If the stochastic process is not isotropic, the optimum grid geometry favors a rectangular grid. To account for the anisotropic nature of the plume, the sample spacing is adjusted to provide more samples along the major axis of the plume (Yfantis, 1985). This adjustment is easier to implement with a rectangular grid than with a triangular grid. Without prior knowledge of the spatial structure of the contaminant plume, the recommended pattern is a rectangle. In addition, the square pattern provides more "closest neighbors" (four versus three) and less sample screening than the equilateral triangular grid (Burgess, 1981). In practice, a square grid is often preferred as a matter of convenience.

To ensure the use of a sampling approach typically used at a site and to ensure that the isotropy of the network was not altered as the number of samples was changed, a square pattern was used in this study. This allowed changes in the number of samples, while holding the sampling area constant and keeping the longitudinal sample spacing equal to the transverse sample spacing. Equal sample spacing

eliminated the possibility that the test of the sensitivity or error as a function of sampling density would be influenced by an introduction of sampling anisotropy.

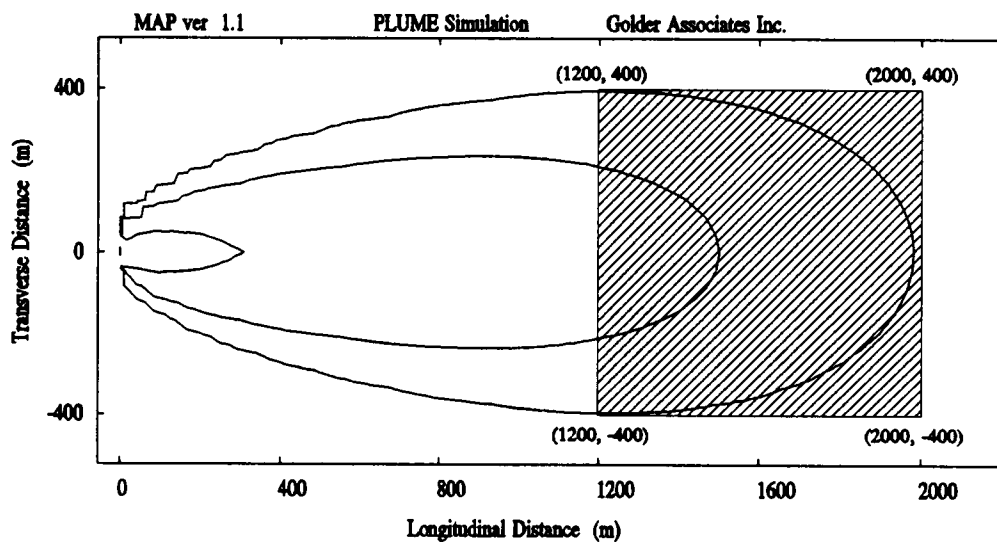
The location of the sampling grid in relation to the contaminant plume is shown in Figure IV-1. Since corner sampling locations were not moved during the study, the sampling grid location remained fixed for all calculations. This location ensured the interpolators would have to provide estimates over the most complex portion of the contaminant plume.

The location of the estimate in relation to the samples can influence the quality of the estimate. Typically, the closer the estimate point is to a data point, the better the estimate (McBratney, 1981). For this study, this influence of sample-to-estimate distance was investigated by moving the sample locations rather than the estimate locations (this is discussed in the next section on sample location variance).

Since there was no added benefit in moving both the estimate and sample locations, the same estimate locations were used throughout the study. The estimate locations were randomly positioned within the squares defined by a six-by-six node pattern, producing 25 estimate points. The random location was used to avoid potential systematic bias of a non-random pattern. The estimate positions used in this study are shown in Figure IV-2.

Evaluation Variables

There are many more variables, and combinations of variables, than can be investigated in a limited study. The objective of this section is to define the variables



Contours at: $0.001 C_0$, $0.01 C_0$, $0.1 C_0$

Advection time = 15.00 years

Average contaminant velocity = 2.5×10^{-6} m/s

Width of line source = 20.0 m

Longitudinal dispersivity = 70.0 m

Transverse dispersivity = 10.0 m

First-order decay constant = 0

Diffusion coefficient = 0

Sampling grid



Figure IV-1. Relationship of Sampling Grid to Plume Contours

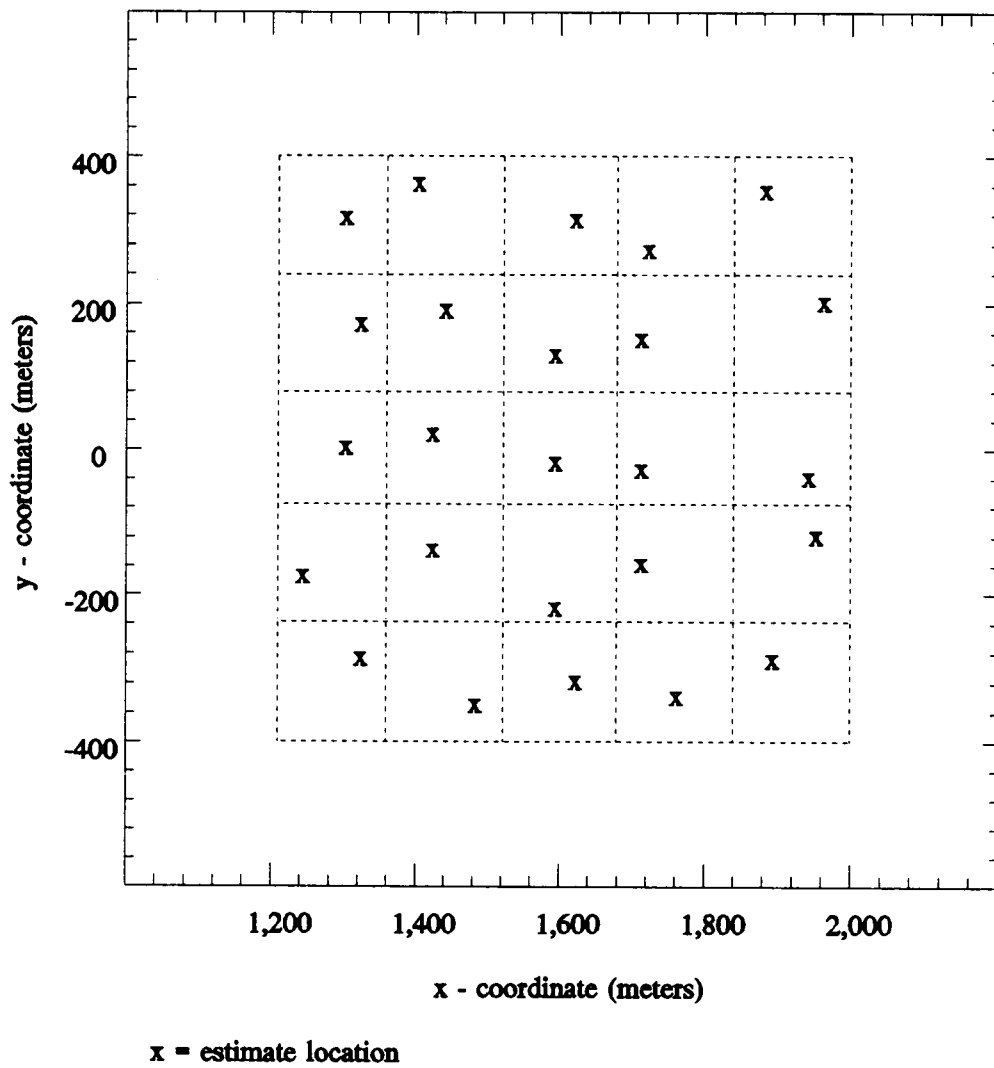


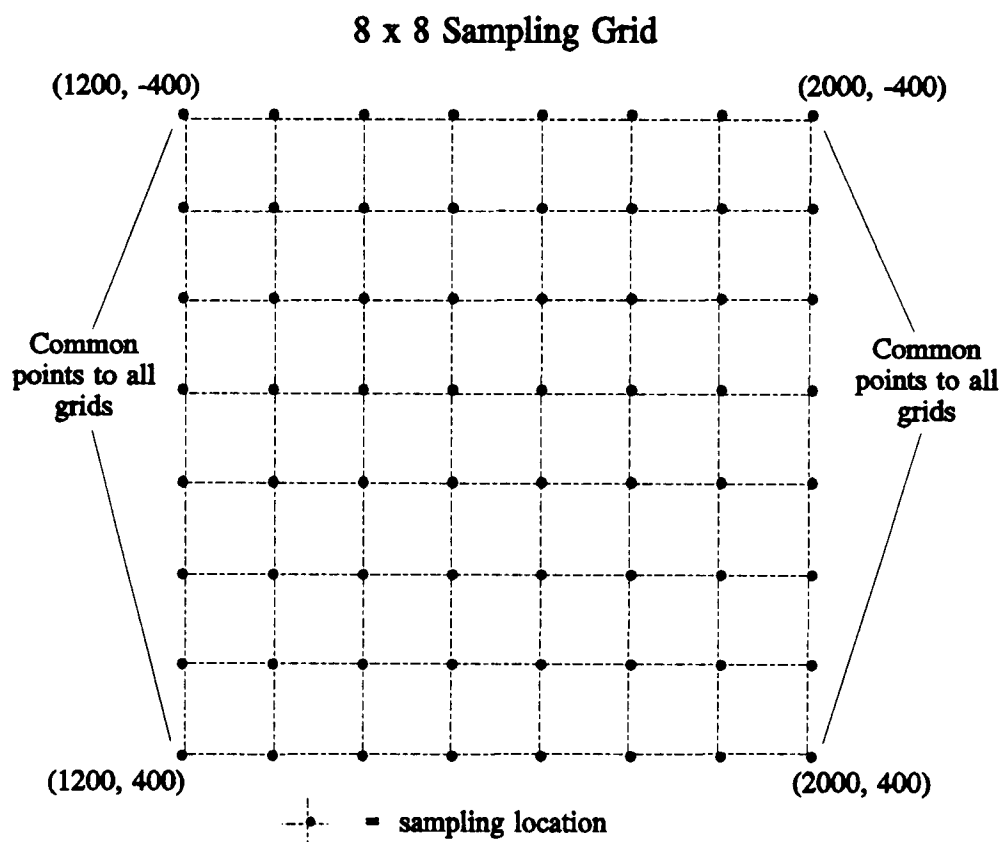
Figure IV-2. Estimate Grid

used in the interpolation tasks and the ranges for those variables. For this thesis, the interpolation methods were evaluated against each other over the range of four variables: (1) sample density; (2) sample location tolerance or position variance, (3) data quality, and (4) network age or plume shape. These variables, along with the sample and estimate grid geometry, defined the structure of the evaluation process.

Sample Density

The cost of a monitoring network is primarily driven by the number of wells. The number of wells not only determines the network construction and development costs, but it also determines the number of samples per sampling cycle. Usually, the life cycle cost of a monitoring program is driven by the analytical costs rather than the construction costs (Nielsen, 1991). In this study, the sample area was held constant; therefore, the terms "well number" and "well density" can be used interchangeably.

Given a square sampling grid, the number of samples can be easily adjusted by adding or deleting a row and a column in each increment. If the locations of the four corner samples are fixed, the network isotropy and sample area are constant for each sampling grid. A literature review indicates that from 30 samples (Cooper, 1988) to 100 samples (Samper, 1989) are required for good kriging estimates. Based on these values, an adequate range of sample densities was used to ensure that the kriging results showed both a significant drop in quality for the lowest values of sample density and a leveling-off of quality at high sample density values. Using a square grid, six sample sets were used containing from 16 (4×4) to 196 (14×14) samples. An example of the sample grid is shown in Figure IV-3.



<u>Matrix</u>	<u>Samples</u>	<u>Matrix</u>	<u>Samples</u>
14 x 14	196	8 x 8	64
12 x 12	144	6 x 6	36
10 x 10	100	4 x 4	16

Figure IV-3. Example of a Sample Grid (Location Variance = 0)

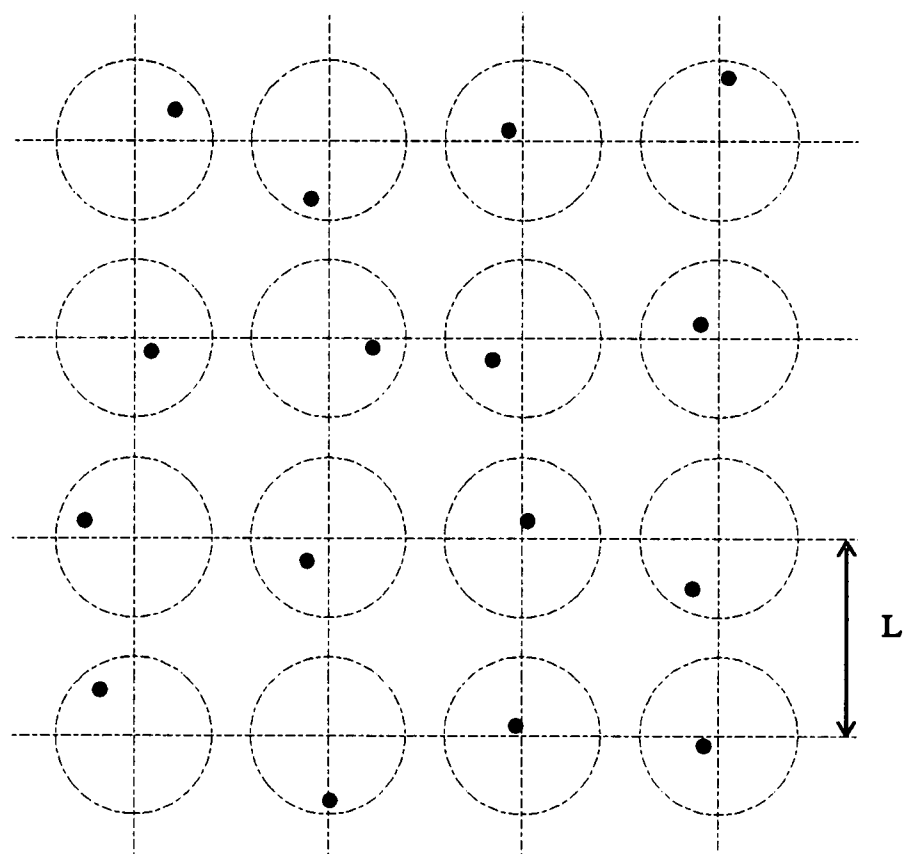
Sample Location Variance

At most sites, the sampling well locations are limited by various factors such as geography, geology, safety, structures, public relations, and politics. The sample "location variance" refers to how close the well must be located to the grid node. The greater this variance, the easier the network is to physically construct and the greater the potential for the network to approach a random design.

In this study, sample location variance was modeled by allowing the sample to be located on a random basis within a specified radius around the desired location. The radius of the circle is the "location variance" and is a function of the spacing between grid nodes (L). Variances for this study ranged from 0 to 0.5 times the node spacing. An example of a section of a sampling grid with non-zero variance is shown in Figure IV-4.

Data Quality

The reported result of a measurement is often taken at face value as representative of the actual contaminant concentration at the sampling location. In reality, there are many factors in the sampling process that can influence the quality of that measurement. Among these factors are heterogeneity of the plume or media, well construction quality, sampling procedures, transportation conditions, laboratory procedures, and human error. For sample screening or preliminary site investigations, where ultimate data quality is not required, the data quality may be reduced intentionally to reduce analysis costs.



- + = desired sample location (grid nodes)
 • = random sample location (variance = $0.4 L$)

Range of variance values for evaluation (variance value equals radius of circle):

0.0 L	0.3 L
0.1 L	0.4 L
0.2 L	0.5 L (maximum without overlap)

Figure IV-4. Example of a Sample Grid (Location Variance = $0.4 L$)

The objective of the data quality variable was to investigate the sensitivity of each interpolation method to data quality or "noise" in the data. To produce a range of data quality, a random noise component was added to the true concentration value for each sample. The equation for the "adjusted" data is as follows:

$$Z(X,n) = Z(X) + nR Z(X) \quad (4.1)$$

where

$Z(X,n)$ = the sample value adjusted for random noise

$Z(X)$ = the true sample value

n = fraction of $Z(X)$ available for adjustment, ranging from 0 to 1.00

R = a random number between -1 and 1

Network Age

Rapid completion of the cleanup may not be an achievable objective of a remedial action. Also, sampling wells, once constructed, cannot be moved. The network age variable investigated how the estimate quality varied as the plume shape varied with time. This also indicated the sensitivity of each method to the complexity of plume contours.

The initial age for the plume equation was set at 15 years to produce a plume large enough for a maximum network of 196 wells to appear realistic. The plume was allowed to "grow" by changing the time constant in the solute transport equation. Graphical presentation of the change in plume geometry with increasing age is shown in Figures IV-5 and IV-6.

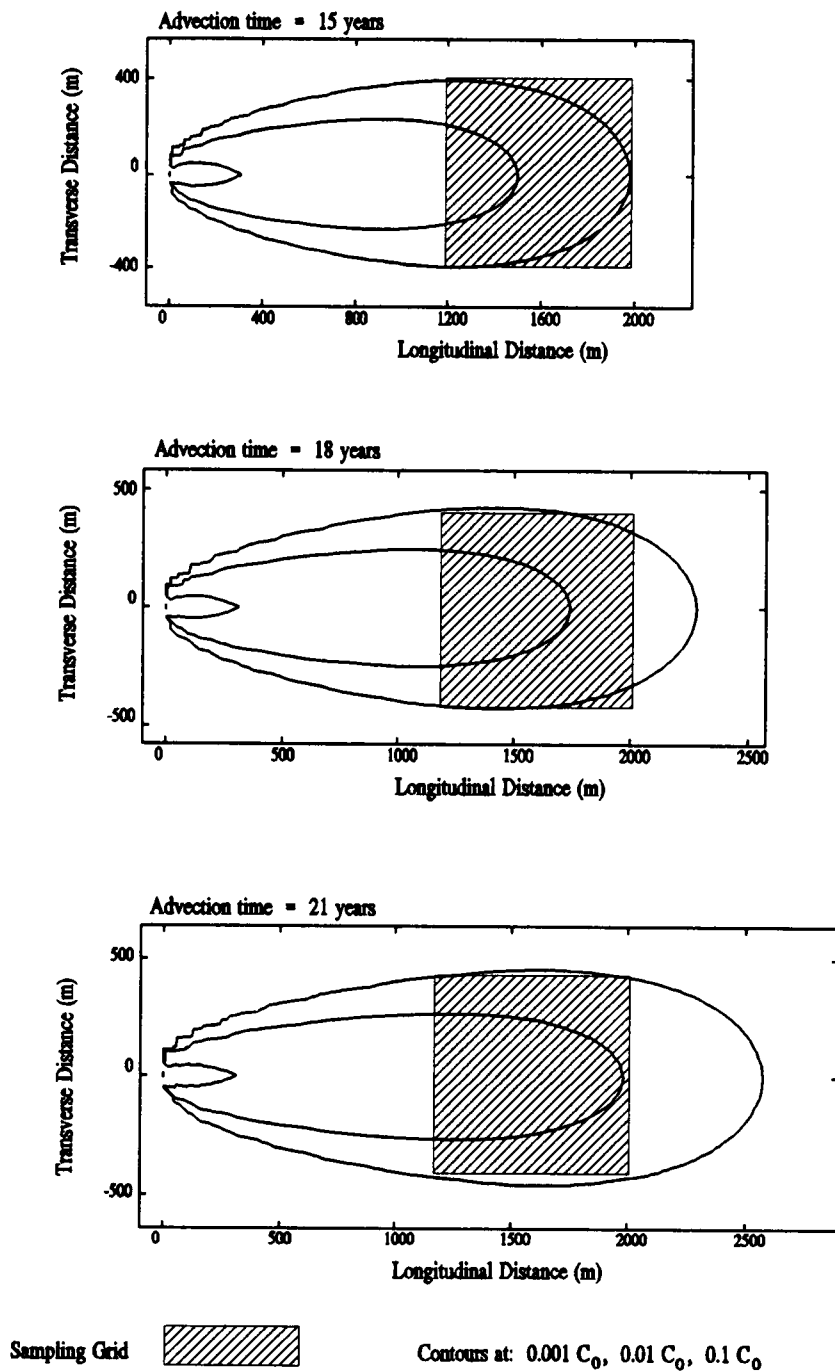


Figure IV-5. Plume Migration (15 to 21 years)

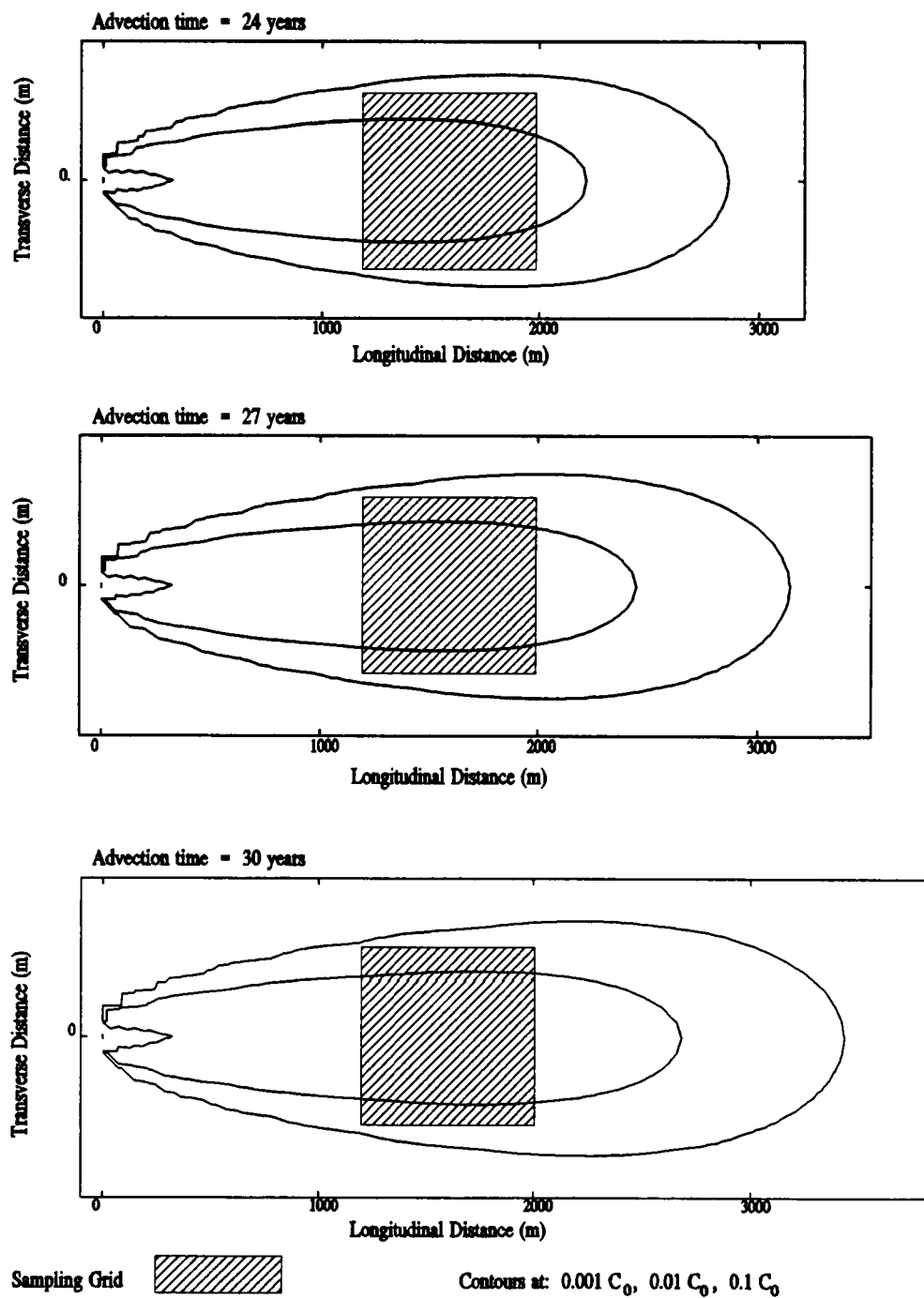


Figure IV-6. Plume Migration (24 to 30 years)

Plume Definition

Although actual sampling data provides a degree of reality not available through analytical models, real sampling networks do not provide the opportunity to place wells in any desired configuration or to randomly move well locations. Also, tracer tests are usually performed using a discrete rather than a continuous release (Freyberg, 1986). To provide a truth model that was infinitely variable over the range of sample number and locations, could provide sample values with zero error, could be "aged" as required, and that best modeled a continuous release, an analytical model was used to generate the "true" sample values.

