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MONITORING NETWORK DESIGN FOR RISK-BASED GROUNDWATER REMEDIATION

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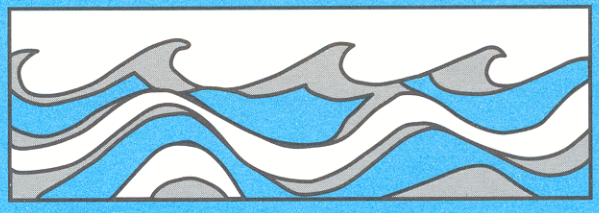

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Monitoring Network Design for Risk-Based Groundwater Remediation

by

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Abstract

Groundwater contamination at hazardous waste sites is a pervasive problem in the United States. Remediating contaminated sites is expensive and remediation depends on groundwater monitoring data that are themselves expensive. Observations of groundwater quality are inherently imprecise, due both to the necessity to characterize a three dimensional spatial process with point observations, and due to measurement error.

In this study, computer simulation models are used to establish the relationship between the site characterization and remedial effectiveness. A two-dimensional contaminant flow and transport model is used to simulate aquifer contamination. Three monitoring strategies are contrasted: a random strategy, a sequential strategy using error propagation, and a sequential strategy using Fourier domain shape analysis (FDSA). In each method, simulated measurements of the concentration of a conservative solute are used to estimate parameters describing the plume geometry and flow characteristics. A hypothetical pump and treat remediation is then designed, based on capture zone analysis, to remove the inferred plume. Finally, remedial effectiveness is quantified in terms of the duration of the simulated remediation, the fraction of solute that is remediated and the total volume of water that must be extracted. The procedure is iterated in a Monte Carlo framework to provide statistical estimates of the remediation effectiveness for different measurement variances.

Sequentially designed networks using error propagation performed significantly better than either the random networks or those designed using FDSA. Under the assumed model conditions, adequate remedial results were obtained with networks of 10 or more wells using error propagation. FDSA remediations began to improve with 15 well networks suggesting that the method may be viable where extensive data sets are available.

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CHAPTER 1: INTRODUCTION

1.1 Overview

Contamination of groundwater resources is a widespread problem that has attracted increasing attention from the public, federal and state agencies, and private industry over the last decade. Shallow aquifers, in the vicinity of hazardous waste sites are at particular risk since direct pathways for contaminant migration from surface facilities to these aquifers are often present. Congress charged the United States Environmental Protection Agency (EPA) with identifying hazardous waste sites and overseeing the process of remediating those sites under the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) of 1980. As of March, 1990 EPA had placed 1218 hazardous waste sites on the National Priority List (NPL) (*Federal Register*, 1990), most of which had associated groundwater contamination. The potential for groundwater contamination exists at as many as 27,000 additional sites (*National Research Council*, 1990) due to a variety of risks including abandoned oil and gas wells and leaky underground storage tanks.

The process of identifying sites in need of remediation and initiating the remedial process is often extremely slow and costly. The cost of characterizing and remediating each NPL site is expected to average between $20-30 million dollars (*U.S. House of Representatives,* 1989). Remediating Department of Energy facilities alone is expected to cost well in excess of 100 billion dollars, due to their physical size and the nature of the contaminants at these sites. As noted in a hearing on the progress of the Superfund program (*U.S. House of Representatives,*

1989) despite EPA expenditures in excess of $1 billion dollars during fiscal years 1987 and 1988, remediation had been completed at only 28 NPL sites by December, 1989. The poor success of CERCLA in promoting timely remediation of hazardous waste sites has fostered interest in improving the process, both from a policy perspective, and with regards to the technical steps required to investigate a site.

The general approach to hazardous waste site remediation that has evolved under EPA guidance is as follows: First, EPA prioritizes sites under National Contingency Plan (NCP) regulations as summarized in the *Federal Register* [1990] by carrying out a cursory site inspection and analyzing existing data. EPA uses these data within the framework of the Hazard Ranking System to estimate potential human health risks based on factors including waste volume, waste toxicity, proximity to population centers and potential for aquifer contamination. Sites scoring over an (arbitrarily selected) value of 28.5 are designated as Superfund sites and are placed on the National Priority List. Superfund sites are subject to remediation as specified by CERCLA, the Superfund Amendments and Reauthorization Act (SARA) of 1986, and appropriate state regulations. Ultimately, EPA and state agencies attempt to find the principal responsible parties (PRPs) who, as a result of their past activities at the site, are liable for the remediation cost.

The next step in the process is a remedial investigation/feasibility study (RI/FS). The RI/FS is usually conducted by a consultant to EPA or under the guidance of the designated state agency. Detailed data are collected during the remedial

investigation to define the extent of the problem including the source(s) of contamination, possible migration pathways for the contaminant and the extent of health risks to human population. At this stage, the number and location of monitoring wells, frequency of sampling, and required accuracy of the physical and chemical measurements must be determined.

These data are interpreted and used as the basis for designing specific remedial alternatives for the site. At this stage, the key issues are estimation of the current spatial distribution of the contaminant and its likely future movement, both without remediation and under alternative remediation approaches. The chemical nature of the contaminant and the hydrogeologic environment will also dictate possible alternative technologies for site restoration. In addition, the likely effectiveness of alternative remedial approaches, and the uncertainty in projections of effectiveness, should be evaluated, (although this is rarely done at present in an objective manner). EPA selects one of the remedial technologies put forth in the feasibility study in what is known as the record of decision (ROD). Design engineers then finalize an engineering and construction plan since designs made during the feasibility study are usually preliminary in nature. Engineering specifications for the remedial facilities and predictions of system performance depend directly on data acquired during the remedial investigation.

The above process of site characterization and remedial design for a hazardous waste site is complicated and lengthy. The remediation itself can take several years depending on the complexity and scale of the problem. Remedial efforts usually include removal of existing facilities, treating and/or removing

contaminated soils and restoring contaminated aquifers. In this report only problems related to aquifer restoration are considered.

Currently, the most prevalent restoration method for contaminated aquifers involves pumping contaminated water from the aquifer and treating it in a surface facility ("pump and treat"). In the case of pump and treat alternatives, important variables are the number, location and pumping rates for the extraction and/or injection wells. Because of uncertainty about the extent of contamination and the performance of remediation alternatives, future data needs and mechanisms for adapting the selected remediation approach as additional data become available are an important consideration on the remedial design. At present though, objective methods for incorporation of such uncertainties in the design process are rarely applied.

1.2 Monitoring network design and aquifer remediation

The interaction between the amount and quality of monitoring data and the successful remediation of an aquifer is intuitively clear, but has not been studied in detail. Allocation of resources between the different remediation stages will impact both ultimate costs and remedial effectiveness. In particular, increasing the amount and quality of monitoring data collected during site characterization should improve the overall effectiveness of the remedial design but will increase costs and may delay implementation of a remedial plan. From a practical standpoint, a site can never be fully characterized due to measurement errors, spatial parameter variations and the inherent ambiguity of groundwater systems

(*Massmann and Freeze*, 1987a,b). Increasing the number of monitoring wells can be expected to reduce the risk of remediation failure. Conceptually, the value of monitoring data at the site characterization stage can be analyzed using cost-benefit methods. While properly designed monitoring strategies will reduce the uncertainties under which remediation alternatives must be designed and compared, a certain level of ambiguity is inevitable and should be incorporated in the final remediation. From an economic standpoint, optimal remediation should weigh the cost of monitoring and site characterization data against the risk of unsuccessful or incomplete remediation.

1.3 Research Objective

The objective of this report is to investigate the tradeoff between site characterization monitoring design, monitoring cost, and remedial effectiveness (defined as the complement of failure risk) for a pump and treat remediation design. The techniques described are meant to represent a framework for studying the interaction between monitoring and remedial effectiveness rather than to define a specific approach for studying individual sites. Thus, for example, a simple analytical model is used to facilitate isolation of the effect of key variables and to control computational requirements. The design variables for the problem are the number, position, and pumping rates for the extraction wells used to remediate the aquifer. The objective was taken to be the minimization of the total cost of remediation, as measured by a surrogate variable, the volume of water to be treated. Additional measures of system performance that are considered include the duration of the remedial activity and the fraction of a

contaminant plume that is remediated given data from a particular monitoring network.

The remainder of this report addresses the specific issues of data collection network design and aquifer remediation as follows: Chapter 2 reviews the literature that is most applicable to this study. Chapter 3 outlines the methods used in a FORTRAN computer program (DEMON, for DEsign MOonitoring Networks), written for this study to simulate the interaction between monitoring network design and remedial effectiveness. In Chapter 4 simulation results for different monitoring strategies evaluated with DEMON are summarized. Finally, in Chapter 5 conclusions based on the model studies are presented along with recommendations for extensions of this work.

CHAPTER 2: BACKGROUND

In Chapter 1, the general procedure for hazardous waste site characterization that is required under CERCLA and related legislation was described as well as some of the shortcomings in the procedure. The interest in hazardous waste site remediation over the last decade has resulted in a body of literature applicable to the problem in general and to the interaction between site characterization monitoring and pump and treat remedial effectiveness. This chapter reviews past research that is most relevant to the topic of this report.

2.1 Monitoring network design

Historically, groundwater monitoring networks have been used to provide data about the quantity and quality of water that could be pumped from regional aquifers. A number of studies have addressed the design of such networks, see for example (*Candela, et al.*, 1988, *Hsueh and Rajagopal*, 1988, and *Olea*, 1984). More recently, as concern for groundwater contamination associated with hazardous waste sites has grown, research directed towards problems associated with smaller, site-specific issues has developed. In this setting, fewer wells are generally available and the distribution of chemical constituents, becomes the focal point of the study, e.g. *(Meyer and Brill*, 1988, *Pfannkuch*, 1982, *Loaiciga*, 1989). Three categories of monitoring network design have been widely applied in recent years. These are: geostatistical methods (*Olea*, 1984, *Carrera, et al.*, 1984, *Rouhani and Hall,* 1988) simulation and optimization methods (*Andricevic*, 1990, *McLaughlin and Graham*, 1989) and finally methods that deal explicitly with risk and uncertainty, often using components of the first two techniques (*Neptune et al.,*

1990, *Massmann and Freeze*, 1987a,b). Each of these will be reviewed in detail after a brief discussion of the purpose of ground water monitoring networks.

Monitoring wells provide the most important hydrogeological and chemical data for most hazardous waste sites. Observations of piezometric head are used to establish the geometric configuration of the water table in both a static and dynamic sense. Concurrent measurements taken at a number of wells lead to an understanding of the preferred flow direction at an instant in time. A sequential sampling program over a period of days, weeks, or years can reveal changes in piezometric head that may reflect important boundary conditions such as variations in streamflow, tides, or anthropogenic impacts. These oscillations can have an important influence on the design of monitoring networks or on the design of remedial programs.

Chemical analyses of groundwater samples collected at monitoring wells provide the other key element for understanding the nature of aquifer contamination at hazardous waste sites. The spatial pattern of concentration of a given constituent is governed by the geometry of the contaminant source, the dispersivity of the media, degree of heterogeneity of the aquifer and the chemical properties of the substance with respect to both the surrounding fluid and mineralogy of the aquifer.

A properly designed monitoring system will provide the maximum amount of information relevant to remediation at a minimum cost. In addition to estimating the variable of interest, whether it is piezometric head or level of contaminant

concentration, it is highly desirable to be able to specify the likely error in an estimate, for instance by placing confidence bounds on the estimate.

The simplest monitoring strategies are those that are specified prior to commencing the data collection phase based on spatial statistical considerations alone. For example, different monitoring strategies including, random sampling, regular grids, stratified random sampling and polygons of influence, were used by *McArthur* [1987] to estimate the total mass of a contaminant around a simulated source of pollution. The drawback with random monitoring strategies is that a large number of measurements are required to adequately sample a plume. In most settings, budgetary constraints would preclude the use of such techniques. More sophisticated network design strategies are often sequential; data available at a given phase in the network development are used to guide decisions about where and when to sample next.

2.1.1 Geostatistics

Geostatistical methods, developed in the mining industry to analyze the spatial distribution of ore bodies, have been adopted during the past fifteen years by groundwater hydrologists. Geohydrologists have used these techniques to describe the spatial variability of aquifer parameters including transmissivity, leakance and chemical content. Kriging, which forms the backbone of geostatistics, accounts for the spatial correlation of closely spaced measurements of a "regionalized" random variable. Kriging is capable of estimating the expected value of the variable and it can be used to estimate the variance of the estimate as a function

of its position. These capabilities have led investigators to use kriging as a technique for monitoring network analysis and design. For example *Olea* [1984] used maximum and average sampling error as measures of sampling efficiency to select among competing sampling densities and patterns for an aquifer in Kansas. A stratified version of an existing monitoring network was formed with an 81 percent reduction in the number of wells with virtually no information loss.

Lognormal kriging was applied to model chloride concentration in a coastal aquifer in Spain by *Candela, et al.* [1988] as an aid to assessing the efficiency of a monitoring network. The actual monitoring network in this case had 120 wells; stratified sampling was used to eliminate 21 wells from the network while maintaining essentially the same network quality. The quality of the network was defined as either the maximum or average kriging error over the region.

Rouhani and Hall [1988] used kriging to design monitoring networks based on variance reduction analysis, and risk reduction analysis. In their study, the variance reduction potential of each of a number of candidate well locations were compared; the location that provided the greatest reduction in variance was used for the next well. They also studied risk-reduction which incorporated both the measurement variance and its magnitude. The technique was applied to design a network for predicting leakance from a shallow contaminated aquifer into an underlying artesian aquifer, (*Rouhani and Hall*, 1988).

Kriging has several important limitations for application to groundwater contamination problems. First, *Journel and Huijbregts* [1978] suggest that at least

30 points are required to estimate the spatial correlation function adequately. This is larger than the number of wells in many hazardous waste site investigations. Secondly, the mathematical form of the semi-variogram must be assumed (based on an analysis of the data) and different forms of the solution can lead to different predictions for the variable.

2.1.2 Simulation and optimization

Simulation and optimization have been used to design monitoring networks by a number of authors. *Meyer and Brill* [1988] describe a method for optimally placing monitoring wells in a network given uncertain longitudinal and transverse dispersivities and flow direction. They used a simulation model to generate a large number of plumes. Monitoring wells were installed over a grid downgradient from the source to detect the plumes if possible. A small number of monitoring locations were selected from all the possible locations, such that the selected wells maximize the probability of detection.

On a regional scale, monitoring decisions can be based on allocation of limited resources to maximize the benefits while protecting the most sensitive locations (*Rajagopal*, 1986, *Hsueh and Rajagopal, 1988*). Integer programming was used in these studies to select sampling frequencies and locations based on potential for population exposure to hazardous substances. The variability of preexisting measurements and budgetary constraints were included in the models.

In a recent study by *Andricevic* [1990] well locations within a groundwater monitoring network were selected to maximize the statistical monitoring power, or

conversely to minimize the network cost. The network was specified by the number of monitoring wells and the sampling frequency at each well. Kalman filtering was used to propagate piezometric head errors through an aquifer. Finally, a network of wells was selected from a finite number of alternatives to either minimize the network cost or maximize the monitoring power of the network.

2.1.3 Risk-based monitoring

Several studies have addressed groundwater monitoring issues from a risk-based perspective. *Massmann and Freeze* [1987a,b] analyzed the installation of a new landfill from a risk-cost-benefit point of view. The value of risk-reduction efforts including installation of monitoring wells, double liners and site selection based on surficial hydraulic conductivity were compared in terms of the probability of causing groundwater contamination. Monitoring wells installed in a spatially variable aquifer were one of the alternatives. Detecting a plume at a monitoring well was assumed to provide protection for a down-gradient compliance surface. However, other safeguards such as installing double liners or siting the facility on low permeability clays were found to be more effective in risk reduction.

Neptune, et al. [1990] considered the potential for adverse health effects from a Superfund site by assigning risks to different "exposure units" (EUs) within the site. Remedial action would be undertaken for EUs with a health risk greater than 10^{-4}. Their study explicitly addressed uncertainty, defined as the probability of reaching an incorrect conclusion for the estimated health risks, for both false

positive and false negative scenarios. They compared different combinations of sampling densities and sample compositing to find a solution that was consistent with an acceptable level of risk.

