COST EFFECTIVE LONG-TERM GROUNDWATER MONITORING DESIGN USING A GENETIC ALGORITHM AND GLOBAL MASS INTERPOLATION

BY

PATRICK MICHAEL REED

B.S., University of Missouri at Rolla, 1997

THESIS

**Submitted in partial fulfillment of the requirements
for the degree of Master of Science in Environmental Engineering in Civil Engineering
in the Graduate College of the
University of Illinois at Urbana-Champaign, 1999**

Urbana, Illinois

Acknowledgments

Firstly, I would like to thank my wife Christy for her perpetual encouragement, understanding, and patience. I would like to thank my advisor Dr. Barbara Minsker for giving me the chance to participate in the entirety of this research project. Dr. Minsker allowed me to feel at ease, encouraging open discussions while guiding both my research and writing efforts.

I would like to thank Dr. Albert Valocchi for his participation in this research project. Dr. Valocchi contributed a great deal of time in the development of this research project, as well as providing invaluable insights into numerical fate-and-transport modeling. I would also like to acknowledge graduate student Brett Schmidt for his help in developing the management model application.

Additionally, I would like to thank Dr. Wayland Eheart for his open door policy. Dr. Eheart readily answered my questions and provided me with useful insights into environmental systems modeling. I would like to express gratitude to Dr. David Goldberg for his advice in the use of genetic algorithms when solving this problem. His practical approach to genetic and evolutionary computation has served as guide in decomposing this problem and will benefit my future research efforts.

I would like to acknowledge the Illinois Water Resources Center and the United States Geological Survey for funding this research effort. Also, I would like to acknowledge Dr. David Carroll for use of his genetic algorithm driver. Lastly, I would like to thank my parents and family for their constant encouragement and substantial support.

Table of Contents

List of Tables

List of Figures

1 Introduction

The *National Research Council* (NRC) has estimated that 300,000 to 400,000 sites in the United States have contaminated groundwater [1993]. The estimated cost of remediating these sites ranges from $480 billion to $1 trillion, or an average cost of $8,000 per household in the United States [*NRC*, 1993]. Early legislative efforts leading to the Resource Conservation and Recovery Act (RCRA) and the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) focused on restoring these resources to their natural states. Cost and technology limitations have since resulted in a shift in the design paradigm for groundwater remediation from resource recovery to long-term risk management.

Risk-based Corrective Action (RBCA) is a direct result of this shifting emphasis [*American Society for Testing and Materials (ASTM)*, 1995]. RBCA uses a tiered approach to remediation, where the cost and level of remediation efforts are controlled by the human health and ecological risks posed by the contaminated resources. The increasing use of RBCA is expected to result in more contaminants being left in place that will require long-term monitoring [*NRC*, 1999]. Long-term monitoring is particularly important for monitored natural attenuation, in which contaminants are mitigated by the natural processes of dilution, dispersion, and degradation. Long-term monitoring at many sites can require decades of expensive sampling at tens or even hundreds of existing monitoring wells, resulting in hundreds of thousands or millions of dollars of costs for sampling and data management per year. This paper presents a new methodology for identifying cost-effective sampling plans to reduce costs at sites with numerous existing monitoring wells.

Although monitoring network design has been studied extensively in the past, previous studies have primarily focused on two problems: (1) the use of geostatistics to augment or design

monitoring networks for site characterization [for a review, see *ASCE Task Committee on Geostatistical Techniques*, 1990b] and (2) the use of optimization and numerical simulation for screening monitoring plans for plume detection at landfills and hazardous waste sites [for a review, see *Loaiciga et al*., 1992]. Approaches using geostatistics for site characterization can be further classified as being either local or global in nature.

The local approach to monitoring design for site characterization uses geostatistics to augment monitoring networks by analyzing the effectiveness of adding sampling points to the network [*ASCE Task Committee on Geostatistical Techniques*, 1990b]. Additional sampling points are added based on an analysis of which locations will maximally decrease the estimation variance attained in geostatistical interpolation [*Rouhani*, 1985]. *Rouhani and Hall* [1988] build on this localized approach by modifying the objective to also include the magnitude of contaminant concentrations within the modeled domain. These studies present methodologies that can be used to enhance monitoring schemes for site characterization, which is an inherently different problem from the long-term monitoring design problem addressed in this study. This study assumes that once sites enter the long-term monitoring phase of remediation, site characterization will be essentially complete and monitoring networks will already exist that can sufficiently capture future plume migration.

The global approach to site characterization uses geostatistics to evaluate the performance of potential monitoring network designs still in their planning stage [*ASCE Task Committee on Geostatistical Techniques*, 1990]. These studies consider several spatial configurations and densities of monitoring wells, each of which are evaluated using the global estimation variance for each potential monitoring network [*Olea*, 1984; *Yfantis et al*., 1987; and *Christakos and Olea*, 1988]. These methods can exactly compute a unique estimation variance for well clusters

with regular geometries and rapidly evaluate the expectation of the variance for random configurations [*ASCE Task Committee on Geostatistical Techniques*, 1990b]. The global estimation variance is minimized within these studies to improve the accuracy of potential network designs. The global approaches have primarily been used in the design of networks that do not yet exist or to redesign pre-existing monitoring networks. The objectives of these studies are also significantly different from the objectives of long-term monitoring design, which does not involve siting new monitoring wells. The methodology developed in this study identifies optimal subsets of sampling points in a pre-existing monitoring network and is not intended to be used for siting new wells. Although the methodology of this study could be considered a global approach, the subsets of sampling points are judged on their ability to yield accurate global mass estimates and not on minimizing the global estimation variance.