The truth generation model used in this study was based on a three-dimensional analytical transport model presented by Domenico and Robbins (1985). The model assumes that the contaminant is released along a continuous source in a uniform aquifer, and predicts relative concentrations as a function of location and time. The equation for the model is as follows:

$$\begin{aligned} \frac{C(x,y,z,t)}{C_0} = & (1/8) \exp \{ (xv/2D_x) [1 - (1 + 4kD_x/v^2)^{0.5}] \} \\ & \operatorname{erfc} \{ [x - vt(1 + 4kD_x/v^2)^{0.5}] / 2(D_x t)^{0.5} \} \\ & \{ \operatorname{erf} [(y + Y/2)/2(D_y t/v)^{0.5}] - \operatorname{erf} [(y - Y/2)/2(D_y t/v)^{0.5}] \} \\ & \{ \operatorname{erf} [(z + Z/2)/2(D_z t/v)^{0.5}] - \operatorname{erf} [(z - Z/2)/2(D_z t/v)^{0.5}] \} \end{aligned} \quad (4.2)$$

where

$C(x,y,z,t)$ = concentration at x,y,z at time t

C_0 = source concentration

x, y, z = downgradient, transverse, and vertical distances from the source

k = first-order decay constant

Y = transverse width of the source

Z = vertical depth of the source

v = average contaminant velocity

D_x, D_y, D_z = longitudinal, transverse, and vertical dispersion coefficients

t = time from start of release

erf = error function

erfc = complementary error function

The average contaminant velocity used in the transport equation is calculated by the following:

$$v = \frac{K}{nR} \frac{\Delta h}{\Delta l} \quad (4.3)$$

where

K = the hydraulic conductivity

$\Delta h/\Delta l$ = the groundwater gradient

R = the retardation factor

n = the effective porosity

The dispersion coefficients are functions of the average contaminant velocity, the dispersivities, and the molecular diffusion coefficient for the contaminant, as shown below:

$$D_x = \alpha_x v + D_m \quad (4.4)$$

$$D_y = \alpha_y v + D_m \quad (4.5)$$

$$D_z = \alpha_z v + D_m \quad (4.6)$$

where

α_x = the longitudinal dispersivity

α_y = the transverse dispersivity

α_z = the vertical dispersivity

D_m = the molecular diffusion coefficient for the contaminant through the media

The model assumes uniform hydrologic and transport properties and a uniform hydraulic gradient over the area of the plume. The first requirement was satisfied by assuming a homogeneous and isotropic media. Also, a uniform hydraulic gradient was used for this study. The model assumes that the volume of the leachate is small when compared to the groundwater volume (usually the case in groundwater contamination) and does not influence the characteristics of the liquid. (Golder Associates, 1992)

Since this study was concerned with the static nature of the plume and not how it formed (as long as it is representative of a contaminant plume), the basic solute transport model could be reduced for this study by using the following simplifying assumptions:

- The plume is to be modeled in two dimensions only
- The contaminant is conservative ($k = 0$)
- The molecular diffusion coefficient is small compared to the advection term and can be neglected ($D_m = 0$)
- The contaminant travels at the groundwater velocity ($R = 1$)

Using these assumptions and substituting in the above equations, (4.2) through (4.6) become:

$$\frac{C(x,y,t)}{C_0} = (1/4) \operatorname{erfc} \{(x - vt)/2(D_x t)^{0.5}\} \quad (4.7)$$

$$\{\operatorname{erf} [(y + Y/2)/2(D_y t)^{0.5}] - \operatorname{erf} [(y - Y/2)/2(D_y t)^{0.5}]\}$$

$$v = \frac{K}{n} \frac{\Delta h}{\Delta l} \quad (4.8)$$

$$D_x = \alpha_x v \quad (4.9)$$

$$D_y = \alpha_y v \quad (4.10)$$

To use the transport model for interpolator evaluation, values for the variables in the model had to be assigned. These values determined the boundaries and contours of the contaminant plume. Typical hydraulic and contaminant values which might be found at a contaminated site are shown in Table IV-1. Additional assumptions for the remaining values, such as source width, were made to approximate an abandoned waste site. Using these values, the model was used to generate sample values and truth values for the evaluation.

Table IV-1. Transport Model Input Values

Parameter	Value	Comments
Assigned Values		
Width of Source (Y)	20 m	MAP default value
Hydraulic Conductivity (K)	10^{-4} m/s	Hydraulic conductivity of clean sand ranges from 10^{-2} m/s to 10^{-6} m/s
Groundwater Gradient ($\Delta h/\Delta l$)	0.01	
Effective Porosity (n)	0.4	Porosity for unconsolidated sand ranges from 0.25 to 0.50
Longitudinal Dispersivity (α_x)	70 m	Consistent with field studies on contaminant plumes in sandy aquifers
Transverse Dispersivity (α_y)	10 m	Consistent with laboratory tests indicating $\alpha_y = 0.01 \alpha_x$ to $0.2 \alpha_x$
Time (t)	15 years (4.73×10^8 s)	Assigned to provide a plume at least 1 km in length
Calculated Values		
Advection Velocity (v)	2.5×10^{-6} m/s	$v = (K/n)(\Delta h/\Delta l)$
Longitudinal Dispersion Coefficient (D_x)	1.8×10^{-4} m ² /s	$D_x = \alpha_x v$
Transverse Dispersion Coefficient (D_y)	2.5×10^{-5} m ² /s	$D_y = \alpha_y v$

References: Freeze, R. Allan, and John A. Cherry, 1979. Groundwater, Prentice-Hall, Englewood Cliffs, New Jersey.

Golder Associates, 1992. Monitoring Analysis Package (MAP) User's Guide, Golder Associates, Redmond, Washington.

Evaluation Metrics

The primary measure of the quality of an interpolator is how representative the estimates are of the true values. The mechanics of obtaining a numerical value for this relationship is called the "metrics" of a measurement. For this evaluation, the mean normalized absolute error (MNAE) was used as the evaluation metric for the total grid of estimates. The MNAE for the grid provides a single number as a measure of the overall performance of the interpolator under one set of conditions.

The individual estimate errors, when considered as a function of estimate location, provide an indication of the influence on the estimate of the estimate location within the plume. The performance measurements presented in Chapter V (Results) were calculated using the following equations (Hughes, 1981):

$$\text{Estimate Error} = Z^*(X_0) - Z(X_0) \quad (4.11)$$

$$\text{Normalized Absolute Error (NAE)} = \frac{|Z^*(X_0) - Z(X_0)|}{Z(X_0)} \quad (4.12)$$

$$\text{Mean Normalized Absolute Error (MNAE)} = \frac{1}{N} \sum \frac{|Z^*(X_0) - Z(X_0)|}{Z(X_0)} \quad (4.13)$$

where

$Z^*(X_0)$ = the estimated value at X_0

$Z(X_0)$ = the true value at X_0

N = the number of samples in the grid

Work Flow

The order of events in the evaluation process is shown in Figure IV-7. This study did not consider the interaction between variables; therefore, each evaluation could proceed independent of the other evaluations. To ensure that the network provided an adequate number of samples for each of the methods, the influence of sample density was conducted first, and that knowledge was used to establish the grid size for the three remaining variables.

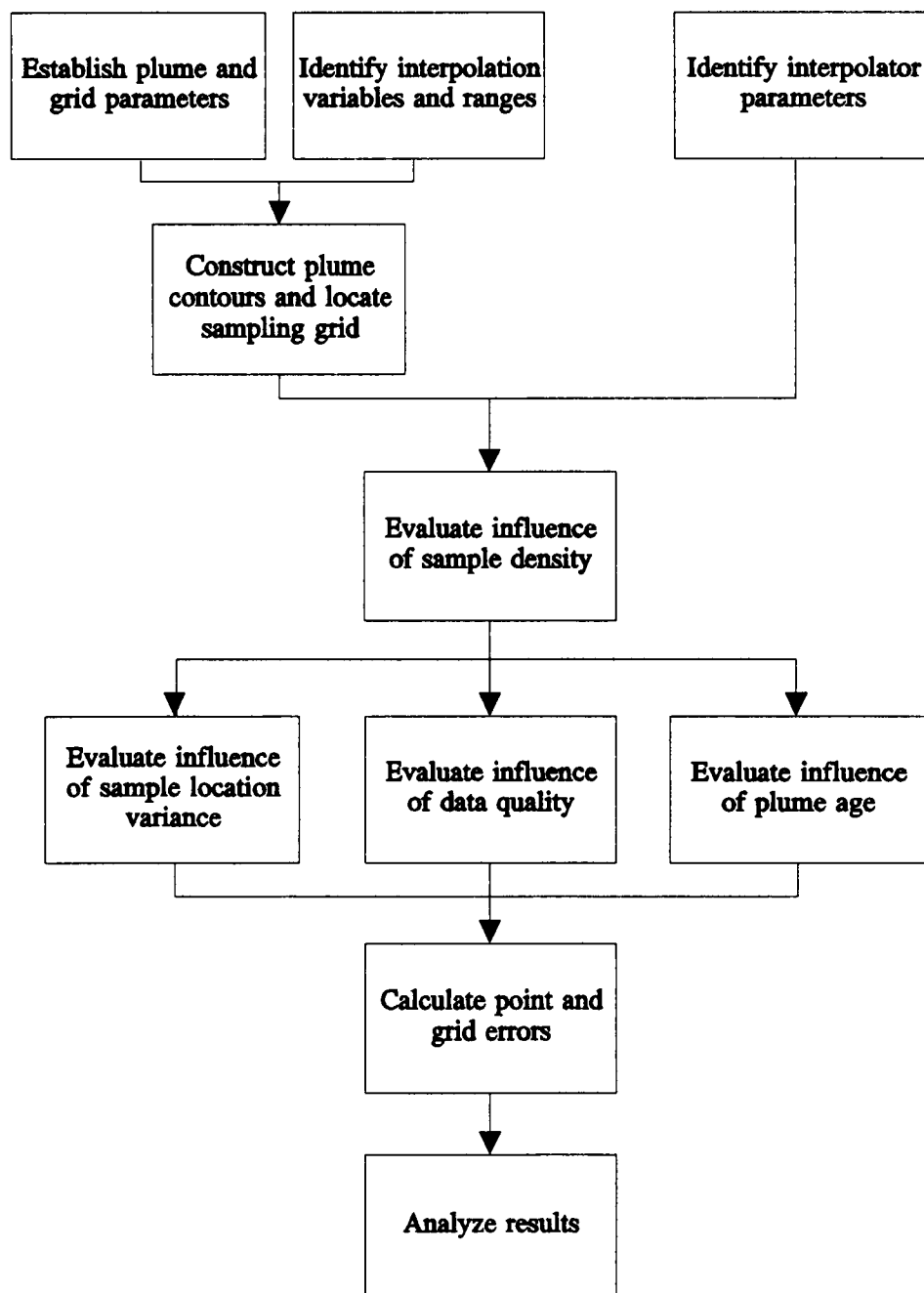


Figure IV-7. Work Flow Schematic

CHAPTER V

INTERPOLATION METHOD PARAMETERS

As discussed in Chapters II and III, with each of the interpolation methods there are subjective decisions that must be made to finalize the form of the interpolation equation. The results of these decisions narrow the designation of the interpolation methods from the generic methods discussed in Chapter II to a single equation or approach appropriate for use in the evaluation. This section discusses those decisions and presents the final form of the three interpolators.

Distance-Weighting Method

Definition of the distance-weighting method required two decisions: (1) selection of the form of the interpolation equation, and (2) development of a function to select the samples to be used (the search function). The first was the least subjective of the two decisions. In a two-dimensional field, the concentration of a contaminant away from a release point decreases as the inverse-square of the radial distance from the release point. This follows from the requirement that mass be conserved as the area increases with the square of the radius. Using this logic, a contaminant plume could be expected to follow a general inverse-square relationship. The inverse-square relationship has been successfully applied to the interpolation of hydrogeological phenomena (Rouhani, 1986).

Although the inverse-square relationship is routinely applied to physical phenomena, this does not ensure that the relationship is appropriate for the contaminant plume since the contaminant transport process is not a radial transport process (as it would be if diffusion were dominant). To test the applicability of an inverse-square function to the plume, a series of computations were made using the evaluation methodology described in Chapter IV and a 10 x 10 sample grid. The results were as follows:

<u>Inverse Power</u>	<u>Mean Normalized Absolute Error (MNAE)</u>
-1	0.073
-2	0.046
-3	0.061
-4	0.086

From these numbers, the inverse-squared relationship appeared to be the best model for contaminant concentration among the powers considered. Fractional powers are not normally used and were not considered. Therefore, the distance-weighting interpolator used an inverse-square relationship.

A desired characteristic of any estimator is that the estimator be unbiased. An estimator is unbiased if the expected value of the estimator is the true value. This does not guarantee that the individual estimates are always equal to the true value, but that there is no systematic over- or under-estimation. In the unbiased form, the inverse-square equation is as follows (Haan, 1977):

$$Z(X_0) = \frac{\sum Z(X_i)/(h_i - h_0)^2}{\sum 1/(h_i - h_0)^2} \quad (5.1)$$

where

$Z(X_0)$ = the estimated value

$Z(X_i)$ = the value at sample point i

$(h_i - h_0)$ = the distance between point i and the location of the estimate

The search function determines which samples are used for each estimate. Typically, the search function is expressed as a "moving neighborhood" consisting of at least the nearest three samples, the minimum number for triangulation (Davis, 1986). Since this study used a square grid rather than a triangular grid for the sampling pattern, the search function was defined such that the result was the selection of the nearest four samples. Because of the geometry of the sampling pattern, this also ensured that one sample will be selected from each of the quadrants around the point to be estimated. This guaranteed that no direction was over- or under-represented in the estimation and the estimate was not biased with respect to direction.

Regression Method

The form of a regression equation is determined by the selection of the order of the polynomial to be fitted to the sample data. In general, the higher the order of the polynomial, the better the fit (Lancaster, 1986). Unfortunately, the higher the order, the more costly the regression calculation in terms of computational resources and the

greater the effect of multicollinearity (linear dependency) among the independent variables (Walpole, 1989). Also, with higher-order polynomials, although the sample points are faithfully reproduced, this is accomplished at the expense of the accuracy of the estimated values since the fitted equation may exhibit significant deviations between samples (Rouhani, 1986).

The simplest trend model used in hydrogeology is the second-degree polynomial (Haan, 1977). This model allows delineation of a simple maximum or minimum yet does not exhibit the mathematical extremes of higher-order models. Typically, use of a higher-order polynomial produces only a slightly better fit. This is demonstrated by the following data obtained from polynomial trend-fitting to hydraulic head data (Rouhani, 1986):

<u>Order of Polynomial</u>	<u>Terms in Equation</u>	<u>Correlation Coefficient</u>
1	3	0.895
2	6	0.983
3	10	0.986

Unfortunately, a good fit to the sample data does not ensure adequate estimate quality; therefore, the correlation coefficient (or other quantification of the regression error) is not necessarily an indication of the quality of the interpolator. Within the literature reviewed, the degree of the polynomial is seldom mentioned; however, one contouring routine that is currently in use for commercial applications uses a fifth-order polynomial for a groundwater contaminant plume (Moltyaner, 1991). Using the

evaluation methodology from Chapter IV and a 10 x 10 sample grid, the following results were obtained:

<u>Order</u>	<u>Terms in Equation</u>	<u>Mean Normalized Absolute Error (MNAE)</u>
2	6	0.915
3	10	0.279
4	15	0.293
5	21	0.163

The selection of the polynomial was a compromise between the decreased error in higher-order polynomials and the increase in computational resources required to handle the regression calculations. Since the contaminant plume may exhibit irregularities that a lower-order polynomial could not model and the fifth-order polynomial produced the lowest MNAE, the fifth-order polynomial was used for the evaluation.

Since use of a higher-order polynomial decreases the number of degrees of freedom available for the regression calculations, a small sample set may not be sufficient. The lower the number of degrees of freedom, the higher the variance in the results, indicating less confidence in the fit. The number of degrees of freedom equals $n-k-1$, where n is the number of samples and k is the number of terms in the regression equation (Walpole, 1989).

The interpolation equation used in the evaluation is as follows:

$$\begin{aligned}
Z(X_0) = & \lambda_0 + \lambda_1 x + \lambda_2 y + \lambda_3 x^2 + \lambda_4 xy + \lambda_5 y^2 \\
& + \lambda_6 x^3 + \lambda_7 x^2 y + \lambda_8 xy^2 + \lambda_9 y^3 + \lambda_{10} x^4 \\
& + \lambda_{11} x^3 y + \lambda_{12} x^2 y^2 + \lambda_{13} xy^3 + \lambda_{14} y^4 + \lambda_{15} x^5 \\
& + \lambda_{16} x^4 y + \lambda_{17} x^3 y^2 + \lambda_{18} x^2 y^3 + \lambda_{19} xy^4 + \lambda_{20} y^5
\end{aligned} \tag{5.2}$$

where $\lambda_0, \dots, \lambda_{20}$ are the regression coefficients.

Kriging

The validity of a kriging estimate depends primarily on the quality of the variogram. Since the parameters that define the variogram are determined through examination of the sample data, the final form of the kriging interpolator cannot be expressed uniquely as part of the methodology. The subjective judgements inherent with variogram development were part of the kriging process and could not be predetermined without invalidating the process itself. The two decisions that could be made as part of the study methodology are (1) identification of the type of kriging to be used, and (2) sizing of the neighborhood.

Simple kriging is not applicable to groundwater contamination since the true mean is unknown. Ordinary kriging is applicable, but only if there is little or no drift. The alternative to ordinary kriging is universal kriging. In groundwater contaminant applications, universal kriging offers no clear advantage over ordinary kriging, but

requires much more user involvement and computing time (Zirschky, 1985).

Therefore, ordinary kriging was used as the kriging interpolation method.

To make estimates using kriging, there must be enough samples in the neighborhood to obtain a stable solution of the kriging equations yet the spatial extent of the samples must not violate the assumption of a stationary mean. A typical number of samples is 10 to 12, with a maximum of 16. No significant improvement is seen by adding samples beyond the closest 16 samples (Sophocleous, 1982). Since, in this study, the square sample grid provided a consistent sample increment at 12 samples with increasing radius, the maximum neighborhood size was selected to be 12 samples as shown in Figure V-1.

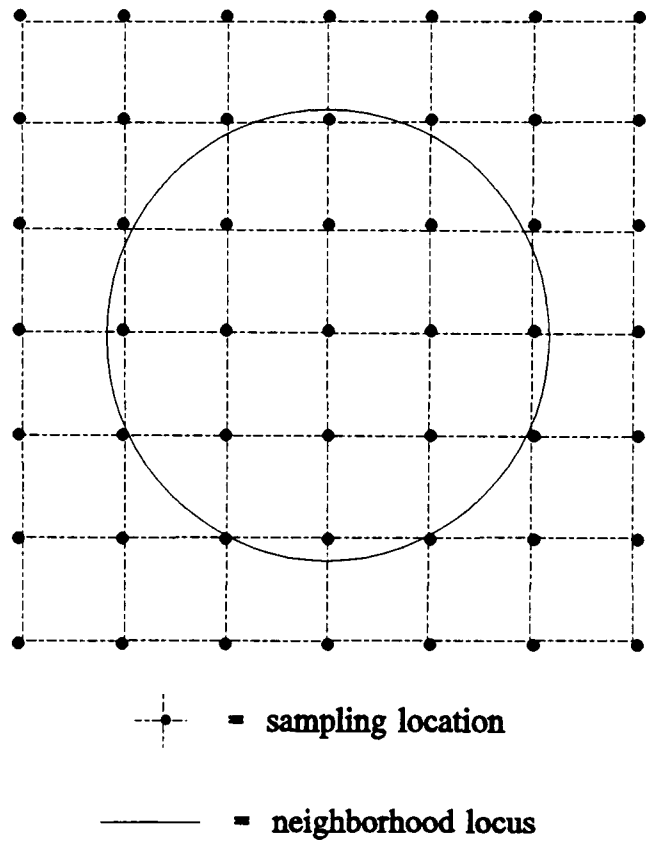


Figure V-1. Depiction of Kriging Neighborhood

CHAPTER VI

RESULTS

This chapter documents the results of the application of the methodology presented in the previous chapter. In this chapter, discussion and analysis are limited to those observations concerning the application of individual interpolation methods. A comparative analysis of the results is provided in Chapter VIII.

During the generation of the data, inspection of the results showed a marked increase in the mean normalized absolute error (MNAE) along the outer rows of the estimate grid. A "row" is defined as a line of estimates that parallels the advection vector of the plume. The outer row corresponds to the gaussian edge of the plume where the contaminant concentration exhibits rapid change as shown in Figure VI-1.

Since this gaussian edge is a common characteristic of contaminant plumes (Domenico, 1985), the results are presented to show normalized errors associated with the inner and outer rows, as well as those associated with the total sample grid. Each graph is composed of three sets of data: (1) the composite MNAE, (2) the MNAE of the outer two rows, and (3) the MNAE of the inner, or central, three rows.

