OPTIMAL DESIGN OF GROUNDWATER QUALITY MONITORING NETWORKS

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ABSTRACT OF DISSERTATION
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This research focuses on the optimal design of groundwater quality monitoring networks. The optimization technique developed allows for incorporation of both the model structure, data error, and model parameter uncertainty into the monitoring network design, with concurrent determination of sampling frequency and well locations.
Particular emphasis has been placed on the use of stochastic models to describe groundwater quality data in order to incorporate both the deterministic and random behavior of groundwater quality in the model evaluation and monitoring network design processes.

A protocol is developed for the evaluation of model applicability and the design of monitoring networks. This protocol was developed based on the results of a simulation study, with the developed protocol tested against field data. The simulation study provided a method of evaluating the performance of various model applicability tests and monitoring network designs against a known correct model. The performance of the protocol could therefore be evaluated for correct models with different magnitudes and types of error (additive and multiplicative normal and lognormal errors were considered), as well as for incorrect models with different magnitudes and types of error.

The results of this research strengthen the importance of a detailed statistical evaluation of model applicability prior to the use of a model as a tool for describing groundwater quality behavior or prior to the design of monitoring networks. The model applicability evaluation should include the use of a variety of statistical tests to assess model applicability, and more importantly, should include the evaluation of the behavior of statistical tests compared to the theoretical expected behavior of the statistical tests for a correct model under conditions of varying sampling frequency, record length, and sampling density. In addition, the optimal monitoring network was found to be highly dependent on the sampling locations used to fit the model and to the monitoring locations identified to be considered for inclusion in the monitoring network.

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1. INTRODUCTION

Groundwater monitoring programs are being undertaken at numerous sites across the country. These groundwater monitoring programs are used to either increase the understanding of a groundwater system or to verify the effectiveness of remedial actions. The monitoring programs are heavily influenced by the requirements of government regulators; however, these requirements are often not based on a quantitative physical or statistical analysis of groundwater information from the site. In addition, the groundwater monitoring programs are most commonly not optimized to meet the information goals of the monitoring program. This results in a rather arbitrary number of wells and frequency of sampling. In addition, the data collected can often be misinterpreted because there is not a clear understanding of how groundwater quality is expected to change over time or what degree of variability is expected in the data.

Current methods used to design groundwater monitoring systems rely predominantly on either physical or statistical data analysis techniques. However, neither physical nor statistical data analyses performed separately provide an optimal basis for the design of groundwater monitoring networks. Physical analysis of data from a site can provide information on aquifer properties from which a model can be developed to predict changes in groundwater conditions. However, purely deterministic approaches to physical modeling provide little insight to the effects of expected variability in groundwater quality, i.e., no measure of the uncertainty level is obtained. Statistical data analyses provide information on the variability of the data, but do not often provide information with which to predict groundwater quality trends in the future. This research focuses on using both physical and statistical analyses conjunctively such that the maximum benefit of the available data can be realized and a more optimal groundwater monitoring network can be designed.

1.1 Objective.

The objective of this research is to develop a protocol for the optimal design of groundwater quality monitoring systems which result in more efficient and effective monitoring networks. The premise of this research is that the optimal groundwater quality monitoring network is dependent on the expected behavior of the groundwater quality. Due to the complex behavior of groundwater quality in response to physical, chemical, and biological processes, the processes which affect those changes must be incorporated explicitly in the design process. In addition, due to the non-deterministic behavior of groundwater quality and due to the error in data collection and analysis, the expected variability of the groundwater quality must also be explicitly incorporated into the design. Therefore, the objective of this research is to develop a protocol for the design of groundwater quality monitoring networks which incorporates information on the deterministic and non-deterministic processes affecting groundwater quality.

1.2 Scope and Limitations.

The monitoring network design protocol developed in this research is not intended to be a rigid methodology for designing groundwater quality monitoring networks. Rather, the protocol is intended to be a general procedure for the design of site-specific monitoring networks. The application of the protocol is expected to be continually evolving as the field of groundwater quality data analysis and monitoring network design evolves.

The specification of a groundwater quality monitoring system depends on the system's information expectations and includes the locations of the groundwater monitoring wells, the sampling frequency, and the selection of constituents for analysis. The selection of appropriate constituents to be analyzed will not be included in this design methodology. However, it is recognized that additional efficiencies in the monitoring network design may be realized by incorporating this last factor into the design process.

The focus of the monitoring network optimization is to design a monitoring network with which to assess the effectiveness of long-term groundwater remedial actions. In order to meet the objective of this type of verification information goal, it is necessary that sufficient information exist (i.e., data is available) to quantify the model structure with an uncertainty level which is consistent with the information goals of the groundwater monitoring system. Rather than to continue to extensively monitor the groundwater system, the purpose of the groundwater monitoring network optimization is to replace groundwater monitoring efforts with groundwater modeling efforts. The premise of this effort to improve the design of groundwater quality monitoring systems is that monitoring has been underway long enough to result in a data record that can support development of the physical and statistical descriptions necessary to reduce the sampling at a site and not reduce the information obtained.

These physical and statistical processes are incorporated into a groundwater quality model. The focus of this research is not the development of groundwater quality models. However, the focus of this research is the development of groundwater quality monitoring networks based on the used of groundwater quality models to explain the processes affecting groundwater quality behavior. Therefore, it is necessary to evaluate the applicability of groundwater quality models and how the structure and uncertainty in the model affect the design of groundwater quality monitoring networks.

The development of a model of a system encompasses four steps: system representation, data measurement, model parameter estimation, and model validation [Mendel, 1973]. For this research, only mathematical statistically-based or physically-based models will be used to represent the groundwater quality system. Evaluation of the data measurement process is not addressed specifically in this research but it is assumed to introduce error into the data and therefore reduce the ability to accurately model the groundwater system. Model parameter estimation techniques are reviewed and statistical tests are evaluated relative to the analysis of model applicability. Lastly, the model is validated by the use of model prediction analyses.

The ability to represent and validate an appropriate model depends on site-specific conditions and information available. The decision as to whether additional effort should be placed on increasing the understanding of a system (additional modeling or data acquisition) or maintaining the current understanding of a system (optimization of the existing monitoring network) is based on the confidence in the understanding of the system dynamics and is based on whether the confidence in the system dynamics is sufficient to meet the information goals of the monitoring network.

Regardless of whether the specific monitoring objective is to increase or validate the understanding in a system, the protocol for groundwater monitoring network design developed in this research can be used to evaluate the uncertainty associated with a given model structure and data set. These models can then be incorporated explicitly into the monitoring network design process to define an optimal groundwater quality monitoring network. Ongoing collection of data from this network can cause a reevaluation of the model and/or a redesign of the groundwater monitoring network. A schematic of this general design process is included as Figure 1.1.

1.3 Approach.

The development of the protocol for groundwater quality monitoring network design is based on the results of a simulation study; i.e., a simulation study is used to develop a procedure for designing groundwater quality monitoring networks. The use of a simulation study allows for testing the performance of different data evaluation techniques and monitoring network design protocol against a known correct model. To assess the applicability of the protocol developed, the procedures are applied to field case studies.

The organization of this dissertation is as follows:

Chapter 2 - Literature Review: summarizes current methods for groundwater quality data analysis and monitoring network design and specifies the limitation of those methods

Chapter 3 - Simulation of Data Records: describes the method used to simulate groundwater quality data using a two-dimensional advection-dispersion model and a superimposed random error

Chapter 4 - Model Parameter Estimation: discusses and compares methods for model parameter estimation

Chapter 5 - Analysis of Model Applicability: assesses the ability of goodness-of-fit and predictive tests to discriminate between models; evaluates

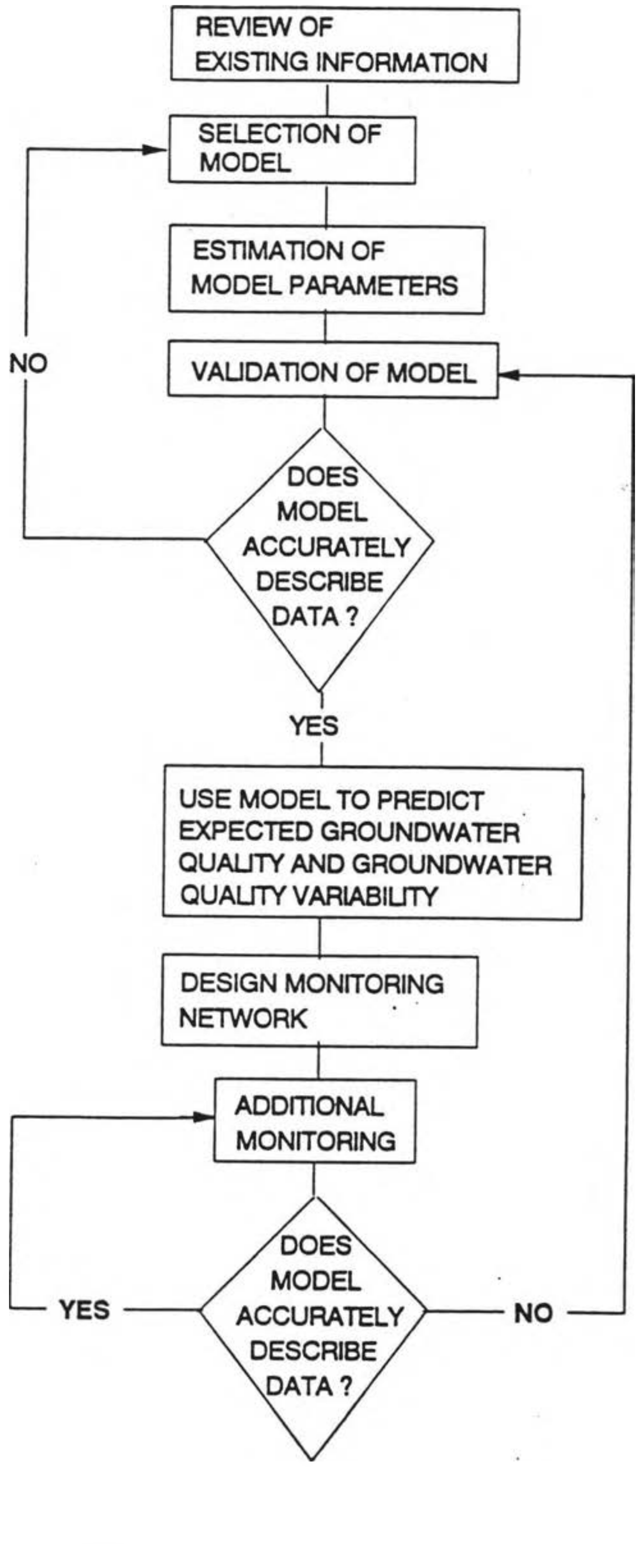


Figure 1.1 Monitoring Network Design Process Flow Chart

behavior of selected statistics for a correct model

Chapter 6 - Error Prediction Propagation: evaluates the propagation of predicted error based on model structure and assumed error distributions

Chapter 7 - Design of Optimal Monitoring Networks: develops method for the design of monitoring networks (frequency and location of samples) based on the model structure and the model/data uncertainty

Chapter 8 - Results of Simulation Study: summarizes the applicability of the statistical tests and monitoring network optimization procedures based on a simulation study; focuses on the results for one incorrect model structure relative to the correct model structure

Chapter 9 - Monitoring Network Design Protocol: summarizes the monitoring network design protocol proposed based on the simulation study performed

Chapter 10- Case Studies: summarizes the application of the monitoring network design protocol to groundwater quality data collected at the IBM facility in East Fishkill, New York

Chapter 11- Summary, Conclusions, and Recommendations: summarizes the research conducted, conclusions made, and recommendations for future work

For the reader who wishes to bypass the theoretical basis for the protocol, a condensed applications approach can be obtained by reading the following sections of this dissertation:

Chapter 9 - Monitoring Network Design Protocol
Chapter 10 - Case Studies - Area C (pp. 200-239)
Chapter 11 - Summary, Conclusions and Recommendations

2. LITERATURE REVIEW

Data collected from water quality monitoring networks have historically been analyzed either statistically, with little attention to physical processes causing the observations, or physically, with little attention to the statistical variability of the data or uncertainty in model structure and model parameters. This research focuses on the combined physical/statistical analysis of groundwater quality monitoring data and how that analysis affects the design of groundwater quality monitoring networks. The following literature review is concentrated in two main areas: 1) Legal Basis for Water Quality Monitoring, and 2) Data Analysis and Design of Water Quality Monitoring Networks.

Regulations regarding water quality specify the objectives for monitoring and have been an influence on the analysis of water quality data and on the design of monitoring networks. The analysis of water quality data and the design of monitoring networks are discussed concurrently. These two topics can not be dissociated because the design of the monitoring network is influenced by the methods of data analysis. The three general methods for data analysis and monitoring network design are: 1) statistical, 2) physical, and 3) combined statistical/physical. These three general categories of methods for water quality data analysis and monitoring network design are reviewed and the limitations of these existing methods are discussed.

2.1 Legal Basis for Water Quality Monitoring.

Two general legal approaches exists for controlling water quality; these are: 1) controlling the receiving water quality and 2) controlling the effluent quality. The first approach, maintaining a specified quality of receiving water, is dependent on effluent standards for meeting the specified water quality. Based on the beneficial use of the water, the number and types of effluent discharges to the water, and area-specific conditions, these effluent standards need not be uniform. The second approach is to control the quality of effluent based on the best available technology (BAT). This approach however does not necessarily arrive at meeting "acceptable " receiving water quality. Frequently, a combination of these two approaches are employed.

Prior to the mid 1960's, water quality laws in the United States (the Refuse Act of 1899, the Oil Pollution Act of 1924, and the Water Pollution Control Act of 1948) were substantially ineffective in controlling water pollution. During the 1960's an increase in public awareness of the environment occurred, as evidenced by the popularity of Rachel Carson's 1962 book, Silent Spring. This increased environmental concern resulted in the enactment of a series of more effective environmental pollution regulations.

In 1965, the Federal Water Quality Act (Public Law (PL) 89-234) was passed. Under this act, surface water quality was controlled by the establishment of stream standards. These standards were set individually by each state and were allowed to vary within the state, depending on the defined use of the water. The focus of this act on in-stream conditions made it difficult to associate in-stream conditions with actions of dischargers due to the complex relationship between sources of discharge and the water bodies.

Due to the delay in states setting water quality standards and problems in enforcement, the Federal Water Pollution Control Act was enacted in 1972 (PL 92-500). This act was amended by the Clean Water Act of 1977, which is how this Act is commonly named. The objective of the Clean Water Act is to restore and maintain the chemical, physical, and biological integrity of the Nation's waters. This act requires that a combination of stream or groundwater and effluent standards be used as the basis for water quality monitoring. The effluent standards are primarily technology based and rely on a permit system, the National Pollution Discharge Elimination System (NPDES), for enforcement. Under the NPDES, every discharger is required to obtain a permit prior to discharge of a pollutant. The requirements of the NPDES permit focus on effluent standards. Evaluation of data in determining whether these effluent standards are being met, as well as the design of a monitoring network to meet these requirements can often best be met by the use of statistical tests since the physical/chemical/biological relationship between the effluent and the receiving water is not required to be known.
During the mid to late 1970s, the focus in environmental monitoring was directed toward hazardous wastes. It was realized that the regulatory authority over hazardous wastes was spread over several agencies. This resulted in the enactment of the Resource Conservation and Recovery Act (RCRA) in 1976. RCRA required the United Stated Environmental Protection Agency (EPA) to develop regulations governing all aspects of the generation, use, transportation and disposal of hazardous wastes, a "cradle to grave" regulation. This law, like the amended Federal Pollution Control Act, monitored water quality based on acceptable discharge levels from the facility to the environment. As for the NPDES permit, this type of regulation focuses on the evaluation of extreme conditions (or standard violations). These type of information goals are often best met by statistical tests.

During the 1980s, the emphasis of environmental monitoring continued to be focused on hazardous wastes. In 1980, the Comprehensive Environmental Response, Compensation and Liability Act (CERCLA) was passed to address the inadequacies of RCRA in cleaning up abandoned hazardous waste disposal facilities. CERCLA, also known as the Superfund Act, establishes mechanisms for cleaning up abandoned hazardous waste facilities. The clean-up requirements for a hazardous waste site are often set by EPA. These requirements are frequently based on both BAT and receiving water goals. To evaluate BAT for a groundwater system, the physical processes affecting the chemical of concern in the environment need to be addressed. This has caused an increase interest in the evaluation of groundwater quality data and on the design of groundwater quality monitoring networks based on the incorporation of physical system processes.

As a result of these acts, a lot of water quality data has been generated. Generally, this data has been collected to meet specific monitoring requirements specified in laws (often discharge only), rather than meeting the objectives of the law (of maintaining specific quality of the receiving water). However, there is more of a focus now on meeting the objective of these laws. To do this, both a physical understanding of the transport processes is needed to associate discharge levels with receiving water quality as well as an understanding of the statistical variability of the data.

2.2 Data Analysis and Design of Monitoring Networks.

Monitoring networks are designed to meet specific information goals regarding water quality. Four primary water quality monitoring objectives are the detection of:

1) average conditions,
2) better definition of existing conditions,
3) changing conditions, and
4) extreme conditions.

The last objective, which focuses on standard violations, is not addressed in this research. However, as discussed in Section 2.1, this type of information objective can generally best be met by the design of monitoring networks and evaluation of data based on the application of statistical tests.

In order to meet the information goals of a groundwater quality monitoring network, hypotheses regarding expected groundwater quality behavior must be made and tests specified for evaluating whether that behavior occurs. The data needs for the tests results in the specification of a monitoring network. The design of the monitoring network includes the determination of sampling locations, selection of water quality variables, and determination of sampling frequencies.

In the last ten years, research has focused on improving the design of monitoring systems in order to better understand the behavior of water quality. This has led to the design of data analysis and monitoring systems in a more systematic manner. A number of researchers have recommended different steps for the systematic design of water quality monitoring systems [Sanders, et al ,1983; Schillerpoot and Groot ,1983; Ward ,1986; Ward, Loftis and McBride ,1986; Ward and McBride, 1986]. These methods concentrate on establishing procedures for the design of a monitoring network that will meet specified monitoring objectives. They stress the incorporation of physical or statistical factors as the basis for design. In addition to purely statistical or deterministic physical bases for design, recently there has been an interest in the use of stochastic models for data analysis. However, there has been little effort in applying these stochastic models to the design of monitoring networks. The use of statistical, physical, and combined physical/statistical techniques for evaluation of water quality data and the design of monitoring networks are discussed below.

2.2.1 Statistical Basis for Groundwater Quality Data Analysis and Network Design.

The use of statistics in water quality data analysis and network design is promoted by many [eg. Palmer and MacKenzie, 1985; Provost, 1984; Schweitzer and Black, 1985; Steele, 1986; and Ward and Loftis, 1986]. The sophistication of the recommended statistical methods depends on the monitoring objectives, the data availability, and the assumptions concerning the statistical distribution of the data.

Generally, purely statistical bases for groundwater quality data analysis and network design are applicable where the information goal is either to verify that no changes in groundwater quality are occurring with time or to better define existing conditions which are expected to change negligibly within the time period of interest. For a specified information objective, the selection of the appropriate statistical method of analysis depends on the characteristics of the data set including the distribution of the data, seasonality and correlation of the data, existence of missing values, and the number of values reported below the detection level.

One method used for evaluating whether changes in groundwater quality are occurring is the two-sample t-test, as used by Sanders and Ward [1979], Loftis and Ward [1986], and Loftis, Harris, and Montgomery [1987]. The two-sample t-test is based on separation of a data record into two subsets and then testing whether the mean of the two subsets is significantly different. This test can be applied at a particular point in space or over a larger area which does not exhibit any spatial non-homogeneous variability in groundwater quality. Given a desired confidence level and a known data variability, the required number of samples can be specified for a monitoring network.

Loftis, Porter and Settembre [1987] used the two-sample t-test for evaluating differences in the means of monthly averaged wastewater data (averaging was performed to eliminate serial correlation; values were paired annually to remove the effects of seasonality). A corollary non-parametric test which can be used if the data is non-normally distributed is the Wilcoxon test.

If the information goal of the monitoring network is a better definition of an existing condition in which spatial variability exists and the data is temporally stationary, spatial correlation techniques such as kriging can be used. Kriging is a statistical method in which estimates of a variable at a non-measured location are made based on a weighted sum of observed measurements at other locations. The weights are determined based on the spatial data correlation. Sophocleous, Paschetto, and Olea [1982] used kriging to evaluate the variability of groundwater levels. This variability was used to assess the optimal groundwater level monitoring network. Carrera, Usunoff, and Szidarovsky [1984] used kriging to design a groundwater quality monitoring network for fluoride, where no trend was observed in the data.

The last information goal for which statistical tests are commonly used for evaluating data and designing monitoring networks is the evaluation of changing conditions. Rather than try to evaluate the physical reasons for change, statistical models are often employed to describe observed trends in data. Spectral or time series analyses are statistical techniques often suggested for assessing trends in water quality data and for the design of monitoring networks. Gunnerson [1966] applied spectral analysis to the design of a monitoring system in a tidal estuary and Munn [1981] reviews the use of spectral analysis for the detection of trends in air quality monitoring. Sanders and Adrian [1978] used an Autoregressive Moving Average (ARMA) time series model to evaluate river flow (found to be highly correlated with water quality), and then used this ARMA model to calculate variances for given sampling frequencies. Kontur [1982] used time series analysis to predict groundwater levels based on a 40-year record of mean annual water levels. Tabios [1984] used different time series models to evaluate dissolved oxygen trends in a river.

Non-parametric methods can be used for non-normally distributed data. Slack and Smith [1982], van Belle and Hughes [1984], and Herricks, et al [1985] strongly recommend the use of non-parametric statistics based on the observation that most water quality records are non-normally distributed. Some non-parametric techniques for trend detection are the Mann-Whitney (step t-test), the Spearman Rho (linear trend test), and the Seasonal Kendal Tau test, as reviewed by Ward and Loftis [1986].

The problem with the use of these statistical models to predict changing conditions in water quality is that often the driving force for change is not included in the statistical model and therefore there is a high level of uncertainty in the use of the model as a predictive tool. Therefore, these statistical techniques are all limited in their applicability to the design of groundwater quality monitoring networks in that they assume that future behavior will mimic past behavior. Statistical techniques are better suited to detection of standard violations for spatially and temporally stationary systems rather than meeting the objective of the majority of groundwater quality monitoring systems which is to detect non-linear changing conditions.

2.2.2 Physical Basis for Groundwater Quality Data Analysis and Network Design.

Subsurface hazardous waste legislation in the 1970s focused groundwater quality data analysis and the design of monitoring networks on the understanding of the physical processes which cause changes in groundwater quality. These physically-based groundwater quality models allow for non-uniform changing behavior based on expected changes in physical conditions affecting the groundwater system. Therefore, instead of a statistically-based model, physically-based groundwater quality models may be used to predict changes in groundwater quality under changing conditions.

For groundwater flow and groundwater contaminant transport models, the parameters in the deterministic physical model can be estimated by either a trial and error procedure or by the use of statistical fitting techniques. The trial and error approach is now used infrequently in favor of statistical techniques. However, because the mathematical problem of parameter identification is improperly posed, an infinite number of solutions exist. A variety of methods have been developed to solve this problem referred to as the inverse problem (or the Cauchy problem), including least squares [Hughes and Lettenmaier, 1981; Kashwap and Chandra, 1982; Bruch, 1974], time series analysis, kriging [Binsariti, 1980; Kitanidis and Vomvoris, 1983; Hoeksema and Kitanidis, 1984; Bruch, 1974], nonlinear regression

[Neuman and Yakowitz, 1979; Knopman, 1987; Knopman and Voss, 1987 and 1988], mini-max and linear programming [Yeh, 1975; Neuman, 1973; Gorelick et al, 1983], gradient search [Vemuri and Karpluy, 1969], quasi-linearization [Yeh and Tauxe, 1971a and 1971b; Lin and Yeh, 1974], maximum principle, and influence coefficient. The use of these different statistical techniques for estimating model parameters may result in different levels of uncertainty in the parameter estimates depending on the applicability of the method to the specific data available.

Although the parameters of these deterministic models are often estimated by statistical methods, deterministic physical models only include specific parameter values. Whereas these deterministic physical models may be better at predicting expected groundwater quality conditions, they do not provide an evaluation of the uncertainty in those predictions. The design of a water quality monitoring network based on a deterministic physical model is often used to identify sampling locations. However, since no uncertainty is included in the model, no estimate of confidence in the monitoring network can be made.

2.2.3 Physical/Statistical Basis for Groundwater Quality Analysis and Network Design.

The focus in the late 1980s towards remediating sites contaminated with hazardous wastes has focused groundwater quality data analysis on the use of models to predict groundwater quality under changing conditions. The prediction of future conditions and the evaluation of the confidence in those predictions requires the use of a combination of physical and statistical data analysis and monitoring design techniques as discussed in this section.

Frequently, physical factors are incorporated into the design of a water quality monitoring network based on observations or experience (empirically), with statistical considerations incorporated explicitly. For example, Erlebach [1979] defines the sampling frequency for a surface water quality monitoring network based on a time series analysis from a pilot study, and incorporates the sampling location and number of sampling sites based on the expected physical representativeness of the location. In the design of a network for evaluating long-term mean precipitation and mean annual rainfall from a storm event, Rodriguez-Iturbe and Mejia [1974] model rainfall as a stationary process in which space and time can be separated. Their method is essentially statistical, although the estimation of the parameters in the spatial correlation structure are dependent on the type of storm event. Bradford and Iwatsubo [1979] designed a water quality monitoring network for San Francisco Bay in which statistical analysis of flow was used to identify stable water quality locations.

Eccles and Nicklen [1979] describe physical factors to consider in designing groundwater quality monitoring networks, but do not propose any method for including these factors explicitly into the monitoring network design. Tinlen and Everett [1979] also emphasize the importance of the consideration of physical factors in their proposed 15-step methodology for monitoring groundwater quality. However, they too do not provide any explicit method of incorporating these factors into the design of groundwater quality monitoring networks. Todd, et al [1976] discuss that the groundwater monitoring network must take into account the physical processes affecting the transport of pollutants through the subsurface, although they conclude that the determination of a sampling frequency often involves trial-and-error procedures.

Because these models empirically include physical processes, there is no physical causal relationship incorporated explicitly into the monitoring network design process. In the last ten years, increased emphasis has been placed in explicitly incorporating the physical attributes of the system and the spatial variability of the data into a model. Two principle types of stochastic models are used:

1) stochastic physical models with deterministic parameter estimates

2) stochastic physical models with stochastic parameter estimates.

These two types of models are discussed below relative to the evaluation of groundwater quality data and to the design of groundwater quality monitoring networks.

2.2.3.1 Stochastic Physical Models with Deterministic Parameter Estimates. Stochastic physical models are frequently developed in which the parameters are considered to be deterministic. The variability of the system is modeled by a separate random term in the model. One common type of stochastic model used in the design of groundwater quality monitoring networks is the kalman filter.

Kalman filtering is a means of evaluating the uncertainty of an estimation based on a physical and statistical understanding of a system. Kalman filtering is based on two equations: 1) the state equation and 2) the measurement equation. The state equation consists of a deterministic physical model plus a random system error term. The measurement equation includes a measurement error which is assumed independent from the system error. Based on these equations, the quality of a monitoring network can be defined based on the confidence of predictions at arbitrary locations. By incorporating a physical model in the state equation, the kalman filtering bases the correlation structure on the process dynamics rather that the statistics of the data. However, the correlation structure can only be determined a priori if the state equation is linear. For nonlinear state equations, the covariance matrix depends on the actual state vector.

The application of kalman filtering to water quality modeling necessitates the approximation of the nonlinear equations describing the solute transport with linear equations. Van Geer [1982 and 1987], van Geer and van der Kluet [1986], and Schillerpoot and Groot [1983] propose the use of kalman filtering for monitoring network design. Pimentel [1975] uses kalman filtering to maximize the time between samples for a specified error based on a purely diffusive contaminant transport problem. He utilizes separation of variables to reduce the partial differential equations (PDEs) to ordinary differential equations (ODEs) and solves the problem in two sub-problems: 1) the specification of model, variables to measure, measuring devices, and spatial distribution of sampling sites, and 2) the sequencing of measurements in time.

Lettenmaier and Burges [1977] use the extended kalman filter (an approximate solution when the process dynamics are nonlinear) to design a river water quality monitoring network. An iterative solution method was used for determining the optimal sample station locations. Sivakumaran [1989] utilized a kalman filtering approach in the design of an estuary water quality monitoring system.

All kalman filtering is limited in that the state system does not incorporate uncertainty in the model parameters. That is, it uses a stochastic model with deterministic parameter values.

2.2.3.2 Stochastic Physical Models with Stochastic Parameter Estimates. The models discussed above treated data error separately from the physical model. During the past ten years, there has been an increased focus in groundwater quality research in the incorporation of variability of parameter estimates into physical models. These models are frequently used to evaluate model behavior relative to assumed model parameter behavior. These models are rarely used for designing a monitoring network or for developing a method of evaluating data collected from an existing network.

Freeze [1975] evaluated the distribution of hydraulic heads based on the results of 500 Monte Carlo simulations where the hydraulic conductivity (K) was assumed to be lognormally distributed. For the steady-state case with known boundary conditions, the heads were normally distributed in the middle of the simulated area and skewed near the boundaries. The largest variance was in the center. With unknown boundary conditions, the variance increased at the boundaries and was approximately normal everywhere. To analyze the transient case, the porosity and compressibility were assumed to be normally and lognormally distributed, respectively. This resulted in a non-normally distributed head distribution.

Frind, et al [1987] ran a contaminant transport model in which the two-dimensional hydraulic conductivity (k) field had been randomly generated in order to verify the theory of the scale dependence of dispersion. Due to the extensive computer time required to run this micro-scale model, only three realizations of the K field were generated. The authors concluded that the effective longitudinal dispersivity converges to a macroscopic value within approximately 50 correlation lengths. At early time, the plume for one realization had a distinct transverse component due to molecular diffusion under a strong gradient. Because only three realization were made, the statistical significance of the scale and time dependence of the dispersion and the effects of this distribution on network design could not be assessed.

This type of work has also been done by other researchers. Bakr et al [1978] assess the head variance produced by specified hydraulic conductivity variances. Smith and Freeze [1979a and 1979b], Delhomme [1979], and Gutjahr [1984] also investigated the covariance between heads and log hydraulic conductivity.

Some work has been conducted to use these stochastic models to design monitoring networks. Knopman and Voss [1987] developed general groundwater quality monitoring design criteria for better defining an appropriate model and model parameters based on the use of a stochastic one-dimensional advection-dispersion model. The authors concluded that observations should be taken at points in time and space that were highly sensitive to model parameters. The determination of these points depends on the form of the model, the estimation of the parameters, and the type of error in the data. In order to design an optimal monitoring network, they conclude that a multi-objective approach is required.

Dawdy and Moore [1979] developed a water quality sampling program for rivers using a one-dimensional advection model. Sources of uncertainty (initial conditions, boundary conditions, waste sources, tributary inflow, model structure itself, and parameters in model) were characterized using time series analysis. Based on given costs for sampling, dynamic programming was used to identify a cost-effective sampling design.

Moore, Dawdy and DeLucia [1976] use a stochastic eutrophication model to describe the uncertainty in water quality variables and then used the model to determine sampling frequencies. They compute the mean and variance of the state variables directly using expectations of the stochastic process. Tung [1986] uses a stochastic groundwater management model where the transmissivity and storage coefficients are assumed random. He then uses first-order analysis to estimate the mean and variance of drawdown at each control point.

Most recently, Loaiciga [1989] developed a method for optimizing the design of groundwater quality monitoring networks based on a stochastic physically-based model. The objective function was to minimize the sum of the variance of expected concentration estimation errors at sampled locations subject to an unbiasedness constraint which required that the mean of all sampling locations be equal to the mean concentration over the region of interest. This optimization constraint placed unrealistic demands on the monitoring network for general application. However, the application of this methodology is the first time that monitoring networks have been designed incorporating physical and statistical knowledge of the variable of interest.

This research focuses on the development of an optimization procedure which incorporates knowledge of the model structure and model uncertainty explicitly into the monitoring network design. Stochastic physically-based models are used which provide a mechanism for predicting non-uniform changes in groundwater quality based on changing physical conditions and for evaluating the confidence level associated with data interpretation and predictions. The optimization procedure allows for a wide spectrum of information goals by not constraining that the samples be unbiased (as developed by Locaigia). In addition, this research focuses on the use of model applicability/discrimination tools in the model selection process and in the use of the information obtained from the model applicability evaluation in the optimization of the monitoring network.

3. SIMULATION OF DATA RECORDS

Groundwater quality data was simulated for this study using a physically based two-dimensional advection-dispersion solute transport model and a superimposed random error. Since the focus of this research is not the discrimination between various physical models, but rather the development of an appropriate data analysis and network design protocol for designing monitoring networks, no other deterministic model was considered for data simulation. Four types of random error were considered: 1) additive normal; 2) multiplicative normal; 3) additive lognormal; and 4) multiplicative lognormal. These deterministic and random components of the simulated data record are discussed below. Rather than performing Monte Carlo simulations, the statistics of interest were evaluated using expectations. The derivation of these statistics is discussed in Chapter 5.

3.1 Physical Model.

The partial differential equation describing solute transport in saturated porous media is derived based on the law of mass conservation, where [Freeze & Cherry, 1979, p.389]

$$\begin{Bmatrix}\text{net rate of}\\ \text{change of mass}\\ \text{of solute}\\ \text{within element}\end{Bmatrix} = \begin{Bmatrix}\text{flux of}\\ \text{solute out}\\ \text{of the}\\ \text{element}\end{Bmatrix} - \begin{Bmatrix}\text{flux of}\\ \text{solute}\\ \text{into the}\\ \text{element}\end{Bmatrix} + \begin{Bmatrix}\text{loss/gain}\\ \text{of solute}\\ \text{mass due to}\\ \text{reactions}\end{Bmatrix}$$

The transport of solutes in groundwater occurs due to both advective transport and dispersion. Advective transport is the movement of chemicals due to bulk groundwater flow, where the average rate of transport is equal to the average linear groundwater velocity. Dispersion is a result of mechanical mixing and molecular diffusion. Mechanical dispersion is caused by the tortuosity of the pore channels, varying pore sizes, and by drag at the pore surfaces. Molecular diffusion is the movement of chemicals due to concentration gradients.

In addition to fluxes due to advection and dispersion, losses or gains of the solute may occur as a result of chemical or biological processes or radioactive decay.

Combining constitutive relations with the law of mass conservation yields the general equation for advective-dispersive transport in a homogeneous, isotropic, saturated porous media:

$$\frac{\partial C}{\partial t} = -\mathrm{div}(C\underline{V} - \underline{D}\ \mathrm{grad}\ C) - R\lambda C \tag{3.1}$$

where,

R = retardation factor
C = mass concentration of constituent
$\underline{V}$ = the average fluid velocity vector
$\underline{D}$ = hydrodynamic dispersion tensor
λ = radioactive decay constant

This partial differential equation can be simplified for a two-dimensional problem in which the groundwater flow is unidirectional and steady state and the direction of flow is oriented along the x axis of a Cartesian coordinate system. The equation describing this flow system is:

$$D_L \frac{\partial^2 C}{\partial x^2} + D_T \frac{\partial^2 C}{\partial y^2} - v \frac{\partial C}{\partial x} - R\lambda C = R \frac{\partial C}{\partial t} \tag{3.2}$$

where,

D_L = longitudinal dispersion coefficient
D_T = transverse dispersion coefficient
v = average pore water velocity in x-direction

To derive an analytical solution to this equation, the initial and boundary conditions must be specified. For this simulation, a finite-width decaying source is specified at the source X_0, Y_0, with initial and boundary conditions given as:

$$C(0,y,t) = C_0 e^{-\alpha t} \qquad -a \le y \le a$$

$$C(0,y,t) = 0 \qquad \text{other values of } y$$

$$\lim_{y \to \pm\infty} \frac{\partial C}{\partial y} = 0$$

$$\lim_{x \to \pm\infty} \frac{\partial C}{\partial x} = 0$$

$$C(x,y,0) = 0$$

where,

$$X = X' - X_0 \text{ and } Y = Y' - Y_0$$

X', Y' are observed values.

The analytical solution to this partial differential equation with initial and boundary conditions as specified above, is:

$$C(x,y,t) = \{(C_0 x)/[4(\pi D_L)^{1/2}]\} * \exp[(vx/2D_L)-\alpha t] \tag{3.3}$$

$$* \int_0^{t/R} \exp\{-[\lambda R - \alpha R + v^2/(4D_L)]\tau - x^2/(4D_L\tau)\}\tau^{-1.5} *$$

$$\{[\mathrm{erf}((a-y)/(2(D_T\tau)^{1/2}))] + \mathrm{erf}[(a+y)/(2(D_T\tau)^{1/2})]\}\, d\tau$$

Using dimensional analysis, it can be shown that this solution is equivalent for all problems in which

1) v/D_L
2) v/D_T
3) v/R
4) α
5) λ
6) a

are equivalent. This means that for similar boundary conditions, systems with equivalent relative flow velocities (v/R, v/D_T, and v/D_L) will have the same non-dimensional solution.

A computer program was modified from Javandel, et al [1984] and Ferziger [1981] to calculate the ratio of C/Co for any point downgradient from the source of contamination, at any point in time. A copy of the computer code (ANAL) is included in Appendix A.

For the simulation study, the parameters of the model were defined as follows:

v/R = 0.5 meters/day
v/D_L = .025 meters^2/day
v/D_T = .25 meters^2/day
α = 0.001 /day
λ = 0.0 /day
a = 30 meters

Using the computer program developed, solutions were calculated at X = 40 to 400 meters, at 40 meter intervals, and at Y = -80 to 80 meters at 40 meter intervals. Solutions were calculated at biweekly intervals for 10 years. Figure 3.1 is a schematic of the idealized aquifer and monitoring system. Figure 3.2 illustrates the concentration at the source. The relative concentrations (C/C_0) predicted by this analytical model are plotted in Figures 3.3, 3.4 and 3.5 for wells at Y=0 meters, Y=40 meters, and Y=80 meters, respectively.

3.2. Distribution and Magnitude of Error Component.

Errors in water quality data records are derived from two sources:

1) laboratory error, and

2) sampling error.

Therefore, the

$$\begin{Bmatrix}\text{Measured}\\ \\ \text{Value}\end{Bmatrix} = \begin{Bmatrix}\text{"True"}\\ \\ \text{Value}\end{Bmatrix} \pm \begin{Bmatrix}\text{Laboratory}\\ \\ \text{Error}\end{Bmatrix} \pm \begin{Bmatrix}\text{Sampling}\\ \\ \text{Error}\end{Bmatrix}$$

If a model is used to simulate the measured values, an additional error is introduced in the analysis, that of the model. That is, neglecting laboratory and sampling error, an error is introduced because a model cannot predict exactly what occurs in a natural system. Therefore,

$$\begin{Bmatrix}\text{Measured}\\ \\ \text{Value}\end{Bmatrix} = \begin{Bmatrix}\text{Model}\\ \\ \text{Value}\end{Bmatrix} \pm \begin{Bmatrix}\text{Model}\\ \\ \text{Error}\end{Bmatrix} \pm \begin{Bmatrix}\text{Laboratory}\\ \\ \text{Error}\end{Bmatrix} \pm \begin{Bmatrix}\text{Sampling}\\ \\ \text{Error}\end{Bmatrix}$$

Research has been conducted to investigate the statistical distribution of these three sources of error. Laboratory error is the most clearly defined with both additive and multiplicative random normal errors being most commonly assumed (Porter, 1985). The relative magnitude of sampling versus laboratory errors was reviewed by McBean and Rovers [1984] via the analysis of sample duplicates and laboratory replicates. For the site chosen for analysis, these authors found that the laboratory error variance was three to fifty times less than the sampling error variance.

The error introduced by the use of a deterministic physical model has been investigated by Gelhar [1977], Gutjahr [1984], Vomvoris and Gelhar [1986], and Frind et al [1987], among others. For water levels, Gelhar [1977] found that the variance of the water level was much smaller than the variance of the hydraulic conductivity. Vomvoris and Gelhar [1986] developed an analytical expression for the variance of the concentration as a function of the mean concentration gradient, variance, and correlation scales of the log-hydraulic conductivity field and local dispersivity values. The derived covariance function of the concentration field involves the evaluation of a three-dimensional integral which in general cannot be solved analytically. The field is in general spatially and temporally variant. Via

Monte Carlo simulation, Frind [1987] showed that the concentration distribution approached a normal distribution after mature development of a contaminant plume.

The combined contribution from all three sources of error was investigated by Loftis et al [1987] for groundwater quality variables. In the data sets analyzed, many of the water quality variables were non-normally and non-symmetrically distributed. After review of available data, Harris [1988] used normal and log-normal additive errors to simulate groundwater quality data.

For this simulation, the three sources of errors (sampling, laboratory, and model) were combined into one error component. Four types of error were considered: 1) additive normal distribution $\epsilon \sim N(0, \sigma_e^2)$; 2) multiplicative normal distribution $\epsilon \sim N(0, C\sigma_e^2)$ (where C = concentration); 3) additive lognormal distribution $\epsilon \sim LN(0, \sigma_e^2)$; and 4) multiplicative lognormal distribution $\epsilon \sim LN(0, C\sigma_e^2)$.

Therefore,

$$\left\{ \begin{array}{c} \text{Simulated} \\ \text{Value} \end{array} \right\} = \left\{ \begin{array}{c} \text{Analytical} \\ \text{Solution} \end{array} \right\} + \epsilon$$

where,

ϵ is distributed as described above.

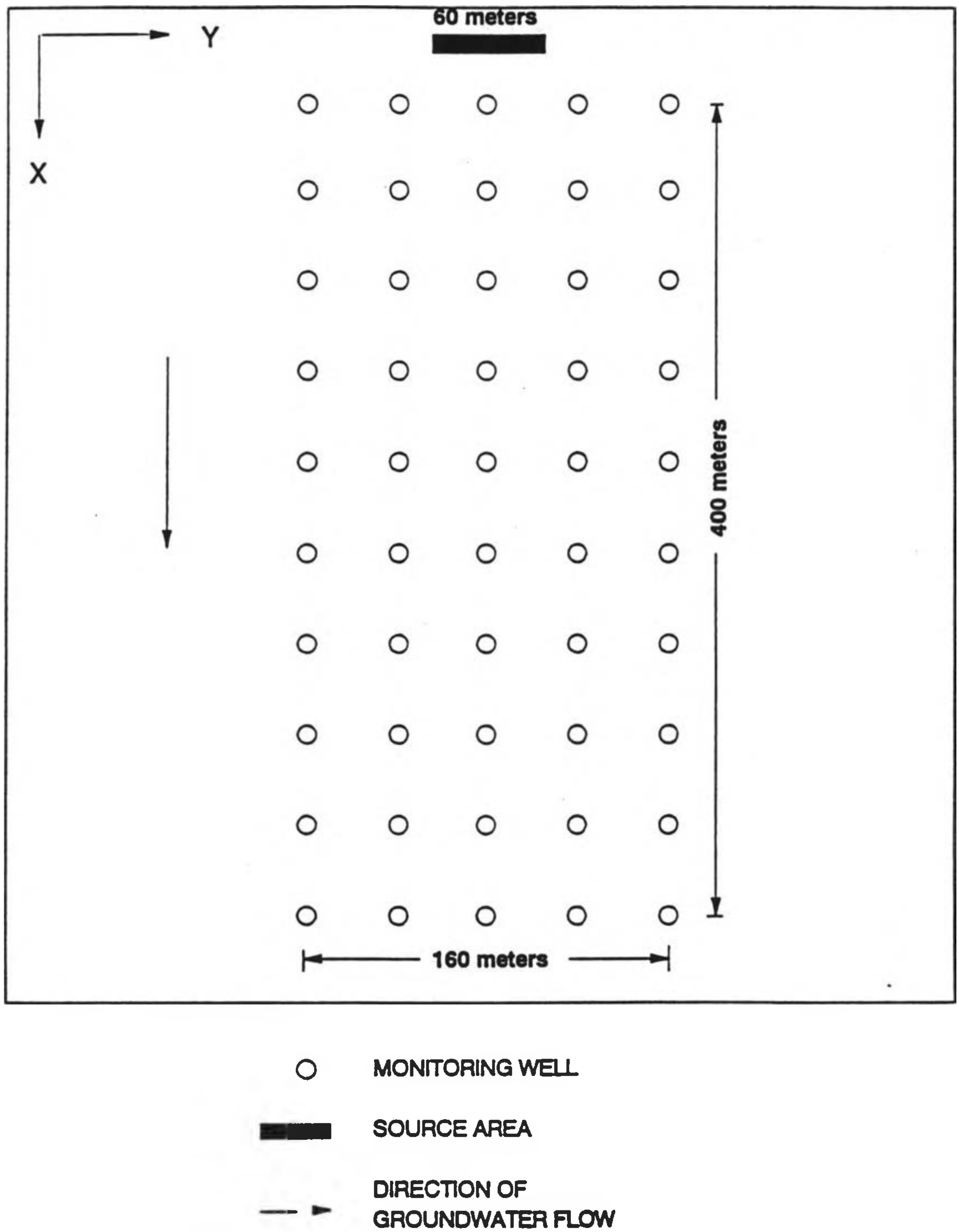


Figure 3.1 Schematic of Simulated Aquifer and Monitoring Network

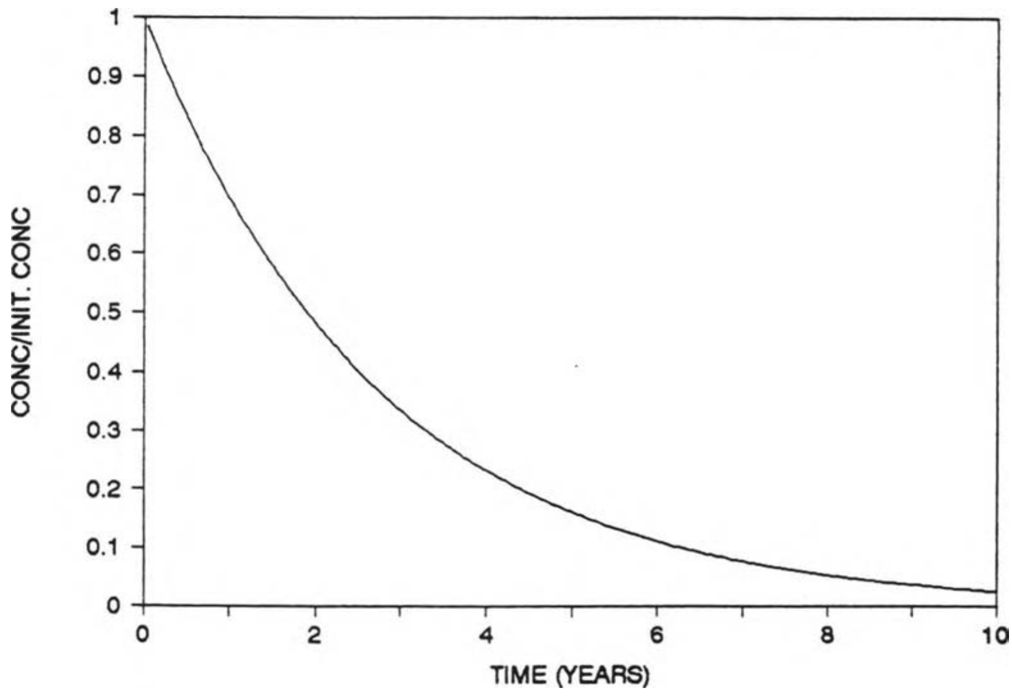


Figure 3.2 Concentration of Contaminant at Source (C) Relative to Initial Concentration at Source (C_o)

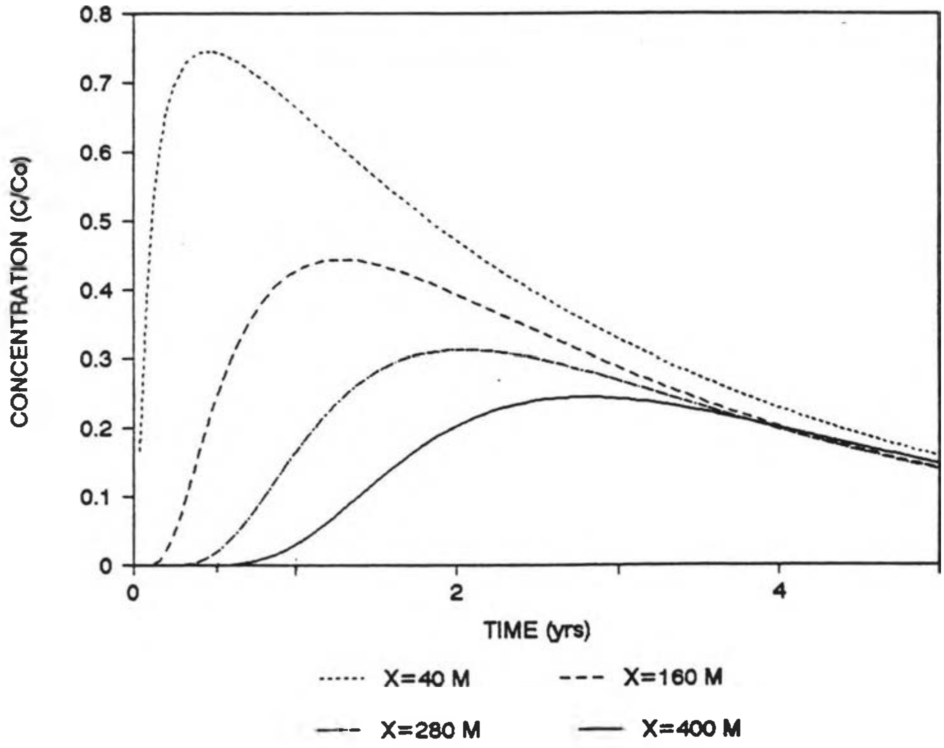


Figure 3.3 Simulated Concentrations at Y=0 Meters

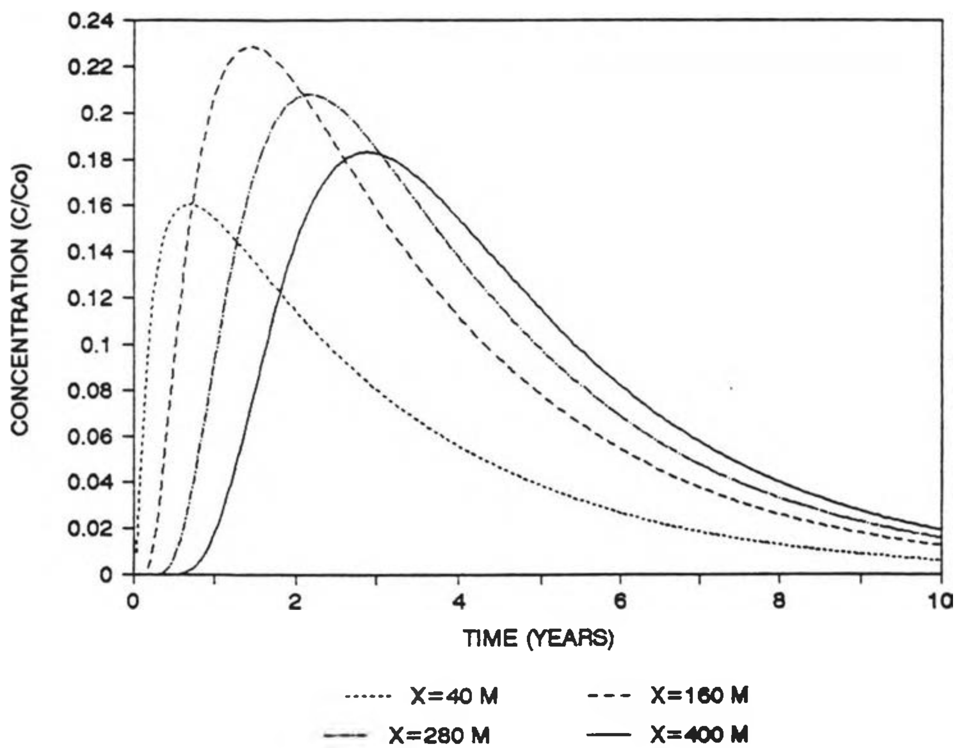


Figure 3.4 Simulated Concentrations at Y = 40 Meters

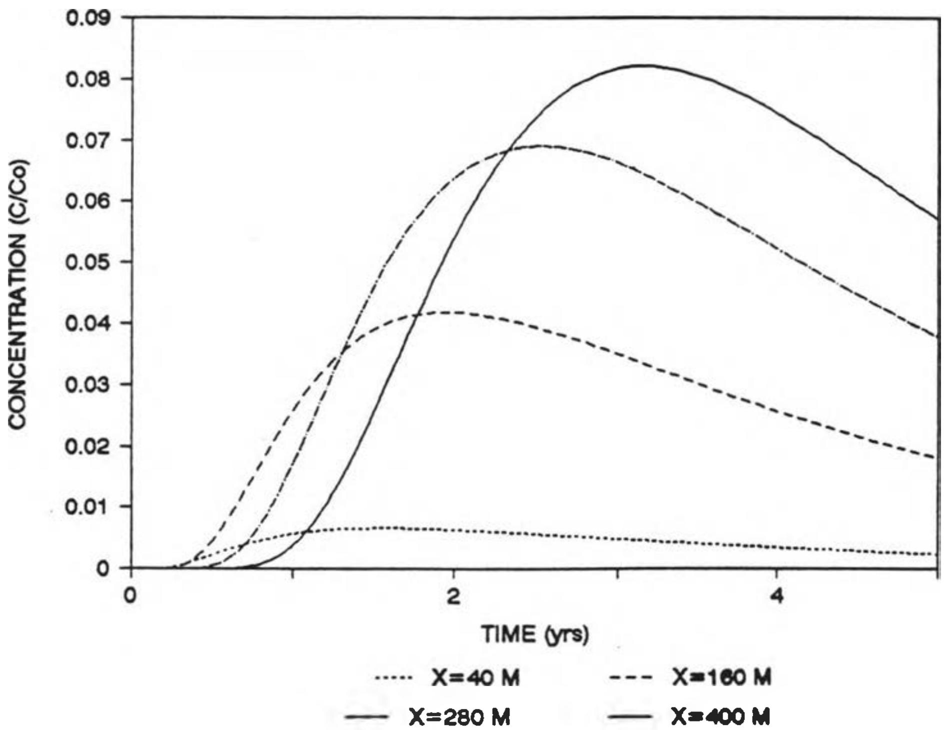


Figure 3.5 Simulated Concentrations at Y = 80 Meters

4. MODEL PARAMETER ESTIMATION

Data can be fit to models using a variety of estimation techniques. Four of the most common techniques are:

1) least squares,
2) weighted least squares,
3) method of moments, and
4) method of maximum likelihood.

The appropriateness of the estimation technique can be evaluated by the efficiency, consistency and sufficiency of the estimator. An efficient estimator is unbiased and has minimum variance. An estimate is unbiased if the expectation of the estimator equals the estimator; bias is an estimate of the systematic error in an estimator. The variance of an estimator measures random error. If a parameter estimate approaches the true parameter value as the sample size increases, then it is a consistent estimator. Lastly, a sufficient estimator contains all the relevant information from a sample. It is desirable to use a parameter estimation method which produces efficient, consistent, and sufficient estimators.

The four common parameter estimation methods listed above are described below in light of these properties.

4.1 Method of Least Squares.

The method of least squares minimizes the square of the differences between observations and model predictions. The least squares estimators are found by solving the following set of simultaneous equations:

$$\partial/\partial\beta_j \sum_{i=1}^{n} (C_i' - \hat{C}_i)^2 = 0 \quad \forall j,\ j = 1,\ldots,p \tag{4.1}$$

where,

p	= number of model parameters
n	= number of observations
C_i'	= observed concentration at time t
$\hat{C}_i$	= concentration predicted by model at time t
β_j	= model parameters

For a linear model ($\underline{C} = \underline{X\beta} + \underline{\epsilon}$), these equations can be solved explicitly, where

$$\underline{\beta} = (\underline{X}'\underline{X})^{-1}\,\underline{X}'\underline{C} \tag{4.2}$$

$$\underline{\beta} = (\underline{X}'\underline{X})^{-1}\,\underline{X}'(\underline{X\beta} + \underline{\epsilon})$$

Taking expectations results in

$$E(\underline{\beta}) = E[(\underline{X}'\underline{X})^{-1}\,\underline{X}'\,(\underline{X\beta})] + E[(\underline{X}'\underline{X})^{-1}\,\underline{X}'\underline{\epsilon})] \tag{4.3}$$

For a zero mean error,

$$E(\underline{\beta}) = \underline{\beta} \tag{4.4}$$

Therefore, the linear squares estimation method will provide unbiased estimators regardless of the error distribution as long as the error is a zero mean process.

To be an efficient estimate, the variance of the estimator must also be a minimum. The variance of the estimators is defined as follows (Farebrother, 1988):

$$VAR(\underline{\beta}) = E(\beta^2) - E^2(\beta)$$

$$VAR(\underline{\beta}) = E[(\underline{X}'\underline{X})^{-1}\,\underline{X}'\,E(\underline{\epsilon\epsilon}')\underline{X}(\underline{X}'\underline{X})^{-1}] \tag{4.5}$$

For an additive normal or lognormal error

$$E[\underline{\epsilon\epsilon}'] = \sigma^2_e\,\underline{I}$$

where,

σ^2_e = variance of error

$\underline{I}$ = identify matrix

For a multiplicative normal or lognormal error

$$E[\underline{\epsilon\epsilon}'] = \sigma^2_e\,\underline{IC}$$

Therefore, for an additive error

$$VAR[\underline{\beta}] = \sigma^2_e I(\underline{X}'\underline{X})^{-1} \qquad (4.6)$$

and for a multiplicative error

$$VAR[\underline{\beta}] = (\underline{X}'\underline{X})^{-1}\,\underline{X}'(\sigma^2_e\,\underline{IC})\underline{X}(\underline{X}'\underline{X})^{-1} \qquad (4.7)$$

For the variance to be a minimum, $\partial VAR(\beta)/\partial\beta = 0$. For an additive error, since $VAR(\beta) \neq f(\beta)$, $\partial VAR(\beta)/\partial\beta = 0$ regardless of the distribution of the error. According to Yevyevich [1972], for the method of least squares to yield an efficient parameter estimate, the residuals should be normally or at least symmetrically distributed, mutually independent, and exhibit constant variance. As shown by the previous analysis, the normality or symmetric requirement is unnecessary. For a least squares estimator where the error is additive, the variance of the parameter estimates decreases with an increase in sample size. In addition, since all the available data is utilized, the least squares estimation technique provides an efficient, sufficient and consistent estimator for models with zero mean additive errors.

For multiplicative errors, the variance of the parameters is a function of the parameters ($VAR(\beta) = f(\beta)$) and therefore the variance of the estimator may not be a minimum. Furthermore, the condition of independence is important for assuring an efficient estimator when using least squares regression.

For a nonlinear model, the variance of the parameters may be solved using the same equations as for a linear model, where $\underline{X}$ is substituted by $\underline{G}$ where

$$\underline{G} = \frac{\partial \underline{C}}{\partial \underline{\beta}}$$

For a nonlinear model, the least squares equations cannot be solved explicitly, but must be solved iteratively. If the initial estimate is close to the true solution, then this iterative procedure will converge to the true solution.

4.2 Method of Weighted Least Squares.

The least squares method of parameter estimation weights all variables equally. If variables are of different dimensions or some observations are less reliable than others, then the estimation of model parameters should be modified. One way of doing this is by weighting the errors. If the model equations are linear in the parameters or the number of observations is large, the inverse of the covariance matrix of the errors can be used. This method of analysis would be appropriate for multiplicative errors in which case the weights would be the inverse of the predicted concentrations.