2.2 Aquifer remediation

There are almost always conflicting objectives for groundwater remedial designs. Liable parties are most interested in minimizing the total cost of a remedial action while regulatory or environmental groups may desire removal of essentially all hazardous substances (e.g. to a non-detectable level). In addition, constraints such as a specific time horizon for remediation or a requirement that the contaminant must spread no further down-gradient to protect a water supply often must be considered. These elements have been incorporated into remedial designs either through ad hoc comparisons of alternative techniques or more recently through mathematical optimization routines. The automated methods differ in the allowable complexity of the hydrogeological environment, solution technique, specification of the objective function and constraints. In all cases reviewed here, the design variables for a pump and treat system are the location and number of extraction and or injection wells and the pumping rates for each of the wells.

Historically, extraction well parameters have been chosen through a trial and error process. *Freeberg, et al.* [1987] tested different combinations of well locations and pumping rates for remediating an aquifer and simulated the response of the aquifer over the life of the remedial program. The "optimal" solution was the

combination of parameters that minimized either the total cost or treatment time. *Tsai and Zielen* [1985] examined different pump and treat strategies for remediating an ammunition plant in Nebraska that had contaminated a shallow aquifer. They chose the final remedial solution from an arbitrary list based on the expected remedial duration and volume of water to be treated.

One approach to quantifying the solution to aquifer remediation is through the use of what *Javandel and Tsang* [1986] refer to as capture-zone analysis. In this analysis, the radius of influence of a pumping well can be calculated for uniform flow in a homogeneous isotropic aquifer of constant thickness based on estimates of aquifer parameters. Within this radius, all groundwater flow is directed towards the pumping well. If the pumping rate is selected so that the radius of influence encompasses the entire contaminant plume, the well can be used to remove all of the contaminant. Multiple well systems can be used if the pumping rate for a single well remedial design would cause an unacceptably large drawdown.

The concept of directing flow from a plume to a set of wells has also been called hydraulic gradient control. *Atwood and Gorelick* [1985] studied alternatives for remediation of groundwater contamination at the Rocky Mountain Arsenal outside of Denver, via hydraulic gradient control. Using a simulation-management model, they attempted to minimize the cleanup time at the site by varying the pumping rate and location of injection wells surrounding the plume. The optimization was implemented by first calculating the system response due to a single well in what they termed the matrix-response method. Drawdowns from

various combinations of pumping and injection wells were added based on the superposition principle. Once a matrix was set up for all possible well locations, they adjusted the flow rates using linear programming until an optimal solution was found. Additional flexibility was incorporated by allowing for multi-stage remedial design. Thus, pumping rates and the selection of wells could be varied over time based on an updated understanding of the aquifer response to the remediation process during the previous time interval.

At some sites remedial design may be driven by the total restoration time rather than costs. *Lefkoff and Gorelick* [1986] studied rapid aquifer restoration constrained by treatment capacity, the capacity of pumping and injection wells and allowable drawdown in the aquifer using linear and quadratic programming. They found that the time constraint imposed on the problem necessitated pumping approximately 10 times the original volume of contaminated water.

Nonlinear programming has been used with some success to address remedial design. *Gorelick, et al.* [1984] posed the problem in terms of minimizing the total volume of water pumped from a site subject to constraints on groundwater quality at various locations and maximum drawdown at the wells. Several experiments demonstrated the flexibility of the method for analyzing management decisions during aquifer remediation. *Ahlfeld, et al.* [1986] accounted for the interaction between contaminant transport and the variable pumping rates using a similar problem formulation with slightly different constraints. Non-linear solutions tend to be computationally intensive but are best able to model adaptive extraction systems.

Greenwald and Gorelick [1989] used the plume capture technique in combination with an optimization routine to determine both pumping and injection rates that minimized the cost of a remediation program under various constraints. A unique feature of their study was the inclusion of a function describing costs as a function of pumping rates. Most researchers have used pumping rates as a surrogate for costs when trying to design a minimum cost remediation program (see for example: *Freeburg, et al., 1987; Ahlfeld, et al.*, 1986; *Satkin and Bedient*, 1988).

Greenwald and Gorelick [1989] simulated plume remediation by tracking the travel time from the plume boundary to one of the remedial wells using a simulation model developed by *Javandel, et al.* [1984]. In their method, the velocity at each point in the aquifer is estimated from the linear combination of the regional flow field and the flow induced by each pumping well. Particles are tracked by integrating numerically along each pathline. The plume is considered to be removed when the last particle arrives at a pumping well. They found that in some cases the cheapest alternative involved higher pumping rates, especially when costs were discounted over time.

Studies that directly model the effectiveness of a remedial design based on groundwater monitoring network design are notably absent from the literature. This report attempts to combine ideas from some of the studies referred to above to study the impact of monitoring design on the ultimate effectiveness of a hazardous waste site remediation. Chapter 3 describes the components of a computer model developed to study the influence of monitoring design on remedial effectiveness.

CHAPTER 3: EXPERIMENTAL DESIGN

3.1 Overview

The relationship between groundwater monitoring network design and hazardous waste site remedial effectiveness could be investigated in at least three ways: through field studies, laboratory studies and computer simulations. Although a computer simulation approach was used in this report, each method has specific advantages and disadvantages that are worth mentioning.

The first category of experiment would entail choosing a contaminated site with sufficient existing monitoring wells to characterize both the aquifer flow regime and contaminant distribution. A pump and treat extraction system designed from all of the available monitoring data could be used as a standard for the experiment. Various subsets of the monitoring wells could be used to simulate alternative monitoring network strategies. Remedial systems designed from each sub-network could then be contrasted with the standard system. Such an approach would be realistic with respect to the quality of the data, complexity of the aquifer and distribution of the monitoring wells. Unfortunately, few sites are adequately monitored to provide enough permutations on the network patterns to reach definitive statistical conclusions. Additionally, the available data provide only one realization from the populations that define the sampling and measurement error distributions, thus limiting the generality of the results. Finally, the results would be site specific, and applicability to other sites with different hydrogeological and contaminant characteristics would be problematic.

A laboratory scale model of a contaminated aquifer is the next type of experiment. In this case, the nature of the aquifer and contaminant could be rigorously controlled and the experiment could be run using different aquifer configurations. Monitoring patterns could be easily altered and scale model pumps could be used to test remedial effectiveness of different extraction systems. Such an experiment seems quite attractive and is worthy of pursuit. However, if not well designed the experiments could be extremely time-consuming and expensive and scaling problems may limit the validity of the results.

Computer simulation is the final category of experiment. Computer models allow a level of flexibility that is generally not possible in either field or laboratory studies. Different combinations of observation errors, different criteria for network design, different numbers of monitoring wells and different measures of remedial effectiveness can all be investigated with relative ease. Since the components of the model are either chosen from available software packages or written based on specific model assumptions, complete control over the nature of the simulated aquifer and the mode of the contamination event are possible. Thus, if it is desirable to apply the model to a specific site whose characteristics are not consistent with the model, those parts of the model that are inconsistent can be modified within the overall framework established here. A disadvantage of computer studies is that one must assume that the model is a reasonable representation of the true subsurface problem.

Figure 1 shows the components of the computer model developed for this study in schematic form. The rest of this chapter outlines the theory behind the components of the computer program (DEMON) written for this study.

3.2 Plume generation

In this report, aquifer contamination is simulated using a plume generation module which models the "true" movement of water and contaminant in the aquifer. For this analysis, the truth model is governed by the following assumptions: uniform steady two dimensional flow and transport of a vertically mixed contaminant in a constant thickness, homogeneous aquifer. A continuous, vertical line source was used to simulate aquifer contamination based on an analytical solution to the advective dispersive equations as described by *Wilson and Miller* [1978]. Their solution is valid for contaminant transport in a homogeneous constant thickness aquifer with confined flow.

In the Wilson-Miller model, the concentration at any point in space is given by:

$$C = \frac{f_m \, e^{(x/B)}}{4\pi\eta(D_x D_y)^{1/2}} \; W\left(u, \frac{r}{B}\right) \qquad 3.1$$

in which:

$$B = \frac{2D_x}{V}, \qquad 3.2$$

$$\gamma = 1 + \left(\frac{2B\lambda}{V}\right), \qquad 3.3$$

$$u = \frac{r^2}{4\gamma D_x t}, \qquad 3.4$$

$$r = \left[\left(x^2 + \frac{D_x}{D_y} y^2\right)\gamma\right]^{1/2} \qquad 3.5$$

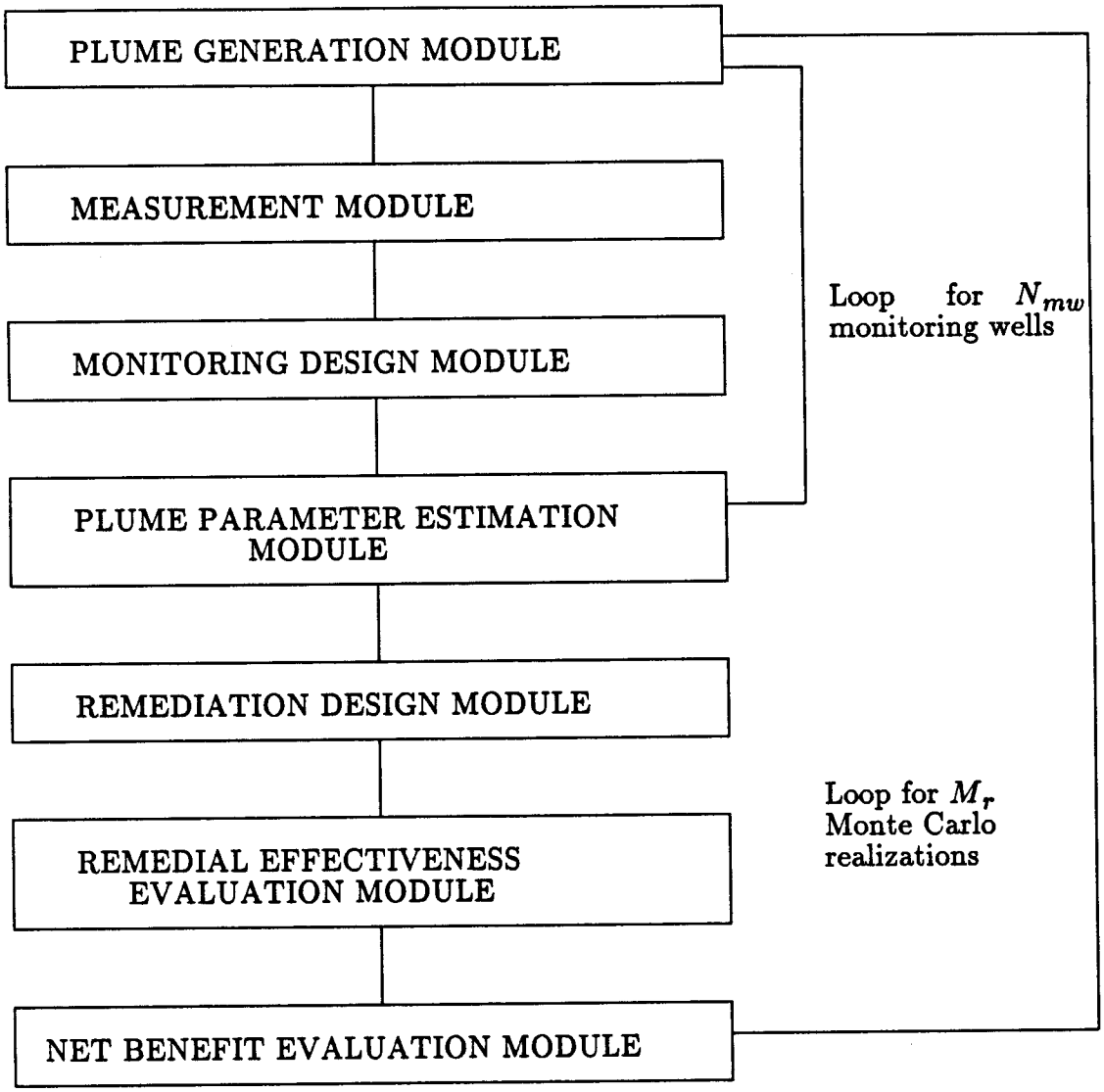

Figure 1) Conceptual flow chart for the FORTRAN program DEMON.

and

$$W\left(u,\ \frac{r}{B}\right) \approx \left(\frac{\pi B}{2r}\right)^{1/2} e^{(-r/B)}\ \text{erfc}\left(-\frac{\frac{r}{B} - 2u}{2u^{1/2}}\right) \qquad 3.6$$

where erfc is the complimentary error function. $W\left(u,\ \frac{r}{B}\right)$ is known as the Hantush well function. Equation 3.6 is an approximation of the well function that is accurate to within ten percent for $r/B > 1$ and to within one percent for $r/B > 10$ (*Wilson and Miller*, 1978).

3.3 Measurement simulation

A measurement submodel is used to simulate the estimation of concentrations at arbitrary locations within the aquifer from direct measurements. The measurement submodel corrupts the true values with random noise to simulate field and laboratory measurement errors. These errors are added to the true concentration data in log space as follows:

$$\log_{10}(C_{obs}) = \log_{10}(C_{true}) + \epsilon_c \qquad 3.7$$

where:

$$\epsilon_c = \sigma_c * \text{Z}(0,1) \qquad 3.8$$

σ_c is the magnitude of the standard deviation of the concentration errors in log space scaled by a mean 0, variance 1 normally distributed random variable Z.

3.4 Parameter Estimation

Based on the error-corrupted measurements, an optimization routine is invoked (*Nelder and Mead*, 1965) to estimate the aquifer transport and dispersion parameters that are assumed to be unknown. The optimization routine can be used in unconstrained mode, where the parameters are allowed to take on any value. Alternatively, upper and lower bounds can be specified for any individual parameter. These bounds can be used to ensure positive flow velocities in an aquifer for instance, or to specify that the lateral dispersion coefficient is smaller than the longitudinal dispersion coefficient. The objective function for the parameter estimation algorithm is minimization of the sum of the squared differences between the logarithm of the measured concentration values and the logarithm of the concentration values generated using the estimated parameters. A FORTRAN implementation of the Nelder-Mead algorithm provided by *Press, et al.* [1986] proved convenient.

The convergence criterion used in the Nelder-Mead algorithm can be specified in several ways. First, if the change in the objective function is small between iterations, convergence may be deemed to have occurred. Secondly, convergence may be specified by the lack of change in parameter values between steps in the search. Occasionally, the algorithm may fail to meet either criterion, in which case the parameter values at the end of 500 iterations are taken as the "optimal" solution.

3.5 Monitoring network design

One of the key goals of site characterization is to establish the outermost limits of the plume. A heuristic approach to plume extent estimation was used in an earlier study by *Wagoner and Lettenmaier* [1989] to place a series of monitoring wells down-gradient from the contaminant source until the concentration of the contaminant falls below a threshold (e.g. detection level) at one of the wells. A similar procedure was used to establish the lateral and up-gradient extent of contamination. A pattern of wells positioned up-gradient, down-gradient, and perpendicular to the plume axis was used in the earlier study as the basis for plume extent estimation through application of the Wilson-Miller algorithm as described in Section 3.2. Subsequent wells were placed in groups of four on a specified (threshold) concentration contour, which was estimated from the model fit to the previously sampled concentration data. This method was appealing in its simplicity and its close relationship to the way that many site investigations are undertaken. However, the monitoring algorithm was heuristic, so the specified loaction for the next well was not "best" in any statistical sense.

Two methods that can be used for predicting the uncertainty in an estimate of a detection level contour were investigated for this report. The first propagates parameter uncertainty through the model to estimate uncertainty in the models' prediction. The second method relies on a Fourier series approach and formulates the problem in terms of shape analysis. The details of each method are described in the following two sub-sections.

3.5.1 First Order Error Propagation

First order error propagation or moment propagation as described by *Benjamin and Cornell* (1970) and *Cornell* (1972) is an approximate method for estimating the mean and variance of a function of random variables. The method has found hydrologic application in stream quality modeling (*Burges and Lettenmaier*, 1975) and in flood plain mapping (*Burges* 1979). In the first study uncertainty in initial dissolved oxygen concentrations and BOD levels were propagated though the Streeter-Phelps equation to estimate uncertainty in the predicted values for DO and BOD at a later time. In the second case, uncertainty in water depth is propagated through a hydraulic routing model to derive an estimate of uncertainty in the width of a flood-plain of a hypothetical river.