Inverse Distance Squared Results

The results of interpolation using the inverse distance squared method are shown in Figures VI-2 through VI-5. Application of this method was greatly

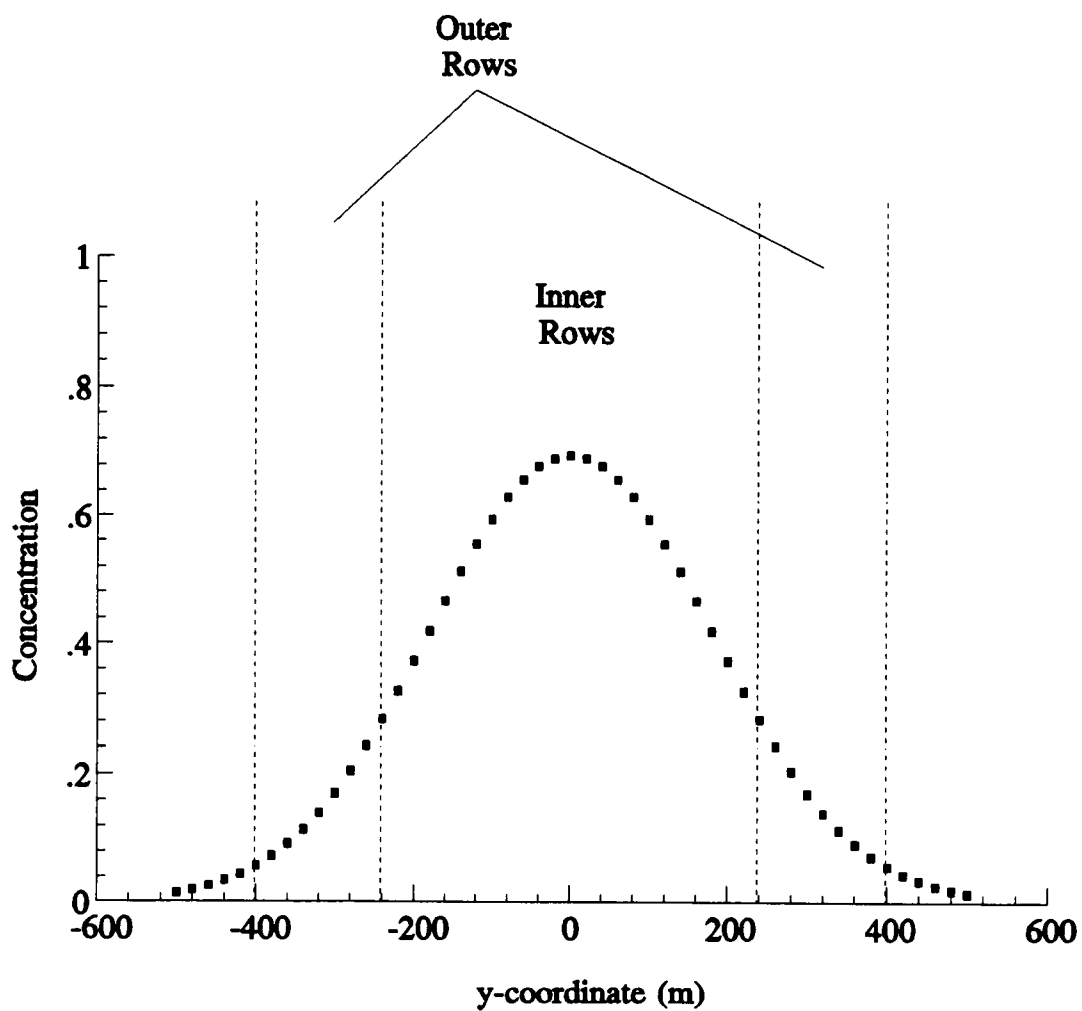


Figure VI-1. Plume Transect at 1600 meters

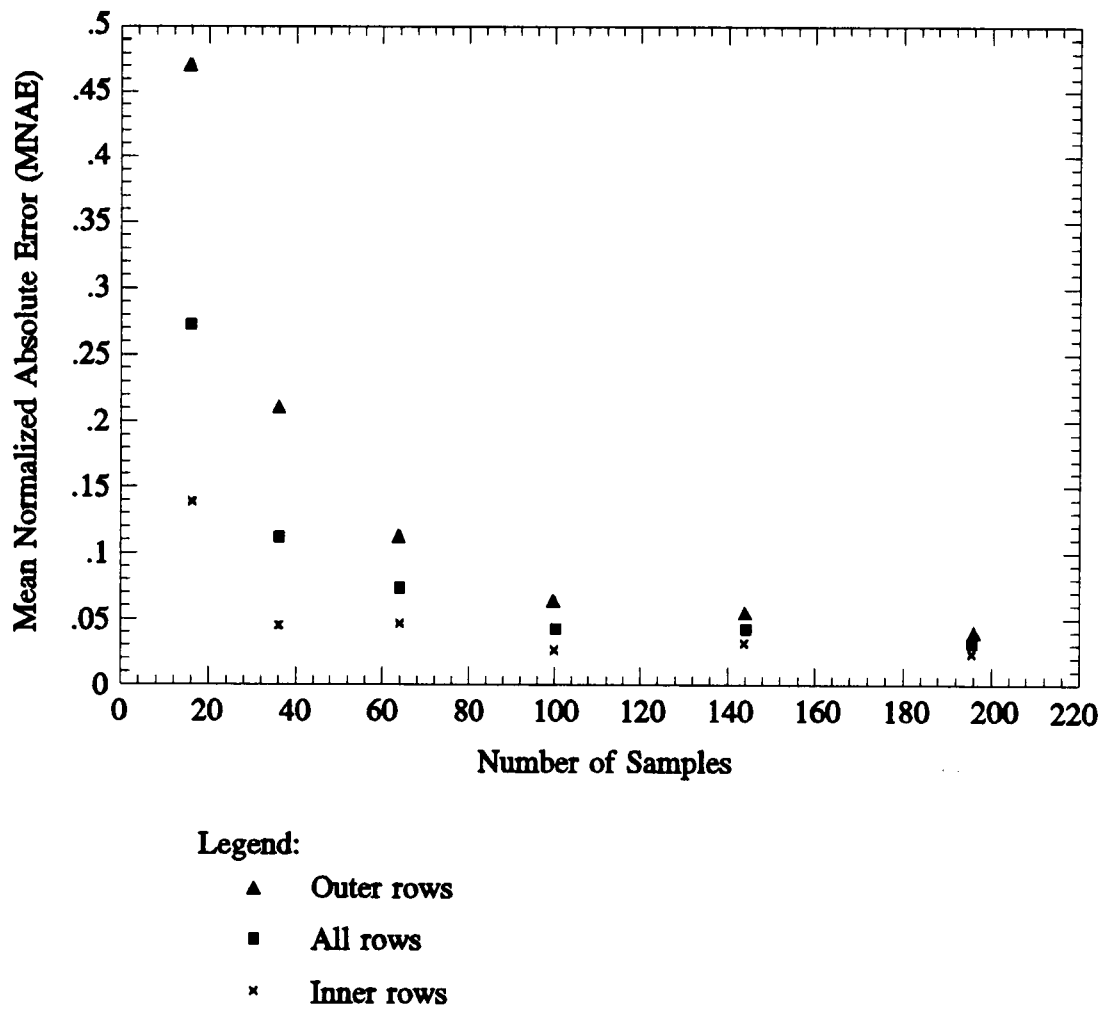


Figure VI-2. Inverse Distance Squared Results (Sample Density)

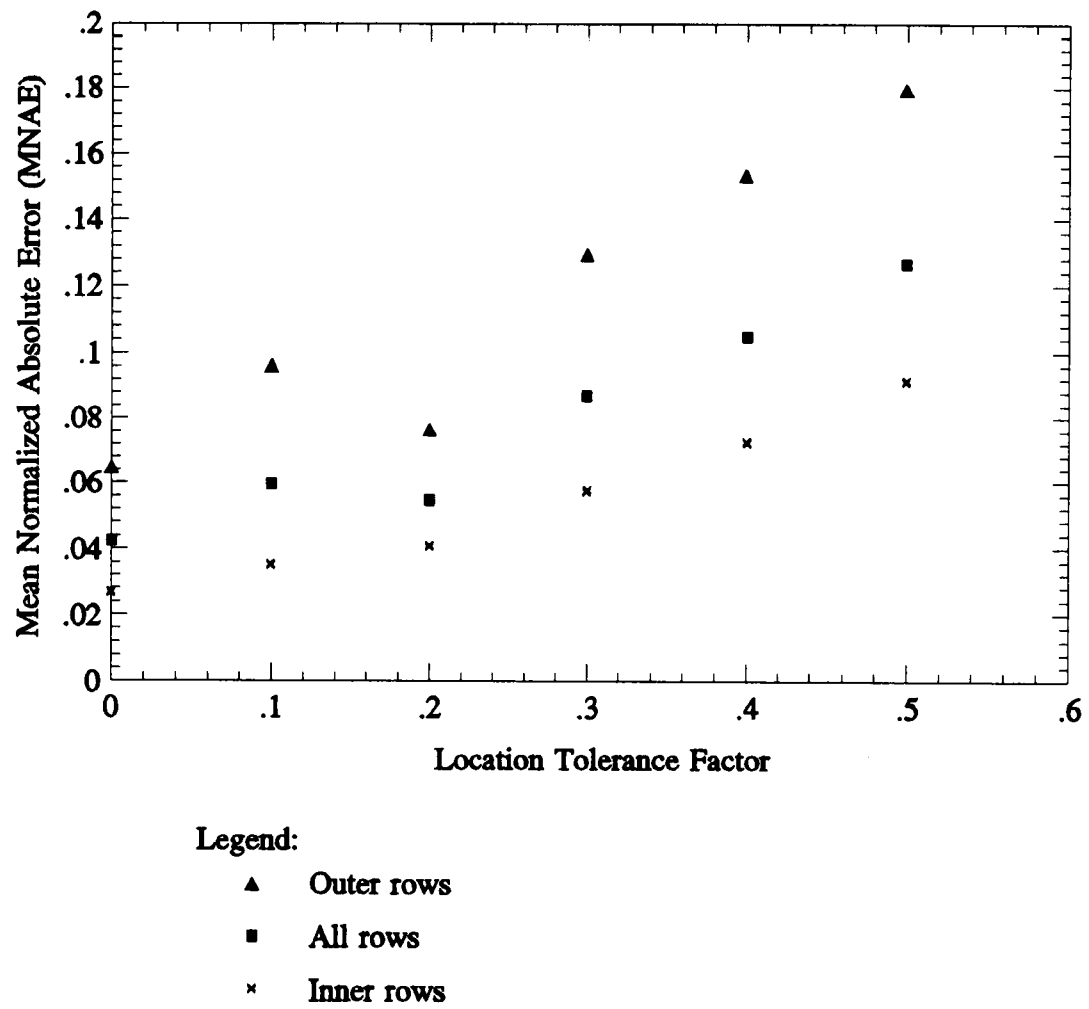


Figure VI-3. Inverse Distance Squared Results (Location Tolerance)

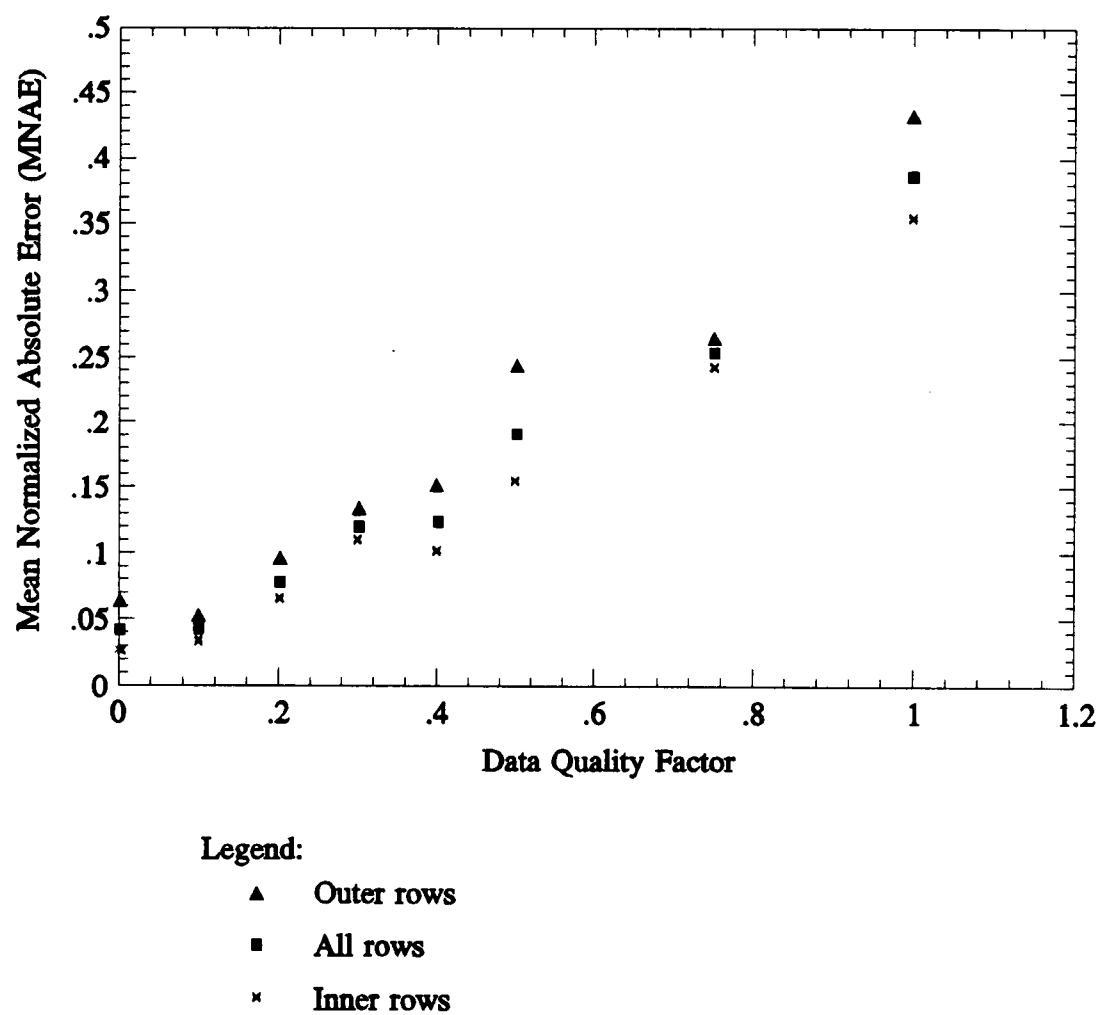


Figure VI-4. Inverse Distance Squared Results (Data Quality)

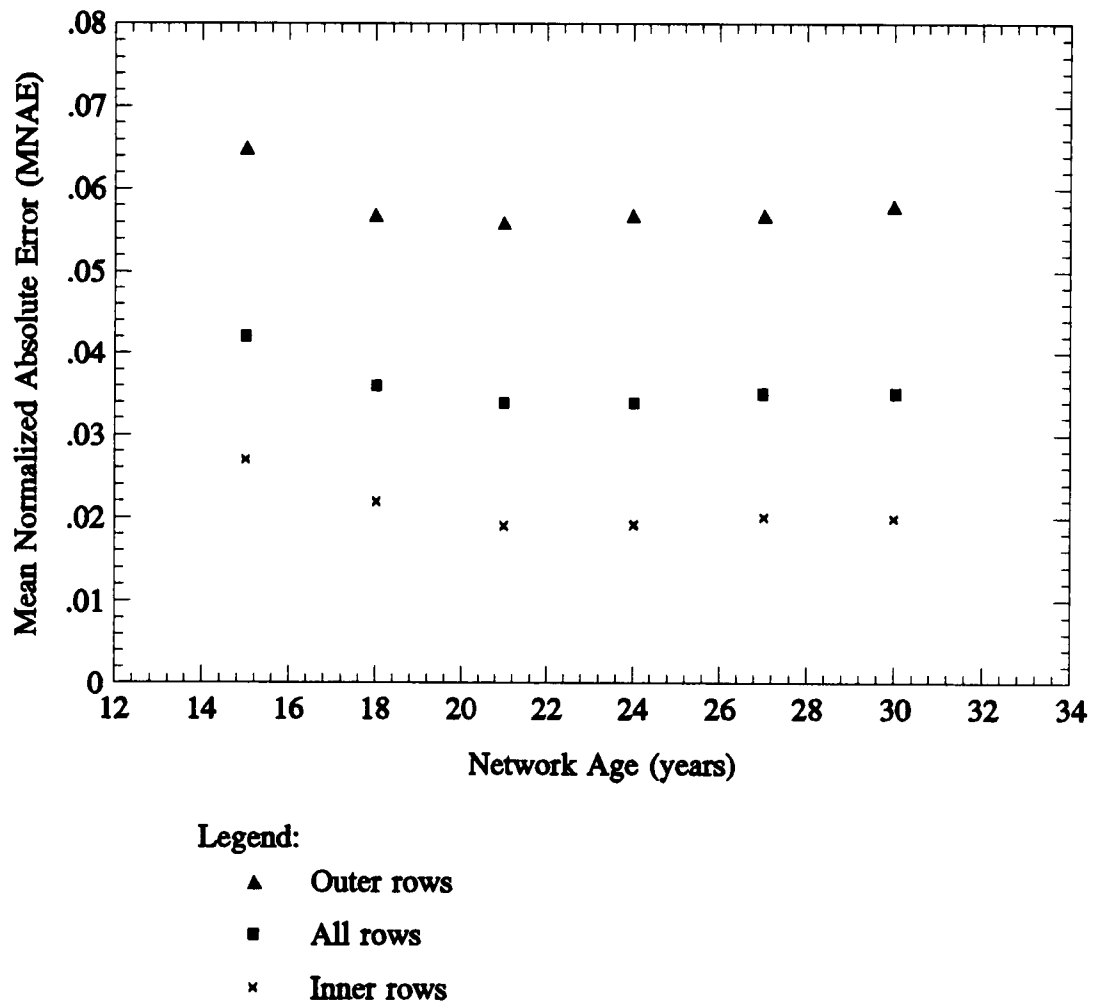


Figure VI-5. Inverse Distance Squared Results (Network Age)

facilitated by the regular pattern of the sampling grid. This reduced the identification of the four samples to be used in the interpolation equation (one in each quadrant) to a simple task of observation. The selection process was slightly complicated as the sample locations deviated from the sample grid nodes under the scenario of varying sample location tolerances. The problems associated with application of the search function with an irregular or random grid are evident in the case study discussed in Chapter VIII.

Figure VI-2 shows the type of response to varying sample density anticipated from a method that returns the sample value when the sample location and estimate location are the same. For synthetic data with no error, as the sample density approaches infinity, all three trends approach zero. For actual sample data, the data would approach some positive number indicative of the variability of the data.

Figures VI-3 and VI-4 also show anticipated results. The MNAE increases with decreased data quality (represented by an increasing data quality factor) and with degeneration of the grid pattern (represented by increasing location tolerance). Figures VI-3 and VI-4 also show considerable scatter in the results indicating individual estimate sensitivity to sample quality and location. This effect is more visual in these two graphs because a random process was used to generate the data for the data quality factors and location tolerances.

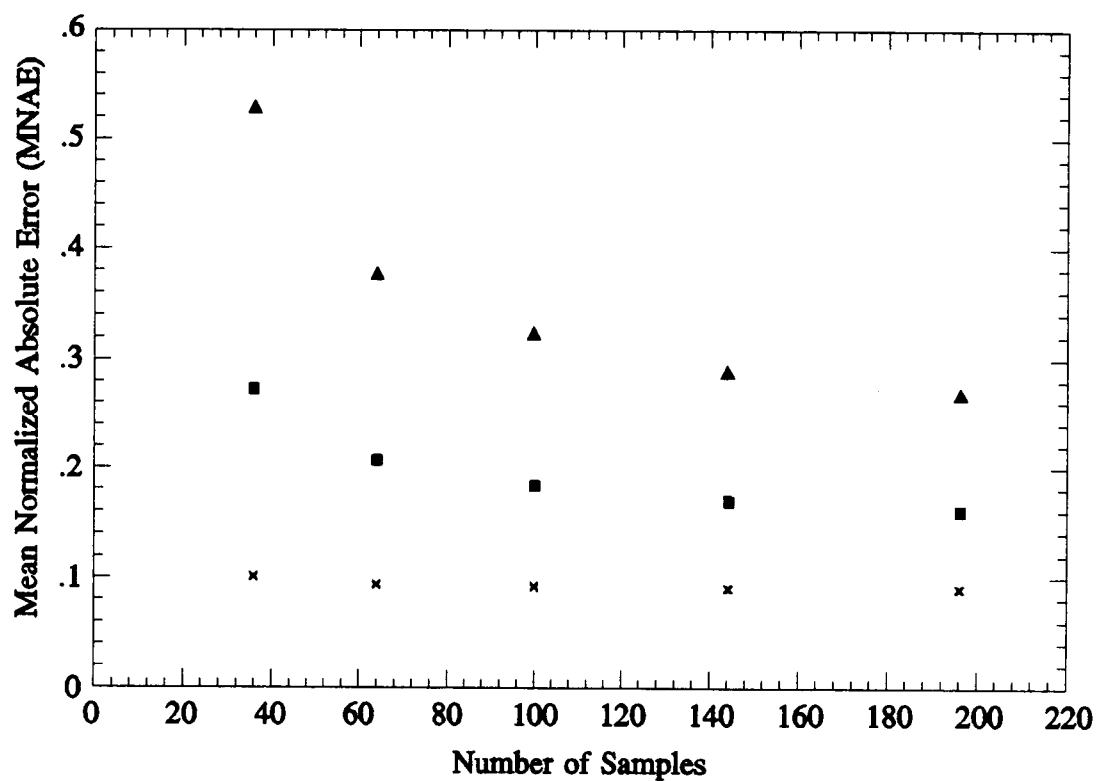
Since a different set of random numbers was used for each value of the variable, the amount of scatter changes with each value. A large number of estimates, such as the number required for contouring, would smooth out the variations. In this study, a grid of 25 estimates was not large enough to dampen the variability caused by this

process, resulting in a larger degree of scatter in the data. If the estimates were recalculated using a different set of random numbers, a different scatter pattern would be obtained. Therefore, caution should be exercised before inferring meaning to outliers.

Regression Method Results

Figures VI-6 through VI-9 show the results of interpolation calculations using the regression method with a fifth order polynomial. Figure VI-6 shows that although the overall error is sensitive to sample density, the error along the inner rows is not. This demonstrates a major problem with the regression approach. Good results can be obtained in the central area of the plume where the concentration is not rapidly changing; however, the higher concentration gradient at the plume edge requires a higher sample density to define the concentration profile. The polynomial is unable to adequately model this area without more samples.

Figure VI-6 also shows that the MNAE of the regression approach does not approach zero. Even on the relatively flat central portion of the plume, the MNAE approaches a value of approximately 0.1 (10% average error). This limit represents the error associated with the best approximation that a fifth order polynomial can make to a gaussian plume. Once the "best fit" has been reached, additional samples will have no influence on the regression coefficients. If a higher order polynomial were used, the overall MNAE would approach a lower, but still non-zero, limit.



Legend:

- ▲ Outer rows
- All rows
- × Inner rows

Note: 4 x 4 sample grid does not provide minimum number of data points required for the regression equation.

Figure VI-6. Regression Method Results (Sample Density)

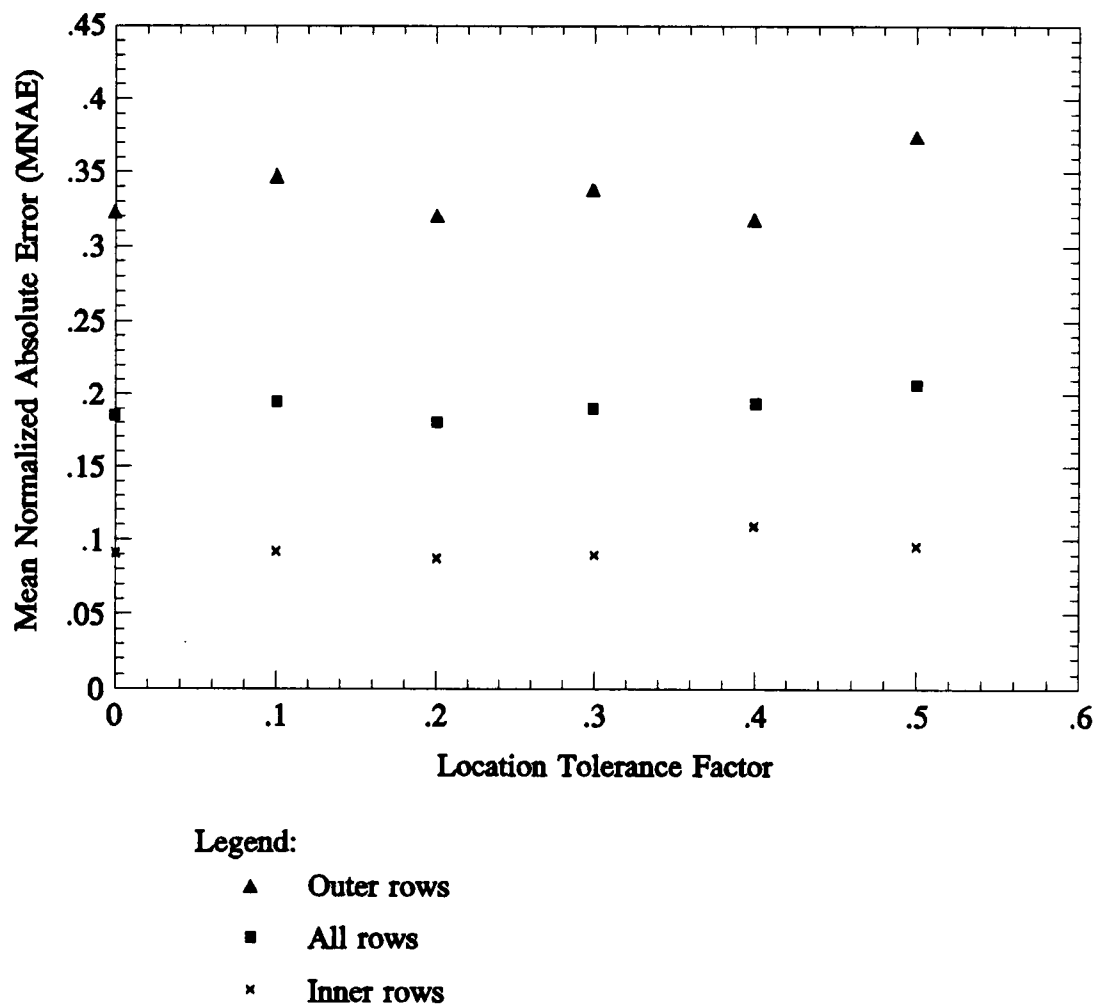
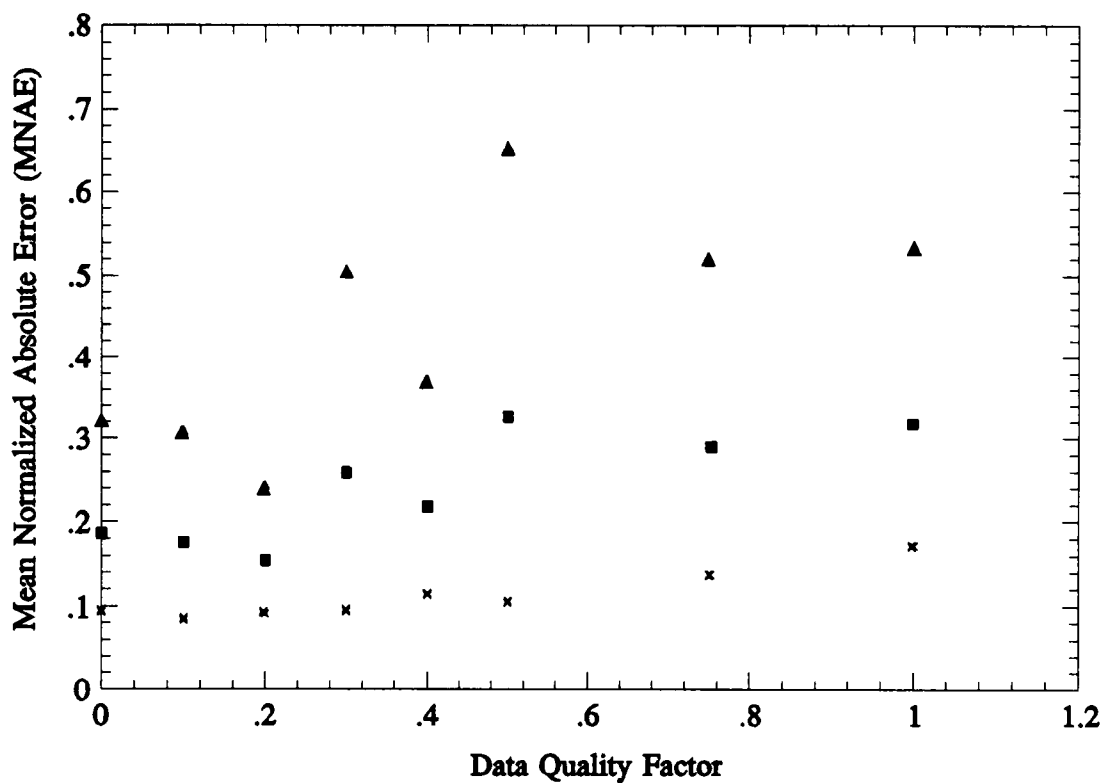