Using weighted least squares, the expected value of the estimators are

$$\underline{\beta} \quad = (\underline{X}'\underline{W}\underline{X})^{-1}\,\underline{X}'\underline{W}\underline{Y} \tag{4.8}$$

$$E(\underline{\beta}) \quad = \underline{\beta} \text{ (unbiased estimators)}$$

Unlike for the ordinary least squares, the variance of the parameter estimates would be equivalent for the additive and multiplicative errors of the same relative error variance.

$$VAR(\underline{\beta}) = E[(\underline{X}'\underline{X})^{-1}\,\underline{X}'\underline{W}E(\underline{\epsilon\epsilon}')\underline{X}'(\underline{X}'\underline{X})^{-1}] \tag{4.9}$$

For additive errors,

$$\underline{W} = \underline{I}$$

$$VAR(\underline{\beta}) = \sigma^2\underline{I}(\underline{X}'\underline{X})^{-1} \tag{4.10}$$

For multiplicative errors,

$$\underline{W} = \underline{I}\underline{C}^{-1} \text{ and } E(\underline{\epsilon\epsilon}') = \underline{C}\,\sigma^2$$

$$VAR(\underline{\beta}) = \sigma^2\underline{I}(X'X)^{-1} \tag{4.11}$$

Therefore, the weighted least squares results in efficient estimators. However, because the predicted values depend on the parameter estimates, this method requires an iterative estimation procedure.

4.3 Method of Moments.

The method of moments equates theoretical population moments with sample moments (the expected value of a random variable to the rth power is the rth population moment of the random variable). In this method, the first p population and sample moments are equated, where p is the number of parameters in the model. When the underlying distribution is normal, the method of moments provides asymptotically efficient estimators. This is generally not true for skewed variables for which method of moments results in biased parameter estimates [Salas, et al, 1980].

4.4 Method of Maximum Likelihood.

The method of maximum likelihood maximizes the likelihood function of the parameters in a model. The likelihood function is the joint probability of the model errors where $L(\cdot) = \prod C(\epsilon/\underline{\beta})$, where

$C = f(\underline{\beta}) + \epsilon.$

The maximum likelihood estimators are calculated solving the following simultaneous equations:

$$\frac{\partial \underline{L}(\cdot)}{\partial \underline{\beta}} = 0$$

These maximum likelihood estimators are asymptotically efficient. However, for certain functions, the equations used are nonlinear and the solutions can only be approximated. The maximum likelihood method is equivalent to the least squares method when the error is normally distributed, independent, zero mean and constant variance.

4.5 General Discussion.

If a model is correct and the errors are distributed with zero mean and constant variance, then the least squares parameter estimation method provides efficient estimators. If the errors are not distributed with constant variance, the least squares estimators are unbiased with minimum variance among all linear squares estimators, but they are not efficient. If the variance of the residuals is not constant, least squares does not provide minimum variance estimators.

If the distribution of the errors are known and are non-normal, maximum likelihood estimators may be used. The maximum likelihood estimator does provide a minimum variance estimator, although this method often needs to be solved by trial and error. An alternative method to maximum likelihood when the errors are multiplicative, is a weighted least squares estimation technique. For this case, the weights would be the inverse of the covariance matrix.

Least squares, weighted least squares, method of moments, and maximum likelihood estimators all may be used to estimate model parameters. The effect of the estimation techniques on model fit is not evaluated in this study. This work is reserved for future research but has been mentioned herein so as not to imply that the parameter estimation method chosen, least squares, is necessarily the best method to use for a given data set and model.

5. ANALYSIS OF MODEL APPLICABILITY

A wide spectrum of models are available for modeling water quality. The statistical and physical models considered for this study and the statistical tools used to evaluate model applicability are discussed below.

5.1 Description of Models Considered.

5.1.1 Statistical Models.

Spectral analysis and ARMA models are commonly used for statistical analysis of water quality data as discussed in Chapter 2. However, because of the limited data available in most groundwater quality records, the use of these models for statistical data analysis is rarely applicable. Instead, the data is often fit to some simpler statistical distribution for trend detection. The statistical analysis of water quality data sets frequently concentrates on the detection of linear trends in order to assess whether long-term deterioration of groundwater quality is occurring. However, in many groundwater problems, particularly in the remediation of site specific groundwater contamination problems, it is rare to expect a linear trend in groundwater quality. Therefore, in this study, in addition to linear trend models, higher order polynomial trends were also fit to both individual wells and groups of wells (trend surfaces).

The polynomial models for individual wells were of the form:

$$C(T) = \sum_{i=0}^{p} B_i T^i$$

The trend surface models were of the form (example for quadratic):

$$C(X,Y,T) = B_o + B_1{*}X + B_2{*}Y + B_3{*}T + B_4{*}X{*}Y + B_5{*}X{*}T + B_6{*}Y{*}T + B_7{*}X^2 + B_8{*}Y^2 + B_9{*}T^2$$

where,

C = concentration of constituent of concern

B_i = least squares fitted parameter

X = X location of well

Y = Y location of well

T = time of observation

p = model order

5.1.2 Physical Models.

The general class of physical models considered are two-dimensional advection-dispersion models. This model is described in Chapter 3.1. The same form of the model as that used to simulate the deterministic component of the simulated data was considered for model fit. This model will be fit to subsets of the data set based on sampling frequency and sampling density.

5.2 Model Applicability Evaluation.

To discriminate between the applicability of the various models considered, the models were evaluated for goodness-of-fit and predictive capabilities. The statistical tests utilized are described in the following two sections.

5.2.1 Goodness-of-fit Tests.

To assess the goodness-of-fit of the models evaluated, three statistical techniques were utilized: 1) an analysis of variance, 2) an analysis of model parameter behavior, and 3) an analysis of residuals. In this analysis, no non-parametric methods were used since the focus of the research is not the discrimination of various tests. The specific tests used in each of these three categories are discussed below.

5.2.1.1 Analysis of Variance. An Analysis of Variance (ANOVA) is based on separation of the total variance into various components. ANOVA tests whether the variance about the model is different than the variance in the observations, i.e., it tests the hypothesis (H_0) and the alternative (H_1):

H_0: $\sigma^2 = \sigma^2_{yx}$

H_1: $\sigma^2 \neq \sigma^2_{yx}$

where,

σ^2_{yx} = variance about the model.

The statistic used to test this hypothesis is the F-test. The F-test is a test to determine equality of variances, assuming that the variances are normally distributed. This assumption implies that both the deviation of the model about the mean and the deviation of the model predictions about the observations are normally distributed.

The F statistic for the regressions is calculated as follows:

$$F\ stat = \frac{MSR}{MSD} \tag{5.1}$$

where,

MSR = Mean Square Residual

MSD = Mean Square Deviation

$$MSR = \frac{SSR}{(P-1)} \tag{5.2}$$

$$MSD = \frac{SSD}{(N-P+1)} \tag{5.3}$$

where,

SSR = Sum of Square Residual

SSD = Sum of Square Deviation

$$SSR = \sum_{i=1}^{N} (\hat{C} - \bar{C})^2 \tag{5.4}$$

$$SSD = \sum_{i=1}^{N} (\hat{C} - C')^2 \tag{5.5}$$

where,

N = number of samples

$\bar{C}$ = average of observations

$\hat{C}$ = predicted values of model

C' = observations

p = the number of parameters in the model

The F-test can also be used to test the significance of higher order models. The F-test statistic calculated to determine if the model of order P added significantly to the model, is

$$F\ add = \frac{(SSR_p - SSR_{p-1})}{SSD_p / (N-P+1)} \tag{5.6}$$

where the subscript designates the order of the model.

This statistic can be evaluated for the simulated data by using expectations. For a stochastic model,

$$C' = C + \epsilon$$

where

C' = observed value,

C = true value, and

ϵ = error.

The expected value of the F-test function can be evaluated as follows:

$$E[FTEST] = E\left\{\frac{MSR}{MSD}\right\}$$

For a nonlinear function, the expectation of the F-test function can be approximated using a Taylor series expansion as:

$$E[FTEST] = \frac{E[MSR]}{E[MSD]}$$

where,

$$E[MSR] = E[SSR]/(P-1)$$

$$E[MSD] = E[SSD]/(N-P+1)$$

The sum of squares residuals (SSR) is unaffected by the error in the data or model, therefore E[MSR] = MSR. However, the sum of squares deviation (SSD) is increased by error in the data or in the model. Therefore, the expected value of the F-test statistic decreases when an error is introduced. The sum of squares deviation can be expanded to:

$$SSD = \sum\hat{C}^2 - 2\sum\hat{C}C' - 2\sum\hat{C}\epsilon + \sum C^2 + 2\sum C\epsilon + \sum\epsilon^2 \tag{5.7}$$

Taking expectations, this reduces to:

$$E[SSD] = \sum(\hat{C}-C)^2 + E[\sum\epsilon^2] \tag{5.8}$$

For additive normal or lognormal errors,

$$E[SSD] = \sum(\hat{C}-C)^2 + N\sigma_e^2 \tag{5.9}$$

This expression is the same for either the normal or lognormal errors since only second order moments are considered in the expectation of the F-test statistic. Therefore, for an additive error,

$$E[FTEST] = \frac{(N-P+1)\sum(\hat{C} - C)^2}{[\sum(\hat{C} - C)^2 + N\sigma_e^2]\,(P-1)} \tag{5.10}$$

For multiplicative normal or lognormal errors,

$$C' = C + \epsilon$$

where, $\epsilon \sim N(0, C\sigma_e^2)$ or $\epsilon \sim LN(0, C\sigma_e^2)$

$$E[SSD] = \sum(\hat{C} - C)^2 + \sigma_e^2\,\Sigma C \tag{5.11}$$

Therefore, for a multiplicative error,

$$E[FTEST] = \frac{(N-P+1)\sum(\hat{C} - C)^2}{[\sum(\hat{C} - C)^2 + \sigma_e^2\sum C]\,(P-1)} \tag{5.12}$$

With no data error and a perfect model, the F-test value equals infinity, regardless of the length of record, frequency of sampling, or number of wells. When an additive normal or lognormal error is present, the expected value of the F-test statistic is:

$$E[F\ Test_A] = \frac{SSR\ (N-P+1)}{(P-1)N\ \sigma_e^2} \tag{5.13}$$

When a multiplicative normal or lognormal error is present, the expected value of the F-test statistic is:

$$E[F\ Test_M] = \frac{SSR\ (N-P+1)}{(P-1)\sigma_e^2\ \sum C} \tag{5.14}$$

It is clear by the form of equations 5.13 and 5.14 that as the sampling frequency or number of wells is increased, the expected value of the F-test value is increased. This is because theoretically, SSR is constant for a specified period. However, it is important to note that the F-test may increase or decrease with the length of record because of the variability of SSR temporally. Therefore, increasing the sampling frequency or the density of wells sampled should increase the expected value of the F-test for a correct model, for a specified record length. Theoretically, it does not matter whether the sampling frequency or the number of wells is increased. Either one will increase the expected value of the F-test statistic by a factor of $(N+n-P+1)/(N-P+1)$, where n equals the number of additional samples. This assumes that SSR is not affected by the addition of new samples and that the samples are independent. Therefore, the selection of well locations and sampling frequency should be made so as to estimate SSR most accurately. To do this, it is necessary to select locations and sampling frequencies such that

$$(1/N)\int C^2 - [(1/N)\int C]^2 = (1/N)\sum C^2 - (\sum C)^2/N$$

Clearly an increase in data error will reduce the F-test statistic and the significance of a specified model. The difference between the additive and multiplicative error on the F-test statistic is

$$\frac{E[F\ test_A]}{E[F\ test_M]} = \frac{\sigma_M^2\ \sum C}{\sigma_A^2\ N} \tag{5.15}$$

Therefore, if the average variances are equivalent for the two errors, i.e.,

$$\sigma_A^2 = \frac{1}{N} \sigma_M^2 \sum C \qquad (5.16)$$

then the expected value of the F-test calculated will be the same, regardless of whether the error is additive or multiplicative.

For a correct model, it is also true that this increase in F-test value with an increase in sampling frequency or density of the network will be linear where

$$F_T(N+n) = F_T(N) * \left(1 + \frac{n}{N-p+1} \right) \qquad (5.17)$$

where,

$F_T(N+n)$ = F-test with N+n samples for specified record length

$F_T(N)$ = F-test with N samples for specified base record length

p = number of model parameters

5.2.1.2 Model Parameter Analysis. For a correct model, as the data size increases, the model parameter estimates should converge towards the "true" model parameter values. As shown in Chapter 4, for a zero mean error process,

$$E(\underline{\beta}) = \underline{\beta}$$

and for a nonlinear model, the variance of the parameter estimates can be approximated using a first-order approximation, as

$$VAR(\beta) = \sigma^2(\underline{X}'\underline{X})^{-1}I \qquad \text{for additive errors}$$

$$= (\underline{X}'\underline{X})^{-1}\underline{X}'(\sigma^2 I\underline{C})\underline{X}'(\underline{X}'\underline{X})^{-1} \qquad \text{for multiplicative errors}$$

where

$$\underline{X} = \underline{G} = \partial\underline{C}/\partial\underline{\beta} \qquad \text{for nonlinear models}$$

Therefore, the behavior of the model parameters should be evaluated relative to this expected behavior for a correct model. Upper and lower error bounds can be defined, assuming a normal distribution to the parameter values, using the student t-test. The error bounds are defined as:

$$\beta = \beta \pm t_{\alpha/2,n-1}\, \sigma/\sqrt{n} \qquad (5.18)$$

5.2.1.3 Residual Analyses. The correlation of residuals was evaluated to assess whether any systematic error existed, i.e., whether the errors exhibited any non-random behavior indicative of improper model selection. To assess this, the temporal lag-one and spatial lag-zero (for multi-site models) correlation of the residuals were calculated. The hypothesis of normality of the residuals was evaluated by use of the skewness test. These tests are described below.

5.2.1.3.1 Correlation of Residuals. The correlation of the residuals (RHO) is defined as

$$RHO = \frac{\sum R'_1 R'_2 - (\sum R'_1 \sum R'_2)/N}{[\sum R'^2_1 - (\sum R'_1)^2/N]^{1/2} * [\sum R'^2_2 - (\sum R'_2)^2/N]^{1/2}} \tag{5.19}$$

where,

R'_i = residual of series i = $R_i + \epsilon$

N = number of samples

R_i = $\hat{C}_i - C_i$

For the lag-one temporal correlation, series one is summed from 1 to (N-1) and series two from 2 to N, at the same well. For the lag-zero temporal correlation, R_1 and R_2 are summed from 1 to N.

The expected value of the correlation function can be approximated using a first order approximation as:

$$E[RHO] = \frac{E[\sum R'_1 R'_2] - E(\sum R'_1 \sum R'_2)/N}{E\{[\sum R'^2_1 - (\sum R'_1)^2/N]^{1/2} * [\sum R'_{22} - (\sum R'_2)^2/N]^{1/2}\}} \tag{5.20}$$

The calculation of the expected value of the residual variance (in the denominator of equation 5.20) is an extension of the Sum of Squares Deviation analysis discussed previously (pp. 52-53), in that

$$E[\sum R'^2_1 - (\sum R'_1)^2/N] = \sum R^2_1 - (\sum R_1)^2/N + N * \sigma^2_e \tag{5.21}$$

for additive normal and lognormal errors, and

$$E[\sum R'^2_1 - (\sum R'_1)^2/N] = \sum R^2_1 - (\sum R_1)^2/N + \sigma^2_e * \sum C \tag{5.22}$$

for multiplicative normal and lognormal errors.

The expected value of the covariance of the residuals (the numerator of equation 5.20 times (N-1)) is unaffected by an error in the model since the error is assumed to be uncorrelated in time and space, i.e.,

$$E[\sum R_1'R_2' - \sum R_1'\sum R_2'/N] = \sum R_1R_2 - \sum R_1\sum R_2/N \tag{5.23}$$

Therefore,

$$E[RHO] = \frac{\sum R_1R_2 - \sum R_1\sum R_2/N}{[\sum R^2_1 + \sum E(\epsilon_1^2)]^{1/2} * [\sum R^2_2 + \sum E(\epsilon_2^2)]^{1/2}} \tag{5.24}$$

The variance of the residual correlation can be approximated as:

$$VAR[RHO] = E(RHO^2) - E^2(RHO)$$

This results for an additive error in

$$VAR[RHO] = \frac{\sigma_e^2(\sum(R_1-\sum R_1/N)^2 + \sum(R_2-\sum R_2/N)^2 + (N-1)\sigma_e^2)}{[\sum R^2_1 + N\sigma_e^2] * [\sum R^2_2 + N\sigma_e^2]} \tag{5.25}$$

and for a multiplicative error

$$VAR[RHO] = \frac{\sigma_e^2 \{\sum(R_1\surd C_2 - \sum R_1\surd C_2/N)^2 + \sum(R_2\surd C_1 -}{[\sum R_1^2 + \sigma_e^2\sum C_1] * [\sum R_2^2 + \sigma_e^2\sum C_2]} \tag{5.26}$$

$$\frac{\sum R_2\surd C_1/N)^2 + \sigma_e^2\sum(C_1C_2)(1-2/N) + \sigma_e^2\sum C_1\sum C_2/N^2\}}{}$$

Theoretically, the correlation of the residuals should be zero for a correct model. This is easily seen by setting R = 0 ($R=\hat{C}-C$) in equation 5.24. In addition, for a correct model, the variance of the residual correlation is expected to be $\sigma_e^2(N-1)/N^2$ for additive errors and $\sigma_e^2\{(N-2)\sum C_1C_2/N\sum C_1\sum C_2 + 1/N^2\}$ for multiplicative errors. This shows that the variance reduces with an increase in sample size and therefore the residual correlation will converge towards zero with an increase in sample size. The hypothesis (H_o) and the alternative (H_1) to be tested are:

H_o : RHO = 0

H_1 : RHO $\neq$ 0

The significance of the correlation of the residuals can be tested for independence by the limits given by:

$$r = \frac{\pm u_{1-\frac{1}{2}\alpha} * \sqrt{N-2}}{N-1} \qquad (5.27)$$

where,

$u_{1-\frac{1}{2}\alpha}$ = the $1-\frac{1}{2}\alpha$ quantile of the standard normal distribution

N = sample size

α = the probability level ($\alpha = 0.05$ is used for all statistics in this research)

5.2.1.3.2 Skewness of Residuals. The skewness of the data was also calculated to test the assumption of normality of the residuals. The skewness coefficient (K) for the residuals is defined as:

$$K = \frac{1/N \sum(R' - \sum R'/N)^3}{[1/N \sum(R' - \sum R'/N)^2]^{3/2}} \qquad (5.28)$$

The expected value of the skewness coefficient can be approximated using a first-order Taylor series expansion. For a least squares fit ($E(\Sigma R'/N)=0$), the approximate expected value of the skewness coefficient is therefore:

$$E(K) = \frac{1/N \sum E(R'^3)}{[1/N \sum E(R'^2)]^{3/2}} \qquad (5.29)$$

where,

$$E(R'^3) = E(R^3) + 3E(R^2\epsilon) + 3E(R\epsilon^2) + E(\epsilon^3) \qquad (5.30)$$

$$E(R'^2) = E(R^2) + E(R\epsilon) + E(\epsilon^2) \qquad (5.31)$$

For a zero mean process,

$$E(R'^3) = E(R^3) + 3E(R\epsilon^2) + E(\epsilon^3) \qquad (5.32)$$

$$E(R'^2) = E(R^2) + E(\epsilon^2) \qquad (5.33)$$

Therefore, the expected value of the skewness coefficient for the four error types (AN = additive normal; MN = multiplicative normal; ALN = additive lognormal; MLN = multiplicative lognormal) considered are:

$$E(K_{AN}) = \frac{1/N\sum R^3 - 3/N^2 \sum R\sum R^2 + 2/N^3 (\sum R)^3}{[1/N \sum(R^2) - 1/N^2 (\sum R)^2 + \sigma_e^2(1-1/N)]^{3/2}} \tag{5.34}$$

$$E(_{MN}) = \frac{1/N\sum R^3 - 3/N^2\sum R\sum R^2 + 2/N^3(\sum R)^3}{[1/N \sum(R^2) - 1/N^2 (\sum R)^2 + \sigma_e^2[\sum C/N(1 - 1/N)]^{3/2}} \tag{5.35}$$

$$E(K_{ALN}) = E(K_{AN}) + \frac{\mu_3(1-3/N+2/N^2) + 3\sigma_e^2/N *}{[1/N \sum(R^2) - 1/N^2 (\sum R)^2 + \sigma_e^2(1-1/N)]^{3/2}} \tag{5.36}$$

$$\frac{(\sum RC-\sum R\sum C/N)(N-2)/N}{}$$

$$E(K_{MLN}) = E(K_{MN}) + \frac{\mu_3 (1 - 3/N + 2/N^2)}{1/N\sum(R^2) - 1/N^2(\sum R)^2 + \sigma_e^2\sum C/N(1-1/N)]^{3/2}} \tag{5.37}$$

Unlike the F-test statistic and the correlation of the residuals, the expected value of the skewness coefficient is affected by the third order moment of the error and therefore the skewness coefficient is different for normal versus lognormal errors.

For a correct model, if the error is normally distributed, the expected value of the residual skewness is zero. The skewness coefficients of the residuals for the lognormally distributed errors are dependent on the variance, skew, and the groundwater quality concentration values (in the case of multiplicative error).

The skewness coefficient for a normal variable is zero. If the series comes from a normal distribution, γ_e is asymptotically normally distributed with mean zero and variance 6/N (Snedecor and Cochran, 1967, p.86). The (1-α) probability limits on γ_e are therefore:

$$\pm\ u_{1-\frac{1}{2}\alpha} * \sqrt{6/N}. \tag{5.38}$$

5.2.2 Predictive Tests.

The ultimate test of a models applicability is its ability to accurately predict future behavior. To assess the predictive capabilities of the models, the average bias of the prediction deviations was used. The average prediction bias is defined as:

$$BIAS = (1/N) * \sum(C' - \hat{C}) \tag{5.39}$$

For a correct model, the expected bias is zero. Therefore, a systematic bias is indicative of an improper model. A negative bias indicates that the model overpredicts groundwater quality concentrations and a positive bias indicates that the model underpredicts groundwater quality concentrations. Because the average bias is a first order moment statistic, it is unaffected by the assumption of model error for a zero mean error.

The expected value of the bias is as shown

$$E(BIAS) = 1/N \sum(C - \hat{C}) \tag{5.40}$$

The variance of the bias is defined as:

$$\begin{aligned} VAR(BIAS) &= E(BIAS^2) - E^2(BIAS) \\ &= E\,[1/N \sum(C'-\hat{C})^2] - \{E[1/N \sum(C'-\hat{C})]\}^2 \\ &= 1/N \sum E(\epsilon^2) + VAR(C-\hat{C}) \end{aligned} \tag{5.41}$$

For additive normal or lognormal errors,

$$E(\epsilon^2) = \sigma^2_e$$

For multiplicative normal or lognormal errors,

$$E(\epsilon^2) = \sigma^2_e C$$

The significance of the bias can be evaluated using the student t-test where

$$t = \frac{BIAS}{\sqrt{VAR(BIAS)/N}} \tag{5.42}$$

If $t \geq t_{critical}$, then the bias is significant. For the correct model, the expected prediction bias is zero with a variance of σ_e^2/N for additive errors and $(\sigma_e^2/N)\sum C$ for multiplicative errors. That is, the variance decreases with an increase in data. Since the expected value of the bias is zero for a correct model, the expected value of the t-test would be infinity.

6. ERROR PREDICTION PROPAGATION

The groundwater quality model, selected by the model applicability analyses described in Chapter 5, is used to predict expected groundwater quality and variability in groundwater quality predictions. The expected value of the groundwater quality is the value of the deterministic model for models with independent parameters and error. The expected variability of a linear model may be calculated explicitly, whereas for a nonlinear model, the expected variability must often be approximated. The methods for calculating expected variability for these two general types of models are discussed below.

6.1 Expected Variability of Linear Models.

A linear model may be generalized as

$$\underline{Y} = \underline{X\beta} + \underline{\epsilon} \tag{6.1}$$

For a future state of interest X., we would like to predict Y. (Ŷ.) and estimate the variability of Ŷ. about Y..

$$\underline{Y}. = \underline{X}.\underline{\beta} + \underline{\epsilon}. \tag{6.2}$$

$$\hat{\underline{Y}}. = \underline{X}.\underline{\beta} = \underline{X}.\underline{\beta} + \underline{X}.(\underline{X}'\underline{X})^{-1}\underline{X}'\underline{\epsilon} \tag{6.3}$$

$$E[\hat{\underline{Y}}.] = \underline{X}.\underline{\beta} \tag{6.4}$$

$$VAR[\hat{\underline{Y}}.] = X.V_{\beta}X.' \tag{6.5}$$

where,

$$V_{\beta} = \sigma^2 I(\underline{X}'\underline{X})^{-1} \text{ for additive errors} \tag{6.6}$$

$$V_{\beta} = (\underline{X}'\underline{X})^{-1}(\underline{X}'\underline{Y}I\sigma^2\underline{X})(\underline{X}'\underline{X})^{-1} \text{ for multiplicative errors} \tag{6.7}$$

(see Chapter 4 for these derivations)

The prediction error, ζ, is defined as the difference between the observed and predicted values.

$$\underline{\zeta} = \underline{Y}. - \hat{\underline{Y}}. \tag{6.8}$$

$$E[\underline{\zeta}] = E[\underline{Y}.] - E[\hat{\underline{Y}}.] = 0 \tag{6.9}$$

$$VAR[\underline{\zeta}] = \underline{X}.V_\beta\underline{X}'. + V_y. \tag{6.10}$$

where,

$$V_y. = E[\underline{\epsilon}^*\underline{\epsilon}^{*\prime}] \tag{6.11}$$

If the model error is additive and $\underline{\epsilon}. \sim \underline{\epsilon}$, then

$$VAR(\underline{\zeta}) = \sigma^2(\underline{X}.I(\underline{X}'\underline{X})^{-1}\underline{X}. + I) \text{ for an additive error} \tag{6.12}$$

$$VAR(\underline{\zeta}) = (\underline{X}'\underline{X})^{-1}(\underline{X}'\underline{Y}I\sigma^2\underline{X})(\underline{X}'\underline{X})^{-1} + \sigma^2\underline{Y}.) \text{ for a multiplicative error} \tag{6.13}$$

6.2 Expected Variability of Nonlinear Models.

The expected variability of nonlinear models may be evaluated using prediction error propagation theory. There are three general methods used to predict error propagation for nonlinear models, namely:

1) evolution of probability density function of the system with time,

2) Monte Carlo simulations, or

3) first (or higher) order error analysis.

The evolution of the probability density function (pdf) involves the solution of a Fokker-Plank or Kolmogorov forward equation. However, the computational effort and complication of deriving a solution for a nonlinear model are formidable [Beck, 1987].

Due to this complexity, the first order error analysis will be used to estimate the first and second moments. First order error analysis was chosen over using a Monte Carlo simulation in order to have an analytical function to incorporate explicitly into the optimization of a groundwater quality monitoring network. First order error analysis is a statistical sensitivity analysis using the first order partial derivatives of the model function with respect to the model parameters. The analysis may provide inaccurate results if the errors in a system are relatively large or if significant non-linearities exist in the system. These inaccuracies can generally be overcome by using higher order error analysis.

In this method, the sources of error attributable to the initial state of the system (model selection), inputs to the model, parameters of the model, and unmeasured input disturbances or other errors are incorporated into prediction of future error.

The total prediction error is defined as:

$$\zeta(x,y,t,\underline{\beta}) = \hat{C}_*(x,y,t,\underline{\beta}) - C_*(x,y,t,\underline{\beta}) \qquad (6.14)$$

where,

ζ = prediction error

$C_*(x,y,t,\underline{\beta})$ = true state of system in future

$\hat{C}_*(x,y,t,\underline{\beta})$ = predicted state of system in future

$\underline{\beta}$ = true model parameters

$\underline{\beta}$ = predicted model parameters

If $\underline{\beta}$ is assumed to be random and not deterministic, the first and second order moments of ζ can be estimated. The variance of the error can be approximated by:

$$VAR\,[\zeta] = E\,\{[\zeta(\bar{\underline{\beta}} + \delta\underline{\beta}) - \zeta(\bar{\underline{\beta}})]^2\} \qquad (6.15)$$

where,

ζ = predicted error

$\delta\underline{\beta}$ = perturbation in $\underline{\beta}$

$\bar{\underline{\beta}}$ = deterministic model parameters

Linearization of $\zeta(\underline{\beta} + \delta\underline{\beta})$ about $\underline{\beta}$ using a taylor series expansion yields

$$VAR\,[\underline{\zeta}] = \underline{X}_* V_\beta \underline{X}'_* + V_{c*} \qquad (6.16)$$

where,

$V_{c*} = E[\underline{\epsilon}^* \underline{\epsilon}^{*\prime}]$

$\underline{X}_*$ = $\partial\underline{C}/\partial\underline{\beta}$ matrix for nonlinear functions evaluated at the predicted values

V_β = parameter variance matrix, as defined in Chapter 4 (equation 4.3 for additive errors and equation 4.4 for multiplicative errors)

For the two-dimensional advection dispersion model (equation 3.3), where the parameters and model variables are assumed independent,

$$C(x,y,t) = \{(C_o x)/[4(\pi D_L)^{1/2}]\} * \exp[(vx/2D_L)-\alpha t]$$

$$* \int_0^{t/R} \exp\{-[\lambda R - \alpha R + v^2/(4D_L)]\tau - x^2/(4D_L\tau)\}\tau^{-1.5} *$$

$$\{[\mathrm{erf}((a-y)/(2(D_T\tau)^{1/2})] + \mathrm{erf}[(a+y)/(2(D_T\tau)^{1/2}]\} \, d\tau$$

the partials of the equation with respect to the parameters can be calculated as follows:

$$\frac{\partial C}{\partial C_o} = \frac{C}{C_o} \tag{6.17}$$

$$\frac{\partial C}{\partial D_L} = C * \left(\frac{-1}{2D_L^2} - \frac{vx}{2D_L^2} \right) + \tag{6.18}$$

$$B \int A * [(v^2\tau/(4*D_L^2) + (x^2/4D_L^2\tau)] \, d\tau$$

where,

$$A = \exp\{-[\lambda R - \alpha R + v^2/(4D_L)]\tau - x^2/(4D_L\tau)\}\tau^{-1.5} * \tag{6.19}$$

$$\{[\mathrm{erf}((a-y)/(2(D_T\tau)^{1/2})] + \mathrm{erf}[(a+y)/(2(D_T\tau)^{1/2}]\}$$

$$B = \frac{C_o x}{4(\pi D_L)^{1/2}} * \exp \left(\frac{vx}{2D_L} - \alpha t \right) \tag{6.20}$$

$$\frac{\partial C}{\partial D_T} = B * \int \exp\{-[\lambda R - \alpha R + v^2/(4D_L)]\tau - x^2/(4D_L\tau)\}\tau^{-1.5} *$$

$$\{-(a-y)/(2D_T^{1.5}(\pi\tau)^{1/2}) * \exp[-(a-y)^{1/2}/(4D_T\tau)] +$$

$$-(a+y)/(2D_T^{1.5}(\pi\tau)^{1/2}) * \exp[-(a-y)^{1/2}/(4D_T\tau)]\} \, d\tau \tag{6.21}$$

$$\frac{\partial C}{\partial v} = C \left(\frac{x}{2D_L} \right) + B \int A\,[-2v\tau/(4D_L)]\, d\tau \,\} \tag{6.22}$$

$$\frac{\partial C}{\partial a} = B * \{\int \exp\{-[\lambda R - \alpha R + v^2/(4D_L)]\tau - x^2/(4D_L\tau)\}\tau^{-1.5} * $$
$$[1/(D_T\pi\tau)^{½}] * \{\exp[-(a-y)^2/(4D_T\tau)] + \exp[-(a+y)^2/(4D_T\tau)]\}\, d\tau \tag{6.23}$$

$$\frac{\partial C}{\partial R} = B * \{ \int A\,(-\lambda\tau + \alpha\tau)d\tau + A\Big|_{\tau = t/R} * (-t/R^2)\} \tag{6.24}$$

$$\frac{\partial C}{\partial \lambda} = B * \int A\,(-R\tau)\, d\tau \tag{6.25}$$

$$\frac{\partial C}{\partial \alpha} = C * (-t) + B \int A\,(R\tau)\, d\tau \,\} \tag{6.26}$$

$$\frac{\partial C}{\partial X_o} = B * \int A[2x/(4DL\tau)]d\tau + [-Bv/(2D_L) - 1/x] \int A d\tau \tag{6.27}$$

$$\frac{\partial C}{\partial Y_o} = B * \{\int \exp\{-[\lambda R - \alpha R + v^2/(4D_L)]\tau - x^2/(4D_L\tau)\}\tau^{-1.5} * $$
$$[1/(D_T\pi\tau)^{½}] * \{\exp[-(a-y)^2/(4D_T\tau)] - \exp[-(a+y)^2/(4D_T\tau)]\}\, d\tau \tag{6.28}$$

The variance of the nonlinear model parameters are calculated as described in Chapter 5, where the total model error variance, σ_e^2, is calculated as

$$\sigma_e^2 = \left(\frac{\sum (C_i - \hat{C}_i)^2}{(N - P + 1)} \right) \tag{6.29}$$

where,

N = number of observations

P = number of model parameters

7. DESIGN OF OPTIMAL GROUNDWATER MONITORING NETWORKS

The design of any monitoring network is based on the objective of maximizing information for a specified cost, or alternatively, minimizing the cost of a monitoring system for specified information goals. The quantification of the objective and information goals into an objective function and constraints in the design of a monitoring system is critical to the success of the monitoring program. The objective function and constraints used for this optimization are discussed below.

7.1 Definition of Objective Function.

For this analysis, the objective of the monitoring network is to minimize the total costs of monitoring. The basic form for this objective function is as follows:

$$\text{MIN } Z = \sum_{i=1}^{n} C_i F_i + \sum_{j=1}^{n_n} C_j$$

where,

Z = objective function

n = total number of wells monitored

n_n = number of new wells, $n_n \leq n$

F_i = sampling frequency for monitoring well i

C_j = cost of installing well j

C_i = cost of sampling and laboratory analysis for sample i

This objective function can be substantially simplified if it is assumed that the cost of installing a well is constant for all wells (C_w) and that the unit price of sample collection and laboratory analysis (C_s) is constant for all samples. A more complex objective function could accommodate more realistic costs for installation and sampling of wells; however, since this is not the focus of this research, this simplified form of the objective function will be utilized. This results in the following objective function:

$$\text{MIN } Z = C_s \sum F_i + C_w n_n$$

For systems where only existing wells will be utilized, this objective function simplifies to

$$\text{MIN } Z = \sum_{i=1}^{n} C_e F_i \quad \text{or simply}$$

$$\text{MIN } Z = \sum_{i=1}^{n} F_i$$

since C_e = a constant and does not affect the minimization

7.2 Optimization Constraints.

The focus of this research is to design monitoring networks in order to evaluate the effectiveness of remedial actions, that is, to design networks that will verify whether expected conditions, developed based on existing information, are or are not occurring. At a particular point in space and time, these future conditions can be expressed in a number of ways, including:

1) expected value,
2) expected variance,
3) expected coefficient of variation, or
4) expected correlation.

The future conditions can be in reference to either concentrations or errors in predicted concentrations. The expected value of the groundwater quality does not incorporate information on the expected variability of the system. In addition, the expected value of the concentration error is zero for a correct model. Therefore, the expected value will not be used as a means of evaluating an information goal for the design of a monitoring network.

The definition of the monitoring network involves the definition of the sampling frequency and the spatial density of the wells. The selection of the sampling frequency and well locations is based on constraints applied to the objective function. Constraints used for the frequency and well location selection are discussed below.

7.2.1 Sampling Frequency.

The frequency of sampling required at a particular location depends on the expected behavior of groundwater quality. Specifically, we are interested in the expected confidence we have in a prediction at a particular time in the future. This can be expressed as either a variance, coefficient of variation, or correlation, relative to either a future concentration or a future concentration error. These functions are all dependent on the frequency of sampling, which is a decision variable in the monitoring network design problem. Any of these measures could be appropriate depending on the representation of goals for the monitoring network system. For this study, however, the expected variance of prediction error was selected to constrain the sampling frequency. This statistic incorporates information on the model structure and model uncertainty into the monitoring network design process.

As shown in Chapter 6, equation 6.10, if we assume a model with stochastic model parameters, the variance of the prediction error can be expressed as

$$VAR[\zeta] = X.V_{\beta}X'. \; + \; V_{c}. \tag{7.1}$$

7.2.2 Sampling Locations.

Groundwater quality at different sampling locations varies in expected behavior. The relationship between locations can be expressed as a spatial correlation. The correlation of the predicted error concentration was used to restrict the spatial density of the monitoring network. This function can be expressed as:

$$CORR(\zeta^*_1,\zeta^*_2) = \frac{COV(\zeta^*_1,\zeta^*_2)}{[VAR(\zeta^*_1)\;VAR(\zeta^*_2)]^{1/2}} \tag{7.2}$$

where,

$$\begin{aligned} COV(\zeta^*_1,\zeta^*_2) &= E[(\bar{\zeta}^*_1 - \zeta^*_1)(\bar{\zeta}^*_2 - \zeta^*_2)] \\ &= E(\zeta^*_1\;\zeta^*_2) \\ &= E[(X^*_1(X'X)^{-1}X'\epsilon)((X^*_2(X'X)^{-1}X'\epsilon)'] \\ &= X^*_1V_{\beta}X^{*\prime}_2 \end{aligned} \tag{7.3}$$

7.3 Optimization Procedure.

The optimization of the monitoring network needs to incorporate both the spatial location and temporal frequency constraints described above. For a specified number of potential sampling locations and sampling frequencies, a branch and bound optimization technique can be utilized to meet this objective. This technique is summarized below and applied to an example problem for illustration purposes.

7.3.1 Branch and Bound Optimization Technique.

The optimization of a groundwater quality monitoring network can be made by using a modified branch and bound technique where the objective function (Z_i) is expressed as:

$$MIN\ Z_i = \sum_{i=1}^{n} VAR(I) * VL(I)$$

where,

n	=	number of wells
i	=	index on well number
VAR(I)	=	predicted variance at well i for sampling frequency F_i
VL(I)	=	binary variable indicating whether well is or is not being sampled; 1 = sampled, 0 = not sampled

The objective function minimizes the number of wells sampled for a specified sampling frequency. The wells are selected based on the following constraint:

$$CORR(I,J) \geq CORRMIN\ \forall\ J = 1,N \text{ and at least one } I \text{ where } VL(I) = 1$$

where,

CORR(I,J) = predicted correlation between wells i and j

CORRMIN = user specified minimum correlation

This form of the objective function imbeds the sampling frequency constraint. In addition, it requires that all possible well locations be specified. It is not required that these well locations have been sampled in the past. Therefore, a different combination of wells could be identified as optimal for each sampling frequency, minimum spatial correlation, and potential monitoring network chosen. The networks resulting from different sampling frequency selection can then be compared and an optimal network selected from among those frequencies and potential wells considered.

In the branch and bound optimization technique, all wells to be considered in the network need to be specified. The branch and bound method employs an enumeration technique which can be applied to integer programming problems. This technique partitions the set of all feasible solutions into subsets. For each subset, a lower bound is calculated for the objective function of the solutions within that subset. If the lower bound in that subset exceeds the current "best objective function", it is excluded from further consideration. An excluded subset is said to be fathomed. This partitioning and fathoming continues until an optimal feasible solution is found. This process is summarized below in four principle steps:

Initialization Step: Begin with entire set of solutions (equivalent to sampling all wells) and apply bound and fathom to the entire set. Calculate an upper bound on the solution Z_u.

Branch Step: Use some branch rule to select one of the remaining subsets (a feasible solution) and partition it

Bound Step: Calculate a lower bound Z_l for the feasible solutions in the subset

Fathom Step: For each subset, compare Z_l to Z_u, exclude it from further consideration if

1) $Z_l > Z_u$; or
2) Subset is an infeasible solution

If $Z_l < Z_u$, then reset $Z_u = Z_l$ and store this as the incumbent solution

Stopping Rule: Stop when there are no remaining unfathomed subsets

For the design of a monitoring network, $Z_l = \sum VAR(I) * VL(I)$. The set is feasible if there exist at least one $CORR(I,J) \geq CORRMIN$ for $VL(J) = 1 \ \forall I \neq J$, when $VL(I) = 0$.

A brief example is shown below to illustrate the application of the branch and bound technique to a monitoring network design.

7.3.2 Example Application of Branch and Bound Technique to a Monitoring Network Design.

Five wells are located on a site. For a specified sampling frequency of 30 days, the prediction error variance for these five wells is:

Location	Prediction Error Variance
MW-1	0.15
MW-2	0.4
MW-3	0.3
MW-4	0.1
MW-5	0.25

The correlation between the predicted concentration errors at these five wells is:

	MW-1	MW-2	MW-3	MW-4	MW-5
MW-1	1.0	0.8	0.85	0.7	0.5
MW-2	0.8	1.0	0.85	0.8	0.55
MW-3	0.85	0.85	1.0	0.9	0.9
MW-4	0.7	0.8	0.9	1.0	0.95
MW-5	0.5	0.55	0.9	0.95	1.0

For a desired minimum correlation of 0.85 for all wells (CORRMIN = 0.85), the following steps outline the branch and bound optimization technique for this data set.

1) Select a subset equal to all wells being sampled

$$Z_u = \sum_{i=1}^{n} VAR(I) * VL(I) = 1.20$$

$$VL(I) = 1 \quad \forall \quad I = 1,..,5$$

2) Apply a Branch Step: delete all wells in order from 1 to n

First Branch (delete Well Number 1, lower branch):

1-5

1/2-5[1] (Z_{lm} = 0.2)

2-5

First Bound Step:

- lower branch is feasible since CORR(1,J)*VL(J) ≥ CORRMIN for J=3; therefore, set VL(1) = 0 and proceed with lower branch

- upper branch is feasible; hold in reserve with Z_{lm} = 0.2 (Z_{lm} equals the minimum lower bound where $Z_{lm} = \sum VAR$ for all solutions where i = all wells denoted to the left of the slash)

Second Branch:

2-5

2/3-5 (Z_{lm} = 0.4)

3-5

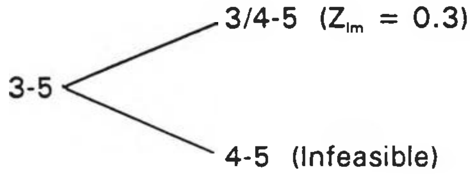
Second Bound:

- lower branch is feasible since CORR(2,J)*VL(J) ≥ CORRMIN for J=3; therefore continue with lower branch and set VL(2) = 0

[1] A/B: "A" signifies that these wells are to be sampled; "B" wells are not yet specified

- upper branch is feasible; hold in reserve with $Z_{lm} = 0.4$

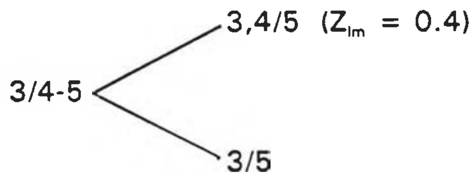
Third Branch:



Third Bound:

- lower branch is infeasible since CORR(3,J)*VL(J) < CORRMIN for J=4 and J=5; therefore proceed with upper branch

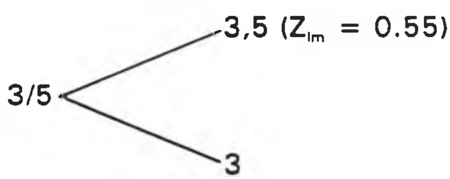
Fourth Branch:



Fourth Bound:

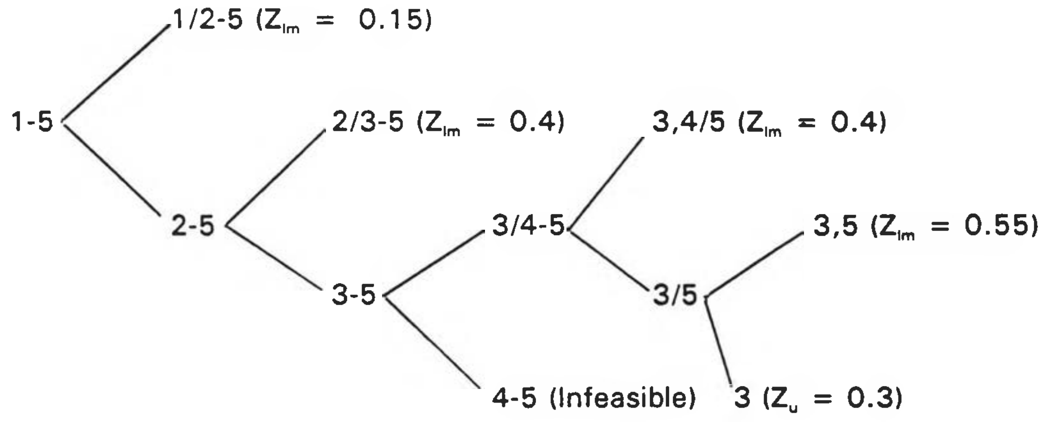
- Lower branch is feasible; therefore proceed with lower branch
- upper branch is feasible; hold in reserve with $Z_{lm} = 0.4$

Fifth Branch:



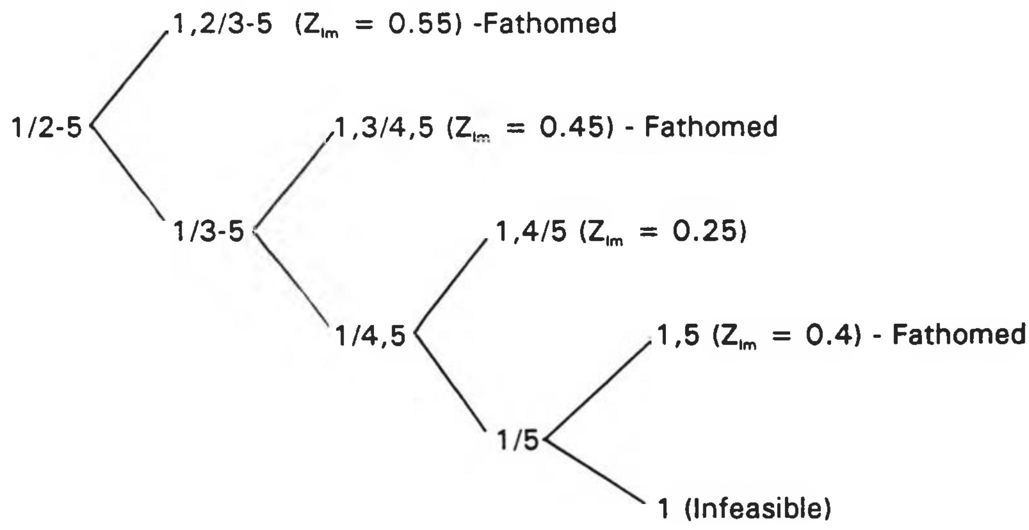
- lower branch is feasible and $Z_l = 0.3$; therefore revise $Z_u = 0.3$ and set VL(I) = 0,0,1,0,0 to the incumbent solution
- upper branch is feasible; hold in reserve with $Z_{lm} = 0.4$

At the completion of this first branch and bound procedure, the following set of fathomed subsets exists:



3) Proceed backward through branches and check for any $Z_{lm} < Z_u$. If Z_{lm} is less then Z_u, than fathom that subset of the data.

In the second, third, fourth,and fifth branches Z_{lm} > Zu. In the first branch, Z_{lm} =0.15; therefore, proceed to the first branch and branch and bound as follows:



On the last branch the lower branch is infeasible. The only upper branch which is feasible and not fathomed is VL(I)=1,0,0,1,0. Therefore, proceed to this branch and continue branching as follows:

$$
\text{1,4/5} \begin{cases} \text{1,4,5 } (Z_l = 0.5) \\ \text{1,4 } (Z_l = 0.25) \end{cases}
$$

The lower branch is feasible and $Z_l < Z_u$, therefore set $Z_u = 0.25$ and VL(I) = 1,0,0,1,0 as the incumbent solution. At this point, all possible subsets have been fathomed and the optimal solution is to sample MW-1 and MW-4. The objective function value for this optimal solution is 0.25.

This branch and bound optimization technique was used to evaluate monitoring network designs for this study. A Fortran 77 computer code, BB.FOR was developed and used for these analyses. A copy of this code is included in Appendix C.

7.4 Evaluation of Optimal Monitoring Network.

Application of this branch and bound optimization to the design of groundwater quality monitoring networks results in the identification of monitoring wells for a specified sampling frequency which minimizes the prediction error variance at sampled wells and insures a minimum spatial error correlation between sampled and non-sampled wells. Sampling at the optimal monitoring network reduces the prediction error variance at non-sampled well locations. This prediction error variance surface can be used to evaluate the uncertainty in the understanding of the system and the locations of the optimal sampling locations relative to the uncertainty surface.

The prediction error variance surface can be expressed as

$$VAR(\zeta) = X.V_\beta X.' + V_y.$$

The reduced error variance surface using the optimal monitoring network can be expressed as

$$VAR(\zeta_N) = X.V_{\beta N} X.' + v_Y.$$

where

$$V_\beta = (X_k X_k')^{-1} \sigma^2 I$$

$$V_{\beta N} = (X_{k+i} X_{k+i}')^{-1} \sigma^2 I$$

k = sampling points in existing monitoring network

i = sampling points in optimal monitoring network

8. SIMULATION STUDY

A simulation study was performed as a basis for the development of a groundwater quality monitoring network design protocol. The methods used in the development of the groundwater monitoring network protocol have been discussed in Chapters four through seven. Specifically, the simulated groundwater quality data was fit to groundwater quality models (Chapter 4) and the applicability of the models was evaluated (Chapter 5). The prediction error was propagated (Chapter 6) and based on these errors, monitoring networks were designed (Chapter 7).

This chapter discusses the results of the simulation study. Evaluation of model applicability is discussed in Section 8.1. The design of the monitoring network based on this evaluation is discussed in Section 8.2.

8.1 Model Applicability.

Models with incorrect structure are used to evaluate the ability of the statistical model applicability tests to identify incorrect models. The correct physical model used to generate the simulated data is used as a basis of comparison. The effect of different types and magnitudes of error on the model applicability tests is evaluated based on the inclusion of additive and multiplicative normal and lognormal data errors in the simulated data.

The two classes of incorrect model structures which are examined relative to the correct model structure are the multi-site polynomial (trend surface) models, and the single-site polynomial models. In addition, the physical model applied to individual wells is used as an additional basis of comparing single-site to multi-site models. Linear, quadratic, and cubic polynomials were considered for the polynomial single-site and trend surface models. The detailed results of the model applicability tests applied to these models are included as Appendix G. General conclusions regarding the ability of the statistical tests to identify incorrect models are discussed herein. However, in this chapter, detailed results are only included for the linear trend surface model.

For the multi-site models (trend surface and multi-site physical), the models were fit to data from different combination of sampling locations, specifically to wells at 40 meter intervals (50 wells), wells at 80 meter intervals (15 wells), and wells at 120 (direction parallel to flow) by 80 meter (direction perpendicular to flow) intervals (9 wells). For all models evaluated, sampling frequencies of biweekly (24 samples/year), monthly (12 samples/year), bimonthly (6 samples/year), quarterly (4 samples/year), triannual (3 samples/year) and biannual (2 samples/year) were considered with record lengths ranging from two to ten years.

To perform the model applicability analyses described in Chapter 5, the following computer codes were written:

1) SWT - fits and evaluates goodness-of-fit and predictive test statistics for single-site polynomial models

2) AWT - fits and evaluates goodness-of-fit and predictive test statistics for trend surface models

A copy of each of these programs is included in Appendix B. Each of the models considered was evaluated for model applicability via goodness-of-fit tests and predictive tests, as discussed below in Sections 8.1.1 and 8.1.2, respectively.

8.1.1 Goodness-of-fit Tests.

As discussed in Chapter 5, to evaluate the goodness-of-fit of the models, analysis of variance, analysis of model parameter behavior, and analysis of residuals were used, as described below.

8.1.1.1 Analysis of Variance. An analysis of variance (ANOVA) was used as a measure of testing the applicability of a model for describing the observed behavior in a specific data set. As discussed in Chapter 5, the ANOVA tests whether the variance about the model is different than the variance in the observations. The F-test is used to test the equality of the variances. Using least squares regression (as discussed in Chapter 4), the statistical models were fit to the simulated data.

For a correct model with no error, the expected value of the F-test statistic equals infinity. With data error present, the expected value of the F-test can be evaluated from a non-distributional approach where $\epsilon \sim N(0,\sigma_{er}^2)$ and

$$\sigma_{er}^2 = \sigma_{ea}^2 \text{ for additive errors, and}$$

$$\sigma_{er}^2 = \sigma_{em}^2 \sum C/N \text{ for multiplicative errors.}$$

An error coefficient of variation can be defined as

$$CV_e = \frac{\sigma_r}{C} \tag{8.1}$$

where the error coefficient of variation (CV_e) is a dimensionless parameter. Substituting equation 8.1 into either equation 5.10 or equation 5.12 results in the following expression for the expected value of the F-test statistic:

$$E[F\text{-test}] = \frac{(N-P+1)\sum(\hat{C}_o - C)^2}{(P-1)\, CV_e^2\, (1/N)(\sum C)^2} \tag{8.2}$$

This relationship can be used to calculate the maximum error coefficient of variation allowable for identification of the correct physical model using the F-test analysis. Figures 8.1 and 8.2 illustrate this relationship. Clearly, as the data set increases in size (either due to an increase in sampling frequency or sampling density), a higher error coefficient of variation is allowable for detection of the correct physical model. For example, for an error coefficient of variation of 10.0, the correct physical model would be correctly identified using the F-test with the following approximate sampling density, record length, and sampling frequency combinations:

Number of Wells	Record Length (Years)	Sampling Frequency	Total Number of Samples
50	<2	Biweekly/Monthly	<1200
50	4.5	Bimonthly	1350
50	6.6	Quarterly	1300
50	7.8	Triannual	1150
50	9.5	Biannual	950
15	5	Monthly	900
9	8	Monthly	850

For this example, the least number of samples required in order to detect that the physical model is significant using the F-test analysis is associated with the monitoring network of 9 wells sampled monthly for 8 years. This however is probably not an unacceptable solution due to the length of record required. Therefore, a denser network would facilitate the early identification of the correct model.

In general, for this example, a fairly high relative error needs to be present in the data before the correct model is misidentified. It must be emphasized that this identification is based on the change in the system over the period of interest relative to the sampling locations and sampling frequency. Since the expected value of the F-test statistic is increased by an increase in SSR, the F-test will be maximized by collecting samples where the expected groundwater quality will maximize $\sum(\hat{C} - C)^2$. This means that samples should be collected spatially covering the entire zone of contamination with location and lengths of record chosen such that $\sum C = \int C$. In addition, due to the non-stationary nature of the plume, this means that the optimal network is dependent on the period of interest and the expected plume distribution for that period. Therefore, significantly more information can be obtained from 9 wells spaced uniformly across a plume than 9 wells clustered at the center of mass of the plume or at the plume boundaries.

The expected value of the F-test statistic is increased for an incorrect model relative to the correct model. The sum of squares deviation (SSD) is the sum of squared deviations between the predicted concentrations and the observed concentrations.

$$E[SSD] = \sum (\hat{C} - C')^2 \tag{8.3}$$

For an incorrect model,

$$\hat{C} = C'' + C$$

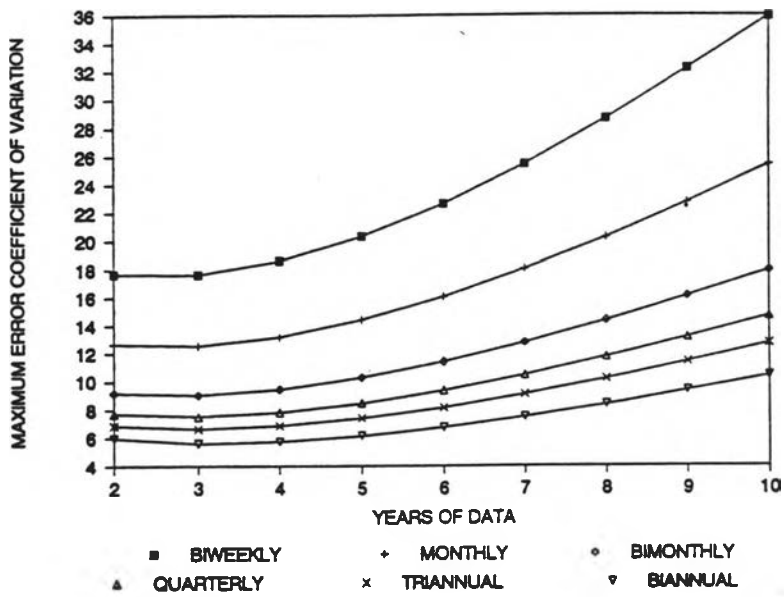


Figure 8.1 Maximum Error Coefficient of Variation for Detection of Correct Physical Model Fit to 50 Wells Based on Expected Value of F-test

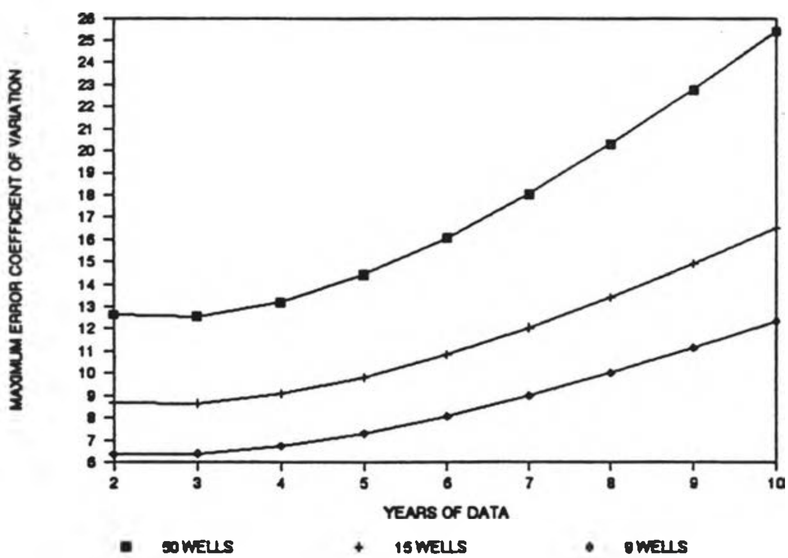


Figure 8.2 Maximum Error Coefficient of Variation for Detection of Correct Physical Model Fit to Monthly Data Based on Expected Value of F-test

$$C' = C + \epsilon$$

where $C'' \neq 0$

Therefore, for an incorrect model,

$$E[SSD] = E(C'')^2 + E(\epsilon^2) \tag{8.4}$$

For a correct model,

$$E[SSD] = E(\epsilon^2) \tag{8.5}$$

For a correct model with incorrect parameters, C" should converge towards zero, thereby reducing the SSD toward the minimum variance. However, for an incorrect model structure, C" will not converge towards zero. The behavior of the expected value of the squared model error deviations ($E[C''^2]$) with time depends on the particular correct and incorrect models, but should increase with time and therefore decrease the F-test statistic.