For the current study, the goal is to estimate uncertainty in the position of a detection level contour, or equivalently, to estimate uncertainty in the predicted concentration as a function of position. The variance in the unknown parameters and the distance and direction from existing monitoring wells are used in the analysis. The model describing the system is developed as follows. From the monitoring data available at a given stage in the network evolution, the flow and transport parameters are estimated using the simplex algorithm (*Nelder and Mead*, 1965). These parameters specify a model that can be used to predict the level of contamination anywhere in the flow domain, in particular the position of the detection level contour can be found in various locations. Presumably, the estimates of this contour are better when a well location is close to the concentration contour of interest; the estimates should degrade as the distance

away from control data increases. A functional relationship describing this prediction process can be written:

$$\log_{10}(C_{dl}) \;=\; f\left(\log_{10}(C_{obs}),\, \vec{a},\, \vec{r}\right) \qquad 3.9$$

where:

C_{dl} is the detection level concentration

C_{obs} is the observed concentration at the nearest monitoring well

$\vec{a}$ is a parameter vector that describes the transport model

and

$\vec{r}$ is the displacement vector from the monitoring well to the C_{dl} contour

The function f describes the decay of the magnitude of the solute concentration moving towards the C_{dl} contour from a monitoring well. In this expression, C_{obs} and the parameters in the vector $\vec{a}$ are taken to be random variables while $\vec{r}$ is considered to be deterministic. The variance in the prediction of the C_{dl} contour can now be approximated following *Benjamin and Cornell* (1970) as:

$$\mathrm{Var}[\log_{10}(C_{dl})] \;\approx\; \sum_{i=1}^{n}\sum_{j=1}^{n} \frac{\partial f}{\partial x_i}\Big|_{\overline{x}_i} \frac{\partial f}{\partial x_j}\Big|_{\overline{x}_j} V[x_i, x_j] \qquad 3.10$$

The overbar notation indicates that the partial derivatives are evaluated at the mean value of the parameters in question. In Equation 3.10 $\vec{x}$ is a vector containing the random parameters, (C_{obs} and $\vec{a}$) while n is the number of

parameters. The variance of C_{obs} is taken as the variance of the additive noise that was originally applied to the data. In general, the covariance matrix $V[\vec{x}]$ is not explicitly available and must be estimated from the model.

Fisher (1956) developed a method for estimating the covariance matrix from what he called the information matrix. *Box and Jenkins* (1976) presented a lucid description of the procedure, which is closely followed here. $S(\vec{x})$ is defined as the sum of squares function which describes the degree of fit between the observed data and that predicted by the model in a least squares sense. The covariance matrix can be written as:

$$\mathrm{V}[\vec{x}] \approx \{ -\mathrm{E}[l_{ij}] \}^{-1} \qquad 3.11$$

where $\mathrm{E}[l_{ij}]$ is the expectation operation taken over the log likelihood of the model. The elements of l_{ij} can be approximated as:

$$l_{ij} \approx -\frac{Sij}{2\sigma_a^2} \qquad 3.12$$

where

$$\mathrm{S}_{ij} = \frac{\partial^2 S(\vec{x})}{\partial x_i \, \partial \mathrm{x}_j} \qquad 3.13$$

and σ_a^2 is the residual variance, unexplained by the model.

Combining these equations gives:

$$\mathrm{V}(\vec{x}) \approx 2\,\sigma_a^2 \{S_{ij}\}^{-1} \qquad 3.14$$

For example the expression for a 2 parameter model is,

$$V(\vec{x}) \approx 2\,\sigma_a^2 \begin{bmatrix} \frac{\partial^2 S(\vec{x})}{\partial x_1^2} & \frac{\partial^2 S(\vec{x})}{\partial x_1 \partial x_2} \\ \frac{\partial^2 S(\vec{x})}{\partial x_1 \partial x_2} & \frac{\partial^2 S(\vec{x})}{\partial x_2^2} \end{bmatrix}^{-1} \qquad 3.15$$

An estimate of the model variance is,

$$\sigma_a^2 = S(\hat{\vec{x}})/n \qquad 3.16$$

The partial derivatives in Equation 3.15 were numerically approximated using a central difference approach. The matrix was inverted using a LU decomposition algorithm from *Press, et al.* (1986).

The information matrix describes the curvature of the objective function at the location defined by the optimal parameters. High curvature for a given combination of parameters implies sensitivity to those parameters and thus a relatively high variance.

Error propagation is used to position wells sequentially in the following way. The existing monitoring data at a given stage of the network is used to estimate the flow and transport parameters. The position of the detection level contour is then calculated at 10 degree increments using the estimated parameters. The variance of each parameter is estimated from the Fisher information matrix. Finally,

parameter variances are propagated into estimates of uncertainty of the position of the detection level contour using error propagation. Areas on the contour with high uncertainty are poorly controlled and thus represent good locations for subsequent monitoring wells.

3.5.2 Fourier Domain Shape Analysis

Fourier domain shape analysis provides a framework for conveniently describing the extent of a contaminant plume, in terms of a specified detection level contour for a given contaminant. Additionally, the variance of the estimated position of the contour can be estimated, which provides a mechanism for selecting the position of subsequent wells. Shape analysis using Fourier techniques has been used successfully in other fields including electrical engineering, meteorology, chemical engineering and material science (see, for example, *Zahn and Roskies*, 1972; *Chandrasekar et al.*, 1990; *Beddow and Meloy*, 1980; *Luerkens et al.*, 1982). The methodology has recently been applied in hydrology by *Kumar and Foufoula-Georgiou*, [1990] for describing the boundary of irregular storms. The method relies on a parametric representation of the boundary of a shape which is then expanded in a Fourier series. Three different parametric representations can be used to describe various curves. These are the complex plane method (*Persoon and Fu*, 1977), the angular direction method (*Zahn and Roskies*, 1972) and the polar coordinate method (*Kumar and Foufoula-Georgiou*, 1990). While each method has advantages, the polar coordinate method is clearest conceptually and is outlined below.

Plume contours are typically plotted and dealt with in map view, i.e. in a cartesian coordinate system. These same data can be transformed into polar coordinates using a suitable origin, for instance the centroid of the plume (see Figure 2). A function describing the polar coordinate form of a closed curve is $R(\theta)$ where R, the radius, is a single-valued function of θ. This can be expanded in an infinite Fourier series:

$$R(\theta) = a_o + \sum_{n=1}^{\infty} (a_n \cos n\theta + b_n \sin n\theta) \qquad 3.17$$

where a_n and b_n are the n^{th} coefficients for the harmonics of the Fourier series expansion of $R(\theta)$. The function $R(\theta)$ is a periodic function with period 2π defined by a finite number of (R, θ) pairs corresponding to sampled locations on the plume. The goal is to use a Fourier series expansion to fit a function through those points that adequately describes the plume (Figure 2a). Since a finite number of points are available, the infinite Fourier series given in Equation 3.17 will be replaced by a finite approximation for $2\,N$ points:

$$R(\theta) = \frac{A_o}{2} + \sum_{n=1}^{N-1} (A_n \cos n\theta + B_n \sin n\theta) + \frac{A_N}{2} \cos N\theta \qquad 3.18$$

The coefficients A_n and B_n are determined from the following relationships:

$$A_n = \frac{1}{N} \sum_{p=1}^{2N-1} R(\theta_p) \cos n\theta_p \qquad 3.19$$

$$B_n = \frac{1}{N} \sum_{p=1}^{2N-1} R(\theta_p) \sin n\theta_p \qquad 3.20$$

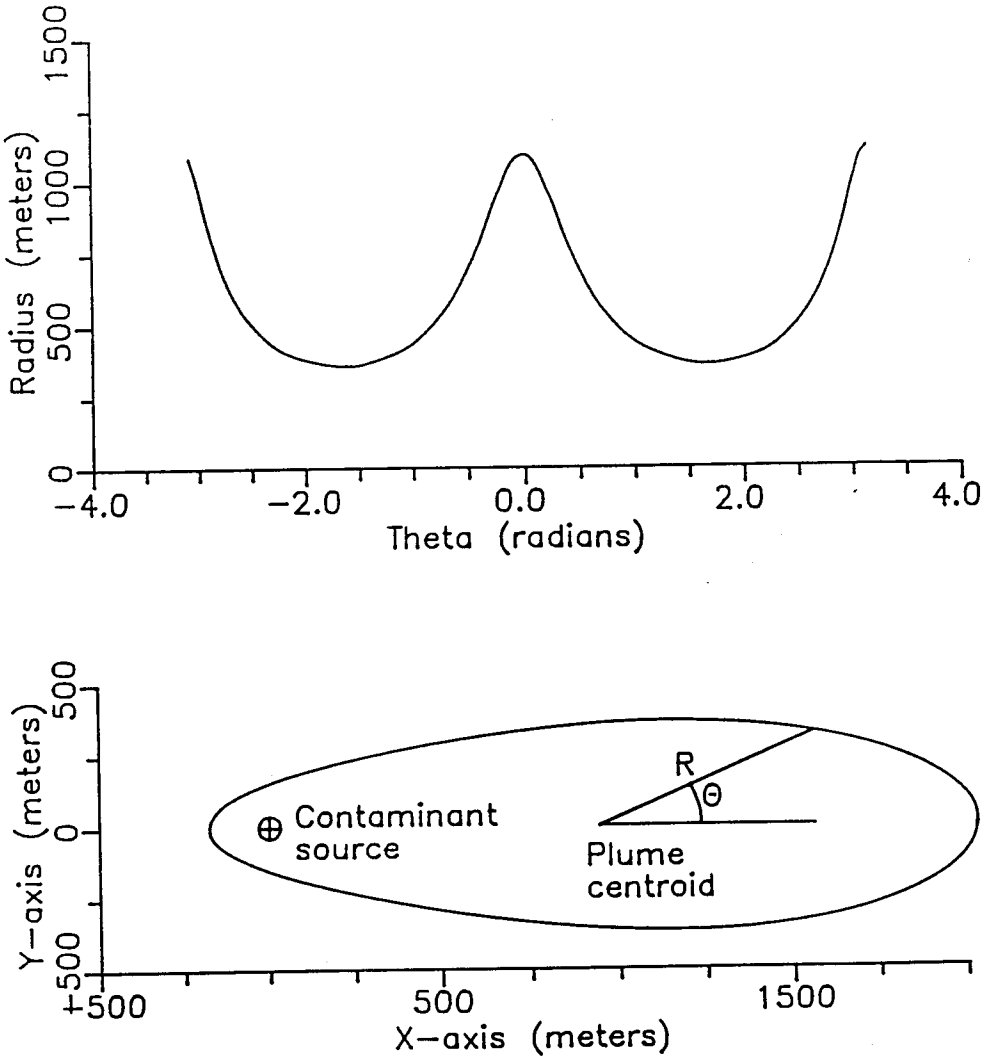

Figure 2) Cartesian representation of a contaminant plume (bottom), and its polar coordinate representation (top).

Given R sampled at equal intervals of θ, Equations 3.19 and 3.20 would usually be solved with a Fast Fourier Transform (FFT) routine. However, for contaminant transport applications θ will not necessarily be specified on equal increments, and an alternate method must be used to solve for the A_n and B_n coefficients.

The solution to Equation 3.17 can be approached using least squares estimation methods (*Lawson and Hanson*, 1974). In this context, the goal is to find the coefficients A_n and B_n that minimize the sum of the squared errors between the observed R's and the estimated $\hat{R}$. In matrix notation, Equation 3.17 can be written:

$$\vec{\hat{R}} = X\,\vec{\beta} \qquad 3.21$$

where $\vec{\hat{R}}$, is an (nx1) column vector of estimated radii, X is an (nxm) matrix containing sine and cosine terms evaluated at θ_i , and $\vec{\beta}$ is an (mx1) column vector of unknown coefficients. Equation 3.21 can be solved using standard techniques for least squares analysis to give an estimate for the coefficients,

$$\vec{\beta} = (X^{T}X)^{-1}X^{T}\vec{R} \qquad 3.22$$

A benefit of solving for the unknown coefficients using regression theory is that the variance of the response variable (estimates of R), can be estimated for a given input matrix X, e.g., (*Milton and Arnold*, 1986). If $\vec{x_o}$ is a vector containing the predictor variables of interest, the variance of any estimate $\vec{\hat{R}}$ can be written:

$$\mathrm{Var}(\hat{R}|\,\vec{x_o}) = \sigma^2\,\vec{x_o}^{T}\,(\mathbf{X}^{T}\,\mathbf{X})^{-1}\,\vec{x_o} \qquad 3.23$$

The variance of the model σ^2, is unknown but can be estimated from the sum of the squared residuals (SSE), between the observed and predicted data. An unbiased estimator can be written,

$$\hat{\sigma} = S^2 = SSE/(n-m-1) \qquad 3.24$$

Equation 3.24 can be used to provide confidence bounds for a given contour and in a procedure to locate the position on a contour with the largest variance.

3.6 Aquifer Remediation- capture zone analysis

Currently, the most prevalent treatment method for contaminated aquifers is referred to as pump and treat. The objective of this type of system is to extract the contaminated water using one or more pumps and treat the water in a surface installation. The treated water is then reinjected into the aquifer, released to a body of surface water or introduced into a municipal waste water system. The design of such a treatment system depends on a number of factors, most of which can not be controlled by the designers. Of particular importance is the volume of contaminated groundwater which directly controls the size of the treatment plant. The local hydraulic gradient is also important since the total drawdown created by the ensemble of wells should be sufficient to completely contain the plume. If this condition is not met, the plume will continue to expand regardless of the duration of the remedial efforts. Hydrogeology must also be taken into consideration, heterogeneities may create preferential pathways for groundwater flow or conversely, the aquifer may be too impermeable to support a sustained pumping program and alternatives such as trenches must be considered. The

chemical nature of the contaminant determines the specific nature of the surface treatment facility including, which components are necessary, and the treatment rate and required retention time in the system. Additionally, corrosive fluids may require the use of nonreactive components like PVC or stainless steel.

For the extraction system in particular, the main design issues are the number, location, and pumping rates of the wells. If hydraulic gradient control is used as the primary criteria, capture zone analysis as described by *Javandel and Tsang* [1986] can be used to design the remedial extraction system for simple aquifers (uniform flow, heterogeneous properties, infinite flow domain); with extraction wells only (injection wells must be dealt with using more sophisticated methods). Capture zone analysis can also be used to obtain an order of magnitude solution for sites that do not exactly adhere to the assumptions of the model.

Capture zone analysis is based on the application of complex potential theory for a homogeneous, isotropic aquifer with a uniform thickness. The goal is to create an area within the aquifer where the drawdown, induced by a system of pumps, encloses the contaminant plume as shown in Figure 3. Starting with a single extraction well, the pumping rate is specified based on the width of the plume, thickness and porosity of the aquifer, and the flow direction and steady-state velocity of the regional flow field. The down-gradient edge of the plume must also be specified since the wells are positioned a specified distance up-gradient from that point. Type curves for various combinations of flow velocity and aquifer thickness given by Javandel and Tsang are used to specify the pumping rate. However, Equation 1 of *Javandel and Tsang* [1986] can be manipulated to allow direct solution for the well discharge rate, Q.