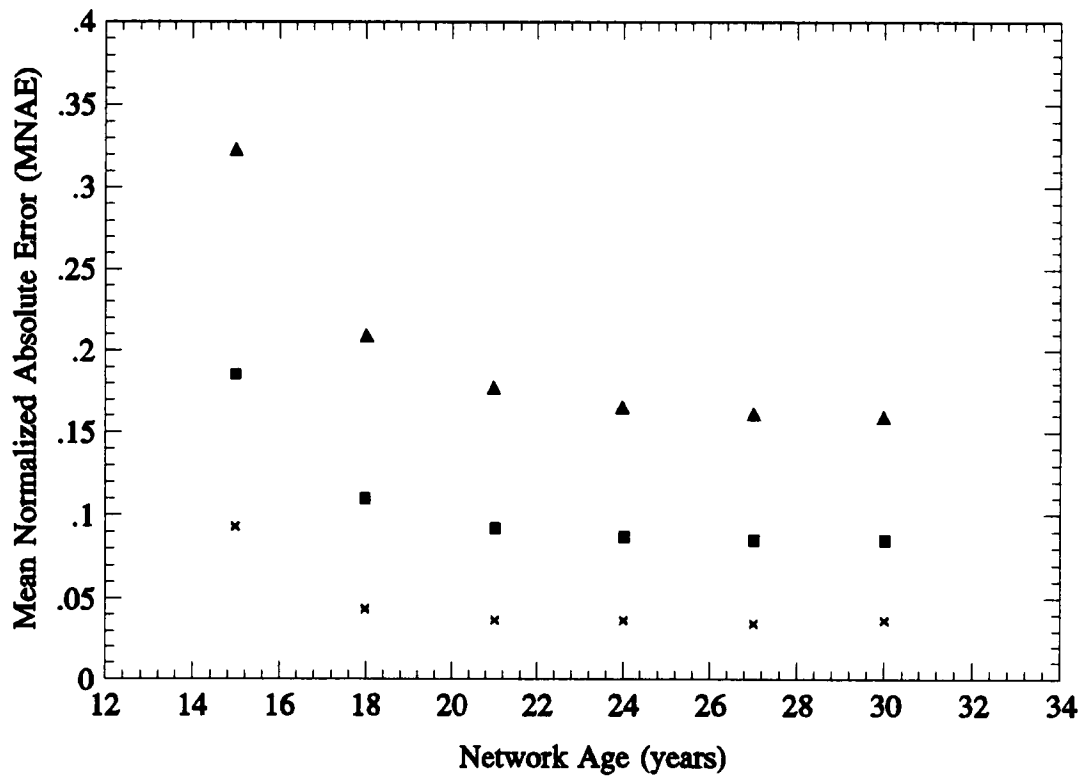
Figure VI-7. Regression Method Results (Location Tolerance)



Legend:

- ▲ Outer rows
- All rows
- × Inner rows

Figure VI-8. Regression Method Results (Data Quality)



Legend:

- ▲ Outer rows
- All rows
- × Inner rows

Figure VI-9. Regression Method Results (Network Age)

Figure VI-7 shows that the regression method is relatively insensitive to the location of the samples. If the samples have a reasonably diverse distribution over the plume, the resulting regression coefficients are similar for different sets of sample locations. This insensitivity does not apply to variances in data quality. Figure VI-8 shows that the regression method is sensitive to the quality of the data, affecting both the value of the MNAE and the scatter of the data.

The poor correlation between estimate quality and goodness-of-fit is demonstrated by comparing the coefficients of determination (R^2) with the interpolation results. For all calculations, except those for varying data quality, the coefficients of determination were greater than 0.97, indicating an excellent fit. However, a good fit did not indicate high estimate quality.

Figure VI-9 demonstrates the problem that the regression method has with interpolation in areas of rapidly changing values. The sample grid is located to include the leading edge of the contaminant plume after 15 years of migration. As the plume continues to migrate, this edge moves away from the sample grid until, at approximately 24 years, it no longer influences the samples. Figure VI-9 shows a distinct decrease in MNAE until the leading edge is clear of the sample grid, beyond which there is no further decrease in the MNAE.

Kriging Results

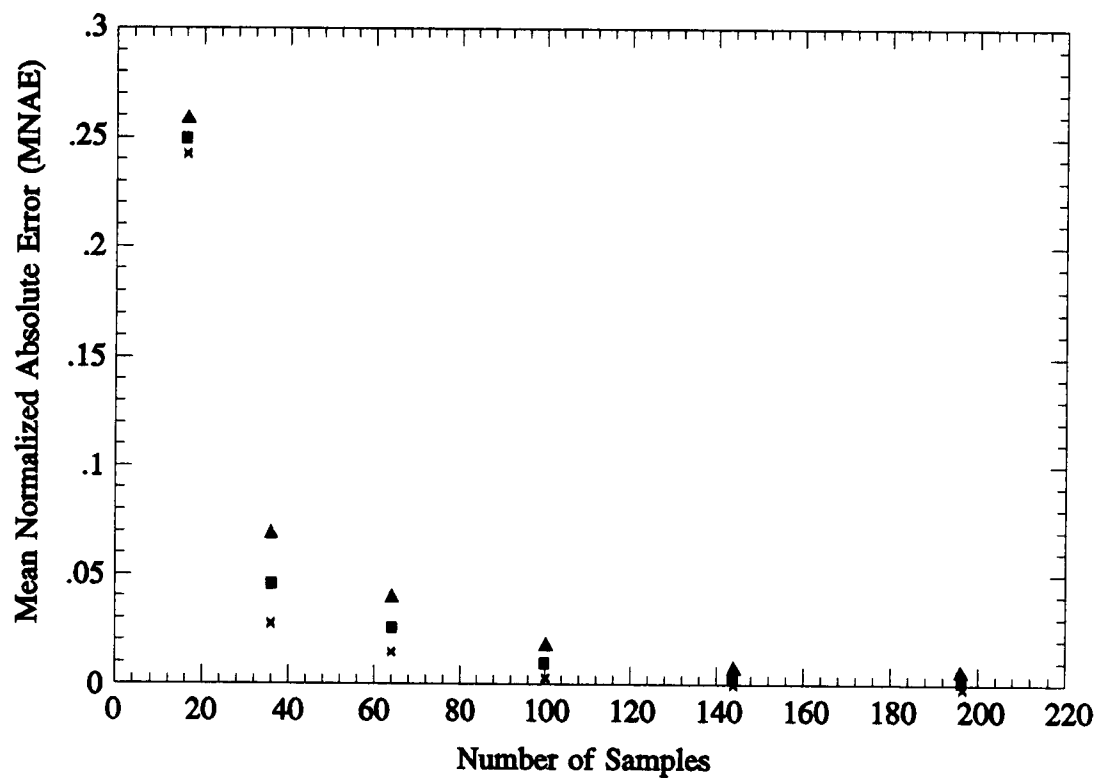
The presentation of the kriging calculations is divided into two areas: (1) the final results, similar to those already presented, and (2) the details of the kriging

process used to generate the results. The interaction between the investigator and the kriging process makes kriging unique among the three interpolation methods. The decisions made during the kriging process (such as variogram selection and neighborhood definition) are tailored to each data set. Therefore, application of kriging to any single set of data by different investigators may not result in a single, unique result. The final results alone have limited utility without knowledge of the details of the process.

Results

The results of the kriging calculations are provided in Figures VI-10 through VI-13. Figure VI-10 shows the problem most commonly associated with kriging, rapid degeneration of estimate quality at low sample densities. This problem is caused by two primary factors: (1) low sample densities do not provide sufficient sample pairs to accurately determine the variogram, and (2) the lack of samples close to the estimate point requires the use a larger neighborhood to obtain the minimum number of samples for the kriging equations, resulting in violations of the stationarity requirement.

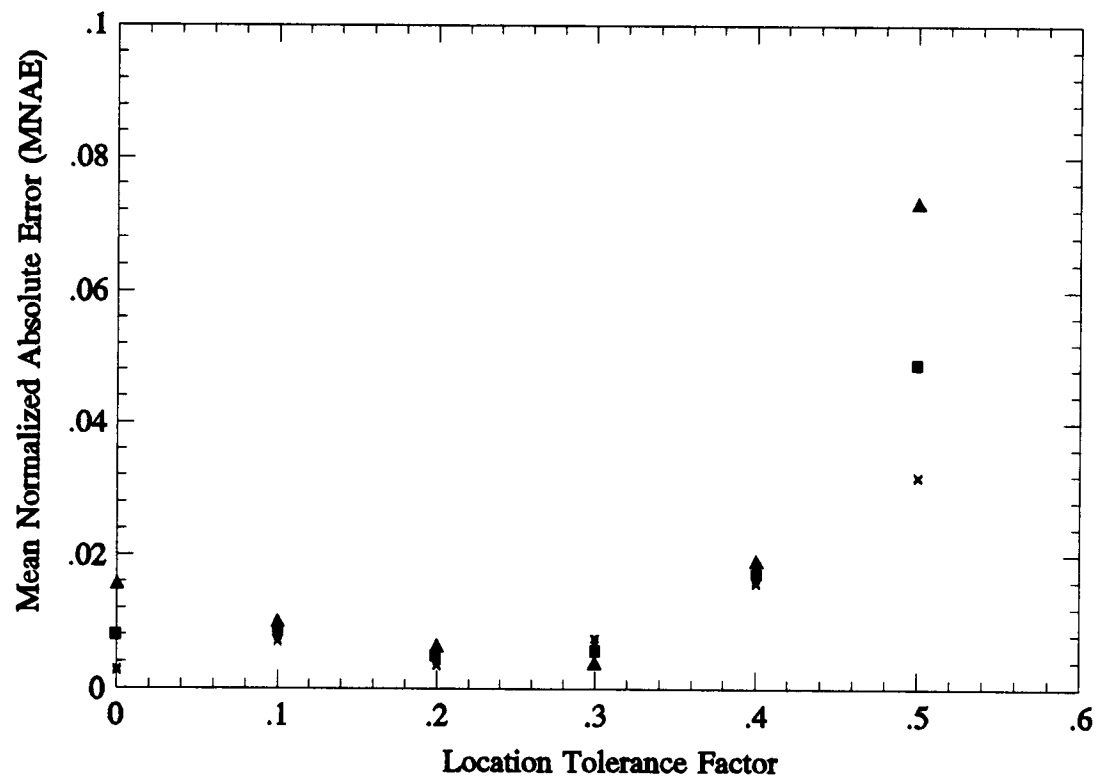
The kriging results are insensitive to minor variations of sample location with respect to the sample grid as shown in Figure VI-11. An argument could be made that some variability in sample location is desired since this would produce a more diverse set of sample pairs with respect to distance and Figure VI-11 could be interpreted to support such a position. However, given the scatter in the data, a single plot is insufficient to verify this hypothesis.



Legend:

- ▲ Outer rows
- All rows
- × Inner rows

Figure VI-10. Kriging Results (Sample Density)



Legend:

- ▲ Outer rows
- All rows
- × Inner rows

Figure VI-11. Kriging Results (Location Tolerance)

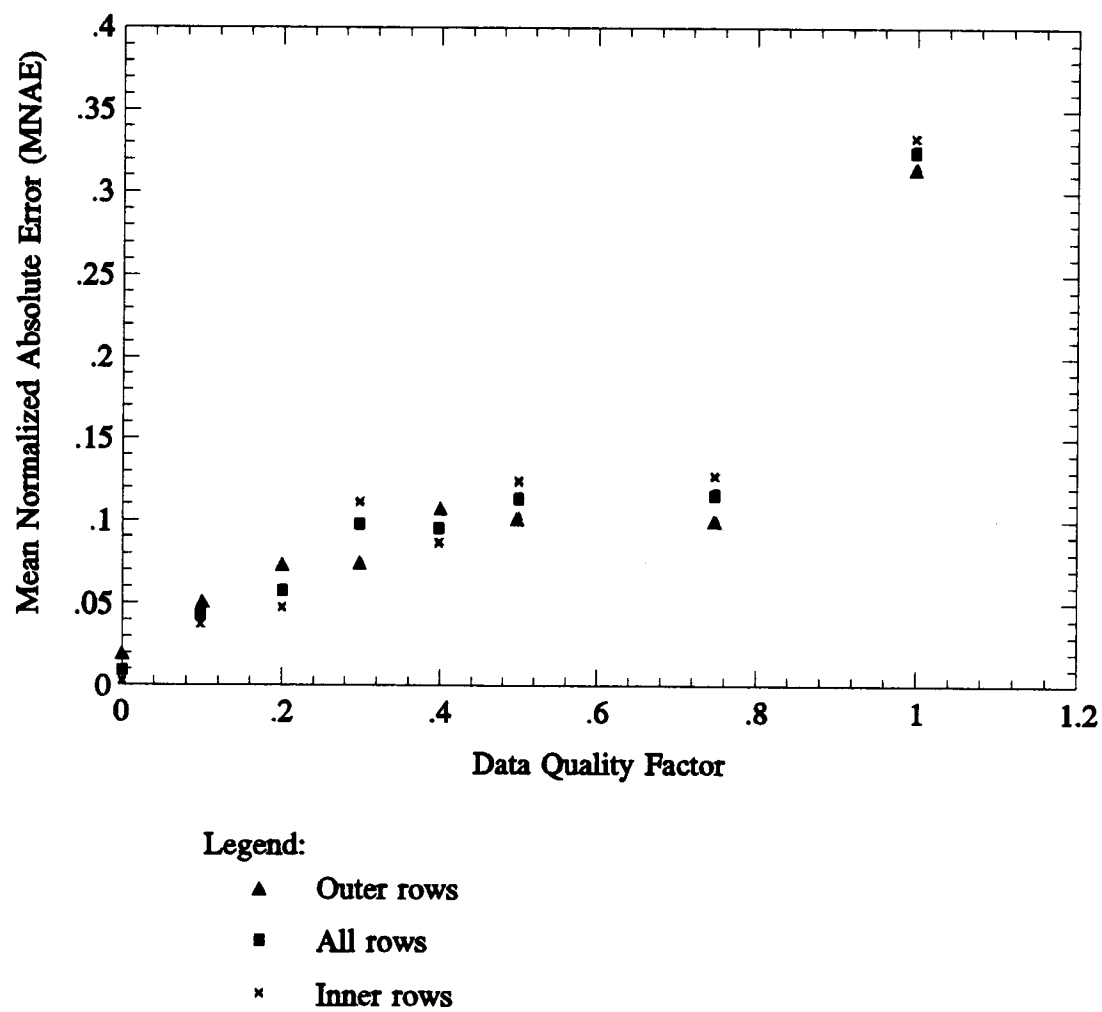
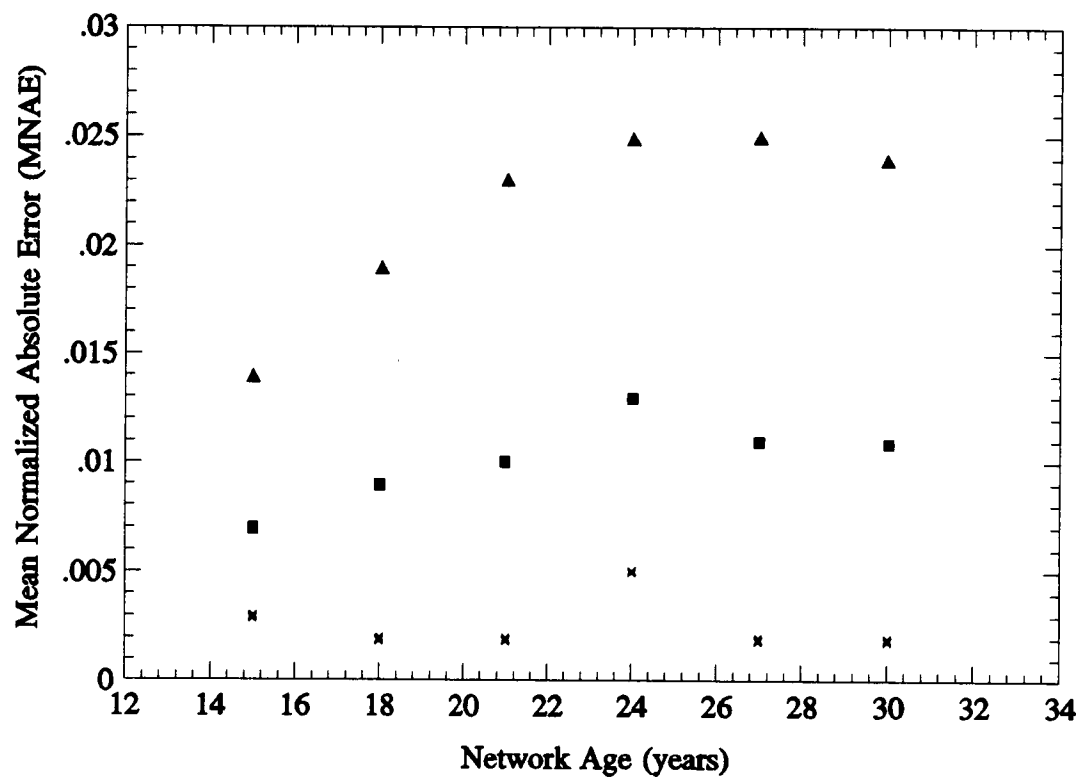


Figure VI-12. Kriging Results (Data Quality)



Legend:

- ▲ Outer rows
- All rows
- × Inner rows

Note: The above plot shows an atypical response for the outer row MNAE. See the text for discussion.

Figure VI-13. Kriging Results (Network Age)

Figure VI-12 shows a decrease in estimate quality with a decrease in data quality, as expected. The unusual feature of this plot is lack of definition between the data for the inner and outer rows. For some values, the inner and outer row error relationships are inverted, with the outer rows showing the lower MNAE. This indicates that the relationship between the errors for inner and outer rows is a weak function of data quality as compared with the relationships demonstrated on other plots. However, what appear to be inversions of the normal inner-outer row relationship may be the result of random data scatter rather than an actual trend.

Figure VI-13 appears to indicate that the kriging estimate quality for the outer rows decreases as the plume migrates and the leading edge moves out of the sample grid. This is contrary to the argument that removal of the leading edge should improve the estimate quality. An inspection of the individual estimates reveals that over 50% of the error is caused by one estimate location that is the most distant from the plume centerline and is close to the lower inflection point on the gaussian curve. This point is also at the extreme edge of the sampling grid with few sample locations beyond this point from which kriging can identify a change in the spatial correlation of the samples.

As the plume migrates, the inflection point moves slightly, resulting in a change in the MNAE of the problem location. Although all three methods show high errors for this location, since the kriging errors are small, this slight change is translated into a significant change in the outer row MNAE in the kriging results, but not in the results of the other two methods which show higher overall errors. Edge effects such

as this are commonly seen in data interpolation. The overall error trend should be considered a more typical example of kriging response to network age.

The Kriging Process

The kriging process is a series of four steps in which the investigator analyzes available information and makes decisions that will eventually influence the quality of the kriging estimates. All of the steps were performed using the Geostatistical Environmental Assessment Software (GEO-EAS), which is available through the Environmental Protection Agency's Environmental Monitoring Systems Laboratory (USEPA, 1991). The steps are as follows:

- (1) Inspection of raw data
- (2) Identification of the components of the variogram (type, range, sill, and major and minor axes)
- (3) Cross-validation of the variogram
- (4) Generation and solution of the kriging equations

For this study, the first step was performed once. Upon inspection, the data distribution was easily recognized as gaussian which is the desired form; therefore, no data transformation was required. This result was not unexpected since application of the truth equation results in the generation of a two-dimensional gaussian plume.

Once the data distribution was determined to be in an acceptable form, the variogram was constructed. A separate variogram was constructed for each data set, ensuring that knowledge of the parameters of a previous variogram did not overly

influence decisions on other data sets. Construction of the variogram was a trial-and-error process using various combinations of values for the type (gaussian, spherical, exponential or linear), sill, nugget and range. The values were first determined assuming isotropic conditions.

Figure VI-14 shows the variogram for the 10 x 10 sampling grid used in the sample density plot (Figure VI-10). The top figure shows the variogram over the entire range of pair distances. The bottom figure focuses on the portion of the variogram that will be used for the calculations. The portion to be used was determined by the size of the neighborhood. In this study, the neighborhood was typically limited to 200 meters in each direction although distances up to 300 meters were permitted if necessary to capture sufficient sample points. That portion of the variogram outside the neighborhood did not have to fit the data since it was never used in the calculations. Using areas beyond approximately 300 meters from the estimate location could have resulted in a violation of the stationarity requirement.

The next step in the variogram development was to determine if the data was anisotropic and to adjust the "omnidirectional" variogram as required. This was accomplished by limiting the selection of data pair vectors to (1) those within a 22.5° angle about a line parallel to the advection vector and (2) those within a 22.5° angle about a line perpendicular to the advection vector. The variogram was adjusted for each case using only the range value (a restriction of the GEO-EAS software). The two directional variograms are shown in Figure VI-15. The range values represent the major and minor axes of the variogram. The GEO-EAS program assumes the directional variogram ranges form an elliptical pattern.