Using a linear trend surface model as an example of an incorrect model structure, Table 8.1 summarizes the F-test results for the linear trend surface model fit to the simulated data with no error from monitoring networks of 50, 15, and 9 wells. The F-test did consistently increase with an increase in the sampling frequency and with an increase in monitoring well density, as illustrated by Figure 8.3 for the linear

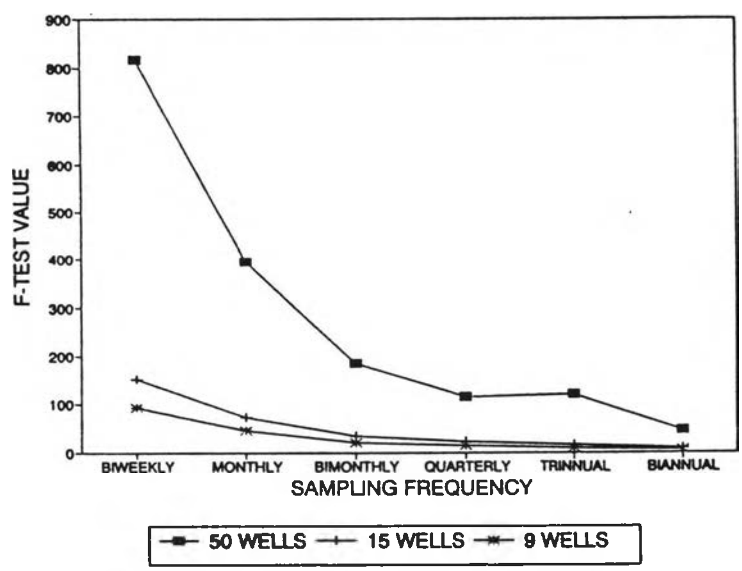


Figure 8.3 F-test Results for Linear Trend Surface Model Fit to Deterministic Data

Table 8.1 F-Test Results for Linear Trend Surface Model Fit to Deterministic Data

50 WELLS

YEARS[a]	BIWEEKLY	MONTHLY	BIMONTHLY	QUARTERLY	TRIANNUAL	BIANNUAL
2	237.0454	121.3795	63.4433	44.1031	34.4234	24.7543
3	186.4653	97.2285	53.2172	38.6155	47.1998	24.6710
4	86.8890	46.6866	26.8211	20.4377	26.1658	14.8956
5	21.1426	11.5033	6.9460	5.6707	7.8457	5.2188
6	29.6961	12.9760	4.8659	2.4056	2.0527	0.7367
7	123.2865	56.7892	23.7799	13.0277	11.7660	3.0611
8	295.9511	140.1669	62.5117	36.8807	36.3940	12.0546
9	533.2402	229.2628	117.6888	71.8188	73.6320	26.7778
10	817.1028	395.5283	184.9554	115.0046	120.677	45.9400

15 WELLS

YEARS[a]	BIWEEKLY	MONTHLY	BIMONTHLY	QUARTERLY	TRIANNUAL	BIANNUAL
2	52.87393	26.82855	13.78474	9.38431	7.153795	4.903283
3	46.6837	24.11769	12.84187	9.073751	7.193333	5.343843
4	27.07912	14.2198	7.8236	5.714241	4.679226	3.706742
5	11.08819	5.831526	3.255012	2.430925	2.046879	1.73109
6	8.59423	4.056823	1.853165	1.158906	0.8396	0.583559
7	22.95242	10.66826	4.604502	2.61844	1.651004	0.744104
8	53.49017	25.38204	11.4196	6.794122	4.497849	2.260843
9	97.4891	46.8739	21.66992	13.28204	9.099033	4.970928
10	151.4847	73.43607	34.52096	21.54774	15.06208	8.622322

9 WELLS

YEARS[a]	BIWEEKLY	MONTHLY	BIMONTHLY	QUARTERLY	TRIANNUAL	BIANNUAL
2	34.36651	18.42738	8.935874	6.089182	4.642464	3.130548
3	30.16461	15.60672	8.329202	5.900434	4.680270	3.442648
4	16.75223	8.84826	4.915828	3.617918	2.976714	2.351949
5	5.735729	3.083971	1.790124	1.382794	1.196938	1.042505
6	3.601407	1.672295	0.746088	0.474950	0.361014	0.283329
7	12.43817	5.719257	2.403223	1.347696	0.843851	0.372598
8	31.76589	15.01169	6.688004	3.974208	2.643599	1.335245
9	59.81982	28.69895	13.19793	8.106728	5.584185	3.068868
10	94.30384	45.63411	21.37276	13.36707	9.383489	5.404370

(a) Record Length for Model Fit

trend surface model fit to ten years of data. As for the correct model, it is true that as the sampling frequency or the number of wells increased, that the linear trend surface model becomes more significant. This behavior was not observed for the quadratic and cubic order trend surface models nor for the single-site polynomial models, as summarized in Appendix G. This non-consistent trend in the F-test for the quadratic and cubic trend surface models is indicative of an improper model fit.

The model significance evaluations discussed above were based on fitting the statistical models to errorless data. The effect of data error on model significance is illustrated by Figure 8.4 for a linear trend surface model fit to simulated data from 50 wells. This figure illustrates that the maximum allowable relative error (expressed as an error coefficient of variation) in the data increases with an increase in the sampling frequency. Excluding the six year record length, the linear model

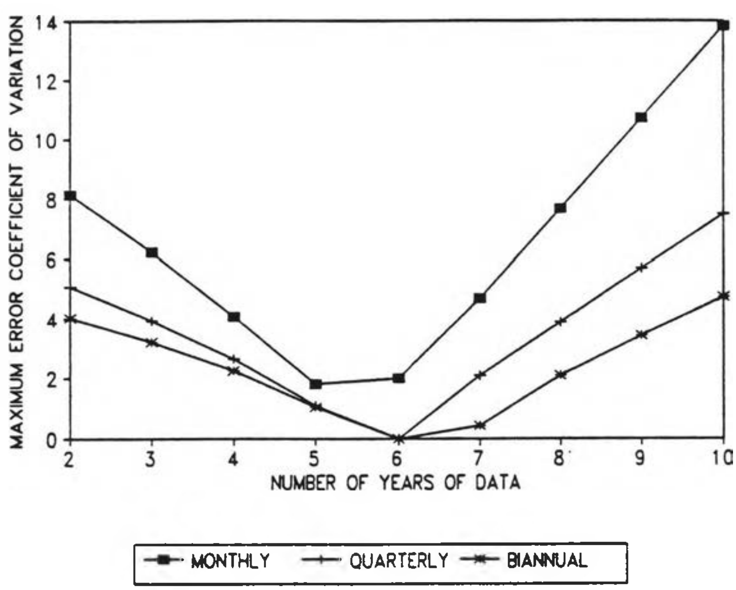


Figure 8.4 Maximum Error Coefficient of Variation for Detection of Significant Linear Trend Surface Model Fit to Data from 50 Wells Based on Expected Value of F-test

was significant for all sampling frequencies and record lengths considered with error coefficients of variation less than 1.0. Comparison of Figure 8.4 to Figure 8.1 (page 87) illustrates the increase in allowable error for the detection of a correct physical model relative to the incorrect linear trend surface model.

To evaluate the trend in the F-test statistic relative to the theoretical linear increase in the F-test statistic for a correct model (as discussed in Chapter 5), the F-test values were fit to linear models with the independent variable being the number of additional samples (n) and the dependent variable being the calculated F-test values. The slope of the calculated linear trend β was compared to the theoretical slope, β, of $F_T(N)/(N-p+1)$. The t-test statistic was used to evaluate whether the slope of the calculated linear trend was significantly different than the theoretical slope for a correct model where t = (β- β)/(√VAR(β)/N).

These t-test statistics are summarized for the exemplary linear trend surface model in Table 8.2 for well densities of 50, 15, and 9 wells and record lengths ranging from two to 10 years of data. For the linear
trend surface models, the only two t-test statistics which were significant were for record lengths of three years with network densities of 15 and 9 wells. The inclusion of data error would reduce the significance of these tests. Therefore, it appears that this test is insensitive to an incorrect model structure. The insensitivity of this test to detecting an incorrect model structure was also evident for the quadratic and cubic trend surface models, as summarized in Appendix G.

Table 8.2 T-Test Statistics[a] on Linear Trend in F-Test Statistics for Linear Trend Surface Model Applied to Deterministic Data

	SAMPLING DENSITY (NUMBER OF WELLS)			
YEARS[b]	50	15	9	ALL[c]
2	-1.07216	-0.47156	-0.08290	0.00289
3	-0.01299	-4.44597	-4.16507	-0.00958
4	-0.01418	-0.56459	-1.55558	-0.01711
5	-0.01503	-0.18303	-0.36520	-0.02557
6	0.01301	0.02225	0.00535	0.00674
7	0.01540	0.17540	0.19091	0.01409
8	0.00788	0.31185	0.29278	0.01045
9	0.00288	0.44889	0.35122	0.00751
10	0.00326	0.69374	0.38370	0.00648

(a) t-test statistics significant at $\alpha = 0.05$ confidence level are highlighted

(b) Record Length for Model Fit

(c) F-tests from all combination of well densities

In summary, the F-test can be used to help identify a correct model. The F-test should be applied to subsets of the available data, both in frequency of sampling and number of wells. For a correct model, an increase in either the sampling frequency or network density should result in an increase in the F-test statistic, with the increase proportional to the increase in the number of samples. In addition, the correct model will continue to be significant under conditions of higher data error.

8.1.1.2 Model Parameter Analysis. The behavior of the estimated model parameters was evaluated using confidence limit bounds about the mean parameter values as defined in Chapter 5, where

$$\beta = \beta \pm t_{\alpha/2,n-1}\sqrt{(VAR_\beta/n)} \tag{8.6}$$

For the correct model structure, the variance of the parameter estimates decreases with an increase in the record length, sampling frequency, or sampling density. This results in a convergence of the parameter estimates towards the true parameter values.

As discussed in Chapter 4, using a least squares regression to fit the correct model to the simulated data will result in the expected value of the parameter estimates being equal to the true parameter values for all types of zero mean errors. In addition, the variance of the parameter estimate decreases with an increase in data size or a reduction in data error.

For an incorrect model structure, the parameter estimates do not necessarily converge towards a single value, but vary with the record length and sampling frequency. Figure 8.5 illustrates the variability of parameters A, B, C and D for the linear trend surface model fit to the simulated data with no superimposed error. As illustrated by this figure, the parameter estimates do not fall within a specified confidence interval which decreases with sample size as do the parameter values

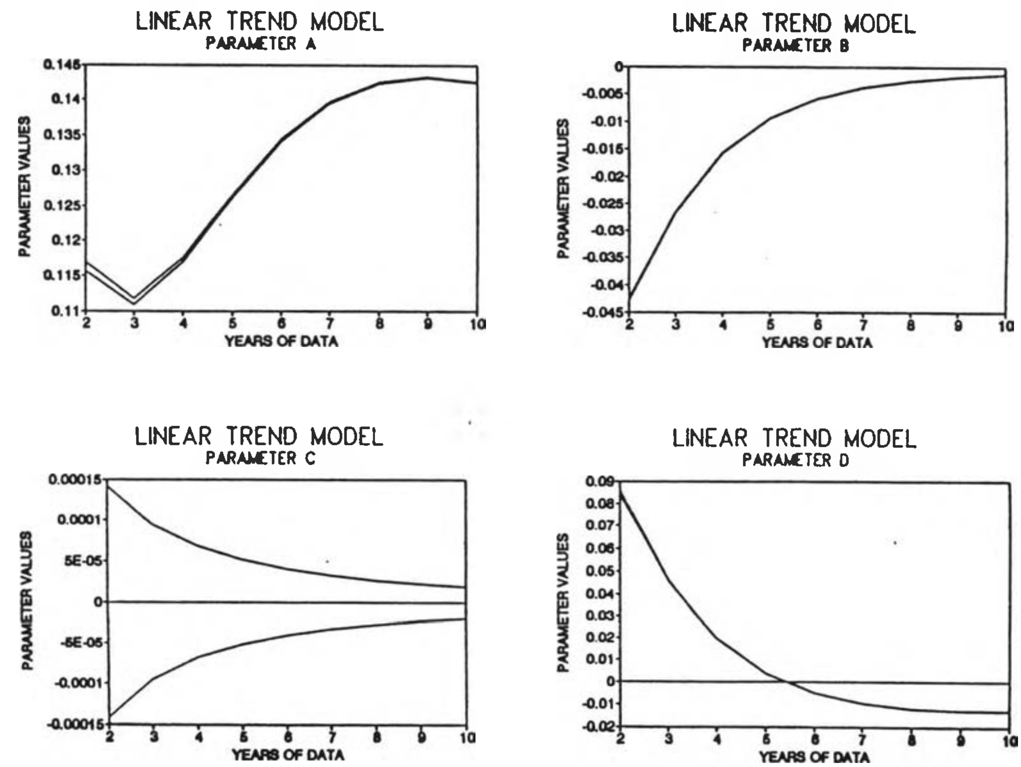


Figure 8.5 Upper and Lower 95% Confidence Limits on Parameter Estimates for Linear Trend Surface Model Fit to Deterministic Data

for a correct model. This parameter behavior was also exhibited by the quadratic and cubic trend surface models, as summarized in Appendix G.

The effect of error on the parameter behavior can be evaluated using the estimate for the parameter variance. For an additive error,

$$VAR(\beta) = \sigma^2 (X'X)^{-1} I$$

where

$$\sigma^2 = \sigma_m^2 + \sigma_e^2$$

σ_m^2 = model error

σ_e^2 = data error

Figure 8.6 illustrate the increase in the upper and lower 95% confidence limits on the parameter estimate A for a linear trend surface model fit to the simulated data with error coefficients of variation of 1.0 and 10.0. Clearly, the ability to detect an incorrect model is reduced with shorter record lengths. However, as the length of the record increases, the behavior of the parameter estimates still indicates an incorrect model, even with significant data error. Therefore, this parameter behavior test appears to be robust and a good method of evaluating model applicability.

8.1.1.3 Residual Analyses. Systematic error in the residuals indicates an improper model fit. Correlation of the residuals was used to assess non-random behavior and skewness of the residuals was used to test the distribution of the data errors, as discussed below.

The correlation of the residuals, RHO, can be used to identify non-random behavior. The expected value of the residual correlation for a correct model is zero, with the variance decreasing with an increase in data size. For an incorrect model, the expected value of the residual correlation is not zero and should be greater than for a correct model. The value of RHO will depend on the behavior of the correct model relative to the incorrect model.

For a linear trend surface model fit to the simulated data with no error present, Table 8.3 summarizes the average lag-one temporal and lag-zero spatial residual correlations. As the sampling frequency and record length increase, the temporal residual correlation increases. There is however no observable correlation between the average spatial residual correlation and either the record length or the sampling frequency. However, the spatial correlation was generally high where the record length and the sampling frequency were relatively high. The residual correlations significant at the 5% confidence limit are highlighted on Table 8.3. Clearly, when no data error is present, the detection of an incorrect model is easily identified using the residual correlations.

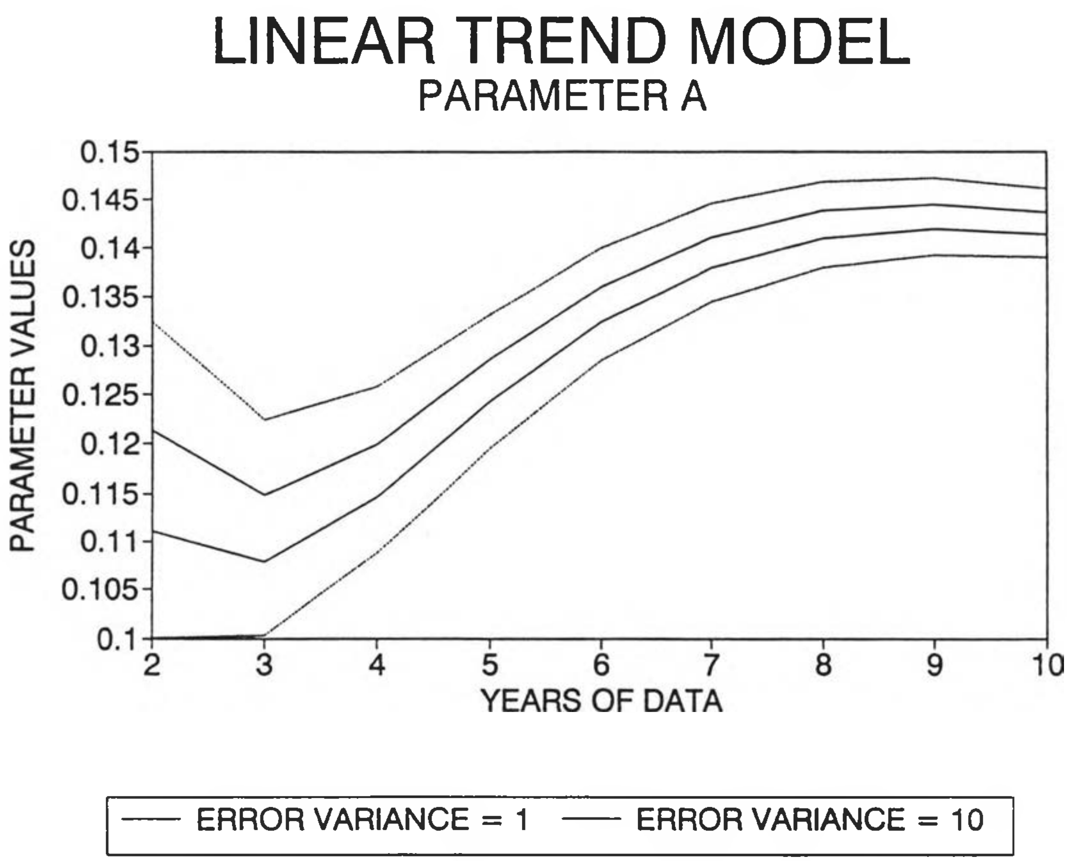


Figure 8.6 Upper and Lower 95% Confidence Limits on Parameter Estimate A For Linear Trend Surface Model Fit to Stochastic Data

The introduction of error to the simulated data greatly reduces the correlation of the residuals. The average temporal and spatial residual correlations are plotted against the error coefficient of variation in Figures 8.7 and 8.8, respectively. These two figures illustrate that, in general, if the error coefficient of variation is greater than 1.0, no significant residual correlation will be detected for a monitoring network of 50 wells sampled monthly fit to a linear trend model. However, despite the insignificant correlation of the residuals when data error is present, evaluation of trends in the residuals can often still be useful in identifying an appropriate model structure.

The skewness of the residuals is assessed to determine whether the error is normally distributed. For a correct model, if the error is normally distributed, the expected value of the residual skewness is zero. The skewness coefficients of the residuals for lognormally distributed errors are dependent on the variance, skew, and, for a multiplicative data error, the groundwater quality concentration values.

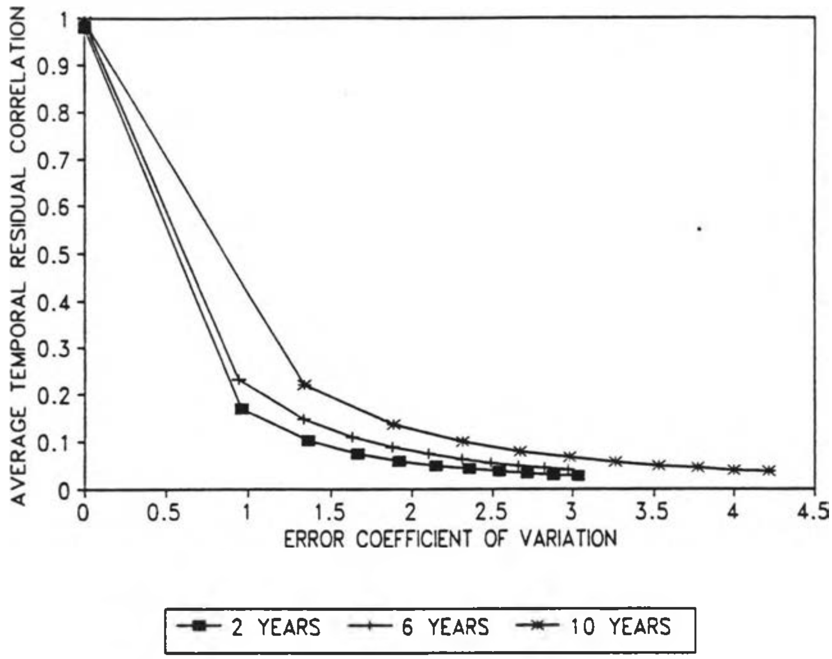


Figure 8.7 Effect of Error Coefficient of Variation on Average Temporal Residual Correlation from Linear Trend Surface Models Fit to Monthly Data at 50 Wells

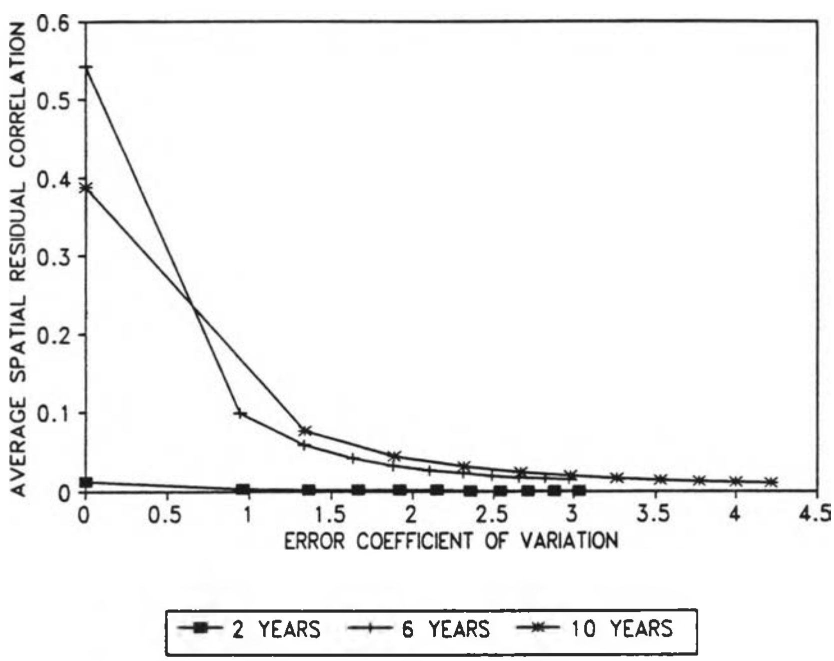


Figure 8.8 Effect of Error Coefficient of Variation on Average Spatial Residual Correlation for Linear Trend Surface Models Fit to Monthly Data at 50 Wells

Table 8.3 Average Residual Temporal and Spatial Correlations[a] for Linear Trend Surface Model Fit to Deterministic Data from 50 Wells

RESIDUAL TEMPORAL CORRELATION

	SAMPLING FREQUENCY					
YEARS[b]	BIWEEKLY	MONTHLY	BIMONTHLY	QUARTERLY	TRIANNUAL	BIANNUAL
2	.9948	.9794	.9191	.8244	.7009	.4053
3	.9967	.9870	.9505	.8947	.8225	.6371
4	.9973	.9894	.9582	.9076	.8384	.6538
5	.9978	.9912	.9663	.9274	.8764	.7432
6	.9982	.9928	.9719	.9382	.8910	.7635
7	.9983	.9934	.9747	.9462	.9096	.8152
8	.9983	.9935	.9754	.9481	.9141	.8309
9	.9983	.9936	.9757	.9489	.9158	.8369
10	.9984	.9937	.9762	.9498	.9173	.8405

RESIDUAL SPATIAL CORRELATION

	SAMPLING FREQUENCY					
YEARS[b]	BIWEEKLY	MONTHLY	BIMONTHLY	QUARTERLY	TRIANNUAL	BIANNUAL
2	.0120	.0119	.0131	.0157	.0193	.0287
3	.1530	.1461	.1325	.1193	.1065	.0820
4	.3747	.3715	.3637	.3539	.3418	.3112
5	.5245	.5199	.5131	.5180	.5037	.4951
6	.5285	.5424	.5710	.6016	.6349	.6505
7	.4679	.4790	.5013	.5240	.5470	.5949
8	.4282	.4383	.4582	.4781	.4979	.5379
9	.3995	.4088	.4511	.4453	.4634	.4994
10	.3786	.3872	.4041	.4280	.4375	.4707

(a) correlations significant at the $\alpha = 0.05$ confidence level are highlighted

(b) Record Length for Model Fit

For an incorrect model structure, the expected value of the residual does not equal zero and therefore the expected value of the skew will be greater than for a correct model. The skewness of the residuals for a linear trend surface model fit to the simulated data without any superimposed error is summarized in Table 8.4. The residual skewness coefficients were significant for approximately one-half of the data subsets evaluated. These significant skewness coefficients are indicative of an incorrect model structure.

Table 8.4 Average Residual Skewness[a] for Linear Trend Surface Model fit to Deterministic Data from 50 Wells

YEARS[b]	SAMPLING FREQUENCY					
	BIWEEKLY	MONTHLY	BIMONTHLY	QUARTERLY	TRIANNUAL	BIANNUAL
2	.0619	.0666	.0785	.0897	.0976	.1018
3	.0110	.0161	.0267	.0373	.0469	.0611
4	-.0550	-.0475	-.0314	-.0147	.0021	.0345
5	-.1290	-.1209	-.1032	-.0843	-.0647	-.0243
6	-.2067	-.1991	-.1820	-.1630	-.1426	-.0983
7	-.2838	-.2775	-.2627	-.2456	-.2262	-.1812
8	-.3512	-.3470	-.3363	-.3226	-.3058	-.2634
9	-.3997	-.3980	-.3922	-.3831	-.3701	-.3333
10	-.4228	-.4237	-.4232	-.4191	-.4107	-.3819

(a) significant skew at the $\alpha = 0.05$ confidence level are highlighted

(b) Record Length for Model Fit

The effect of error on the expected value of the residual skewness is illustrated by Figure 8.9 for a normal error and Figure 8.10 for a lognormal error. For a normally distributed error, the significant skew of the residuals for an incorrect model fit to record lengths of 6 and 10 years is obliterated by relatively small data errors. Therefore, it is unlikely that skew can be used to identify an improper model. For a lognormal error, the skew of the residual increases with an increase in data error. Since the skew of the residual for a correct model also increases with an increase in data error, the detection of a significant residual skew may therefore be a good indicator of non-normality of the data error, but not a good indicator of an improper model structure.

8.1.1.4 Summary of Goodness-of-fit Tests. The three criteria used to determine the goodness-of-fit of a model, the F-test, parameter behavior, and residual behavior, have been discussed above. For a correct model, an increase in the sampling frequency, sampling density, or record length increases the ability to detect a correct model structure (except for the F-test which varies with an increase in the record length). This is not necessarily true for an incorrect model, as exemplified by fitting the linear trend surface model to different subsets of the

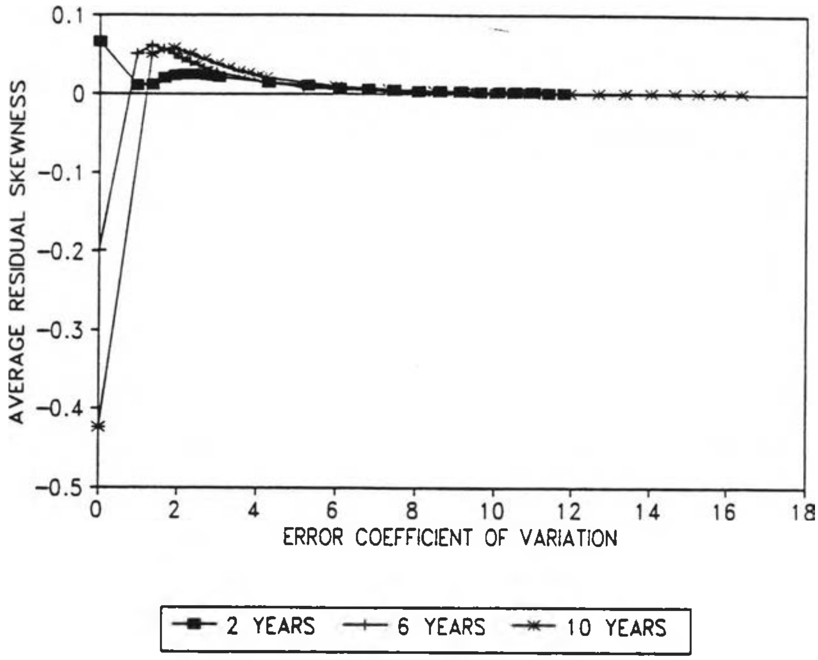


Figure 8.9 Effect of Error Coefficient of Variation on Average Residual Skewness from Linear Trend Surface Model Fit to Monthly Data at 50 Wells with Normal Error Variance

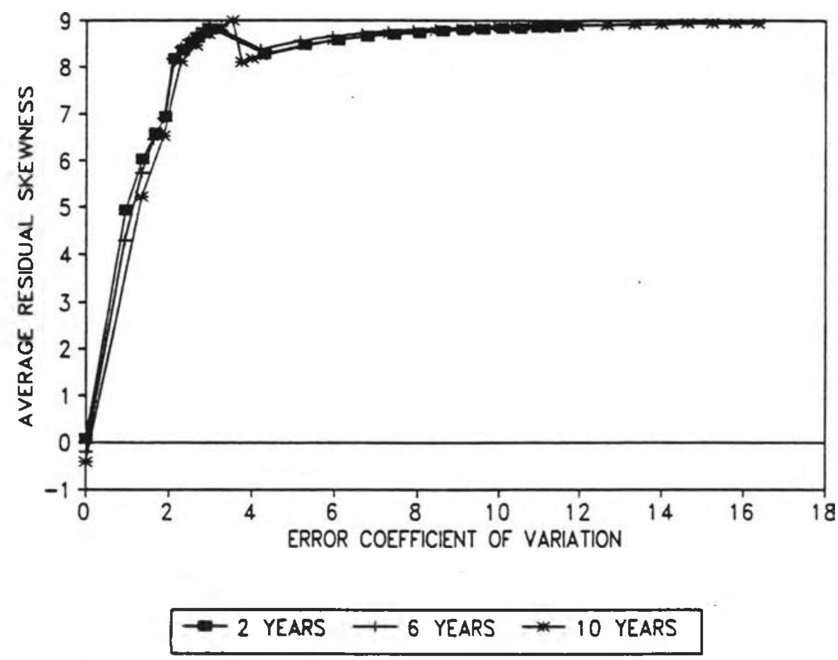


Figure 8.10 Effect of Error Coefficient of Variation on Average Residual Skewness from Linear Trend Surface Model Fit to Monthly Data at 50 Wells with Lognormal Error Variance

simulated data. Therefore, it is important to look at the behavior of these model applicability statistics under the conditions of varying sampling frequency, sampling density, and record length.

In addition to the convergent behavior of each of the individual statistics for a correct model, it is important to use a combination of statistics. This is exemplified by comparison of the range of error coefficients of variation allowed for evaluating the significance of the correct physical model versus the incorrect linear trend surface model based on the results of the F-test, parameter behavior, and residual behavior.

For detection of a significant model based on the F-test, the error coefficient of variation must be less than the error coefficient of variation lines shown on Figures 8.11 and 8.12 for a correct physical model and for an incorrect linear trend surface model, respectively. For the detection of a significant linear trend surface model based on the parameter estimate behavior or the residual behavior, the error coefficient of variation must be greater than the error coefficient of variation lines shown on Figure 8.12. Since the expected value of the parameter estimates should converge towards a single value and since the expected value of the residual temporal and spatial correlation is zero for a correct model, the data error should not limit the ability of these tests to detect the correct model. The shaded region on each figure illustrates the range of error allowable for detection of a significant model based on the use of all the goodness-of-fit statistics evaluated. Figures 8.11 and 8.12 illustrate that the F-test and parameter behavior analyses are more robust

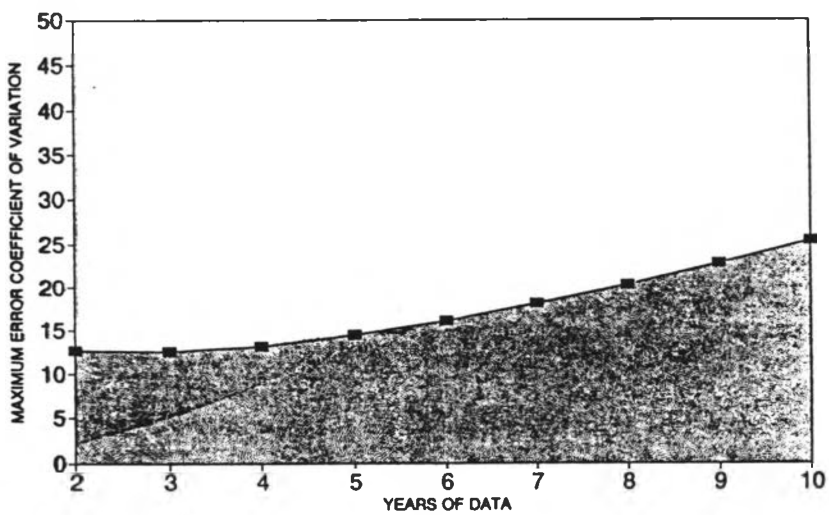


Figure 8.11 Error Coefficient of Variation for Detection of Significant Physical Model Fit to Monthly Data from 50 Wells

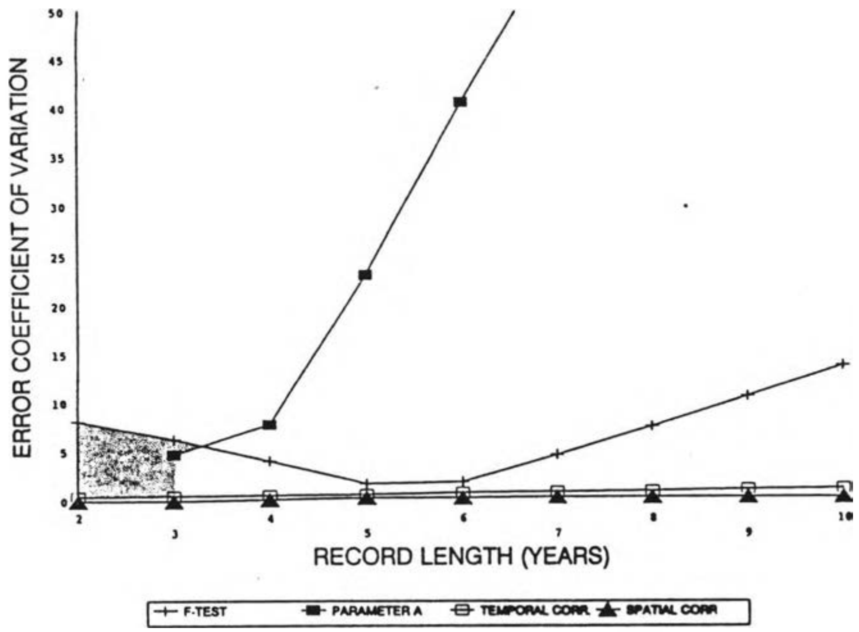


Figure 8.12 Error Coefficient of Variation for Detection of Significant Linear Trend Surface Model Fit to Monthly Data From 50 Wells

tests for model significance evaluation than are the residual tests. In addition, the combined use of goodness-of-fit statistics significantly aids in the model discrimination process. This is exemplified by Figure 8.12 for which, when using all model applicability statistics, the linear trend surface model would only be incorrectly identified as significant with

approximately three or less years of data with an error coefficient of variation between approximately one and seven. Lastly, the residual skew may be used to identify non-normal data errors, but is generally not effective at discriminating between models.

8.1.2 Predictive Tests.

For a correct model, the expected value of the prediction bias is zero, and the variance of the prediction bias decreases with an increase in data. For an incorrect model structure, the expected value and variance of the prediction bias is greater than for a correct model. The systematic behavior of the bias should be evident in the prediction error residuals.

Table 8.5 summarizes the average one-year prediction bias, variance, and associated t-test of the prediction error for a linear trend surface model fit to the simulated data without superimposed errors from 50 wells. The average one-year prediction bias varies in magnitude with an

Table 8.5 Average One-year Prediction Bias, Variance and Associated t-test for Linear Trend Surface Model Fit to Deterministic Data from 50 Wells

ONE-YEAR PREDICTION BIAS

YEARS[a]	SAMPLING FREQUENCY					
	BIWEEKLY	MONTHLY	BIMONTHLY	QUARTERLY	TRIANNUAL	BIANNUAL
2	-.0781	-.0784	-.0790	-.0795	-.0801	-.0812
3	-.0891	-.0903	-.0923	-.0951	-.0975	-.1022
4	-.0789	-.0805	-.0836	-.0867	-.0898	-.0961
5	-.0612	-.0627	-.0659	-.0690	-.0722	-.0787
6	-.0428	-.0442	-.0471	-.0501	-.0530	-.0590
7	-.0264	-.0277	-.0302	-.0328	-.0355	-.0409
8	-.0126	-.0137	-.0159	-.0182	-.0205	-.0253
9	-.0012	-.0022	-.0042	-.0061	-.0081	-.0124

VARIANCE

YEARS	SAMPLING FREQUENCY					
	BIWEEKLY	MONTHLY	BIMONTHLY	QUARTERLY	TRIANNUAL	BIANNUAL
2	.01540	.01553	.01576	.01596	.01613	.01638
3	.00893	.00907	.00933	.00958	.00982	.01022
4	.00441	.00449	.00465	.00480	.00494	.00521
5	.00208	.00211	.00219	.00227	.00234	.00218
6	.00097	.00099	.00103	.00106	.00109	.00116
7	.00046	.00047	.00048	.00050	.00052	.00054
8	.00022	.00023	.00023	.00024	.00025	.00026
9	.00011	.00011	.00012	.00012	.00012	.00012

T-TEST

YEARS	FREQUENCY OF SAMPLING					
	BIWEEKLY	MONTHLY	BIMONTHLY	QUARTERLY	TRIANNUAL	BIANNUAL
2	-21.80125	-15.41012	-10.89958	-8.899502	-7.724333	-6.344525
3	-32.66199	-23.22521	-16.5509	-13.74082	-12.05021	-10.1094
4	-41.15744	-29.42716	-21.23442	-17.69756	-15.64799	-13.31388
5	-46.48474	-33.43505	-24.39068	-20.481	-18.27995	-16.85569
6	-47.60456	-34.40965	-25.41926	-21.76205	-19.66112	-17.323
7	-42.63985	-31.29727	-23.8752	-20.74454	-19.06656	-17.60056
8	-29.42726	-22.1275	-18.15908	-16.61425	-15.87923	-15.69039
9	-3.96347	-5.138093	-6.640783	-7.875066	-9.056075	-11.3196

(a) Record Length for Model Fit

increase in record length but does decrease with an increase in sampling frequency. The fact that the bias does not converge towards zero with both an increase in sampling frequency or record length is indicative of an incorrect model structure.

The significance of the bias can be evaluated using the Student t-test, where

$$t = \frac{E(BIAS)}{\sqrt{(VAR(BIAS)/N)}} \tag{8.7}$$

At the 5% significance level, there is a significant bias in all the one-year predictions based on the linear trend surface model fit to errorless data from 50 wells.

For the multi-year prediction bias (i.e. average prediction bias more than one year into the future), in general, the magnitude of the prediction bias increases with the number of years predicted, as summarized in Table 8.6 for the linear trend surface model fit to the simulated data without superimposed errors. The non-convergence of the bias towards zero is indicative of an improper model fit. Table 8.7 summarizes the t-test statistics associated with these multi-year prediction biases. All the prediction biases are significant at the $\alpha = 0.05$ level with the significance of the bias increasing with an increase in the number of years predicted.

The introduction of error to the data reduces the significance of the bias. Figure 8.13 illustrates the maximum error coefficient of variation for detection of a one-year significant prediction bias for a linear trend surface model fit to 50 wells. As the record length or sampling frequency increases, the maximum error coefficient of variation tends to generally decrease (excluding less than four year of data). Therefore, with a larger data set, the ability to detect significant bias in the predictions decreases.

In summary, use of the prediction bias and associated t-test statistic to evaluate the significance of the bias appear to be good tools when data error is low, the data record is significant in length, or change

is rapid relative to sampling density. When data error is present, evaluation of trends in the prediction bias resulting from fitting the model to subsets of the available data should still aid in model discrimination.

8.1.3. Summary of Model Applicability.

In general, for a correct model, increasing the sampling frequency, sampling density, or record length will result in

- an increase in the F-test statistic (excluding record length),
- a decrease in parameter estimate uncertainty,
- a reduction in residual correlation,
- convergence in residual skewness, and
- a reduction in prediction bias.

Table 8.6 Average Multi-year Prediction Bias for Linear Trend Surface Model fit to Monthly Deterministic Data from 50 Wells

50 WELLS

YEARS[a]	NUMBER OF YEARS PREDICTED							
	1	2	3	4	5	6	7	8
2	-.0784	-.1362	-.1999	-.2521	-.3073	-.3605	-.4120	-.4261
3	-.0903	-.1300	-.1675	-.2025	-.2355	-.2668	-.2967	
4	-.0805	-.1034	-.1240	-.1426	-.1595	-.1752		
5	-.0627	-.0742	-.0838	-.0918	-.0988			
6	-.0442	-.0485	-.0513	-.0531				
7	-.0277	-.0275	-.0264					
8	-.0137	-.0109						
9	-.0022							

15 WELLS

YEARS	NUMBER OF YEARS PREDICTED							
	1	2	3	4	5	6	7	8
2	-.0921	-.1421	-.2890	-.3644	-.4173	-.4893	-.5020	-.5321
3	-.1004	-.1360	-.1875	-.2243	-.2886	-.3115	-.4043	
4	-.0988	-.1109	-.1334	-.1506	-.1627	-.1833		
5	-.0882	-.0932	-.1138	-.1223	-.1331			
6	-.0613	-.0721	-.0854	-.0902				
7	-.0305	-.0314	-.0404					
8	-.0221	-.0229						
9	-.0102							

9 WELLS

YEARS	NUMBER OF YEARS PREDICTED							
	1	2	3	4	5	6	7	8
2	-.0998	-.1662	-.2994	-.3767	-.4253	-.5088	-.5533	-.5990
3	-.1133	-.1411	-.1905	-.2445	-.2017	-.3265	-.4154	
4	-.1004	-.1178	-.1459	-.1663	-.1804	-.2002		
5	-.0921	-.0988	-.1155	-.1243	-.1445			
6	-.0661	-.0725	-.0883	-.0921				
7	-.0317	-.0356	-.0467					
8	-.0223	-.0323						
9	-.0031							

(a) Record Length for Model Fit

Table 8.7 T-test Statistic Associated with Multi-year Prediction Bias from Linear Trend Surface Model Fit to Monthly Data

50 WELLS

YEARS	T-STATISTIC ASSOCIATED WITH PREDICTION OF							
	1 YR	2 YR	3 YR	4 YR	5 YR	6 YR	7 YR	8 YR
2	-15.41	-36.15	-58.40	-74.86	-90.03	-103.13	-114.72	-115.43
3	-23.23	-47.47	-70.85	-90.94	-107.94	-122.52	-135.26	
4	-29.43	-56.15	-82.36	-105.92	-126.36	-144.26		
5	-33.44	-61.27	-89.44	-116.51	-142.61			
6	-34.41	-60.55	-86.71	-113.00				
7	-31.30	-50.21	-65.77					
8	-22.13	-28.14						
9	-5.14							

15 WELLS

YEARS	T-STATISTIC ASSOCIATED WITH PREDICTION OF							
	1 YR	2 YR	3 YR	4 YR	5 YR	6 YR	7 YR	8 YR
2	-6.34	-16.03	-26.92	-37.01	-45.79	-53.40	-60.11	-66.14
3	-9.96	-21.44	-33.50	-44.62	-54.32	-62.75	-70.12	
4	-12.86	-25.43	-38.48	-50.86	-62.02	-71.96		
5	-14.75	-27.56	-40.97	-54.20	-67.02			
6	-15.36	-27.21	-39.24	-51.65				
7	-14.25	-23.38	-31.33					
8	-10.96	-15.15						
9	-4.77							

9 WELLS

YEARS	T-STATISTIC ASSOCIATED WITH PREDICTION OF							
	1 YR	2 YR	3 YR	4 YR	5 YR	6 YR	7 YR	8 YR
2	-5.42	-13.60	-22.40	-30.24	-36.92	-42.64	-47.66	-52.17
3	-8.51	-18.17	-27.96	-36.68	-44.07	-50.39	-55.86	
4	-10.90	-21.47	-32.20	-42.08	-50.75	-58.29		
5	-12.46	-23.33	-34.53	-45.68	-55.95			
6	-13.03	-23.22	-33.74	-44.62				
7	-12.20	-20.39	-27.62					
8	-9.59	-13.66						
9	-4.46							

(a) Record Length for Model Fit

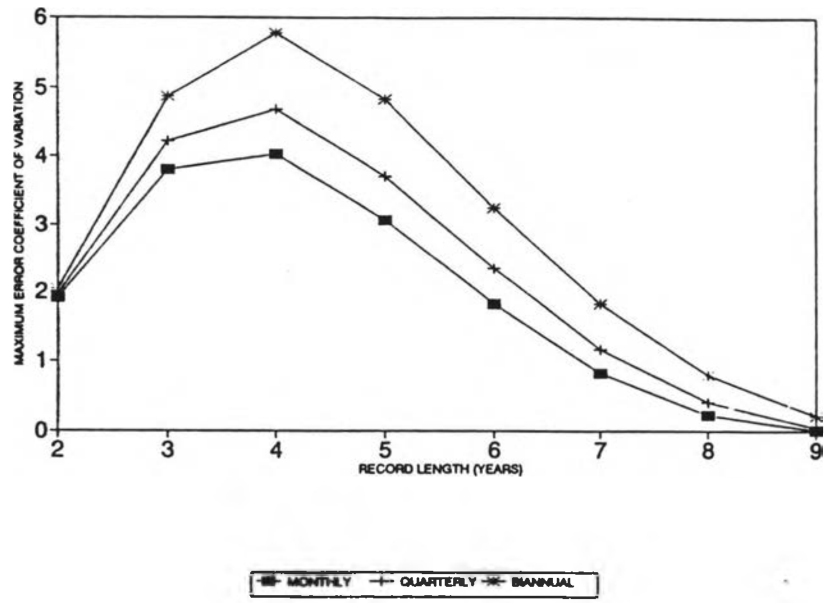


Figure 8.13 Effect of Error on One-Year Prediction Bias for Linear Trend Surface Model Fit to Data from 50 Wells

For an incorrect model, these statistics will not all behave as described above. Due to the sensitivity of the power of individual statistical tests in the presence of data error, it is important to look at a combination of goodness-of-fit and predictive test statistics and most important, to look at the behavior of these statistics as the sampling frequency, record length, and sampling density varies. The consistency of these statistics is an important tool due to the ability of error to reduce the significance of individual tests.

8.2. Optimization of Monitoring Networks

The design of optimal monitoring networks based on the results of the model applicability analyses is discussed in this section. The objective function and constraints for the monitoring network optimization are expressed as:

$$\text{MIN } Z_I = \sum_{i=1}^{n} \text{VAR(I)} * \text{VL(I)}$$

Subject to,

$$\text{CORR(I,J)} \geq \text{CORRMIN} \;\forall\; \text{J} = 1,\text{N and at least one I where VL(I)} = 1$$

where,

CORR(I,J) = predicted correlation between wells i and j
CORRMIN = minimum spatial correlation
n = number of wells
i = index on well number
VAR(I) = predicted variance at well i for sampling frequency F_i
VL(I) = binary variable indicating whether well is or is not being sampled; 1 = sampled, 0 = not sampled

The variance of the expected error (ζ) is developed in Chapter 6 and shown to be:

$$VAR[\zeta] = X.V_{\beta}X. + V_{c}. \tag{8.8}$$

As for all models, the expected variance of the predicted error at a well is a minimum at the beginning of the prediction period. However, the prediction error variance is not necessarily monotonically increasing for a nonlinear function.

The correlation between expected errors was shown in Chapter 7 to be:

$$CORR(\zeta^*_1,\zeta^*_2) = \frac{X._1V_{\beta}X._2'}{[(X._1V_{\beta}X._1' + V_{c}._1)(X._2V_{\beta}X._2' + V_{c}._2)]^{½}} \tag{8.9}$$

The sampling density for the multi-site models is defined based on meeting minimum specified spatial prediction error correlations and minimizing the sum of the expected error variance at the sampled wells. Based on the equation for predicted error variance, every location would have a different optimal sampling frequency with that frequency changing over time. A widely varying sampling frequency is impractical to apply, therefore a single sampling frequency was specified and the optimal location of wells for that frequency determined. Therefore, it is guaranteed that the minimum allowed prediction variance is met at all sampling points for the first sampling event.

Ideally, the model should be reevaluated after each sampling event and the sampling frequency and sampling locations redefined. This is also an impractical constraint. Therefore, it is assumed that the defined sampling network will be monitored for some user-specified interval prior to reevaluation.

Computer models were written to calculate the optimal sampling frequencies for the single-site models and sampling frequencies and sampling locations for the multi-site models based on the branch and bound technique discussed in Chapter 7. These programs, included in Appendix C, are:

VARASS - calculates parameter variance matrix (V_{β}) for single-site polynomial models

VARATS -	calculates parameter variance matrix (V_β) for trend surface models
VARP -	calculates parameter variance matrix (V_β) for physical model
OPTASS -	calculates prediction error variance ($X.V_\beta X.'$) for a specified frequency for single-site polynomial models
OPTATS -	calculates prediction error variance ($X.V_\beta X.'$) for a specified frequency for trend surface models
OPTAP -	calculates prediction error variance ($X.V_\beta X.'$) for a specified frequency for physical model
BB -	performs branch and bound optimization

The optimal monitoring network for the correct physical model (Section 8.2.1) is compared to the optimal monitoring network for a linear trend surface model (Section 8.2.2), selected as an example of an incorrect model structure. Optimal monitoring networks for other incorrect model structures are discussed in detail in Appendix G.

8.2.1 Optimization Based on a Physical Model

The design of a monitoring network is dependent on the model structure and on the fit of the model to the data. The optimal monitoring network is reduced with an increase in the confidence of a model. This is expressed as a reduction in the sampling frequency, number of wells, and/or objective function value. This is exemplified by the results of the monitoring network optimization for the physical model fit to monthly data, as summarized in Table 8.8. As shown in Table 8.8, the objective function value decreases and the sampling density decreases with an increase in the data set used to fit the model.[21] Therefore, the increase in the data set is associated with a decrease in the uncertainty of the model.

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[2] The value of the objective function decreases with an increase in sampling frequency used to fit the model, where the lower frequencies include the same samples. That is, the objective function based on the monitoring network sampled biweekly is less than the objective function for the same network sampled monthly which is less than for the objective function for the same network sampled bimonthly which is less than the objective function for the same network sampled triannually. However, since the monitoring network comprised of triannual samples contains different samples than does the monitoring network sampled biannually, the triannual monitoring network does not necessarily result in a lower objective function than does the biannual network from the same wells. This is due to the dependence of V_β on the specific data used to fit the selected model to the data.

Table 8.8 Objective Function[a] and Number of Monitoring Wells for Physical Model fit to 50 Wells;
Minimum Spatial Error Prediction Correlation = 0.9;
Future Monthly Sampling Frequency

	EXISTING MONITORING NETWORK SAMPLED					
YEARS[c]	BIWEEKLY	MONTHLY	BIMONTH	QUARTER	TRIANN	BIANN
2	1.0002[a]	5.4830	5.5690	15.2924	541.113	17.786
	1[b]	4	4	4	5	4
3	1.00008	1.1839	2.4802	3.3403	261.657	5.2947
	1	1	2	2	4	3
4	1.00002	1.0016	1.0039	1.1468	82.834	2.4680
	1	1	1	1	4	2
5	1.00001	1.00003	1.00004	1.10109	42.258	1.00004
	1	1	1	1	4	1
6	1.00000	1.00001	1.00001	1.00004	22.414	1.00004
	1	1	1	1	4	1
7	1.00000	1.00000	1.00000	1.00001	16.863	1.00001
	1	1	1	1	4	1
8	1.00000	1.00000	1.00000	1.00000	8.9529	1.00001
	1	1	1	1	3	1
9	1.00000	1.00000	1.00000	1.00000	7.0719	1.00000
	1	1	1	1	3	1
10	1.00000	1.00000	1.00000	1.000000	3.7687	1.00000
	1	1	1	1	2	1

(a) Value shown * Data Error Variance equals the Objective Function for the Designed Monitoring Network

(b) Number of monitoring wells in network

(c) Record Length for Model Fit

The results of this optimization indicate that after two years of monthly sampling from 50 wells, the monitoring network could be reduced to four wells sampled monthly. After three years of the same 50 wells sampled monthly, the monitoring network could be reduced to a single well sampled monthly. Therefore, the monitoring network could be significantly reduced by using a physical model to explain the correlation of samples spatially and temporally. A spatial error correlation of 0.9 would be maintained between the sampled and non-sampled wells, with an uncertainty represented by the objective function value.

This uncertainty associated with the sampled and non-sampled wells can be illustrated graphically by plotting the prediction error variances calculated for use in the optimization. The error prediction variances for the physical model fit to two years of monthly data from 50 wells associated with the objective function value of 5.4830 in Table 8.8 are plotted and contoured on Figure 8.14a. The reduced prediction error variances based on the optimal monitoring network is plotted as Figure 8.14b.

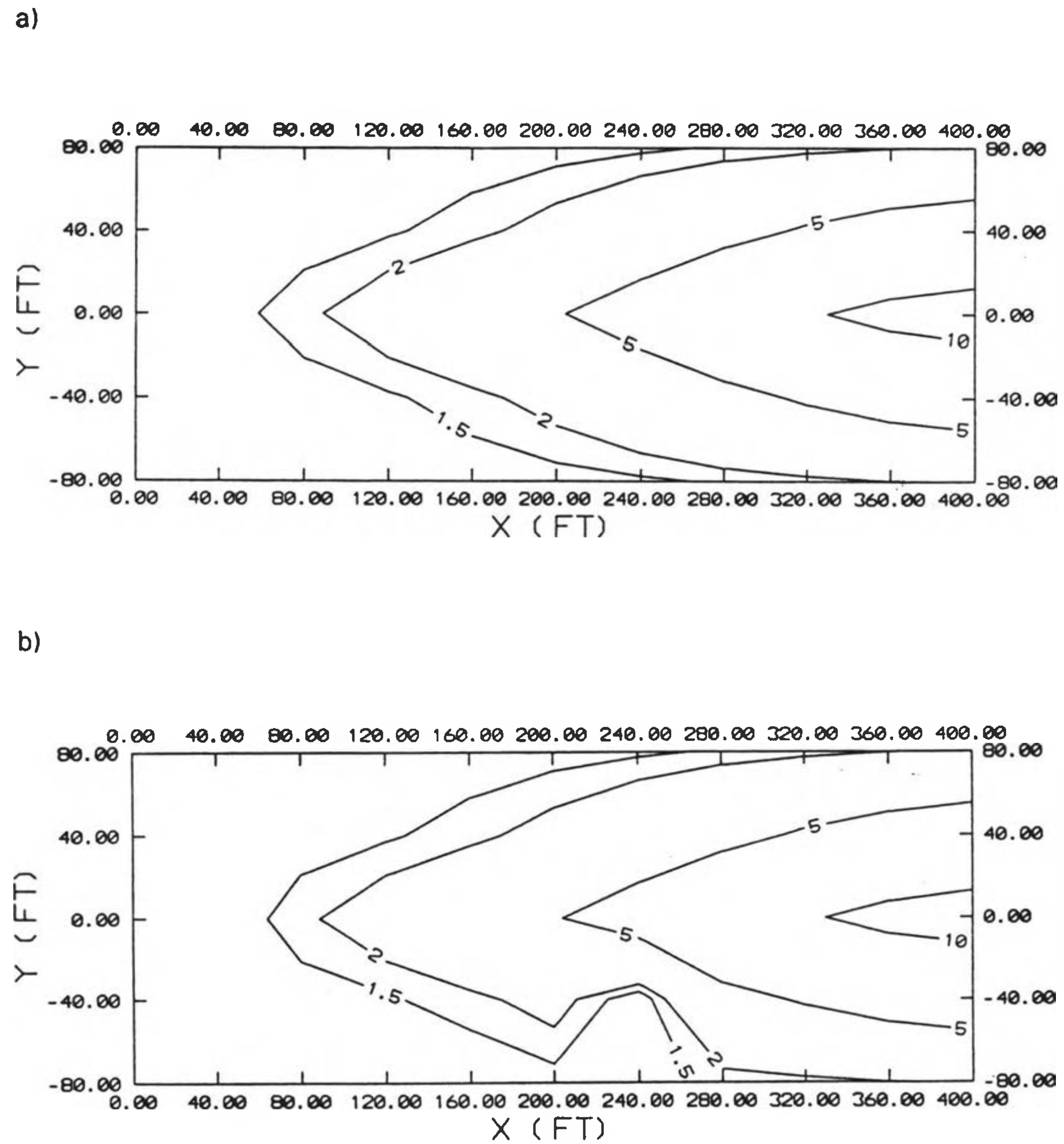


Figure 8.14 Prediction Error Variance for Physical Model a)prediction b) with optimal sampling network

An alternative means of representing the uncertainty in the system is by plotting the confidence bounds on a specified concentration of interest. These confidence bounds can be defined based on the prediction error variances as follows:

$$C^* = E[C^*] \pm t_{\alpha/2,n-1} \sqrt{VAR(\zeta)/n}$$

This surface is plotted for a concentration of 100 ppb (relative to a source concentration of 1000 ppb) in Figure 8.15 for the physical model fit to two years of monthly data from 50 wells with an error coefficient of variation equal to 5% and a 5% ($\alpha = 0.05$) significance level. Figure 8.15 is an alternative representation of Figure 8.14b. The shaded region on FIgure 8.15 illustrates the 95% confidence limits on the 100 ppb concentration. The confidence bounds illustrated in Figure 8.15 can be calculated for any concentration of interest and are informative in evaluating the confidence associated with a given model and a given monitoring network. If the uncertainty in the optimally designed monitoring system, as represented by either Figure 8.14b or Figure 8.15, is unacceptable to the groundwater quality monitoring manager, then the required minimum spatial correlation (CORRMIN) can be increased which will result in additional sampling and a reduction in the uncertainty interval for a given concentration of interest.

The example optimal monitoring networks described above were for a specified future monthly sampling frequency. Increasing the future sampling frequency does

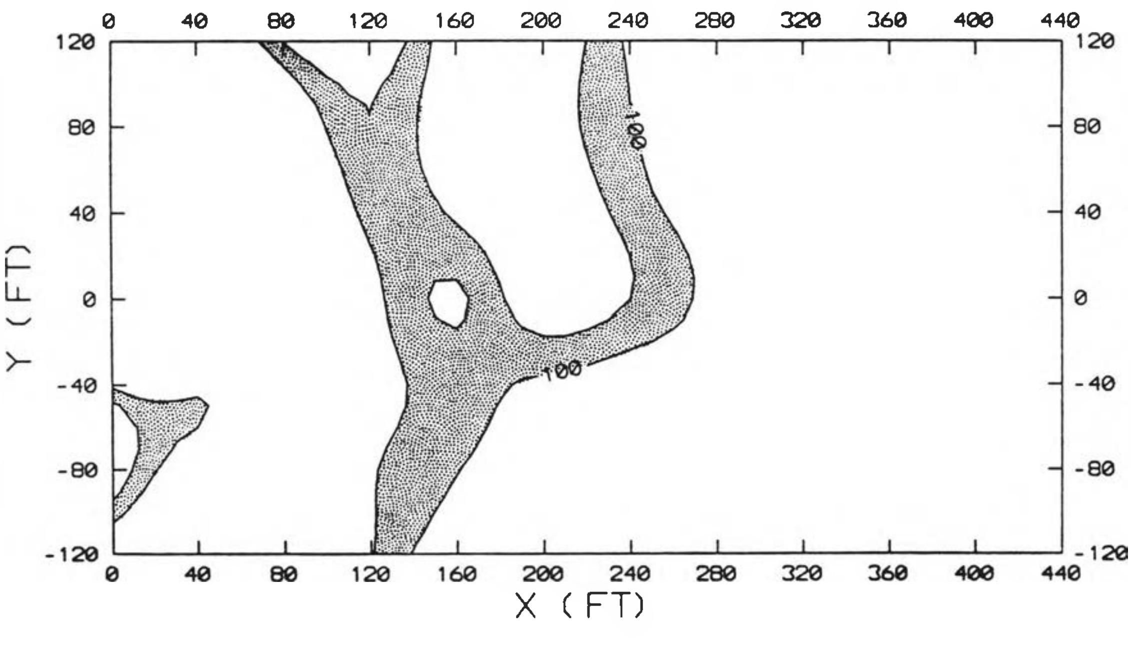


Figure 8.15 Predicted Concentration Estimates with Confidence Limits for Physical Model Fit to Two Years of Monthly Data at 50 Wells with Optimal Sampling

not necessarily decrease the sampling density or the value of the objective function, as summarized in Table 8.9. The number of monitoring wells required to be sampled does not change with an increase in the future sampling frequency and therefore the cost would be reduced by sampling less frequently. This is due to the functions for the correlation and variance of the prediction error not being monotonically decreasing and increasing functions, respectively. For this case, an additional alterative sampling constraint may be prudent to be imposed regarding the expected maximum change in expected behavior of the variable of interest or some other constraint which may constrain the frequency or density of sampling.