The second monitoring network design problem that has been studied in the literature involves screening monitoring plans for plume detection at landfills and hazardous waste sites, primarily using optimization and/or numerical simulation. Much of the research in this area builds on the work of *Massmann and Freeze* [1987a,b], who present a guide for landfill monitoring design that uses a conditional simulation approach to calculate the probability of detection for a particular monitoring network. *Meyer and Brill* [1988] built upon this work by combining Monte Carlo simulation with an optimization model, which was formulated as a maximal covering location problem. Analytical optimization formulations have since been used in several studies to identify monitoring network designs at landfill sites that maximize the likelihood of intercepting plumes from leaking landfill leachate [*Hsueh and Rajagopal*, 1988; *Loaiciga*, 1989; *Hudak and Loaiciga*, 1993]. *Hudak and Loaiciga* [1992] present a heuristic approach using facility location theory to augment pre-existing monitoring networks. The

approach was proposed as an alternative to the geostatistical methods described above. More recent studies have incorporated uncertainty and/or multi-objective optimization to design cost-effective monitoring networks that maximize the probability of plume detection at landfills and hazardous waste sites undergoing remediation [*Meyer et al*., 1994; *James and Gorelick*, 1994; *Cieniawski et al.*, 1995; and *Storck et al*., 1997]. The fundamental objective of all of these studies is to design monitoring networks that will maximize the probability of detecting a plume, which is substantially different from the objectives of this study. This study assumes that the plumes at sites undergoing long-term monitoring have already been detected and the goal of the monitoring is to track the progress of remediation using global contaminant mass estimates.

Unlike the studies discussed above, the methodology developed in this work is specifically designed for sites with extensive pre-existing monitoring networks from the site characterization phase of remediation. The method does not augment or design the monitoring networks using the local or global estimation variance and is not intended for plume detection. The method uses a numerical simulation model to predict future plume location. A genetic algorithm then searches for sampling plans using kriging and inverse-distance weighting interpolation to calculate global mass estimates for candidate subsets of wells within the existing monitoring network. Global mass estimates are used in this study to show changes in the dissolved contaminant mass between successive monitoring periods, which have recently been shown to be a more effective indicator of natural attenuation than concentration-based methods [*Nyer et al*., 1998]. The method could easily be modified to design for local concentration estimates if desired, however.

2 Management Model

The management model developed for this study has three primary components: (1) groundwater fate-and-transport simulation, (2) global mass estimation, and (3) optimization using a genetic algorithm (GA). These components were combined to satisfy the goal of this study, which is to minimize sampling costs while accurately quantifying the mass of contaminant present at a site. Figure 1 shows how each of these components are combined to find an optimal subset of sampling locations. The fate-and-transport model (1) is used to project the migration and mass of dissolved contaminants from some initial time t_0 to some future time t_n, assuming that a sufficient amount of historical data exists to allow for simulation and calibration of a numerical fate-and-transport model. Note that the methodology can also be applied strictly using historical data if such an approach is preferred. The coordinates and predicted contaminant concentrations of every potential sampling location within the domain are then encoded into a specified number of randomly generated sampling plan designs. Each of these designs are then evaluated in terms of their cost and global mass estimation (2) error. The cost and mass estimation error are combined, using the objective function and constraints described in section 2.1, to compute a fitness (or measure of the quality) of each potential sampling design. Fitness values are then used by the GA (3) to determine which individual sampling designs are allowed to reproduce and evolve in later generations. The management model undergoes several iterations of evolving new populations of potential sampling plans until the GA converges to several optimal or near-optimal sampling designs. More details on this methodology are given in Sections 2.1 and 2.2.The methodology developed in this study assumes that an initial baseline at time t_o will be established using historical data and/or samples taken from all available monitoring points being considered. This initial baseline will then serve as a foundation for the