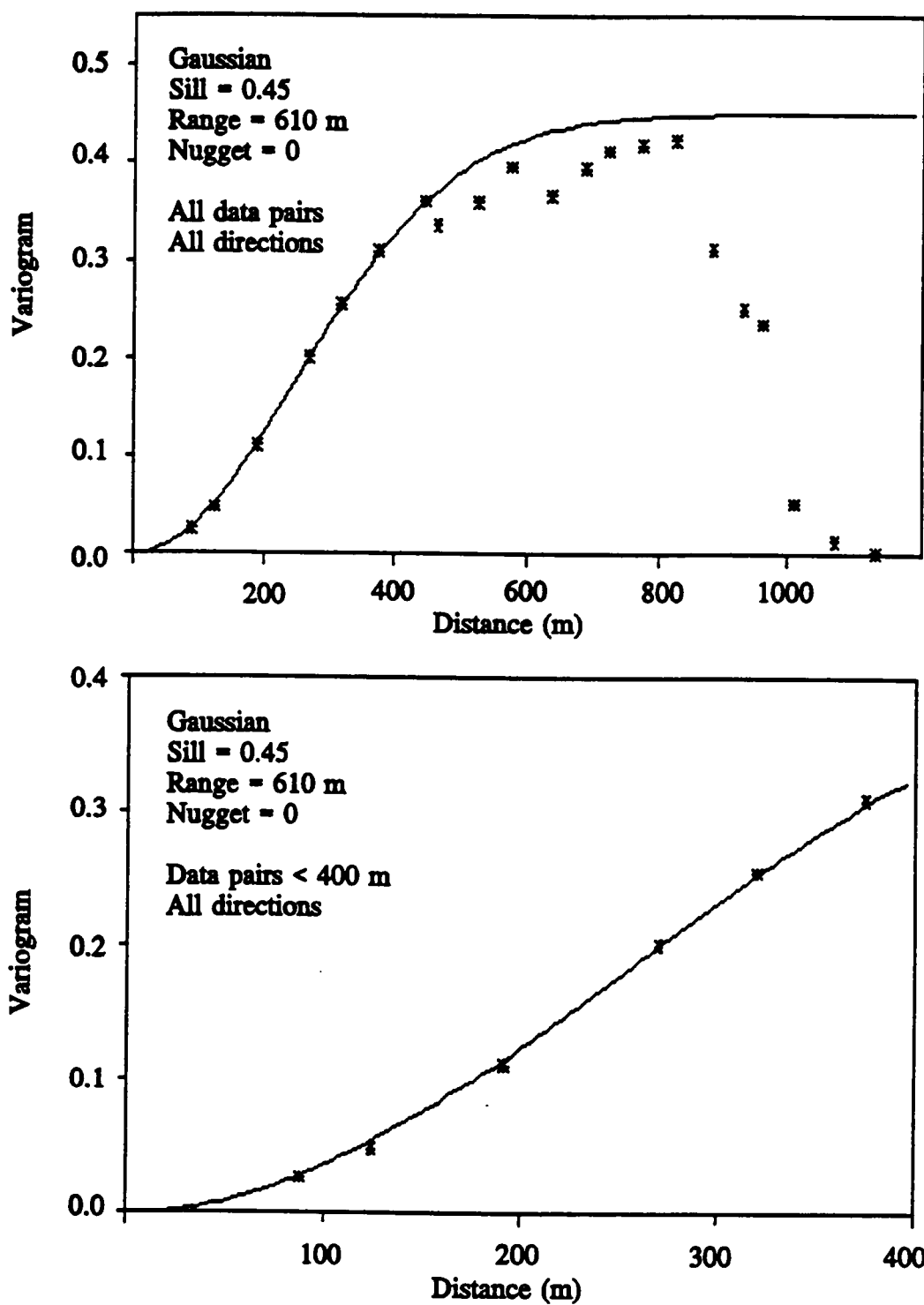


Figure VI-14. Variograms for 10 x 10 Sample Grid (Isotropic)

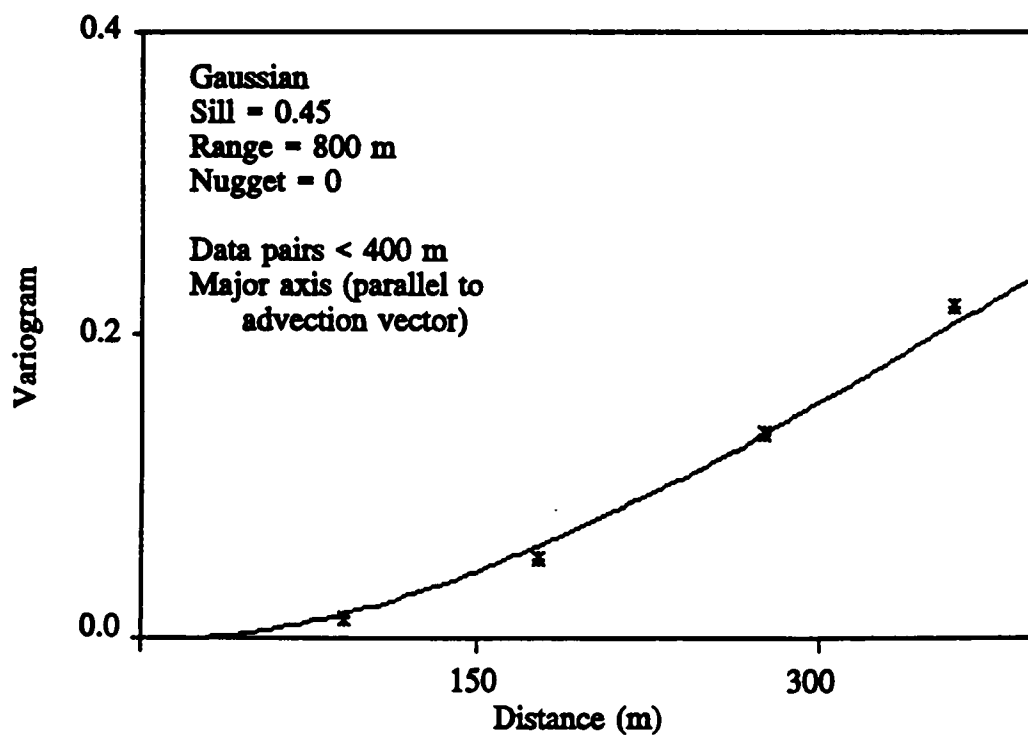
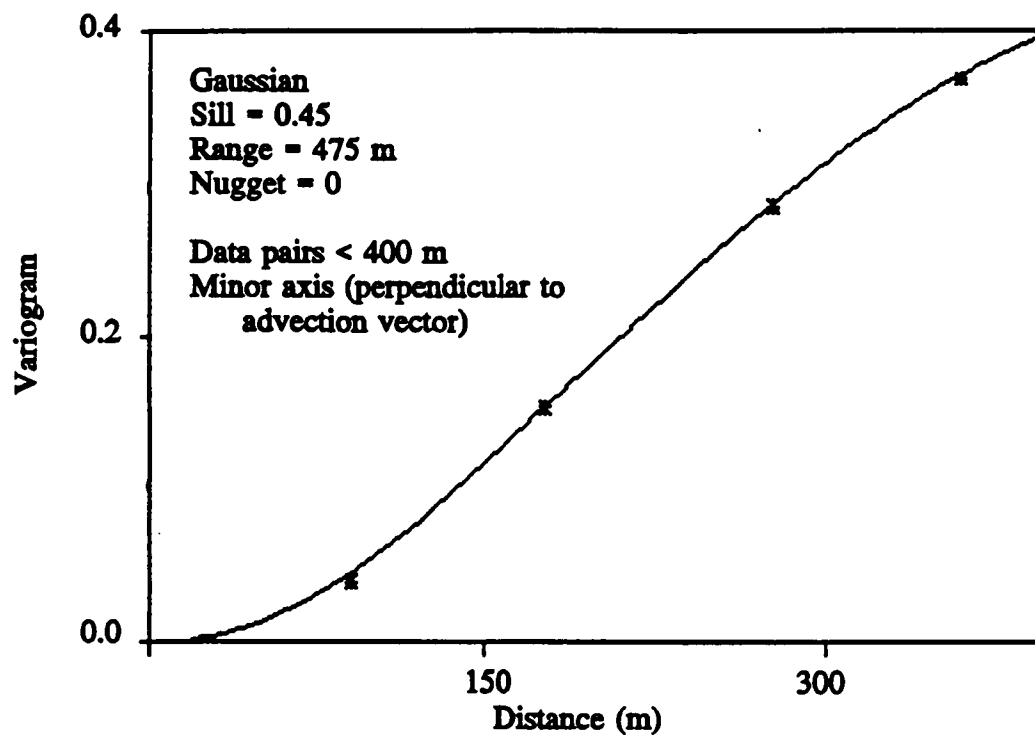


Figure VI-15. Variograms for 10 x 10 Sample Grid (Anisotropic)

The third step in the kriging process is cross-validation. Cross-validation involves estimating values at each sampled location while excluding the value of the point to be estimated. This provides a measure of how well the variogram and neighborhood search function will accurately reproduce the spatial variability of the observed data. Cross-validation was performed for one data set. Since minor variations in the variogram had no observable effect on the kriging results, a visual fit of the variogram proved to be more than adequate.

The final step in the kriging process is the generation and solution of the kriging equations. At this point, the only parameter left to finalize was the search parameters which define the neighborhood. For all of the data sets, except for the extremely low sample density runs, this was set as a circular search pattern with a 200-meter radius. This provided between 8 and 12 samples for each estimate. For the low sample density runs, the search radius was expanded to 300 meters and the minimum number of samples was reduced from 8 to 4.

Throughout the kriging process, the variable having the most influence on the quality of the kriging estimates was the variogram. Since all of the data were generated using the same "truth" equation, the "true" variogram never changes (except for the network age variable). The variance in the variogram parameters can be used as a indication of the error introduced by the variation of the sample density and location, data quality, and network age. Tables VI-1 through VI-4 provide a listing of all of the variograms used to generate the kriging data in this chapter. The variance in variogram parameters shows good agreement with the variance in MNAE shown in Figure VI-10 through VI-13.

Table VI-1. Variogram Parameters (Sample Density)

Variograms for Sample Density Variable					
Sample Grid Size	Type	Sill	Nugget	Major Range	Minor Range
14 x 14	Gaussian	0.45	0	820	495
12 x 12	Gaussian	0.45	0	800	485
10 x 10	Gaussian	0.45	0	800	475
8 x 8	Gaussian	0.45	0	830	475
6 x 6	Gaussian	0.60	0	1025	550
4 x 4	Gaussian	0.60	0	1100	600

Table VI-2. Variogram Parameters (Location Tolerance)

Variograms for Location Tolerance Variable					
Location Tolerance Factor	Type	Sill	Nugget	Major Range	Minor Range
0.0	Gaussian	0.5	0	850	520
0.1	Gaussian	0.5	0	860	520
0.2	Gaussian	0.5	0	880	600
0.3	Gaussian	0.5	0	860	540
0.4	Gaussian	0.5	0	880	540
0.5	Gaussian	0.5	0	860	520

Table VI-3. Variogram Parameters (Data Quality)

Variograms for Data Quality Variable					
Data Quality Factor	Type	Sill	Nugget	Major Range	Minor Range
0.0	Gaussian	0.45	0	800	475
0.1	Gaussian	0.50	0	850	520
0.2	Gaussian	0.45	0.005	900	530
0.3	Gaussian	0.45	0.01	850	450
0.4	Gaussian	0.45	0.04	800	430
0.5	Gaussian	0.45	0.04	820	465
0.75	Gaussian	0.57	0.07	760	430
1.0	Exp	0.44	0.02	700	270

Table VI-4. Variogram Parameters (Network Age)

Variograms for Network Age Variable					
Network Age (years)	Type	Sill	Nugget	Major Range	Minor Range
15	Gaussian	0.5	0	840	525
18	Gaussian	1.0	0	950	450
21	Gaussian	1.5	0	1100	400
24	Gaussian	2.0	0	1350	375
27	Gaussian	2.5	0	1500	375
30	Gaussian	3.0	0	1700	375

CHAPTER VII

METHOD COMPARISON

The previous chapter focused on the results of individual extrapolation methods without any comparison of the methods to each other. This chapter presents the interpolation results in a form suitable for comparison and discusses the similarities and differences of the methods. Presentation of conclusions on the merits and applicability of the three methods is reserved for the final chapter.

Inspection of the data included in this chapter supports an argument that, within the range of variables used in this study, kriging consistently provides more accurate estimates than the inverse distance squared method which, in turn, consistently provides more accurate estimates than the regression method. The only condition for which this pattern failed to hold was for a data quality factor of 1.0. The significance of this single deviation from the pattern is debatable due to the considerable amount of scatter in the data associated with the data quality variable.

Figures VII-1 through VII-3 and Table VII-1 show that the response to sample density is similar for each method. Each method shows (1) a region in which the sample quantity is insufficient to support the estimation function, resulting in a rapid decrease in estimate quality, (2) a region of increasing estimate quality with increasing sample number, and (3) a region of diminishing returns, where additional data provide marginal increase in quality.

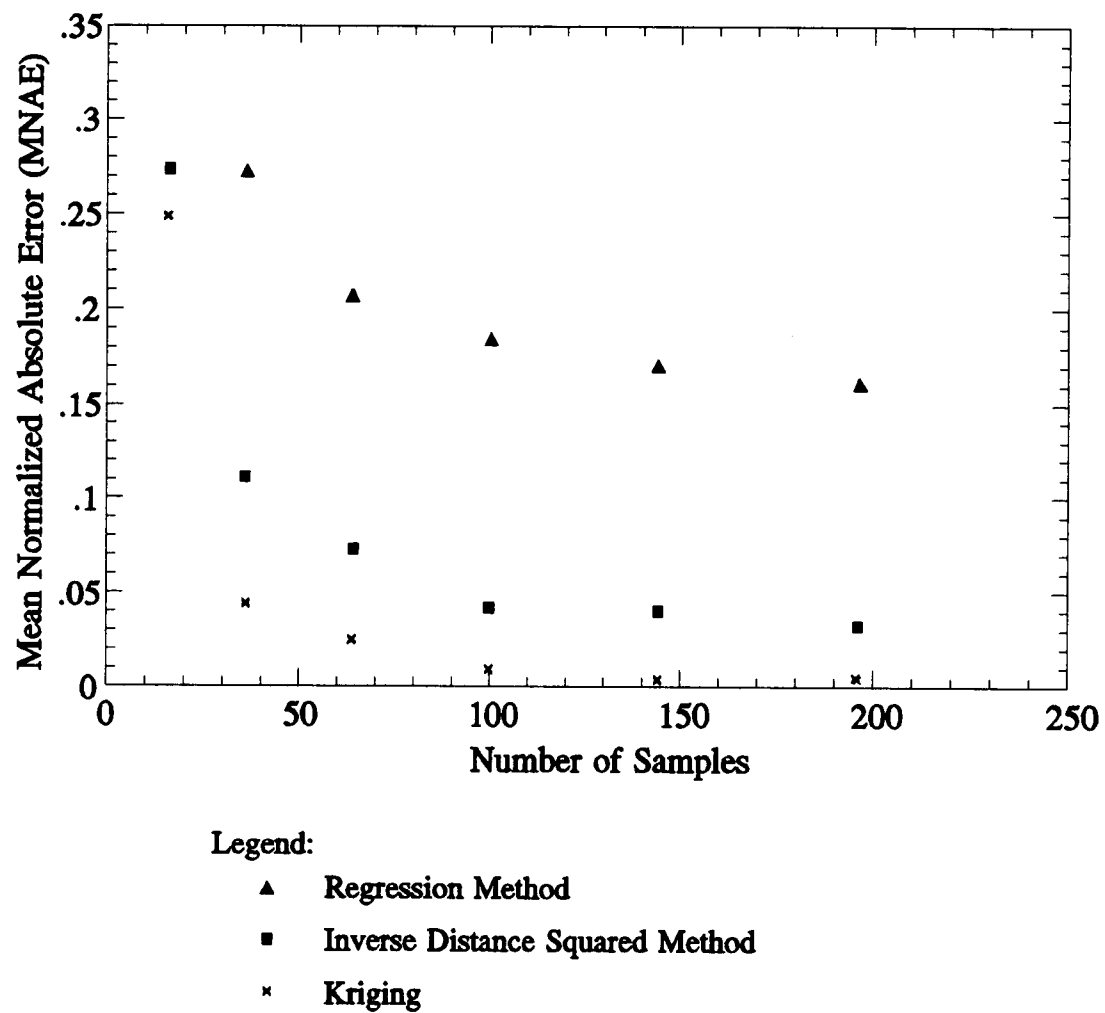


Figure VII-1. Mean Normalized Absolute Error Comparison (Sample Density)

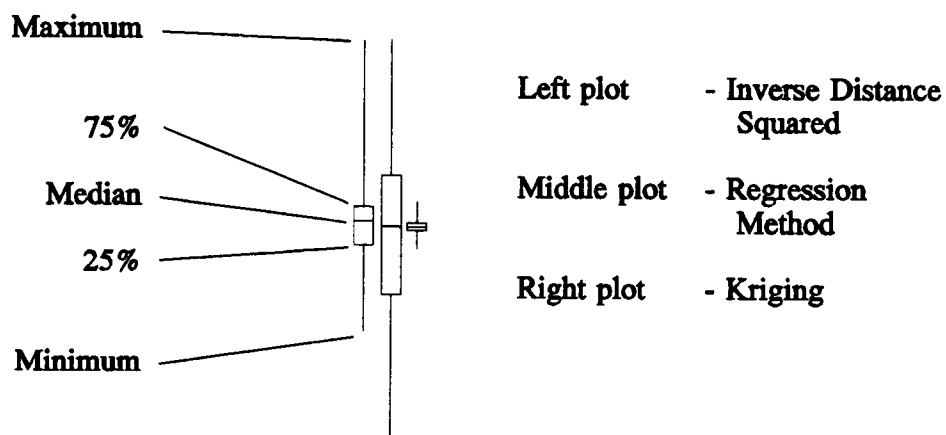
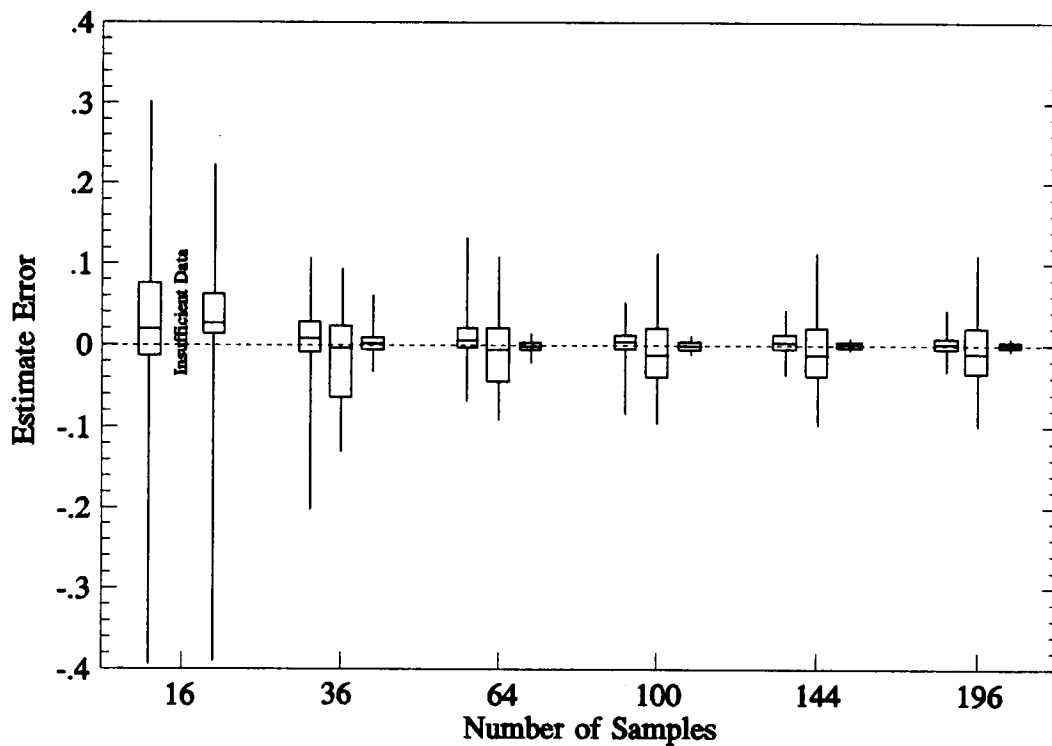


Figure VII-2. Estimate Error Comparison (Sample Density)

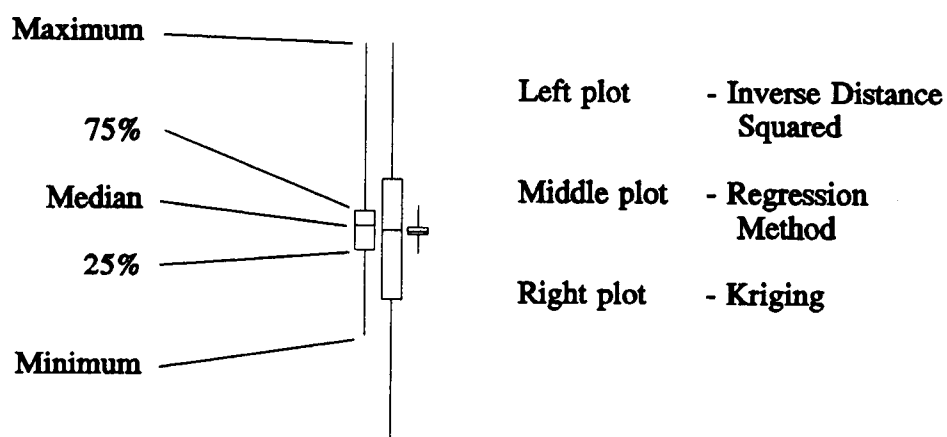
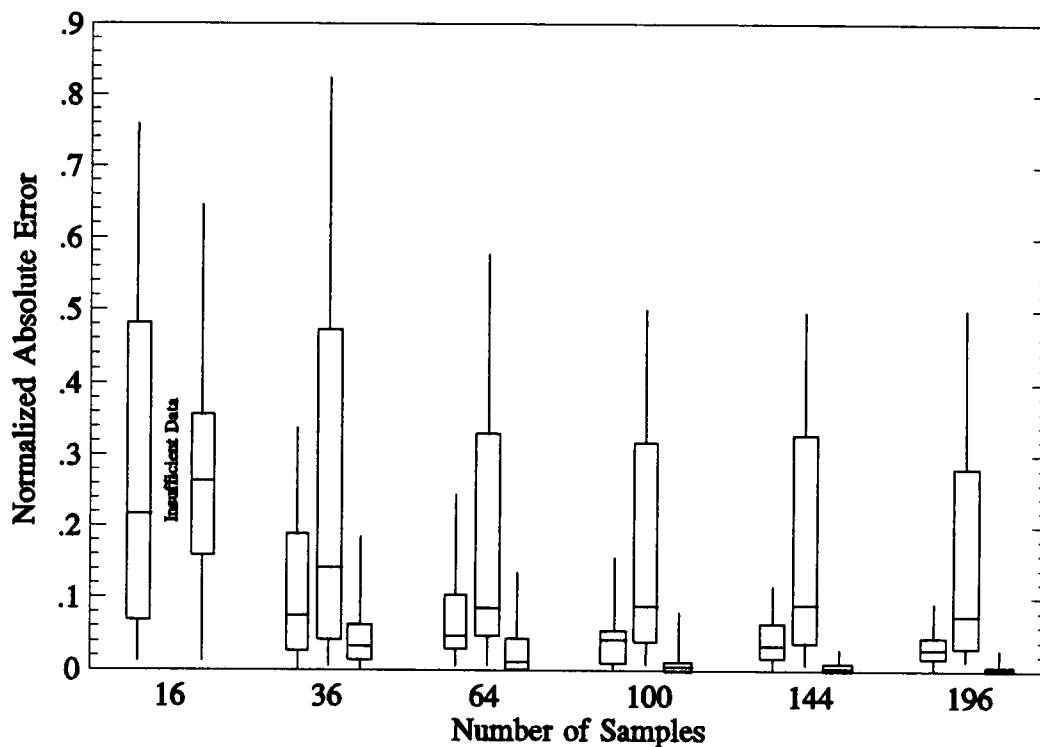


Figure VII-3. Normalized Absolute Error Comparison (Sample Density)

Table VII-1. Summary Statistics (Sample Density)

Interpolation Method	Number of Samples	Normalized Absolute Error Distribution				
		Mean	Median	Min.	Max.	Std. Dev.
Inverse Distance Squared	16	0.273	0.239	0.017	0.753	0.236
	36	0.111	0.101	0.001	0.340	0.096
	64	0.073	0.044	0.005	0.246	0.061
	100	0.042	0.046	0.001	0.155	0.037
	144	0.041	0.041	0.002	0.114	0.028
	196	0.033	0.034	0.003	0.082	0.023
Regression Method	16	(insufficient samples)				
	36	0.273	0.155	0.008	0.824	0.287
	64	0.208	0.130	0.004	0.577	0.204
	100	0.185	0.122	0.009	0.497	0.179
	144	0.171	0.104	0.012	0.496	0.165
	196	0.162	0.088	0.013	0.500	0.158
Kriging	16	0.249	0.264	0.011	0.646	0.151
	36	0.045	0.030	0.0	0.185	0.046
	64	0.025	0.008	0.0	0.137	0.036
	100	0.009	0.003	0.0	0.081	0.018
	144	0.003	0.0	0.0	0.030	0.008
	196	0.004	0.0	0.0	0.030	0.009

The kriging data support previous research findings indicating that kriging begins to show significant deterioration of estimate quality with less than approximately 30 samples (Cooper, 1988). Since both kriging and the inverse distance squared method return the sample value when the sample and estimate locations coincide, their estimate error will approach zero as the number of samples approaches infinity. For practical applications with a finite number of samples, each of the methods has reached its minimum estimate error at or before 196 samples. It should be noted that any reference to a specific number of samples (or a sample density) applies only to the plume profile and sample area used in this study. Different spatial distributions will require different sample quantities (or sample densities) to achieve the same estimate quality.