Table 8.9 Objective Function[a] and Number of Monitoring Wells for Physical Model Fit to Monthly Data from 50 Wells; Minimum Spatial Error Prediction Correlation = 0.9

	FUTURE SAMPLING FREQUENCY (IN DAYS)						
YRS[b]	15	30	45	60	90	120	180
2	5.6484 3	5.5690 3	7.1802 3	6.9559 3	6.7993 3	6.5465 3	5.7277 3
3	2.4927 2	2.4802 2	2.4682 2	2.4566 2	2.4344 2	2.4135 2	2.3750 2
4	1.0041 1	1.0039 1	1.0038 1	1.0037 1	1.0025 1	1.0002 1	1.0001 5 1
5	1.00004 1	1.00004 1	1.0004 1	1.0003 1	1.0003 1	1.00003 1	1.0000 3 1
6	1.00001 1	1.00001 1	1.0001 1	1.00001 1	1.00001 1	1.00001 1	1.0000 1 1
7	1.00000 1	1.00000 1	1.00000 1	1.00000 1	1.00000 1	1.00000 1	1.0000 0 1
8	1.00000 1	1.00000 1	1.00000 1	1.00000 1	1.00000 1	1.00000 1	1.0000 0 1
9	1.00000 1	1.00000 1	1.00000 1	1.00000 1	1.00000 1	1.00000 1	1.0000 0 1
10	1.00000 1	1.00000 1	1.00000 1	1.00000 1	1.00000 1	1.00000 1	1.0000 0 1

(a) Value shown * Data Error Variance equals the Objective Function for the Designed Monitoring Network

(b) Record Length for Model Fit

These additional constraints can be easily incorporated in the branch and bound optimization technique used herein.

The effect of the choice of minimum spatial correlation is summarized in Table 8.10 for existing monitoring networks of 50, 15, and 9 wells sampled monthly, with a future monthly sampling frequency specified. The value of the objective function increases with a decrease in the network density and with an increase in the minimum spatial correlation. The number of wells required to be sampled also increased with an increase in the minimum spatial correlation.

Clearly, the monitoring network optimization is highly dependent on the data used to fit the model. This can be seen by comparing the monitoring network optimization for three different monitoring networks each composed of 9 wells, as summarized in Table 8.11. Monitoring network A consists of 9 wells at X = 120, 240, and 360 meters and at Y= -80, 0, and 80 meters. Monitoring network B consists of 9 wells at X = 80, 240, and 400 meters and at Y = -80, 0 and 80 meters. Monitoring network C consists of 9 wells at X = 80, 120, and 240 meters and at Y = -40, 0 and 40 meters. The objective function value generally decreases with a more equally spaced existing monitoring network. The prediction error variances predicted by these three monitoring networks are plotted on Figure 8.16. The reduction in these prediction error variance surfaces, based on the optimal monitoring networks, are illustrated in Figure 8.17. Due to the low minimum achievable spatial correlation, the prediction error variance surface is affected relatively little by the optimal monitoring network.

In addition to being sensitive to the data used to fit the model, the monitoring network optimization is also sensitive to the potential wells to be included in the optimal monitoring network. Therefore, additional well locations were considered for the optimal future monitoring network based on the physical model fit to one and two years of data. All wells within the predicted extent of the groundwater plume (defined as 5 ppb relative to a source concentration of 1000 ppb) were considered for the future monitoring network. This introduced potentially twenty new monitoring wells into the monitoring network design. The spacing of any new wells considered was consistent with the existing network used to define the plume.

Optimal monitoring networks were determined for a maximum spatial correlation of 0.8 and a specified future monthly sampling frequency. The results for these optimizations are summarized in Table 8.12. The objective function values and number of wells required generally increase with a reduction in the sampling frequency or record length. The prediction error variances for the wells are plotted in Figure 8.18a for the physical model fit to one year of monthly data. Figure 8.18a illustrates the predicted error variance without monitoring and Figure 8.18b illustrates the reduction of the prediction error variance with the specified optimal monitoring network.

An alternative representation of this uncertainty is represented by Figure 8.19. Figure 8.19 illustrates the 95% upper and lower confidence limits on the 100 ppb concentration contour with and without the sampling from the optimal monitoring

Table 8.10 Objective Function[a] and Number of Monitoring Wells for Physical Model Fit to Monthly Data from 50 Wells; Future Monitoring Network Sampled Monthly

	MINIMUM SPATIAL CORRELATION OF WELLS SPECIFIED NUMBER OF WELLS IN EXISTING MONITORING NETWORK								
YRS[b]	0.90			0.95			0.99		
	50	15	9	50	15	9	50	15	9
2	5.569[a] 3[d]	20.634 3	IS[c]	13.51 9 6	IS	IS	IS	IS	IS
3	2.4802 2	IS	IS	4.072 3 3	IS	3.307 6 2	IS	IS	IS
4	1.0039 1	1.1560 1	2.6067 2	1.045 5 1	2.310 8 2	2.613 0 2	IS	IS	IS
5	1.0004 1	1.0055 1	1.1077 1	1.000 0 1	1.051 8 1	1.080 1 1	1.010 7 1	3.190 2 3	IS
6	1.0000 1	1.0003 1	1.0006 1	1.000 0 1	1.000 3 1	1.005 7 1	1.000 0 1	2.030 4 2	2.084 0 2
7	1.0000 1	1.0001 1	1.0002 1	1.000 0 1	1.000 1 1	1.000 9 1	1.000 0 1	1.004 2 1	1.010 8 1
8	1.0000 1	1.0000 1	1.0001 1	1.000 0 1	1.000 0 1	1.000 0 1	1.000 0 1	1.000 0 1	1.000 1 1
9	1.0000 1	1.0000 1	1.0000 1	1.000 0 1	1.000 0 1	1.000 0 1	1.000 0 1	1.000 0 1	1.000 0 1
10	1.0000 1	1.0000 1	1.0000 1	1.000 0 1	1.000 0 1	1.000 0 1	1.000 0 1	1.000 0 1	1.000 0 1

(a) Value shown * Data Error Variance equals the Objective Function for the Designed Monitoring Network

(b) Record Length for Model Fit

(c) IS = Impossible Solution: minimal spatial correlation cannot be achieved

(d) Number of Monitoring Wells in Network

Table 8.11 Objective Function[a] and Number of Monitoring Wells for Physical Model Fit to Three Different 9-Well Monitoring Networks Sampled Monthly;
Minimum Spatial Prediction Error Correlation = 0.8

	EXISTING MONITORING NETWORK		
YEARS[b]	MN A[c]	MN B[d]	MN C[e]
2	1.64347 1	11.5565 5	IS[f]
3	1.68760 1	2.64725 2	5.95210 3
4	1.24089 1	1.17654 1	1.35845 1
5	1.00064 1	1.01212 1	1.00166 1
6	1.00024 1	1.00342 1	1.00058 1
7	1.00009 1	1.00112 1	1.00022 1
8	1.00001 1	1.00037 1	1.00005 1
9	1.00001 1	1.00010 1	1.00002 1
10	1.00000 1	1.00004 1	1.00001 1

(a) Value shown * Data Error Variance equals the Objective Function for the Designed Monitoring Network

(b) Record Length for Model Fit

(c) Monitoring Network A Well Locations: X @ 120,240,360 meters; Y @ -80,0,80 meters

(d) Monitoring Network B Well Locations: X @ 80,240,400 meters; Y @ -80,0,80 meters

(e) Monitoring Network C Well Locations: X @ 80,120,240 meters; Y @ -40,0,40 meters

(f) IS = Impossible Solution: minimal spatial correlation cannot be achieved

network (relative to a source concentration of 1000) for this same one-year monitoring period. This graphical means of representing the uncertainty in the groundwater quality system is extremely informative to the groundwater manager. As discussed earlier, this represent the allowed quantified uncertainty (expressed as

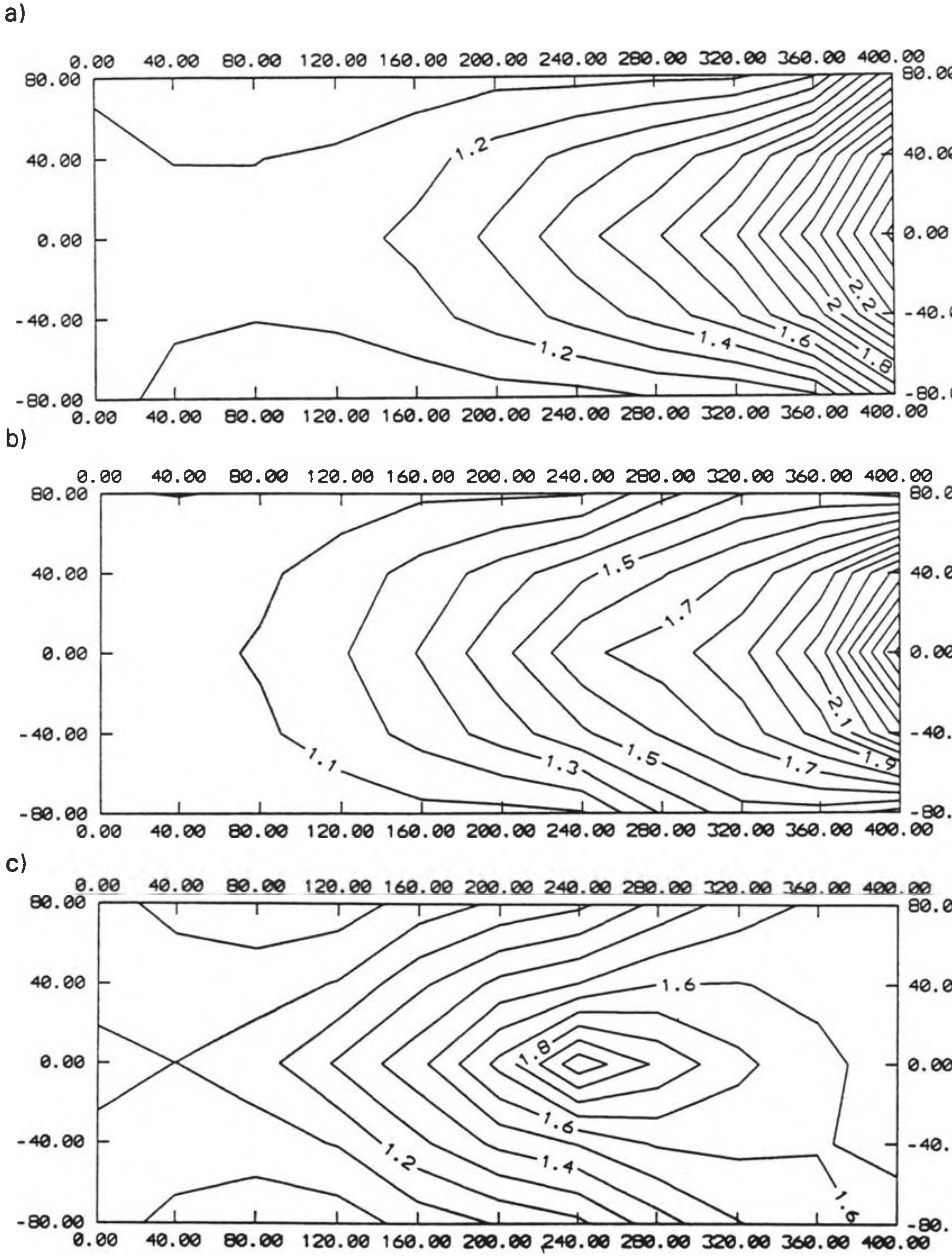


Figure 8.16 Prediction Error Variances for Physical Model Fit to Three 9-Well Monitoring Networks: a) Monitoring Network A: X=120,240,360 meters; Y =-80,0,80 meters; b) Monitoring Network B: X=80,240,400 meters; Y =-80,0,80 meters; c) Monitoring

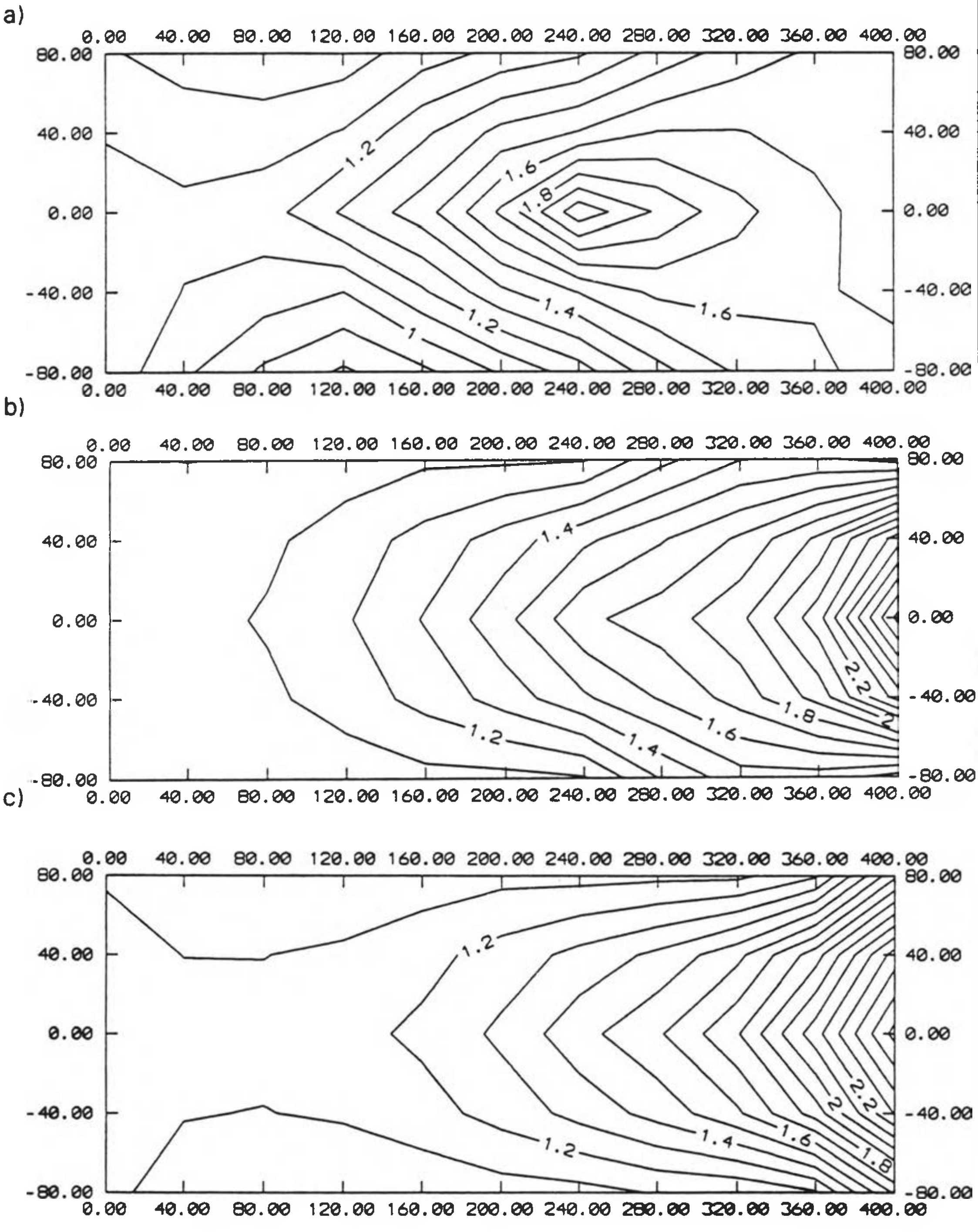


Figure 8.17 Reduced Prediction Error Variance for **Physical Model Fit to Three** 9-Well Monitoring Networks with Optimal Sampling: **a) Monitoring** Network A: X = 120,240,360 meters; Y = -80,0,80 **meters; b)** Monitoring Network B: X = 80,240,400 meters; Y = -80,0,80 meters; c) Monitoring Network C: X = 80,120,240 meters; Y = -40,0,40 meters

Table 8.12 Objective Function[a] for Physical Model Fit to Monthly Data from 50 Wells; Increased Size of Potential Future Monthly Frequency Monitoring Network; Minimum Spatial Error Prediction Correlation = 0.8;

SAMPLING FREQUENCY	RECORD LENGTH 1 YEAR	2 YEARS
Biweekly	20.154[b]	1.03889
	4[c]	1
Monthly	19.156	5.606
	3	3
Bimonthly	31.923	5.583
	3	3
Quarterly	65.379	10.043
	4	4
Triannual	203.848	234.690
	7	5
Biannual	58.169	12.415
	5	4

(a) Sampling Frequency for Model Fit

(b) Value shown * Data Error Variance equals the Objective Function for the Designed Monitoring Network

(c) Number of monitoring wells in network

a minimum spatial correlation) used in the branch and bound optimization of the groundwater quality monitoring network.

8.2.2 Optimization Based on a Linear Trend Surface Model.

In addition to evaluation of the optimal monitoring networks for the correct physical model, optimal monitoring networks for the incorrect trend surface models and single-site polynomial models were evaluated. The optimization of a monitoring network based on the linear trend surface model was selected as an example of the optimization for an incorrect model. The detailed results for the monitoring network optimization for the quadratic and cubic trend surface models and for the single-site polynomial models are discussed in Appendix G.

For an existing monitoring network of 50 wells, with a required minimum spatial correlation of 0.9, the resulting optimal monitoring networks for the linear trend surface model fit to different sampling frequency and record length data subsets are reported in Table 8.13. Table 8.14 summarizes the optimal monitoring networks for the linear trend surface model fit to monthly data from networks consisting of

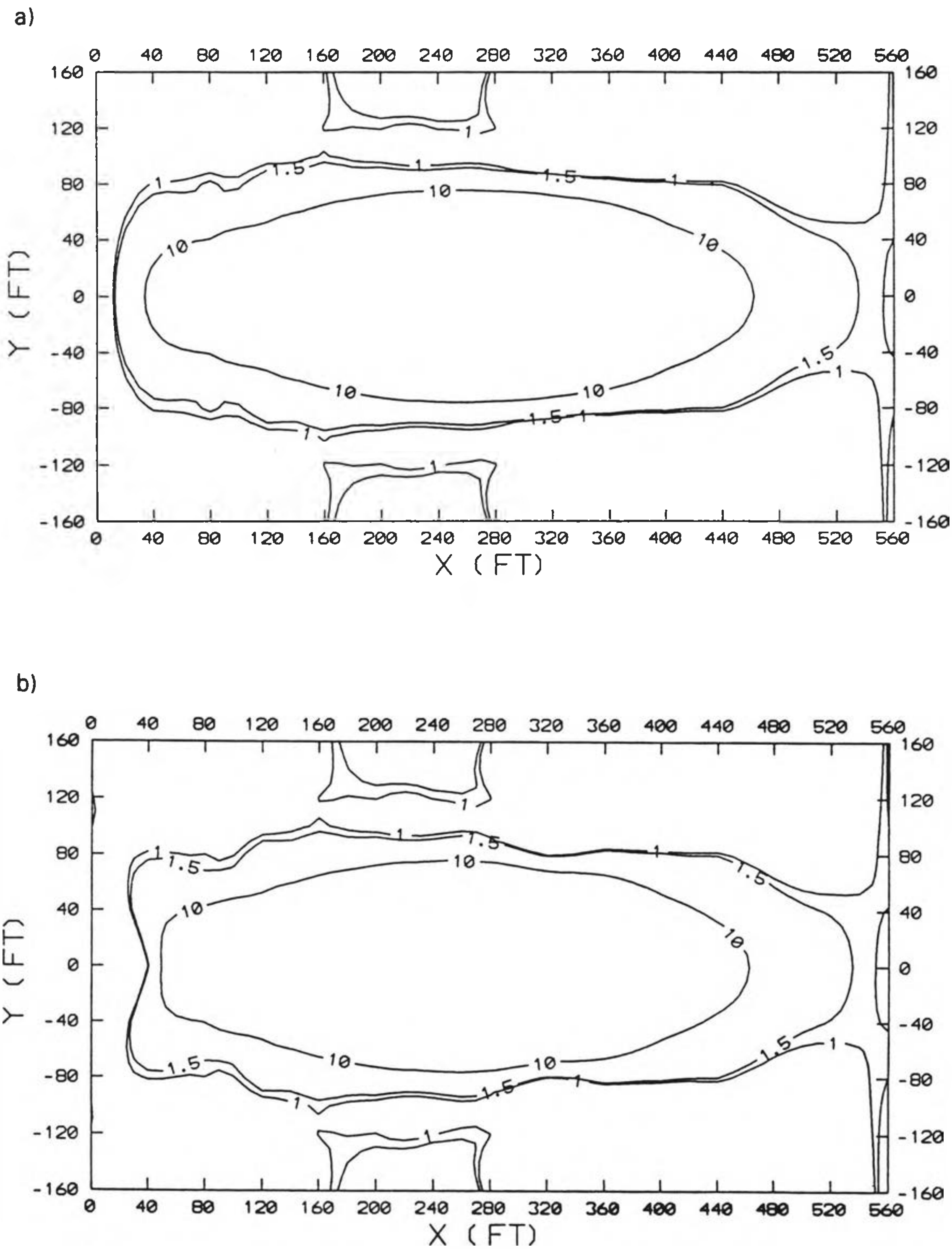
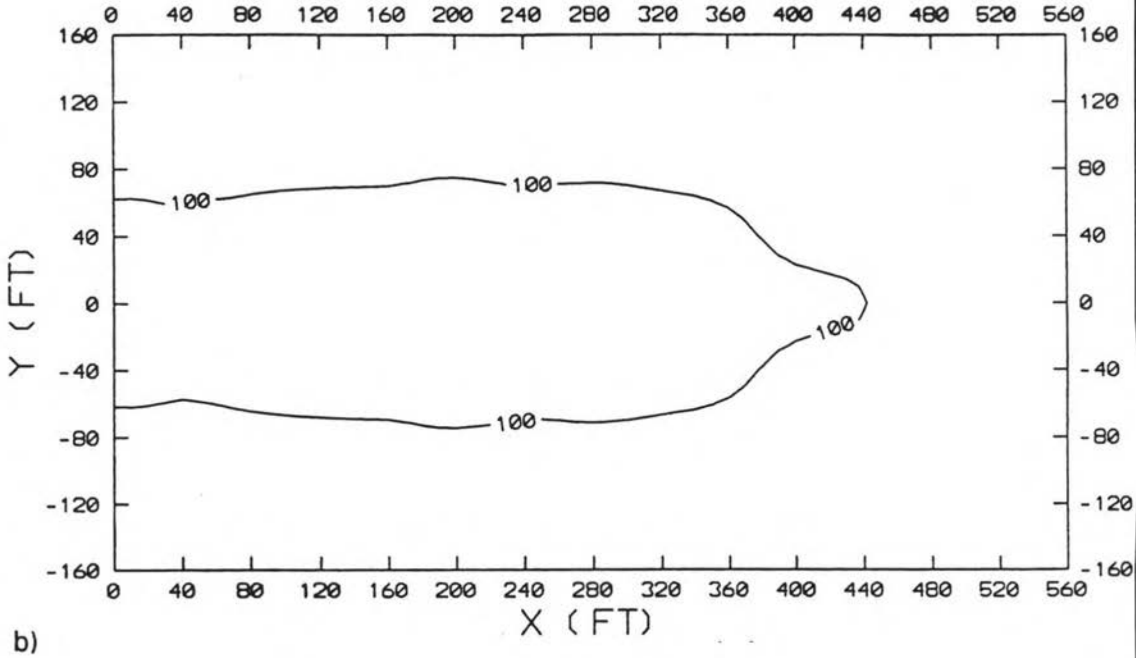


Figure 8.18 Prediction Error Variance for Increased Potential Monitoring Network Based on Physical Model Fit to One Year of Monthly Data From 50 Wells: a) prediction; b) with optimal monitoring network

a)



b)

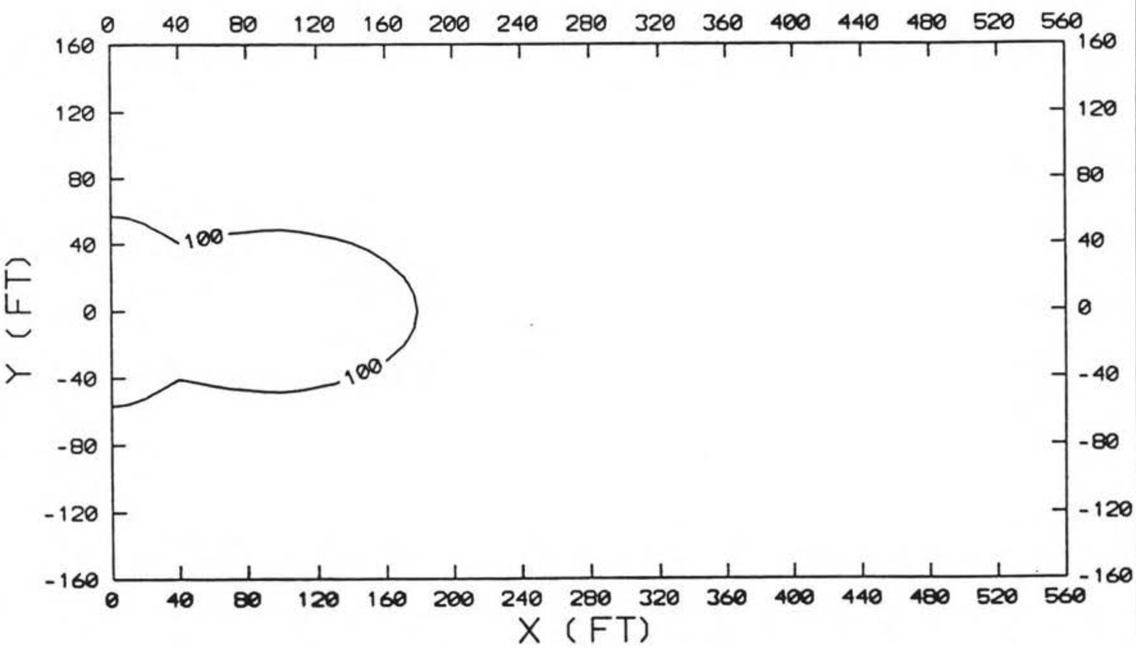


Figure 8.19 Predicted Upper and Lower 95% Confidence Bounds on 100 ppb Concentration Based on Physical Model Fit to One Year of Monthly Data From 70 Wells

Table 8.13 Objective Function[a] for Linear Trend Surface Model Fit to Monitoring Network of 50 Wells; Minimum Spatial Error Prediction Correlation = 0.9; Future Monthly Sampling Frequency

	EXISTING MONITORING NETWORK SAMPLED					
YEARS[b]	BIWEEK	MONTHLY	BIMONTH	QUARTER	TRIANN	BIANN
2	1.0070	1.0134	1.0242	1.0325	1.0480	1.0507
3	1.0045	1.0089	1.0165	1.0233	1.0352	1.0387
4	1.0033	1.0066	1.0125	1.0181	1.0278	1.0312
5	1.0026	1.0052	1.0100	1.0145	1.0230	1.0257
6	1.0021	1.0043	1.0083	1.0146	1.0196	1.0219
7	1.0018	1.0037	1.0071	1.0122	1.0170	1.0192
8	1.0016	1.0032	1.0062	1.0105	1.0151	1.0171
9	1.0014	1.0029	1.0055	1.0093	1.0135	1.0153
10	1.0013	1.0026	1.0050	1.0083	1.0123	1.0139

(a) Value shown * Data Error Variance equals the Objective Function for the Designed Monitoring Network

(b) Record Length for Model Fit

Table 8.14 Objective Function[a] for Linear Trend Surface Model Fit to Existing Monitoring Network Sampled Monthly; Minimum Spatial Prediction Error Correlation = 0.9; Future Monthly Sampling Frequency

	EXISTING MONITORING NETWORK		
YEARS[b]	50 WELLS	15 WELLS	9 WELLS
2	1.0134	1.0480	1.0912
3	1.0089	1.0318	1.0605
4	1.0066	1.0232	1.0451
5	1.0052	1.0188	1.0358
6	1.0043	1.0156	1.0297
7	1.0037	1.0133	1.0255
8	1.0032	1.0116	1.0222
9	1.0029	1.0103	1.0197
10	1.0026	1.0093	1.0177

(a) Value shown * Data Error Variance equals the Objective Function for the Designed Monitoring Network

(b) Record Length for Model Fit

50, 15, and 9 wells. Only one monitoring well was required for the linear trend surface model fit to all combinations of record lengths, sampling frequencies, and sampling densities considered with a minimum spatial correlation of 0.9. As the sampling frequency, sampling density or record length increased, the objective function value consistently decreased. This is unlike the objective function value for the correct model and is due to the prediction error variance function being a monotonic increasing function and the correlation function being a monotonic decreasing function for the polynomial models. In addition, the objective function value increased with an increase in the specified future sampling frequency, as summarized in Table 8.15. It is important to note however, that this decrease in the objective function value with an increase in sample size for a specific model does not mean that the model structure is necessarily correct, but that the confidence in the model parameters has increased.

The prediction error variance for the linear trend surface model fit to ten years of monthly monitoring data from 50 wells is plotted as Figure 8.20a. The reduction of the prediction error variance surface for the optimal sampled network at X=40, Y=0 meters is illustrated by Figure 8.20b. Comparison of these two figures illustrates the relatively small reduction in error variance immediately surrounding the sampling well. At a distance from the well, no observable decrease in the error prediction variance is apparent.

An alternative representation of this uncertainty in the system is illustrated by Figures 8.21a and 8.21b which show the upper and lower 95% confidence limit concentrations for this same monitoring network. These figures illustrate the low confidence associated with the linear trend surface model, such that the model is essentially uniform spatially with large relative error bounds on the predicted concentration.

8.2.3 Comparison of Optimal Monitoring Networks

A comparison of the monitoring network optimization for the physical and statistical models considered in the simulation study was made based on an analysis of an existing monitoring network of 50 wells sampled monthly. The objective function value for the optimal monitoring networks are summarized in Table 8.16.

Using these objective function values and the model error variances calculated for the models in Section 8.1, Table 8.17 shows which model provides the minimal objective function value, assuming different data error variances. Clearly, as the data set increases in size, the validity of the correct model becomes more apparent, and will result in significantly less prediction uncertainty.

This behavior is also exhibited in the maximum prediction error variance at a single location. Table 8.18 summarizes the maximum error variance at a single location for the four multi-site models considered. Table 8.19 summarizes which model provides the minimum prediction error variance at a single location under the conditions of different data error variances.

Table 8.15 Objective Function[a] for Linear Trend Surface Model Associated with Different Future Sampling Frequencies; Existing Monitoring Network of 50 Wells Sampled Monthly; Minimum Spatial Error Prediction Correlation = 0.9

	FUTURE SAMPLING FREQUENCY (IN DAYS)						
YRS[b]	15	30	45	60	90	120	180
2	1.0131	1.0134	1.0138	1.0141	1.0148	1.0156	1.0171
3	1.0087	1.0089	1.0090	1.0092	1.0095	1.0098	1.0105
4	1.0065	1.0066	1.0067	1.0068	1.0069	1.0071	1.0075
5	1.0052	1.0052	1.0053	1.0053	1.0054	1.0056	1.0056
6	1.0043	1.0043	1.0044	1.0044	1.0045	1.0047	1.0047
7	1.0037	1.0037	1.0037	1.0037	1.0038	1.0039	1.0040
8	1.0032	1.0032	1.0033	1.0033	1.0033	1.0034	1.0034
9	1.0029	1.0029	1.0029	1.0029	1.0029	1.0030	1.0030
10	1.0026	1.0026	1.0026	1.0026	1.0026	1.0027	1.0027

(a) Value shown * Data Error Variance equals the Objective Function for the Designed Monitoring Network

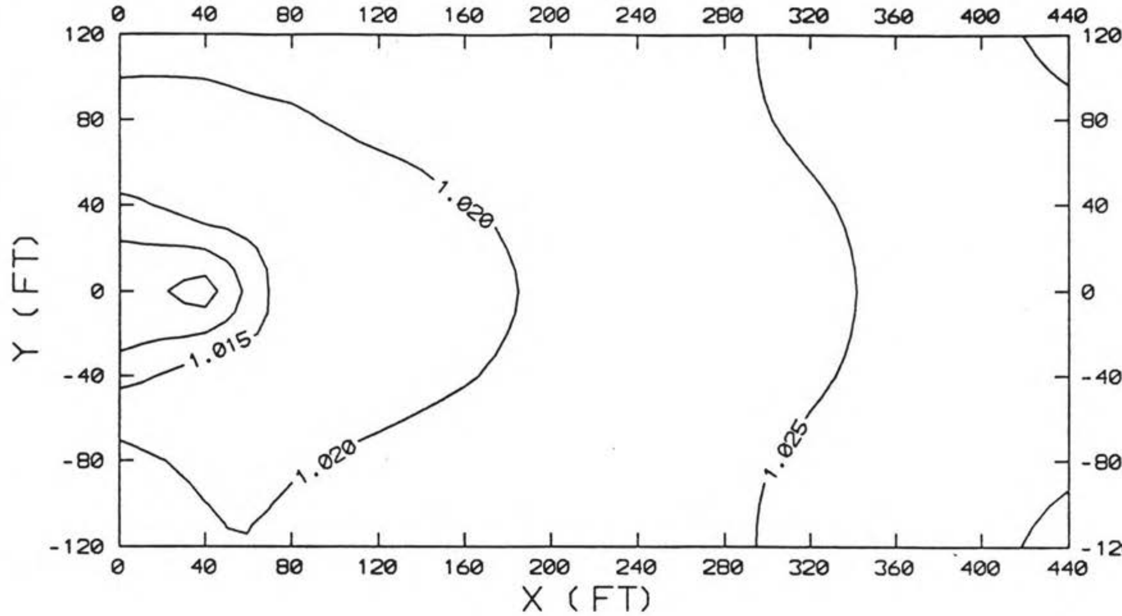
Table 8.16 Comparison of Prediction Error Variance[a] for Alternative Multi-site Models; Existing Network of 50 Wells Sampled Monthly; Future Monthly Sampling Frequency; Minimum Spatial Error Prediction Correlation = 0.9

YEAR[b]	LINEAR TREND	QUADRATIC TREND	CUBIC TREND	PHYSICAL
2	1.0134	1.3485	26.351	5.5690
3	1.0089	1.2149	18.571	2.4802
4	1.0066	1.1522	14.128	1.0039
5	1.0052	1.1184	11.462	1.0004
6	1.0043	1.0965	9.7117	1.0001
7	1.0037	1.0819	8.0107	1.00000
8	1.0032	1.0709	7.8162	1.00000
9	1.0029	1.0624	3.7018	1.00000
10	1.0026	1.0557	3.4077	1.00000

(a) Value shown * (Model Error Variance + Data Error Variance) equals the sum of prediction variance for the designed monitoring network

(b) Record Length for Model Fit

a)



b)

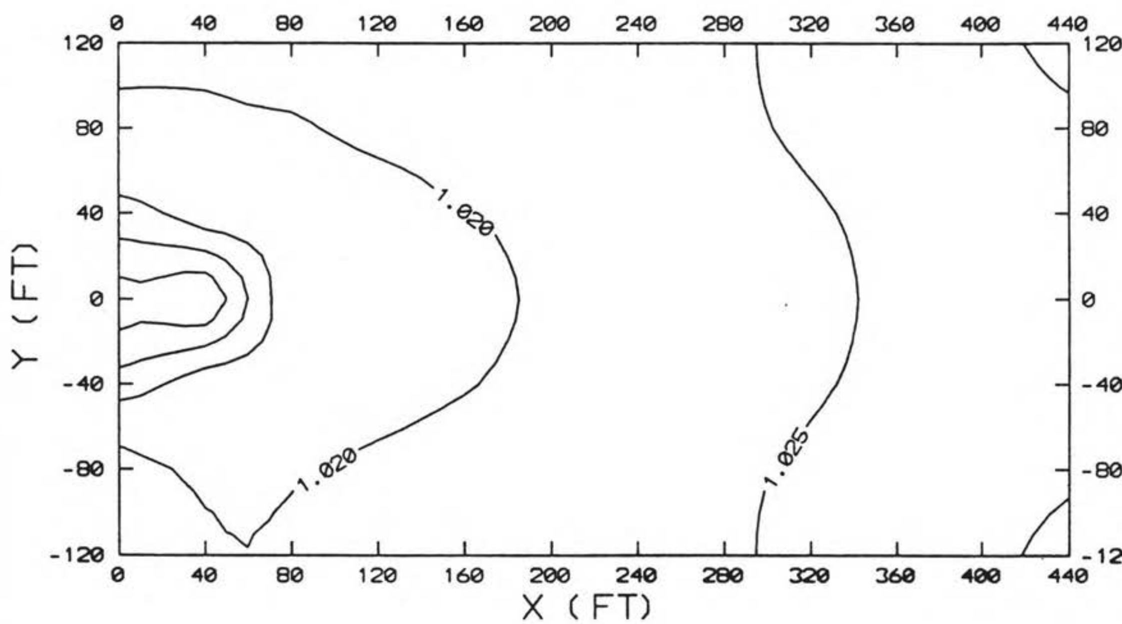


Figure 8.20 Prediction Error Variance for Linear Trend Surface Model Fit to Ten Years of Monthly Data from 50 Wells; a) predicted; b) with optimal sampling network

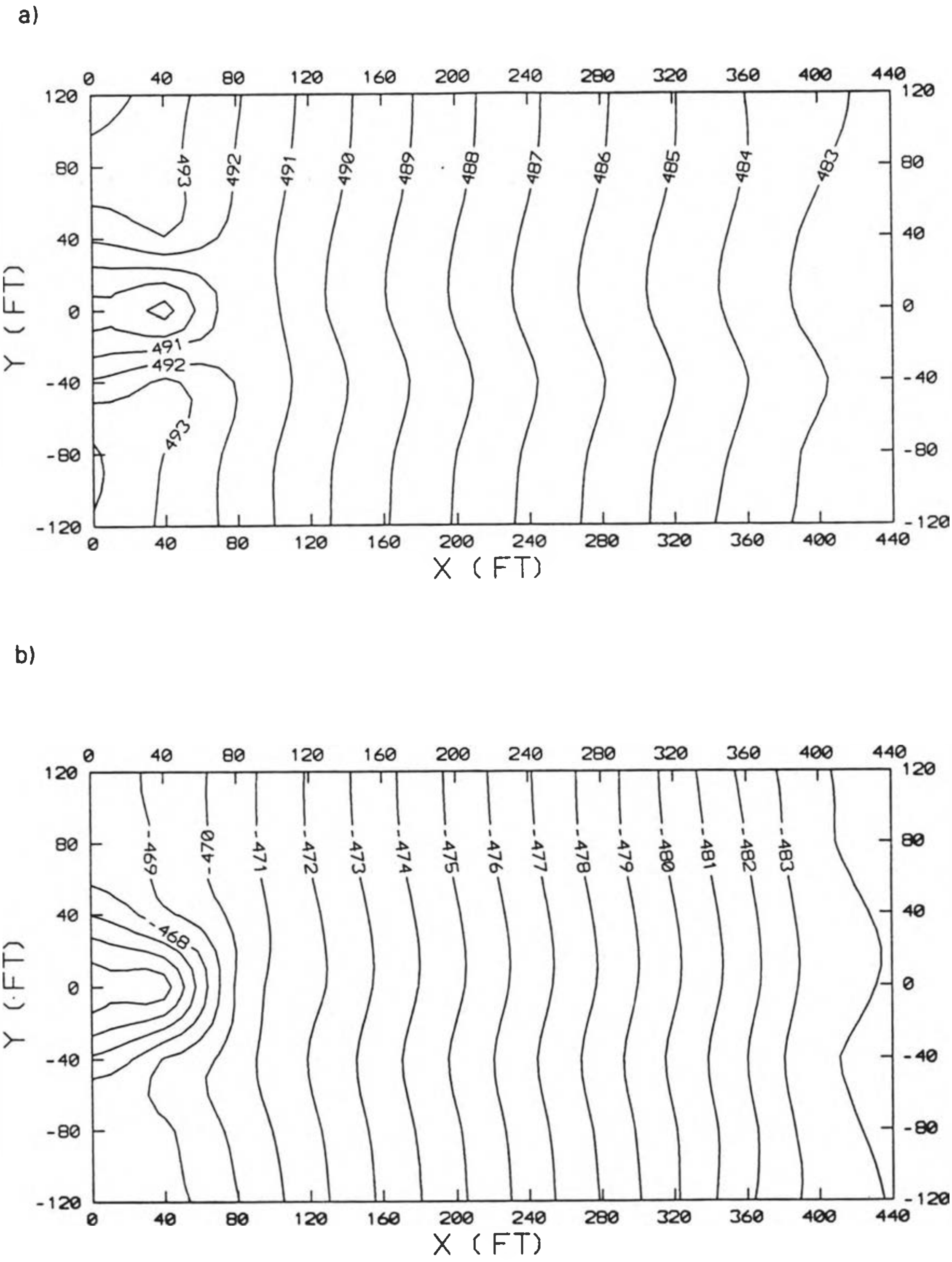


Figure 8.21 Upper (a) and Lower (b) 95% Confidence Bounds on Predicted Concentrations for Linear Trend Surface Model Fit to 10 Years of Monthly Data

Table 8.17 Data Error Variance over which Model Provides "Best" Predictor

YEAR[a]	LINEAR TREND	QUADRATIC TREND	CUBIC TREND	PHYSICAL
2	> .0116	< .0016 & > .0029	None	< .0029
3	> .0356	< .0356 & > .0029	None	< .0055
4	None	None	None	All
5	None	None	None	All
6	None	None	None	All
7	None	None	None	All
8	None	None	None	All
9	None	None	None	All
10	None	None	None	All

(a) Record Length for Model Fit

These differences in the monitoring network optimization for the correct physical model versus incorrect linear trend surface model are illustrated by a comparison of the predicted plume, with confidence limits defined based on the prediction error variance for the model fit to two years of data with an error coefficient of variation equal to .05. Figures 8.22a and 8.22b illustrate the upper and lower 95% confidence concentration contour plots for the linear trend surface model. These

Table 8.18 Comparison of Maximum Single Prediction Error Variance[a] at a Well for Existing and Future Monthly Sampling Frequency; Minimum Spatial Error Prediction Correlation = 0.9

YEAR[b]	LINEAR TREND	QUADRATIC TREND	CUBIC TREND	PHYSICAL
2	1.0230	1.8312	30.679	11.528
3	1.0165	1.5511	20.960	3.0257
4	1.0123	1.4080	15.769	1.2698
5	1.0098	1.3230	12.660	1.0566
6	1.0082	1.2670	10.606	1.0157
7	1.0070	1.2280	9.1921	1.0060
8	1.0061	1.1988	8.1234	1.0019
9	1.0054	1.7614	7.2961	1.0007
10	1.0049	1.1580	6.6373	1.0003

(a) Value shown * (model Error Variance + Data Error Variance) equals the sum of prediction variance for the designed monitoring network

(b) Record Length for Model Fit

Table 8.19 Data Error Variance over which Model Provides "Best" Minimum Single Well Location Error Prediction Variance

YEAR[a]	LINEAR TREND	QUADRATIC TREND	CUBIC TREND	PHYSICAL
2	> .00157	None	None	< .00157
3	> .00961	<.00961 & >.00798	None	< .00798
4	> .05642	None	None	< .05642
5	> .2772	None	None	< .2772
6	> 1.5343	None	None	<1.5343
7	None	None	None	All
8	None	None	None	All
9	None	None	None	All
10	None	None	None	All

(a) Record Length for Model Fit

figures can be compared to Figure 8.15 for the physical model fit to the same data set. Clearly, the incorrect linear trend surface model has a larger uncertainty associated with it then does the physical model and results in a monitoring network with a lower confidence level.

Regardless of the model selected to simulate the behavior of the data, the optimization technique explicitly incorporates information on the model structure and uncertainty in the model into the monitoring network design process. The optimization requires that the groundwater quality manager specify a minimum desired spatial correlation. The uncertainty in predicted groundwater quality can be plotted for the resulting optimal network. This uncertainty surface can be used by the manager to adjust the required minimum spatial correlation to achieve the desired confidence in the monitoring as required by the information goals.

Clearly, as available data increases, the uncertainty in the model reduces, as does the data needs in the monitoring network. Therefore, confidence in the model structure can replace monitoring of wells. The uncertainties associated with the model can be quantified and incorporated in the monitoring network design process by using the techniques described herein. If the uncertainty associated with a parameter variance matrix is too high, as represented by a large objective function value or a low minimum spatial error correlation, then the optimal monitoring network should be designed to minimize V_β rather than the prediction error variance. This can be done by sampling where the prediction error variance is a maximum. The same branch and bound technique can be used where

$$\mathrm{MAX}\ Z_j = \sum_{i=1}^{n} \mathrm{VAR(I)} * \mathrm{VL(I)}$$

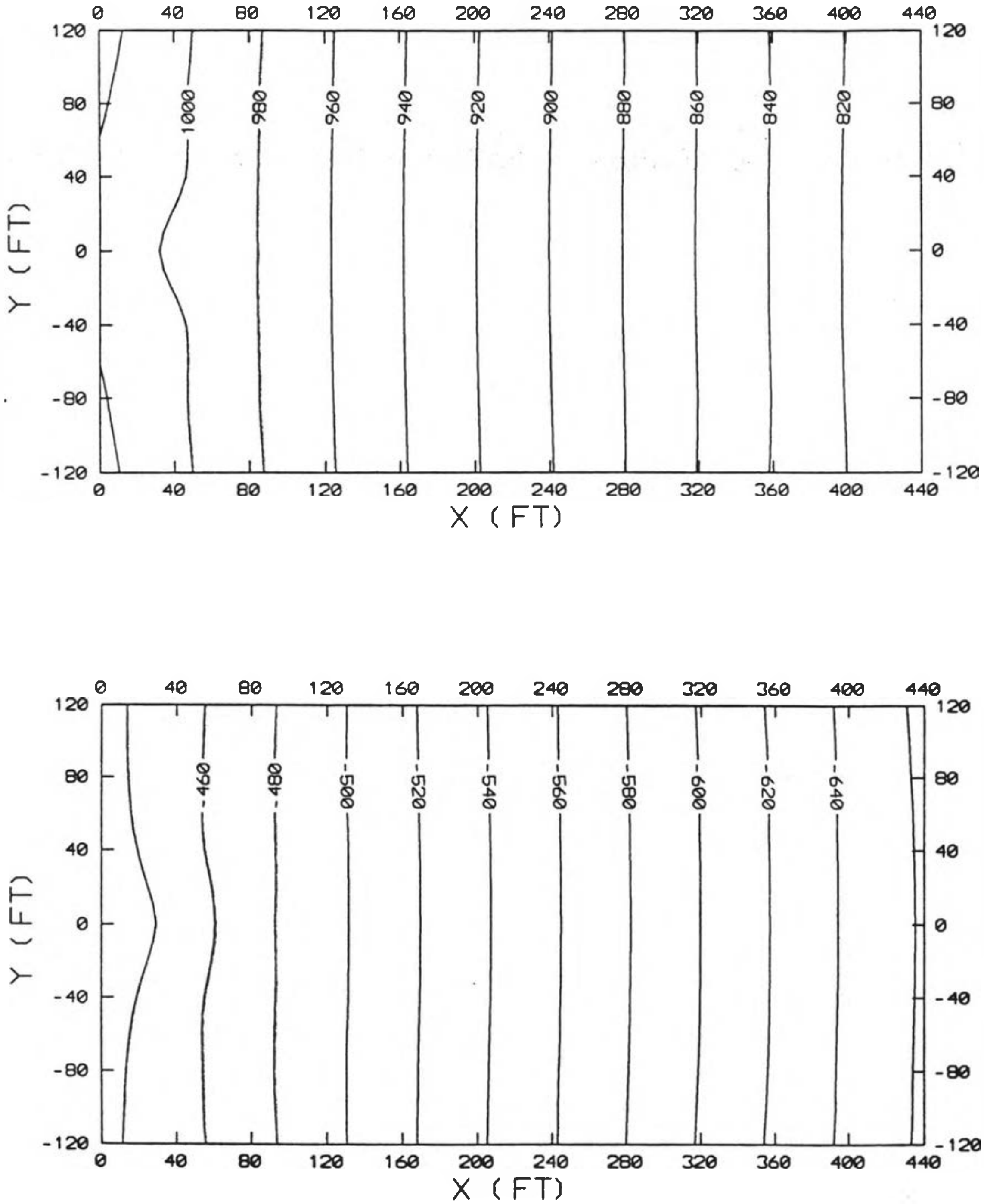


Figure 8.22 Predicted Upper (a) and Lower (b) 95% Confidence Bounds on Concentration Based on Linear Trend Surface Model Fit to Two Years of Monthly Data from 50 Wells

Subject to,

$$CORR(I,J) \leq CORRMIN \; \forall \; I \text{ and } J \text{ where } VL(I) = 1 \text{ and } VL(J) = 1$$

Either objective goal can be met by using a form of the prediction error variance and some form of spatial correlation in the branch and bound optimization technique. In some cases, a combination of these goals may be appropriate.

9. MONITORING NETWORK DESIGN PROTOCOL

The design of a groundwater quality monitoring network includes the definition of well locations, sampling frequency, and the designation of analytes. This study has focused on the determination of the first two monitoring network design components. The determination of these two components is dependent on the information objectives of the monitoring network relative to the groundwater quality data behavior. The information objectives of a groundwater quality monitoring network are generally to either increase the understanding of the system or to maintain a specified level of understanding in the system. This "understanding" can be expressed as a confidence in the existing system and in future conditions of the system.

The simulation study discussed in Chapter 8 reviewed statistical methods used to assess the applicability of a model to both describe and predict groundwater quality. In addition, the structure of the selected models as well as uncertainty in the models were incorporated explicitly into the design of monitoring networks. Based on this simulation study, the five principal steps recommended for a monitoring network design protocol are:

1) select model(s) and divide record into subsets based on record length, sampling density, and sampling frequency,
2) fit model to data subsets,
3) calculate and evaluate model goodness-of-fit,
4) calculate and evaluate model predictions, and
5) design optimal monitoring network.

The interactive nature of these steps is outlined in Figure 9.1. Each of the steps is described in more detail below.

9.1 Step 1 - Select Model.

A model of a groundwater system is selected based on the review of available information. The ability to select an appropriate model structure is dependent on the amount of data available. The simplest structure applicable should be applied first to the data. Subsequent refinements to the three-dimensionality of the model structure and to the non-homogeneity of the model parameters should be made as confidence in the model increases or as the data needs from the monitoring network system become more complex. Generally, a class or group of related models may be selected which may be appropriate for further consideration.

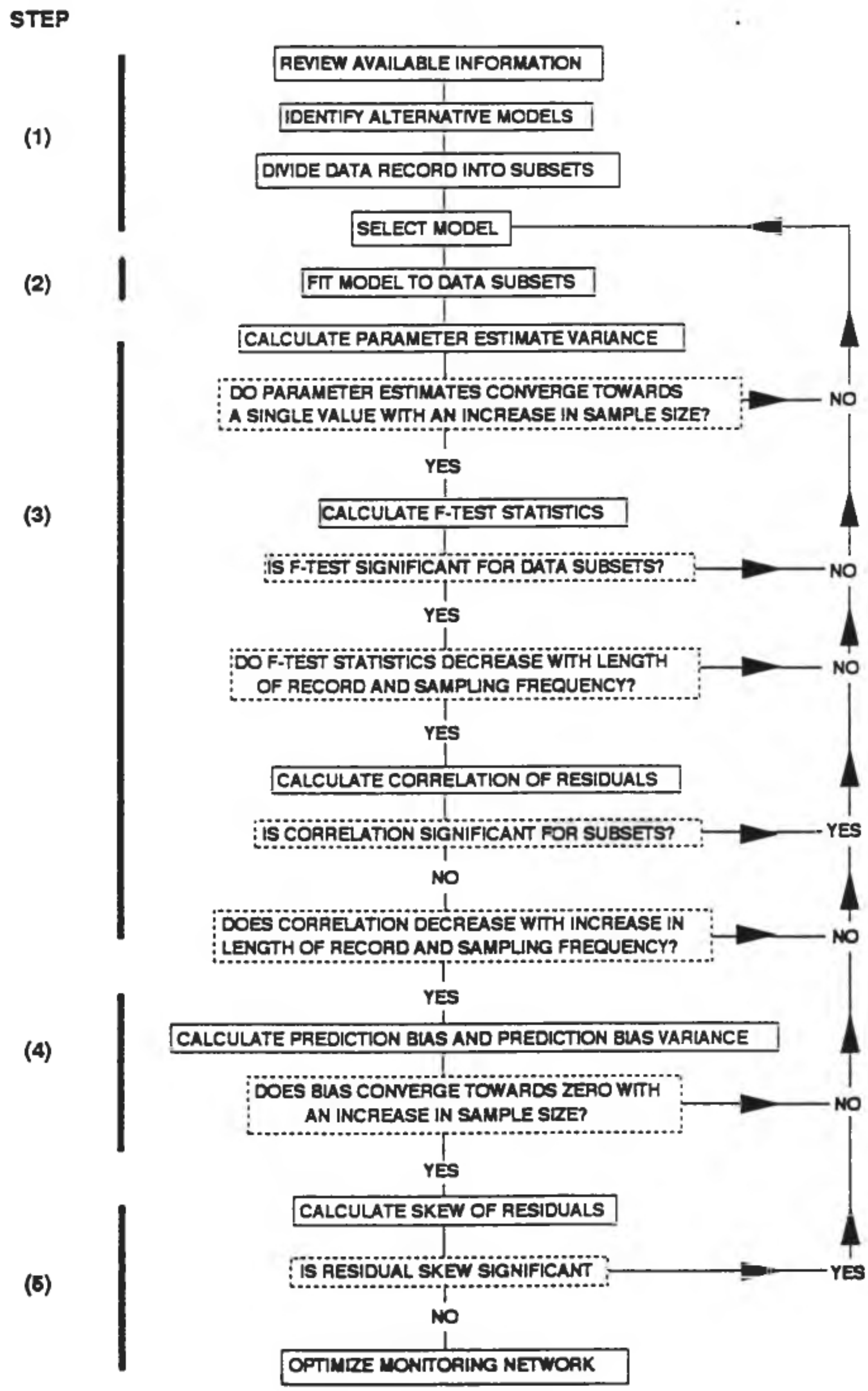


Figure 9.1 Monitoring Network Design Protocol

In evaluating the applicability of a model, it is important to evaluate the fit of the model to a number of data subsets. Consistency in the statistics' behavior is more important than the significance of a single statistic. This was shown in the simulation study (Chapter 8) where a model could be significant based on the results of the model applicability analysis for the model fit t o a single data set, but be incorrect. However, for these incorrect models, the statistical tests did not consistently become more significant as the record length, sampling frequency, or sampling density increased. Therefore, the ability to identify that a model is incorrect is based on the behavior of the statistic as the sampling frequency, sampling density, and record length increase, rather than the significance of the numeric value of the statistic itself. Therefore, the first step in designing a monitoring network includes the subdivision of the existing data into multiple subsets based on sampling frequency, sampling density, and record length.

9.2 Step 2 - Fit Model to Data Subsets.

The model parameters for a selected model structure can be estimated using a variety of techniques as described in Chapter 4. In this study, a least squares regression was used to fit the models to the data. As shown in Chapter 4, this least squares regression parameter estimation technique provides efficient, consistent, and sufficient parameter estimates for the correct model when the errors are zero mean and additive. The parameter estimates can also be made to be efficient, sufficient and consistent by using a weighted least square regression when the error is data-dependent (non-additive). However, the relationship of the dependence must be known so as to properly weight the data.

9.3 Step 3 - Evaluate Model Goodness-of-fit.

The significance of the model needs to be evaluated by goodness-of-fit tests. Three classes of model applicability tests are recommended: analysis of variance, model parameter behavior, and residual behavior. The F-test statistic, used to evaluate the analysis of variance, should be significant and should increase with an increase in sampling frequency or number of wells. The parameter estimates should converge towards the "true" parameter values within specified confidence limits as defined by the parameter variance. Lastly, the residuals should not be significantly correlated and should converge towards zero as the data set increases. If these conditions are not met, then the selection of model structure should be reevaluated. If any of the statistical tests fail the criteria for model goodness-of-fit, then the behavior of the failed statistical tests should be carefully evaluated in order to identify potential alternative model structures.

9.4 Step 4 - Calculate and Evaluate Prediction Statistics.

As for the goodness-of-fit tests, the important aspect of the prediction test is the behavior of the prediction bias. Specifically, the prediction bias should converge towards zero, the prediction bias variance should decrease as the data set increases, and the prediction bias should not be significant. If any of these behaviors are not observed, then the model structure or the assumed error distribution should be reevaluated. As for the goodness-of-fit tests, the non-systematic behavior of the prediction bias can be used to help identify other more appropriate model structures for consideration.

9.5 Step 5 - Monitoring Network Design.

If the model meets both the goodness-of-fit and prediction tests as described above, then the data is consistent with the hypothesized model structure and a monitoring network can be designed based on the model structure, model parameter estimates, parameter uncertainty, and data error uncertainty. The information goal of the monitoring network will be to either increase or maintain the confidence in the understanding of the groundwater quality system. The certainty in the system can be quantified via the model prediction uncertainty. A monitoring network can then be designed to meet the required confidence in the groundwater quality system.

Prior to optimizing the model network, the skew of the residual should be evaluated. If the skew is significant, the behavior of the skew with an increase in data should be evaluated to aid in error distribution distinction. This error distribution can be incorporated in the optimization, or the model can be refitted to the data using a weighted least squares regression to account for the error distribution.

The tradeoff between optimization of an existing monitoring network and additional modeling or additional data collection is dependent on the required confidence in the model to meet the information goals of the monitoring network. If there is insufficient certainty in the model as described by either the model error or model parameter variance matrix, then a system should be designed to increase the model certainty. The limitations of the optimization based on the certainty of the model can be realized by evaluating the maximum spatial correlation obtainable for a given data set as well as evaluating the prediction error variance function, as described in Chapter 8. For instance, a desired minimum spatial correlation may not be realized with the existing monitoring network. The branch and bound technique can be used to identify additional sampling locations and sampling frequencies to meet a desired spatial correlation of errors, or samples.