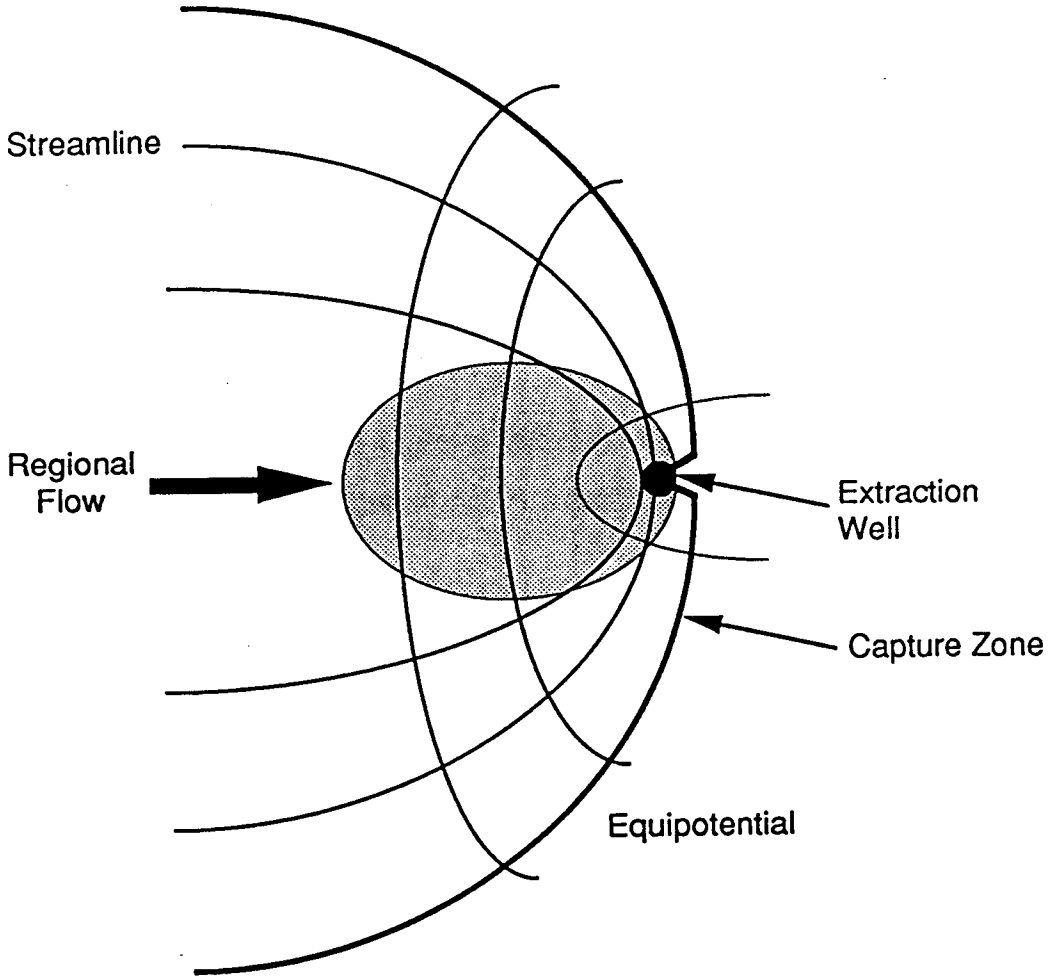

Figure 3) Illustration of the capture-zone for a contaminant plume, after Greenwald and Gorelick [1989].

While the flow obtained using the single well solution may theoretically remediate the aquifer, physical constraints imposed by pump capacities or allowable drawdowns may make this solution untenable. If an (arbitrary for this study) maximum flow rate is exceeded, the algorithm proceeds to a multiple well solution. Two and three well remedial strategies that position extraction wells on a line perpendicular to the regional flow, near the down-gradient edge of the plume, are also presented by *Javandel and Tsang* [1986]. The solution of the multiple-well problem was given in type-curve format which was not convenient for computer implementation. Instead, the relevant equations were solved using Gauss Siedel iteration to obtain the flow for each well and the distance between the extraction wells as follows: Equation 9 in the subject paper was solved for d, which is one-half of the distance between the pumping wells, to give:

$$d \leq \frac{Q}{\pi b V} \tag{3.25}$$

where b is the aquifer thickness and V is the seepage velocity. The pumping rate Q was determined by rewriting Javandel and Tsang's equation 10 as follows:

$$Q = \frac{bVY}{\left[1 - \frac{1}{2\pi}\left\{\tan^{-1}\left(\frac{y-d}{x}\right) + \tan^{-1}\left(\frac{y+d}{x}\right)\right\}\right]} \tag{3.26}$$

The value of Q obtained from the single well solution was used as an initial estimate in Equation 3.25 to solve for d; this value is then used in Equation 3.26 to solve for Q. The process is repeated until the change in Q is small between successive iterations. If the flow rate is still too large, the algorithm installs a third well such that all three wells are on a line perpendicular to the flow

direction, symmetrically spaced about the main axis of the plume. As with the two well case, the well spacing and flow for each well are also obtained using the Gauss Siedel method. Although the method can be generalized for additional wells, only the 1, 2 or 3 well solutions were used in this study. If the flow for the three well solution was still above the specified maximum, it was set equal to that maximum to avoid unrealistically high pumping volumes. In these cases, it is to be expected that the inability to remediate the inferred plume with three or fewer wells will be reflected by reduction of the remedial effectiveness. However, the position(s) and well discharge rates are established based on estimates of the down-gradient edge and width of the plume and the appropriate flow parameters.

3.7 Remedial Effectiveness

A particle tracking scheme, suggested by *Greenwald and Gorelick* [1989] for estimating the remedial effectiveness of an extraction system was used for the same purpose in this study. A computer model developed by *Javandal, et al.,* [1984] called RESSQ is capable of tracking particles under steady-state pumping conditions though a constant-thickness two-dimensional aquifer. Streamlines initiated from 18 points on each of 4 contours on the true plume were tracked from their starting locations for a maximum of 15 years. Streamlines that reached one of the extraction wells within this time limit corresponded to portions of the plume that would be remediated by the extraction system. Streamlines that did not reach the extraction wells, either because the wells were mispositioned relative to the actual plume or because the flow rate designed for the wells was inadequate, correspond to portions of the plume that were unremediated by the extraction system.

The extraction wells may be poorly located with respect to the plume because of a poor estimate of the true plume geometry. In this situation, the capture zone created by the extraction wells may not fully enclose the plume and some contaminant may escape down-gradient, carried by the regional flow field. In this situation, a numerical integration is performed over the unremediated portion of the plume and the ratio of this volume of contaminant to the total volume of contaminant is calculated. In an actual site remediation one would be unsure of the total contaminant mass. Therefore it would not generally be possible to estimate the fraction of mass that was remediated. However, the unremediated mass could become significant if it reached a compliance surface after the remedial program was supposed to have been completed. Three measures of remedial effectiveness are used in this report to gauge the monitoring networks.

The first measure is remedial duration. As discussed in *Geenwald and Gorelick* [1989] and *Lefkoff and Gorelick* [1986] the duration of a remedial action can be of importance in aquifer restoration for several reasons. First, the anticipated duration of a site remediation is a key element in a present-value cost estimate for a project. Secondly, legal or policy requirements may stipulate a maximum allowable remedial period. The performance measure used for the simulations in this report was the simulated remedial duration normalized by the nominal remedial period (the time required to remediate the plume in the case where the plume was known exactly).

The second measure of remedial effectiveness is the ratio of mass that is remediated, M_r to the total contaminant mass M_t. The total mass is known from the input data, while the portion of the plume that is remediated is obtained by

numerical integration. The integral is calculated by overlaying a rectangular grid onto a polygon defined by the portion of the plume that is unremediated. An algorithm which specifies whether a grid node is within or on the polygon (Hacker, 1962; Shimrat, 1962) is then used to determine which cells contribute to the sum. Figure 4 shows a portion of a plume that is unremediated, bounded by the C_1 and C_2 contours, with a grid overlay. Nodes at the center of each grid cell are checked to see where they fall with respect to the polygon. The circles are representative nodes showing three possibilities. The concentration value for nodes located within the polygon (solid circles) contribute to the integral. Nodes located outside the polygon (open circles) do not contribute to the integral. Finally, nodes that happen to fall on a vertex of the polygon or along one of its edges are assigned a value of 1/2 of the concentration at that node (half-filled circles).

The final measure of remedial effectiveness used in this study is based on the total volume of contaminated water that must be treated during remediation. Treatment volume (V_t) is simply the product of the number of extraction wells, the pumping rate per well and the treatment period. A normalized treatment volume is formed by dividing the volume of water treated in each experiment by the total volume of contaminated water.

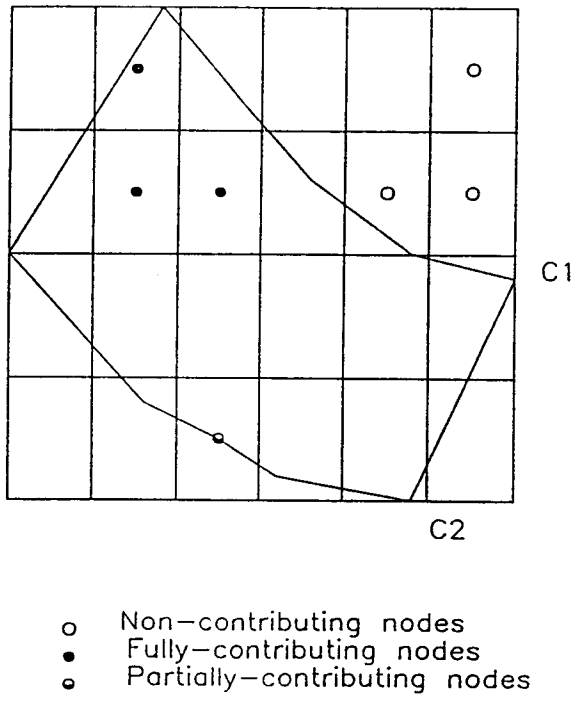

Figure 4) Integration graticule for estimating remedial effectiveness.

CHAPTER 4: SIMULATION RESULTS

In this chapter, the computer simulations made with the program DEMON are detailed. As described in Chapter 3, and shown schematically in Figure 1, the model must be initiated with a known plume. The truth model used for this report was patterned after a hazardous waste site described by *Wilson and Miller*, [1978]. That site was an aircraft plant in New Jersey where approximately 24 kg/day of chromium was discharged into waste pits between 1942 and 1949. The pits directly overlaid a thick porous aquifer and the chromium entered the aquifer and spread with the regional groundwater flow some 1200 meters down-gradient where the aquifer intersected a stream. The average porosity of the aquifer was 35 percent with a saturated thickness of 34 meters. Other characteristics of the aquifer that were reported in the *Wilson and Miller* [1978] study are summarized in Table 1.

4.1 Random network design

A sequence of simulations using randomly installed monitoring wells were used as a base case for comparison purposes. These computer runs provide a standard against which the results from the iterative network design algorithms, presented later in this chapter, can be judged. In the preliminary tests, a number of wells were randomly positioned within a window surrounding the contaminant source and error-corrupted contaminant concentration measurements were simulated. Flow and transport parameters were estimated from the concentrations and a

Table 1) Model parameters and allowable ranges for optimization routine

Parameter	Symbol	Default	Minimum	Maximum	Units
Longitudinal dispersivity	(D_x)	21.3	5.0	40.0	m
Ratio of longitudinal to lateral dispersivity	(D_x/D_y)	5.0	2.0	10.0	—
Seepage velocity	(V)	0.46	0.10	1.0	m day^{-1}
Source strength	(f_m)	0.72	0.20	1.5	kg day^{-1} m^{-1}
Flow azimuth	(θ)	0.0	$-20.$	20.	degrees
Porosity*	(η)	0.35	—	—	—
Contamination period*	(T_c)	7.7	—	—	years
Aquifer thickness*	(b)	33.	—	—	m
Retardation factor*	(R_d)	1.0	—	—	—
Source location*	$(x_o\ ,\ y_o)$	(0,0)	—	—	(m,m)

* Note: these parameters were assumed to be known exactly.

remedial extraction system was designed based on a plume consistent with those parameters. The extraction system was then used to remediate the true plume. Finally, the effectiveness of the remediation was evaluated.

Two hundred Monte Carlo iterations of this experiment, for a given number of monitoring wells in the network, and a given level of measurement error, provide solutions that represent possible outcomes under different patterns of randomly located wells and with different random measurement errors. Taken together, these data were used to evaluate the performance of different network design strategies. Table 2 shows the combinations of networks sizes (N_{mw}) and measurement error levels (σ_c) that were used for the random well positioning experiments as well as for the subsequent network designs.

Table 2. Trial values for N_{mw} and σ_c

N_{mw}	8	10	12	15	
σ_c	0.00	0.25	0.50	0.75	1.0

As described in Section 3.7, three measures of remedial effectiveness were used to evaluate each remedial strategy. Each measure was referenced to an optimal remediation, as calculated when the plume parameters were assumed to be known exactly. In the optimal case, the plume was completely decontaminated in 8.4 years by three extraction wells. During that time, 10.5 million cubic meters of

water were extracted from the wells. This corresponds to 3.2 times the volume of water enclosed by the 10 $\mu g/l$ contour. Table 3 shows the number of trials, out of 200 experiments that led to extraction designs that did not remediate a significant portion of the plume within the (arbitrarily imposed) maximum remedial duration of 15 years. In Table 3 there is a general trend towards fewer failed remediations as the monitoring network is expanded. Deviations from this trend are probably related to the relatively small number of simulations (200). The 15 year time limit was imposed for computational reasons: streamlines that missed an extraction well would in theory travel forever within the two-dimensional, infinite model aquifer. From a practical standpoint, a real extraction system that failed to pump out any contaminant would also be terminated, although probably in less than 15 years.

Table 3) Number of non-remediations, out of 200, for the random well placement strategy.

		σ_c				
		0.00	0.25	0.50	0.75	1.00
N_{mw}	8	39	46	34	39	36
	10	39	35	42	32	40
	12	41	42	44	41	37
	15	35	34	35	27	26

The means and standard deviations for each of the three remedial measures resulting from the random network design experiments are shown in Table 4.

Table 4) Summary statistics for the random network design experiments (tabulated as mean/standard deviation).

a) Normalized remediation duration

		σ_c				
		0.00	0.25	0.50	0.75	1.00
N_{mw}	8	1.27/.36	1.28/.37	1.23/.36	1.22/.37	1.21/.36
	10	1.23/.36	1.24/.35	1.23/.36	1.21/.34	1.24/.38
	12	1.23/.35	1.25/.35	1.27/.36	1.24/.35	1.25/.36
	15	1.20/.34	1.19/.34	1.23/.34	1.22/.33	1.22/.34

b) Fraction of contaminant removed

		σ_c				
		0.00	0.25	0.50	0.75	1.00
N_{mw}	8	.722/.43	.705/.45	.765/.42	.745/.42	.784/.40
	10	.760/.42	.745/.43	.755/.42	.785/.40	.745/.42
	12	.735/.44	.737/.44	.714/.44	.747/.43	.756/.42
	15	.786/.40	.784/.41	.767/.42	.804/.39	.809/.39

c) Pore volumes treated

		σ_c				
		0.00	0.25	0.50	0.75	1.00
N_{mw}	8	4.80/2.2	4.78/2.2	4.51/2.2	4.38/2.3	4.30/2.3
	10	4.60/2.1	4.62/2.1	4.55/2.2	4.31/2.2	4.55/2.3
	12	4.59/2.0	4.70/2.1	4.74/2.2	4.63/2.1	4.74/2.2
	15	4.48/1.9	4.39/1.9	4.57/2.0	4.49/2.0	4.46/2.1

Figures 5a-c show the mean behavior of the remedial effectiveness measures as a function of the number of wells in the monitoring network. Figure 5a shows that the remedial duration declines as the networks are enlarged. Figure 5b shows that the average fraction of the contaminated mass that is removed by the extraction system rises as the number of wells increases. Figure 5c shows that as the networks are expanded the volume of water that must be treated declines (recall that 3.2 pore volumes is the optimal solution).

Figures 6, 7 and 8 show the cumulative distribution functions (CDF) for the 3 remedial measures for the random well placement simulations using 8, 10 and 15 monitoring wells, respectively, with σ_c=1.0. The top plot in each figure shows the distribution of treatment durations, normalized by the 8.4 year optimal solution. The middle plot in each figure shows the fraction of contaminant removed by the extraction system. Finally, the bottom plot on each figure shows the number of pore volumes that were extracted by each system. In the context of this experiment, an ideal monitoring network would determine the nature of the true plume for each realization of the experiment. In that case, each CDF would be horizontal with values of 1.0, 1.0 and 3.2, for the top, middle and bottom plots, respectively.