Each of the estimation methods has a slightly different response to deviations of sample location from the nodes of the sample grid as shown in Figures VII-4 through VII-6 and Table VII-2. The regression method is relatively insensitive over the range of location variance allowed and the inverse distance squared method demonstrates sensitivity over the entire range. Kriging shows initial insensitivity with an increase in MNAE beyond a tolerance factor of 0.3. (The tolerance factor represents the amount of random location movement permitted expressed as a fraction of the internodal spacing.)

A tolerance factor of 0.5 is the maximum deviation permitted if the sample locations are arranged according to a pattern or grid. Beyond this point, the spatial distribution of the sample network will show an increasing loss of uniform coverage. As location randomness increases, there will be more sample areas that depend on

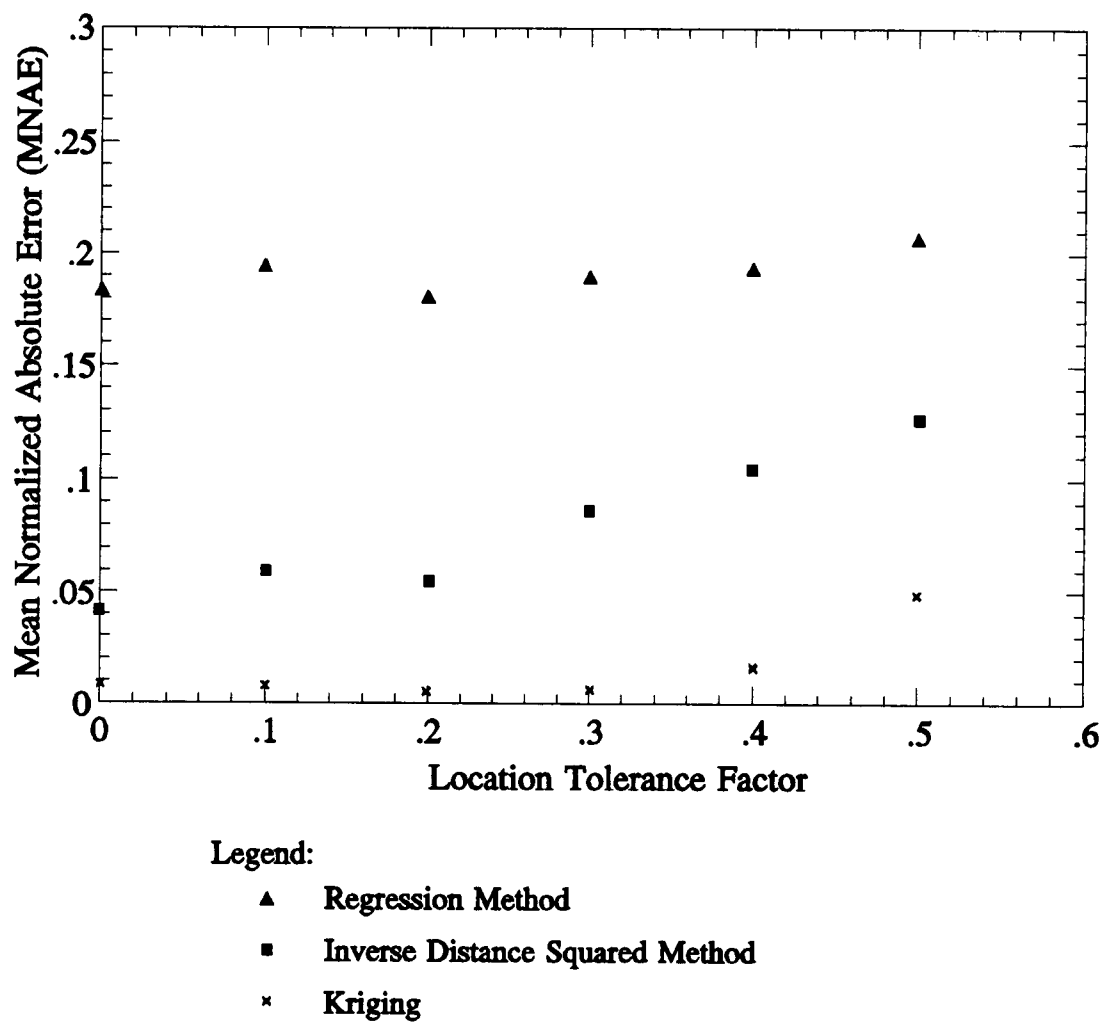


Figure VII-4. Mean Normalized Absolute Error Comparison (Location Tolerance)

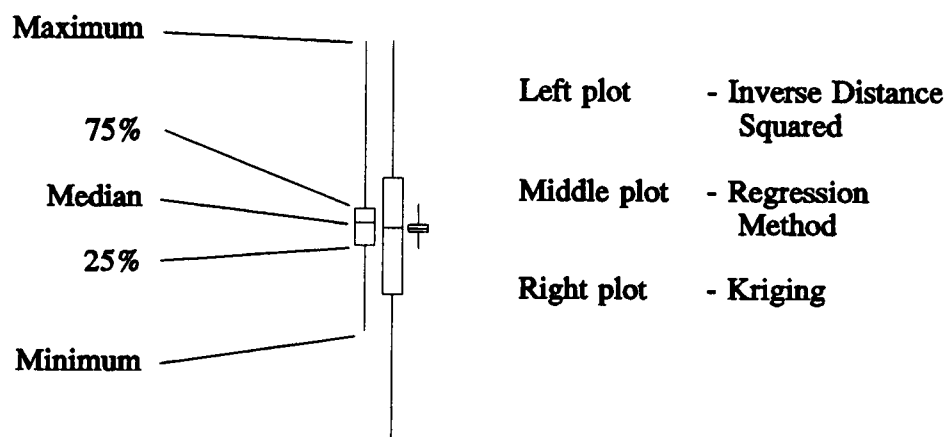
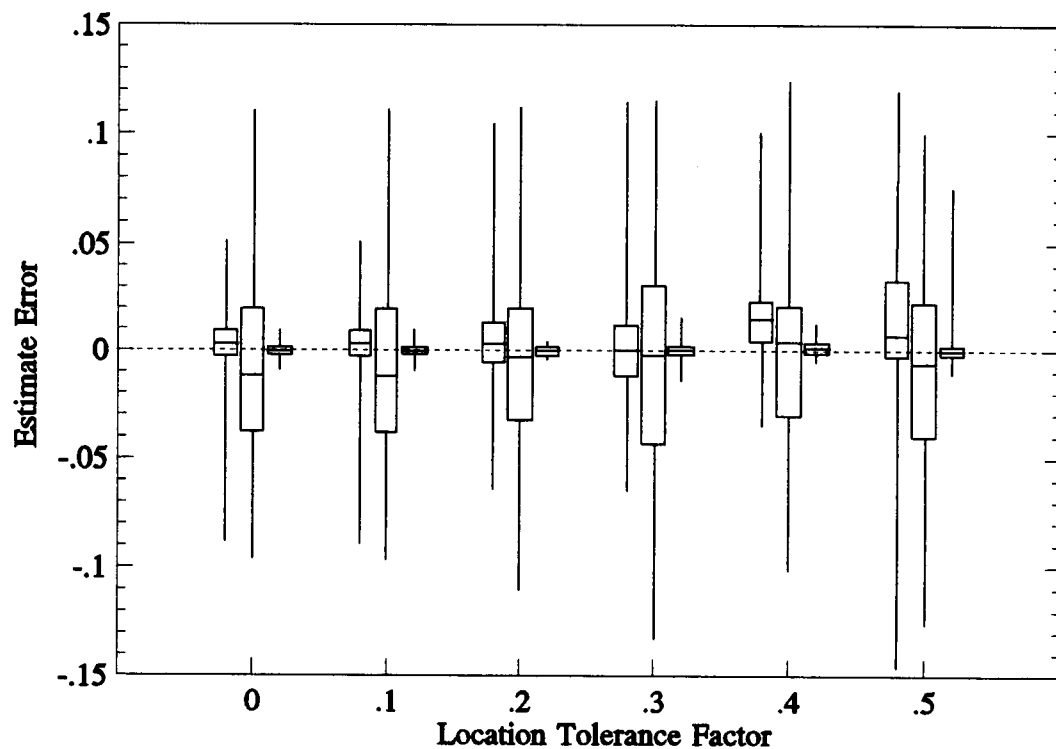


Figure VII-5. Estimate Error Comparison (Location Tolerance)

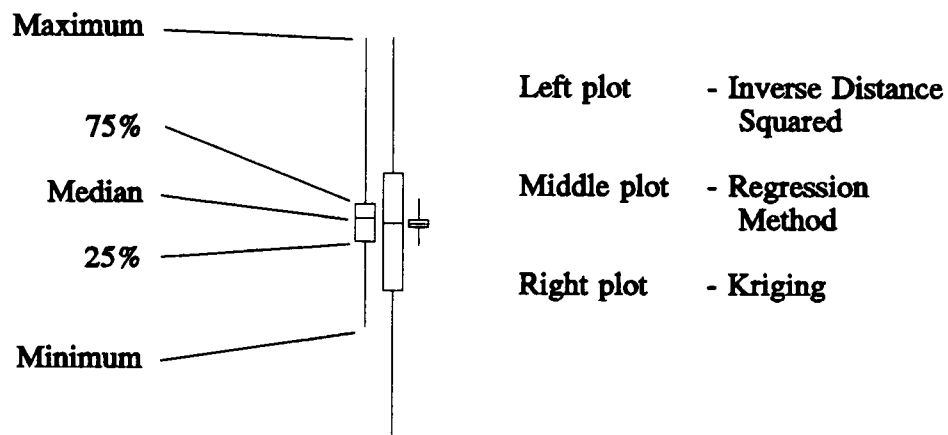
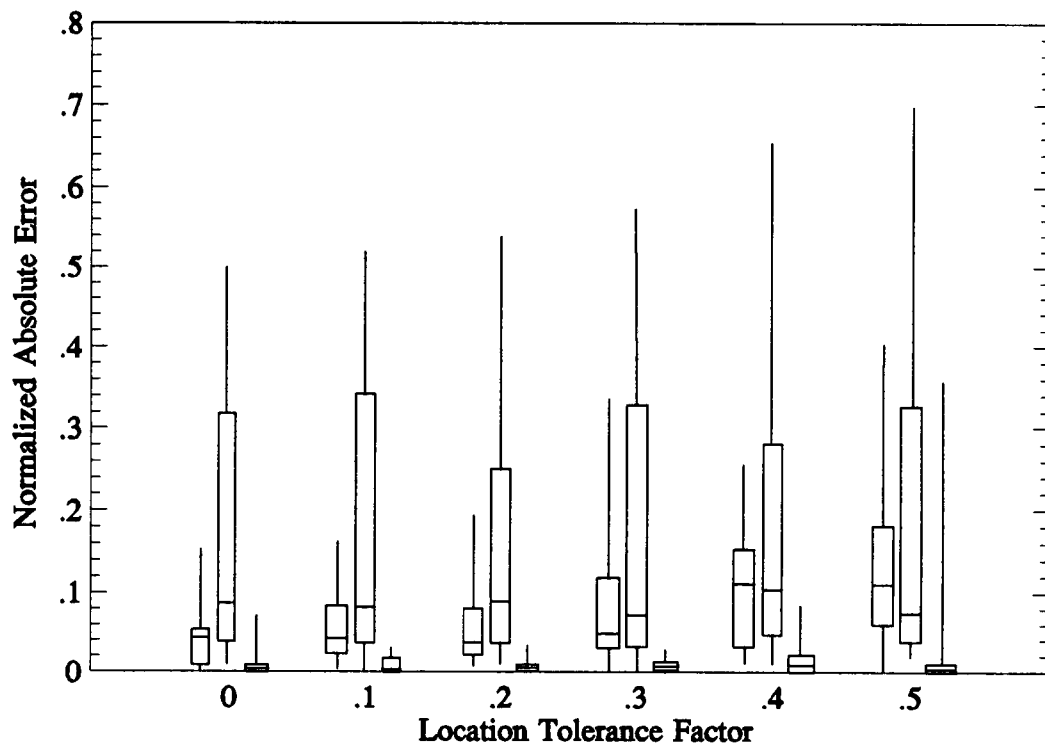


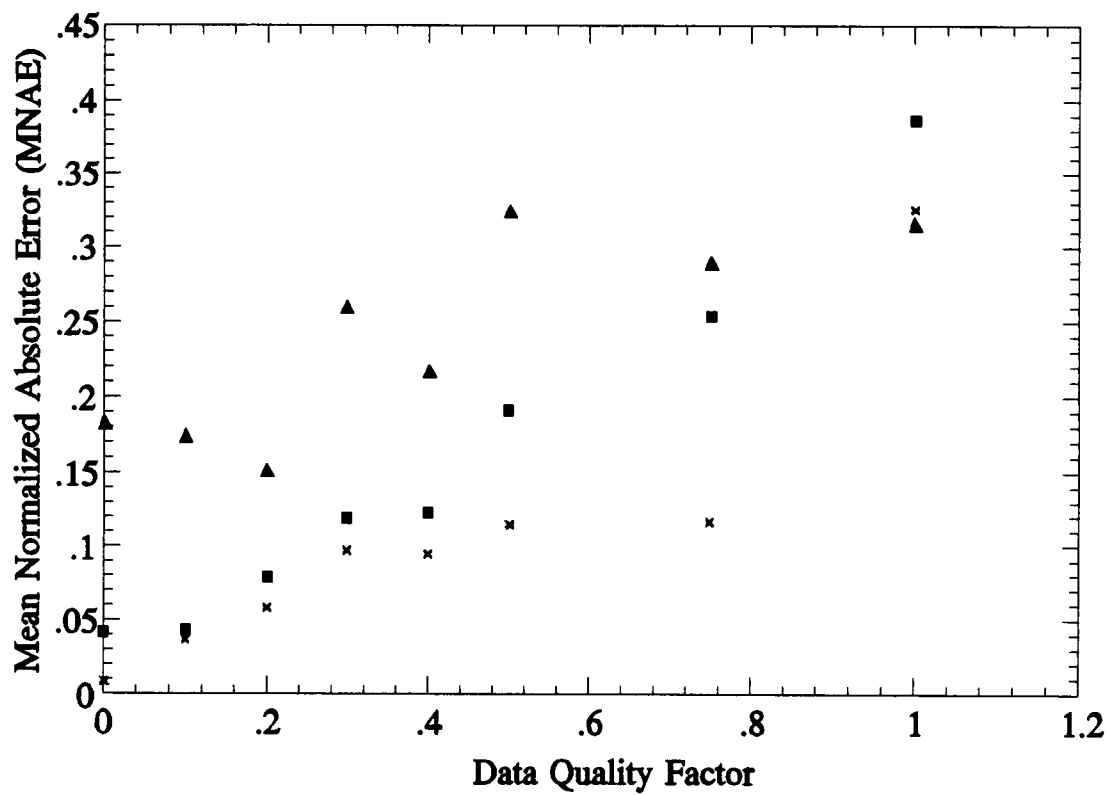
Figure VII-6. Normalized Absolute Error Comparison (Location Tolerance)

Table VII-2. Summary Statistics (Location Tolerance)

Interpolation Method	Location Tolerance Factor	Normalized Absolute Error Distribution				
		Mean	Median	Min.	Max.	Std. Dev.
Inverse Distance Squared	0.0	0.042	0.046	0.001	0.155	0.037
	0.1	0.060	0.048	0.004	0.159	0.048
	0.2	0.055	0.038	0.007	0.195	0.046
	0.3	0.087	0.072	0.0	0.339	0.089
	0.4	0.105	0.120	0.008	0.253	0.074
	0.5	0.127	0.124	0.0	0.402	0.095
Regression Method	0.0	0.185	0.122	0.009	0.497	0.179
	0.1	0.195	0.142	0.002	0.524	0.187
	0.2	0.181	0.089	0.012	0.539	0.190
	0.3	0.190	0.091	0.001	0.577	0.188
	0.4	0.194	0.110	0.010	0.649	0.205
	0.5	0.207	0.080	0.019	0.697	0.217
Kriging	0.0	0.009	0.003	0.0	0.081	0.018
	0.1	0.008	0.005	0.0	0.030	0.010
	0.2	0.005	0.002	0.0	0.030	0.008
	0.3	0.006	0.004	0.0	0.028	0.008
	0.4	0.017	0.009	0.0	0.082	0.022
	0.5	0.049	0.002	0.0	0.356	0.107

distant samples for estimate calculations. A visual extrapolation of Figure VII-4 would imply that at some level of location randomness, the estimate quality of kriging and the inverse distance squared method will degenerate to the level of the regression method. Although such extrapolations must be used with caution, the implied result is reasonable since both kriging and the inverse distance squared method assign near samples higher leverage than distant samples. Without the presence of near samples, the distant samples (which may not have high spatial correlation) have a greater impact on the estimate. The regression method gives all sample locations the same weight and, therefore, is not as sensitive to sample location. The case study presented in the next chapter provides additional insight into this relationship.

Figures VII-7 through VII-9 and Table VII-3 show the relationship between estimate quality and the data quality factor. The data quality factor represents the maximum amount of random error permitted in the sample value normalized to the sample value. Kriging and the regression method demonstrate similar relationships between estimate quality and data quality. This is expected since both methods use a sufficient number of samples to dampen the influence of random noise. However, the inverse distance squared method uses only four samples per estimate. One sample with a large amount of error has more impact on the inverse distance squared estimate than on an estimate from the other two methods. If extrapolated, the inverse distance squared error can be expected to exceed that of the regression method. However, this would not be characteristic of actual application since such poor data quality (over 100% error) is not typical of properly designed monitoring networks (Nielsen, 1991).



Legend:

- ▲ Regression Method
- Inverse Distance Squared Method
- × Kriging

Figure VII-7. Mean Normalized Absolute Error Comparison (Data Quality)

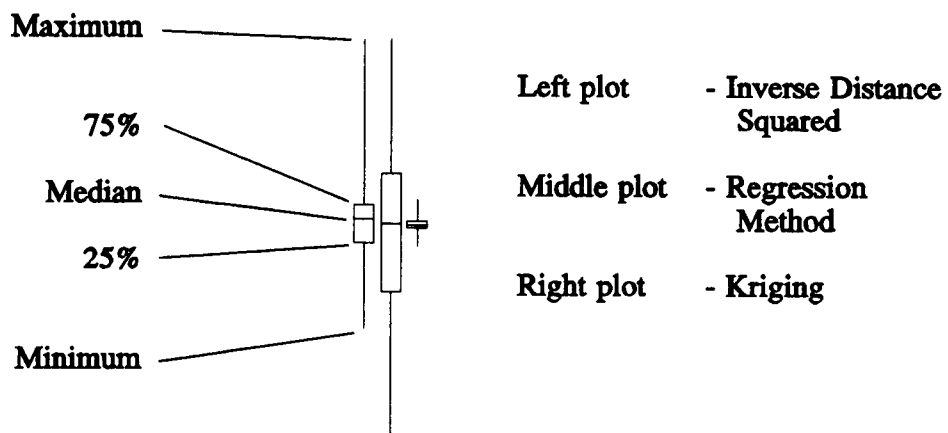
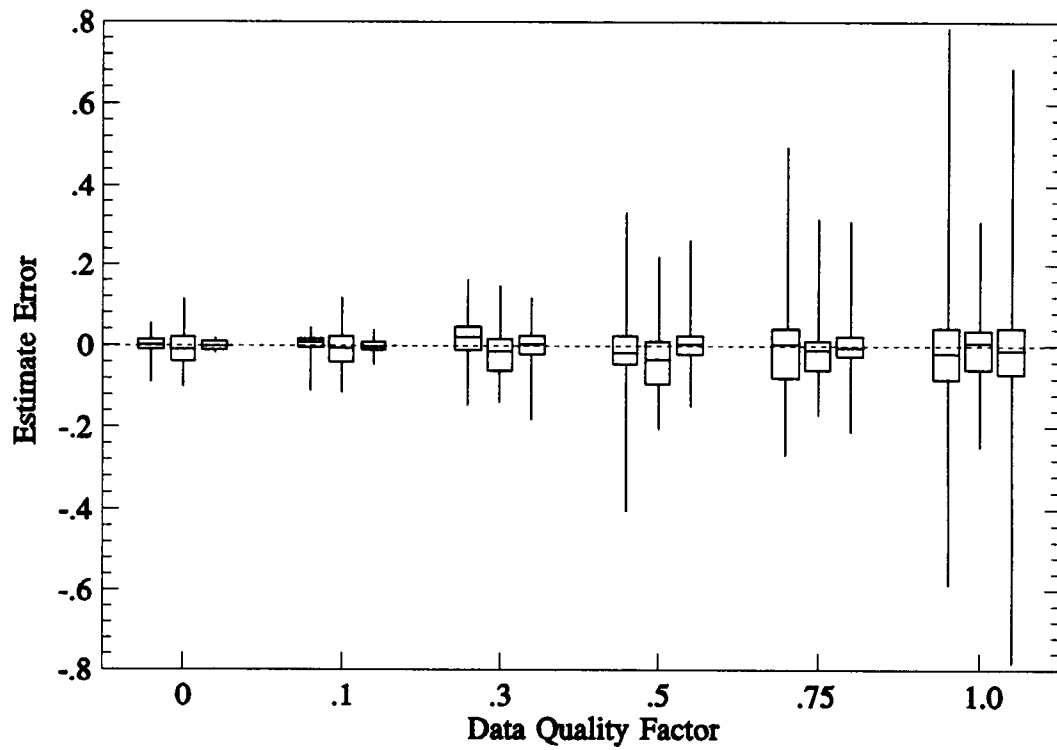


Figure VII-8. Estimate Error Comparison (Data Quality)