If the certainty in the model is sufficient to meet the specified information objectives, the branch and bound optimization technique can be used to design a system which maintains a specified confidence level in the model. Specifically, the optimal monitoring networks for different future sampling frequencies can be compared and evaluated relative to the prediction error variance surface predicted.

The design of a monitoring network is not a static system, but must always be reevaluated for adequacy as new data is collected. The frequency of these reevaluations should be considered when designing the monitoring network so as to optimize the network for that period of time given the information objective(s) of the system.

10. CASE STUDIES

The monitoring network design protocol, developed based on the results of the simulation study, as summarized in Chapter 9, was applied to groundwater quality data collected at the IBM facility in East Fishkill, New York. The purpose of this case study evaluation was not to necessarily identify the best model for the data, but rather to test the general applicability of the monitoring network design procedures developed.

IBM's facility in East Fishkill, New York manufactures semiconductors. The facility employees over 10,000 people and occupies 750 acres. All the process and potable water required on site is obtained from groundwater underlying the site. To meet the corporate environmental policy to "...meet or exceed all environmental regulations", a site-wide investigation of groundwater was initiated in 1978. This investigation identified three principal areas on the site with groundwater quality concerns, identified as Areas A, B, and C, on Figure 10.1. In all three areas, the

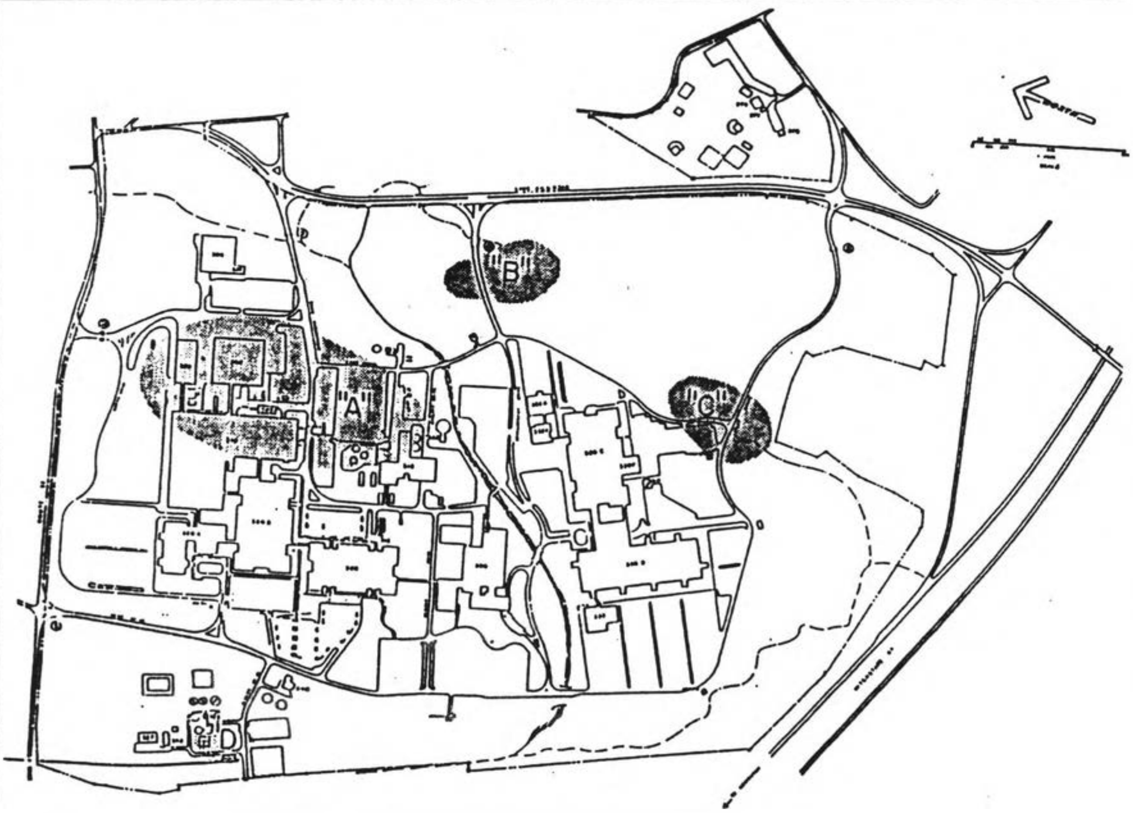


Figure 10.1 IBM East Fishkill Facility Site Location

most prevalent of the chlorinated hydrocarbons detected in groundwater is perchloroethylene (PCE), with levels ranging from non-detectable to 10 mg/l.

The discovery of chemicals of concern in groundwater instigated a groundwater quality monitoring program in 1979 which included periodic groundwater sampling and additional hydrogeologic investigations. The investigation of the distribution and movement of the chlorinated hydrocarbons in the subsurface at the East Fishkill facility has resulted in a groundwater database consisting of over 470 well points. Currently, approximately 100 of those well points are sampled on a routine basis for water quality.

Two areas, designated as Areas A and C, were selected for application of the monitoring network design protocol at the IBM East Fishkill facility. As of January 1988, eighty-three (83) groundwater wells had been installed in Area A and twenty-seven (27) wells had been installed in Area C. These wells have been sampled for periods ranging from one to nine years, with frequencies ranging from approximately biweekly to biannual. The constituent Perchloroethylene (PCE) was selected for analysis since this chemical is the most prevalent at the site.

The model applicability analyses and monitoring network optimization for the PCE groundwater quality data are discussed below for Areas A and C on the IBM East Fishkill facility. The evaluation is consistent with the protocol summarized in Chapter 9, and follows the following five steps:

1) Select Model(s) and Divide Data Record into Subsets
2) Fit Model(s) to Data Subsets
3) Calculate and Evaluate Model Goodness-of-fit
4) Calculate and Evaluate Model Predictions
5) Design Optimal Monitoring Network

The physical and statistical models discussed in the simulation study were selected as candidate models for describing the groundwater quality data collected at the IBM facility. The models were fit to data subsets consisting of record lengths ranging from one (1980) to nine (1980-1988 inclusive) years of data, with sampling frequencies consisting of all the available data as well as reduced frequencies of bimonthly, quarterly, triannual and biannual. All wells available for a specific record length were included in the data subsets. No vertical segregation of the data was performed.[31]

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[3] It is recognized that the subsurface is characterized by two primary geologic units: the fractured bedrock and the overburden. However, rather than dividing the data vertically into these two zones, the models were applied to the data assuming a vertically homogeneous environment. The purpose of this case study evaluation was to evaluate the protocol rather than to identify the best model for the data used.

The statistical models were fit to the data using linear least-squares regressions. Two Fortran Computer codes, FDSWT and AWT, were written to calculate the best-fit parameter values and goodness-of-fit and predictive test values for the single-site polynomial and trend surface models, respectively. These codes are included in Appendix D. For a highly variable data set, convergence is often difficult for a non-linear model. Therefore, limitations on the ranges of the parameter values were imposed on the physical model parameter values based on additional site information. The computer code FDP (also included in Appendix D) was written to fit the physical model to the data.

The models were considered for application in order of most simple (single-site polynomial) to most complex (physical). The results of the goodness-of-fit and predictive tests were used to select a candidate model. Monitoring networks were then designed for all models considered based on error prediction and optimization techniques, as developed in Chapters 6 and 7, and as applied to the simulated data in Chapter 8. The fortran computer code, PARV, was written to calculate the parameter variance matrix for the physical model, as included in Appendix E. A series of computer codes were written to perform the optimization procedure for the various models considered, as follows:

VARFSS -	calculates the parameter variance matrix for the single-site polynomial models, field data
VARFTS -	calculates the parameter variance matrix for the trend surface models, field data
VARFP -	calculates the parameter variance matrix for the physical model, field data
OPTFSS -	calculates the prediction error variance for the single-site polynomial models, field data
OPTFTS -	calculates the prediction error variance for the trend surface models, field data
OPTFP -	calculates the prediction error variance for the physical model, field data
BBFTS -	performs the branch and bound optimization procedure for the trend surface models, field data
BBFP -	performs the branch and bound optimization procedure for the physical model, field data

These computer codes are included as Appendix F.

The results of the model goodness-of-fit tests (Protocol - Step 3) and model prediction tests (Protocol - Step 4) are discussed for each model applied to the data in Area A (Section 10.1.1) and Area C (Section 10.2.1). The design of optimal montioring networks (Protocol - Step 5) is then evaluated for each of the models in (Area A - Section 10.1.2 and Area C - Section 10.2.2).

10.1 Area A.

Area A is shown on Figure 10.1. The source of PCE in this area is believed to have been leaks and spills associated with solvent storage and handling.

10.1.1 Model Selection.

The selection of a model (from among those models used in the simulation study) for describing the PCE groundwater quality in Area A is based on the protocol outlined in Chapter 9. Specifically, goodness-of-fit is evaluated based on the results of F-test analyses, model parameter behavior, and residual behavior. Model prediction capabilities are then evaluated using prediction bias, prediction bias variance, and the associated t-test statistic.

10.1.1.1 Single-site Polynomial Models. The F-test results for the significant single-site polynomial models fit to the data from Area A are summarized in Table 10.1. For the single-site polynomial models, approximately one-half of the wells in Area A did not exhibit any significant linear trend. Those wells that did exhibit significant polynomial trends tended to be significant at lower orders. The behavior of the estimated parameters was not evaluated for those wells which exhibit significant polynomial trends due to the relatively small data sizes.

The residuals were evaluated for the single-site polynomial models fit to all the data for each well. Because sampling frequencies were not consistent in time, temporal lag-one residual correlations were calculated assuming all samples were equally spaced. Table 10.2 summarizes the residual temporal correlations for the significant polynomial models significant based on the results of the F-test analysis. None of the residual correlations were significant at the $\alpha = 0.05$ confidence level. In addition, as the record length increased, the residual correlations tended to decrease, which is consistent with the expected behavior for a correct model. However, since the residual correlations were also not significant for data from wells with an insignificant polynomial trend, the evaluation of the residual correlation did not aid in model discrimination.

The skewness of the residuals for the significant single-site polynomial models is summarized in Table 10.3. Those record lengths which exhibited a significant model fit based on the results of the F-test and residual behavior are highlighted. None of the residual skewness statistics were significant at the $\alpha = 0.05$ confidence level. In addition, there was no observable trend to the skewness of the residuals with an increase in record length. Therefore, based on the results of the simulation study, it is inferred that the error in the data is not non-normally distributed and the F-test statistics are valid.

Based on the results of the goodness-of-fit tests, the single-site polynomial model appears to be a relatively good model for some wells and record lengths as exhibited by a significant F-test value and insignificant residual correlation and residual skew.

Table 10.1 F-test Results for Significant Single-site Polynomial Models Fit to Data From Area A

			F Test Results		
Well	Number	Years of	Period of Significance[a]		
No.	of Samples	Data[a]	Linear	Quadratic[b]	Cubic[b]
11	52	1980-87	1980-81	1981	1981
12	32	1980-85	1982	NS	(d)
13	26	1980-86	1980-81	NS	(d)
15	63	1980-87	1986	NS	(d)
16	65	1980-88	1986-87	NS	(d)
17	65	1980-88	1980,1985-87	198	1985
18	27	1980-87	1982-83	198	NS
19	49	1980-87	1980-83	1982-83	1982-83
20	51	1980-87	1986	NS	(d)
21	51	1980-87	1980,83-84,87	NS	(d)
22	62	1980-87	1980-82	1981-82	1982
39	10	1980-87	1985,1987	NS	(d)
44	12	1980-83	1984-86	NS	(d)
74	15	1982-84	1983	NS	(d)
103	35	1981-87	1983-84,1986	1983,1986	NS
105	17	1981-87	1983	NS	(d)
106	19	1981-87	1982-83	NS	(d)
109	19	1981-88	1983-87	1983,1985-87	(e)
117	27	1981-87	1985-87	NS	(d)
118	24	1981-87	1985-87	NS	(d)
126	9	1981-86	1985,1987	1985	1985
129	8	1982-87	1983	(e)	(e)
130	10	1981-87	1983,1986-87	NS	(e)
731	4	1987	1987	(e)	(e)
734	4	1987	1987	(e)	(e)
752	4	1987	1987	(e)	(e)
822	7	1982-86	1983	NS	NS
823	11	1982-87	1987	NS	(d)
934	14	1984-87	1987	NS	(d)
965	7	1985-87	1986-87	1986-87	1986-87

a) Record Length for period from 1980 through year noted
b) F-test addition over lower order polynomial
c) NS = not significant
d) lower order model not significant
e) insufficient data record length

Table 10.2 Residual Temporal Correlations[a] for Single-Site Polynomial Models Fit to Data from Area A

Linear Model

	RECORD LENGTH (years)							
Well No.	1980	80-81	80-82	80-83	80-84	80-85	80-86	80-87
11	0.0364	0.0402	0.0343	0.0253	0.0200	0.0151	0.0145	0.0142
12	0.0249	0.0249	0.0258	0.0164	0.0056	0.0048		
13	0.0107	-0.0163	-0.0130	-0.0003	-0.0000	-0.0002	-0.0006	
15	0.0059	-0.0040	-0.0002	-0.0051	-0.0028	-0.0018	-0.0012	-0.0003
16	-0.0596	-0.0056	-0.0021	-0.0002	0.0014	0.0014	0.0012	0.0011
17	-0.0044	0.0329	0.0290	0.0234	0.0164	0.0126	0.0107	0.0099
18			-0.1493	-0.0583	-0.0064	-0.0043	-0.0033	-0.0029
19	-0.0370	-0.0370	0.0303	0.0052	0.0182	0.0143	0.0140	0.0137
20	-0.0066	0.0101	0.0117	0.0093	0.0024	-0.0028	-0.0017	-0.0008
21	-0.0918	0.0350	0.0287	0.0208	0.0116	0.0105	0.0001	-0.0001
22	-0.0183	0.0079	0.0220	-0.0027	-0.0004	-0.0002	-0.0001	-0.0001
39	-0.0724	-0.0724	-0.0668	-0.0520	-0.0520	-0.0271	-0.0271	-0.0015
44			-0.1690	-0.0984	-0.0634	-0.0634	-0.0634	-0.0354
74			-0.0671	-0.0108				
103			-0.0195	0.0081	0.0265	0.0323	0.0240	
105			-0.0460	-0.0264	-0.0327	-0.0203	-0.0166	
106			-0.0385	-0.0257	-0.0210	-0.0129	-0.0103	
109			-0.0917	-0.0128	0.0045	0.0079	0.0057	
117			0.0463	0.0160	0.0046	0.0046	0.0044	
118			-0.0438	-0.0015	0.0176	0.0158	0.0142	
126			-0.0040	-0.0408	0.0422	0.0105		
129				-0.0456	-0.0501	-0.0107	0.0055	
130			-0.1734	-0.0401	-0.0169	-0.0151	-0.0174	
716						-0.0990		
731						-0.0930		
734						-0.1890		
752						-0.2011		
822			-0.1597	-0.0568	-0.0568	-0.0635		
823			-0.0593	-0.0842	-0.0399	-0.0321	-0.0243	
934					0.0261	0.0123		
965					-0.0082	-0.0279		

continued

Table 10.2, continued

Quadratic Model

Well No.	RECORD LENGTH (years) 1980	80-81	80-82	80-83	80-84	80-85	80-86	80-87
11	0.03933	0.02527	0.02086	0.02529	0.02529	0.01992	0.01437	0.01416
17	-0.0092	-0.0131	0.02925	0.02057	0.02057	0.01428	0.01063	0.00940
18			-0.0816	-0.0816	-0.0060	-0.0036	-0.0039	
19	-0.0265	-0.0265	0.02261	0.00505	0.00505	0.01019	0.00796	0.00781
22	-0.0353	-0.0154	0.00596	-0.0028	-0.0028	-0.0016	-0.0003	-0.0005
103			-0.1808	-0.04	-0.0400	0.00845	0.02713	0.02192
			-0.1831	-0.1831	-0.0205	0.02220	0.01712	
126			-0.1110	-0.1110	-0.0245	-0.0055	0.00320	
965					-0.0478	-0.0760		

Cubic Model

Well No.	RECORD LENGTH (years) 1980	80-81	80-82	80-83	80-84	80-85	80-86	80-87
11	-0.0254	0.0209	0.02384	0.01763	0.01955	0.01500	0.01431	0.01416
17	-0.0145	-0.0375	0.00462	0.01829	0.01416	0.01173	0.00920	0.00940
19	-0.0237	-0.0237	-0.0295	0.00451	0.00621	0.00822	0.00775	0.00781
22	-0.0359	-0.0169	-0.0148	-0.0088	-0.0022	-0.0007	-0.0006	-0.0005
965					-0.1285	-0.0760		

(a) correlations significant at the $\alpha = 0.05$ level are highlighted

Table 10.3 Residual Skewness[a] for Single-site Polynomial Models Fit to Area A Data

Linear Model

	RECORD LENGTH (years)							
Well No	1980	80-81	80-82	80-83	80-84	80-85	80-86	80-87
11	0.0093	0.0290	0.0686	0.0675	0.0652	0.0580	0.0569	0.0556
12	0.0891	0.0891	0.0657	0.0132	0.0203	0.0185		
13	-0.0366	0.0175	0.0898	0.0962	0.0925	0.0740	0.0533	
15	-0.0161	0.1905	0.1726	0.1034	0.0933	0.0816	0.0719	0.0636
16	0.1962	0.1746	0.1636	0.1170	0.0796	0.0631	0.0560	0.0530
17	0.0797	0.0668	0.0704	0.0457	0.0353	0.0287	0.0258	0.0229
18	0.1172	0.0648	0.1038	0.1398	0.1783	0.1515	0.1488	0.1480
19	0.0648	0.0952	-0.0660	-0.0005	0.0106	0.0156	0.0154	0.0154
20	0.0844		0.0932	0.0852	0.1044	0.0484	0.0343	0.0364
21	0.0189	-0.0198	-0.0190	-0.0160	0.0015	0.0579	0.1247	0.1073
22	-0.1150	0.0111	-0.0031	0.1698	0.1596	0.1400	0.1270	0.1207
39	-0.0965	-0.0965	-0.1523	-0.1376	-0.1376	-0.0903	-0.0903	-0.0420
44			0.0354	-0.0009	0.0309	0.0309	0.0309	0.1105
74			0.1258	0.1091	0.1856			
103			-0.1455	0.0449	-0.0073	0.0500	0.0189	0.0469
105			-0.2454	-0.1402	0.1335	0.0847	0.0977	0.0891
106			0.0368	0.0223	0.1698	0.1801	0.1852	0.1610
109				-0.1283	0.0005	0.0187	0.0844	0.0981
117			0.0087	0.0503	-0.0046	-0.0437	-0.0437	-0.0459
118				0.2546	0.0851	0.0070	0.0069	0.0000
126				0.1580	0.1432	0.0194	0.0727	
129				0.2353	-0.0084	0.0930	0.1646	0.1771
130			0.0145	-0.0058	0.0929	0.0660	0.0812	0.0477
731							-0.2311	
734							0.1535	
752							-0.1839	
822				-0.0197	0.0786	0.0786	0.2571	
823				-0.0747	0.0515	0.0930	0.0730	0.0681
934						-0.0564	-0.0288	
965						-0.1207	0.0591	

Table 10.3, continued

Quadratic Model

Well No	RECORD LENGTH (years) 1980	80-81	80-82	80-83	80-84	80-85	80-86	80-87
11	0.03016	.01790	-0.0300	0.06482	0.06482	0.05824	0.05044	0.04927
17	0.08352	0.11558	0.06678	0.04333	0.04333	0.03254	0.02571	0.02144
18			0.06910	-0.1029	-0.1029	0.18603	0.15165	0.14522
19	0.07282	0.07282	-0.0706	0.00176	0.00176	-0.0135	-0.0035	-0.0058
22	-0.1206	0.00902	0.00592	0.16759	0.16759	0314647	0.12143	0.11255
103			0.19309	-0.1998	-0.1998	-0.0082	-0.0129	0.03402
109				0.16629	0.16629	-0.1236	-0.0460	-0.0380
				0.19989	0.19989	-0.0749	0.05864	-0.0174
65							-0.0665	0.02671

Cubic Model

Well No.	RECORD LENGTH (years) 1980	80-81	80-82	80-83	80-84	80-85	80-86	80-87
11	0.06427	0.01261	-0.0022	0.02345	0.05541	0.05018	0.05237	0.04927
17	-0.0308	0.0959	0.09990	0.06562	0.03005	0.02877	0.02173	0.02144
19	0.06740	0.0674	-0.0237	-0.0025	-0.0043	-0.0041	-0.0051	-0.0058
126				-0.1300	-0.1274	-0.0742	-0.0174	-0.0174
965							-0.0945	0.02671

(a) skewness coefficients signficant at the $\alpha = 0.05$ level are highlighted

For these significant single-site polynomial models based on the goodness-of-fit tests, the average one-year prediction bias and associated t-test statistics are summarized in Table 10.4. Those biases associated with record lengths which exhibited a significant polynomial trend based on the results of the F-test and residual behavior are highlighted. T-test statistics significant at the $\alpha = 0.05$ level are also highlighted. Many of the one-year prediction biases were significant for the wells and record lengths which exhibited significant polynomial trends. However, as the record lengths increased, the significance of the prediction bias for the significant models based on the F-test analysis tended to decrease. From these predictive tests, it appears that the single-site polynomial models are, in general, poor models for describing the observed PCE groundwater behavior in Area A. Those wells which did exhibit significant polynomial trends based on the goodness-of-fit tests generally exhibited significant prediction biases. These results suggest that another model would be more appropriate at describing the data.

10.1.1.2 Trend Surface Models. Linear, quadratic and cubic trend surface models were fit to the data from Area A. The F-test results for the multi-site models fit to the data from Area A are summarized in Table 10.5. The linear trend surface model was significant for all record lengths considered when fit to all the available data for a specific record length (i.e., no sampling frequency reduction). The quadratic and cubic trend surface models were significant for all record lengths considered, excluding the five-year period from 1980 through 1985 in which a linear trend

Table 10.4 One-Year Prediction Bias[a] and Associated t-tests[b] for Single-site Polynomial Models Fit to Area A Data

Linear Model

Well	1980		1980-81		1980-82		1980-83		1980-84		1980-85		1980-86	
No.	Bias	T-test	Bias	T-test	Bias	T-test	Bias	T-test	Bias	T-test	Bias	T-test	Bias	T-test
11	116.96	6.97	184.77	1.31	106.18	0.71	-84.62	-9.93	-26.41	-3.8	-36.65			
12					-4351		-1944	-0.62	-10	-0.03				
13	-77696	-1.78	-3E+05		-1E+05	-8.19	-28935		-2E+05		150570			
15	44597	1.03	-84288	-2.39	38273	0.36	-42267	-18	-19969	-7.74	998.43	0.43	33281	4.47
16	524.24	5.94	273.01	5.33	-180.8	-5.97	-192.4	-8.2	-82.95	-3.87	-61.38	-47.6	-9.95	-1.27
17	2433	3.13	-747.9	-1.14	-693.2	-4.71	-767.6	-3.54	-446.6	-5.26	400.07	3.85	-274.5	-1.32
18					-71.56		-1.79	-0.12	429.36	0.77	-162.8	-18.2		
19			-449.1	-3.68	-188.4	-1.96	-471.4	-5.34	-219.6	-3.8	-314.3	-70.3		
20	5.02	4.06	3.14	7.7	1.78	1.71	12.11	1.11	6.14	0.63	3.3	0.49	-9.31	-1.63
21	54.46	10.23	3.5	15.66	-9.39		4.7	1.01	51.65	2.75	242.26	1.08	-100.5	-10.6
22	153.26	3.18	199.01	10.65	2033.5	1.14	-437.4	-169	-149.5	-116	-22.43	-3.48	-3.74	-0.48
39			-6.28		0.46				3.05					
44					-1.78	-9.74	0.95	6.73						
74					13387		218412	1.42						
103					-25.79	-3.65	19.65				161.48	4.97	-291	-8.65
105					-0.48	-1.55	1.73		2.74		-1.82	-12.9	-0.25	
106					0.95	0.37	1.95		-5.38		-3.8	-26.9	1.03	1.3
109							42.53		41.66		50.59	22.35	19.1	16.75
117					-2509	-0.11	34670	3.15	912.37	0.04				
118							-40306		79841	3.76	-256.7	-0.03	-25159	-0.69
126							-5.71		120.56					
129							10.76		-20.9					
130					4.06		-0.89		2.01					
823					-11837	-2.2	-5000		-3424					
934													-1.69	

(continued)

Table 10.4, continued

Quadratic Model

Well No.	1980 Bias	1980 T-test	1980-81 Bias	1980-81 T-test	1980-82 Bias	1980-82 T-test	1980-83 Bias	1980-83 T-test	1980-84 Bias	1980-84 T-test	1980-85 Bias	1980-85 T-test	1980-86 Bias	1980-86 T-test
11	232.85	5.58	35.57	0.41	-571.9	-2.27	-64.68	-7.59	14.55	2.09	2.7			
17	1981.8	2.85	-6559	-2.86	-376.8	-2.29	451.24	1.42	618.72	7.28	995.53	7.41	-83.74	-0.46
18					-64.4		50.09	3.76	450.83	0.81	-130.6	-11.9		
19			313.3	1.78	-715.4	-40.2	-481.2	-5.46	318.18	4.21	114.19	5.23		
22	-33.64	-1.12	-586.9	-3.14	1768.1	0.97	-328.9	-40.3	239.23	8.45	205.59	11.13	164.47	5.64
103					40.52		76.75				84.12	2.69	-399.1	-7.77
109							-17.73		-26.04		-49.85	-11	-23.44	-5.98
126							4.28		2.45					

Cubic Model

Well No.	1980 Bias	1980 T-test	1980-81 Bias	1980-81 T-test	1980-82 Bias	1980-82 T-test	1980-83 Bias	1980-83 T-test	1980-84 Bias	1980-84 T-test	1980-85 Bias	1980-85 T-test	1980-86 Bias	1980-86 T-test
11	-1137	-3.13	116.4	0.87	-947.6	-2.72	417.73	3.27	169.79	10.91	35.04			
17	-8560	-3.44	130.9	0.17	8243.3	5.02	1781.7	3.28	162.82	1.92	46.52	0.45	-1377	-2.91
19			-6368	-5.82	-1824	-7	-377.7	-4.8	755.42	6.66	61.49	5.2		
126							40.19		-172.8					

(a) biases associated with wells and record lengths which exhibited a significant trend based on the results of F-test analysis and residual behavior are highlighted

(b) t-test values significant at the $\alpha = 0.05$ level are highlighted

Table 10.5 F-test Results and Associated T-tests for Multi-site Models Fit to Data from Area A

Record Length	Model	FREQUENCY OF SAMPLING All	Bimonthly	Quarterly	Triannual	Biannual	t-test
1980	Linear	6.564	4.781	4.781	3.766	2.148	-0.01878
	Quadratic	2.877 2.199	1.529	2.458	1.117	-0.32739	
	Cubic	5.359	3.905	2.766	3.587	3.709	-1.61468
	Physical	5008.8	10,263.5	1578.1	42335.0	11689.2	-0.08698
	Size	135	82	82	51	37	
1980-81	Linear	9.831	6.372	4.134	4.533	3.104	-0.21767
	Quadratic	9.831	2.875	1.745	1.891	1.305	0.30785
	Cubic	8.364	5.118	2.989	3.098	1.792	0.97995
	Physical	747.5	3992.9	3,1800,000	523.88	5892.6	-0.00884
	Size	222	141	96	92	68	
1980-82	Linear	14.742	10.308	8.226	7.741	5.933	0.06071
	Quadratic	6.104	4.386	3.278	3.057	2.386	0.41598
	Cubic	9.879	6.787	4.931	4.587	3.478	0.66023
	Physical	1488.1	834.9	2152.2	481.22	700.5	-0.00750
	Size	324	237	185	169	135	
1980-83	Linear	20.760	15.387	12.431	11.386	8.594	0.18654
	Quadratic	8.414	6.312	5.013	4.609	3.591	0.07840
	Cubic	14.602	10.392	8.366	7.541	5.854	0.11970
	Physical	1260.2	717.6	30,015.6	1063.4	551.8	-0.00277
	Size	499	521	312	283	215	
1980-84	Linear	4.481	3.245	2.502	2.292	1.873	0.07322
	Quadratic	1.939	1.544	1.319	1.253	1.056	-0.71679
	Cubic	2.948	2.212	1.725	1.643	1.293	0.01145
	Physical	1786.7	843.1	2705.0	841.6	699.9	-0.00128
	Size	683	626	423	380	302	

Table 10.5, continued

Record Length	Model	All	Bimonthly	Quarterly	Triannual	Biannual	t-test
		FREQUENCY OF SAMPLING					
1980-85	Linear	6.047	3.851	2.727	2.411	1.853	0.17061
	Quadratic	2.300	1.484	1.059	0.941	0.738	0.15171
	Cubic	3.412	2.173	1.530	1.297	0.956	0.26766
	Physical	47098.9	9352.7	2307.4	2163.4	2613.9	0.02154
Size		842	626	499	446	355	
1980-86	Linear	7.782	5.137	3.633	3.190	2.444	0.16797
	Quadratic	3.013	2.007	1.414	1.243	0.965	0.15938
	Cubic	4.504	2.676	1.894	1.620	1.208	0.23376
	Physical	1096840.	1077.1	2735.1	2494.8	732.2	0.01484
Size		965	724	575	514	408	
1980-87	Linear	8.794	5.828	3.948	3.451	2.523	0.19497
	Quadratic	3.397	2.282	1.554	1.418	1.044	0.16392
	Cubic	3.908	2.640	1.888	1.631	1.214	0.20403
	Physical	44564.6	2803.2	5272.2	915.6	1217.9	0.01291
Size		1149	869	685	629	491	
1980-88	Linear	8.863	5.869	3.972	3.490	2.547	0.19879
	Quadratic	3.466	2.341	1.608	1.472	1.097	0.15809
	Cubic	3.916	2.623	1.854	1.627	1.202	0.19999
	Physical	38143.5	1877.4	57437.9	26460.3	3911122.3	-0.01732
Size		1162	881	607	641	503	

(a) F-tests significant at α=0.05 level are highlighted surface model was significant but higher order trend surface models were not significant.

As the sampling frequency reduced, the significance of the model reduced for a given record length. This is consistent with the expected behavior of a correct model. The t-test statistics on the linear trend in the F-test values were not significantly different than the theoretical trend for a correct model for either the linear, quadratic or cubic trend surface models. Therefore, based on the F-test analyses, the trend surface models appear to be good models at describing the observed PCE groundwater quality data.

The behavior of selected model parameter estimates are illustrated in Figures 10.2, 10.3, and 10.4 for linear, quadratic and trend surface models, respectively. These figures show that the model parameter estimates converge towards single values within the 95% confidence limit bounds. This behavior is consistent with the expected behavior for a correct model structure.

The average lag-one temporal and lag-zero spatial residual correlations for the multi-site models are summarized in Table 10.6. The lag-one temporal correlations were calculated as described for the single-site polynomial models. The lag-zero spatial correlations between Station 1 and Station 2 were calculated by selecting the sample at Station 2 which was the closest in time to the date of the sample

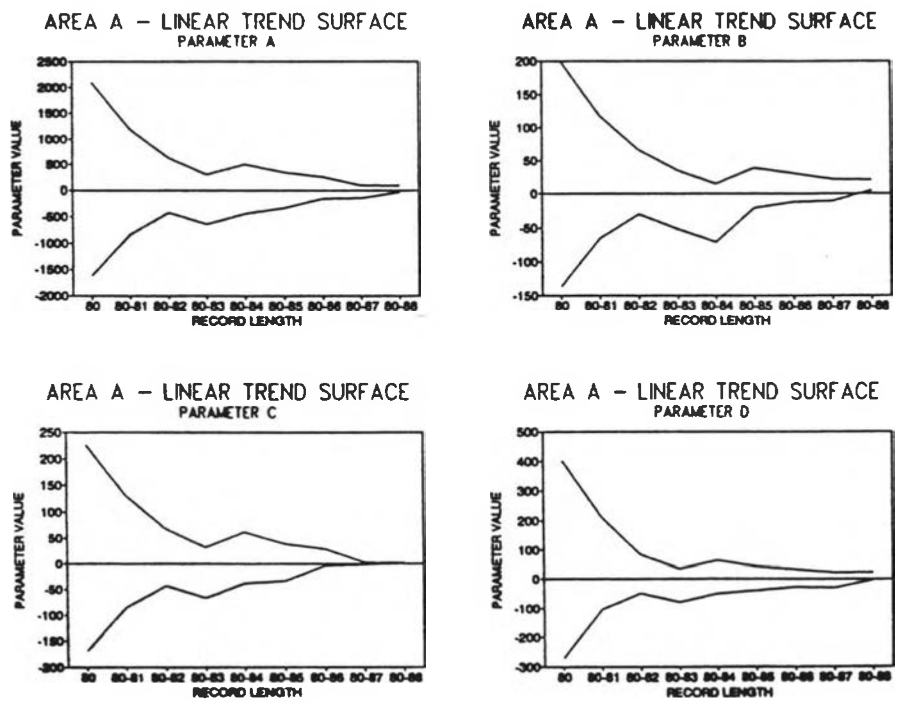

Figure 10.2 Upper and Lower Confidence Limits of Parameter Estimates for Linear Trend Surface Model Fit to All Data in Area A

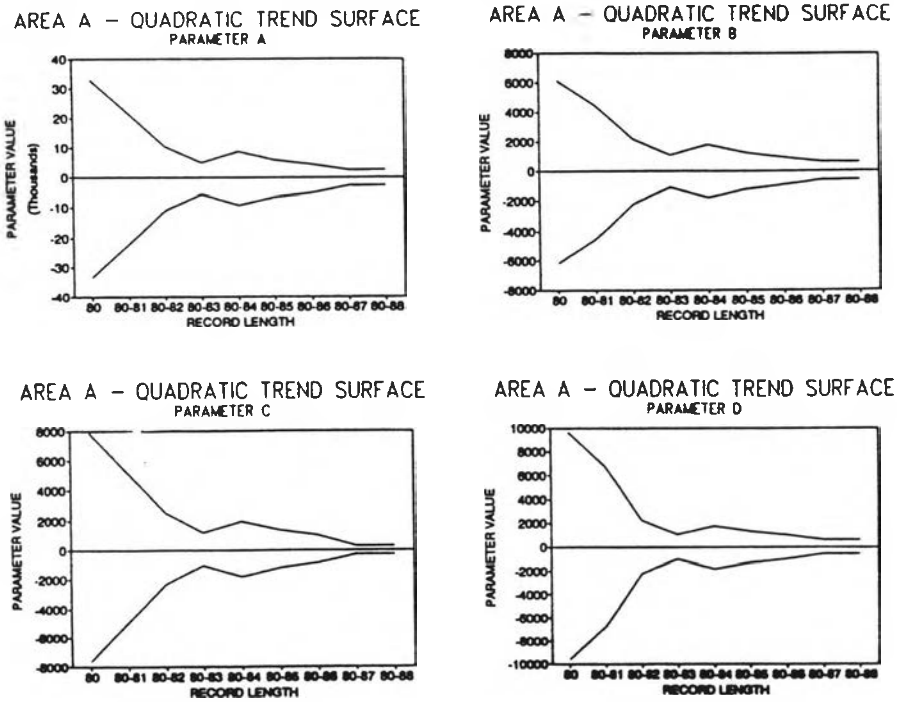

Figure 10.3 Upper and Lower Confidence Limits of Selected Parameter Estimates for Quadratic Trend Surface Model Fit to All Data in Area A

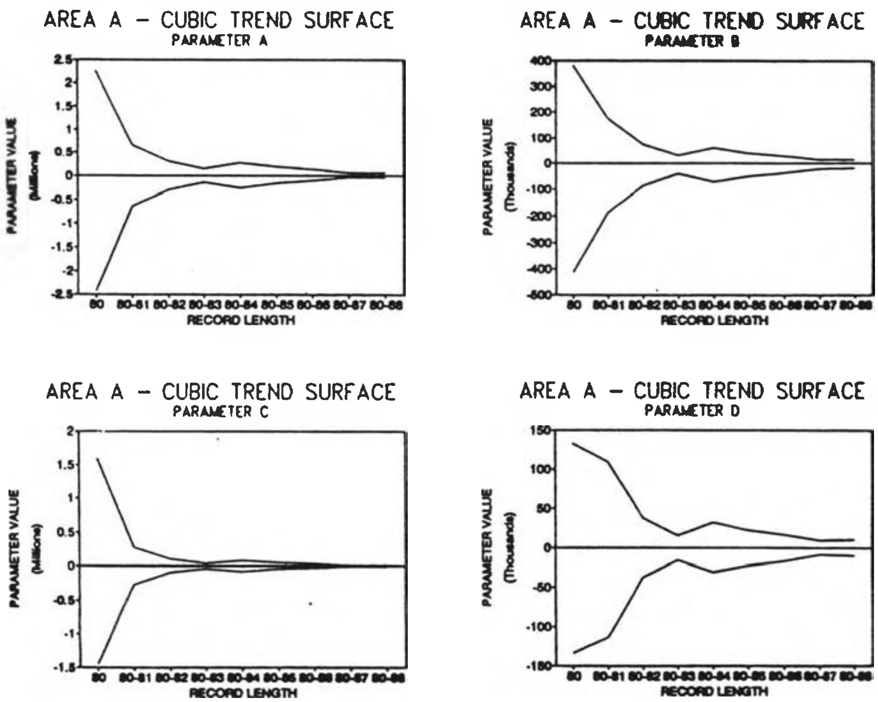

Figure 10.4 Upper and Lower Confidence Limits of Selected Parameter Estimates for Cubic Trend Surface Model Fit to All Data in Area A

Table 10.6 Average Residual Temporal and Spatial Correlations[a] for Multi-Site Models Fit to Data from Area A

Temporal Residual Correlation

YEAR	LINEAR	QUADRATIC	CUBIC	PHYSICAL
1980	.8336	.6028	.5210	.1184
1980-81	.7984	.7626	.7642	.0864
1980-82	.6097	.7138	.5520	.0263
1980-83	.5901	.6368	.6457	.0425
1980-84	.4666	.5776	.5012	-.0358
1980-85	.3808	.4211	.4995	.0465
1980-86	.3355	.4805	.5233	.0121
1980-87	.5557	.5916	.5548	.0743
1980-88	.5643	.5849	.5251	.1267

Spatial Residual Correlation

YEAR	LINEAR	QUADRATIC	CUBIC	PHYSICAL
1980	.5336	.3726	.0736	.0581
1980-81	.5339	.4531	-.0289	.0707
1980-82	.2582	.2721	.4363	.0604
1980-83	.4692	.3845	.1779	.0457
1980-84	.3848	.5483	.4598	.0412
1980-85	.2546	.0817	.1167	.0572
1980-86	.1961	.0101	.0508	.0462
1980-87	.4464	.4188	.1124	.0515
1980-88	.4450	.4507	.0780	.0496

(a) residual correlations significant at the $\alpha = 0.05$ confidence level are highlighted

was the closest in time to the date of the sample collected from Station 1. The average residual temporal correlations are significant at the $\alpha = 0.05$ level for all trend surface models and record lengths. In addition, the average spatial residual correlation is significant for approximately 50% of the trend surface models and data sets considered. These significant residual correlations indicate that there is a systematic behavior to the residuals which the trend surface models are unable to explain. Based on the highly significant correlation of the residuals, subsets of the data were not reviewed for trends.

The skewness of the residuals resulting from fitting the multi-site polynomial models to the data from Area A is summarized in Table 10.7. The results in Table 10.7

Table 10.7 Residual Skewness[a] for Multi-Site Models Fit to Data from Area A

YEARS	LINEAR	QUADRATIC	CUBIC	PHYSICAL
1980	-.2529	-.0026	-.1350	1.737
1980-81	.0323	.2028	.0156	1.699
1980-82	-.0477	-.0420	-.0347	1.623
1980-83	-.1512	-.0883	-.1866	1.045
1980-84	-.0562	.0503	-.4173	1.2442
1980-85	.0498	.0864	-.0576	1.4441
1980-86	.0682	.1164	-.0507	1.5116
1980-87	-.0946	-.1480	.0353	1.4791
1980-88	-.1336	-.1593	.0694	1.4934

(a) skewness coefficients significant at the $\alpha = 0.05$ confidence level are highlighted

show that the data error is not significantly non-normally distributed and therefore the F-test statistics are not invalidated.

Based on the results of the goodness-of-fit tests, the trend surface models do not pass the test of being good models for describing the PCE groundwater quality data in Area A. Specifically, both the temporal and spatial residuals are highly correlated indicating a systematic behavior in the data not accounted for by the model.

The prediction capabilities of these trend surface models were then evaluated. The average one-year prediction biases resulting from the trend surface models applied to the Area A data is summarized in Table 10.8. The significance of these prediction biases was evaluated using the t-test, as summarized in the same table. At the $\alpha = 0.05$ significance level, approximately one-half of the trend surface models do not pass the test of a non-biased prediction.

Based on the F-test statistics and the behavior of the parameter estimates, the trend surface models are generally good models at describing the PCE groundwater quality behavior. A significant improvement was realized over the single-site models. However, the significance of the temporal correlation of the residuals as well as the significance of the prediction bias for approximately one-half of the models, indicates that another model may be more appropriate for describing this data.

10.1.1.3 Physical Model. The last model considered for describing the PCE groundwater quality in Area A is the physically-based two-dimensional advection-dispersion model, as described in Chapter 3. The range of possible values for the model parameters was constrained based on additional information, as summarized in Table 10.9.

Table 10.8 One-Year Prediction Bias and Associated t-test for Multi-Site Models Fit to Data from Area A

BIAS

YEAR	LINEAR	QUADRATIC	CUBIC	PHYSICAL
1980	5264.0	38,009.6	172,447.9	457,428
1980-81	-28,083.4	39,434.9	112,423.3	500,558
1980-82	-10,277.3	14,086.6	-8,699.7	-76,145
1980-83	21,162.4	40,194.9	8,190.3	355,799
1980-84	-11,962.8	-45,594.9	-136,117.0	158,569
1980-85	-1908.1	-15.7	14,201.4	283,026
1980-86	-778.2	-356.5	1,601.7	73,173
1980-87	-17,626.3	-275.76	14,441.6	1115

T-TEST ON BIAS

YEAR	LINEAR	QUADRATIC	CUBIC	PHYSICAL
1980	.4510	3.2971	7.9929	10.620
1980-81	-2.5851	5.7841	3.9678	15.40
1980-82	-2.2585	3.4924	-2.2727	-.977
1980-83	0.8837	1.6752	0.3456	5.431
1980-84	-2.5450	-9.4567	-23.5195	8.963
1980-85	-0.3828	-0.0318	0.7649	23.658
1980-86	-1.7738	-0.8320	0.4132	7.228
1980-87	-2.7930	-0.5625	1.2393	6.392

(a) t-tests significant at α = 0.05 confidence level are highlighted

Based on site history, the earliest time which a source of PCE could have been introduced to the subsurface in Area A was 1964. Given that separate phase product is still observed in the source area, α, the source decay constant, was set equal to zero, thereby forcing the concentration at the source to be a constant.

Values for the retardation coefficient, R, and the decay constant, λ, were defined based on theoretical values for these parameters. The retardation coefficient, R, is defined as:

$$R = 1 + \frac{\rho_b K_d}{n} \tag{10.1}$$

where,

Table 10.9 Constraints on Physical Model Parameters for Area A

	Parameter	Definition	Range Information
C_0	Initial Source Concentration	200,000 - 1,500,000	minimum concentration based on observed concentrations in source area; maximum concentration based on solubility of PCE
t_0	initial time of source introduction	1964 - on	site history
R	Retardation coefficient	2.5	Theoretical (discussion follows)
λ	decay constant	0.0	Theoretical (discussion follows)
α	source decay constant	0.0	separate phase source still observed in source area;, therefore concentration at source is a constant
X_0	location of source	7400-7800	Identification of Source based on historical use information and observed separate phase product
Y_0	location of source	4600-5000	

ρ_b = bulk density

K_d = distribution coefficient

n = porosity

These parameters can be estimated using the following formulas:

$$n = 1 - \rho_b/\rho_s \quad (10.2)$$

$$K_d = f_{oc}K_{oc} \quad (10.3)$$

where,

ρ_s = 2.65 gm/cm^3 for an average porous medium

f_{oc} = fraction of organic carbon in soil

K_{oc} = organic carbon normalized soil/water partition coefficient

For PCE, K_{oc} values ranging from approximately 200 to 370 have been cited in the literature [Schwarzenbach and Westall, 1981; Callahan, et al, 1979]. Assuming the soil has a porosity of 0.3 ($n=0.3$) and an organic content of 0.1% ($f_{oc}=0.001$), then a retardation coefficient of approximately 2.5 ($R \approx 2.5$) can be calculated using equations 10.1, 10.2, and 10.3. Rather than using R directly in the parameter estimation routine, R was set equal to one (no retardation) and the non-dimensional approach discussed earlier was used, using the relative velocity (v/R) and relative dispersion coefficients (D_L/R and D_T/R).

Based on laboratory studies, PCE is not expected to significantly biodegrade or adsorb to sediments [Bouwer and McCarty, 1983; Callahan, et al, 1979]. Therefore, the decay constant, λ, was set equal to zero.

The F-test statistics for the physical model fit to all available data are summarized in Table 10.5 along with the other multi-site models. The physical model was significant for all record lengths based on the results of the F-test analyses. In addition, the F-test statistics for the physical model were higher than the F-test statistics for the statistical trend surface models considered. As shown in Table 10.5, the F-test does not necessarily increase with an increase in sampling frequency. The trend of these F-test statistics was evaluated relative to the theoretical slope for a correct model as discussed in Chapter 8. These results do not indicate that the trend in the F-test is different than the trend for a correct model. However, with limited data, it is difficult to use this test for model discrimination, as discussed in Chapter 8 for the simulation study.

Table 10.10 summarizes the results of the best-fit parameters for record lengths ranging from one to nine years of data and frequencies ranging from approximately monthly (all data) to biannual. This table shows that the parameter estimates do not appear to converge towards a single value. The behavior of selected model parameter estimates for the physical model fit to all available data for the periods ending 1985 through 1989 are illustrated in Figure 10.5.[42] Figure 10.5 illustrates the non-convergent behavior of the model dispersion coefficients. The behavior of these parameter estimates is indicative of an incorrect model structure.

The average residual temporal and spatial correlations for the data in Area A fit to the physical model are summarized in Table 10.6. Unlike the trend surface models, none of the correlations were significant, consistent with a correct model and parameter estimation procedure.

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[4] Due to the sensitivity of the inversion of the nearly singular matrix and due to the high variance for the models fit to record lengths of less than five years and to data sets with reduced sampling frequencies, parameter variances could only be calculated with five or more years of data.

Table 10.10 Best-fit Physical Model Parameter Estimates[a] for Area A

YEARS OF RECORD	SAMPLING FREQUENCY	PARAMETER C_o	D_L	D_T	V	A
1980	All	290,000	.02	.003	.33	55
	Bimonthly	400,000	.02	.002	.14	55
	Quarterly	410,000	.10	.003	.30	55
	Triannual	400,000	.10	.003	.30	55
	Biannual	340,000	.07	.003	.68	55
80-81	All	320,000	.02	.002	.26	55
	Bimonthly	450,000	.02	.003	.20	55
	Quarterly	400,000	.04	.003	.29	55
	Triannual	560,000	.03	.003	.23	50
	Biannual	390,000	.05	.003	.30	55
80-82	All	280,000	.04	.003	.50	55
	Bimonthly	320,000	.04	.003	.40	55
	Quarterly	330,000	.04	.003	.49	50
	Triannual	340,000	.04	.003	.47	50
	Biannual	510,000	.03	.003	.46	50
80-83	All	260,000	.04	.003	.45	50
	Bimonthly	280,000	.02	.001	.15	50
	Quarterly	250,000	.04	.003	.41	50
	Triannual	260,000	.04	.003	.42	50
	Biannual	250,000	.04	.003	.46	50
80-84	All	250,000	.13	.002	.27	50
	Bimonthly	260,000	.14	.001	.21	50
	Quarterly	250,000	.04	.003	.46	50
	Triannual	260,000	.04	.003	.45	50
	Biannual	220,000	.04	.003	.46	50
80-85	All	250,000	.11	.003	.03	50
	Bimonthly	250,000	.04	.003	.45	50
	Quarterly	240,000	.04	.003	.45	50
	Triannual	250,000	.04	.003	.45	50
	Biannual	220,000	.04	.003	.45	50
80-86	All	250,000	.08	.003	.06	50
	Bimonthly	250,000	.04	.003	.43	50
	Quarterly	250,000	.04	.003	.42	50
	Triannual	260,000	.04	.003	.42	50
	Biannual	230,000	.04	.003	.42	50

Table 10.10, continued

YEARS OF RECORD	SAMPLING FREQUENCY	PARAMETER C_0	D_L	D_T	V	A
80-87	All	250,000	.12	.003	.04	50
	Bimonthly	250,000	.14	.001	.13	50
	Quarterly	250,000	.03	.001	.29	50
	Triannual	250,000	.03	.002	.27	50
	Biannual	230,000	.03	.002	.27	50
80-88	All	250,000	.12	.003	.04	50
	Bimonthly	250,000	.13	.002	.13	50
	Quarterly	250,000	.03	.002	.28	50
	Triannual	260,000	.05	.003	.27	50
	Biannual	240,000	.35	.003	.08	50
TOLERANCE (b)		±10,000	±.01	±.001	±.01	±5

(a) parameter estimates for X_0 and Y_0 were 7690 and 4850 feet, respectively, for all data subsets

(b) tolerance for each parameter estimate for model fit

The skewness of the residuals are summarized in Table 10.7. The skewness of the residuals were significantly different from zero at the $\alpha = 0.05$ confident level. This may indicate a non-additive data error or an incorrect model structure.

The physical model exhibited variable model goodness-of-fit characteristics. The F-test statistics were significant and the residual were uncorrelated. However, the parameter estimate did not converge towards single values and the skew of the residuals was significant. The physical model fit is therefore non-ideal.

The physical model with the estimated best-fit model parameters was used to evaluate prediction bias. As summarized in Table 10.8, the prediction bias was significant using the physical model for the majority of data subsets considered.

Based on the model applicability test considered, the physical model was highly significant based on the analysis of variance and residual correlations. However, the parameter behavior and significance of the prediction bias indicates the model is not appropriate for describing the PCE groundwater data in Area A.

10.1.1.4. Summary of Model Selection. None of the models considered for describing the PCE groundwater quality behavior in Area A met all the criteria for

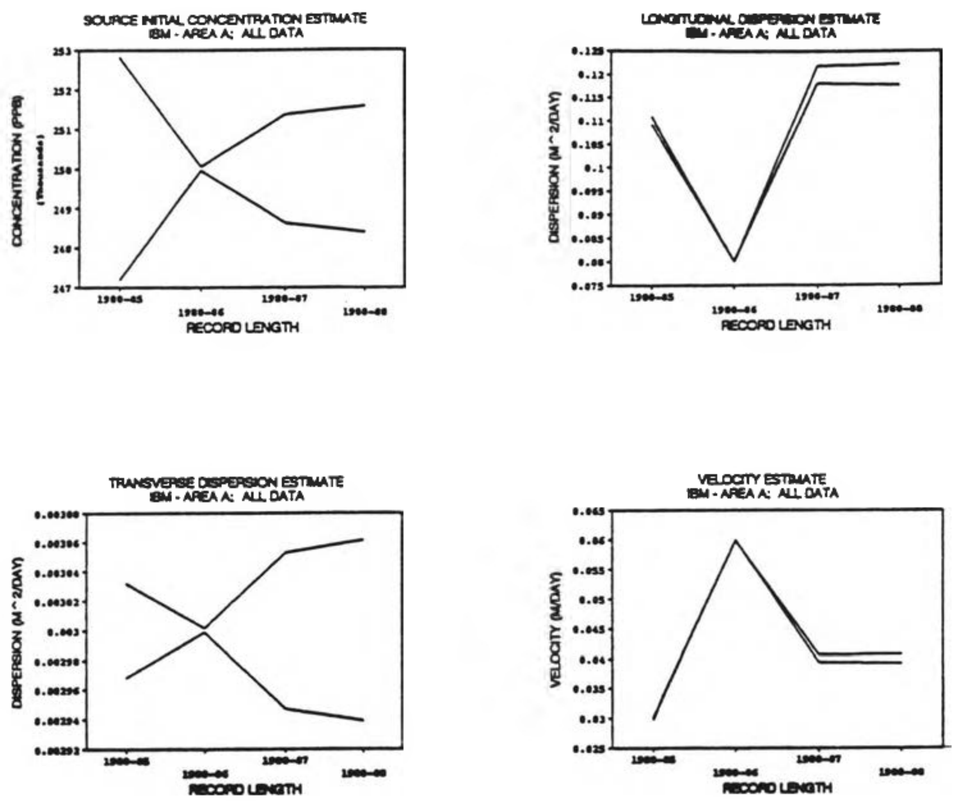

Figure 10.5 Upper and Lower Confidence Limits of Selected Parameter Estimates for Physical Model Fit to All Data in Area A

model applicability, as outlined in Chapter 9 (Protocol - Steps 4 and 5). Clearly, the multi-site models exhibited superior behavior over the single-site models in their general ability to both consistently describe and predict groundwater quality behavior. The trend surface models exhibited both significant model fit based on analysis of variance and parameter behavior; however, the residuals exhibited systematic error and the prediction biases were significant. The physical model was more highly significant than the trend surface models based on the analysis of variance (ANOVA) and exhibited insignificant residual correlation. However, the parameter behavior was indicative of an incorrect model and the prediction bias was more significant than for the trend surface models. Overall, of the models considered, the linear trend surface model exhibited the best model applicability characteristics. Under further consideration, a different physical model should be considered. Given the high D_L/D_T ratio and other geologic data available for the site, a fractured flow model may be more appropriate at describing this data, with the data segregated vertically to account for the overburden versus bedrock characteristics.

10.1.2 Monitoring Network Optimization.

The optimization of monitoring networks was evaluated for all the models considered, regardless of the results of the goodness-of-fit tests, in order to evaluate the behavior of the error prediction variance and the optimal monitoring networks for the various models considered relative to the goodness-of-fit and prediction tests.

10.1.2.1 Single-Site Polynomial Models. Only the sampling frequency can be optimized for the single-site models since no structure exists to describe the spatial interdependence of the wells. For a specified frequency, a prediction error variance can be calculated for each well (or conversely, for a specified error variance a sampling frequency could be calculated). Table 10.11 summarizes the error prediction variance at the wells in Area A for a monthly future sampling frequency. The error prediction variances generally tended to decrease with an increase in record length. In addition, the prediction error variance increased as the model order increased. This indicates a higher uncertainty with the higher order models, consistent with the F-test analyses which indicated that in general, the higher order single-site models are not significant for the data.

The prediction error variance also varied with location. Figure 10.6 illustrates the spatial variability of the prediction error variance based on a single-site linear model applied to all available data from 1980 through 1988. These results are compared to the results for the multi-site models in the following sections.

10.1.2.2 Trend Surface Models. For the trend surface models, Table 10.12 summarizes the prediction error variances at the individual wells in the multi-site network. Comparing Table 10.12 to Table 10.11 illustrates the clear advantage in incorporating information on the spatial interdependence of the data in a model. For the majority of the wells, the error prediction variance at the individual well based on the trend surface model was lower than the prediction error variance at that well for the single-site polynomial model. As for the single-site polynomial models, the prediction error variance at individual wells was higher with the higher order trend surface models.

Figure 10.7 illustrates the prediction error variance surface for the linear trend surface model applied to all available data from 1980-88. The difference between the prediction error variances at individual wells based on the linear trend surface versus single-site linear models is illustrated by comparison of Figure 10.7 to Figure 10.6. The "uncertainty surface" is clearly more uniform for the linear trend surface model than it is for the single-site linear models.

The resulting optimal monitoring networks for the trend surface models are summarized in Table 10.13. Due to the high correlation of the model structure, the optimal monitoring networks with a specified minimum spatial correlation of 0.9, consists of only one well. The sampling at these "optimal" locations results in a reduction in the prediction error variance surface. Figure 10.8 illustrates the reduction in the prediction error variance for the linear trend surface model applied to the data from 1980 through 1988. Comparison of Figure 10.8 to Figure 10.7 illustrates the reduction in the topographical prediction error highs as wells as the reduction at the sampling wells (appearing as "bulls-eyes").