Differences between Figures 6, 7 and 8 are related to the statistical power of larger networks. First, the fraction of mass that was removed increased as the number of monitoring wells was increased. Secondly, the pore volume approached the optimal solution of 3.2 pore volumes for a larger percentage of the solutions as the

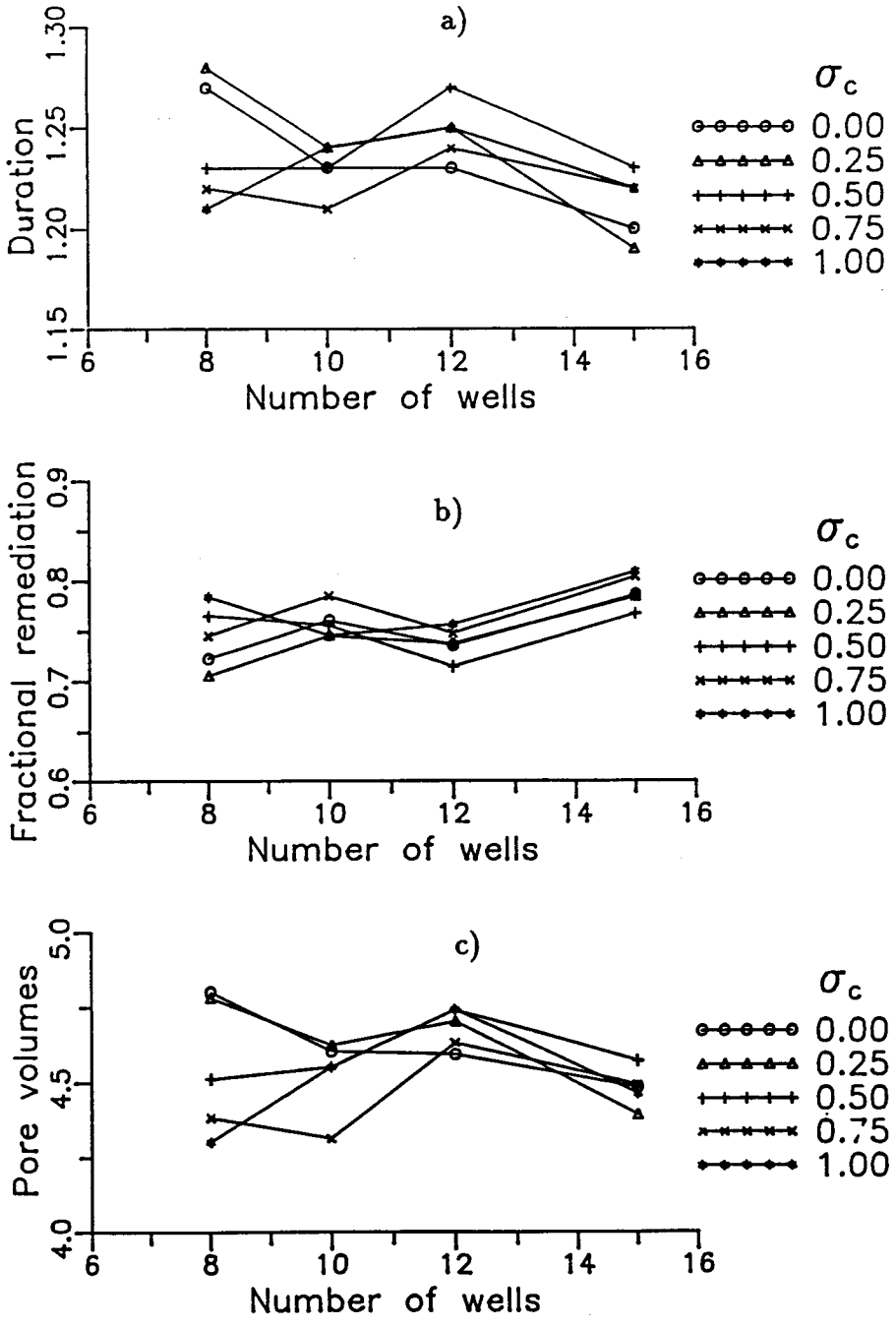

Figure 5) Mean remedial effectiveness as a function of network size (random network design).

number of wells was increased (the bottom curve in each figure became more horizontal when the number of wells was increased).

4.2 Network design using error propagation

The first network design method tested in this study that used existing data to control the position of subsequent wells in an iterative mode used the error propagation method as outlined in Section 3.5.1. The experiments performed for this portion of study were similar to those described in the previous section except for the following features. An initial array of 5 random wells was installed at the beginning of each Monte Carlo run. Measurements taken at these wells were used for parameter estimation and the covariance matrix $V[\vec{x}]$ of the parameters was calculated numerically and the uncertainty in the value of the $\log_{10}(C)$ (inferred from the current estimate of the flow and transport parameters) was estimated using first order error propagation. These estimates were made on the C_{dl} contour at 10 degree angular increments. The next monitoring well was then located on the contour where the uncertainty was the highest. Wells were added sequentially by repeating the above process until the allocated number of wells were installed in the network. The permutations of σ_c and N_{mw} that were used in the error propagation simulations are shown in Table 2.

Table 5 contains the number of computer runs that were unable to remediate any of the plume without violating the 15 year (T_{max}) constraint. The results shown in Table 5 are superior to those shown in Table 3. Also, the trend for fewer failures with larger networks is more apparent. A cursory comparison of Table 5

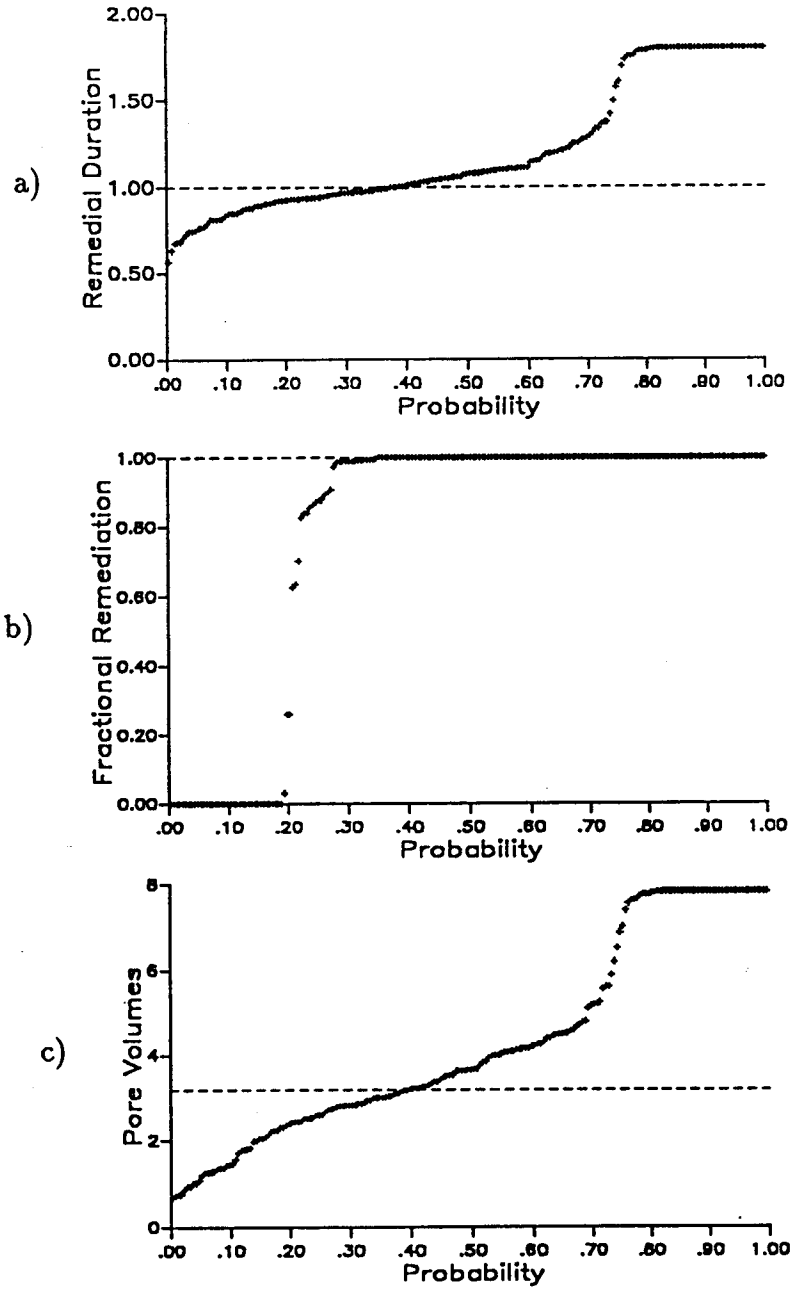

Figure 6) Cumulative distribution functions for 200 iterations, $\sigma_c = 1.00$, for 8 randomly positioned wells.

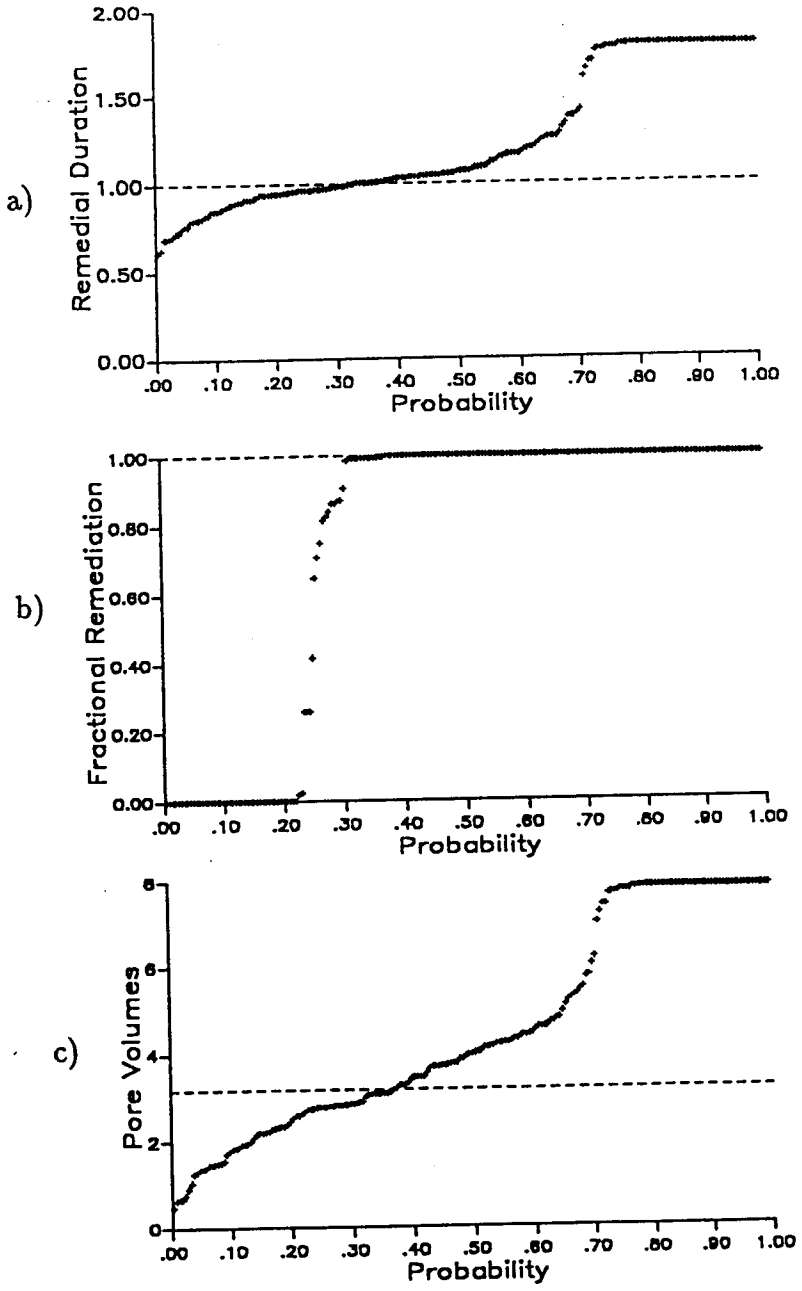

Figure 7) Cumulative distribution functions for 200 iterations, $\sigma_c = 1.00$, for 10 randomly positioned wells.

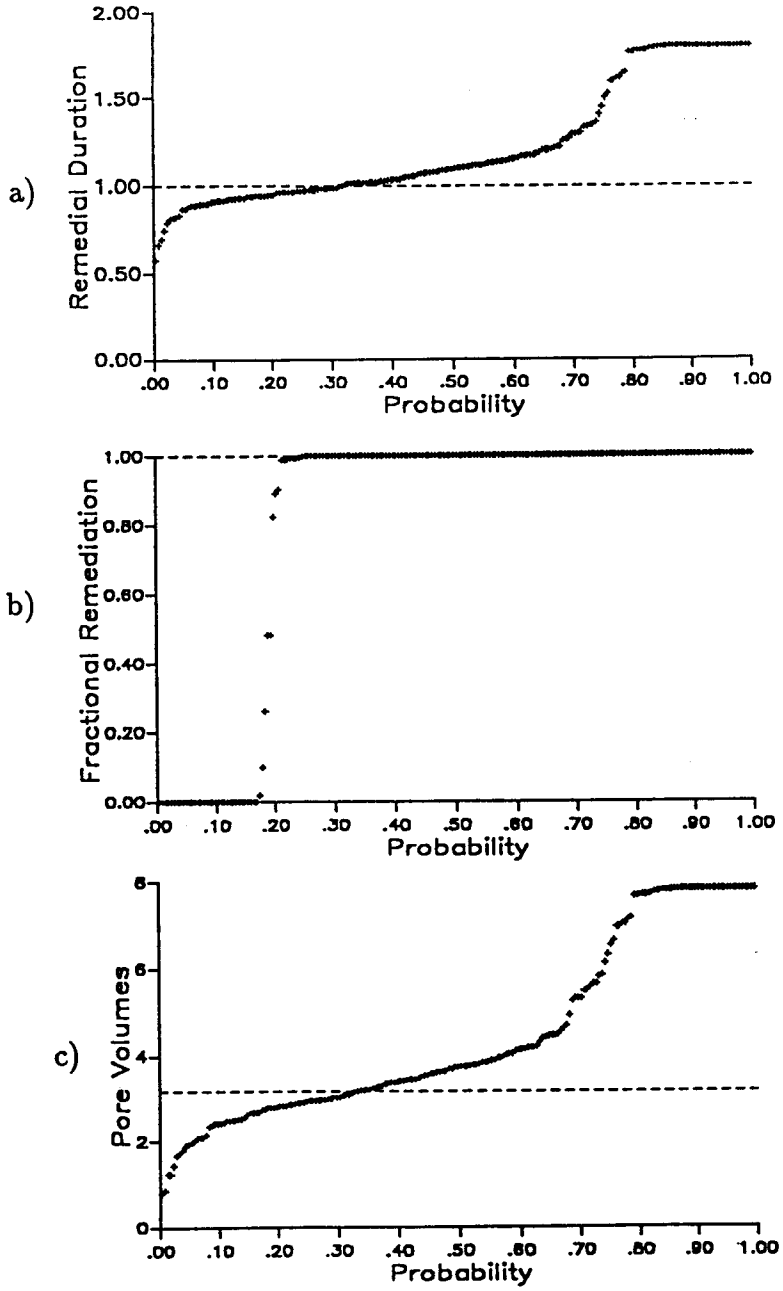

Figure 8) Cumulative distribution functions for 200 iterations, $\sigma_c = 1.00$. for 15 randomly positioned wells.

and Table 3 shows the superior effectiveness of the error propagation approach in eliminating solutions that were completely incapable of remediating the plume. This fact is especially striking for the larger networks. Consider for example, that nearly 16 percent of the 15 well random networks led to non-remediations while only 0.1 percent of the error propagation trials failed in this fashion.

Table 5) Number of non-remediations, out of 200, for networks designed using error propagation.

		σ_c				
		0.00	0.25	0.50	0.75	1.00
N_{mw}	8	5	3	8	10	13
	10	1	3	7	5	6
	12	1	3	1	4	4
	15	0	0	0	0	1

Figures 9, 10 and 11 are the CDFs for the 8, 10 and 15 well error propagation experiments. These plots comparable to Figures 6, 7 and 8 for the random networks. Figure 9 is generally similar to Figure 6 which implies that the first three wells installed using error propagation do not dramatically improve the remedial performance. For the 10 well simulations, improvements can be seen when Figure 10 is compared with Figure 7. Note for instance, that a greater number of the error propagation solutions led to 100 percent remediations while fewer realizations led to non-remediations. Also, a larger fraction of the both the remedial duration and pore volumes treated were near the optimal solutions of 1.0

and 3.2, respectively using error propagation. The results of the 15 well error propagation solution (Figure 11) were dramatically better than the 15 random well solution (Figure 8). Note for instance, how flat the remedial duration and pore volumes treated CDFs are in Figure 11.

The summary statistics for the error propagation experiments are given in Table 6. Again, the improvement over the random networks is clear both in the mean response and the smaller spread of the data, as shown by the standard deviation statistics. Figure 12 shows the mean response of the remedial effectiveness measures as a function of the number of wells in the network. The vertical axes are scaled the same as in Figure 5 but have been shifted. All three subplots in Figure 12 approach the optimal values of 1.0, 1.0 and 3.2 much better than did the equivalent plots on Figure 5.

4.2.1 Numerical considerations for error propagation

Numerical problems were occasionally encountered while inverting the information matrix to calculate the parameter covariance matrix in the error propagation routine. This occurred when one or more of the optimal parameters were located at either the upper or lower bounds as specified in Table 1. This behavior can be seen by studying plots of the sum of squares function ($S(\vec{x})$ from Section 3.5.1) in the neighborhood of the optimal solution as a function of two parameters at a time. Since there were five adjustable parameters in the model, 10 different contour maps could be generated for all combinations of these parameters.