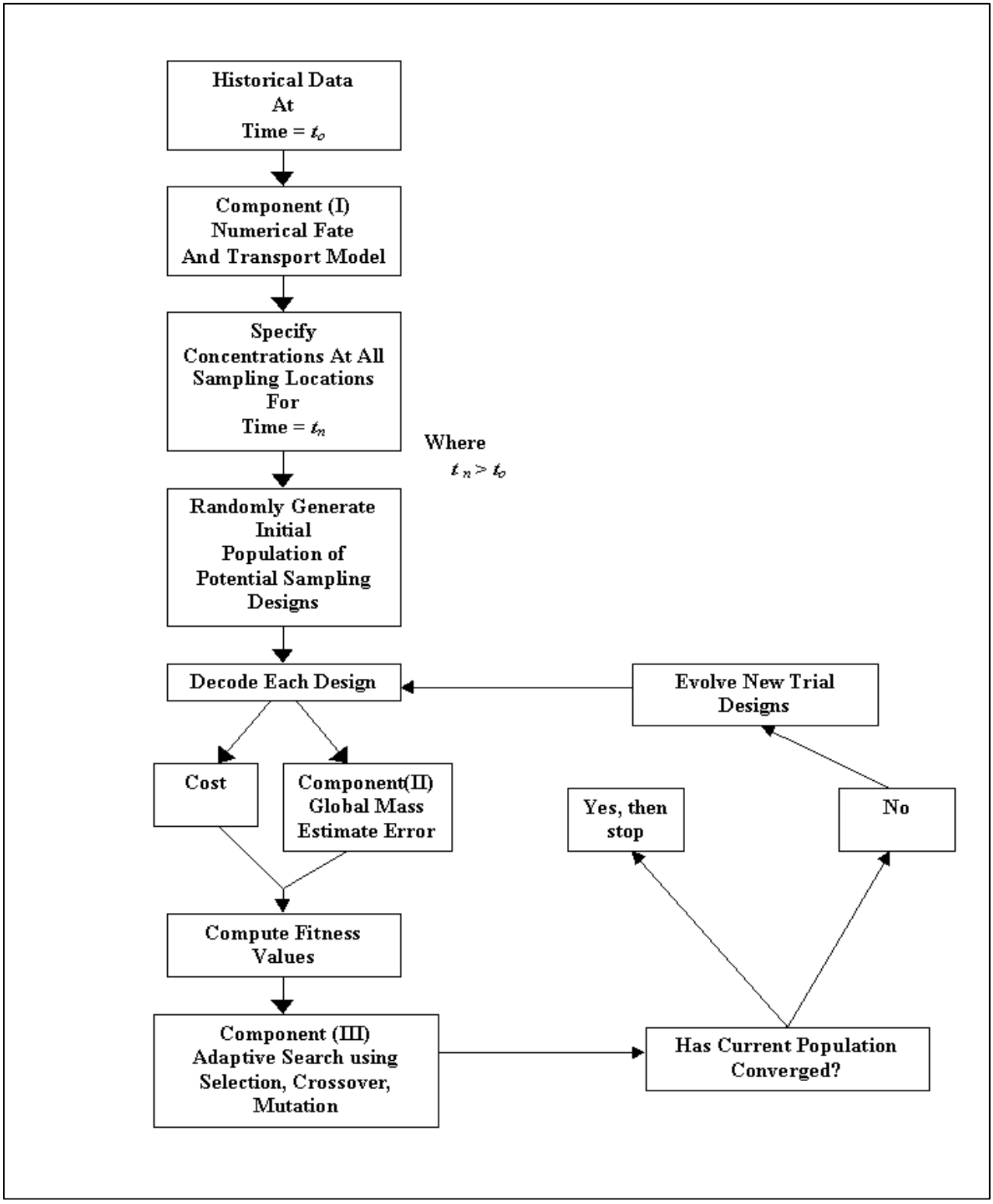

Figure 1. Management model schematic

predictive modeling that projects contaminant migration from the initial time, t_o, to some final time, t_n. The management model is then used to identify optimal sampling designs for multiple monitoring periods between times t_o and t_n. After time t_n has passed, it is assumed that a new baseline will be established and the entire process repeated for the full duration of the long-term monitoring program.

2.1 Objective Function and Constraints

Equation (1) represents the primary objective of this study of reducing long term monitoring costs. $C(x_i)$ represents the cost of one round of sampling at a single monitoring well. The index i represents each of the n potential sampling locations. The variable x_i is set equal to 1 if monitoring location i is sampled and 0 otherwise. The objective function is simply the summation of the total cost for sampling n_s monitoring wells, which are a specified subset of n (the total number of potential sampling locations). Note that equation (1) assumes that each round of monitoring will involve sampling for all constituents included in the cost $C(x_i)$. Selection of which constituents to sample is not considered at this time.

$$Minimize \sum_{i=1}^{n} C(x_i) x_i \tag{1}$$

Subject to:

$$\left\{ E \le E_{accept} \right\} \tag{2}$$

Equation (2) represents the global mass estimation error constraint. This constraint specifies that the error E in the estimate of the total dissolved mass of contaminant must be less than or equal to the magnitude of acceptable error, E_{accept}. Equation (3) shows how the global mass estimation error, E, is calculated.

$$E = abs\left[\left(\frac{Mass_{All} - Mass_j}{Mass_{All}} \right) \right] * 100 \tag{3}$$

$Mass_{All}$ is the best mass estimate based on sampling all available monitoring points in the model domain. Equation (3) is the absolute relative difference between $Mass_{All}$ and the mass estimate, $Mass_j$, for the sampling plan design j being evaluated. The mass estimation constraint represented by equation (2) was implemented using a linear penalty function shown in equation (4).

$$Penalty = \frac{\left(E_{accept} - E\right)}{E_{accept}} I \tag{4}$$

This penalty function, which is added to equation (1) to determine the fitness of each design j, assigns large penalties for errors in the mass estimates greater than the specified level of acceptable error, E_{accept}, and it rewards solutions with errors less than the specified acceptable error. The variable I is a large integer constant used to scale the magnitude of the penalty function.

2.2 Fate-and-Transport Simulation

Prediction of the contaminant plume's future behavior was done using the Reactive Transport in 3-Dimensions (RT3D) simulation package code developed at the Pacific Northwest National Laboratories [*Clement et al.*, 1998]. RT3D is a 3-dimensional finite difference code that models the advection, dispersion, and reaction or biodegradation of contaminants in the subsurface. RT3D was developed to serve as a modeling tool for sites implementing intrinsic bioremediation, but it can also be used to evaluate contaminant fate-and-transport under many other reactive or non-reactive conditions. The current version of RT3D has several reaction packages, which include instantaneous aerobic decay of benzene, toluene, ethyl benzene, and xylene (BTEX), degradation of BTEX using multiple electron acceptors, rate-limited sorption reactions, a double Monod kinetic model, and sequential degradation of perchloroethylene

(PCE). It is also possible for the user to add customized packages for specific aqueous contaminant reactions of interest.

RT3D must be coupled with a groundwater flow simulator. Flow simulation is used to determine the hydraulic heads required in the calculation of contaminant transport velocities. Groundwater flow was modeled using MODFLOW (for more details on MODFLOW see *McDonald and Harbaugh*, [1988]). RT3D's role in the methodology is to use current site data to predict contaminant concentrations in a future sampling period at all existing monitoring well locations. The predicted concentrations are then assumed to be representative of the actual site conditions that will be encountered at the next sampling period at some future time, t_n.