An alterative method of representing the uncertainty in the model is by plotting upper and lower confidence limits to desired concentrations of interest. Figure 10.9

Table 10.11 Error Prediction Variance at Individual Wells for Single Site Polynomial Models Fit to Data in Area A with Future Monthly Sampling Frequency

LINEAR MODEL

WELL	RECORD LENGTH								
NO.	1980	80-81	80-82	80-83	80-84	80-85	80-86	80-87	80-88
7	954.8	57.72	22.27	6.606	5.495	5.2021	3.8385	2.9488	2.9488
11	218.6	136.4	710.9	602.8	383.2	223.12	206.3	199.94	199.94
12	3E+06	6E+06	9E+05	5E+05	6E+05	391825	391825	391825	391825
13	8E+07	4E+08	5E+08	4E+08	3E+08	3.3E+08	3.2E+08	3.2E+08	3.2E+08
14	3E+09	2E+09	8E+08	7E+08	7E+08	7E+08	7E+08	7E+08	7E+08
15	2E+08	7E+08	4E+08	4E+08	2E+08	1.5E+08	1.1E+08	9.1E+07	9.1E+07
16	2E+05	31464	13684	8433	4382	2538	1815.7	1489.1	1443.3
17	1E+05	2E+05	1E+05	82206	45958	27416	20161	17479	16572
18			65.45	100.3	3152	10299	8882.8	8298.8	8298.8
19	4032	2419	6254	3137	4903	3476.5	3345	3212.1	3212.1
20	19.65	3.26	1.255	0.811	2.237	2.823	3.0542	2.9361	2.9361
21	38.65	41.37	19.09	10.17	7.604	24.294	761.55	662.6	662.6
22	1266	1039	660	42249	23713	12953	8708.3	7092.1	7092.1
26	521.3	312.8	208.5	269.1	47.57	47.567	47.567	47.567	47.567
38	42.08	25.25	16.83	16.83	16.83	16.834	16.834	16.834	16.834
39	7.415	4.449	2.252	1.692	1.692	1.4096	1.4096	1.2953	1.2953
43	13.04	3.674	1.525	1.089	1.089	1.0886	1.0886	1.0886	1.0886
44			10.65	3.907	2.043	2.0427	2.0427	2.0582	2.0582
45	145.5	87.27	27.7	52.29	45.8	45.803	45.803	45.803	45.803
74			3E+07	1E+07	3E+09	3.3E+09	3.3E+09	3.3E+09	3.3E+09
103			229.9	132.2	89.75	296.32	2159.1	1474.3	1474.3
104				2E+06	4E+05	419772	419772	363429	363429
105			1.397	0.439	1.685	1.4799	0.9298	0.6226	0.6226
106			0.807	0.858	9.953	8.6384	5.5795	3.4399	3.4399
108				9.157	6.597	4.7573	1.5415	0.7934	0.7099
109				178.5	241.3	222.61	100.67	58.529	53.419
116					1E+08	1.3E+08	1.3E+08	1.5E+08	1.5E+08
117				2E+08	1E+08	1.7E+08	1.7E+08	1.5E+08	1.5E+08
118				2E+09	2E+09	4.1E+08	3.3E+08	2.9E+08	2.9E+08
126				7.49	708.4	849.58	810.43	810.43	810.43
129					271.8	193.89	183	147.12	147.12
130				7.767	19.51	14.721	11.607	9.9128	9.9128
176				69069	2E+05	159107	159107	159107	159107
700								15684	15684
707								152.54	152.54
708								3241.5	3241.5
716								241698	241698
731								3.607	3.607
734								509.79	509.79
737								16747	16747
751								0.7436	0.7436
752								2.8502	2.8502

(continued)

Table 10.11, continued

LINEAR MODEL

WELL NO.	RECORD LENGTH 1980	80-81	80-82	80-83	80-84	80-85	80-86	80-87	80-88
753								0.3328	0.3328
816				3E+05	7E+05	291998	291998	291998	291998
817					1E+08	9.6E+07	8.8E+07	8.8E+07	8.8E+07
818					8E+08	7.6E+08	5.9E+08	5.9E+08	5.9E+08
819				3E+08	2E+08	1.6E+08	1.3E+08	1.1E+08	1.1E+08
820				1E+05	3E+05	265484	434921	541910	541910
821					1E+09	1.3E+09	2.9E+09	2.9E+09	2.9E+09
822				7E+07	6E+11	5.7E+11	6.6E+11	6.6E+11	6.6E+11
823				3E+06	2E+06	1.5E+06	1.4E+06	1.2E+06	1.2E+06
824				7E+05	4E+05	384065	542976	1.2E+06	1.2E+06
825				2E+06	2E+06	1.4E+06	1.4E+06	1.4E+06	1.4E+06
826				71738	2E+07	2.4E+07	2.1E+07	2.1E+07	2.1E+07
827				3E+05	3E+05	209661	158207	123166	123166
865				4E+06	4E+06	4.2E+06	4.2E+06	4.2E+06	4.2E+06
866				21256	11556	11556	11556	11556	11556
934							8.6777	2.9573	2.9573
965							9.7696	14.454	14.454
966							0.0527	0.0407	0.0407
998									3.1959
999									1.7472

QUADRATIC MODEL

WELL NO.	RECORD LENGTH 1980	80-81	80-82	80-83	80-84	80-85	80-86	80-87	80-88
7	1E+05	3517	659	221.7	158	88.403	54.394	34.478	51.717
11	39428	1744	2164	3737	2338	880.79	1020.9	1213.9	1820.9
12	3E+08	1E+09	6E+07	6E+07	2E+07	1.1E+07	1.7E+07	2.6E+07	3.9E+07
13	2E+10	2E+10	7E+09	3E+09	3E+09	3.4E+09	2E+09	3.3E+09	4.9E+09
14	0	6E+08	5E+08	4E+08	3E+08	2.7E+08	2.7E+08	2.7E+08	2.7E+08
15	5E+08	1E+09	8E+08	4E+08	1E+08	0	-1E+08	-9E+07	-9E+07
16	39335	8814	6676	4358	2114	1213.1	878.45	735.29	714.57
17	6E+05	2E+05	3E+05	70510	20251	-12972	-20366	-25955	-24364
18				54.3	5079	5368.6	4580.5	4234.4	4234.4
19	17629	6495	9578	4938	1372	-924.3	-1712	-2157	-1078
20	86.66	5.349	1.669	0.39	1.054	0	0	-1.497	0
21	171	84.19	40.36	10.62	3.809	0	-341.9	-321.4	-321.4
22	4447	1030	905.9	65937	11796	0	-8741	-10738	-10738
26			113	649.7	69.19	46.125	46.125	46.125	46.125
38	19.44	39.55	28.25	22.6	22.6	16.948	16.948	16.948	16.948
39	52.51	6.804	6.029	3.902	2.927	1.5435	1.5435	1.2176	1.2176
43		5.657	2.031	1.097	1.097	1.0966	1.0966	1.0966	1.0966
44			35.51	6.678	3.382	2.2546	2.2546	1.875	1.875

(continued)

Table 10.11, continued

QUADRATIC MODEL

WELL NO.	1980	80-81	80-82	80-83	80-84	80-85	80-86	80-87	80-88
					RECORD LENGTH				
45			81.72	75.34	78.26	52.172	52.172	52.172	52.172
74			8E+07	3E+07	3E+09	1.6E+09	3.3E+09	3.3E+09	3.3E+09
103				91.44	153.8	177.58	1855.5	699.89	0
104				2E+06	5E+05	181883	363766	393612	393612105
			0.746	1.859	1.0016	0.9868	0.6581	0.6581	
106				1.472	13.38	8.4101	6.0023	1.8185	1.8185
108					6.474	3.6817	1.5833	0.819	0.3667
109					25.67	24.642	21.773	19.275	9.2887
116					9E+07	6E+07	6E+07	7.7E+07	7.7E+07
117				3E+08	2E+08	8.6E+07	0	8E+07	8E+07
118				8E+08	3E+09	4.2E+08	1.7E+08	1.5E+08	1.5E+08
126				7.459	544.8	264.89	869.89	869.89	869.89
129					87.36	219.72	192.32	140.66	140.66
130				13.87	20.37	12.937	12.927	10.265	10.265
176				1E+05	2E+05	103333	103333	103333	103333
716								201880	201880
737								12131	12131
816					1E+06	243701	121851	121851	243701
817									8.6E+07
818					1E+09	8.9E+08	7.1E+08	8.6E+07	8.6E+07
819					5E+08	2E+08	1.4E+08	7.1E+08	7.1E+08
820					3E+05	301384	244387	1.3E+08	1.3E+08
821					2E+09	1.6E+09	1.6E+09	170588	170588
822					3E+11	2.3E+11	6.8E+11	1.6E+09	1.6E+09
823				5E+06	4E+06	1.5E+06	1.2E+06	6.8E+11	6.8E+11
824				1E+06	7E+05	359395	283054	1.1E+06	1.1E+06
825				4E+06	4E+06	1.7E+06	1.7E+06	1.2E+06	1.2E+06
826					1E+07	2.8E+07	2E+07	1.7E+06	1.7E+06
827					4E+05	201037	170448	136288	136288
866					20586	13724	13724	13724	13724
934							5.4126	2.7729	1.3864
965							0.3919	3.041	3.041
966							0.0653	0.0448	0.0448

CUBIC MODEL

WELL NO.	1980	80-81	80-82	80-83	80-84	80-85	80-86	80-87	80-88
					RECORD LENGTH				
7	3E+07	2E+05	2E+05	7271	4636	2956.6	1425.6	848.29	1539.8
11	8E+05	1E+05	1E+05	1E+05	87864	31154	39907	38673	69980
12	5E+10	6E+11	2E+10	1E+09	9E+08	6.1E+08	1.3E+09	2.5E+09	4.6E+09
13	1E+12	1E+12	7E+11	2E+11	1E+11	1.3E+11	5.7E+10	1.1E+11	2E+11
14	7E+10	1E+11	9E+10	8E+10	3E+10	6.9E+10	1.5E+11	3E+11	5.6E+11

(continued)

Table 10.11, continued

CUBIC MODEL

WELL NO.	RECORD LENGTH 1980	80-81	80-82	80-83	80-84	80-85	80-86	80-87	80-88	
15	3E+08	2E+09	6E+08	6E+08	2E+08	1.4E+08	9.8E+07	8.3E+07	8.3E+07	
16	7E+07	2E+06	2E+06	1E+05	50182	19830	11469	6492.9	11186	
17	3E+05	3E+05	3E+05	98052	41214	23771	17457	16826	16001	
18				127.5	7304	0	-9342	-4385	-4385	
19	1E+05	22075	22075	6827	-3447	-10324	-10340	-7717	-5145	
20	336.5	15.97	15.97	1.057	1.064	-2.701	-8.784	-6.76	-5.408	
21	575.7	165.5	165.5	27.67	0	-58.4	-1971	-1956	-1630	
22	25290	3557	3557	98514	0	-39559	-57325	-53717	-50136	26
			505.9	99.39	49.697	74.546	74.546	74.546		
38	182.2	37.56	37.56	15.02	13.15	9.3902	9.3902	9.3902	7.5122	
39	37.22	7.596	7.596	7.977	4.986	3.2605	3.2605	2.7787	2.084	
43	174.8	18.47	18.47	1.979	1.979	1.9793	1.9793	1.9793	1.4845	
44				14.75	6.013	4.8101	4.8101	4.0913	3.0685	
45				173.2	121.8	97.447	97.447	97.447	73.086	
74			1E+08	6E+07	5E+09	3.5E+09	5.3E+09	7.1E+09	5.3E+09	
103				222.4	158	101.6	1929.9	-2303	-5183	
104				4E+06	5E+05	364568	546852	488742	488742	
105				1.829	3.474	1.6646	1.1554	0.9135	0.609	
106				3.56	24.91	13.941	8.5969	3.7051	1.8526	
108					8.648	4.5316	1.7181	0.7027	0	
109					5.565	3.1726	4.1319	3.1302	0	
116								1.2E+08	8.6E+07	
117				4E+08	2E+08	-2E+08	-2E+08	-8E+07	0	
118					2E+08	4.4E+08	-2E+08	-1E+08	-3E+08	
126					255.1	457.08	1267.9	1267.9	950.9	
129						328.47	301.57	305.42	229.07	
130					16.37	30.992	23.453	21.9	16.425	
176					43576	34861	34861	34861	26146	
816					2E+06	260989	260989	260989	260989	
818						4.9E+08	1.7E+09	1.7E+09	1.3E+09	
819						5.1E+08	3.4E+08	2.7E+08	2E+08	
820					2E+05	654990	564773	388983	194492	
821						7.6E+10	2.3E+09	2.3E+09	1.8E+09	
822					9E+10	3.3E+06	6.9E+11	6.9E+11	5.2E+11	
823				5E+06	8E+06	837047	2.6E+06	2.1E+06	1.6E+06	
824				3E+06	1E+06	4E+06	646632	1.3E+06	982770	
825					9E+05	781370	4E+06	4E+06	3E+06	
826					1E+06	4.5E+07	4.6E+07	4.6E+07	3.5E+07	
827					9E+05	500375	351441	268190	201142	
865									35373	
866						44216	35373	35373	26530	
934							8.8014	3.9386	1.3129	
965							0.0441	0.065	0.0433	
966							0.1281	0.0829	0.0553	

Table 10.12 Error Prediction Variance at Individual Wells for Trend Surface Models Fit to Data in Area A with Future Monthly Sampling Frequency

LINEAR MODEL

WELL NO.	1980	80-81	80-82	80-83	80-84	80-85	80-86	80-87	80-88
				RECORD LENGTH					
7	10.225	6.9021	5.1701	3.7665	3.1173	2.8344	2.5683	1.5549	1.549
11	9.9147	6.6881	5.0238	3.6697	3.046	2.7647	2.5066	1.5715	1.5657
12	9.9304	6.6987	5.0314	3.6747	3.0498	2.7681	2.5095	1.5722	1.5664
13	9.8976	6.6782	5.0142	3.6629	3.0399	2.7622	2.5054	1.5568	1.5511
14	9.8961	6.6772	5.0134	3.6624	3.0395	2.7619	2.5051	1.5565	1.5508
15	9.8947	6.6763	5.0127	3.6619	3.0391	2.7616	2.5049	1.5562	1.5505
16	9.7102	6.5544	4.9213	3.6004	2.9906	2.7238	2.4744	1.5223	1.5169
17	9.7095	6.554	4.9209	3.6001	2.9903	2.7237	2.4743	1.5219	1.5165
18	9.6329	6.5015	4.8845	3.5759	2.9723	2.7068	2.4595	1.5228	1.5175
19	9.6348	6.5027	4.8854	3.5765	2.9728	2.7071	2.4598	1.5231	1.5178
20	9.5591	6.453	4.8477	3.5511	2.9526	2.6918	2.4476	1.5074	1.5022
21	9.5558	6.4507	4.8461	3.55	2.9518	2.6911	2.447	1.5072	1.502
22	9.5521	6.4482	4.8443	3.5489	2.9509	2.6903	2.4463	1.5071	1.5019
26	9.5125	6.4148	4.8308	3.541	2.9487	2.6772	2.4313	1.5589	1.5534
38	9.1193	6.1572	4.6341	3.4082	2.8429	2.5982	2.3688	1.469	1.4643
39	9.1218	6.1589	4.6353	3.409	2.8435	2.5988	2.3693	1.4691	1.4643
43	9.8485	6.6538	4.9832	3.6406	3.0179	2.7576	2.5066	1.4824	1.4772
44	10.097	6.8211	5.1046	3.7219	3.0805	2.8104	2.5508	1.5073	1.5018
45	10.101	6.8235	5.1063	3.723	3.0814	2.8111	2.5514	1.5077	1.5021
74			5.009	3.6594	3.0372	2.7599	2.5034	1.5559	1.5502
103		6.7553	5.0653	3.6965	3.064	2.7876	2.5285	1.5424	1.5367
104			5.0653	3.6965	3.064	2.7876	2.5285	1.5424	1.5367
105		6.7585	5.0675	3.6981	3.0652	2.7886	2.5294	1.5427	1.537
106		6.7585	5.0675	3.6981	3.0652	2.7886	2.5294	1.5427	1.537
108		6.6914	5.0121	3.6601	3.0336	2.7691	2.5155	1.4969	1.4915
109		6.6914	5.0121	3.6601	3.0336	2.7691	2.5155	1.4969	1.4915
115						2.7473	2.4926	1.5539	1.5483
116			4.9778	3.6386	3.0214	2.7459	2.4914	1.5531	1.5474
117		6.6276	4.9782	3.6389	3.0216	2.746	2.4916	1.553	1.5473
118		6.6276	4.9782	3.6389	3.0216	2.746	2.4916	1.553	1.5473
126		6.1658	4.6463	3.4171	2.8519	2.5995	2.3677	1.502	1.4971
128				3.3853	2.8256	2.5827	2.3555	1.4666	1.462
129			4.5982	3.3843	2.8248	2.582	2.3549	1.4665	1.4619
130		6.1064	4.5982	3.3843	2.8248	2.582	2.3549	1.4665	1.4619
176		6.7188	5.0467	3.685	3.058	2.7743	2.5144	1.579	1.5731
700					3.057	2.7855	2.5281	1.5218	1.5162
701								1.522	1.5164
702								1.5308	1.5251
703								1.531	1.5254
704								1.5299	1.5242
705								1.5589	1.553
706								1.5587	1.5528
707								1.5641	1.5582

(continued)

Table 10.12, continued

LINEAR MODEL

WELL NO.	1980	80-81	80-82	80-83	80-84	80-85	80-86	80-87	80-88
				RECORD LENGTH					
708								1.5644	1.5585
710								1.5693	1.5634
716								1.5812	1.5754
731								1.532	1.5267
732								1.5323	1.5269
734								1.5125	1.5074
735								1.5003	1.4954
737								1.5001	1.4952
744								1.5771	1.5709
745								1.5773	1.5711
746								1.5655	1.5594
751								1.4965	1.4915
752								1.5066	1.5015
753								1.4967	1.4916
816			5.0591	3.6931	3.0635	2.7811	2.5208	1.5709	1.5651
817			5.043	3.6822	3.0549	2.7744	2.5155	1.5648	1.559
818			5.0287	3.6727	3.0477	2.768	2.5099	1.564	1.5582
819			4.9901	3.647	3.0282	2.7506	2.495	1.5605	1.5548
820			5.0594	3.6933	3.0638	2.7808	2.5205	1.5736	1.5677
821			4.9989	3.6527	3.032	2.7555	2.4997	1.5542	1.5486
822			5.014	3.6628	3.0397	2.7623	2.5056	1.5555	1.5498
823			5.0211	3.6674	3.0428	2.7661	2.5093	1.5509	1.5452
824			5.0094	3.6596	3.0369	2.7609	2.5047	1.5499	1.5442
825			5.0025	3.6549	3.0332	2.7581	2.5025	1.5467	1.541
826			5.0153	3.6639	3.0414	2.7612	2.5037	1.5682	1.5624
827			5.0279	3.6724	3.048	2.7665	2.5081	1.572	1.5661
864				3.6817	3.0548	2.7735	2.5144	1.5688	1.5629
865			5.0395	3.6796	3.0518	2.7748	2.5169	1.5495	1.5438
866			5.066	3.6973	3.0652	2.7868	2.5271	1.5518	1.5461
934					2.9048	2.6503	2.4124	1.494	1.489
965						2.6684	2.431	1.4544	1.4496
966						2.6705	2.4327	1.4549	1.4501
972						2.7639	2.5072	1.5523	1.5466
978							2.4502	1.5142	1.5089
980							2.4828	1.5328	1.5273
994								1.5303	1.5251
996								1.535	1.5297
997								1.5635	1.5575
998								1.5693	1.5633
999								1.9663	1.8637

(continued)

Table 10.12, continued

QUADRATIC MODEL

WELL	RECORD LENGTH								
NO.	1980	80-81	80-82	80-83	80-84	80-85	80-86	80-87	80-88
7	9130.5	5555.2	3857.1	2512.4	1905.4	1589.7	1310.0	810.6	688.87
11	8406.1	5186.6	3609.0	2366.1	1797.5	1495.3	1232.9	857.2	696.94
12	8441.0	5208.0	3624.0	2375.7	1804.7	1501.3	1237.7	859.2	699.11
13	8378.6	5136.6	3569.0	2335.1	1773.6	1477.4	1218.8	696.0	672.58
14	8375.4	5134.2	3567.2	2333.9	1772.6	1476.7	1218.2	695.5	672.04
15	8372.5	5131.9	3565.5	2332.7	1771.8	1475.9	1217.7	694.9	671.52
16	7987.8	4839.7	3352.0	2186.2	1660.2	1386.5	1146.0	628.8	607.52
17	7986.7	4838.0	3350.7	2185.2	1659.5	1385.9	1145.5	628.0	606.74
18	7815.9	4744.1	3286.3	2145.9	1630.3	1360.9	1125.3	625.1	604
19	7819.7	4747.0	3288.4	2147.3	1631.3	1361.8	1126.0	625.7	604.61
20	7668.2	4627.6	3200.7	2086.4	1584.9	1324.6	1096.1	596.2	576.03
21	7661.1	4623.4	3197.7	2084.5	1583.4	1323.4	1095.1	595.8	575.65
22	7653.0	4618.5	3194.3	2082.4	1581.8	1322.1	1094.1	595.4	575.23
26	7518.2	4661.3	3243.0	2133.9	1622.9	1349.1	1114.9	675.7	653.06
38	6762.2	4038.1	2781.5	1811.9	1377.9	1154.1	958.2	512.5	495.12
39	6767.3	4041.2	2783.6	1813.2	1378.9	1154.9	958.9	512.7	495.37
43	8336.3	4954.6	3418.8	2209.7	1672.8	1402.9	1160.1	571.2	551.83
44	8877.5	5311.1	3673.0	2377.3	1799.7	1507.3	1244.4	625.8	604.57
45	8885.2	5316.2	3676.6	2379.7	1801.5	1508.8	1245.6	626.5	605.27
74			3558.1	2328.0	1768.2	1473.0	1215.3	693.9	670.53
103		5251.4	3642.9	2374.6	1801.9	1503.8	1240.7	679.0	656.07
104			3642.9	2374.6	1801.9	1503.8	1240.7	679.0	656.07
105		5258.0	3647.6	2377.6	1804.2	1505.7	1242.2	679.8	656.81
106		5258.0	3647.6	2377.6	1804.2	1505.7	1242.2	679.8	656.81
108		5048.4	3488.0	2258.8	1711.0	1433.4	1184.6	598.1	577.75
109		5048.4	3488.0	2258.8	1711.0	1433.4	1184.6	598.1	577.75
115						1451.6	1198.0	687.2	664
116			3497.1	2289.0	1739.0	1448.6	1195.6	685.3	662.26
117		5035.0	3497.6	2289.3	1739.1	1448.8	1195.7	685.2	662.12
118		5035.0	3497.6	2289.3	1739.1	1448.8	1195.7	685.2	662.12
126		4109.3	2841.9	1862.7	1417.9	1183.6	982.0	564.6	545.56
128				1773.1	1349.0	1129.8	938.6	505.3	488.19
129			2717.3	1771.3	1347.6	1128.7	937.7	504.9	487.81
130		3946.2	2717.3	1771.3	1347.6	1128.7	937.7	504.9	487.81
176		5260.6	3662.8	2402.6	1825.1	1517.5	1250.6	736.5	711.8
700					1771.8	1481.4	1223.0	643.8	621.99
701								644.3	622.44
702								662.2	639.8
703								662.7	640.26
704								660.6	638.23
705								711.9	687.88
706								711.4	687.43
707								722.8	698.47
708								723.6	699.19
710								727.5	702.98

(continued)

Table 10.12, continued

QUADRATIC MODEL

WELL NO.	1980	80-81	80-82	80-83	80-84	80-85	80-86	80-87	80-88
					RECORD LENGTH				
716								735.1	710.44
731								632.9	611.55
732								633.5	612.1
734								596.6	576.44735
							560.9	541.99	
737								560.4	541.48
744								767.9	741.98
745								768.4	742.45
746								744.6	719.43
751								566.0	546.91
752								588.2	568.28
753								577.3	557.79
816			3673.1	2405.6	1827.0	1520.5	1253.3	725.0	700.62
817			3633.9	2378.7	1806.6	1504.1	1240.3	712.8	688.79
818			3606.4	2361.4	1793.6	1493.2	1231.5	709.6	685.75
819			3530.6	2312.9	1757.2	1462.9	1207.0	699.0	675.44
820			3677.5	2409.5	1830.0	1522.6	1254.9	729.4	704.82
821			3537.3	2314.4	1758.0	1464.6	1208.5	689.9	666.67
822			3566.8	2333.2	1772.0	1476.3	1218.0	693.9	670.48
823			3573.2	2335.2	1773.2	1478.1	1219.6	687.3	664.12
824			3550.2	2320.5	1762.3	1468.9	1212.2	684.1	661.07
825			3533.0	2308.5	1753.1	1461.6	1206.3	678.1	655.22
826			3588.2	2351.8	1786.7	1486.7	1226.0	714.7	690.64
827			3617.3	2371.4	1801.5	1498.6	1235.6	722.6	698.26
864				2383.1	1810.1	1506.5	1242.0	719.2	694.99
865			3605.1	2354.3	1787.4	1490.3	1229.5	687.3	664.16
866			3657.5	2387.7	1812.5	1511.2	1246.4	694.6	671.14
934					1496.1	1251.1	1036.7	564.4	545.32
965						1244.7	1031.8	505.2	488.06
966						1248.2	1034.6	506.5	489.27
972						1475.9	1217.8	689.1	665.85
978							1105.2	608.1	587.58
980							1166.4	648.7	626.79
994								617.5	596.67
996								633.2	611.87
997								627.6	704.12
998								639.7	715.34
999								640.4	

(continued)

Table 10.12, continued

CUBIC MODEL

WELL NO.	RECORD LENGTH 1980	80-81	80-82	80-83	80-84	80-85	80-86	80-87	80-88
7	2.3E+09	3.9E+07	1.3E+07	6.5E+06	4.7E+06	3.5E+06	2.7E+06	9E+05	9E+05
11	1.8E+09	3.4E+07	1.2E+07	5.8E+06	4.2E+06	3.1E+06	2.5E+06	9E+05	9E+05
12	1.8E+09	3.4E+07	1.2E+07	5.8E+06	4.2E+06	3.1E+06	2.5E+06	9E+05	9E+05
13	1.9E+09	3.4E+07	1.2E+07	5.7E+06	4.1E+06	3.1E+06	2.4E+06	8E+05	8E+05
14	1.9E+09	3.4E+07	1.2E+07	5.7E+06	4.1E+06	3.1E+06	2.4E+06	8E+05	8E+05
15	1.9E+09	3.4E+07	1.2E+07	5.7E+06	4.1E+06	3.1E+06	2.4E+06	8E+05	8E+05
16	1.8E+09	3.1E+07	1.1E+07	5.3E+06	3.8E+06	2.8E+06	2.2E+06	7E+05	7E+05
17	1.8E+09	3.1E+07	1.1E+07	5.3E+06	3.8E+06	2.8E+06	2.2E+06	7E+05	7E+05
18	1.7E+09	3E+07	1E+07	5.1E+06	3.7E+06	2.7E+06	2.1E+06	7E+05	7E+05
19	1:7E+09	3E+07	1E+07	5.1E+06	3.7E+06	2.7E+06	2.1E+06	7E+05	7E+05
20	1.7E+09	2.9E+07	9.8E+06	4.9E+06	3.6E+06	2.7E+06	2.1E+06	7E+05	6E+05
21	1.7E+09	2.9E+07	9.8E+06	4.9E+06	3.6E+06	2.6E+06	2.1E+06	7E+05	6E+05
22	1.7E+09	2.9E+07	9.8E+06	4.9E+06	3.6E+06	2.6E+06	2.1E+06	7E+05	6E+05
26	1.4E+09	2.8E+07	9.9E+06	4.8E+06	3.5E+06	2.6E+06	2.1E+06	8E+05	8E+05
38	1.4E+09	2.3E+07	8E+06	4E+06	2.9E+06	2.2E+06	1.7E+06	5E+05	5E+05
39	1.4E+09	2.3E+07	8E+06	4E+06	2.9E+06	2.2E+06	1.7E+06	5E+05	5E+05
43	2.2E+09	3.4E+07	1.1E+07	5.5E+06	4E+06	3E+06	2.3E+06	6E+05	6E+05
44	2.4E+09	3.7E+07	1.2E+07	6.1E+06	4.4E+06	3.3E+06	2.5E+06	7E+05	7E+05
45	2.4E+09	3.7E+07	1.2E+07	6.1E+06	4.5E+06	3.3E+06	2.5E+06	7E+05	7E+05
74			1.1E+07	5.7E+06	4.1E+06	3.1E+06	2.4E+06	8E+05	8E+05
103		3.5E+07	1.2E+07	6E+06	4.3E+06	3.2E+06	2.5E+06	8E+05	8E+05
104			1.2E+07	6E+06	4.3E+06	3.2E+06	2.5E+06	8E+05	8E+05
105		3.6E+07	1.2E+07	6E+06	4.3E+06	3.2E+06	2.5E+06	8E+05	8E+05
106		3.6E+07	1.2E+07	6E+06	4.3E+06	3.2E+06	2.5E+06	8E+05	8E+05
108		3.4E+07	1.1E+07	5.7E+06	4.1E+06	3E+06	2.3E+06	7E+05	7E+05
109		3.4E+07	1.1E+07	5.7E+06	4.1E+06	3E+06	2.3E+06	7E+05	7E+05
115						3E+06	2.4E+06	8E+05	8E+05
116			1.1E+07	5.5E+06	4E+06	3E+06	2.3E+06	8E+05	8E+05
117		3.2E+07	1.1E+07	5.5E+06	4E+06	3E+06	2.3E+06	8E+05	8E+05
118		3.2E+07	1.1E+07	5.5E+06	4E+06	3E+06	2.3E+06	8E+05	8E+05
126		2.3E+07	8.1E+06	4.1E+06	2.9E+06	2.2E+06	1.7E+06	6E+05	6E+05
128				3.9E+06	2.8E+06	2.1E+06	1.6E+06	5E+05	5E+05
129			7.7E+06	3.9E+06	2.8E+06	2.1E+06	1.6E+06	5E+05	5E+05
130		2.3E+07	7.7E+06	3.9E+06	2.8E+06	2.1E+06	1.6E+06	5E+05	5E+05
176		3.4E+07	1.2E+07	5.9E+06	4.2E+06	3.2E+06	2.5E+06	9E+05	9E+05
700					4.3E+06	3.2E+06	2.5E+06	8E+05	7E+05
701								8E+05	7E+05
702								8E+05	8E+05
703								8E+05	8E+05
704								8E+05	8E+05
705								9E+05	8E+05
706								9E+05	8E+05
707								9E+05	9E+05
708								9E+05	9E+05

(continued)

Table 10.12, continued

CUBIC MODEL

WELL NO.	1980	80-81	80-82	80-83	80-84	80-85	80-86	80-87	80-88
					RECORD LENGTH				
710								9E+05	9E+05
716								9E+05	9E+05
731								7E+05	7E+05
732								7E+05	7E+05
734								7E+05	6E+05
735								6E+05	6E+05
737								6E+05	6E+05744
							1E+06	1E+06	
745								1E+06	1E+06
746								9E+05	9E+05
751								6E+05	6E+05
752								7E+05	6E+05
753								6E+05	6E+05
816			1.2E+07	5.9E+06	4.3E+06	3.2E+06	2.5E+06	9E+05	9E+05
817			1.2E+07	5.9E+06	4.2E+06	3.2E+06	2.5E+06	9E+05	8E+05
818			1.2E+07	5.8E+06	4.2E+06	3.1E+06	2.5E+06	9E+05	8E+05
819			1.1E+07	5.6E+06	4E+06	3E+06	2.4E+06	8E+05	8E+05
820			1.2E+07	5.9E+06	4.3E+06	3.2E+06	2.5E+06	9E+05	9E+05
821			1.1E+07	5.6E+06	4.1E+06	3E+06	2.4E+06	8E+05	8E+05
822			1.2E+07	5.7E+06	4.1E+06	3.1E+06	2.4E+06	8E+05	8E+05
823			1.2E+07	5.7E+06	4.2E+06	3.1E+06	2.4E+06	8E+05	8E+05
824			1.1E+07	5.7E+06	4.1E+06	3.1E+06	2.4E+06	8E+05	8E+05
825			1.1E+07	5.7E+06	4.1E+06	3E+06	2.4E+06	8E+05	8E+05
826			1.2E+07	5.7E+06	4.1E+06	3.1E+06	2.4E+06	9E+05	8E+05
827			1.2E+07	5.8E+06	4.2E+06	3.1E+06	2.5E+06	9E+05	9E+05
864				5.8E+06	4.2E+06	3.2E+06	2.5E+06	9E+05	9E+05
865			1.2E+07	5.8E+06	4.2E+06	3.1E+06	2.5E+06	8E+05	8E+05
866			1.2E+07	6E+06	4.3E+06	3.2E+06	2.5E+06	8E+05	8E+05
934					3.3E+06	2.4E+06	1.9E+06	6E+05	6E+05
965						2.5E+06	1.9E+06	5E+05	5E+05
966						2.5E+06	1.9E+06	5E+05	5E+05
972						3.1E+06	2.4E+06	8E+05	8E+05
978							2.1E+06	7E+05	7E+05
980							2.3E+06	8E+05	7E+05
994								7E+05	7E+05
996								7E+05	7E+05
997								9E+05	9E+05
998								9E+05	9E+05

Table 10.13 Optimal Monitoring Networks for Trend Surface Models Fit to Area A Data with Minimum Correlation of 0.9, Future Monthly Sampling Frequency

Linear Trend Surface Model

Record Length	Wells in Network	Objective Function
1980	38	9.19935
1980-81	129	6.10638
1980-82	129	4.5982
1980-83	129	3.3843
1980-84	129	2.8248
1980-85	129	2.5820
1980-86	129	2.3549
1980-87	965	1.4544
1980-88	965	1.4496

Quadratic Trend Surface Model

Record Length	Wells in Network	Objective Function
1980	38	6762.16
1980-81	129	3946.17
1980-82	129	2717.33
1980-83	129	1771.32
1980-84	129	1347.64
1980-85	129	1128.71
1980-86	129	937.68
1980-87	129	504.91
1980-88	129	487.81

Cubic Trend Surface Model

Record Length	Wells in Network	Objective Function
1980	26	1.368×10^{9}
1980-81	38	2.347×10^{7}
1980-82	129	7.678×10^{6}
1980-83	129	3.864×10^{6}
1980-84	129	2.801×10^{6}
1980-85	129	2.089×10^{6}
1980-86	129	1.627×10^{6}
1980-87	129	5.191×10^{5}
1980-88	129	4.999×10^{5}

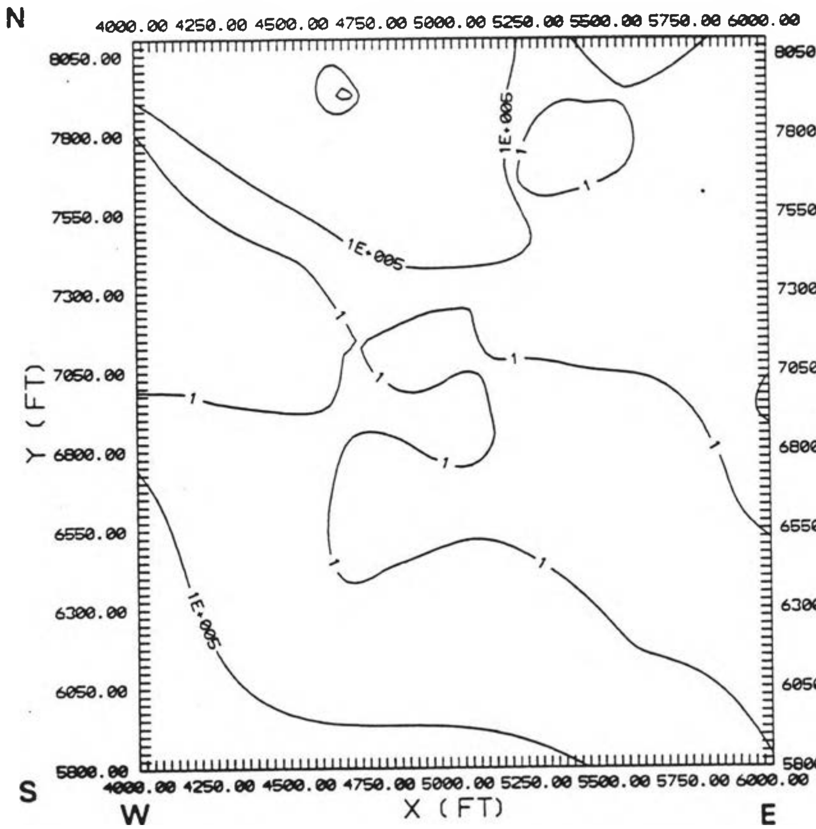

Figure 10.6 Prediction Error Variance at Individual Wells for Single-site Linear Model Fit to All Available Data in Area A

illustrates this uncertainty for contour intervals of 0 ppb, 20,000 ppb, 40,000 ppb, and 60,000 ppb. Both the location of these contours and the uncertainty in the contours can be used by the water quality manager to evaluate the confidence in the model and in the optimally designed monitoring network.

Due to the highly correlated prediction error variances, the optimization of the network using the branch and bound technique resulted in a minimum number of sampling locations.[61] The optimization clearly indicated that the objective function was reduced with an increase in record length for the linear, quadratic, and cubic trend surface models. In addition, use of the multi-site polynomial models over the single-site polynomial models greatly reduces the monitoring network by replacing sampling at all individual well locations with the correlation implied by the multi-site model structure.

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6 A different spatial correlation constraint may be more appropriate for this data

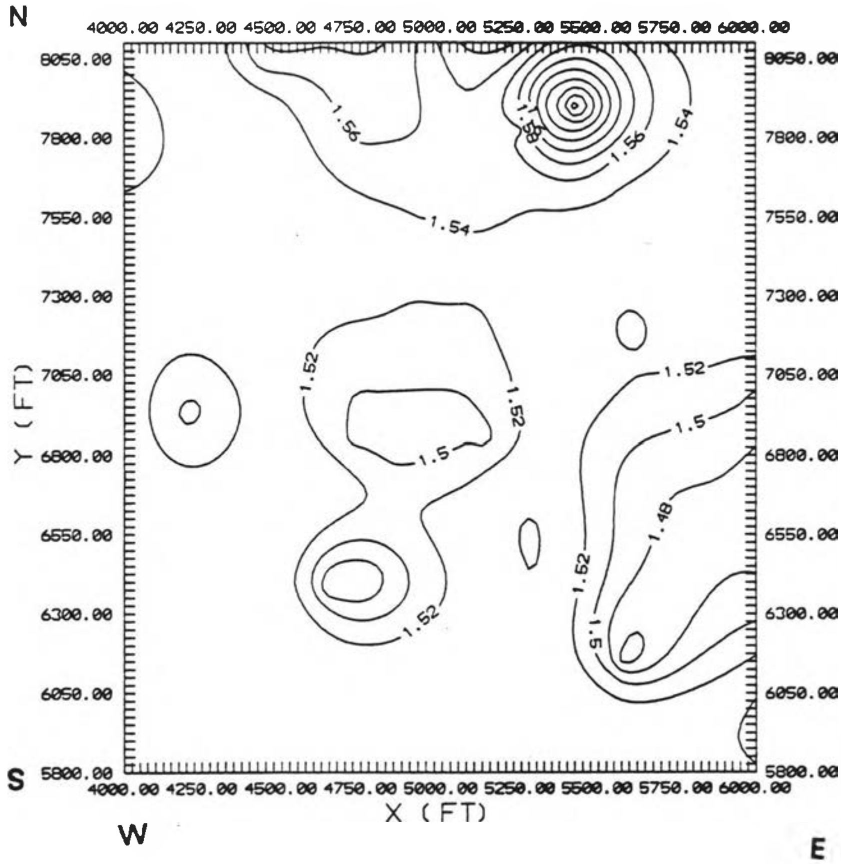

Figure 10.7 Prediction Error Variance at Individual Wells for Linear Trend Surface Model Fit to all Available Data in Area A

10.1.2.3 Physical Model. The error prediction variances at individual wells resulting from the physical model fit to the data from Area A are summarized in Table 10.14 and are plotted in Figure 10.10 for the physical model fit to all available data. Comparison of Figure 10.10 to Figure 10.8 illustrates that the uncertainty for the physical model is more highly variable than for the linear trend surface model. However, the majority of the wells had lower prediction variances based on the use of the physical model, as represented by the larger area contoured between 1.0 and 1.5 for the physical model.

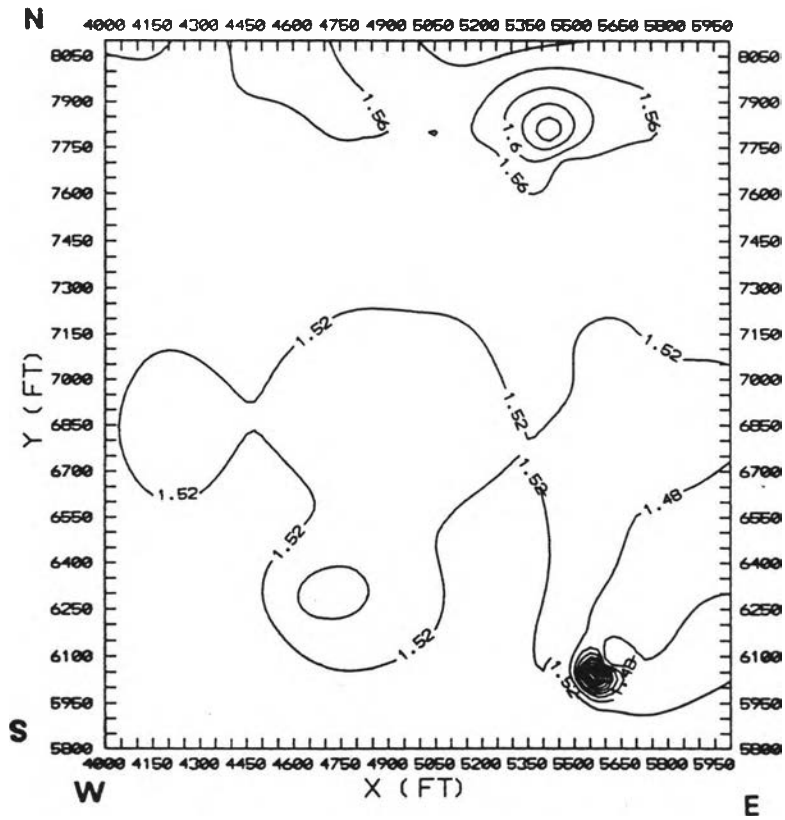

Figure 10.8 Prediction Error Variance Based on Optimal Monitoring Network for Linear Trend Surface Model Fit to All Available Data in Area A

The optimization of the monitoring network based on the physical model for Area A is summarized in Table 10.15.[62] With the existing wells, a maximum spatial correlation of the prediction error variance of 0.3 could only be obtained. Inclusion of additional wells in the network was not considered in this work but would increase the maximum spatial correlation obtainable. Figure 10.11 illustrates the reduction in the prediction error variance surface using the optimal sampling networks for the physical model fit to the data from 1980-88. Comparison of Figure 10.11 to Figure 10.10 illustrates the reduction in the prediction error variance surface after sampling from the optimal monitoring network. Due to the uncertainty

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[6] As discussed for the parameter estimate behavior, the solution of the parameter variance matrix, V_β, was not obtainable for less than five year of data due to the near singularity of the matrix to be inverted.

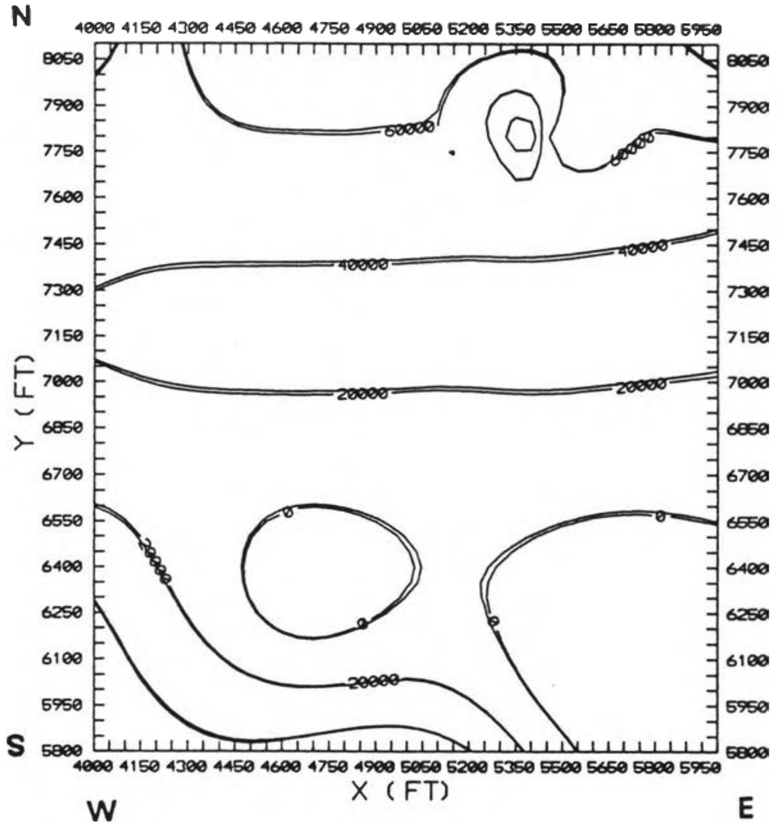

Figure 10.9 Upper and Lower 95% Confidence Limits on Concentrations Bassed on Linear Trend Surface Model Fit to All Available Data in Area A

in the model, this accounts for a generally small reduction in the prediction error variance surface.

An alternative representation of the uncertainty in the model can be realized by plotting confidence limits on concentrations of interest, as shown on Figure 10.12. Concentration intervals of 0, 20,000, 40,000, 60,000, 100,000 and 200,000 were used as a basis of direct comparison to Figure 10.9, the predicted concentration uncertainty intervals for the linear trend surface model. Figure 10.12 illustrates a more concentrated area of elevated levels of PCE, relative to the wider distribution predicted by the linear trend surface model, as shown in Figure 10.9. In addition, the spatial uncertainty in these predicted concentrations is indistinguishable at the scale of the plot for the physical trend surface model.

Table 10.14 Error Prediction Variances at Individual Wells for Physical Model Fit to Data from Area A

WELL NO.	RECORD LENGTH 1980-86	1980-86	1980-87	1980-88
1	28.3147976	9528.1025040	10.2826628	10.5326919
7	5.7732193	3.3532012	59.4745750	59.4667749
11	1.0000000	1.0000000	1.0000000	1.0000000
12	1.0000000	1.0000000	1.0000000	1.0000000
13	57.3753953	4.2333113	196.5267858	196.5275193
14	15.6611168	1.4167402	36.3838967	36.3839792
15	4.1074190	1.0199918	5.9318956	5.9319009
16	1.0000000	1.0000000	1.0000000	1.0000000
17	1.0000000	1.0000000	1.0000000	1.0000000
18	1.0000000	1.0002389	1.0000099	1.0000100
19	1.0000000	1.0001158	1.0000380	1.0000380
20	1.0000000	2.4905597	1.0000000	1.0000000
21	1.0000000	7.4820374	1.0000000	1.0000000
22	1.0000000	4.6477047	1.0000000	1.0000000
26	1.0020691	1.0000041	1.0058085	1.0058099
38	1.0000000	1.0000000	1.0000000	1.0000000
39	1.0000000	1.0000000	1.0000000	1.0000000
43	1.0000000	6.6493893	1.0000000	1.0000000
44	1.0000000	8.7689E+30	1.0000000	1.0000000
45	1.0000000	4.2469E+30	1.0000000	1.0000000
74	244.2130500	6552.1949175	1262.7927450	1262.9379197
103	1.1352807	2.6154992	1.0521954	1.0520993
104	1.0490475	2.6127660	1.0513665	1.0512712
105	1.0496531	3.0089049	1.0735255	1.0734070
106	1.0496531	3.0089049	1.0736799	1.0735612
108	1.0000000	8.84829E+31	1.0000000	1.0000000
109	1.0000000	8.84829E+31	1.0000000	1.0000000
115	27.5619734	18256.6414145	11.5788392	11.8007328
116	27.2904504	22888.0052680	12.3214480	12.5312830
117	27.6172427	23577.9455525	12.4613241	12.6699348
118	27.6480397	23577.9455525	12.4613209	12.6699316
126	1.0000000	2.380E+31	1.0000000	1.0000000
128	1.0000000	1.0000000	1.0000000	1.0000000
129	1.0000000	1.0000000	1.0000000	1.0000000
130	1.0000000	1.0000000	1.0000000	1.0000000
176	1.0000000	1.0000000	1.0000000	1.0000000
700	1.0000000	1.9188190	1.1269741	1.1269620
701			1.3923232	1.3923054
702			1.0000260	1.0000353
703			1.0000434	1.0000576
704			1.0000089	1.0000110
705			19.6310984	19.6289475
706			23.7446039	23.7419315
707			1.0000000	1.0000000
708			1.0000000	1.0000000

(continued)

Table 10.14, continued

WELL NO.	RECORD LENGTH 1980-86	1980-86	1980-87	1980-88
710			1.0000000	1.0000000
716			1.0000000	1.0000000
731			1.0000000	1.0000000
732			1.0000000	1.0000000
734			1.0000000	1.0000000
735			1.0000000	1.0000000
737			1.0000000	1.0000000
744			1.0000000	1.0000000
745			1.0000000	1.0000000
746			1.0000000	1.0000000
751			1.0000000	1.0000000
752			1.0000000	1.0000000
753			1.0000000	1.0000000
816	1.0000000	1.0000000	1.0000000	1.0000000
817	1.0000000	1.0000000	1.0000000	1.0000000
818	1.0000000	1.0000000	1.0000000	1.0000000
819	1.2071539	2.5783953	2.3796683	2.3804162
820	1.0000000	1.0000000	1.0000000	1.0000000
821	27.5377304	17212.2550000	11.4250242	11.6502032
822	1.0000000	1.0000000	1.0000000	1.0000000
823	1.0000000	1.0000002	1.0000000	1.0000000
824	1.0000000	1.0000000	1.0000000	1.0000000
825	1.0000000	1.0000000	1.0000000	1.0000000
826	1.0000000	1.0000000	1.0000000	1.0000000
827	1.0000000	1.0000000	1.0000000	1.0000000
864	1.0000000	1.0000000	1.0000000	1.0000000
865	1.0000000	1.0034251	1.0000319	1.0000319
866	1.0003488	2.0640601	1.0692998	1.0692907
934	1.0000000	1.668E+34	1.0000000	1.0000000
965	1.0000000	1.0000000	1.0000000	1.0000000
966	1.0000000	1.0000000	1.0000000	1.0000000
972	1.0000000	1.0000000	1.0000000	1.0000000
978		1.0000000	1.0000000	1.0000000
980		1.0000000	1.0000000	1.0000000
994			1.0021430	1.0036620
996			1.0053163	1.0053053
997			1.0000000	1.0000000
998			1.0000000	1.0000000
999			1.0000000	1.0000000

10.1.2.4 Summary of Monitoring Network Optimization. The individual sampling frequencies required at individual wells based on the prediction error variances (Tables 10.11, 10.12, and 10.14) are reduced by the use of a multi-site model. Based on the model applicability analyses, the linear trend surface model provided the best description and prediction of PCE groundwater quality behavior of the multi-site models evaluated. Comparison of the optimal monitoring networks and associated objective functions for the multi-site models considered indicates that the objective function is minimized by use of a linear trend surface model. Figure 10.9 illustrates the uncertainty in model predictions using the optimally designed monitoring network based on the linear trend surface applied to all available data in Area A. Given that this uncertainty is acceptable to the groundwater manager, the monitoring network in Area A can be reduced to one well (965) sampled monthly without a loss of information from the monitoring network system.

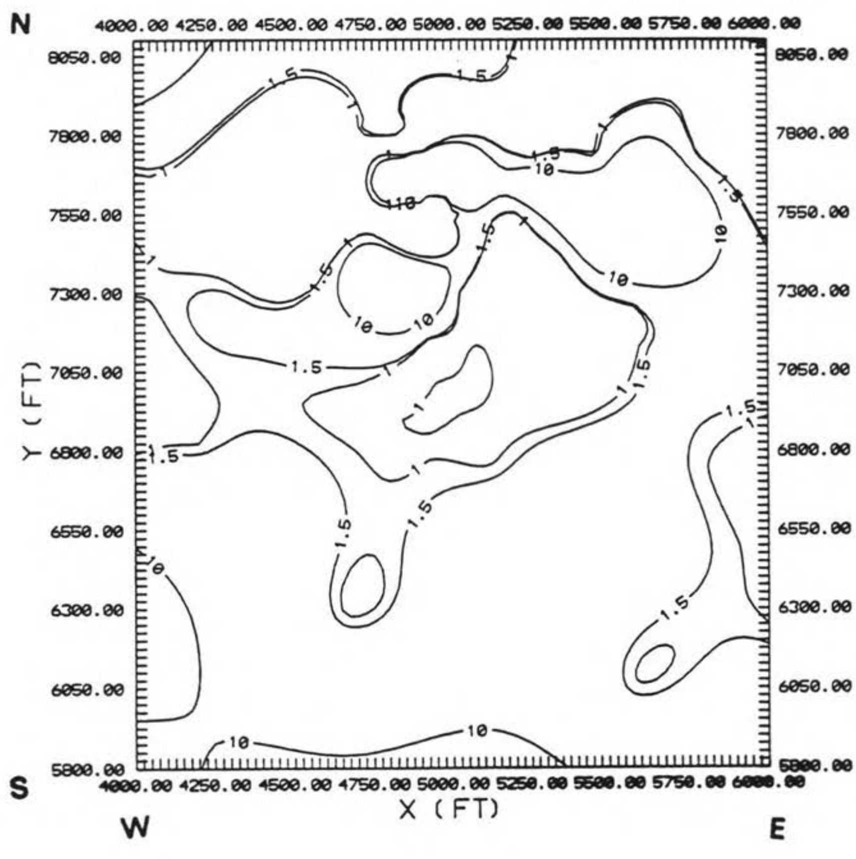

Figure 10.10 Prediction Error Variance at Individual Wells for Physical Model Fit

Table 10.15 Optimal Monitoring Networks for Physical Model Fit to Area A Data; Spatial Correlation = 0.3

RECORD LENGTH	WELLS	OBJECTIVE FUNCTION
1980-1985	15; 818	5.31457
1980-1986	14; 700	3.33556
1980-1987	1; 15; 104	17.26592
1980-88	1; 15; 104	17.51586

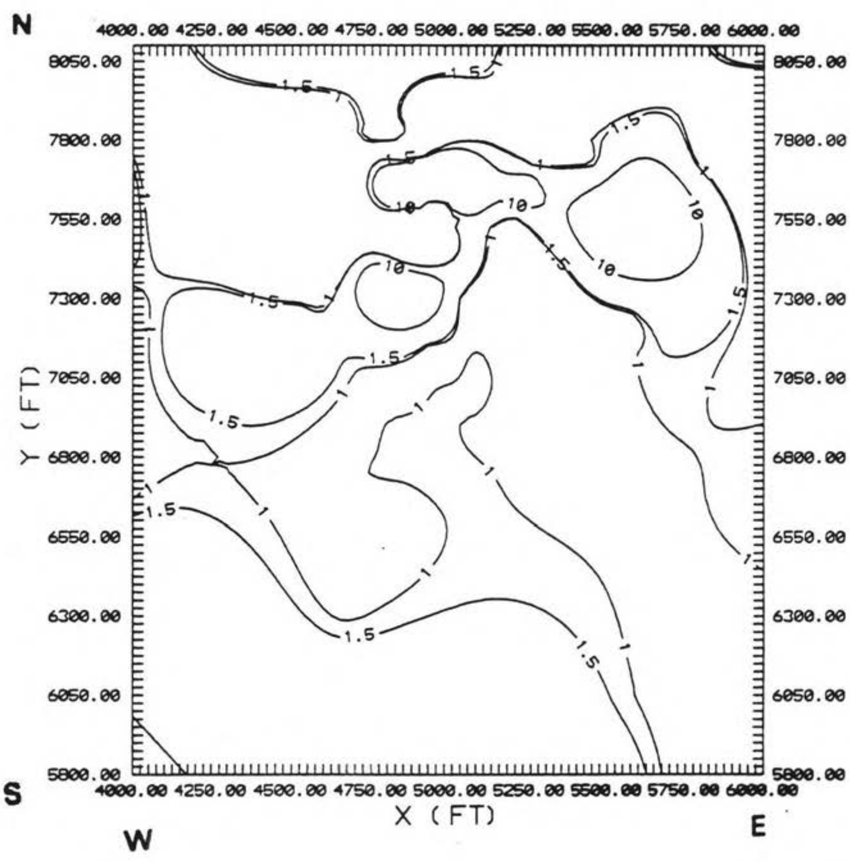

Figure 10.11 Prediction Error Variance for Optimal Monitoring Network Based on Physical Model Fit to All Available Data in Area A

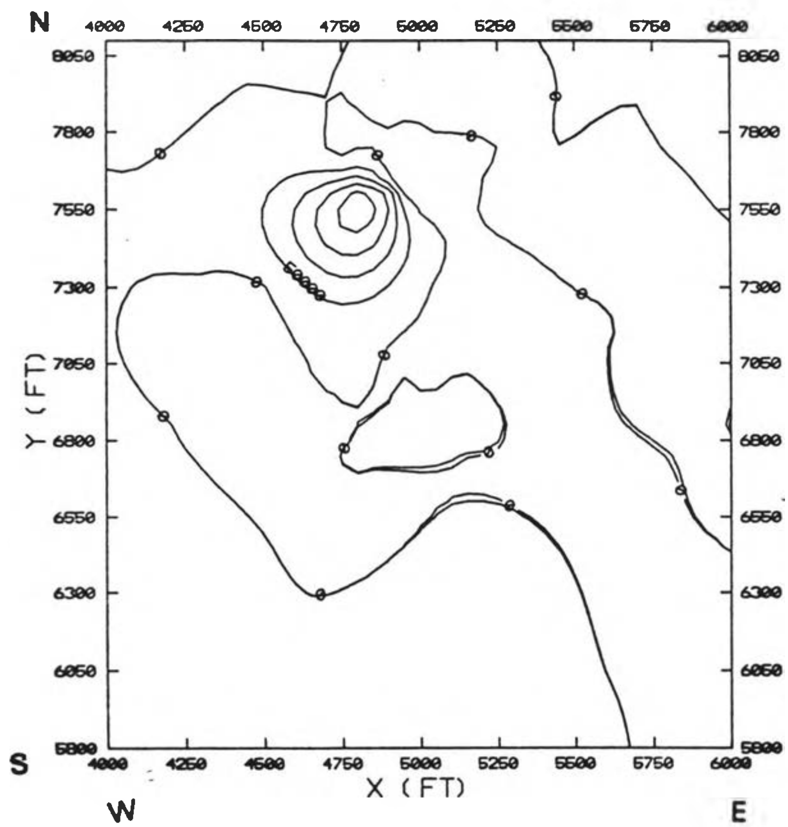

Figure 10.12 Upper and Lower 95% Confidence Bounds on Predicted Concentrations Based on Physical Model Fit to All Available Data

10.1.3 Summary of Model Selection and Network Design for Area A.

The model selection process indicated that the multi-site models were superior to the single-site models in model applicability. This superiority of the multi-site models was also evidenced by the significantly reduced average prediction error variances at individual wells. Of the multi-site models considered, none exhibited "ideal" behavior based on a combination of test statistics. However, based on both model applicability and monitoring network design considerations, the linear trend surface model was superior for the PCE groundwater quality data in Area A. It is highly recommended that a fractured flow type model be considered for further evaluation given the statistical characteristics of the data, the results from the physical porous media model goodness-of fit evaluation, and other site information.

10.2 Area C

Area C is defined by the limits shown in Figure 10.1. The suspected source for PCE in Area C is a construction debris landfill which was used beginning in the early 1970s. Groundwater flow is principally to the south.

10.2.1 Model Selection.

The selection of a model for describing the PCE groundwater quality data in Area C is based on the protocol outlined in Chapter 9. Specifically, goodness-of-fit of the candidate models is evaluated based on an evaluation of F-test statistics, model parameter behavior, and residual behavior. Model prediction capabilities are then evaluated using prediction bias, prediction bias variance, and the associated t-test, as discussed below.

10.2.1.1 Single-site Polynomial Models. Single-site polynomial models were fit to the data from Area C using least-squares regression. The results of the F-test statistics for those wells exhibiting significant polynomial trends are summarized in Table 10.16. Approximately one-third of the wells did not exhibit any significant linear trend. Only two of the ten wells which exhibited significant linear trends, exhibited any significant higher order trends. Lastly, those wells that did show a significant polynomial trend did so only over limited time periods. Parameter behavior was not evaluated due to the limited data length.

Table 10.17 summarizes the residual temporal correlations observed for the significant single-site models based on the results of the F-test analyses. Those correlations associated with record lengths which exhibited significant trends are

Table 10.16 F-test Statistics for Single-site Polynomial Models Fit to Data From Area C

WELL No.	RECORD LENGTH	Available Data	F Test Results - Period of Significance: Linear	Quadratic(a)	Cubic(a)
51	18	1980-82	1980(d)	NS(b)	(c)
53	77	1980-88	1983,1987,1988	NS	(c)
54	73	1980-88	1981,1982	1982	1982
69	41	1980-87	1981	NS	(c)
111	16	1981-87	1981	NS	(c)
835	8	1982-87	1983	NS	(c)
836	8	1982-87	1983	NS	(c)
837	23	1982-88	1982	NS	(c)
922	9	1984-87	1987	1987	NS
923	9	1984-87	1986,1987	NS	(c)

a) F-test addition over lower order polynomial
b) NS = not significant
c) lower order model not significant
d) years indicating period for 1980 through year designated

Table 10.17 Residual Temporal Correlation[a] for Single-Site Polynomial Models Fit to Data from Area C

Linear Model

Well No.	1980	1980-81	1980-82	1980-83	1980-84	1980-85	1980-86	1980-87	1980-88
51	0.0242	0.0351	0.0293	0.0293	0.0293	0.0293	0.0293	0.0293	
53	-0.0050	-0.0030	-0.0063	-0.0040	-0.0016	-0.0010	-0.0008	-0.0007	-.0006
54	-0.0214	-0.0093	-0.0014	-0.0033	-0.0017	-0.0013	-0.0010	-0.0009	-.0009
69	-0.0940	-0.0263	-0.0067	-0.0056	-0.0044	-0.0037	-0.0035	-0.0034	-.0034
111		(a)	-0.1102	-0.0036	-0.0018	0.0187	0.0225	0.0254	
835				(a)	-0.0756	-0.0437	-0.0360	-0.0205	
836				(a)	-0.0756	-0.0437	-0.0360	-0.0205	
837			(a)	-0.0441	-0.0214	-0.0157	-0.0114	-0.0081	-.0073
922							-0.0499	-0.0534	
923							-0.0712	-0.0608	

Quadratic Model

Well No.	1980	1980-81	1980-82	1980-83	1980-84	1980-85	1980-86	1980-87	1980-88
54	-0.0164	-0.0088	-0.0049	-0.0047	-0.0029	-0.0016	-0.0012	-0.0009	-.0009
922							-0.0773	-0.0672	

Cubic Model

Well No.	1980	1980-81	1980-82	1980-83	1980-84	1980-85	1980-86	1980-87	1980-88
54	-0.0350	-0.0089	-0.0059	-0.0099	-0.0030	-0.0019	-0.0015	-0.0012	-.0012

(a) correlations for models which were significant based on the F-test statistics are highlighted

highlighted. None of the residual correlations were significant. In addition, the residual correlations generally decreased with an increase in record length. However, since there was no difference in the residual temporal correlations between the wells which did have significant polynomial trends and those which did not, the evaluation of residuals did not aid in model discrimination.