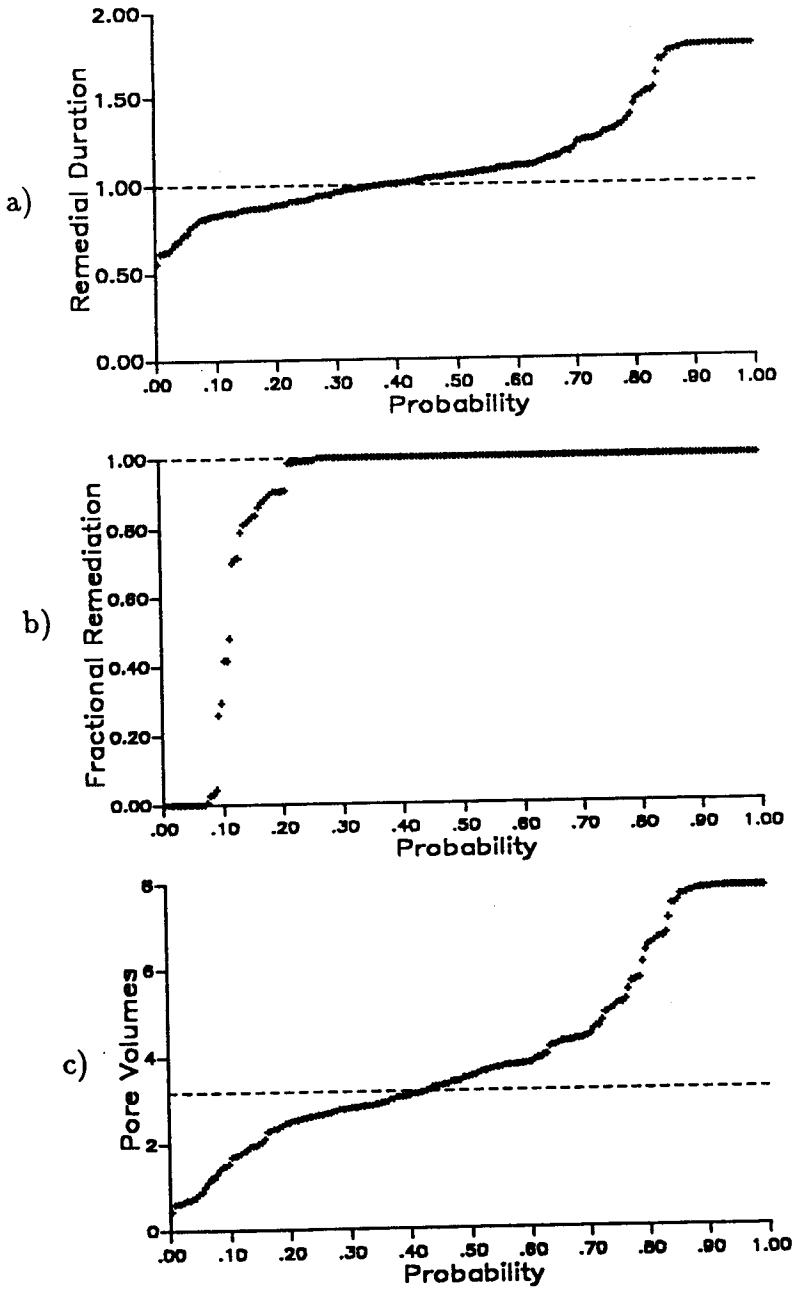

Figure 9) Cumulative distribution functions for 200 iterations, $\sigma_c = 1.00$, 8 well network designed using error propagation.

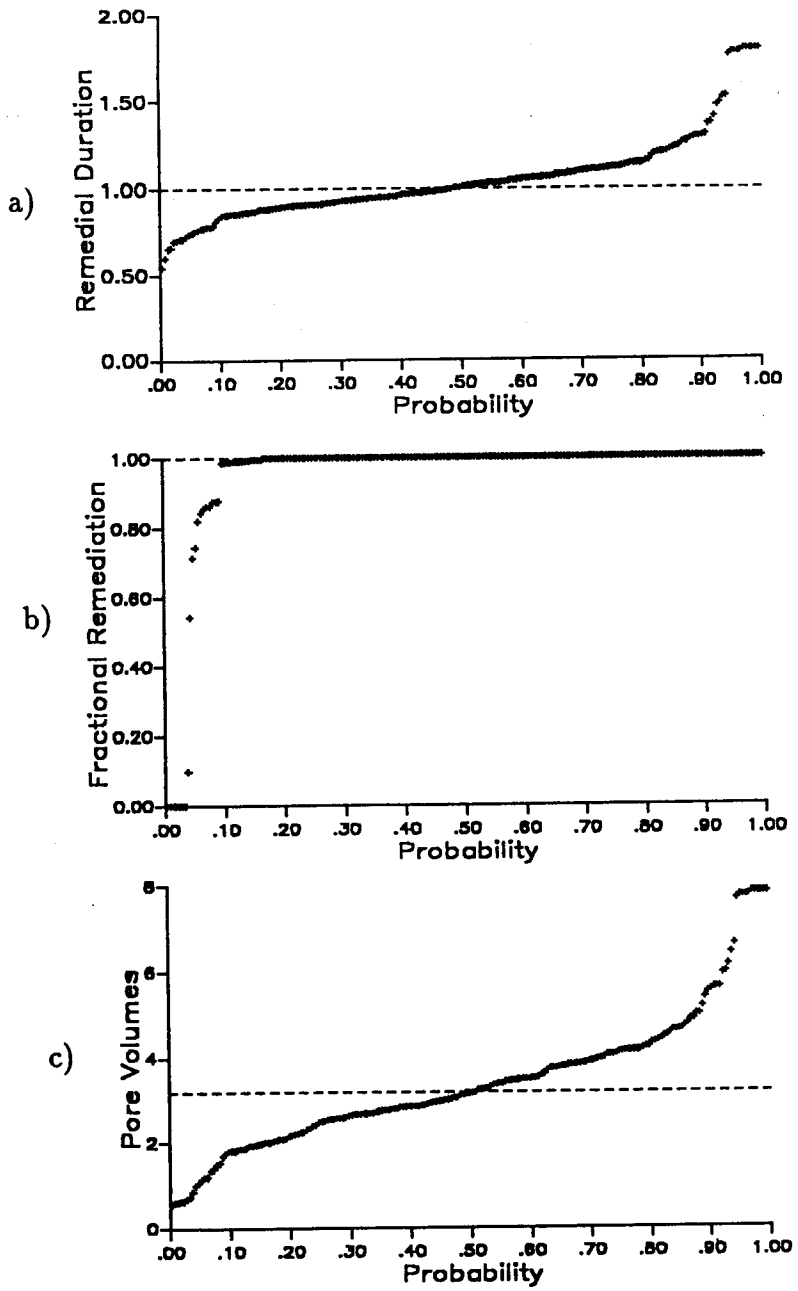

Figure 10) Cumulative distribution functions for 200 iterations, $\sigma_c = 1.00$, 10 well network designed using error propagation.

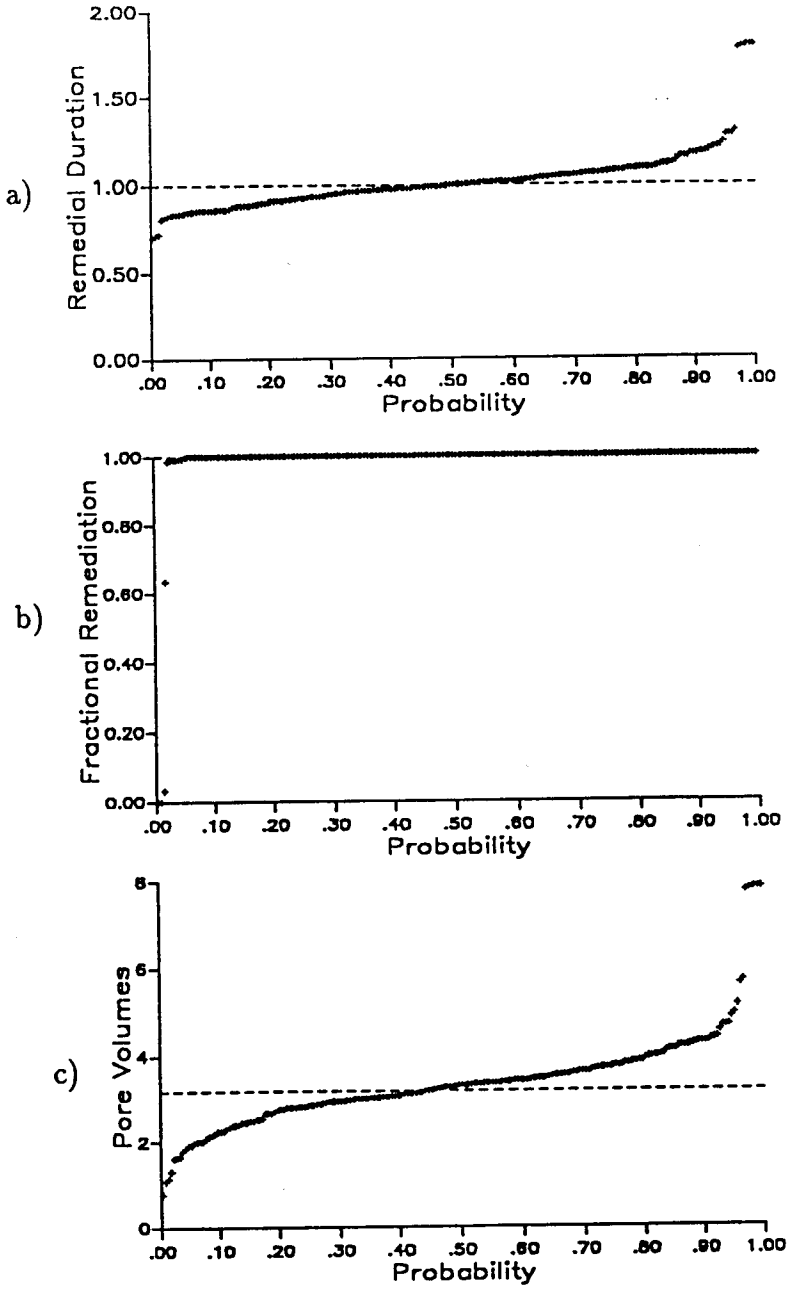

Figure 11) Cumulative distribution functions for 200 iterations, $\sigma_c = 1.00$, 15 well network designed using error propagation.

Table 6) Summary statistics for networks designed using error propagation (tabulated as mean/standard deviation).

a) Normalized remediation duration

		σ_c				
		0.00	0.25	0.50	0.75	1.00
N_{mw}	8	1.05/.19	1.07/.24	1.07/.27	1.12/.29	1.15/.33
	10	1.00/.08	1.03/.17	1.06/.24	1.03/.24	1.05/.24
	12	1.01/.08	1.02/.15	1.01/.18	1.06/.22	1.04/.24
	15	1.00/.01	.997/.10	1.00/.10	1.01/.14	1.02/.17

b) Fraction of contaminant removed

		σ_c				
		0.00	0.25	0.50	0.75	1.00
N_{mw}	8	.958/.18	.944/.21	.927/.24	.927/.24	.879/.30
	10	.994/.07	.975/.15	.950/.20	.948/.21	.949/.20
	12	.990/.10	.978/.14	.985/.10	.964/.17	.955/.18
	15	1.00/0.0	.994/.07	1.00/0.0	.996/.02	.983/.12

c) Pore volumes treated

		σ_c				
		0.00	0.25	0.50	0.75	1.00
N_{mw}	8	3.48/1.2	3.67/1.5	3.65/1.7	3.79/1.9	4.01/2.1
	10	3.38/.52	3.50/1.1	3.57/1.5	3.39/1.5	3.41/1.6
	12	3.42/.45	3.48/.93	3.39/1.2	3.53/1.4	3.36/1.6
	15	3.37/.01	3.35/.64	3.28/.68	3.24/1.0	3.37/1.1

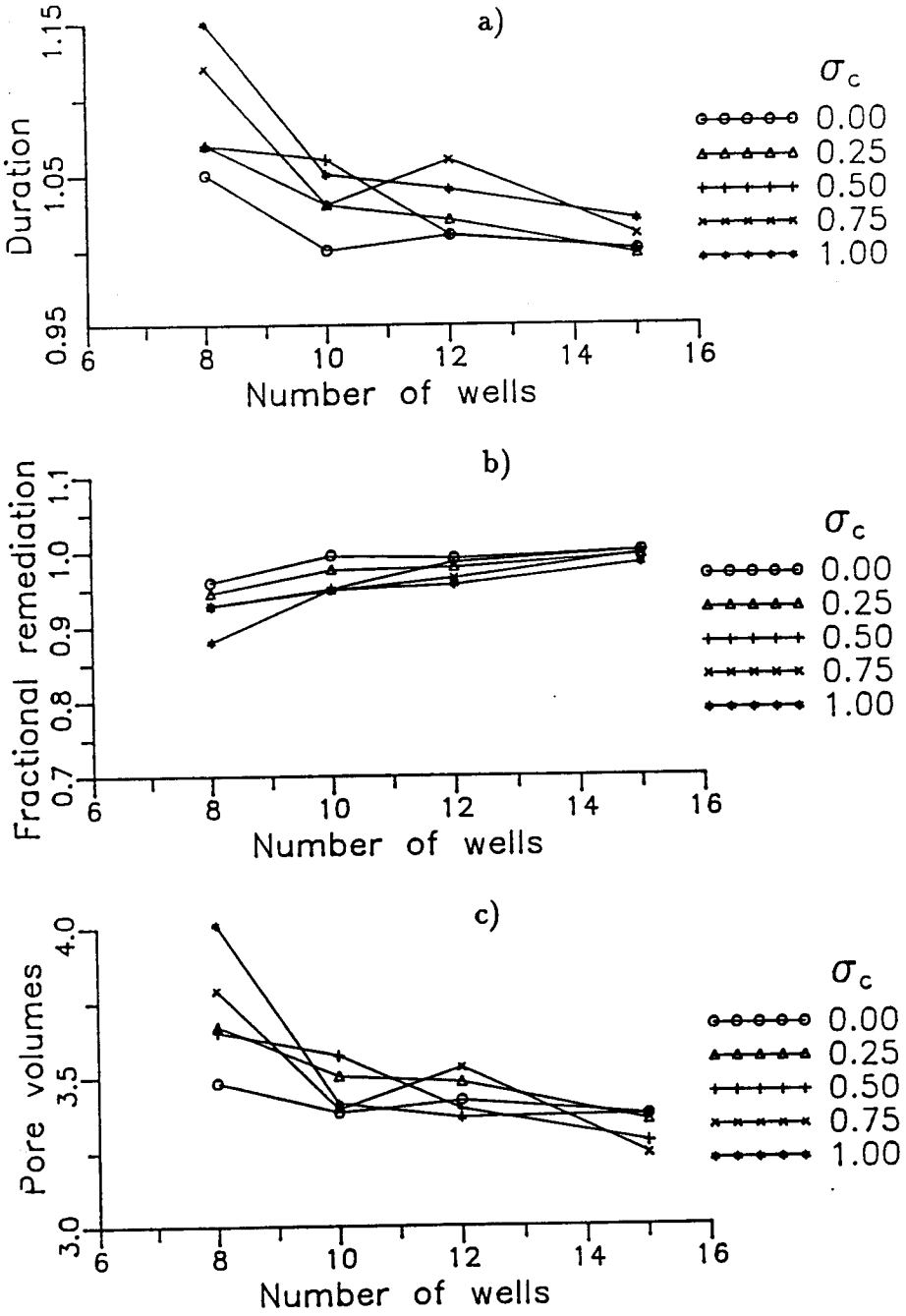

Figure 12) Mean remedial effectiveness as a function of network size, (networks designed using error propagation).

Figure 13 is an example of this type of plot showing flow velocity versus longitudinal dispersivity. The response surface has a minimum at the center of the plot corresponding to the true value of the parameters. On the left edge of the plot (for low flow velocities) the contours are nearly vertical and $S(\vec{x})$ is relatively insensitive to changes in longitudinal dispersivity. In this case, numerical derivatives of the response function with respect to these parameters are often unstable, which leads to elements of the information matrix that vary over several orders of magnitude. This in turn leads to instability in the matrix inversion process (Equation 3.11). In contrast, Figure 14 shows flow direction versus longitudinal dispersivity. Here, the response surface is symmetric with respect to the flow direction and is generally well behaved, i.e. the curvature of the surface varies slowly.