2.3 Global Mass Estimation

RT3D output specifying the future contaminant concentrations at all existing monitoring points is used to evaluate individual sampling plans in terms of the accuracy of their global contaminant mass estimates attained using the methods described below. The global mass estimate is assumed to be a suitable indicator of the goal of the sampling program in this study, but other indicators such as local concentration values could easily be substituted in the methodology. For each potential design, the coordinates and concentrations of sampled points are used to estimate contaminant concentrations at all unsampled nodes within the modeled domain using one of two interpolation methods: kriging or inverse distance weighting. The global mass estimate for a particular sampling plan is then calculated by simply adding all of the mass concentrations and multiplying this value by the total effective pore volume of the aquifer.

2.3.1 Ordinary Kriging

The primary strength of geostatistical methods such as ordinary kriging is that they provide minimum error, unbiased estimates of contaminant concentrations at unsampled

locations using linear combinations of sampled concentrations. *Cooper and Istok* [1988a,b,c] present a comprehensive review of how to properly use geostatistics in problems related to groundwater contamination. The principles presented in these articles serve as the basis for the geostatistics portion of this study, which involves four primary steps.

First, the contaminant concentration data are modified to insure that they are both additive (by converting from contaminant mass per unit volume of groundwater to contaminant mass per unit volume of aquifer) and normally distributed (by taking the log transform of the data). The second and third steps of the analysis are calculation of the experimental semi-variogram and structural analysis. The experimental semi-variogram is a measure of the spatial correlation among contaminant concentrations at sampled locations. It consists of a plot of the covariance of contaminant concentrations versus their separation distances. Structural analysis consists of fitting a mathematical model to the semi-variogram plot. In this study, the semi-variogram is fit using RT3D simulated data within the test case domain and is then applied for all sampling plans evaluated. Any of several semi-variogram models may be used as long as they are positive-definite and non-negative [*Cooper and Istok*, 1988; *Kitanidis*, 1996; *Goovaerts*, 1997]. The final step of the analysis involves estimating contaminant densities at unsampled locations using ordinary kriging.

Kriging is a best linear unbiased estimator that yields the expected value of the contaminant at some unsampled location given a linear combination of known or sampled data. Kriging results in estimates and estimation errors for all points in a domain. The validity of kriged estimates depends on how well the mathematical model used in structural analysis predicts the spatial correlation of contaminant densities. Cross validation is the primary means used to insure the accuracy of the mathematical model. Cross validation consists of sequentially

estimating concentrations at each of the *n* known locations using the remaining *n-1* sampled locations in the domain. An analysis of the residuals between the estimates and actual known concentrations must show that the residuals are normally distributed, independent, and have an expected value equal to zero before the semi-variogram model can be accepted.

The Geostatistical Software Library (GSLIB) [*Deutsch and Journel*, 1992] is used in this study to calculate the experimental semi-variogram and to validate the mathematical model used in structural analysis. The validated model of the semi-variogram is then used as an input for kriging. The kriging subroutines used in this study (also from GSLIB) are very flexible, allowing estimation in two or three dimensions. These subroutines are used to calculate contaminant concentrations at all unsampled points in the modeled domain for each sampling plan considered. The primary drawback in using kriging for interpolation is its computational complexity. The computational effort for kriging grows as a function of $O(mn_s^3)$, where m is the number of nodes requiring interpolation and n_s is the number of sampled (or known) concentrations within the modeled domain. Another drawback to using kriging is that calculating and validating the semi-variogram can require considerable expertise and analytical time. These limitations were the motivation for considering inverse distance weighting as an alternative interpolation method. The inverse distance method could also be used as a screening step to determine whether a detailed geostatistical analysis could result in considerable savings in sampling costs.

2.3.2 Inverse Distance Interpolation

The primary strength of inverse distance-based interpolation is its numerical simplicity. Estimating all unsampled points within the modeled domain using this method has the computational complexity of $O(mn_s^2)$. Equation (5) shows that this interpolation scheme is

simply a matrix multiplication of the inverse distance weights w_{kl} by the vector of n_s sampled concentrations, where n_s is again the number of sampled concentrations. The multiplication results in , which is a vector of m concentration estimates, where m is the total number of nodes requiring interpolation.

$$\hat{C} = \begin{bmatrix} w_{11} & \bullet & \bullet & \bullet & w_{1n_s} \\ \bullet & \bullet & & & \bullet \\ \bullet & & \bullet & & \bullet \\ \bullet & & & \bullet & \bullet \\ w_{m1} & \bullet & \bullet & \bullet & w_{mn_s} \end{bmatrix} \begin{Bmatrix} c_1 \\ \bullet \\ \bullet \\ \bullet \\ c_{n_s} \end{Bmatrix} \tag{5}$$

where

$$w_{kl} = \frac{1}{\left((x_k - x_l)^2 + (y_k - y_l)^2\right)^2}, \; for \; k = 1,...,m \; and \; l = 1,...,n_s \tag{6}.$$

The coordinates for the m nodes requiring interpolation are represented by x_k and y_k. The parameters x_l and y_l, are the coordinates of each of the n_s sampled concentrations.