The skewness of the residuals from the significant polynomial models based on the results of the F-test and residual correlation analyses are summarized in Table 10.18. Those skewness coefficients associated with record lengths which exhibited significant trends based on the results of the F-test and residual correlation analyses are highlighted on Table 10.18. As for the residual correlation, no significant skew was detected. In addition, there was no observable pattern to the residual skew as the record length increased.

Based on these goodness-of-fit statistics, the linear single-site models appears to be good models for describing the PCE groundwater quality at select wells and record lengths. However, the single-site models were not significant for the vast majority of wells and record lengths.

For the single-site models, the average prediction bias and associated t-test statistics for the wells exhibiting significant linear, quadratic, or cubic trends are summarized in Table 10.19. Biases associated with significant single-site models based on the results of the F-test and the residual behavior analyses are highlighted.

In addition, biases which were significant based on the t-test analysis are denoted by highlighted t-test values. As shown by Table 10.19, most of the models significant based on the goodness-of-fit tests, exhibited significant prediction bias. Only the predictions made from a linear model fit to the data from MW-54 did not exhibit a significant bias over the period from 1980-81, as indicated by a highlighted bias and a non-highlighted t-test value.

In summary, the single site polynomial models are not good models for describing the PCE groundwater quality data in Area C. The goodness-of-fit tests only indicate a few wells over limited record lengths which exhibited significant polynomial trends. The statistical behavior was not consistent and does not necessarily improve with record length. In addition, prediction bias is generally significant using these single-site polynomial models.

10.2.1.2 Trend Surface Models. The F-test results for the trend surface models fit to the data are summarized in Table 10.20. For the trend surface models applied to all available data, a linear model was significant for 1980 and 1980-81 (one and two years of data) and periods of 1980-1985 (six years) through 1980 -1988 (nine years). For those periods which the linear model was significant, the quadratic and cubic order models were also significant at the $\alpha = 0.05$ significance level.

As for Area A, a reduction in data was evaluated to assess the behavior of the F-test statistics. The F-test statistics did not consistently decrease with a decrease in sampling frequency as did the statistics for Area A. However, the only t-test statistic which indicated that the trend in the F-test statistics was significantly

Table 10.18 Residual Skewness(a) for Single-Site Polynomial Models Fit to Data From Area C

Linear Model

Well No.	1980	1980-81	1980-82	1980-83	1980-84	1980-85	1980-86	1980-87	1980-88
51	0.0070	0.0314	0.0332	0.0332	0.0332	0.0332	0.0332	0.0332	
53	0.0956	0.0598	0.0405	0.0311	0.1122	0.1015	0.0915	0.0856	0.0851
54	-0.1178	0.0606	0.1056	0.1734	0.1545	0.1299	0.1165	0.1072	0.1064
69	0.0835	0.0960	0.0941	0.0897	0.0888	0.0850	0.0818	0.0807	0.0807
111		(a)	0.2825	0.1689	0.1567	0.1070	0.0907	0.0702	
835				(a)	0.0085	0.0678	0.1481	0.1654	
836				(a)	0.0085	0.0679	0.1481	0.1654	
837			(a)	0.1774	0.1650	0.1460	0.1338	0.1255	0.1231
922							0.2114	0.0240	
923							0.0545	0.0956	

Quadratic Model

Well No.	1980	1980-81	1980-82	1980-83	1980-84	1980-85	1980-86	1980-87	1980-88
54	-0.1433	0.0598	-0.0163	0.1575	0.1393	0.1231	0.1133	0.1060	0.1053
922							0.1700	0.1081	

Cubic Model

Well No.	1980	1980-81	1980-82	1980-83	1980-84	1980-85	1980-86	1980-87
54	-0.0522	0.0754	-0.0676	0.1231	0.1394	0.1191	0.1071	0.0999

(a) skewness for models which were significant based on the F-test statistics are highlighted

Table 10.19 One-Year Prediction Bias[a] and Associated T-test Statistics[b] for Single-site Polynomial Models Fit to Data from Area C

Linear Model

WELL	RECORD LENGTH 1980		1980-81		1980-82		1980-83		1980-84		1980-85		1980-86	
NO.	BIAS	T-TEST	BIAS	T-TEST	BIAS	T-TEST	BIAS	T-TEST	BIAS	T-TEST	BIAS	T-TEST	BIAS	T-TEST
51	**-50.6**	**-5.211**												
53	14.736	1.3145	-3.684	-0.057	-22.72	-0.827	**-15.7**	**-5.68**	-29.47	**-3.718**	-11.38	**-2.322**	-10.93	**-6.676**
54	-10.06	-1.317	2.447	0.5257	**-244.9**	**-18.07**	-45.17	**-27.31**	5.328	0.3486	-5.61	**-19.43**	1.941	1.7422
69	1.812	**4.1353**	**2.556**	**3.3678**	3.912	0.977	-1.643	**-116.2**	-0.692	**-37.9**	-0.08	**-2.53**		
111					-244.1		-12.5		279.89	3.9236				
835							8.596		6.23					
836							8.596		6.23					
837					-25.37	-9.732	-0.28	-8.858	1.302			1.55	6.9318	1.512

Quadratic Model

WELL	RECORD LENGTH 1980		1980-81		1980-82		1980-83		1980-84		1980-85		1980-86	
NO.	BIAS	T-TEST	BIAS	T-TEST	BIAS	T-TEST	BIAS	T-TEST	BIAS	T-TEST	BIAS	T-TEST	BIAS	T-TEST
54	-1.776	-0.232	5.753	1.0184	**-664.2**	**-6.533**	12.432	1.6267	62.752	**3.6719**	22.56	**12.205**	18.52	**-6.686**

Cubic Model

WELL	RECORD LENGTH 1980		1980-81		1980-82		1980-83		1980-84		1980-85		1980-86	
NO.	BIAS	T-TEST	BIAS	T-TEST	BIAS	T-TEST	BIAS	T-TEST	BIAS	T-TEST	BIAS	T-TEST	BIAS	T-TEST
54	-155.1	**-3.769**	-28.42	**-2.147**	**-1446**	**-3.785**	198.32	**5.6625**	68.672	**4.0184**	-11.09	**-6.307**	-17.46	**-8.505**

(a) biases highlighted indicate those models and record lengths which exhibit a significant model fit based on F-test and residual analyses

(b) t-test statistics significant at the $\alpha = 0.05$ confidence level are highlighted

Table 10.20 F-test Results[(a)] and Associated t-tests for Multi-site Models Fit to Data from Area C

Record Length	Model	All	Bimonthly	Quarterly	Triannual	Biannual	t-test
		Frequency of Sampling					
1980	Linear	4.106	5.019	5.666	2.946	3.770	-.04571
	Quadratic	3.209	7.332	18.625	11.152	(b)	(b)
	Cubic	1.920	3.360	(b)	(b)	(b)	(b)
	Physical	480.958	153.976	199.475	25.376		-2.11282
	Size	38	22	14	13	9	
1980-81	Linear	3.397	2.882	2.552	3.101	3.421	-.10144
	Quadratic	30.271	22.210	17.775	15.550	12.951	-4.87063
	Cubic	39.910	43.611	32.929	27.192	22.945	-1.35043
	Physical	1233.793	622.157	2029.275	1435.467	111.935	-0.00928
	Size	79	49	33	30	21	
1980-82	Linear	2.481	1.724	1.332	0.923	0.403	.08201
	Quadratic	16.820	12.138	8.560	7.686	7.365	-1.08114
	Cubic	14.392	12.098	8.956	8.593	11.919	-1.60613
	Physical	54341.38	1330.915	523.84	6322.542	455.859	0.53841
	Size	99	68	49	46	31	
1980-83	Linear	1.158	1.005	0.723	0.507	0.105	.05941
	Quadratic	15.217	13.384	9.816	9.001	5.798	-.15988
	Cubic	11.833	8.834	6.557	5.951	3.836	.22847
	Physical	1027.948	803.96	485.638	1553.328	2544.249	-.86586
	Size	134	95	71	66	47	
1980-84	Linear	1.502	1.729	1.168	1.290	0.403	.04151
	Quadratic	13.769	16.061	12.255	11.473	7.306	-.21771
	Cubic	9.819	12.175	9.048	8.710	5.458	-.21625
	Physical	4082.297	827.887	1189.488	1707.659	519.046	.26382
	Size	181	130	97	94	67	

Table 10.20, continued

Record Length	Model	All	Frequency of Sampling Bimonthly	Quarterly	Triannual	Biannual	t-test
1980-85	Linear	3.578	3.081	2.459	2.628	1.381	.03069
	Quadratic	23.928	23.920	16.838	15.536	10.491	-.08189
	Cubic	13.274	14.234	10.067	9.547	6.4001	-.12344
	Physical	6076.29	908.058	3563.029	1140.936	911.281	.11611
	Size	231	165	124	119	89	
1980-86	Linear	8.476	6.536	4.781	4.604	2.570	.03521
	Quadratic	31.406	28.954	21.227	19.226	13.286	-.07002
	Cubic	19.282	18.691	13.004	12.259	8.317	-.06453
	Physical	1145.618	1468.996	1296.66	5333.695	1040.775	-.07606
	Size	326	235	178	167	123	
1980-87	Linear	11.180	7.770	5.687	5.421	3.070	.02245
	Quadratic	28.285	23.917	17.471	17.292	11.276	-.01760
	Cubic	18.524	16.210	11.647	10.724	7.150	.00930
	Physical	3112.268	4701.232	9290.391	2244.329	1394.134	-.01913
	Size	392	283	220	203	155	
1980-88	Linear	11.209	7.861	5.805	5.547	3.197	.02361
	Quadratic	28.558	24.219	17.753	17.635	11.533	-.01626
	Cubic	18.754	16.484	11.911	10.989	7.392	.01112
	Physical	9671.102	1758.162	2318.713	885.414	4110.417	-.00421
	Size	396	287	224	207	159	

(a) F-test values significant at the $\alpha = 0.05$ level are highlighted

(b) insufficient data to calculate

different than for a correct model was for a quadratic trend surface model fit to data from 1980 through 1981 as indicated by a significant t-test value.
The behavior of selected model parameter estimates is illustrated in Figures 10.13, 10.14, and 10.15 for the linear, quadratic and cubic trend surface models, respectively. The parameter estimates do not converge towards a single value within the specified 95% confidence limits. This is indicative of an incorrect model structure. The average temporal and spatial residual correlations for the multi-site models are summarized in Table 10.21. All correlations significant at the $\alpha = 0.05$ significant level are highlighted. As for Area A, the temporal correlations were more significant than the spatial correlations. In general, the correlations increased with an increase in record length, consistent with an incorrect model structure.

The skewness of the residuals resulting from the trend surface models fit to all available data are summarized in Table 10.22. The skewness coefficients were significant for a majority of the models and record length considered, particularly for the longer record lengths. This could be indicative of either an incorrect model structure or non-additive non-normal data errors.

Based on the F-test analysis, parameter behavior, and residual behavior, the trend surface models do not appear to adequately describe the PCE groundwater quality data in Area C. This is indicated by the inconsistent F-test behavior with an increase in record length, parameter estimates which vary outside specified confidence limits and do not converge towards single values, and significant residual correlations which increase with an increase in data size.

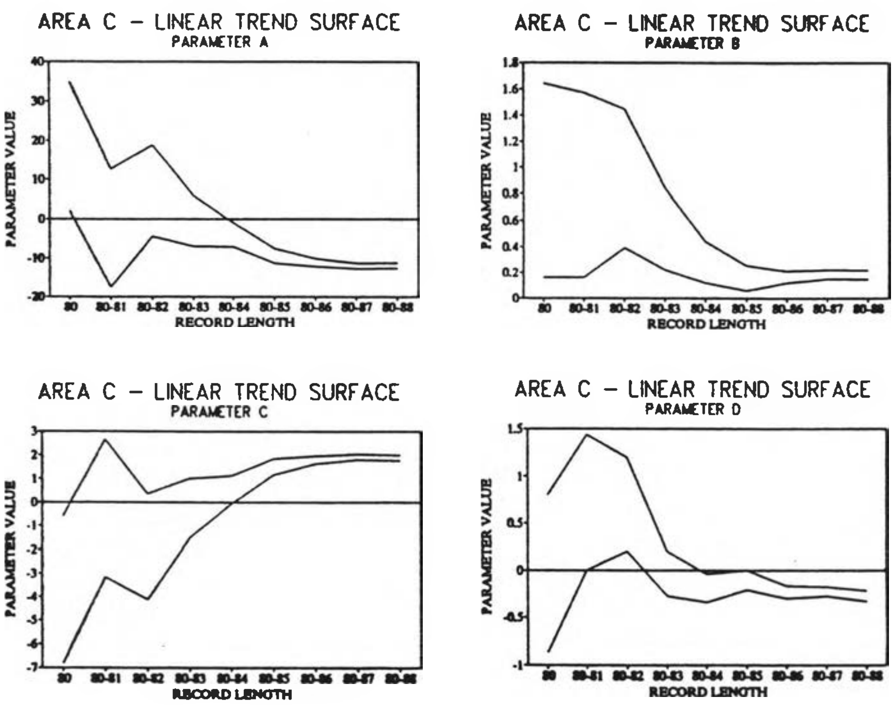

Figure 10.13 Upper and Lower 95% Confidence Limits of Parameter Estimates for Linear Trend Surface Model Fit to All Data in Area C

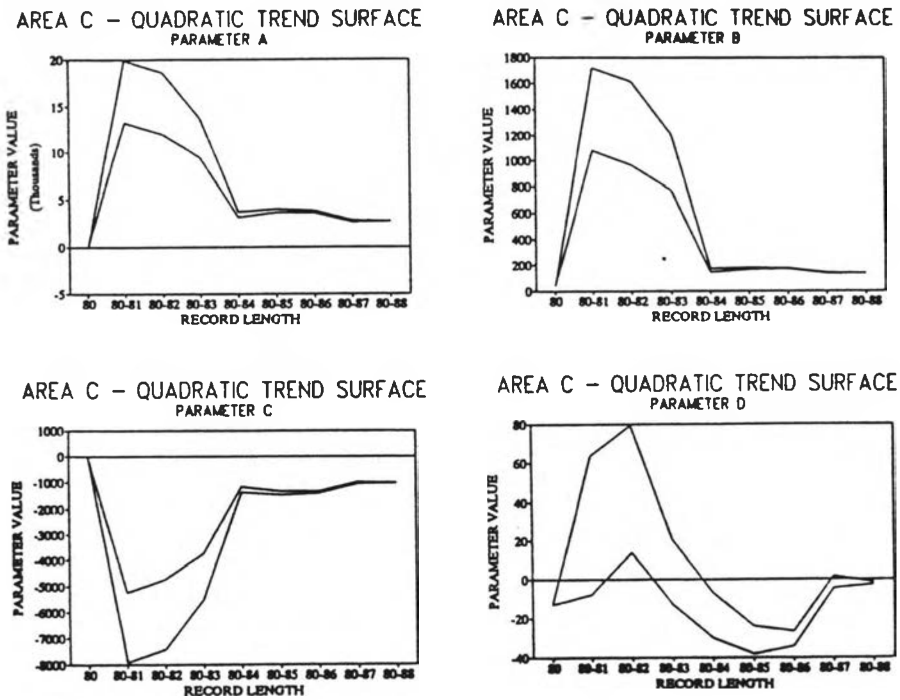

Figure 10.14 Upper and Lower 95% Confidence Limits of Selected Parameter Estimates for Quadratic Trend Surface Model Fit to All Data in Area C

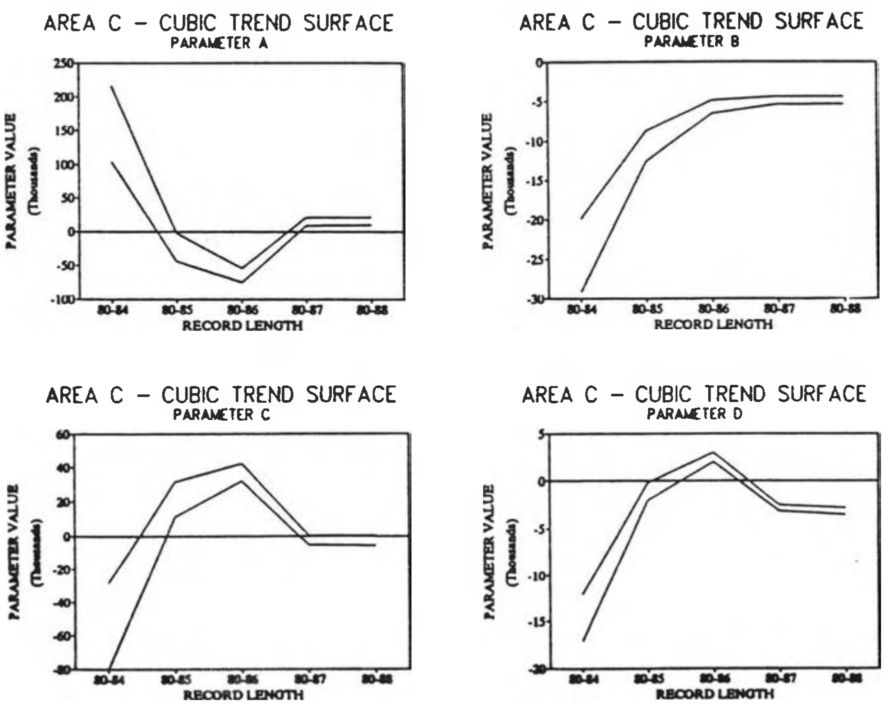

Figure 10.15 Upper and Lower 95% Confidence Limits of Selected Parameter Estimates for Cubic Trend Surface Model Fit to All Data in Area C

Table 10.21 Average Residual Temporal and Spatial Correlation Ranges for Multi-Site Models Fit to Data from Area C

Temporal Residual Correlation

YEAR	LINEAR	QUADRATIC	CUBIC	PHYSICAL
1980	-.0612	.2128	.1586	.00168
1980-81	.6022	.3485	.1948	.13789
1980-82	.1767	.1835	.1980	-.00326
1980-83	-.0028	.2628	.1460	.04646
1980-84	-.0018	.4483	.2085	.3371
1980-85	-.0428	.4697	.4770	.3650
1980-86	.4002	.6041	.5237	.4433
1980-87	.4103	.5586	.5363	.5382
1980-88	.4312	.5553	.5378	.5378

Spatial Residual Correlation

YEAR	LINEAR	QUADRATIC	CUBIC	PHYSICAL
1980	-.0405	-.0017	.0506	-.0341
1980-81	.4251	.0832	-.0401	.05933
1980-82	.1657	.0571	.0542	.01731
1980-83	.0611	.0244	.0457	.14635
1980-84	.1444	.2332	.1155	.1969
1980-85	.1788	.1594	.0182	.0650
1980-86	.4063	.1769	.1010	.01016
1980-87	.3772	.5014	.1946	-.0092
1980-88	.3735	.4686	.1982	-.0083

(a) correlations significant at the $\alpha = 0.05$ level are highlighted

The average prediction biases resulting from the trend surface models are summarized in Table 10.23. The t-test statistics associated with these prediction biases are also summarized in this table. T-test values significant at the $\alpha = 0.05$ significance level are highlighted. The t-test indicates the prediction biases resulting from fitting the linear model to the data are generally not significant (except for the period of 1980-82 which did not exhibit a significant linear trend based on the F-test analysis). The t-test associated with the prediction biases resulting from fitting the quadratic and cubic models to the data are significant for approximately one-half of the record lengths considered.

The trend surface models appear to offer a significant improvement over the single-site models, with the F-test statistic indicating a significant model fit. However, based on the results from the evaluation of parameter behavior, residual behavior,

Table 10.22 Residual Skewness[a] for Multi-Site Models Fit to Data from Area C

YEARS	LINEAR	QUADRATIC	CUBIC	PHYSICAL
1980	.1117	.1092	-.1699	1.01616
1980-81	-.3488	.2194	.7131	0.85078
1980-82	.7942	.4583	.5476	1.13935
1980-83	.9236	1.3876	1.3161	1.11119
1980-84	.9588	2.0564	1.4839	1.24422
1980-85	1.0813	1.8409	1.7418	1.31739
1980-86	.1470	.4604	.1812	0.6235
1980-87	.3780	.8525	.6535	0.4801
1980-88	.3777	.8418	.6541	0.4806

(a) skewness coefficient significant at the $\alpha = 0.05$ level are highlighted

Table 10.23 One-Year Prediction Bias and Associated T-test Statistics[a] for Multi-Site Models Fit to Data from Area C

BIAS

YEAR	LINEAR	QUADRATIC	CUBIC	PHYSICAL
1980	-3.963	77.352	476.001	100.596
1980-81	1.399	-47.375	-230.266	525.0116
1980-82	-78.452	-230.772	-116.834	125.745
1980-83	-15.442	63.615	172.640	283.672
1980-84	13.742	21.495	24.343	50.71144
1980-85	-13.898	21.007	32.635	-110.247
1980-86	3.799	13.163	-20.275	-28.6885
1980-87	-30.505	24.886	6.294	-121.885

T-TEST STATISTICS

YEAR	LINEAR	QUADRATIC	CUBIC	PHYSICAL
1980	-0.8156	7.5957	6.4679	.52161
1980-81	0.0329	-1.1138	-1.9010	NA
1980-82	-5.7492	-10.3752	-1.4314	.29017
1980-83	-0.8362	3.6727	7.5416	.86539
1980-84	0.9462	3.3420	0.9096	.3025
1980-85	-1.5346	2.7603	2.5608	-.2579
1980-86	0.2548	1.4228	-2.6526	-.0654
1980-87	-1.8165	2.2804	1.0571	-.9213

(a) t-test statistics significant at the $\alpha = 0.05$ level are highlighted and predication bias, the trend surface models are inappropriate for describing the behavior observed in the PCE groundwater quality data from Area C.

10.2.1.3 Physical Model. As for Area A, the range of potential physical model parameter values was constrained by both historical site use information and theoretical chemical behavior. The range of potential parameter values for the physically-based two-dimensional model fit to the PCE groundwater quality data from Area C are summarized in Table 10.24.

Table 10.24 Constraints on Physical Model Parameters for Area C

Parameter	Range	Information
C_0	>600	minimum based on observed concentration in source area
t_0	1970-1982	site history: 1970 was earliest use of area as construction landfill; in 1982 the source area was removed
R	2.5	Theoretical (see p. 184)
λ	0.0	Theoretical (see p. 184)
α	> 0.0	no separate phase source detected; therefore modeled as decaying source
X_0	4600-5000	Identification of source location based on historical use
Y_0	7400-7800	

The suspected source area in Area C was a construction landfill which was used since the early 1970s. In 1982, the source area was removed. No separate phase product has been detected in Area C; therefore, it is assumed that there was a decaying source from the early 1970s to 1982 ($\alpha > 0$). The chemical/physical retardation (R) and decay properties (λ) were assumed to be equivalent to those for Area A, as discussed in Section 10.1.1.3.

The F-test results for the physical model fit to the data from Area C are summarized in Table 10.20 along with the results from the other multi-site models. As shown in Table 10.20, the physically-based model is significant based on the F-test for all data subsets considered. In addition, the significance of the fit is an improvement over the results for the multi-site statistical models considered as evidenced by the significantly higher F-test values. Lastly, the trend in the F-test statistics were not significantly different than the theoretical slope of the F-test values for a correct model, as discussed in Chapter 8. Therefore, the F-test results are consistent with a correct model structure.

The parameter values resulting from fitting the physical model to all available data over different record lengths and sampling frequencies are summarized in Table 10.25 for Area C. In addition, Figures 10.16 through 10.20 illustrate the behavior of these estimated parameters for different sampling frequencies. As illustrated by these figures and Table 10.25, the behavior of the parameter estimates is consistent with parameter behavior for a correct model in that the convergence of parameters is maintained within the confidence limits calculated and the parameter estimates converge towards single values as the data set increases in size.

The correlation of the residuals is summarized in Table 10.21 for the physical model fit to all available data over different record lengths. The temporal correlation was significant for longer record lengths, although the spatial correlation was not significant over any record lengths. The effect of data reduction on the residual temporal correlation is summarized in Table 10.26. The increase of these residual temporal correlations with an increase in the data set is consistent with a significant residual correlation. The residual skewness for the physical model fit to the data is summarized in Table 10.22 with the results for the other multi-site models. The skewness coefficients are significant for the physical model fit to all data record lengths. The results from the residual analysis could indicate either an incorrect model structure or a non-additive, non-normal data error.

The goodness-of-fit tests performed for the physical model fit to Area C data indicate that the physical model is relatively good at describing the PCE groundwater quality data. The significance of the residual temporal correlations and residual skew indicates a more complex physical model with consideration of non-normal data my be appropriate for further consideration.

The one-year prediction bias and associated t-test statistics are summarized in Table 10.27 for the physical model fit to the data from Area C. None of the one-year prediction biases based on the model fit to all available data were significant. Some of the prediction biases for the physical model fit to reduced data sets were significant based on the t-test results. However, the prediction biases generally reduced as the frequency of sampling increased. This is indicative of a correct model structure.

The results of the prediction tests for the physical model fit to the data from Area C indicate a significant model. These results strengthen the confidence in the physical model based on the goodness-of-fit tests.

10.2.1.4 Summary of Model Selection

Of the models considered, the trend surface models were a significant improvement over the single-site statistical models in that the F-tests were consistently significant. In addition, the physical model was a significant improvement over the multi-site statistical models in that the parameter behavior and prediction bias behavior was consistent with the expected behavior for a correct model structure. Clearly, of the models considered, the physical model was the best model at describing and predicting the groundwater quality behavior observed. The only non-ideal behavior exhibited by the statistics was

Table 10.25 Best-fit Physical Model Parameter Estimates[a] for Area C

YRS OF RECORD	SAMPLING FREQUENCY	PARAMETER C_0	D_L	D_T	v	α
1980	All	1600	10	1.5	.15	.0010
	Bimonthly	1675	10	1.5	.15	.0048
	Quarterly	1575	10	1.5	.15	.0058
	Triannual	1575	10	1.5	.15	.0041
	Biannual	1500	10	1.5	.15	.0053
80-81	All	1600	10	1.5	.15	.0010
	Bimonthly	1550	10	1.4	.15	.0011
	Quarterly	1575	10	1.5	.15	.0009
	Triannual	1575	10	1.5	.15	.0041
	Biannual	1650	10	1.5	.15	.0008
80-82	All	1550	10	1.5	.16	.0011
	Bimonthly	1625	10	1.4	.15	.0010
	Quarterly	1575	10	1.4	.15	.0008
	Triannual	1600	10	1.5	.15	.0008
	Biannual	1625	10	1.4	.15	.0007
80-83	All	1600	10	1.5	.15	.0011
	Bimonthly	1550	10	1.4	.15	.0010
	Quarterly	1625	10	1.5	.15	.0009
	Triannual	1650	10	1.5	.15	.0009
	Biannual	1525	10	1.5	.15	.0007
80-84	All	1675	10	1.5	.15	.0012
	Bimonthly	1600	10	1.5	.15	.0011
	Quarterly	1675	10	1.5	.15	.0010
	Triannual	1550	10	1.4	.15	.0009
	Biannual	1575	10	1.5	.15	.0008
80-85	All	1600	10	1.5	.15	.0012
	Bimonthly	1600	10	1.5	.15	.0011
	Quarterly	1600	10	1.4	.15	.0010
	Triannual	1625	10	1.5	.15	.0010
	Biannual	1625	10	1.5	.15	.0009
80-86	All	1575	10	1.5	.15	.0011
	Bimonthly	1600	10	1.5	.16	.0011
	Quarterly	1600	10	1.5	.15	.0009
	Triannual	1625	10	1.5	.15	.0009
	Biannual	1525	10	1.5	.16	.0008

(continued)

Table 10.25, continued

YRS OF RECORD	PARAMETER SAMPLING FREQUENCY	C_o	D_L	D_T	v	α
80-87	All	1550	10	1.5	.15	.0013
	Bimonthly	1650	10	1.4	.15	.0010
	Quarterly	1650	10	1.4	.15	.0009
	Triannual	1550	10	1.5	.15	.0008
	Biannual	1525	10	1.5	.15	.0007
80-88	All	1675	10	1.5	.15	.0010
	Bimonthly	1650	10	1.5	.15	.0010
	Quarterly	1650	10	1.5	.15	.0009
	Triannual	1525	10	1.5	.15	.0008
	Biannual	1675	10	1.5	.15	.0008
TOLERANCE[b]		±25	±1	±0.1	±.01	±.0001

(a) parameter estimates for X_0, Y_0 and a were 4800, 6200, and 200 feet,respectively, for all data subsets

that of the significant temporal correlation of the residuals and the skewness of the residuals. None of the models exhibited a temporal residual correlation which was not significant. This information, along with the significant skewness of the residual for the physical model fit to the data could indicate a non-additive, non-normal error rather than an incorrect model structure. Lastly, further refinement of the physical model to address the vertical non-homogeneity of the system should be considered in further model refinement evaluations.

10.2.2 Monitoring Network Optimization.

Optimal monitoring networks were evaluated for all the models considered, regardless of the results of model applicability analyses in order to compare the networks.

10.2.2.1 Single-Site Polynomial Models. As discussed earlier, only sampling frequency can be optimized for single-site polynomial models since there is no spatial correlation implied by the models. Table 10.28 summarizes the error prediction variance at each well in Area C for a specified future monthly sampling frequency. The error prediction variances vary dramatically for the different wells and different record lengths considered. The error prediction variances associated with models significant based on the F-test evaluation (highlighted in

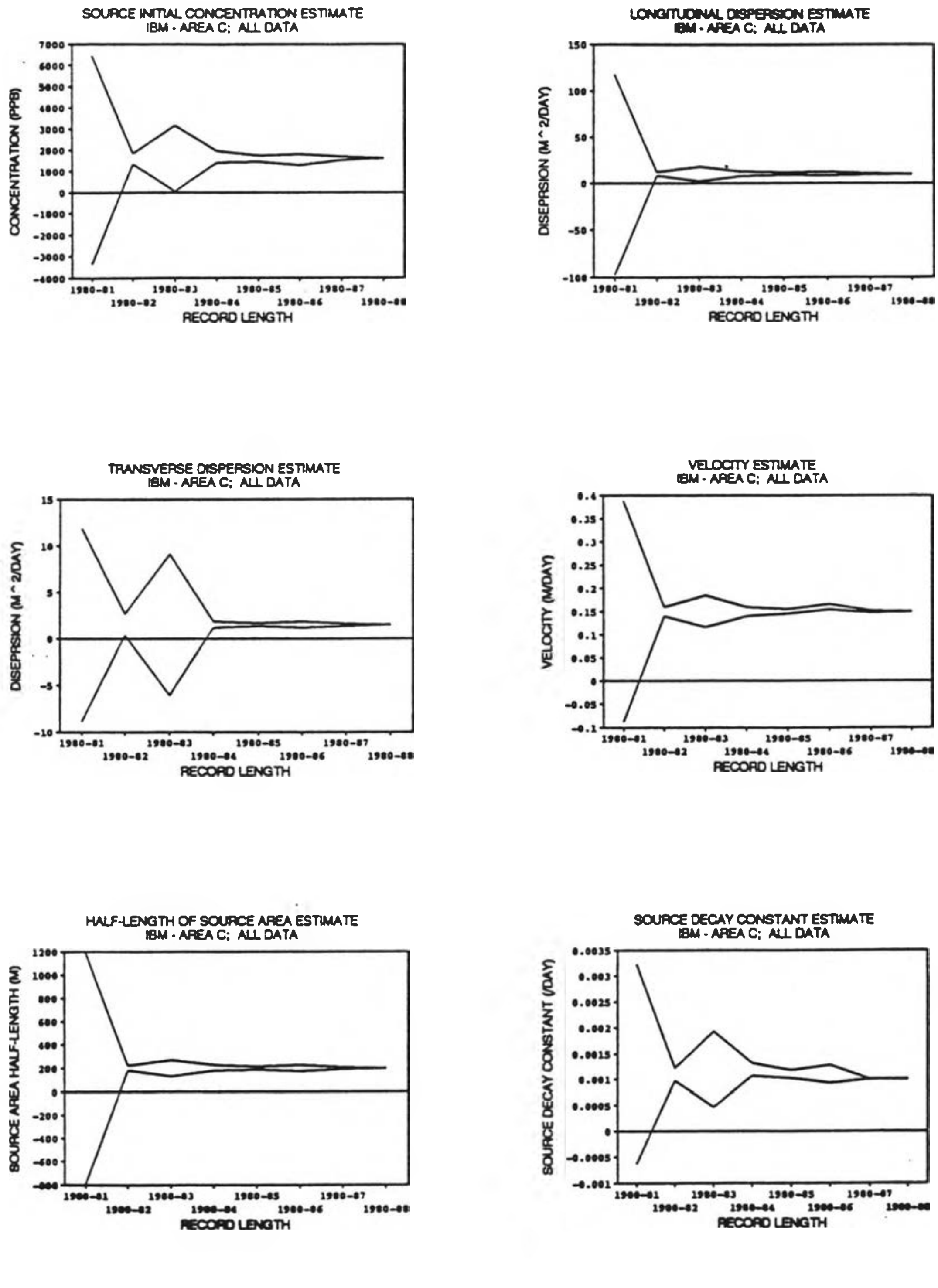

Figure 10.16 Upper and Lower 95% Confidence Limits of Selected Parameter Estimates for Physical Model Fit to All Data in Area C

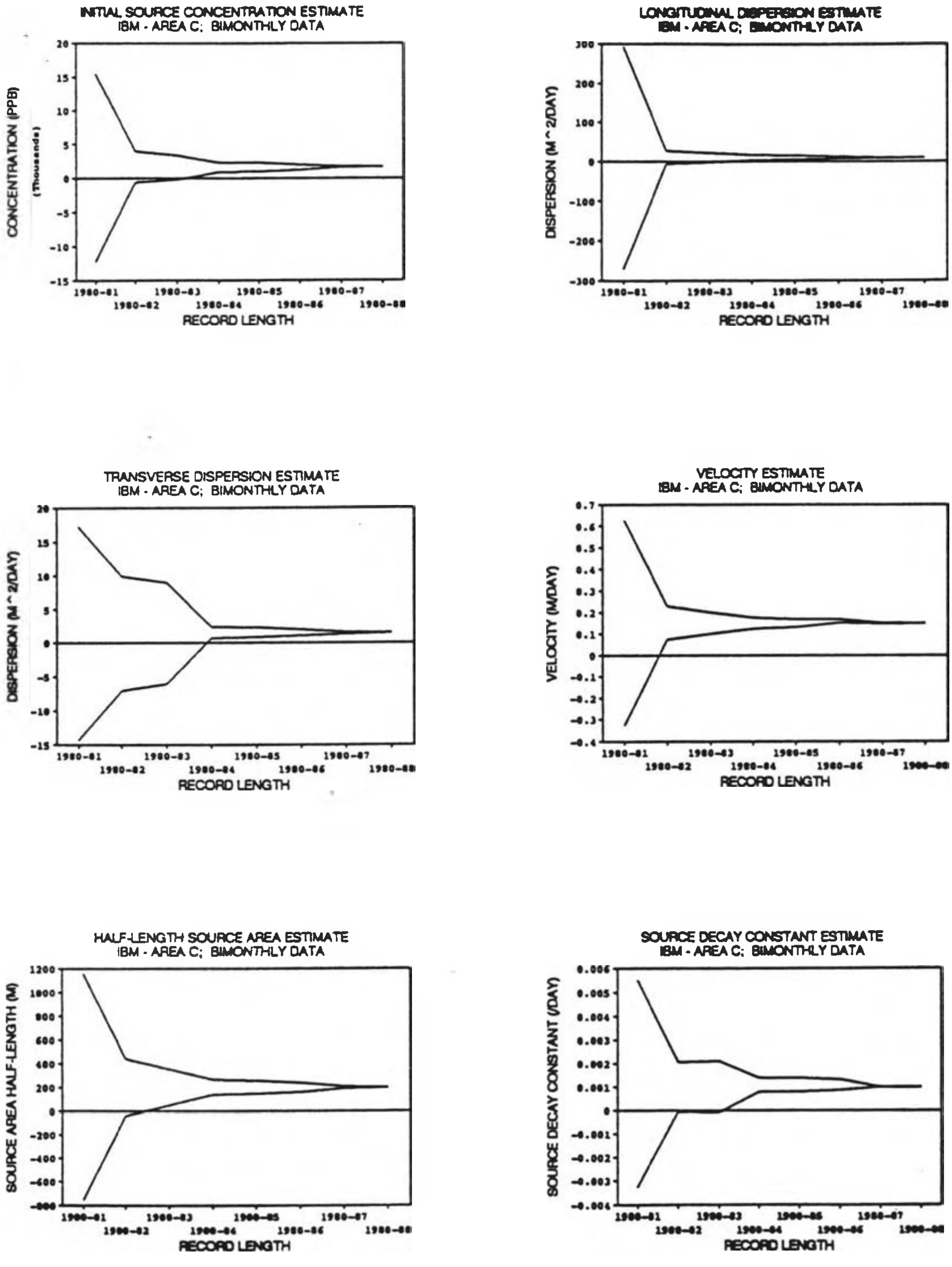

Figure 10.17 Upper and Lower 95% Confidence Limits of Selected Parameter Estimates for Physical Model Fit to Bimonthly Data in Area C

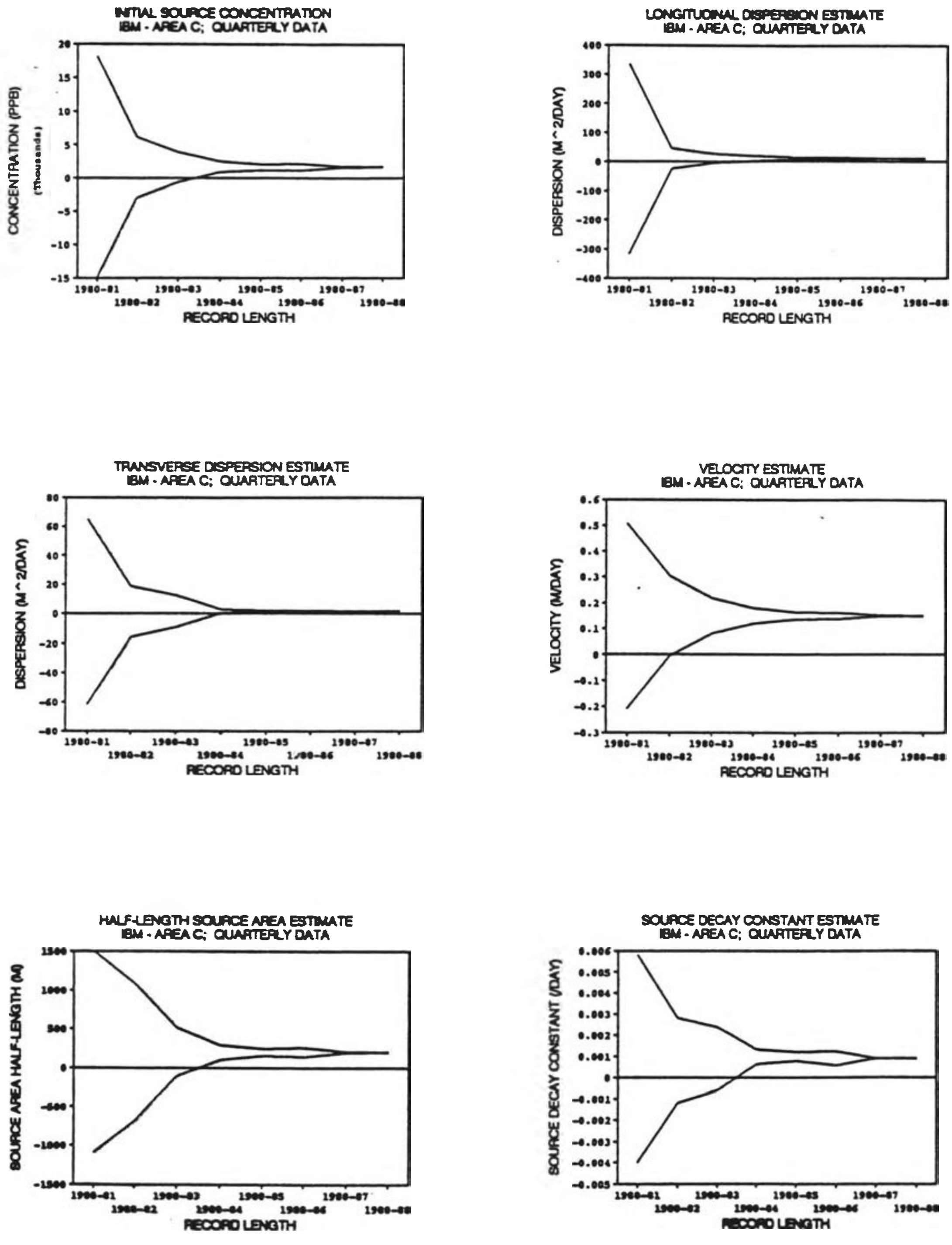

Figure 10.18 Upper and Lower 95% Confidence Limits of Selected Parameter Estimates for Physical Model Fit to Quarterly Data in Area C

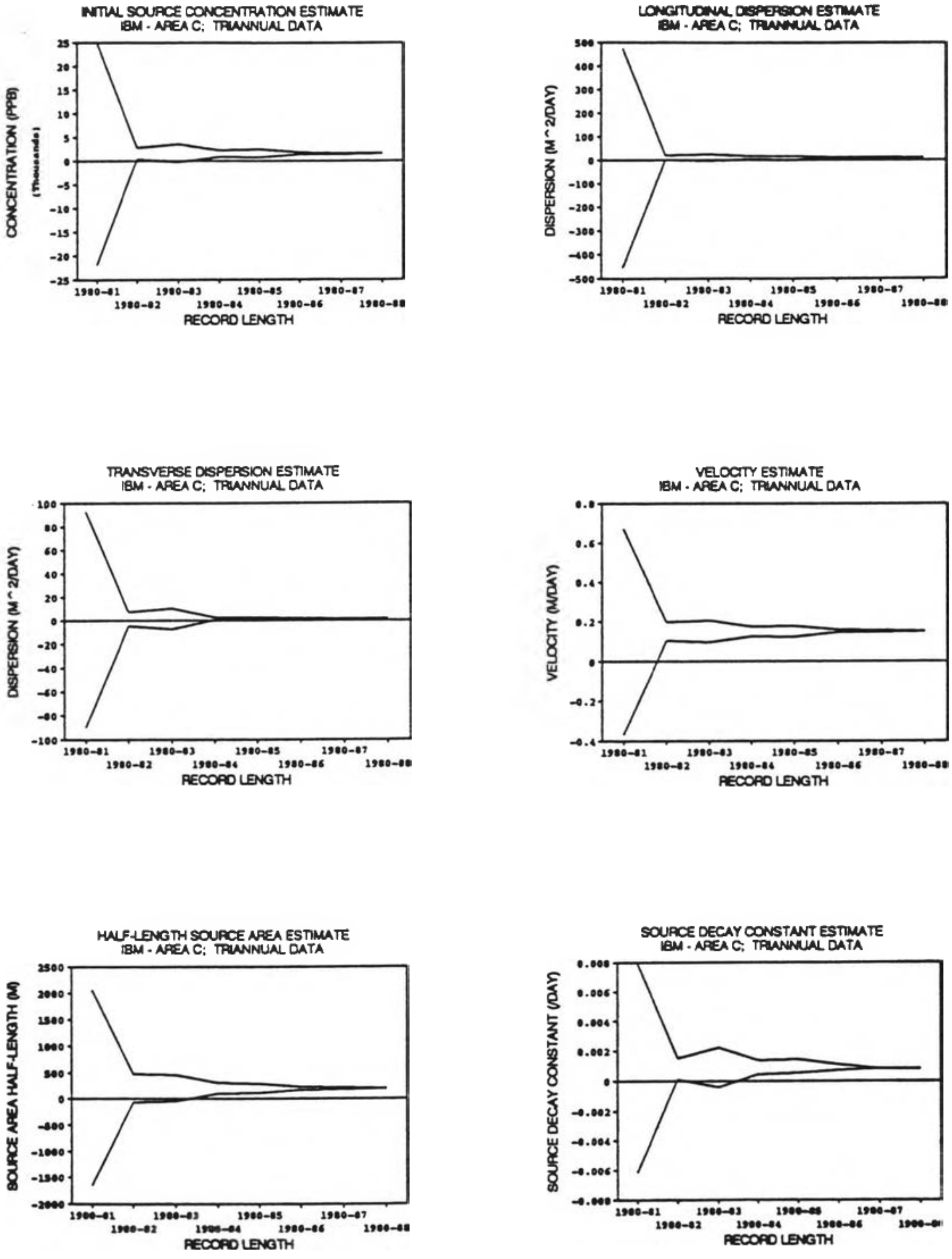

Figure 10.19 Upper and Lower 95% Confidence Limits of Selected Parameter Estimates for Physical Model Fit to Triannual Data in Area C

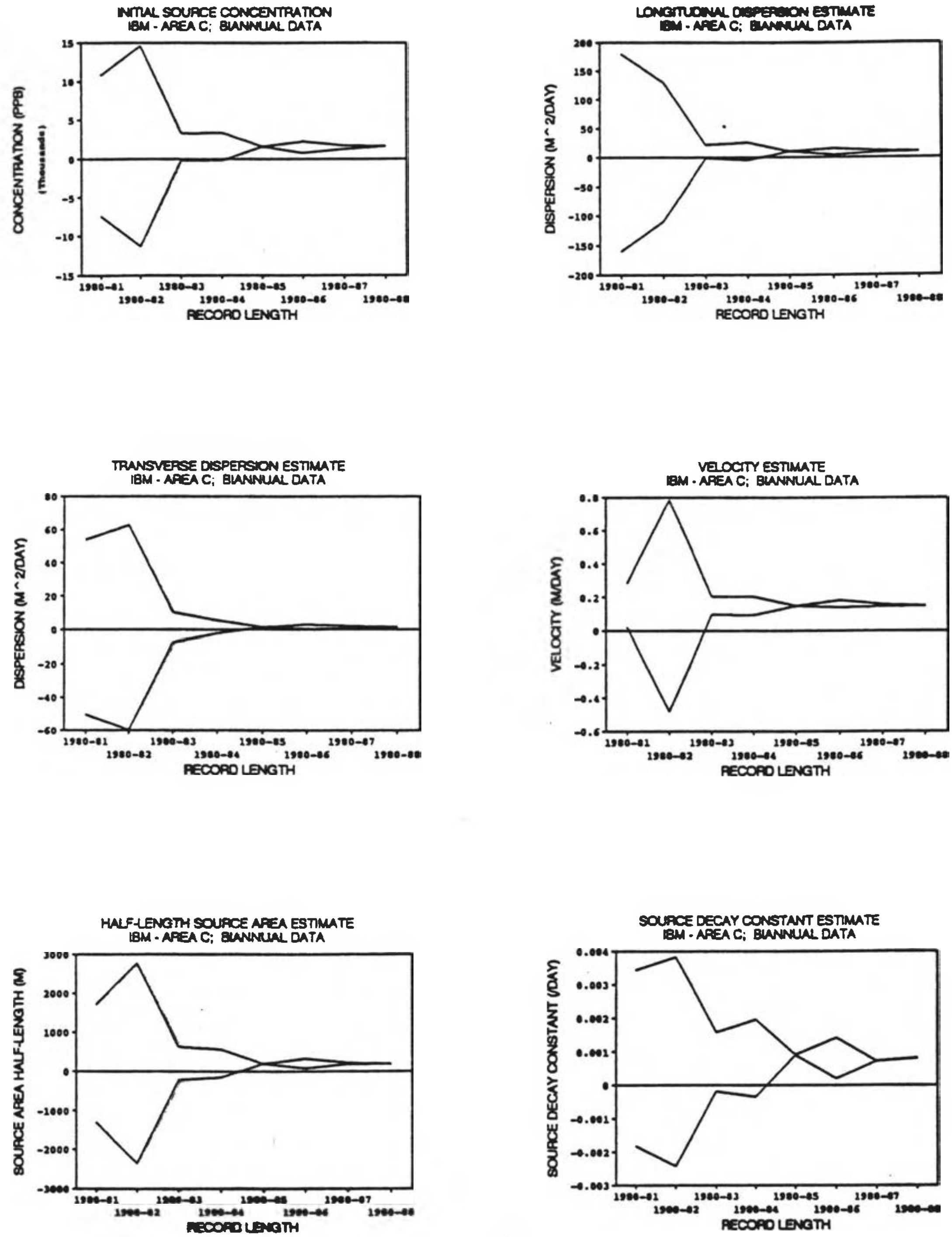

Figure 10.20 Upper and Lower 95% Confidence Limits of Selected Parameter Estimates for Physical Model Fit to Biannual Data in Area C

Table 10.26 Residual Temporal Correlation for Physical Model Fit to Reduced Data Sets from Area C

RECORD LENGTH	ALL	SAMPLING FREQUENCY BIMONTHLY	QUARTERLY	TRIANNUAL	BIANNUAL
1980	.00168	-.3660	(a)	(a)	(a)
1980-81	.13789	.2663	.2913	-.0115	.1627
1980-82	-.00326	.0246	.0515	-.0460	.1264
1980-83	.04646	.0179	.0595	-.0711	-.0910
1980-84	.3371	.2641	.2640	.2269	.2898
1980-85	.3650	.2882	.2898	.2363	.3221
1980-86	.4433	.4510	.4603	.3812	.4136
1980-87	.5382	.5576	.5437	.5289	.5145
1980-88	.5378	.5556	.5406	.5380	.5700

(a) insufficient data to calculate

Table 10.27 One-Year Prediction Bias and Associated t-test[a] for Physical Model Fit to Reduced Data Sets from Area C

PREDICTION BIAS

RECORD LENGTH	ALL	SAMPLING FREQUENCY BIMONTHLY	QUARTERLY	TRIANNUAL	BIANNUAL
1980	100.596	105.068	-406.661	135.825	211.622
1980-81	525.012	111.223	-124.89	-102.382	-206.401
1980-82	125.745	-177.766	-565.065	-561.197	-934.044
1980-83	283.672	-46.14	-194.131	-214.831	-523.417
1980-84	50.711	-189.26	-551.605	-711.849	-951.888
1980-85	-110.247	-162.613	-301.313	-343.176	-570.217
1980-86	-28.689	-80.947	-330.691	-389.141	-296.914
1980-87	-121.885	-127.899	-148.229	-161.550	-192.293

T-TEST OF PREDICTION BIAS

RECORD LENGTH	ALL	SAMPLING FREQUENCY BIMONTHLY	QUARTERLY	TRIANNUAL	BIANNUAL
1980	.5216	3.5938	-7.543	2.7342	4.4214
1980-81	NA	1.1617	-1.0900	-.8107	-1.3808
1980-82	.2902	-2.56482	-7.5263	-7.8484	-4.8218
1980-83	.8654	-.6037	-2.3595	-2.3849	-11.5233
1980-84	.3025	-1.6986	-5.3693	-12.1498	-7.5085
1980-85	-.2579	-2.7020	-4.2433	-.4353	-6.8021
1980-86	-.0654	-.9394	-3.9599	-4.2267	-2.4917
1980-87	-.9213	-1.8592	-2.0641	-2.3600	-2.9560

(a) significant t-test values and associated prediction biases are highlighted

Table 10.28 Error Prediction Variance at Individual Wells for Single-Site Models Fit to Data in Area C with Monthly Sampling Frequency

Linear Model

WELL NO.	1980	80-81	80-82	80-83	80-84	80-85	80-86	80-87	80-88
	RECORD LENGTH FOR MODEL FIT								
51	407.78	56.68	71.46	106.69	141.91	177.14	229.99	300.44	370.9
53	389.63	134.79	119.58	65.73	226.45	133.76	90.63	70.7	68.89
54	64.89	35.84	1368.9	906.68	488.98	284.37	183.19	131.5	127.94
69	6.14	1.68	1.34	1.54	1.45	1.36	1.31	1.29	1.29
110				3540.8	2063	1409.7	1201	2171.2	2171.2
111			21389	7581.4	5689.8	4767.4	8440.9	7353.1	7353.1
835					8.76	7.33	6.7	5.65	5.65
836					8.76	7.33	6.7	5.65	5.65
837				7.38	3.36	2.56	2.12	1.85	1.78
921							1.52	1.42	1.42
922							1.24	1.33	1.33
923							470.76	397.27	397.27
924							3.09	58.17	58.17
932							7.69	7.15	7.15
943							2.59	1.53	1.49

Quadratic Model

WELL NO.	1980	80-81	80-82	80-83	80-84	80-85	80-86	80-87	80-88
	RECORD LENGTH FOR MODEL FIT								
51	61792	3197	5352.4	12302	24352	43513	72102	112758	168427
53	60293	5388.8	1932.1	387.17	1138.8	542.01	365.04	142.28	276.18
54	15.764	13.43	402.82	453.23	241.3	143.36	92.909	67.024	65.233
69	23.104	1.884	1.2914	1.2565	1.4667	1.1856	1.1582	1.1504	1.1504
110				4816.9	3604.4	1453.4	1318.8	1784	1784
111			1176.3	8668.3	8017.7	4492.3	4174.1	4458.8	4458.8
835					5.1355	3.8047	4.5385	3.9954	3.9954
836					5.1355	3.8047	4.5385	3.9954	3.9954
837				11.933	4.8454	1.832	1.5775	1.4247	1.3872
921							1.3431	1.3629	1.3629
922							1.2626	1.2041	1.2041
923							481.69	381.28	381.28
924							2.8252	11.025	11.025
932							8.682	6.8876	6.8876
943							2.7291	1.2713	1.256

(continued)

Table 10.28, continued

Cubic Model

WELL NO.	RECORD LENGTH FOR MODEL FIT 1980	80-81	80-82	80-83	80-84	80-85	80-86	80-87	80-88
53	1.3E+07	439195	146495	27463	43600	17770	9983	142.28	11714
54	33021	3579.5	15031	14526	6678.4	2155.8	917.59	67.024	766.54
69	16.444	2.1681	1.4329	1.7096	1.4052	1.3544	1.1573	1.1504	1.153
110				11123	4538.7	1938.7	2156.4	1784	1759.4
111				1511.9	3038.5	3369.8	4694.1	4458.8	4882
835						2.6701	3.7863	3.9954	3.5124
836						2.6701	3.7863	3.9954	3.5124
837				26.324	6.4483	2.7388	1.6095	1.4247	1.4065
921							1.8481	1.3629	1.3326
922							1.4693	1.2041	1.2319
923							744.86	381.28	400.83
924							3.4194	11.025	5.349
932							10.998	6.8876	7.3912
943							3.7548	1.2713	-0.866

(a) error prediction variance associated with significant models based on F-test analysis are highlighted

Table 10.28) are not necessarily less than for insignificant models. Lastly, the prediction error variance tended to increase with the model order.

Figure 10.21 illustrates the spatial distribution of the prediction error variance at individual wells based on a single-site linear model applied to all available data. This figure illustrates the extreme spatial variability of the prediction error variances for individual wells.

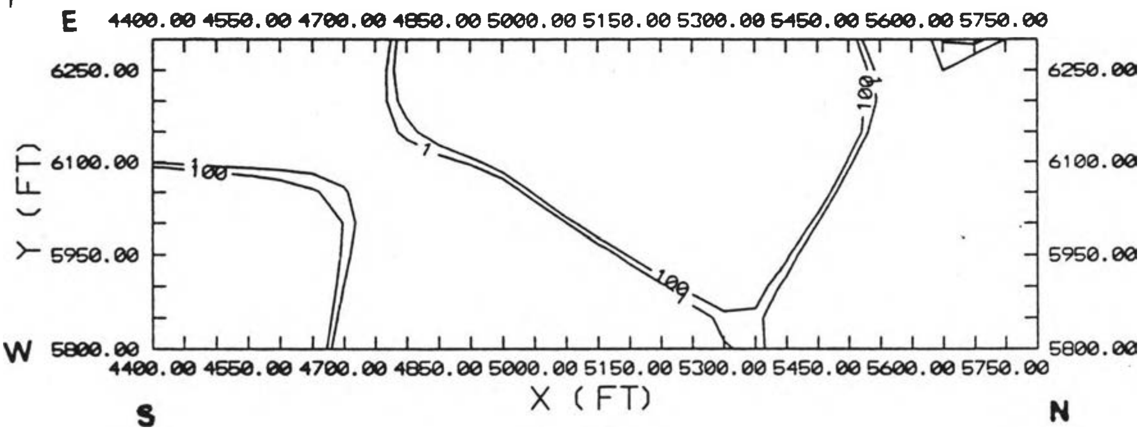

Figure 10.21 Prediction Error Variance at Individuals Wells for Single Site Linear Model Fit to All Available Data in Area C

10.2.2.2 Trend Surface Models. Table 10.29 summarizes the error prediction variances at individual wells based on fitting the trend surface models to Area C data. The error prediction variances at individual wells varied depending on the well location with some variances being significantly less based on the trend surface models and others being significantly more than for the single-site polynomial models. Figure 10.22 illustrates this prediction error variance surface for the linear trend surface model applied to the entire data set. This prediction error variance surface is much more uniform than the prediction error variance surface based on the single-site models as shown in Figure 10.21. As for Area A, this clearly illustrates the advantage of utilizing multi-site models over single-site models.