4.3 Network design using Fourier domain shape analysis

The Fourier domain shape analysis (FDSA) approach for plume estimation provided the greatest flexibility in terms of implemention, which proved to be both an advantage and a liability. In contrast to other fields where shape analysis has been applied to describe a curve, in contaminant hydrology it is highly unlikely that any reasonable number of monitoring wells will be located on the detection level (or any other) contour. Thus, standard techniques for estimating the spectrum of a function can not be readily applied.

In this study several implementations of FDSA were considered. The first method was applied in the following way. Five wells were installed randomly in a window

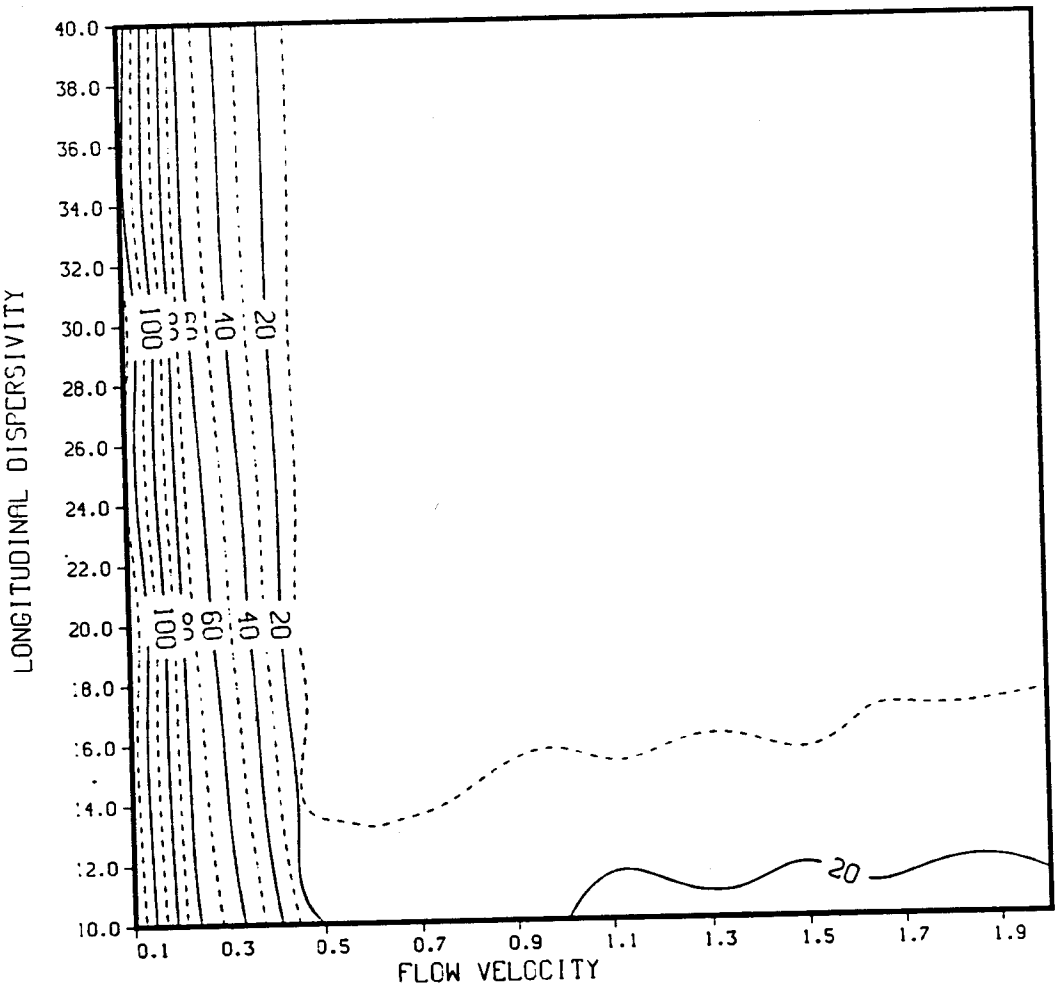

Figure 13) Variation in the residual sum of squares as a function of the velocity (x-axis) and longitudinal dispersivity (y-axis).

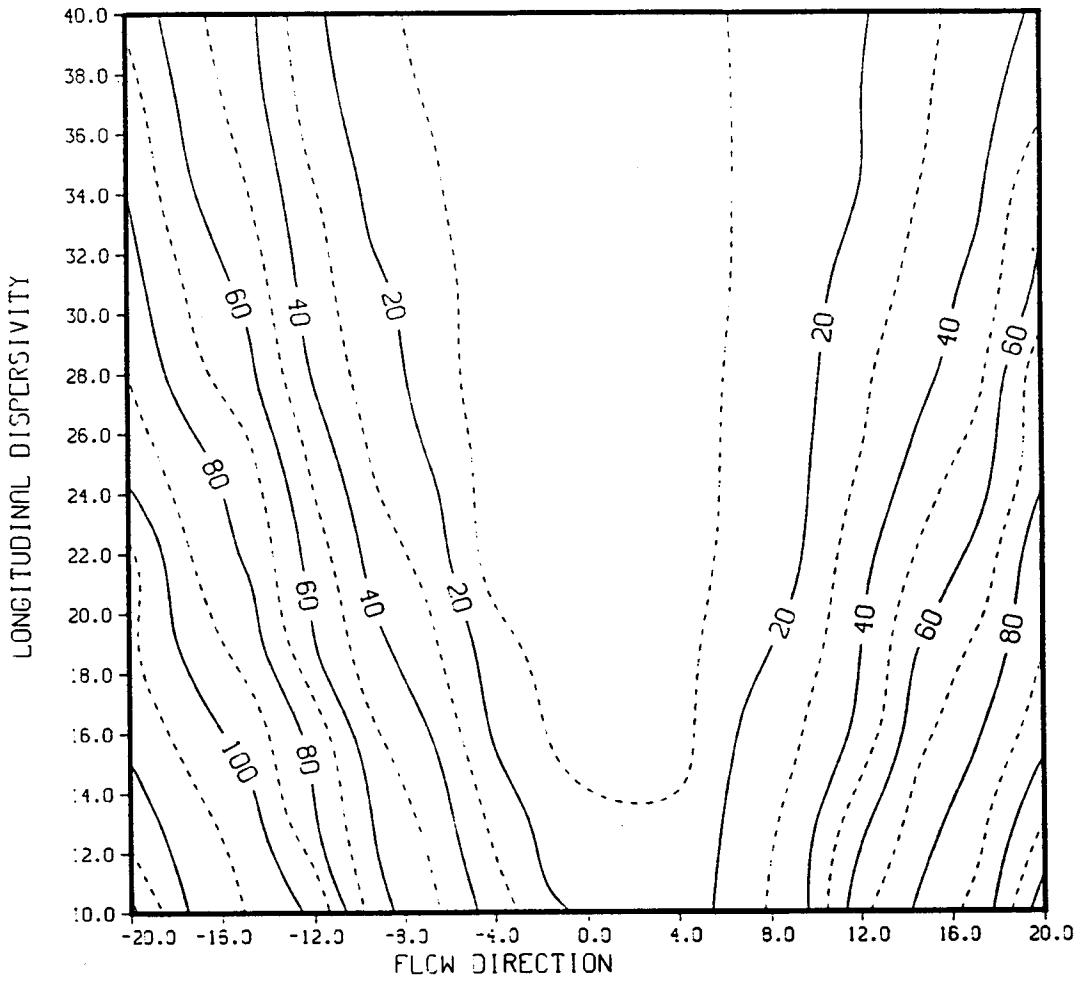

Figure 14) Variation in the residual sum of squares as a function of the flow direction (x-axis) and longitudinal dispersivity (y-axis).

around the contaminant source. Next, the Nelder-Mead algorithm was used to estimate the plume parameters by minimizing the sum of the squared differences between the logarithm of the observed concentrations and the concentrations calculated with the estimated parameters. Each existing monitoring well was extrapolated to the detection level contour in the direction with the highest concentration gradient. The centroid of these points was used as the origin for a polar coordinate transformation. Finally, a Fourier series was fit to the (R, θ) pairs in a least squares sense as described in Section 3.5.2. Confidence intervals on the modeled radii were then used as a criterion for positioning subsequent wells in the network.

The problem with this implementation is that the reconstructed radii tend to be highly oscillatory between the control points. Figure 15 is an example of this behavior, where an 11 term Fourier series was fit through 30 (R, θ) points (top plot). The model curve passes smoothly through the data points where the points are closely spaced. However, where the control is sparse (between 0 and 2 radians), the Fourier series produces a curve that does not resemble a typical plume geometry. This behavior was not acceptable and several alternative formulations for constraining the radii were investigated.

Gill, et al. [1984] describe a linearly constrained least squares optimization procedure for bounding either the parameters or a linear combination of the parameters in a least squares problem. The constraints can be posed either as statements of equality or inequality. In the context of this work, the constraints

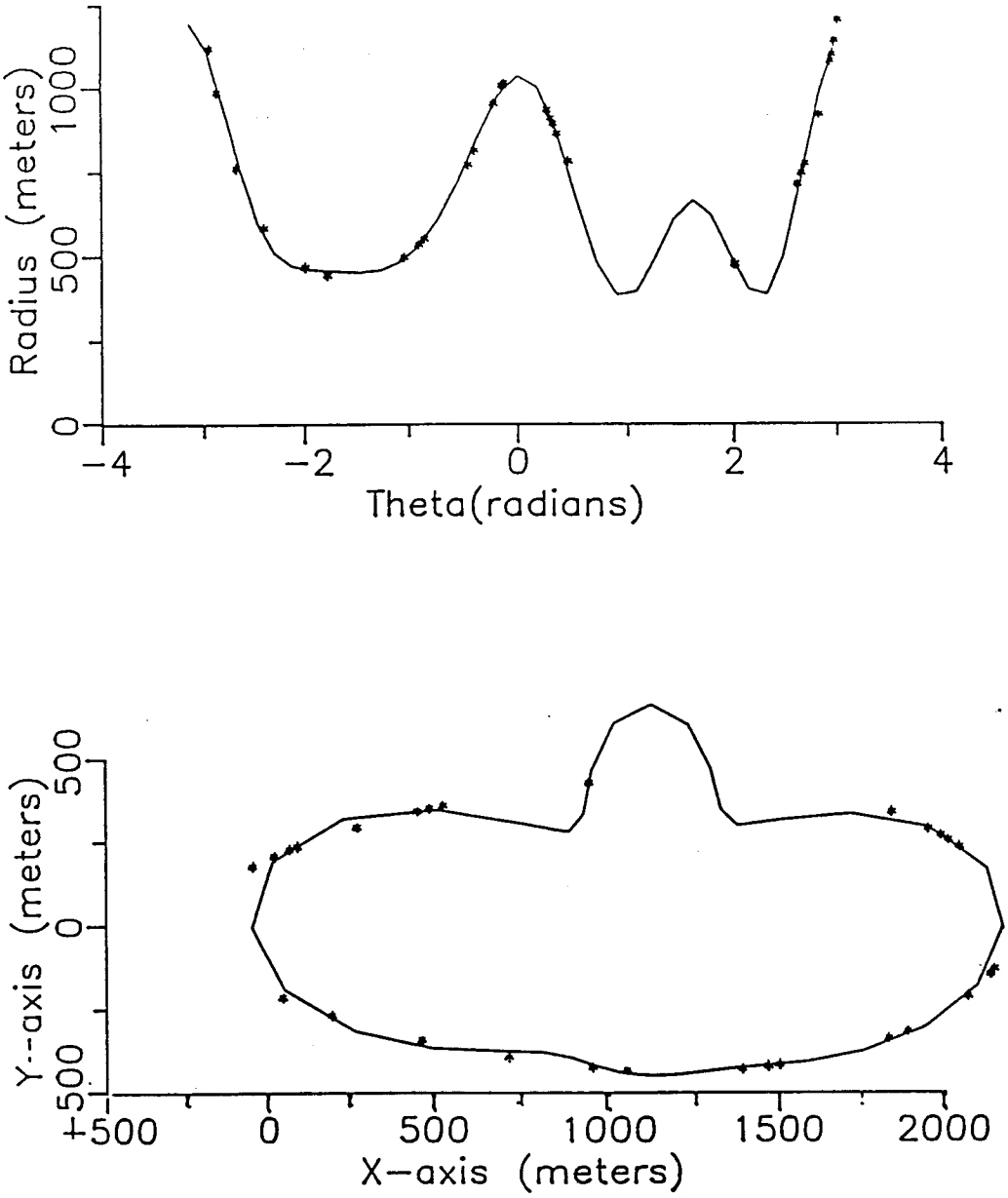

Figure 15) Polar coordinate (top) and cartesian (bottom) representations of a detection level contour using unconstrained FDSA.

maintaining continuous first and second derivatives (*Press, et al.,* 1986). The splined points are allowed to overshoot the observations, and do so occasionally (Figure 20a).

The cubic spline was incorporated in the design algorithm as follows. At a given stage in the network, the existing wells were extrapolated along the direction of maximum gradient and transformed to polar coordinates. A cubic spline was used to interpolate between these points on equal intervals and a Fourier series was fit to the splined points using least squares. A second pass of the least squares algorithm using the extrapolated data only was used to estimate confidence intervals for the splined FDSA contour at equal sample intervals. Next, a well was installed at the angle with the widest confidence bounds. This procedure was then repeated until the specified size of monitoring network was in place. Figure 20 shows an example on a splined contour fit with an 11 term Fourier series expansion and the derived confidence intervals. The relatively smooth nature of the plume boundary in Figure 20b compares favorably with the plume derived using a Fourier series without a cubic spline (Figure 15b).

Another approach that may improve the performance of the FDSA technique is to implement it in conjunction with error propagation. This was pursued by using error propagation to estimate the concentration variance at equal intervals on the detection level contour. Then, the inverse of these variances were used as weights in a standard least squares formulation. Thus, locations with high uncertainty would be down-weighted in the solution procedure. Weighted least squares is

particular phase in a monitoring program probably do not reflect actual extremes. In addition to estimates of radius as a function of angle, the least squares formulation was used to specify confidence intervals for these estimates. Thus, at any stage in the network, the poorest estimate was used as the location for the next well in the system.

As with the error propagation experiments, 5 wells were installed randomly and 8, 10, 12, and 15 well networks were constructed sequentially. This process was repeated 200 times for the levels of additive noise shown in Table 2. Figures 16, 17, and 18 show the CDFs for the 8, 10 and 15 well experiments for $\sigma_c = 1.00$, respectively. Several differences can be seen between these results and those from the previous two sets of experiments.

Table 7 shows the number of non-remediations that resulted from the FDSA experiments, while Table 8 summarizes the mean and standard deviations for each of the remedial effectiveness measures. Based on the number of non-remediations FDSA performed similarly to the random network for the 8, 10, and 12 well experiments. However, in the 15 well experiment there were only one half as many failures using FDSA as with the random network.

Figure 19 shows the mean remedial effectiveness measures as a function of the number of wells in the experimental networks. For the smaller (8, 10, 12) well networks the average remedial duration is relatively long while the fraction of mass that is remediated is low. There is a dramatic improvement is all three performance measures as the network is enlarged to 15 wells.

implemented by pre-multiplying each side of Equation 3.20 by a column vector containing the appropriate weighting constants.

Exploratory results using weighted least squares proved the method to be somewhat unstable. An examination of the weights showed that they occasionally varied by several orders of magnitude, especially for experiments with a high level of additive noise. This line of research was not pursued in great detail, but some form of robust weighting, using the rank of the variances for example, deserves further study.