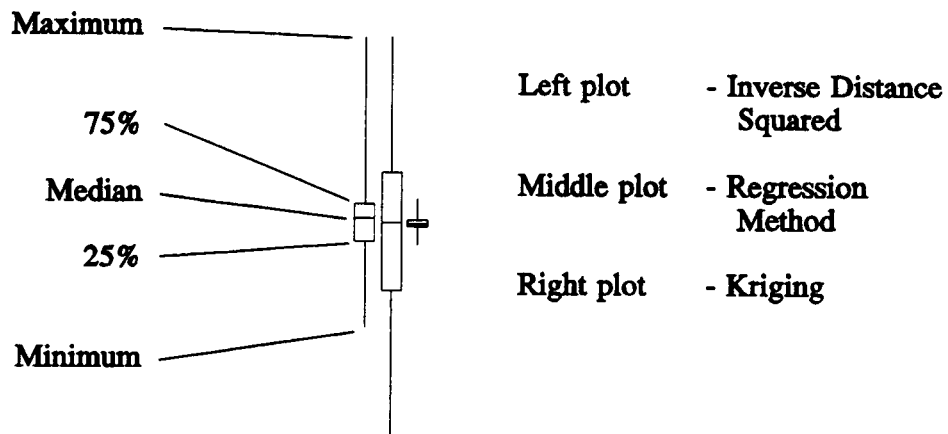
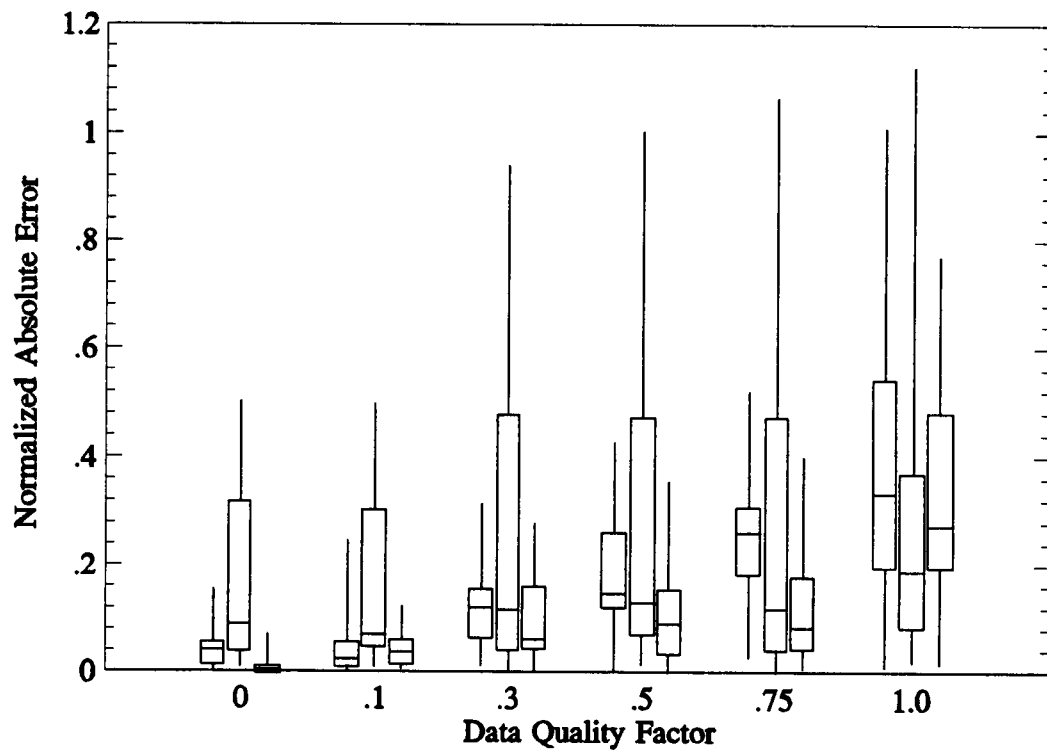


Figure VII-9. Normalized Absolute Error Comparison (Data Quality)

Table VII-3. Summary Statistics (Data Quality)

Interpolation Method	Data Quality Factor	Normalized Absolute Error Distribution				
		Mean	Median	Min.	Max.	Std. Dev.
Inverse Distance Squared	0.0	0.042	0.046	0.001	0.155	0.037
	0.1	0.041	0.027	0.004	0.245	0.052
	0.2	0.078	0.069	0.002	0.303	0.068
	0.3	0.119	0.125	0.013	0.313	0.074
	0.4	0.123	0.094	0.002	0.292	0.089
	0.5	0.191	0.174	0.0	0.425	0.119
	0.75	0.253	0.263	0.032	0.516	0.127
	1.0	0.387	0.399	0.004	1.004	0.247
Regression Method	0.0	0.185	0.122	0.009	0.497	0.179
	0.1	0.176	0.068	0.010	0.493	0.176
	0.2	0.152	0.098	0.0	0.590	0.180
	0.3	0.261	0.145	0.008	0.953	0.295
	0.4	0.218	0.129	0.001	1.000	0.261
	0.5	0.325	0.165	0.012	1.000	0.374
	0.75	0.291	0.127	0.0	1.059	0.366
	1.0	0.318	0.202	0.018	1.118	0.327
Kriging	0.0	0.009	0.003	0.0	0.081	0.018
	0.1	0.042	0.039	0.002	0.123	0.034
	0.2	0.058	0.056	0.003	0.174	0.048
	0.3	0.097	0.061	0.003	0.278	0.084
	0.4	0.095	0.090	0.006	0.290	0.071
	0.5	0.115	0.102	0.0	0.356	0.099
	0.75	0.117	0.118	0.008	0.397	0.098
	1.0	0.326	0.288	0.001	0.772	0.194

Figures VII-10 through VII-12 and Table VII-4 show the response of the three interpolation methods to continued migration of the plume. As mentioned in Chapter VI, the effect of plume migration on a stationary sampling grid is a decrease in the edge effects. As expected, the method most effected by the edge effects, the regression method, shows the most improvement in estimate quality as the plume stabilizes. Kriging and the inverse distance squared method, which are influenced to a lesser degree than the regression method, show relative insensitivity to changes in the plumes spatial distribution caused by migration.

The impact of plume migration on estimate quality can be considered in a spatial rather than a temporal connotation. In this sense, kriging and the inverse distance squared method are relatively insensitive to the location of the sampling area within the plume. However, the regression method will yield different estimate quality depending on whether the sampling network contains areas of rapidly changing values or is located in a region of little change. Since monitoring networks are initially planned with limited information about the exact plume location, this limitation may be a significant factor in the selection of an interpolation method.

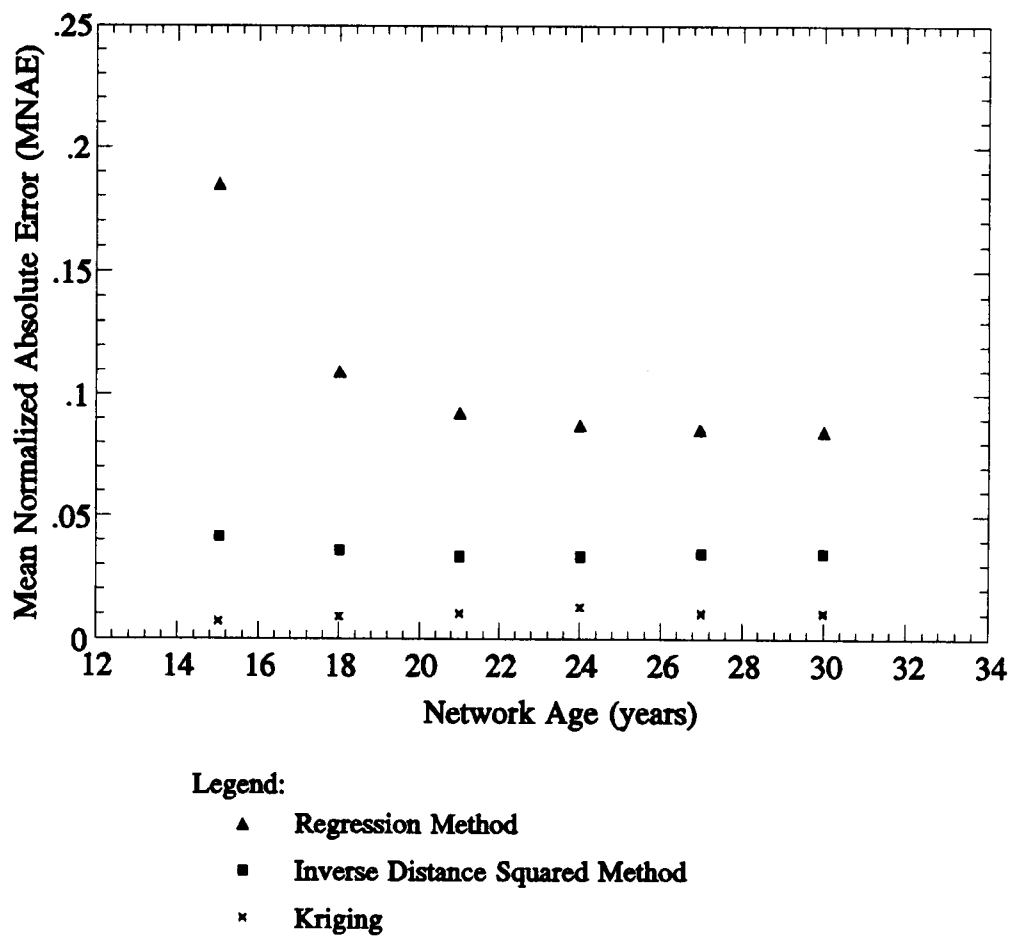


Figure VII-10. Mean Normalized Absolute Error Comparison (Network Age)

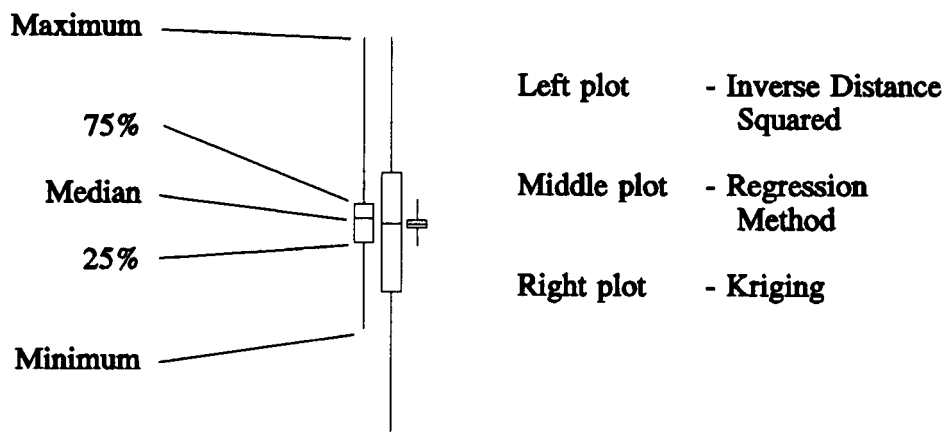
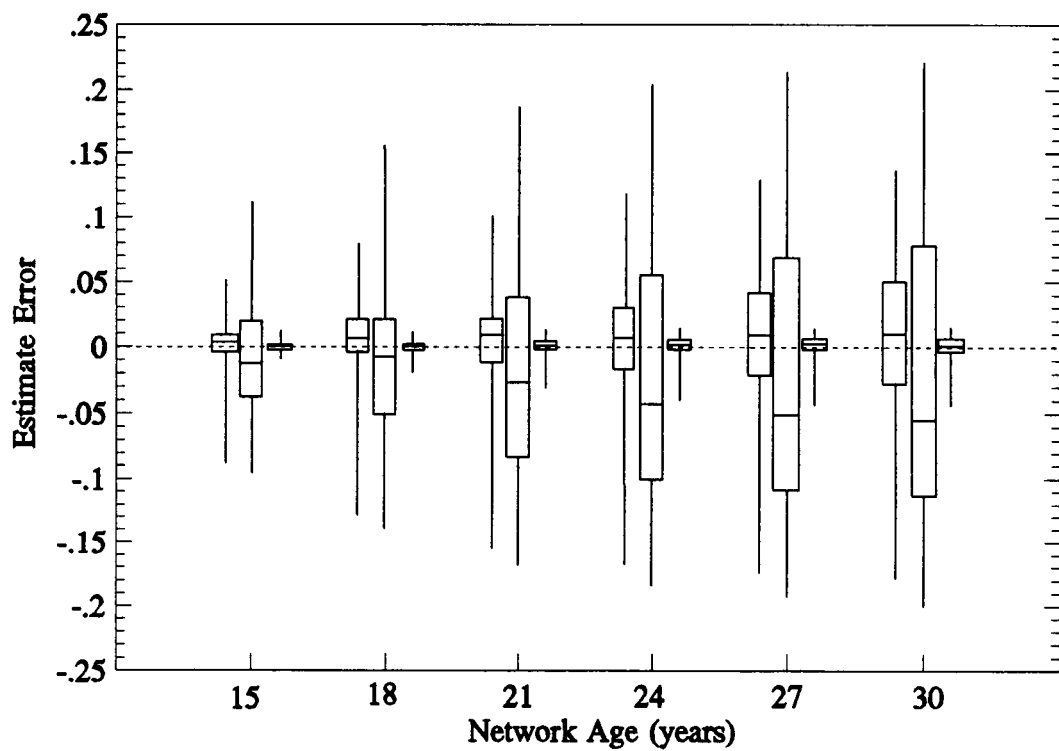


Figure VII-11. Estimate Error Comparison (Network Age)

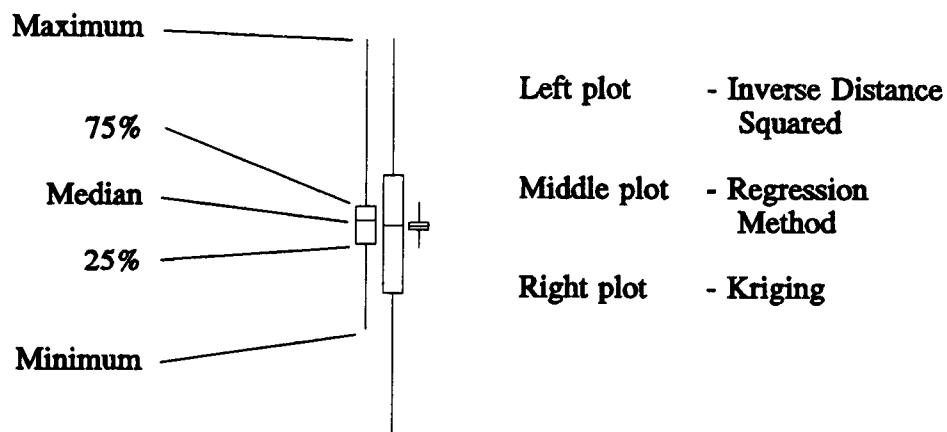
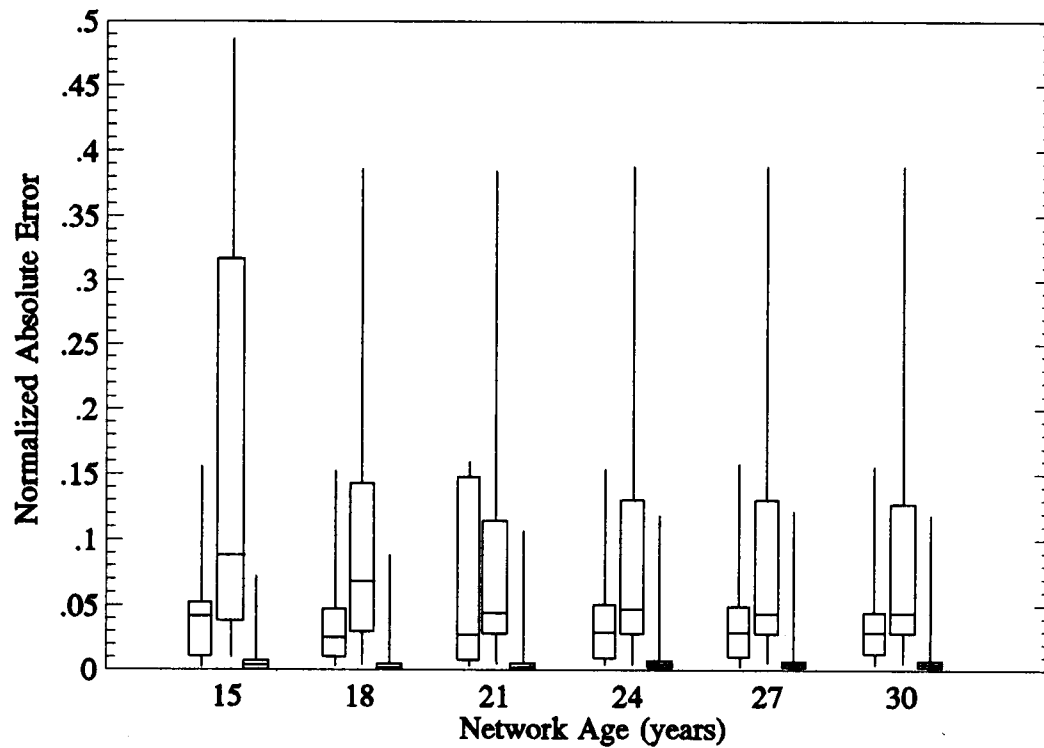


Figure VII-12. Normalized Absolute Error Comparison (Network Age)

Table VII-4. Summary Statistics (Network Age)

Interpolation Method	Network Age (years)	Normalized Absolute Error Distribution				
		Mean	Median	Min.	Max.	Std. Dev.
Inverse Distance Squared	15	0.042	0.046	0.001	0.155	0.037
	18	0.036	0.028	0.003	0.152	0.034
	21	0.034	0.028	0.002	0.152	0.034
	24	0.034	0.029	0.001	0.152	0.035
	27	0.035	0.030	0.001	0.154	0.035
	30	0.035	0.030	0.003	0.155	0.035
Regression Method	15	0.185	0.122	0.009	0.497	0.179
	18	0.110	0.071	0.003	0.388	0.117
	21	0.093	0.056	0.008	0.386	0.104
	24	0.088	0.046	0.0	0.387	0.101
	27	0.086	0.042	0.003	0.388	0.100
	30	0.086	0.043	0.003	0.385	0.099
Kriging	15	0.009	0.003	0.0	0.081	0.018
	18	0.009	0.003	0.0	0.088	0.020
	21	0.010	0.002	0.0	0.107	0.025
	24	0.013	0.003	0.0	0.117	0.028
	27	0.011	0.003	0.0	0.117	0.027
	30	0.011	0.003	0.0	0.114	0.026

CHAPTER VIII

CASE STUDY

To this point, results have been based on synthetically generated sample data to permit tight control over the sample characteristics. The results of interpolation using the synthetic data have been presented in the previous two chapters as general trends for each of the interpolation methods. In this chapter, sampling data from an actual site are used to generate estimates and error measurements, and those results are compared to the trends presented in the previous chapter.

The site description and sample data are taken from a case study by Istok, Smyth, and Flint (Istok, 1993). The site is located near Ontario, Oregon. Nitrate contamination has been detected in a shallow, poorly-confined, sand and gravel aquifer underlying the lower Malheur River basin. The aquifer is in an area of intensive agricultural activity, which has resulted in frequent application of nitrogen fertilizer and the herbicide Dacthal (dimethyl tetrachloroterephthalate) or DCPA. The goal of the original case study was to estimate nitrate and DCPA concentrations throughout the aquifer using cokriging.

The area of concern is a small (16.5 km²) portion of the aquifer selected for detailed study. For the study, samples were collected from 42 wells which were part of an existing groundwater monitoring network. The depth and screened interval varied; however, all wells were screened over the entire thickness of the aquifer. The nitrate concentrations are provided in Table VIII-1.

Table VIII-1. Measured Nitrate Concentrations

Well No.	Coordinates (km)		Nitrate Concentration (mg/l) *	Well No.	Coordinates (km)		Nitrate Concentration (mg/l) *
	x	y			x	y	
1	22.4	21.0	13.6	22	24.6	28.7	0.2
2	22.9	21.0	17.7	23	24.9	28.9	6.2
3	22.7	25.6	24.5	24	24.0	27.8	12.6
4	23.2	25.5	3.2	25	23.6	28.9	17.2
5	24.1	25.7	12.6	26	23.4	28.8	16.0
6	24.5	25.5	0.2	27	23.3	28.0	25.3
7	23.3	24.0	13.6	28	23.7	27.7	16.6
8	19.9	27.5	1.0	29	23.9	27.2	9.8
9	19.5	25.8	10.4	30	21.8	27.7	22.2
10	20.0	24.0	19.9	31	21.6	27.5	23.3
11	19.5	24.0	18.0	32	22.1	26.8	32.0
12	21.9	23.1	20.8	33	21.8	26.0	26.5
13	21.8	22.2	9.9	34	21.5	26.3	21.5
14	20.1	22.6	21.6	35	20.7	26.3	27.4
15	20.2	23.2	14.4	36	23.8	26.0	4.4
16	21	22.0	9.3	37	23.8	26.9	12.3
17	22.7	19.5	0.4	38	22.3	25.2	30.6
18	24.6	29.7	11.8	39	23.6	25.4	0.4
19	20.3	28.4	12.0	40	20.8	25.5	11.0
20	20.0	24.4	12.0	41	21.6	23.5	16.5
21	26.3	26.9	11.0	42	19.4	26.3	1.3

* The nitrate concentration is expressed as nitrogen.

Since the small sample size did not allow segregation of a subset of wells whose values would be estimated from the remaining samples, the method used to generate estimates was the same method used for cross-validation of the variogram. One sample was removed from the sample set and the remaining samples were used to estimate the missing sample. From the total sample set, 25 sample locations were selected to serve as both sample and estimate locations.

The layout of the sample set is shown in Figure VIII-1. Solid lines indicate the approximate concentration contours. The 25 estimates were made for locations within the dashed box using the remaining 41 samples as the sample set. Estimate locations had to remain within the outer bounds of the sample space to prevent the interpolation task from becoming an extrapolation task. Selecting estimate locations from within the box ensured compliance with this requirement.

The regression method was a straight-forward application of linear regression techniques and presented no problems. Use of the inverse distance squared method proved more difficult because the irregular sample pattern did not always produce a sample in each quadrant surrounding the estimate location. In these cases, a subjective decision was made to determine which four samples would be used for the estimate. Where possible, the best compromise between closeness and angular diversity was used. In all cases, the estimate location was contained within the polygon created by the sample locations.

Generation of the kriging estimates generally followed the process used in the Istok, Smyth, and Flint case study (Istok, 1993). The authors judged that the data best fit a gaussian form after a logarithmic transformation. Therefore, the natural

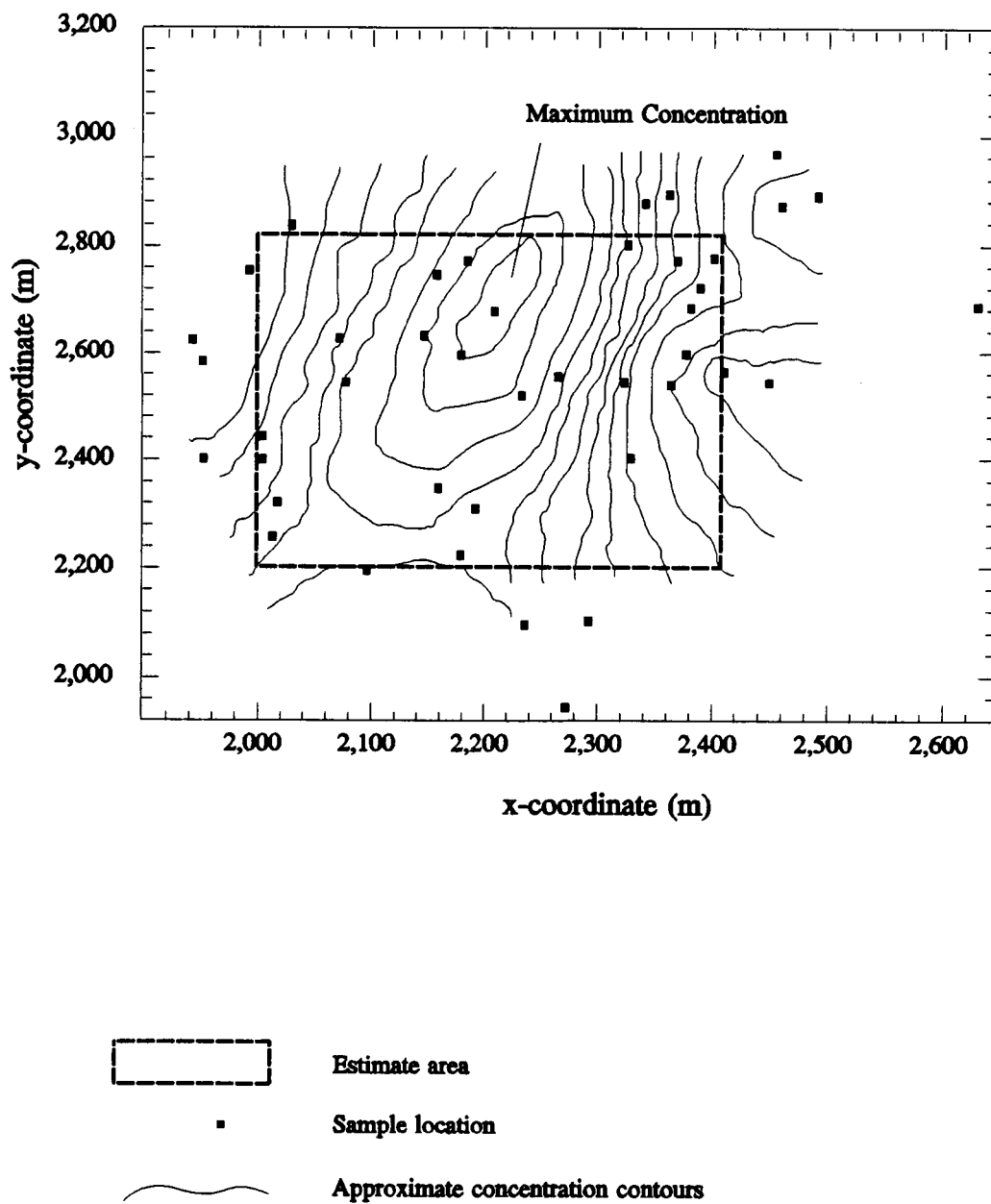


Figure VIII-1. Case Study Sample Locations

logarithms of the sample values were used to construct the variogram and the kriging estimates were generated in the log domain. The inverse log transformation of the estimates was performed to obtain the final kriging estimates. The parameters of the variogram were generated independent of those used in the Istok, Smyth, and Flint study to ensure the decision-making process used for the variogram remained the same throughout this study. More caution was needed in developing the variogram in the log domain since small errors in the log domain can translate large errors in the final kriging estimates due to the inverse log transformation. The variogram parameters were as follows:

- Type: Spherical Model
- Nugget: 0.80
- Sill: 1.20
- Range: 4 km
- Isotropy: Insufficient samples, isotropic assumed

Results of the three methods are shown in Figures VIII-2 and VIII-3 and in Tables VIII-2 through VIII-4. These results show the same general trend observed using the synthetic data. Kriging provides the highest quality estimates (MNAE = 0.361), closely trailed by the inverse distance squared method (MNAE = 0.409), with the regression method providing the lowest quality estimates (MNAE = 0.530).