Table 10.30 summarizes the optimal monitoring networks for linear, quadratic, and cubic trend surface models fit to Area C data. This table illustrates the dramatic increase in prediction error variances with the higher order models. However, despite the higher variance at individual wells for the higher order

Table 10.29 Error Prediction Variances at Individual Wells for Trend Surface Models Fit to Data From Area C with Future Monthly Sampling Frequency

LINEAR MODEL

WELL NO.	RECORD LENGTH 1980	80-81	80-82	80-83	80-84	80-85	80-86	80-87	80-88
51	595.81	278.94	227.46	166.01	69.967	41.625	19.809	15.154	15.029
52	581.22	272.01	221.84	161.84	68.218	40.614	19.379	14.828	14.707
53	575.05	269.08	219.47	160.05	67.446	40.163	19.188	14.682	14.562
54	563.88	263.77	215.16	156.85	66.096	39.381	18.856	14.430	14.312
69	573.99	268.53	219.07	159.69	67.236	40.032	19.132	14.634	14.515
110		277.82	226.57	165.33	69.662	41.446	19.732	15.094	14.971
111		277.82	226.57	165.33	69.662	41.446	19.732	15.094	14.971
558								15.071	14.947
559								15.064	14.94
560								15.064	14.94
561								15.139	15.015
562								15.290	15.164
563								15.290	15.164
835			230.31	168.14	70.877	42.154	20.033	15.325	15.199
836			230.31	168.14	70.877	42.154	20.033	15.325	15.199
837			228.79	167.00	70.399	41.878	19.916	15.236	15.111
921					65.788	39.218	18.788	14.387	14.269
922					65.905	39.286	18.816	14.408	14.29
923					65.666	39.148	18.758	14.364	14.246
924					65.566	39.091	18.733	14.346	14.229
932					67.496	40.192	19.200	14.691	14.570
943						40.167	19.189	14.677	14.557
944						40.124	19.171	14.664	14.544
954						39.006	18.698	14.322	14.205
955						39.047	18.715	14.335	14.218
956						39.096	18.736	14.351	14.234
957							8.754	14.365	14.247

QUADRATIC MODEL

WELL NO.	RECORD LENGTH 1980	80-81	80-82	80-83	80-84	80-85	80-86	80-87	80-88
51	2.6E+14	2.2E+8	1.8E+8	1.5E+8	3.1E+6	2.2E+6	1.7E+6	1.2E+6	1.2E+6
52	2.4E+14	2.1E+8	1.7E+8	1.5E+8	3.0E+6	2.1E+6	1.6E+6	1.1E+6	1.1E+6
53	2.4E+14	2.0E+8	1.7E+8	1.4E+8	3.0E+6	2.1E+6	1.6E+6	1.1E+6	1.1E+6
54	2.3E+14	2.0E+8	1.6E+8	1.4E+8	2.9E+6	2.0E+6	1.5E+6	1.1E+6	1.1E+6
69	2.4E+14	2.0E+8	1.7E+8	1.4E+8	3.0E+6	2.1E+6	1.6E+6	1.1E+6	1.1E+6
110		2.2E+8	1.8E+8	1.5E+8	3.1E+6	2.2E+6	1.7E+6	1.2E+6	1.1E+6
111		2.2E+8	1.8E+8	1.5E+8	3.1E+6	2.2E+6	1.7E+6	1.2E+6	1.1E+6
558								1.2E+6	1.1E+6

(continued)

Table 10.29, continued

QUADRATIC MODEL

WELL NO.	RECORD LENGTH 1980	80-81	80-82	80-83	80-84	80-85	80-86	80-87	80-88
559								1.2E+6	1.1E+6
560								1.2E+6	1.1E+6
561								1.2E+6	1.2E+6
562								1.2E+6	1.2E+6
563								1.2E+6	1.2E+6
835			1.9E+8	1.6E+8	3.2E+6	2.3E+6	1.7E+6	1.2E+6	1.2E+6
836			1.9E+8	1.6E+8	3.2E+6	2.3E+6	1.7E+6	1.2E+6	1.2E+6
837			1.9E+8	1.5E+8	3.2E+6	2.2E+6	1.7E+6	1.2E+6	1.2E+6
921					2.8E+6	2.0E+6	1.5E+6	1.0E+6	1.0E+6
922					2.8E+6	2.0E+6	1.5E+6	1.0E+6	1.0E+6
923					2.8E+6	2.0E+6	1.5E+6	1.0E+6	1.0E+6
924					2.8E+6	2.0E+6	1.5E+6	1.0E+6	1.0E+6
932					3.0E+6	2.1E+6	1.6E+6	1.1E+6	1.1E+6
943						2.1E+6	1.6E+6	1.1E+6	1.1E+6
944						2.1E+6	1.6E+6	1.1E+6	1.1E+6
954						1.9E+6	1.5E+6	1.0E+6	1.0E+6
955						2.0E+6	1.5E+6	1.0E+6	1.0E+6
956						2.0E+6	1.5E+6	1.0E+6	1.0E+6
957							1.5E+6	1.0E+6	1.0E+6

CUBIC MODEL[a]

WELL NO.	RECORD LENGTH 1980	80-81	80-82	80-83	80-84	80-85	80-86	80-87	80-88
51	1.4E+5	8.5E+2	2.7E+4	1.9E+2	3.7E+1	9.7E+0	4.1E+0	1.9E+0	1.9E+0
52	1.3E+5	7.1E+2	2.4E+4	1.7E+2	3.4E+1	9.1E+0	3.8E+0	1.8E+0	1.8E+0
53	1.3E+5	5.6E+2	2.3E+4	1.5E+2	3.3E+1	8.8E+0	3.7E+0	1.7E+0	1.7E+0
54	1.2E+5	4.4E+2	2.1E+4	1.3E+2	3.1E+1	8.3E+0	3.5E+0	1.7E+0	1.6E+0
69	1.3E+5	3.3E+2	2.2E+4	1.3E+2	3.2E+1	8.7E+0	3.7E+0	1.7E+0	1.7E+0
110		7.4E+2	2.6E+4	1.8E+2	3.6E+1	9.6E+0	4.1E+0	1.9E+0	1.9E+0
111		7.4E+2	2.6E+4	1.8E+2	3.6E+1	9.6E+0	4.1E+0	1.9E+0	1.9E+0
558								1.9E+0	1.9E+0
559								1.9E+0	1.9E+0
560								1.9E+0	1.9E+0
561								1.9E+0	1.9E+0
562								2E+0	1.9E+0
563								2E+0	1.9E+0
835			2.8E+4	2.2E+2	3.8E+1	1E+1	4.2E+0	2E+0	2E+0
836			2.8E+4	2.2E+2	3.8E+1	1E+1	4.2E+0	2E+0	2E+0
837			2.8E+4	2.1E+2	3.8E+1	9.9E+0	4.2E+0	2E+0	1.9E+0
921					3.2E+1	8.3E+0	3.5E+0	1.6E+0	1.6E+0
922					3.2E+1	8.3E+0	3.5E+0	1.6E+0	1.6E+0

(continued)

Table 10.29, continued

QUADRATIC MODEL

WELL NO.	1980	80-81	80-82	80-83	80-84	80-85	80-86	80-87	80-88
					RECORD LENGTH				
559								1.2E+6	1.1E+6
560								1.2E+6	1.1E+6
561								1.2E+6	1.2E+6
562								1.2E+6	1.2E+6
563								1.2E+6	1.2E+6
835			1.9E+8	1.6E+8	3.2E+6	2.3E+6	1.7E+6	1.2E+6	1.2E+6
836			1.9E+8	1.6E+8	3.2E+6	2.3E+6	1.7E+6	1.2E+6	1.2E+6
837			1.9E+8	1.5E+8	3.2E+6	2.2E+6	1.7E+6	1.2E+6	1.2E+6
921					2.8E+6	2.0E+6	1.5E+6	1.0E+6	1.0E+6
922					2.8E+6	2.0E+6	1.5E+6	1.0E+6	1.0E+6
923					2.8E+6	2.0E+6	1.5E+6	1.0E+6	1.0E+6
924					2.8E+6	2.0E+6	1.5E+6	1.0E+6	1.0E+6
932					3.0E+6	2.1E+6	1.6E+6	1.1E+6	1.1E+6
943						2.1E+6	1.6E+6	1.1E+6	1.1E+6
944						2.1E+6	1.6E+6	1.1E+6	1.1E+6
954						1.9E+6	1.5E+6	1.0E+6	1.0E+6
955						2.0E+6	1.5E+6	1.0E+6	1.0E+6
956						2.0E+6	1.5E+6	1.0E+6	1.0E+6

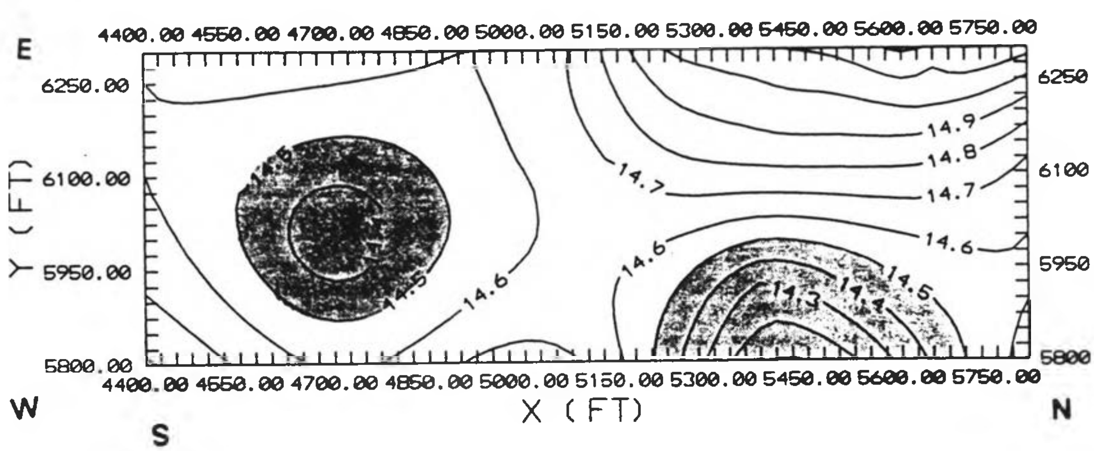

Figure 10.22 Prediction Error Variance for Linear Trend Surface Model Fit to All Available Data in Area C

Table 10.30 Monitoring Networks for Trend Surface Models Fit to Area C Data with Minimum Spatial Correlation of 0.9, Future Monthly Sampling Frequency

Linear Trend Surface Model

Record Length	Wells	Objective Function
1980	54	563.875
1980-81	54	263.767
1980-82	54	215.159
1980-83	54	156.849
1980-84	924	65.565
1980-85	954	39.006
1980-86	954	18.698
1980-87	954	14.322
1980-88	954	14.205

Quadratic Trend Surface Model

Record Length	Wells	Objective Function
1980		
1980-81	54	1.96×10^{8}
1980-82	54	1.63×10^{8}
1980-83	54	1.36×10^{8}
1980-84	924	2.79×10^{6}
1980-85	954	1.95×10^{6}
1980-86	954	1.49×10^{6}
1980-87	954	1.03×10^{6}
1980-88	954	1.01×10^{6}

Cubic Trend Surface Model

Record Length	Wells	Objective Function
1980	53 & 69	2.54×10^{15}
1980-81	51 & 111	1.59×10^{13}
1980-82	836 & 837	5.42×10^{14}
1980-83	836 & 837	4.22×10^{12}
1980-84	54	3.12×10^{11}
1980-85	954	8.16×10^{9}
1980-86	954	3.45×10^{9}
1980-87	954	1.61×10^{9}
1980-88	954	1.57×10^{9}

models, significant reduction in monitoring networks may still be realized by utilizing the high spatial correlation of the data in the multi-site networks.

Figure 10.23 illustrates the reduction in prediction error variance based on the optimal monitoring network for a linear trend surface model applied to all available data. Comparison of the shaded region of prediction error variances less than 14.5 in Figure 10.23 to Figure 10.22 illustrates the reduction in the prediction error variance surface based on the optimal sampling for a linear trend surface model. The most dramatic difference in the surfaces is at the monitoring wells with an overall reduction to all other sampling locations.

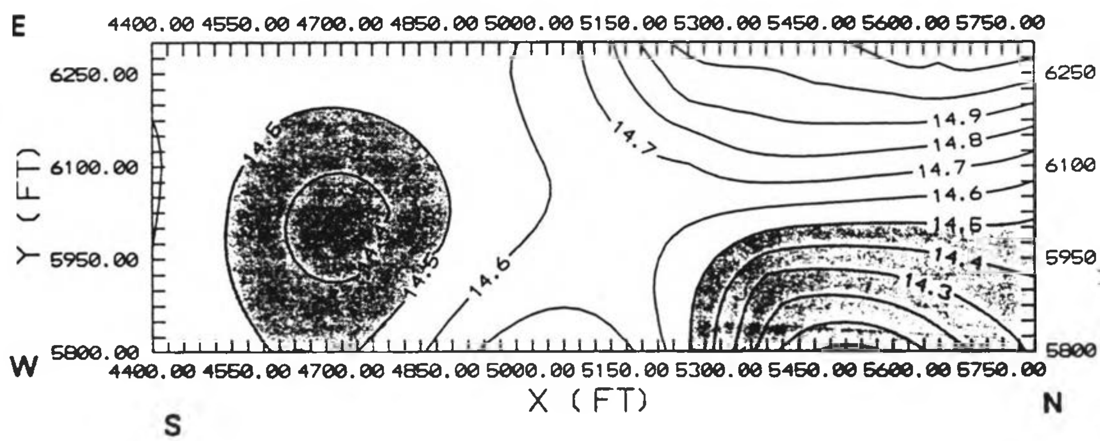

Figure 10.23 Prediction Error Variance Based on Optimal Monitoring Network for Linear Trend Surface Model Fit to All Available Data in Area C

An alternative means of representing this uncertainty in the model and in the optimal monitoring network can be shown by plotting the upper and lower confidence limits on concentrations of interest for the linear trend surface model fit to all available data in Area C, as shown in Figure 10.24. This representation of the linear trend surface model and monitoring network uncertainty can be used by the monitoring network manager to evaluate whether the specified minimum spatial correlation and future sampling frequency arrive at a monitoring network and prediction certainty which will meet the needs of the monitoring network information goals.

10.2.2.3 Physical Model. Table 10.31 summarizes the error prediction variances at individual wells based on the physical model fit to the data in Area C. Comparison of Table 10.31 to Table 10.29 illustrates the improvement in the physical model over the trend surface models at describing and predicting the

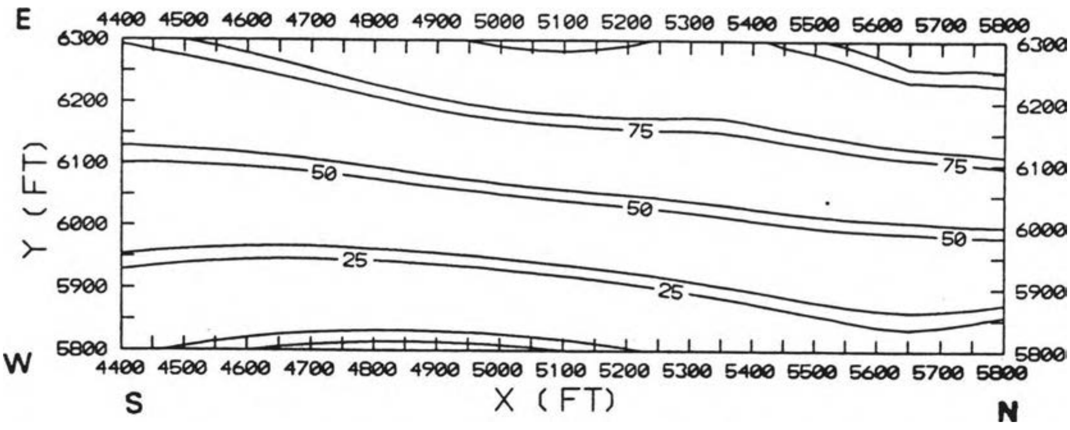

Figure 10.24 Upper and Lower 95% Confidence Limits on Predicted Concentrations Based on Linear Trend Surface Model Fit to All

PCE groundwater quality in Area C. These prediction error variances for the physical model based network are more variable, but on the average, are less than for the linear trend surface models. This is illustrated by comparison of the area with prediction error variances less than 14.5 for the linear trend surface model, as shown on Figure 10.22, to the area with prediction error variance less than 14.5 for the physical model, as shown on Figure 10.25. The shaded area on Figure 10.25 is substantially larger than the shaded area shown on Figure 10.22.

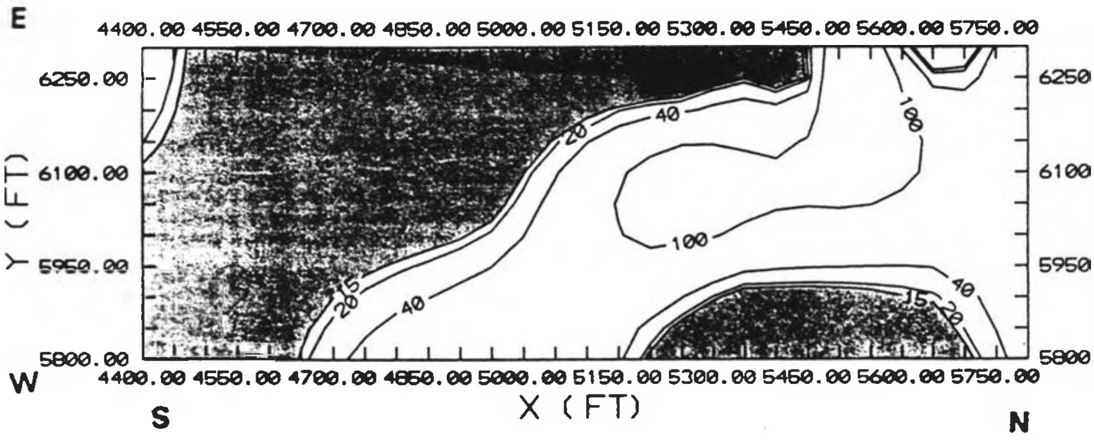

Figure 10.25 Prediction Error Variance for Physical Model Fit to All Available Data in Area C

Table 10.31 Error Prediction Variances for Individual Wells for Data from Area C Fit to Physical Model

WELL NO.	1980	80-81	80-82	80-83	80-84	80-85	80-86	80-87	80-88
				RECORD LENGTH					
51	3.9E5	11365.1	920.78	1216.15	680.79	584.59	554.35	180.69	94.64
52	3.6E5	120274	2386.7	1920.48	708.40	618.32	529.96	135.27	140.4
53	7178	1329.6	53.663	14.0839	2.9702	2.3283	1.4819	1.1814	1.1715
54	72.17	16.191	1.5135	1.16461	1.0186	1.0147	1.0044	1.0008	1.0005
69	20.28	1.9815	1.0590	1.03212	1.0037	1.0030	1.0008	1.0001	1.0001
110		36431.1	396.03	260.878	34.502	54.627	15.996	7.0829	14.437
111		36431.1	396.03	260.878	103.04	54.628	15.996	7.0829	14.437
558					3.1500	5.4274			
559					3.0396	4.8588			
560					3.0396	4.8588			
561					4.8145	16.287			
562					10.443	34.69			
563					10.443	34.69			
835		124.64	129.678	23.653	52.475	19.515	10.706	42.259	
836		124.64	129.678	23.653	52.475	19.515	10.706	42.259	
837		213.758	232.04	31.39	35.558	27.149	8.4800	27.925	
921			5.988	5.5622	2.3868	1.6027	1.9188		
922			4.297	6.4214	2.5581	1.6540	2.0237		
923			3.885	4.3900	2.0551	1.4663	1.6572		
924			3.040	3.9268	1.9644	1.4396	1.6108		
932			2.9945	1.4705	1.1735	1.1822			
943			1.0036	1.0008	1.0001	1.0001			
944			1.0040	1.0009	1.0001	1.0001			
954			3.2882	2.2434	1.6387	2.1175			
955			3.6267	2.406	1.7171	2.2976			
956			4.1162	2.6199	1.8196	2.5433			
957			2.8274	1.9184	2.7905				

Figure 10.26 illustrates the reduction in the prediction error variance based on the optimal sampling network for a physical model applied to ten years of data. Sampling at the wells identified in the optimization results in a significant reduction in the prediction error variance surface for the physical model. The optimal prediction error variance surface is both more uniform and significantly smaller in magnitude.

This reduced uncertainty in the model and in the model predictions can be realized by plotting the upper and lower confidence limits on concentrations of interest, as shown in Figure 10.27 for the physical model fit to all available data. Due to the low error prediction variance, no appreciable observable uncertainty in the predicted concentrations is apparent in Figure 10.27. In addition, comparison of Figure 10.27 to Figure 10.24 illustrates a dramatically different expected distribution of the PCE groundwater quality in Area C.

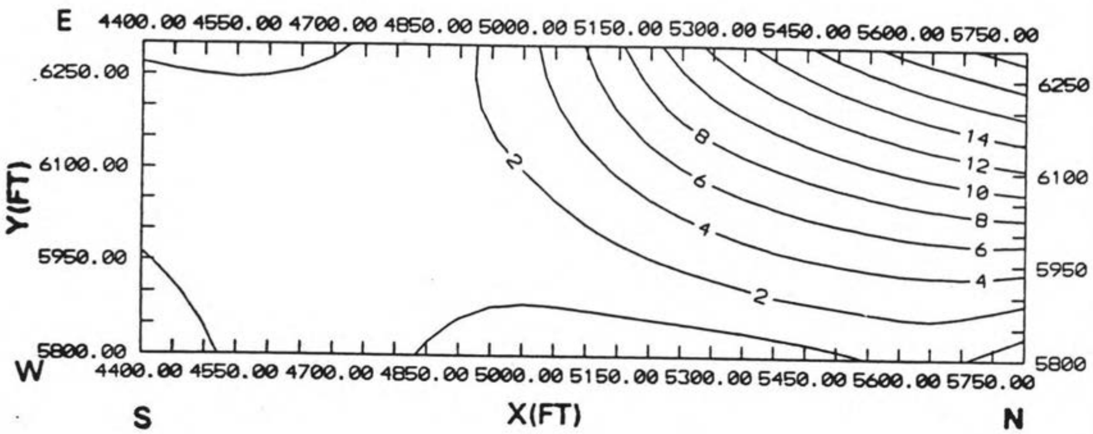

Figure 10.26 Prediction Error Variance for Optimal Monitoring Network Based on Physical Model Fit to All Available Data in Area C

The improvement in the physical model over the trend surface models can also be realized by comparing the optimal monitoring networks. The optimal monitoring networks based on the physical model are summarized in Table 10.32. The maximum spatial correlation achieved ranged from approximately

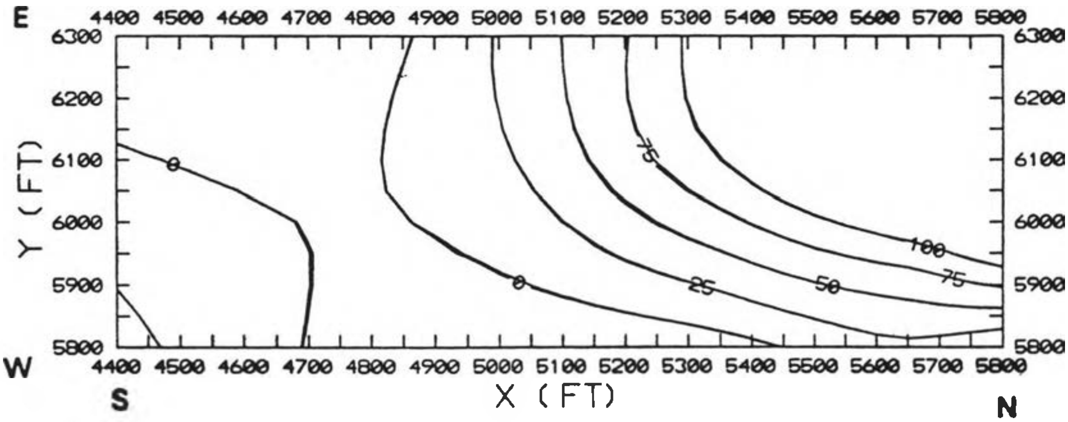

Figure 10.27 Upper and Lower 95% Confidence Limits on Predicted Concentrations Based on Physical Model Fit to All Available Data in Area C

0.4 to 0.7 depending on the record length. These results illustrate that, in general, the objective function is minimized by an increase in record length. In comparison to Table 10.30, for the trend surface models, the physical model is superior in minimizing the objective function for record lengths of two years and longer compared to the linear trend surface model and for all record lengths compared to the quadratic and cubic trend surface models.

10.2.2.4 Summary of Monitoring Network Optimization. The monitoring network optimization for Area C allowed for the evaluation of error prediction propagation and data correlation based on both the physical and statistical data evaluation (for multi-site models). The objective function was minimized by use of a physically-based model. Based on the physical model fit to all available data, the Area C monitoring network could be reduced to a network of two wells (69 and 955) sampled monthly, maintaining a spatial correlation of 0.7. The uncertainty in this optimal monitoring network is illustrated by Figure 10.27. Given that this uncertainty is acceptable to the groundwater manager, the use of a physically-based model to explain the groundwater quality behavior could greatly reduce the current monitoring in Area C.

Table 10.32 Monitoring Network Optimization for Physical Model Fit to All Data in Area C with Future Monthly Sampling Frequency

RECORD LENGTH		MINIMUM CORRELATION BETWEEN ALL WELLS 0.7	0.6	0.5	0.4
1980	Objective Function	(a)	7198.46	7198.46	7198.46
	Wells		53,69	53,69	53,69
1980-81	Objective Function	(a)	(a)	(a)	1345.85
	Wells				53,54
1980-82	Objective Function	(a)	(a)	(a)	126.16
	Wells				54,835
1980-83	Objective Function	(a)	(a)	(a)	15.116
	Wells				53,69
1980-84	Objective Function	(a)	6.9918	3.885	3.885
	Wells		69,922	924	924
1980-85	Objective Function	(a)	4.291	3.288	2.995
	Wells		69,954	954	932
1980-86	Objective Function	(a)	16.997	16.997	1.964
	Wells		110,943	110,943	924
1980-87	Objective Function	8.083	5.815	5.815	1.717
	Wells	69,110	69,561	69,561	955
1980-88	Objective Function	3.298	1.919	1.611	1.611
	Wells	69,955	921	924	924

(a) minimum correlation required cannot be met with existing data base

10.2.3 Summary of Model Selection and Network Design for Area C.

The results of the monitoring network optimization for Area C confirm the results of the model applicability analysis which indicated the superiority of the physical model over the statistical models for describing and predicting the observed PCE groundwater quality behavior in Area C. The optimization allowed for a minimization of error variance with a specified minimum spatial correlation.

Therefore, both the model applicability and network optimization resulted in the selection of the physical model for describing the observed PCE groundwater quality behavior in Area C. Use of the physical model greatly reduced the number of wells required to be monitored to achieve a 0.7 spatial correlation between the sampled and non-sampled well locations.

For future refinement, a reevaluation of the model fit using weighted least squares is recommended to evaluate the systematic residual behavior. In addition, a correlation structure dependent on the predicted PCE concentrations is recommended to constrain the monitoring network spatially., Lastly, refinement of the physical model structure to evaluate the vertical non-homogeneity of the system should be considered.

11. SUMMARY, CONCLUSIONS AND RECOMMENDATIONS

11.1 Summary.

The objective of this research was to develop a method for optimally designing groundwater monitoring networks. The design of an optimal network must incorporate all available information including any physical processes affecting groundwater conditions and any information on natural, sampling, and laboratory error which affects data quality. Therefore, the development of a method for designing groundwater monitoring networks must first evaluate the deterministic processes affecting the variable of interest and the uncertainty in the processes and in the data. This information can than be incorporated into a monitoring network system design. The contribution of this research is the development of a protocol for evaluating the adequacy of a model structure, for quantifying data error, and for explicitly incorporating the system deterministic and random structure into a monitoring network optimization which allows for a wide variety of information goal objectives.

This research was divided into three main components as follows:

1) performance of a simulation study to evaluate model applicability and monitoring network design methods (Chapter 8),

2) development of a monitoring network design protocol based on the results of the simulation study (Chapter 9), and

3) application of the protocol to field data (Chapter 10).

The simulation study was used as a tool to evaluate methods for assessing both model applicability and the design of monitoring networks. The simulation study provided a method of evaluating the performance of various tests against a known correct model (the model used to generate the simulated data). The performance of these tests could therefore be evaluated for correct models with different magnitudes and types of error (additive and multiplicative normal and lognormal errors were considered), as well as for incorrect models with different types of errors. The behavior of the statistical tests considered was evaluated based on the use of expectations rather than using Monte Carlo simulations.

The most important results from the simulation study regarding the evaluation of model applicability were:

1) any single statistical test applied to a single data set may be misleading as a basis for evaluating model applicability,

2) comparison of the behavior in statistical tests to the theoretical expected behavior for a correct model under conditions of varying sampling frequency, record length, and sampling density is a good means of evaluating model applicability, and

3) evaluation of more than one type of statistic provides a means of evaluating consistency in model behavior.

Groundwater monitoring networks were optimized based on the model structure, model parameter uncertainty, and data uncertainty quantified in the model applicability analyses. A branch and bound optimization technique was used which incorporates both the deterministic and random components of the data explicitly into the network design process using prediction error analysis. Knowledge of the degree of uncertainty in the groundwater system is useful for all groundwater monitoring applications. This uncertainty analysis can be applied to either optimizing an existing network (when system uncertainty is less than the maximum uncertainty allowable to meet the information objective) or in identifying information gaps. For either groundwater monitoring objective, the optimization technique allows for a concurrent determination of sampling frequency and well locations to meet specified information goals.

Use of the simulation study to evaluate groundwater monitoring network optimization procedures illustrated the importance of the network density relative to the evaluation of the variable of interest and the design of the monitoring network. The optimal network was highly sensitive to both the sampling locations used to fit the model and to the monitoring locations identified to be considered for inclusion in the optimal monitoring network.

The results of the simulation study were incorporated into a monitoring network design protocol which focuses on the use of a variety of statistical techniques applied over a number of data subsets to evaluated model applicability. The monitoring network optimization allows for designing a network based on the selected model structure and confidence in that model. The maximum spatial correlation obtainable is dependent on the locations identified as potential sampling points as well as the model structure and confidence in that model.

The principle steps in the monitoring network design protocol are as follows:

1) identify alternative models based on the review of available data,

2) divide available data into subsets based on record length, sampling frequency, and sampling density,

3) fit model to data subsets,

4) calculate goodness-of-fit and predictive test statistics for "best-fit" models,

5) evaluate significance of statistical tests and trends in the tests relative to expected behavior for a correct model structure

6) optimize monitoring network including information of model structure and model uncertainty to meet specific information goals for the network.

To evaluate the applicability of the protocol, the protocol was applied to the evaluation of PCE groundwater quality data collected at the IBM East Fishkill facility in New York. Two areas on the facility were selected for evaluation - Areas A and C. Both statistical and physical models were fit to subsets of the PCE data from these two areas and were used to evaluate the applicability of the models. No one model met all the conditions of a "correct model" based on the model applicability tests considered. Evaluation of the field data illustrated the problems in selecting an "ideal model" for a specific data set based on the model applicability analyses. Given unlimited resources, it would always be desirable to collect more data to reduce the uncertainty in the understanding of a groundwater system. However, there is no such thing as unlimited resources. Once a model is identified which adequately explains the deterministic and random nature of a system, then optimization of the monitoring network system should be performed where the deterministic nature of the model can be substituted for monitoring, thereby reducing long-term costs without losing needed information.

For the IBM data, a linear trend surface model was the best model for Area A and a physically-based advection-dispersion model was best for Area C. Based on these models and the level of uncertainty associated with them, the monitoring networks in both areas could be dramatically reduced. The network in Area A could be reduced from 83 wells to one well sampled monthly and the monitoring network in Area C could be reduced from 27 wells to two wells sampled monthly. These results indicate that the use of a model can have tremendous impact on the ability to predict groundwater quality behavior and can result in the ability to significantly reduce a monitoring network. The extensive data analysis required to develop a model and quantitatively evaluate the uncertainty associated with it can be a substantial level of effort. Therefore, a tradeoff is realized between monitoring without extensive data analysis and modeling with extensive data analysis.

These potential reductions to the monitoring networks are based purely on a quantitative evaluation of the available data. The additional factor which is incorporated in the design of monitoring networks is a subjective "comfort level" factor. This includes the comfort of the groundwater manager as well as regulators who often oversee the groundwater monitoring at facilities. These subjective factors often have an overriding influence on the design of monitoring networks.

11.2 Conclusions.

The results of this research strengthen the importance of a detailed statistical evaluation of model applicability prior to the use of a model as a tool for understanding groundwater quality behavior or prior to the design of monitoring networks based on a specified model. Frequently, a specific model fitting technique is utilized with existing data and if the model is significant based on some single test applied to all available data, that model is utilized to make critical decisions on the monitoring network design. This research shows that no one statistical test applied to a single set of data is significant or should be relied on as a basis of model evaluation. Statistical tests which evaluate the fit of a model, consistency in the model fit, residual behavior, and model predictions should all be used to evaluate the applicability of a model. Based on the results of the field data, it is anticipated that frequently no one model will meet the conditions of an "ideal" model. These non-ideal behaviors must be critically evaluated by the groundwater manager in order to determine whether these uncertainties are acceptable in order to meet the information goals of the groundwater monitoring system.

The model structure, as well as the uncertainty in the model, should then be used to design a monitoring network. The model structure should generally be physically-based in order to accommodate changing conditions in the environment. In this manner, the monitoring network optimization protocol can be used to evaluate confidence in the model under these changing conditions and identify the optimal monitoring network under conditions of uncertainty. Depending on the confidence in the model and in the monitoring network information goals, the application of this protocol can result in significant reductions in monitoring networks. The applicability of the methodology developed is dependent on the available data and on the information needs of the monitoring network. Application of the protocol developed herein will however quantify the uncertainty in a system and allow for predictions of uncertainty. These uncertainty predication can be used to evaluate whether the information goals can be obtained given the uncertainty in the system understanding. If the information goals can not be met, then the predicted error uncertainty can be used to focus where information should be optimally collected to reduce uncertainty in the system.

11.3 Recommendations.

As in most research, for every question that is answered, another is raised. These additional questions form the basis for recommendations resulting from this research. Recommendations are made relative to the principle steps in the monitoring network design protocol. These recommendations derive from both the simulation study and from application of the protocol to the field data.

1) Fitting Model to Data Subsets

- A more detailed consideration of the effect of different model fitting techniques on the evaluation of model applicability under different model parameter and model error distributions is warranted. This research selected least-squares regression as a fitting technique rather than focusing on the affect of the selected model fitting technique on the model applicability evaluation.

2) Calculation of Model Applicability Statistics

- Consideration should be given to alternative tests to evaluate the power of various test for model discrimination

3) Optimization of Monitoring Network

- The error prediction correlation structure used to constrain the well locations was restrictive in its application. For future research, it is recommended that a different expression for spatial interdependence such as the correlation of the expected data values be utilized for this constraint.

- The branch and bound optimization technique is limited to integer type problems in which all the possible well locations have been pre-specified. Significant additional research is necessary in the unconstrained optimization process to incorporate new sampling locations efficiently into the monitoring network design.

- A combination of information objectives to both increase the confidence in the model and maintain a specific understanding in the system should be addressed., This could be applied to cases where the uncertainty in a model is acceptable in some regions , but not others.

It is this author's belief that the pursuit of these topics will result in advancing this research and the field of groundwater quality data evaluation and monitoring network design.

12. REFERENCES

Aoki, M., State Space Modeling of Time Series. Springer-Verlag, New York, 1987.

Bakr, A.A., L.W. Gelhar, A.L. Gutjahr, and J.R. MacMillan, "Stochastic Analysis of Spatial Variability in Subsurface Flows, 1. Comparison of 1 and 3-D Flows," in Water Resources Research 14(2): 263-272, 1978.

Ballinger, D.G., "Effluent and Compliance Monitoring Programs Mandated by EPA," in Establishment of Water Quality Monitoring Programs. L.G. Everett and K.D. Schmidt, eds., Proceedings of a Symposium held in San Francisco, California June 12-14, 1978, American Water Resources Association, Minneapolis, Minnesota, 1979.

Bard, Y., Nonlinear Parameter Estimation. Academic Press Inc., London, 1974.

Basta, D.J. and B.T. Bower, eds. Analyzing Natural Systems. Resources for the Future, Washington D.C., 1982.

Bear, J., Hydraulics of Groundwater. McGraw-Hill Inc., New York, 1979.

Beck, M.B., "Water Quality Modeling: A Review of the Analysis of Uncertainty," in Water Resources Research 23(8): 1393-1442, 1987.

van Belle, G. and J.P. Hughes, "Nonparametric Tests for Trend in Water Quality," in Water Resources Research 20(1): 127-136, 1984.

Binsariti, A.A., Statistical Analyses and Stochastic Modeling of Contaro Aquifer in Southern Arizona. Ph.D. Dissertation, Department of Hydrology and Water Resources, University of Arizona, Tucson, 1980.

Bradford, W.L. and R.T. Iwatsubo, "Design of a Primary Monitoring Network for Water Quality in San Francisco Bay, California," in Establishment of Water Quality Monitoring Programs. L.G. Everett and K.D. Schmidt, eds., Proceedings of a Symposium held in San Francisco, California June 12-14, 1978, American Water Resources Association, Minneapolis, Minnesota, 1979.

Bouwer, E.J. and P.L. McCarty, Transformation of 1- and 2-carbon halogenated aliphatic organic compounds under methanogenic conditions, in Applied Environmental Microbiology 45: 1286-1294, 1983.

Bruch, J.C. Jr., C.M. am, and T.M. Simundlich, "Parameter identification in field problems, in Water Resources Research 10(1): 73-79, 1974.

Callahan, M.A., et al, Water-Related Environmental Fate of 129 Priority Pollutants, Vol II, EPA-440/4-79-0296, December 1979.

Carrera,J., E. Usunoff, and F. Szidarovsky, "Method for optimal observation network design for groundwater management," in Journal of Hydrology 73(1/2):147-163, 1984.

Chu, W.-S., E.W. Strecker, and D.P. Lettenmaier, "An evaluation of data requirements for groundwater contaminant transport modeling," in Water Resources Research 23(3); 408-424, 1987.

Close, M.E., "Simulating the Effects of the Waiau Irrigation Scheme on Recharge and Groundwater Levels," in Journal of Hydrology, New Zealand 24(2): 49-63, 1985.

Cochran, W.G., Sampling Techniques, John Wiley and Sons, N.Y., 1977.

Cushman, John C., "On Unifying the Concepts of Scale, Instrumentation, and Stochastics in the Development of Multiphase Transport Theory", in Water Resources Research 20(11): 1668-1676, 1984.

Davis, John C. Statistics and Data Analysis in Geology. John Wiley and Sons, New York, 1973.

Dawdy, G.C. and S.F. Moore, "Water quality sampling programs in rivers," in Journal of the Environmental Engineering Division, ASCE, 105(EE4): 695-712, 1979.

Delhomme, J.P., "Spatial Variability and Uncertainty in Groundwater Flow Parameters: A Geostatistical Approach," in Water Resources Research 15(2): 269-280, 1979.

Diskin, M.H. and E. Simon, "A Procedure for the Selection of Objective Functions for Hydrologic Simulation Models," in Journal of Hydrology, 34: 129-149, 1977.

Eccles, L.A. and R.R. Nicklen, "Factors Influencing the Design of a Groundwater Quality Monitoring Network," in Establishment of Water Quality Monitoring Programs, L.G. Everett and K.D. Schmidt, eds., Proceedings of a Symposium held in San Francisco, California June 12-14, 1978, American Water Resources Association, Minneapolis, Minnesota, 1979.

Eheart, J.W. and A.J. Valocchi, "Multicriteria Management of Groundwater Quality Under Uncertainty," in Water Resources Center Research Report No. 201, University of Illinois, July 1986.

Erlebach, W.E., "A Systematic Approach to Monitoring Trends in the Quality of Surface Waters," in Establishment of Water Quality Monitoring Programs, L.G. Everett and K.D. Schmidt, eds., Proceedings of a Symposium held in San Francisco, California June 12-14, 1978, American Water Resources Association, Minneapolis, Minnesota, 1979.

Farebrother, R.W., Linear Least Squares Computations. Marcel Dekker, Inc., New York, 1988.

Ferziger, J., Numerical Methods for Engineering Application. John Wiley & Sons, New York, 1981.

Freeze, R.A., "A Stochastic Conceptual Analysis of One-dimensional Groundwater Flow in Non-uniform homogenous Media," in Water Resources Research 11(5): 725-741, 1975.

Freeze, R.A. and J.A. Cherry, Groundwater. Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1979.

Freund, R.F. and P.D. Minton, Regression Methods. Marcel Dekker, Inc., New York, 1979.

Freyberg, D.L., D.M. Mackay and J.A. Cherry, "Advection and Dispersion in an experimental Groundwater Plume," in Frontiers in Hydraulic Engineering. ASCE, Cambridge, MA, pp. 36-41, 1983.

Frind, E.O., E.A. Sudicky, and S.L. Schellenberg, "Micro-Scale Modelling in the Study of Plume Evolution in Heterogeneous Media," in Advances in Analytical and Numerical Groundwater Flow and Quality Modelling. NATO Advanced Research Workshop, National Laboratory of Civil Engineering, Lisbon, Portugal, June 1987.

van Geer, F.C., "An Equation Based Theoretical Approach to Network Design for Groundwater Levels using Kalman Filters," in Improvements of Methods of Long Term Prediction of Variations in Groundwater Resources and Regimes Due to Human Activity. Proceedings of the Exeter Symposium, IAHS Publ. No, 136: 241-250, 1982.

van Geer, F.C., Applications of Kalman Filtering in the Analysis and Design of Groundwater Monitoring Networks. TNO Institute of Applied Geoscience, Delft, the Netherlands, June 1987.

van Geer, F.C. and P. van der Kluet, "Tradeoff between Frequency and Density of a Ground-water Measurement Network," in Integrated Design of Hydrological Networks. Proceedings of the Budapest Symposium, July 1986, IAHS Publ. No. 158 : 213-229, 1986.

Gelhar, L.W., Effects of hydraulic conductivity variations on groundwater flows, in Hydraulic Problems Solved by Stochastic Methods. pp. 409-431, Water Resources Publications, Ft. Collins, CO, 1977.

Gelhar, L.W., Stochastic analysis of flow in heterogeneous porous media, in Fundamentals of Transport Phenomena in Porous Media.pp. 673-720, J.Bear and M.Y. Corapcioglu, eds., Martinus Nijhoff Publishers, Dordrecht, the Netherlands, 1984.

Gorelick, S.M., B. Evans and I. Remson, "Identifying Sources of Groundwater Pollution: An Optimization Approach," in Water Resources Research 19(3): 779-790, 1983.

Gorelick, S.M., C.I. Voss, P.E. Gill, W. Murray, M.A. Saunders, and M.H. Wright, "Aquifer Reclamation Design: The Use of Contaminant Transport Simulation Combined with Nonlinear Programming," in Water Resources Research 20(4): 415-427, 1984.

Grisak, G.E., R.E. Jackson and J.F. Pickens, "Monitoring Ground Water Quality: the Technical Difficulties," in Establishment of Water Quality Monitoring Programs, L.G. Everett and K.D. Schmidt, eds., Proceedings of a Symposium held in San Francisco, California June 12-14, 1978, American Water Resources Association, Minneapolis, Minnesota, 1979.

Gunnerson, C.G. "Optimizing Sampling Intervals in Tidal Estuaries," in Journal of the Sanitary Engineering Division, Proceedings of the American Society of Civil Engineers, pp. 103-124, 1966.

Gupta, V.L., Information content of time varying data, in Journal of the Hydraulics Division 92(SA2):103-125, ASCE, 1966.

Gutjahr, Allan, "Stochastic Models of Subsurface Flow: Log Linearized Gaussian Models are "exact" for Covariances", in Water Resources Research, 20(12): 1909-1912, 1984.

Harris, J., Statistical Analysis of Ground Water Quality: Interaction of Deterministic and Stochastic Components, Ph.D. Dissertation, Colorado State University, Fort Collins, CO, March 1988.

Herricks, E.E., D.J. Schaeffer, and J.C. Capsner, "Complying with NPDES permit limits: When is a violation a violation?," in Journal Water Pollution Control Federation 57(2): 109-115, 1985.

Hirsch, R.M., J.R. Slack, and R.A. Smith, "Techniques of Trend Analysis for Monthly Water Quality Data, in Water Resources Research 18(1): 107-121, 1982.

Hoeksema, R.J. and P.K. Kitanidis "An Application of the Geostatistical Approach to the Inverse Problem in 2-D Groundwater Modeling," in Water Resources Research 20(7): 1003-1020, 1984.

Hughes, J.P. and D.P. Lettenmaier, "Data Requirements for Kriging: Estimation and Network Design," in Water Resources Research 17(6): 1641-1650, 1981.

Javandel,I., C. Doughty, and C.F.Tsang. Groundwater Transport: Handbook of Mathematical Models. Washington, D.C.: American Geophysical Union, 1984.

Kashyap, D. and S. Chandra, "Nonlinear Optimization for Aquifer Parameter Estimating with Inadequate Data," in Improvement of Methods of Long Term

Prediction of Variations in Groundwater Resources and Regimes Due to Human Activity. Proceeding of the Exeter Symposium ,July 1982.

Kazmann, R.G., "An Introduction to Ground-Water Monitoring," in Ground Water Monitoring Review. Spring 1981, pp. 28-30.

Kitanidis, P.K. and E.G. Vomvoris, "A Geostatistical Approach to the Inverse Problem in Groundwater Modeling (steady state) and 1-D simulation," in Water Resources Research 19(3): 677-690, 1983.

Knopman, D.S., Discrimination Among One-Dimensional Models of Solute Transport in Porous Media: Implications for Sampling Design. Draft Dissertation, 1987.

Knopman, D.S. and C.I. Voss, "Behavior of Sensitivities in the One-Dimensional Advection-Dispersion Equation: Implications for Parameter Estimation and Sampling Design," in Water Resources Research 23(2): 253-272, 1987.

Knopman, D.S. and C.I. Voss, Discrimination Among One-Dimensional Models of Solute Transport in Porous Media: Implications for Sampling Design, in Water Resources Research 24(2): February, 1988.

Kontur, I., "Long-range Groundwater Level Prediction Based on Time Series Analysis," in Improvements of Methods of Long Term Prediction of Variations in Groundwater Resources and Regimes Due to Human Activity. Proceedings of the Exeter Symposium, IAHS Publ. No. 136: 187-193, 1982.

Lettenmaier, D.P., Design of Monitoring Systems for Detection of Trend in Stream Quality. Technical Report No. 39, Charles W. Harris Laboratory, University of Washington, Seattle, 1975.

Lettenmaier, D.P. and S.J. Burges, "Design of Trend Monitoring Networks," in Journal of the Environmental Engineering Division 103(EE5): 785-802, 1977.

Lin, A.C. and W.W-G. Yeh, Identification of Parameters in an Inhomogeneous Aquifer by Use of the Maximum Principle of Optimal Control and Quasilinearization, in Water Resources Research 10(4): 829-838, 1974.

Loaiciga, "An Optimization Approach for Groundwater Quality Monitoring Network Design," in Water Resources Research 25(8): 1771-1782, 1989.

Loftis, J.C., J. Harris, and R.H. Montgomery, "Detecting Changes in Ground Water Quality at Regulated Facilities," in Ground Water Monitoring Review. Winter 1987.

Loftis, J.C., P.S. Porter, and G. Settembre, "Statistical Analysis of Industrial Wastewater Monitoring Data," in Journal Water Pollution Control Federation. March 1987, pp. 145-151.

Loftis, J.C. and R.C. Ward, "Statistical Tradeoffs in Monitoring Network Design," in Establishment of Water Quality Monitoring Programs. L.G. Everett and K.D. Schmidt, eds., Proceedings of a Symposium held in San Francisco, California

June 12-14, 1978, American Water Resources Association, Minneapolis, Minnesota, 1979.

Loftis, J.C. and R.C. Ward," Evaluating Stream Standard Violations Using a Water Quality Data Base," in Water Resources Bulletin 17(6): 1071-1078, December 1981.

Loftis, J.C. and R.C. Ward, "Water quality monitoring - some practical sampling frequency considerations," in Environmental Management 4(126): 521-526, 1986.

van der Made, J.W., "Determination of the Accuracy of Water Level Observations, in Advances in Hydrometry. Proceedings of the Exeter Symposium, IAHS Publ. No. 134: 173-184, 1982.

McBean, E.A. and F.A. Rovers, "Alternatives for Assessing Significance of Changes in Concentration Levels," in Ground Water Monitoring Review 4(3): 39-41, 1984.
McBean, E.A. and F.A. Rovers, "Alternatives for Assessing Significance of Changes in Concentration Levels," in Ground Water Monitoring Review 4(3): 39-41, 1984.

McLaughlin, D.B. and W.D. Graham, "Design of Cost-effective Programs for Monitoring Ground-water Contamination, " in Integrated Design of Hydrological Networks. Proceedings of the Budapest Symposium, IAHS Publ. No. 158: 231-245, 1986.

Moore, S.F., The Application of Linear Filter Theory to the Design and Improvement of Measurement Systems for Aquatic Environments. Ph.D. Thesis, University of California at Davis, 1971.

Moore, S.F., "Estimation theory applications to design of water quality monitoring systems", in Journal of the Hydraulics Division 99(HY5): 815-831, ASCE, 1973.

Moore, S.F., G.C. Dandy, and R.J. DeLucia, "Describing Variance with a Simple Water Quality Model and Hypothetical Sampling Programs," in Water Resources Research 12(4): 795-804, 1976.

Munn, R.E., "The Estimation and Interpretation of Air Quality Trends, Including some Implications for Network Design," in Environmental Monitoring and Assessment 1: 49-58, 1981.

Nelson, J.D. and R.C. Ward, "Statistical Considerations and Sampling Techniques for Ground-Water Quality Monitoring," in Ground Water 19(6): 617-625, 1981.

Neuman, S.P., Calibration of Distributed Parameter Groundwater Flow Models Viewed as a multiple-objective decision process under uncertainty, in Water Resources Research 9(4): 1006-1021, August 1973.

Neuman, S.P., "Statistical Characterization of Aquifer Heterogeneities: An Overview," in Recent Trends in Hydrogeology, Special Paper 189, Geological Society of America, Boulder, CO, pp. 81-102, 1982.

Neuman, S.P. and E.A. Jacobson, "Analysis of Nonintrinsic Spatial Variability by Residual Kriging with Application to Regional Groundwater Levels," in Mathematical Geology 16: 499-521, 1984.

Neuman, S.P. and S. Yakowitz, "A statistical approach to the inverse problem of aquifer hydrology, 1. Theory,: in Water Resources Research 15(4): 845-860, 1979.

Palmer, R.N. and M.C. MacKenzie, "Optimization of Water Quality Monitoring Networks," in Journal of Water Resources Planning and Management 111(4): 478-493, 1985.

Parker, J.M. and S.S.D. Foster, "Groundwater Monitoring for Early Warning of Diffuse Pollution," in Monitoring to Detect Changes in Water Quality. Series Proceedings of the Budapest Symposium, IAHS Publ. No. 157: 37-46, 1986.

Parkhurst, D.F., "Optimal Sampling Geometry for Hazardous Waste Sites," in Environmental Science and Technology 18: 521-523, 1984.

Pederson, G.L., M.A. Sylvester and H.H. Higgins, "Design of an Integrated Water Quality Monitoring Program for Santa Clara County, California," in Establishment of Water Quality Monitoring Programs. L.G. Everett and K.D. Schmidt, eds., Proceedings of a Symposium held in San Francisco, California June 12-14, 1978, American Water Resources Association, Minneapolis, Minnesota, 1979.

Pimentel, K.D., Toward a Mathematical Theory of Environmental Monitoring: the Infrequent Sampling Problem, Thesis presented to the University of California at Livermore, California, 1975.

Pomeroy, R.D. and G.T. Orlob, Problems of Setting Standards and of a Surveillance for Water Quality Control. Publication No. 36, California State Water Quality Control Board, Sacramento, CA, May, 1967.

Porter, P.S., Statistical Analysis of Water Quality Data Affected by Analytical Limits of Detection. Ph.D. Thesis, Colorado State University, Fort Collins, Colorado, 1986.

Provost, L.P., "Statistical methods in environmental sampling, in Environmental Sampling for Hazardous Wastes. pp. 79-86, American Chemical Society, Washington, D.C., 1984.

Remson,I. and J.R. Randolph, "Application of Statistical Methods to the Analysis of Ground-water Levels," in Transactions, American Geophysical Union, pp. 75-83, 1958.

Rodriguez-Iturbe,I. and J.M. Mejia, "The Design of Rainfall Networks in Time and Space," in Water Resources Research 10(4): 713-728, 1974.

Salas, J.D. et al, Applied Modeling of Hydrologic Time Series. Water Resources Publications, Ft. Collins, CO 1980.

Sanders, T.G. and D.D. Adrian, "Sampling Frequency for River Quality Monitoring," in Water Resources Research 14(4): 569-576, 1978.

Sanders, T.G. and R.C. Ward, "Relating Stream Standards to Regulatory Water Quality Monitoring Practices," in Establishment of Water Quality Monitoring Programs. L.G. Everett and K.D. Schmidt, eds., Proceedings of a Symposium held in San Francisco, California June 12-14, 1978, American Water Resources Association, Minneapolis, Minnesota, 1979.

Sanders, T.G., R.C. Ward, J.C. Loftis, T.D. Steele, D.D. Adrian, V. Yevjevich, Design of Networks for Monitoring Water Quality. Water Resources Publications, Littleton, Co, 1983.

Schilperoort, T. and S. Groot, "Design and Optimization of Water Quality Monitoring Networks," paper presented at the International Symposium on Methods and Instrumentation for the Investigation of Groundwater Systems (MIIGS) Noordwijkerhout, the Netherlands, May 1982, Publication no. 286, 1983.

Schwarzenbach, R.P. and J. Westall, "Laboratory Sorption Studies," in Environmental Science Technology 11(15): 1360-1367, 1981.

Schweitzer, G.E. and S.C. Black, "Monitoring Statistics," in Environmental Science and Technology 19: 1026-1030, 1985.

Schweitzer, G.E. and J.A. Santolucito, Eds., Environmental Sampling for Hazardous Waste. American Chemical Society Symposium Series No. 267, Washington D.C., 1984.

Serrano, S.E., T.E. Unny, and W.C. Lennox, "Analysis of Stochastic Groundwater Flow Problems. Part I: Deterministic Partial Differential Equations in Groundwater Flow. A Functional-Analytic Approach," in Journal of Hydrology 82: 247-263, 1985.

Serrano, S.E., T.E. Unny, and W.C. Lennox, "Analysis of Stochastic Groundwater Flow Problems. Part II: Stochastic Partial Differential Equations in Groundwater Flow. A Functional-Analytic Approach," in Journal of Hydrology 82: 265-284, 1985.

Serrano, S.E., T.E. Unny, and W.C. Lennox, "Analysis of Stochastic Groundwater Flow Problems. Part III: Approximate Solution of Stochastic Partial Differential Equations," in Journal of Hydrology 82: 285-306, 1985.

Sgambat, J.R., K.S. Porter and D.W. Miller, "Regional Ground Water Quality Management," in Establishment of Water Quality Monitoring Programs. L.G. Everett and K.D. Schmidt, eds., Proceedings of a Symposium held in San Francisco, California June 12-14, 1978, American Water Resources Association, Minneapolis, Minnesota, 1979.

Smith, L. and R.A. Freeze, "Stochastic Analysis of Steady State Groundwater Flow in a Bounded Domain, 1. One-Dimensional Simulation," in Water Resources Research 15(3): 521-528, 1979a.

Smith, L. and R.A. Freeze, "Stochastic Analysis of Steady State Groundwater Flow in a Bounded Domain, 2. Two-Dimensional Simulation," in Water Resources Research 15(5): 1543-1559, 1979b.

Smith, L. and F.W. Schwartz, "Mass Transport 1. A Stochastic Analysis of Macroscopic Dispersion," in Water Resources Research 16(2): 303-313, 1980.

Sophocleous, M., J.E. Paschetto, and R.A. Olea, "Ground-Water Network Design for Northwest Kansas, Using the Theory of Regionalized Variables," in Ground Water, Vol. 20, No. 1, pp.48-58, 1982.

Steele, T.D., "Converting Water Quality Information Goals into Statistical Design Criteria, " in Monitoring to Detect Changes in Water Quality. Series Proceedings of the Budapest symposium, IAHS Publ. No. 152: 71-78, July 1986.

Tabios, G.Q. III, Nonlinear Stochastic Modeling of River Dissolved Oxygen. Ph.D. Dissertation, Fall 1984, CSU.

Tinlen, R.M. and L.G. Everett, "Establishment of Ground Water Quality Monitoring Programs" in Establishment of Water Quality Monitoring Programs. L.G. Everett and K.D. Schmidt, eds., Proceedings of a Symposium held in San Francisco, California June 12-14, 1978, American Water Resources Association, Minneapolis, Minnesota, 1979.

Todd, D.K., R.M. Tinlin, K.D. Schmidt, and L.G. Everett, Monitoring Groundwater Quality: Monitoring Methodology. General Electric Company - TEMPO Center for Advanced Studies, US EPA, 1976.

Tung, Y-K., "Groundwater Management by Chance-Constrained Model," in Journal of Water Resources Planning and Management 112(1): 1-19, 1986.

Vansteenkiste, G.C., ed., Modeling,Identification and Control in Environmental Systems. North-Holland, Amsterdam, 1978.

Vemuri, V. and W.J. Karplus, Identification of nonlinear parameters of groundwater basin by hybrid computerization, in Water Resources Research 5(1): 172-185, 1969.

Vomvoris, E.G. and L.W. Gelhar, Stochastic Prediction of Dispersive Contaminant Transport, Report No. EPA/600/2-86/114, U.S. EPA Office of Research and Development, Ada, Oklahoma, 1986.

Ward, R.C., Data Acquisition Systems in Water Quality Management. Report EPA-R5-73-014, EPA, Washington, D.C., 1973.

Ward, R.C., "Framework for Designing Water Quality Information Systems, in Monitoring to Detect Changes in Water Quality. Series Proceedings of the Budapest symposium, July 1986, IAHS Publ. No. 152: 89-95, 1986.

Ward, R.C. and J.C. Loftis, "Establishing Statistical Design Criteria for Water Quality Monitoring Systems: Review and Synthesis," in Water Resources Bulletin 21(5): 759-767, 1986.

Ward, R.C., J.C. Loftis, and G.B. McBride, "The "Data-rich but Information-poor" Syndrome in Water Quality Monitoring," in Environmental Management 10(3): 291-297.

Ward,R.C. and G.B. McBride, "Design of Water Quality Monitoring Systems in New Zealand," Water Quality Centre Publication No. 8, Ministry of Works and Development, Hamilton, New Zealand, 1986.

Ward, R.C., S.R. Nichols and G.V. Skogerboe, Surveillance in water quality management, in Journal of the Water Pollution Control Federation 45(10): 2081-2087, 1973.

Ward, R.C. and L. Russel, Data requirements of a water quality management program, in Water Resources Bulletin 9(6): 1234-1248, 1978.

Ward, R.C. and D.H. Vanderholm, "Cost-effectiveness methodologies for data acquisition in water quality management," in Water Resources Research 9(3): 536-545, 1973.

Willis, R., "A Planning Model for The Management of Groundwater Quality," in Water Resources Research 15(6): 1303-1312, 1979.

Willis,R. and W.W-G. Yeh. Groundwater Systems Planning and Management. Englewood, New Jersey: Prentice-Hall,Inc., 1987.

Yeh, W.W-G., Aquifer parameter identification, in Journal of Hydraulic Division American Society of Civil Engineers 101(HY9): 1197-1209, 1975.

Yeh, W.W-G., Review of parameter identification procedures in groundwater hydrology: the inverse problem, in Water Resources Research 22(2): 95-108, 1986.

Yeh, W.W-G. and G.W. Tauxe, A proposed technique for identification of unconfined aquifer parameters, in Journal of Hydrology 12(2): 117-128, 1971a.

Yeh,W.W-G. and G.W. Tauxe, Quasilinearization and the Identification of Aquifer Parameters, in Water Resources Research 7(2): 375-381, 1971b.

Yeh,W.W-G. and G.W. Tauxe, Optimal identification of aquifer diffusivity using quasilinearization, in Water Resources Research. 7(4): 955-962, 1971.

Yeh, W.W-G. and Y.S. Yoon, Aquifer parameter identification with optimum dimension in parameterization, in Water Resources Research 17(3): 664-672, 1981.

Yevyevich, V., Probability and Statistics in Hydrology, Water Resources Publications, Fort Collins, Colorado, 1972.