2.4 Adaptive Search

The goal of this study is to reduce sampling costs by eliminating data redundancy at sites with numerous sampling locations. This goal is inherently a search problem. It requires the identification of a subset of wells that can be used to quantify the mass of contaminant without appreciably increasing the mass estimation error relative to sampling all available locations. The decision space for this search problem grows as a function of 2^n where n is the total number of available sampling locations being considered. As the number of monitoring wells increases beyond 20, the decision space quickly grows from millions to beyond billions of unique sampling designs that must be considered. The simple GA was chosen in this study because this algorithm efficiently searches large decision spaces using a process analogous to Darwinian natural selection.

GAs have been used successfully for a number of engineering design applications within water resources [see *Wang,* 1991, *Ritzel et al.*, 1994, *McKinney and Lin*, 1994, *Cieniawski et al*., 1995, and *Smalley and Minsker*, submitted 1999]. A principal difference between optimization using a GA versus more traditional methods is that the decision space is searched from an entire population of potential sampling designs. Each potential sampling design is encoded as a binary string (or chromosome), where a value of 1 in the i^{th} digit represents sampling from the i^{th} well at the site. Decoding each chromosome into the sampling plan it represents consists of listing the contaminant concentrations and coordinates of all sampled locations. These data are then used by the interpolation subroutines to estimate contaminant concentrations at all unsampled locations within the domain and the total contaminant mass. From this information, the fitness of the design is then determined using the penalty-based objective function discussed in Section 2.2. The total number of nonzero digits represents the n_s sample points used in the current design.

Once the fitness of each plan is estimated, the GA generates improved sampling plans using three basic operators: (1) selection, (2) crossover (mating), and (3) mutation. First, strings are selected at random to compete in pairwise (binary) tournaments [*see Goldberg and Deb,* 1991]. The string with higher fitness is selected to enter the mating population. Next, the crossover operator couples members of the mating population which then mate with a specified crossover probability (P_c). Mating consists of randomly selecting one or more crossover points at which the strings exchange bit values (alleles) with each other. The crossover operator used in this study produces one child string per mated pair of parent strings. If mating does not take place, the parents are replaced back into the population. Selection and crossover are repeated until a specified population size is reached. Lastly, mutation occurs when random alleles within

the new population are changed with a given probability of mutation (P_m). These three operators act to create a new population (or generation) of individual sampling plans with improved average fitness.

The Schema Theorem is the general theory describing how these three operators combine to evolve high quality, optimal or near-optimal solutions [*see Holland*, 1975 and *Goldberg*, 1989]. It states that highly fit strings are composed of small chunks of information (or building blocks) that are relevant to the solution of the problem. The GA exerts a selection pressure where only highly fit members are allowed to pass their traits or building blocks to the next generation. In this manner, the GA assembles optimal or near-optimal solutions to a problem by combining highly fit building blocks. Convergence to optimal or near-optimal solutions occurs when the change in fitness of the current generation from the previous generation is less than a user-specified tolerance. *De Jong* [1975] showed that GA performance is generally acceptable when P_c is high and P_m is low (P_m approximately equal to N^{-1} where N is again equal to the population size). Appendix A of this study presents a more detailed analysis of the effects of P_c and P_m on the solution quality for a small test case.

3 Management Model Application

3.1 Overview and Site Description

To demonstrate the potential of the management model described in Section 2, a case study has been developed from previous studies of the Hill Air Force Base in Utah [*Wiedemeier et al.*, 1995b and *Lu et al.*, 1999]. These studies used numerical simulation to assess the natural attenuation of BTEX contamination in an unconfined, sandy aquifer that has resulted from an underground storage tank facility located at the site. Adaptations were made to the data presented in *Wiedemeier et al.* [1995b] and *Lu et al.* [1999] to satisfy the assumption of data redundancy, i.e., the assumption that more monitoring points exist than required for an accurate global mass estimate. *Wiedemeier et al.* [1995b] served as the basis for both the historic BTEX concentrations used as the initial conditions for all numerical simulations completed in this study and the 30 monitoring points assumed in this case study (20 of which exist at the site and 10 which were added to ensure data redundancy). It was not the goal of this study to calibrate numerical simulations to exactly replicate BTEX fate-and-transport at Hill Air Force Base. The use of available data from this site is only meant to serve as a basis for the development of a realistic case study that demonstrates the potential efficacy of the management model in reducing long-term monitoring costs.

Section 3.2 further explains the required input and the numerical domain used for fate-and-transport simulation of BTEX. The numerical simulations were used to predict contaminant concentrations at all potential sampling locations 90 days after the historic data presented in *Wiedemeier et al.* [1995b]. The inputs and modeling required for global mass estimates from the RT3D output are discussed in Section 3.3. Lastly, Section 3.4 describes the input parameters that control how the GA searches the decision space.

3.2 Numerical Simulation

3.2.1 Numerical Domain

Lu et al. [1999] used RT3D in a calibrated simulation of BTEX migration under the influence of multiple electron acceptors at the Hill Air Force Base. These simulations served as the primary guide in developing the contaminant fate-and-transport component of this case study. The aquifer is unconfined with a saturated thickness of less than 0.9 meters and a modeled area of approximately 810,000 square meters. Figure 2 shows the two-dimensional numerical domain and the 30 potential sampling locations used in this case study. A two-dimensional domain was assumed to be adequate in our study and in the previous studies [*Wiedemeier et al.*, 1995b and *Lu et al.*, 1999] because of the aquifer's negligible thickness relative to its areal extent. The numerical grid has 6708 cells used to calculate groundwater flow and contaminant transport. The contoured concentrations in the figure represent the total BTEX concentrations 180 days after the initial conditions given in *Wiedemeier et al.* [1995b].