The overall errors for all of the methods are higher than any shown in the previous chapters. The case study strains the capabilities of the interpolation methods

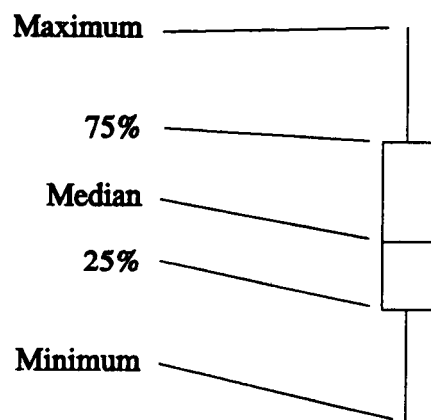
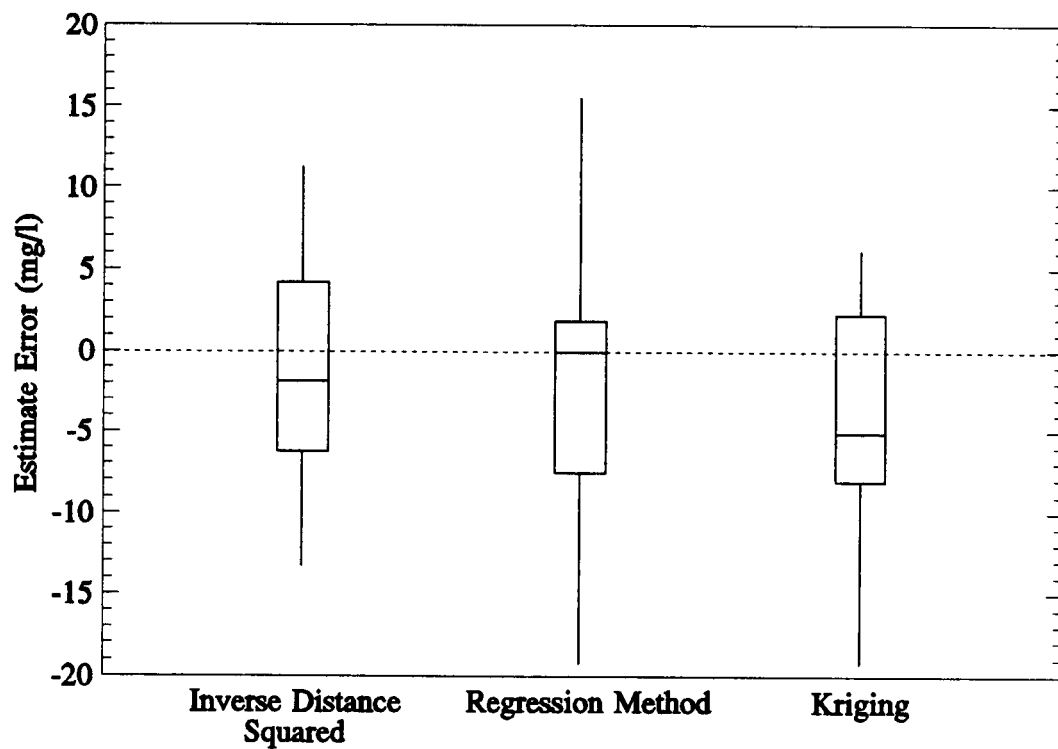


Figure VIII-2. Case Study Estimate Error Comparison

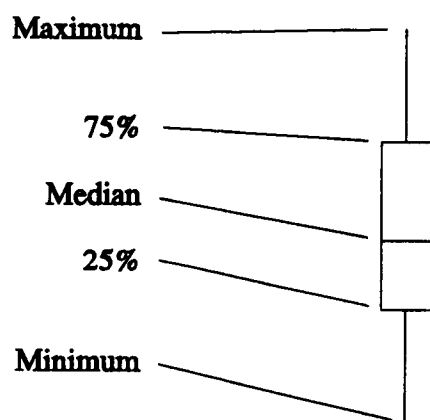
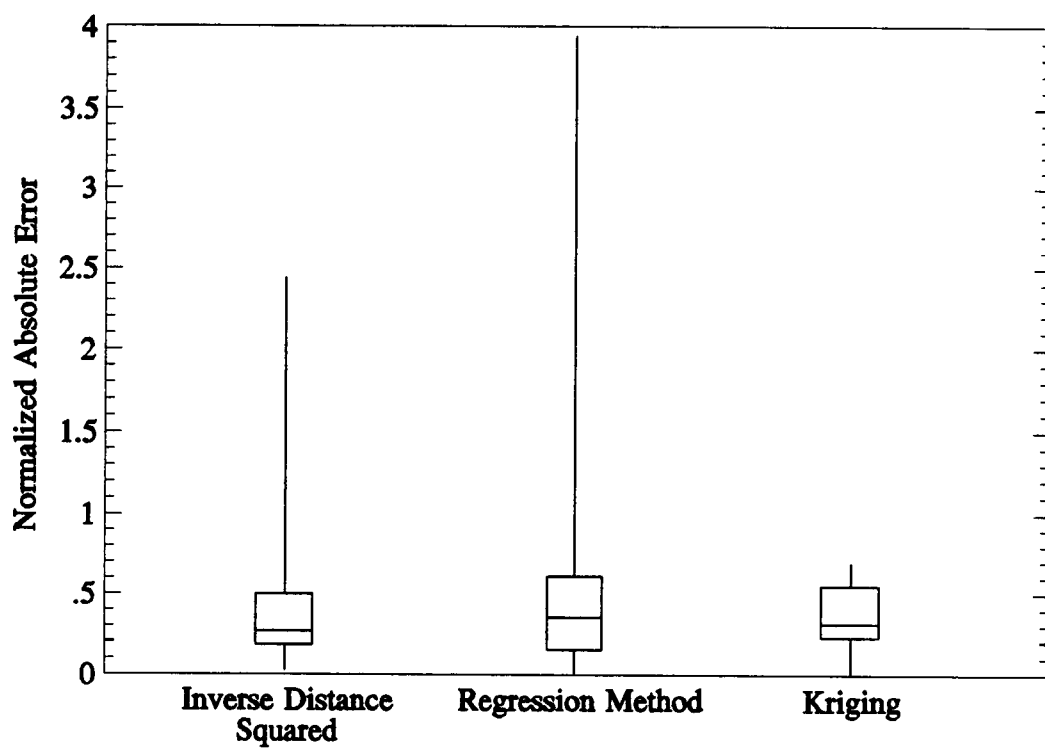


Figure VIII-3. Case Study Normalized Absolute Error Comparison

Table VIII-2. Case Study Estimates (Inverse Distance Squared)

Estimate Coordinates (km)		Measured Value (mg/l)	Estimated Value (mg/l)	Estimate Error (mg/l)	Normalized Absolute Error
x	y				
22.7	25.6	24.5	16.7	(7.8)	0.318
23.2	25.5	3.2	11.0	7.8	2.445
23.3	24.0	13.6	11.1	(2.5)	0.185
20.0	24.0	19.9	14.6	(5.3)	0.264
21.9	23.1	20.8	15.5	(5.3)	0.254
21.8	22.2	9.9	14.7	4.8	0.483
20.1	22.6	21.6	14.4	(7.2)	0.333
20.2	23.2	14.4	19.5	5.1	0.352
21.0	22.0	9.3	14.2	4.9	0.523
20.0	24.4	12.0	18.5	6.5	0.540
24.0	27.8	12.6	14.4	1.8	0.140
23.3	28.0	25.3	16.8	(8.5)	0.335
23.7	27.7	16.6	14.7	(1.9)	0.112
23.9	27.2	9.8	13.3	3.5	0.352
21.8	27.7	22.2	24.0	1.8	0.080
21.6	27.5	23.3	23.2	(0.1)	0.005
22.1	26.8	32.0	25.2	(6.8)	0.211
21.8	26.0	26.5	24.4	(2.1)	0.079
21.5	26.3	21.5	25.7	4.2	0.196
20.7	26.3	27.4	14.1	(13.3)	0.485
23.8	26.0	4.4	8.4	4.0	0.899
23.8	26.9	12.3	10.3	(2.0)	0.162
22.3	25.2	30.6	24.3	(6.3)	0.206
20.8	25.5	11.0	22.4	11.4	1.036
21.6	23.5	26.5	20.1	(6.4)	0.216
MNAE = 0.409					

Table VIII-3. Case Study Estimates (Regression Method)

Estimate Coordinates (km)		Measured Value (mg/l)	Estimated Value (mg/l)	Estimate Error (mg/l)	Normalized Absolute Error
x	y				
22.7	25.6	24.5	9.8	(14.7)	0.599
23.2	25.5	3.2	15.8	12.6	3.932
23.3	24.0	13.6	8.8	(4.8)	0.350
20.0	24.0	19.9	7.8	(12.1)	0.607
21.9	23.1	20.8	12.4	(8.4)	0.402
21.8	22.2	9.9	16.3	6.4	0.642
20.1	22.6	21.6	8.5	(13.1)	0.605
20.2	23.2	14.4	14.5	0.1	0.004
21.0	22.0	9.3	20.1	10.8	1.166
20.0	24.4	12.0	13.3	1.3	0.106
24.0	27.8	12.6	13.4	0.8	0.062
23.3	28.0	25.3	19.3	(6.0)	0.237
23.7	27.7	16.6	13.6	(3.0)	0.183
23.9	27.2	9.8	10.3	0.5	0.050
21.8	27.7	22.2	27.7	5.5	0.247
21.6	27.5	23.3	25.1	1.8	0.079
22.1	26.8	32.0	27.0	(5.0)	0.156
21.8	26.0	26.5	27.7	1.2	0.045
21.5	26.3	21.5	31.2	9.7	0.453
20.7	26.3	27.4	8.1	(19.3)	0.704
23.8	26.0	4.4	6.0	1.6	0.372
23.8	26.9	12.3	6.1	(6.2)	0.505
22.3	25.2	30.6	23.1	(7.5)	0.244
20.8	25.5	11.0	26.5	15.5	1.409
21.6	23.5	26.5	18.1	(8.4)	0.097
MNAE = 0.530					

Table VIII-4. Case Study Estimates (Kriging)

Estimate Coordinates (km)		Measured Value (mg/l)	Estimated Value (mg/l)	Estimate Error (mg/l)	Normalized Absolute Error
x	y				
22.7	25.6	24.5	8.8	(15.7)	0.641
23.2	25.5	3.2	5.4	2.2	0.688
23.3	24.0	13.6	5.3	(8.3)	0.610
20.0	24.0	19.9	14.7	(5.2)	0.261
21.9	23.1	20.8	14.2	(6.6)	0.317
21.8	22.2	9.9	14.6	4.7	0.475
20.1	22.6	21.6	13.5	(8.1)	0.375
20.2	23.2	14.4	17.1	2.7	0.188
21.0	22.0	9.3	15.2	5.9	0.634
20.0	24.4	12.0	14.2	2.2	0.183
24.0	27.8	12.6	8.5	(4.1)	0.325
23.3	28.0	25.3	13.1	(12.2)	0.482
23.7	27.7	16.6	11.5	(5.1)	0.307
23.9	27.2	9.8	10.1	0.3	0.031
21.8	27.7	22.2	22.2	0.0	0.000
21.6	27.5	23.3	18.0	(5.3)	0.227
22.1	26.8	32.0	24.0	(8.0)	0.250
21.8	26.0	26.5	20.5	(6.0)	0.226
21.5	26.3	21.5	24.3	2.8	0.130
20.7	26.3	27.4	8.8	(18.6)	0.679
23.8	26.0	4.4	3.9	(0.5)	0.114
23.8	26.9	12.3	8.4	(3.9)	0.317
22.3	25.2	30.6	11.5	(19.1)	0.624
20.8	25.5	11.0	17.1	6.0	0.555
21.6	23.5	26.5	16.5	(10.0)	0.374
MNAE = 0.361					

with a combination of low sample density and an irregular sample pattern. The data quality factor is unknown. Although both the detection limit and sensitivity of the nitrate analyzer were both below the roundoff error in the data, the amount of error introduced from sampling extraction handling, preservation, transportation, and laboratory procedures could not be determined. Information on the degree of heterogeneity and anisotropy was also unavailable.

The comparative analysis of data from one site is insufficient to completely validate the general trends suggested by the analysis of the synthetic data. However, the results of this case study provides one positive indication that the trends may be applied to actual sites.

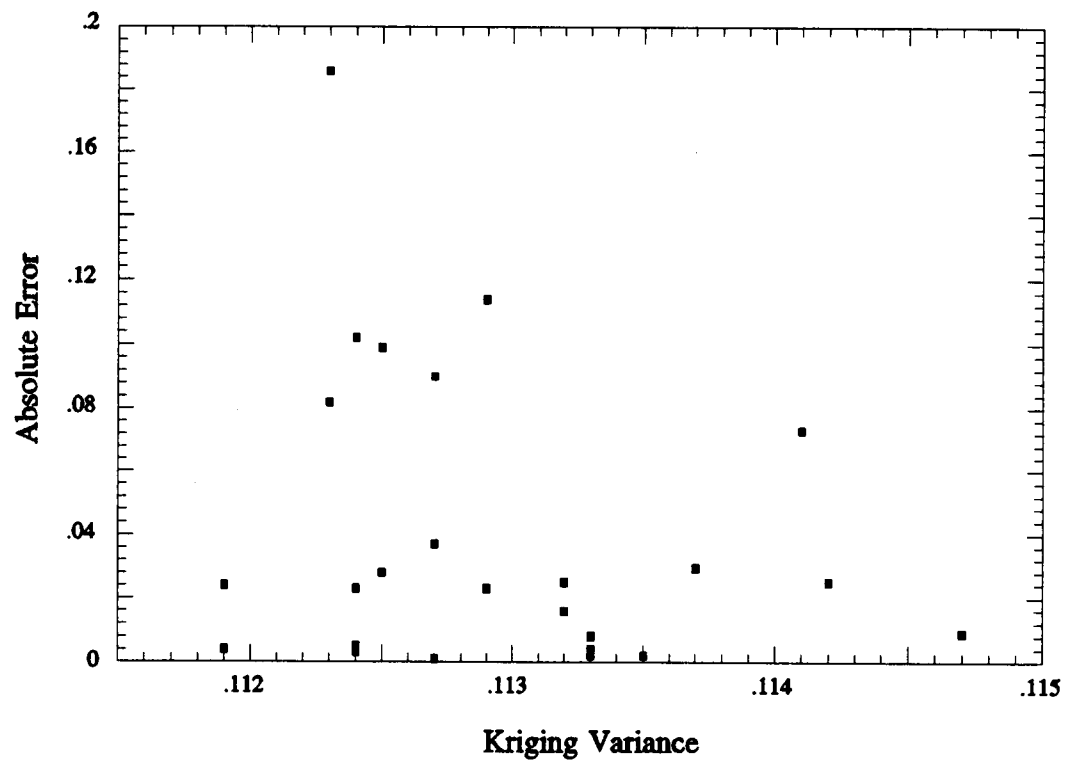
CHAPTER IX

CONCLUSIONS

If estimate quality could be used as the sole measure of an interpolation method, there could be only one conclusion from this study. Over the range of variables investigated, kriging provided the highest quality estimates of all of the methods evaluated and, judged solely on estimate quality, would be the method of choice. However, in actual use, a lower quality estimate may be acceptable in light of the specific advantages offered by a method. This chapter summarizes the advantages and disadvantages of each method as applied to a site investigation.

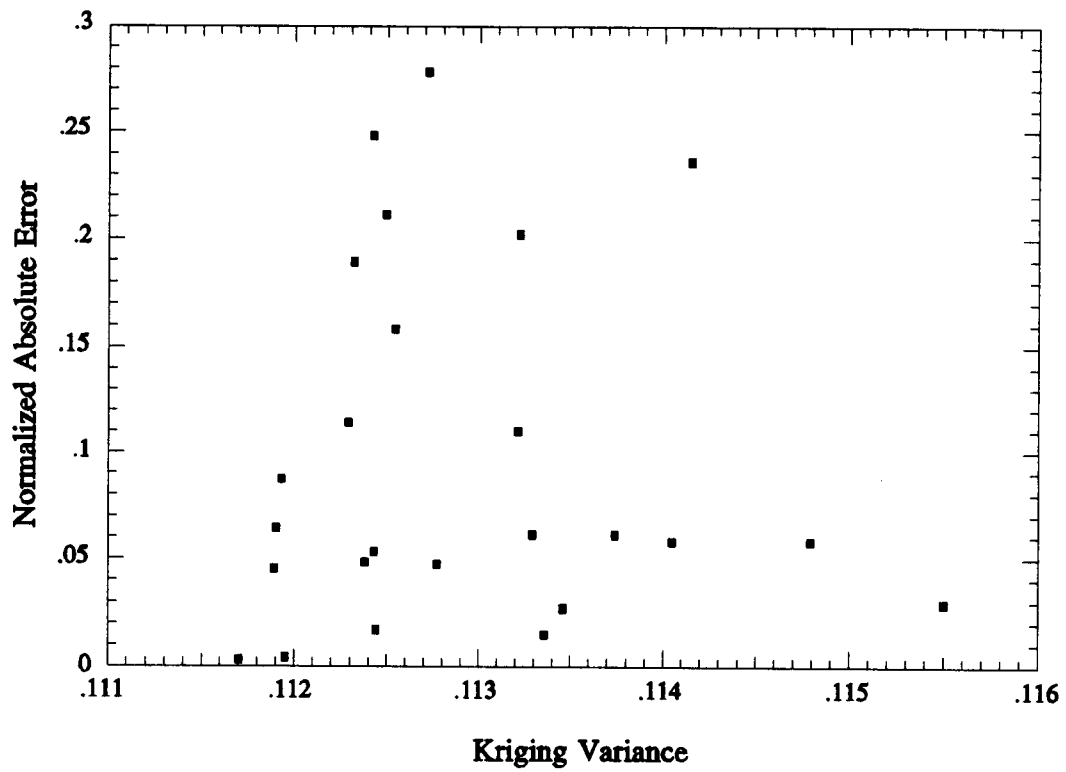
The major advantage of kriging is clearly the quality of the estimates, although the difference in quality is significantly reduced when actual site sample values are used. Kriging also provides the kriging variance as a measure of the confidence interval of the estimate. Although this is not a direct measure of the estimate error (the actual value must be known to calculate actual error), it does have value in determining additional sample locations. The lack of correlation between the kriging variance and the absolute and normalized errors is shown in Figures IX-1 and IX-2. Therefore, caution should be exercised when using the kriging variance in an attempt to improve the estimate quality.

The advantages of kriging are compromised by the need to make numerous subjective decisions during the process. In contrast to decisions made for the other methods, some kriging decisions (such as data transformation, variogram construction



Number of samples = 100
Location tolerance factor = 0.0
Data quality factor = 0.30
Network age = 15 years

Figure IX-1. Absolute Error as a Function of Kriging Variance



Number of samples = 100
Location tolerance factor = 0.0
Data quality factor = 0.30
Network age = 15 years

Figure IX-2. Normalized Absolute Error as a Function of Kriging Variance

and validation, and neighborhood selection) must be made for each data set. These decisions require a level of knowledge of geostatistics that can only come from experience. Also, poor decisions may impact the estimate quality to a degree at which kriging no longer produces the best estimates.

Kriging is also confined by the limitations of the available software packages written for geostatistics, whereas the other two methods can be applied through readily available spreadsheet and linear regression software. For the geostatistical software that is available, little information is provided on the mathematical methods used to develop or solve the kriging equations or on any simplifying assumptions, leaving the investigator at the mercy of the software developer.

The inverse distance squared method is part of a family of interpolation methods commonly applied to physical phenomena and uses simple mathematics to generate the estimates. Because of this, most users will have an intuitive feel for the relationship between the sample values and the estimates. The simplicity of the method allows estimates to be generated with as few as three sample locations and can be performed using a simple scientific calculator. The quality of the estimates was close to the kriging quality for most scenarios included in this investigation, including the case study.

The inverse distance squared method requires two subjective decisions that may impact the estimate quality. The investigator must first determine if "inverse distance squared" is the proper relationship to use rather than another function such as "inverse distance" or "inverse distance cubed." For this study, this decision was made using knowledge of the actual values, knowledge not usually available in actual application.

The second decision must determine how the samples used for each estimate will be chosen. The search function may impact the quality of the estimate. If too many samples are used, the estimate may be based on values that are not spatially correlated with the estimate location. If an insufficient number of samples is used, the estimates will prove to be highly sensitive to data quality. Also, the search function may prove difficult to apply in the network geometry is irregular as demonstrated in the case study. If these are not significant concerns, the inverse distance squared method provides a simple alternative to kriging.

When compared to the other methods, the regression method provides the fewest reasons for selection. The method consistently produced the lowest quality estimates under all conditions and was unable to produce any estimate at low sample densities. The order of the polynomial, and even whether to use a polynomial, must be determined by the investigator without benefit of actual values. The coefficient of determination, one of the few indicators available to the investigator, has been shown to be useless in predicting estimate errors. In addition, the regression equation may produce negative values which may impact overall values if not corrected (such as setting all negative values to zero).

The regression does have one advantage that is unavailable with the other methods. Once the regression equation has been determined, the sample values are no longer needed. This allows the regression equation to be easily incorporated in software or used in programmable calculators without dedicating memory to large sample databases.

The regression method is accepted as a common method for interpolating geophysical phenomena, although the results of this study strongly imply that the application to contaminant plumes can be questioned. The process of fitting a curve to sample data is intuitive and the process itself is rarely questioned except for the form of the regression equation. In addition, the strengths and weaknesses of linear regression have been studied and documented in depth. Although this may provide a false sense of confidence in the method, it also provides the investigator with a significant amount of established information to use in understanding and improving the process.

The advantages and disadvantages discussed in this chapter are summarized in Table IX-1. The final conclusion to be drawn from this study is that no single interpolation method can be proclaimed to be superior without consideration of the specifics of the task to be accomplished. Each method has advantages not gained through any other method and suffers handicaps not faced by the other methods. The most significant subjective decision faced by an investigator, the selection of the interpolation method, is one that must be made based on experience and site-specific knowledge.

Table IX-1. Summary of Advantages and Disadvantages

Interpolation Method	Advantages	Disadvantages
Kriging	• Consistently produces the lowest errors of all the methods • Provides an estimate of the uncertainty in the estimate	• Numerous subjective decisions are required which may impact estimate quality • Process is not intuitive except to a person knowledgeable in geostatistics • Application requires custom software
Inverse Distance Squared	• Produces estimate quality close to that of kriging in most situations • Can be performed in the field with only a simple scientific calculator • Requires only three samples to obtain an estimate • Process is intuitive	• Requires a subjective judgement to determine the degree to which the distance difference will be raised • Requires subjective determination of the search function • Search function may be difficult to apply for irregular networks • Estimates are sensitive to sample errors
Regression Method	• The sample data set is not required once the regression coefficients have been determined • Process is intuitive • Statistics of linear regression are well known	• Requires a subjective decision on the order of the polynomial • Produces the highest errors (both point and grid) of all the methods • Requires the highest minimum number of samples to produce an estimate • Can produce negative values

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