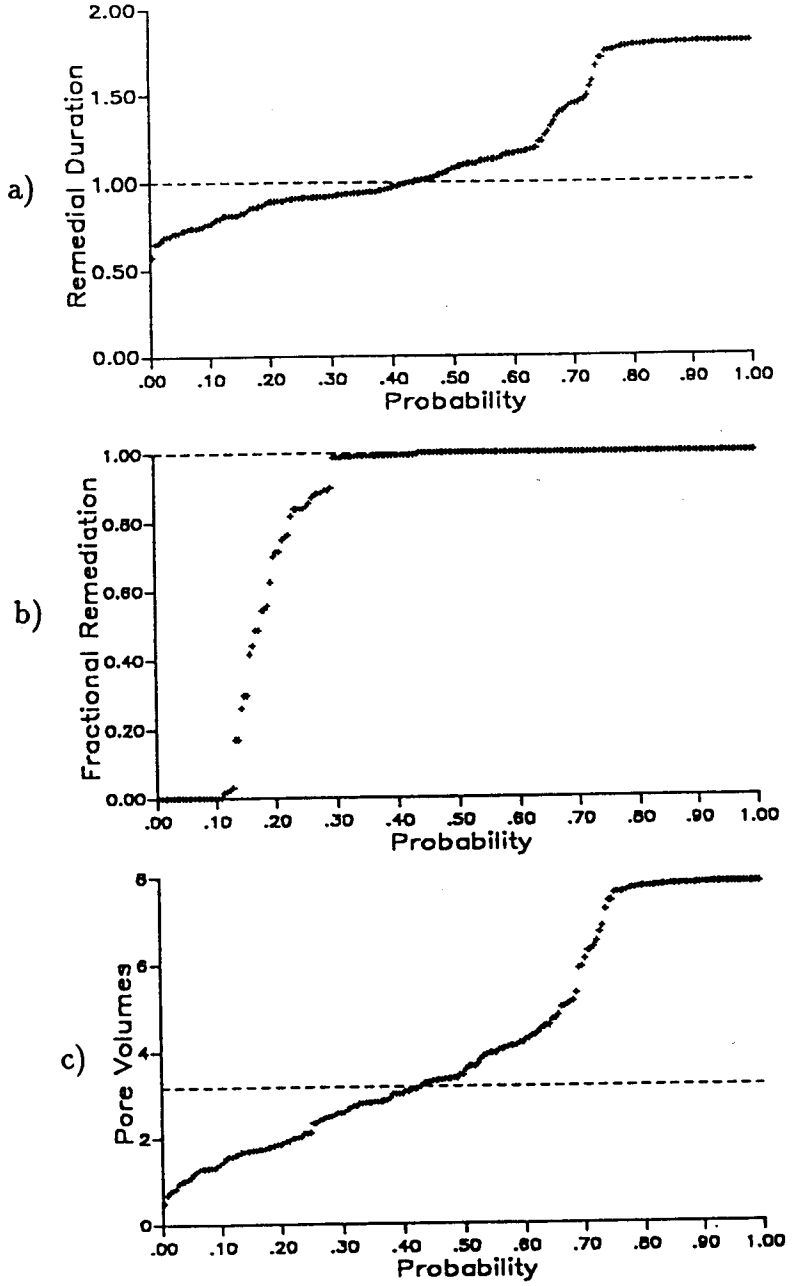

Figure 17) Cumulative distribution functions for 200 iterations, $\sigma_c = 1.00$, 10 well network designed using Fourier domain shape analysis.

contaminated mass extracted by the wells and lastly the volume of water pumped during the extraction program.

Three network design algorithms were compared in a series of Monte Carlo experiments that provided estimates of the remedial effectiveness measures under various levels of measurement errors and with different sized monitoring networks. The first algorithm, which was used as an experimental control, located wells randomly in a window around the contaminant source. The second algorithm used first order error propagation to infer the position on the detection level contour where uncertainty was highest. Subsequent wells in the network were placed on the plume boundary where the uncertainty was highest. The final method used Fourier domain shape analysis (FDSA) to predict the shape of the detection level contour and placed subsequent wells where confidence bounds in the estimate of the contours' position were highest.

5.2 Conclusions

On average, the random networks led to remedial durations between 20 percent to 30 percent longer than an ideal extraction system (designed with prior knowledge of the plume extent). Extraction systems designed using the random networks removed 75 percent to 80 percent of the contaminated mass from the aquifer and pumped between 30 percent and 50 percent more water than required by the optimal solution. As the random networks were enlarged, only minor improvement in these measures was noted.

Table 7) Number of non-remediations, out of 200, for networks designed using Fourier domain shape analysis.

		σ_c				
		0.00	0.25	0.50	0.75	1.00
N_{mw}	8	37	33	41	39	44
	10	39	37	46	27	33
	12	35	40	42	47	37
	15	6	17	11	16	15

4.3.1 Alternate formulations for FDSA

In addition to the relatively poor performance of networks designed using FDSA as detailed in the previous section, the computational burden of the constrained least squares algorithm increased computer run-times by an order of magnitude versus the error propagation approach. In addition to the FDSA approach described above, two variations on the FDSA approach were investigated in a preliminary fashion. These will be briefly reviewed in this section.

As mentioned previously, fitting a Fourier series to radii sampled unequally in the angular direction led to high frequency oscillations in the fitted plume. Fitting a cubic spline to the polar coordinate data was used as a practical way of interpolating between the observed data to establish equally spaced samples. Cubic splines have the property of honoring observation data points exactly while

been established. A number of simplifications were made in performing the work. Perhaps the most significant from a practical standpoint is the use of surrogate measures of network performance. Replacing the surrogates with economic measures should be the topic of subsequent research. Thus, the cost of installing monitoring wells and sampling for chemical constituents could be considered along with construction and operating costs of alternate extraction designs. An extension along these lines would incorporate a penalty function for failing to properly remediate a site. This could be simulated by imposing a fine if contaminated water reached a compliance surface some distance down gradient from the contaminant source.

Several simplifications that were made in this report could be eliminated at the expense of a more complicated model. The aquifer in this study was assumed to be homogeneous and flow was uniform. These restrictions could be eliminated if a numerical flow-transport program was used as a simulation tool. However, major portions of the experimental design would have to be modified if a numerical model was used. For example, for each Monte Carlo realization the analytical transport model was executed hundreds of times in order to estimate transport parameters. This would take many minutes or hours (rather than a few seconds) in a numerical model.

Also worth investigating is the impact of sampling over time in a network. As formulated here, all samples were assumed to be taken instantaneously and the remediation began at that same time. A more realistic situation would entail a monitoring program scheduled over months or years and a remedial action that

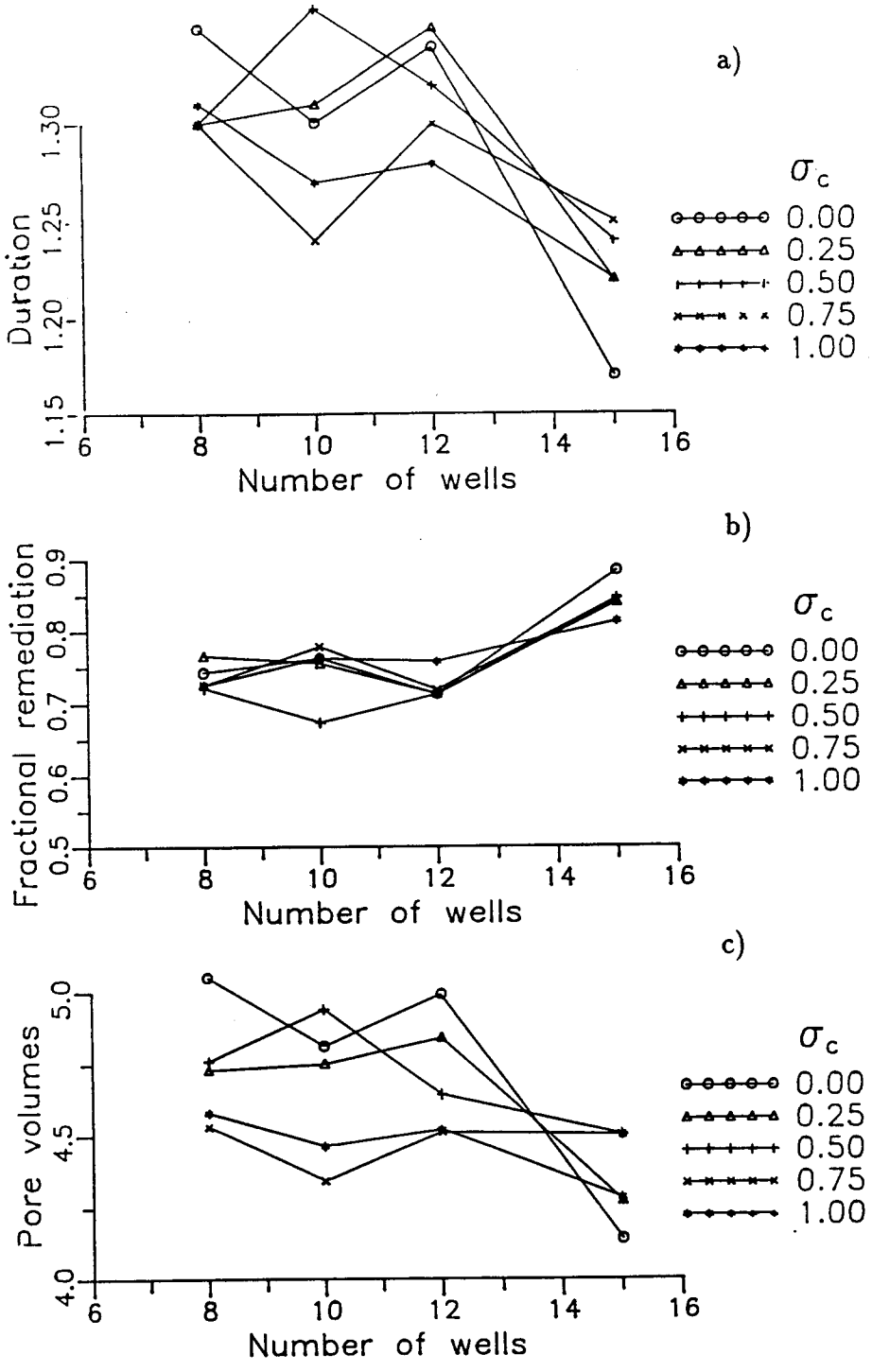

Figure 19) Mean remedial effectiveness as a function of network size (network designed using Fourier domain shape analysis).

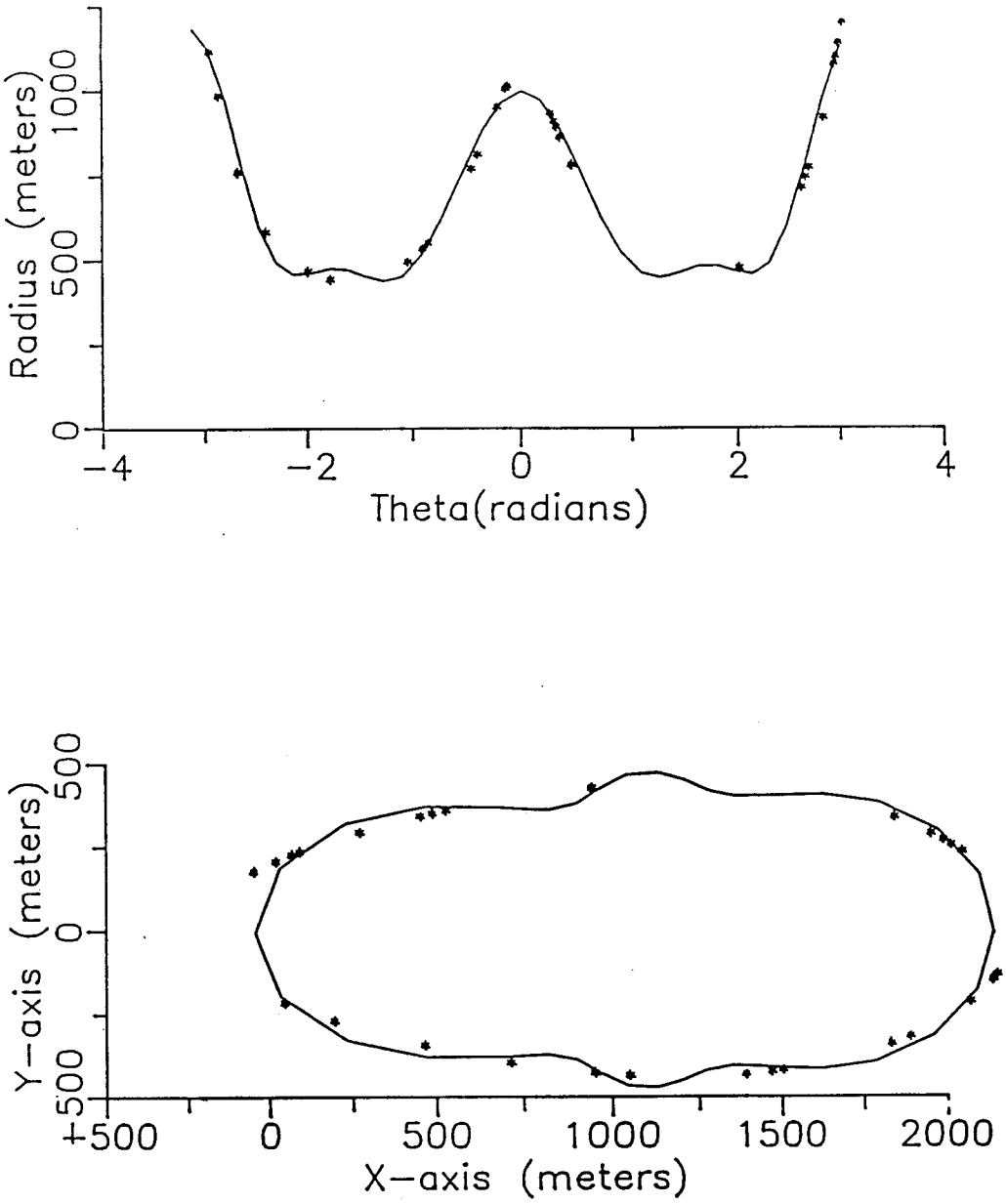

Figure 20) Polar coordinate (top) and cartesian (bottom) representations of a detection level contour using a cubic spline constraint.

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CHAPTER 5: SUMMARY, CONCLUSIONS AND RECOMMENDATIONS

5.1 Summary

Concern over groundwater contamination is growing but the expense of conducting site investigations and remediating sites that are contaminated is enormous. Future site studies and associated remedial efforts will be closely scrutinized for both economic and technical justification. Explicitly establishing the relationship between a network of groundwater monitoring wells and the effectiveness of a remedial action at a contaminated site can demonstrate the need for adequate monitoring networks. Analytical techniques that evaluate the quality of a network at a given stage provide a powerful tool for designing a cost-effective remedial investigation.

In this report an experimental framework for evaluating groundwater monitoring strategies based on the performance of aquifer remediation designed from the monitoring data has been outlined. A FORTRAN program DEMON was written to test the validity of the framework and to compare different network design strategies. In the computer program, simulated contaminant concentration measurements were used to infer the position of a detection level contour in the contaminant plume. A pump and treat extraction system was then designed to capture the inferred plume. The effectiveness of the extraction system was checked by tracking particles from the boundary of the true plume to the extraction wells. The quality of the extraction design was evaluated with three measures: the total duration of the pumping program, the fraction of

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The results of experiments using error propagation were markedly better than those for the random network results. The average remedial duration was within 5 percent to 10 percent of the optimal value. On average over 90 percent of the contaminated mass was removed while 10 percent more water than necessary under ideal conditions was pumped. Most importantly, the the error propagation design algorithm is robust since the experimental results converged rapidly to the ideal solution as the size of the network was increased (recall Figure 12).

The results from the FDSA experiments were clearly inferior to the error propagation results. On average, remedial durations were 20 percent to 35 percent above the optimal solution. The fraction of contaminant removed varied between 70 percent and 90 percent and the required treatment volume was 30 percent to 55 percent above the optimal solution. Worth noting however, is the fact that the results of the FDSA approach improved significantly as the networks were expanded from 12 to 15 wells. It is plausible that the data requirements for FDSA are large and better performance might be seen with networks of 20 wells or more. However, in the framework of this experiment (many repeated simulations) the computational requirements of FDSA would become prohibitive for networks of this size. Additionally, FDSA would not be practical for most field cases if 15 or more wells were required.

5.3 Recommendations

In this report a framework for analyzing the effectiveness of pump and treat systems for aquifer remediation as controlled by monitoring network design has

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commenced at some time after the site investigation ended. In that case, it becomes critical not only where to sample but when to sample. Kalman filtering might prove useful in this context (see for example,Van Geer and Van der Kloet, 1986).

Finally, Fourier domain shape analysis has not been fully investigated. Several properties may make it attractive for plume characterization. These include parsimonious description of complex shapes and the ability to scale the expression of a known contour to describe adjacent contours. For this reason, the suggestions made at the end of the previous chapter are worth implementing more carefully. In particular, the cubic spline seems to be able to overcome some the difficulties associated with unequal sample intervals without increasing computer run times significantly. Weighted least squares, which was briefly tested may also prove to be useful, although a robust method for selecting appropriate weights must be developed.

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