As shown in Figure 2, the groundwater flow direction is to the southwest. Groundwater flow direction was enforced using the constant head boundary conditions shown on the northeastern and southwestern grid cells in Figure 2. The concentration boundary conditions and the BTEX source area were modeled using constant concentration cells.

3.2.2 Model Parameters

Data presented in *Wiedemeier et al.* [1995b] provided the initial conditions for the BTEX plume shown in Figure 2 and the initial conditions for dissolved oxygen (DO), nitrate (NO_3^{2-}), sulfate (SO_4^{2-}), ferrous iron (Fe^{2+}), and methane (CH_4). RT3D assumes first order decay rates for BTEX degradation.

The electron acceptors are modeled using Monod kinetics in combination with an inhibition model to simulate sequential utilization [*Lu et al.*, 1999]. Contour maps of the initial conditions

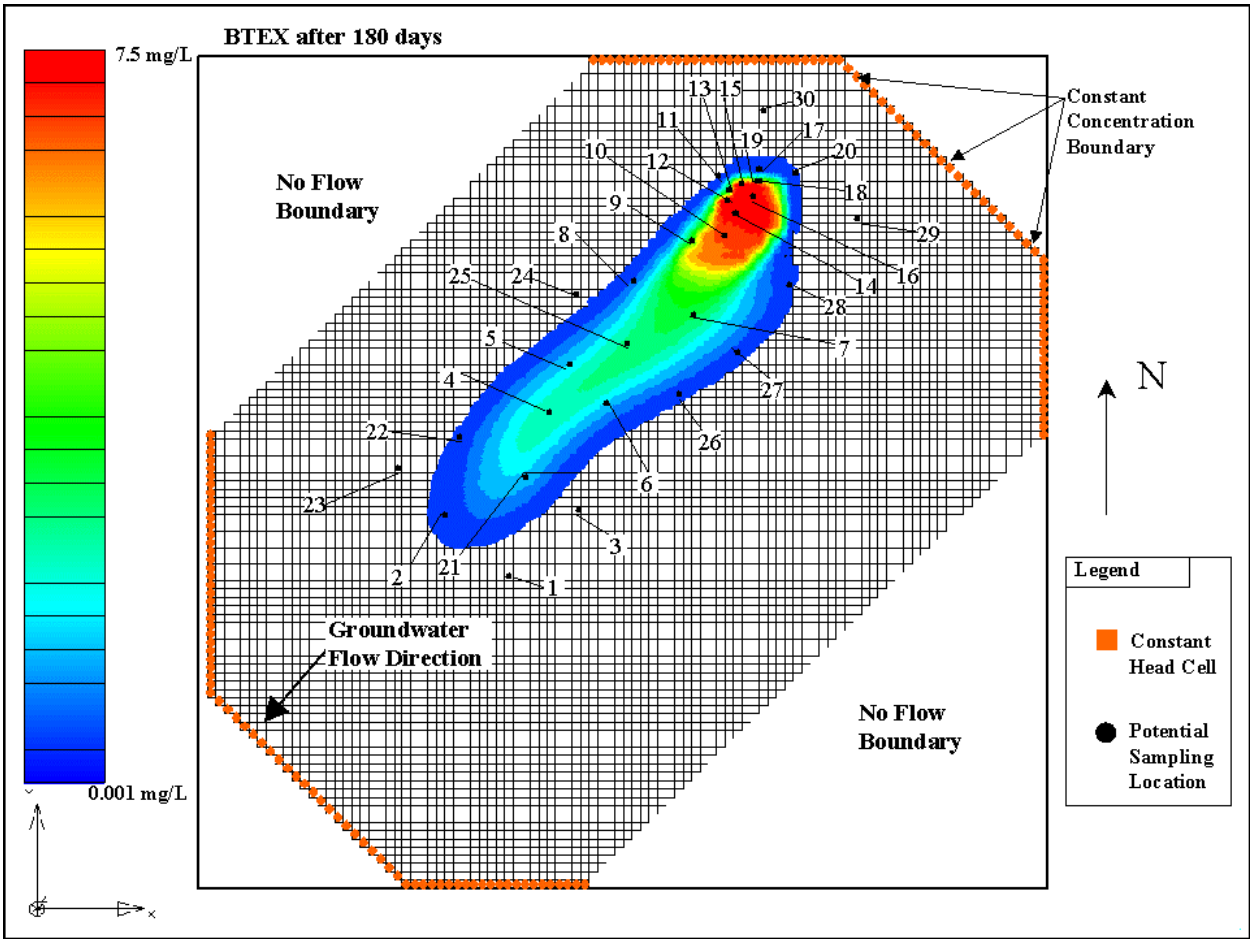

Figure 2. Plan view of numerical domain

from *Wiedemeier et al.* [1995b] can be found in Appendix B. Table 1, adapted from *Lu et al.* [1999], shows the aquifer properties and model parameters used to simulate transport and biodegradation of BTEX. Aquifer properties were assumed to be homogenous and isotropic. As in *Lu et al.* [1999], groundwater flow was assumed to be steady state. To assure that the simulations using RT3D would not be subject to significant numerical errors, the simulation model was checked for convergence as a function of grid size. Square grid cell sizes were decreased from 18.3 to 6.1 meters. It was found that the simulation results did not change

appreciably when cell sizes were changed from 9.14 to 6.1 meters, so the 9.14 meter grid cell size was used in this case study.

Table 1. Aquifer properties and model parameters (adapted from *Lu et al.*, [1999])

PARAMETER	VALUE
Hydraulic conductivity	5.89 meters/day
Porosity	0.25
Longitudinal dispersivity	8.14 meters
Ratio of transverse to longitudinal dispersivity	0.1
Discretization in the x-direction	9.14 meters
Discretization in the y-direction	9.14 meters
Extent of model in x-direction	914 meters
Extent of model in y-direction	914 meters
Aerobic degradation rate	0.051 day^{-1}
Nitrate reduction rate	0.031 day^{-1}
Iron reduction rate	0.0051 day^{-1}
Sulfate reduction rate	0.003 day^{-1}
Methanogenic degradation rate	0.002 day^{-1}
BTEX boundary condition	0 mg/L
Oxygen boundary condition	6.0 mg/L
Nitrate boundary condition	17.0 mg/L
Ferrous iron boundary condition	0.001 mg/L
Sulfate boundary condition	100 mg/L
Methane boundary condition	0.0001 mg/L
Maximum methane	2.045 mg/L
Maximum ferrous iron	50.5 mg/L

3.3 Global Mass Estimation

Recall that the global mass estimate of BTEX is used as an indicator of the performance of potential sampling designs in this case study. The GA calculates the global mass by interpolating BTEX concentrations at all unknown locations within the modeled domain using the sampled points specified in each design. Recall that the computational complexity of kriging and inverse-distance weighting are $O(mn_s^3)$ and $O(mn_s^2)$, respectively. To reduce m (the number of unestimated points in the modeled domain), and hence reduce computational time since m is much larger than n_s (the total number of sampled concentrations), a sub-domain of the original

numerical grid was used for calculating global mass estimates. Subsequent sections describe the sub-domain, the spatial correlation model, and the input parameters used in the calculation of global mass estimates.

3.3.1 Sub-Domain Description

Figure 3 shows the sub-domain used for calculating mass estimates relative to the original numerical grid. The sub-domain consists of a 45 by 15 grid with 13 meter square cells. The numerical grid was reduced from 6708 nodes to 675 nodes within the interpolation sub-domain. The "true" mass of dissolved BTEX within the sub-domain (from RT3D) is assumed to be 37.6 kg. The total mass of BTEX neglected due to the use of the sub-domain was found to be very near zero while the computational effort required to solve this case study was reduced by more than 94 percent.

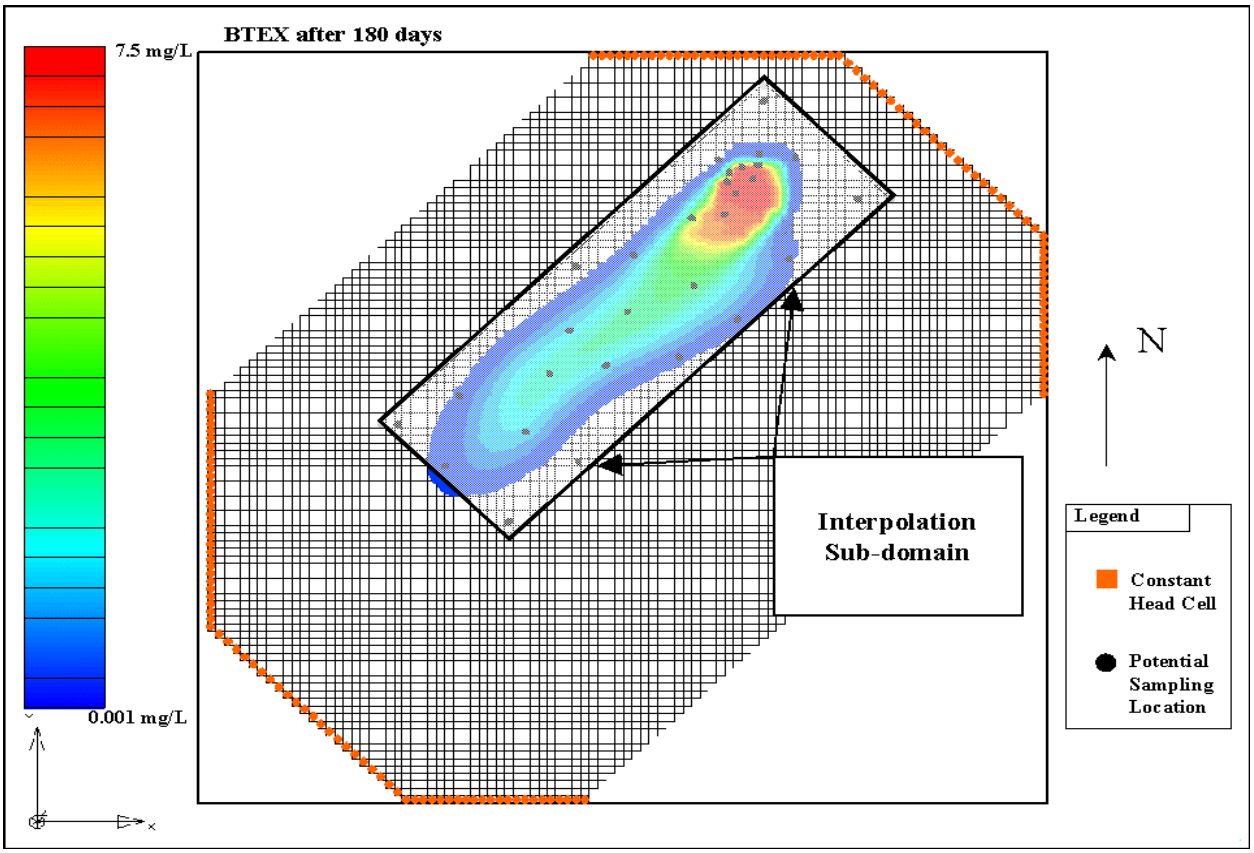

Figure 3. Interpolation sub-domain

3.3.2 Spatial Modeling and Interpolation Parameters

The spatial modeling methodology presented in *Cooper and Istok* [1988a,c] and discussed in Section 2.3.1 consisted of converting the BTEX concentrations to units of mass per cubic foot of aquifer and subsequently transforming them using equation (7) from *Cooper and Istok* [1988a].

$$Y(x) = \ln[Z(x) + A] \tag{7}$$

The transformation yields *Y(x)*, which has an improved fit to the Gaussian distribution relative to the original BTEX concentration data, *Z(x)*. The fit to the Gaussian distribution was further improved using the fitting parameter, *A*, which had a value of 10.2 in this study. The fitting parameter was determined using relationships presented in *Cooper and Istok* [1988a] for the mean and variance of a log-transformed random function.

Once the data were transformed, structural analysis was conducted. The validity of kriging estimates is heavily dependent on the structural analysis, in which a model is chosen to capture the spatial correlation of the BTEX shown in the experimental variogram (steps two and three of the methodology). Equation (8) is the exponential model from *Deutsch and Journel* [1992], which was used to represent the spatial correlation of the BTEX concentrations along the plume's longitudinal axis.

$$g(h) = c\left[1 - \exp(-\frac{h}{a})\right] \tag{8}$$

The semi-variogram, (h), represents the difference between the spatial covariance of BTEX concentrations and the variance of the BTEX data [for reference see *Kitanidis*, 1996]. It is a function of *h*, the separation distance between two points. Equation (8) is an example of a stationary model, where the semi-variogram value approaches the variance of the BTEX data as

h approaches infinity. The parameters *c* and *a* are fitting parameters used to fit this model to the experimental variogram data points. The range of the spatial correlation is represented by the parameter *a* in equation (8), which was found to be 174 meters for this study. The parameter *c* represents the variance in the semi-variogram and was found to be 0.86. The actual variance of the data used in calculating of the experimental variogram was 0.88, showing that the model is closely replicating the statistical properties of the BTEX data. Cross-validation of the model showed that the residuals, which represent the difference between known concentration values and estimates, had a zero mean value. Additionally, the residuals were independent and approximately normally distributed.

Inverse-distance weighting requires the specification of only a single parameter, r_i, which is equal to the maximum distance between any unestimated point and the sample points used for interpolation (i.e., any sample point beyond the distance r_i from an unestimated point is not used to calculate concentrations at that point). Kriging estimates also require specification of a similar parameter, the maximum search radius, r_k. Equation (9) presents a rule-of-thumb recommended by *Cooper and Istok* [1988a] to define r_k.

$$|r_k| < \frac{L}{2} \tag{9}$$

This rule requires that the maximum kriging search radius for unestimated points be less than half of the contaminant plume's length (or *L*) along its longitudinal axis. Equation (10) gives a rule-of-thumb developed by trial-and-error in this work for the maximum search radius for inverse distance weighting.

$$|r_i| < \frac{L}{6} \tag{10}$$

Conservatively, this rule-of-thumb ensures that the sampling plan designs found using the less accurate form of mass estimation will sample more wells than more accurate solutions based on kriging. Note that this rule-of-thumb was developed for the single case shown in this work and has not yet been tested for other cases. In this study, the plume's length was equal to approximately 582 meters.

3.4 Parameter Settings for Adaptive Search

The 30 potential sampling locations included in the case study produce a decision space with nearly 1.1 billion unique sampling plans to be searched by the simple GA. Hence, it is vital that the adaptive search performed by the GA be efficient at exploring this space and not prone to premature convergence. To ensure efficient operation, a time scale analysis was used in this study to define the parameters that control the GA. In addition to this analysis, the results from the GA parameter analysis for a small case study, presented in Appendix A, were also considered. The principal parameters of interest are the population size (N), the probability of crossover (P_c), and the probability of mutation (P_m). All of the results shown in this study used a population size of 100. This value was estimated from the results of equation (11), a population sizing equation for simple GAs [*Harik et al.*, 1997] that is based on the building block theory of the Schema Theorem [for reference see *Goldberg*, 1989].

$$N \geq -2^{K-1} \ln(\alpha) \left(\frac{s_{bb}}{d} \right) \sqrt{p\,(n_{bb} - 1)} \tag{11}$$

Building blocks in this work are the singular binary digits that represent each of the potential sampling locations in the modeled domain, so the order of the building blocks, K, is equal to 1. The building block order represents the minimum number of binary digits that have physical significance to solution of the problem. To insure that the solution converges to a near optimal solution with high certainty, (the probability of failure) was set to 0.01 percent. The variable

$_{bb}$ represents the variance of building block fitness and d is the signal difference between the best and second best building blocks. The ratio of $_{bb}$ to d represents the interference with solution convergence from noise caused by competing building blocks (for more information see [*Goldberg et al.*, 1992 and *Harik et al*., 1997]). Because the building blocks are single digits (representing the simplest case possible), the influence of noise was neglected and this ratio was assumed to equal unity. The final term, n_{bb}, represents the maximum possible number of building blocks, which in this study corresponds with the total number of potential sampling locations, 30. This analysis showed that a population size of greater than 88 members would be required. Based on these results, a population size of 100 was selected.

The remaining GA parameters were estimated using this population size and a time scale analysis of the convergence of a simple GA. P_m was set equal to the reciprocal of population size or 0.01 in accordance with the findings of [*De Jong*, 1975] and the parameter analysis discussed in Appendix A. *Thierens* [1995] investigated the effects that selection and crossover have on solution quality and defined an upper bound on P_c for tournament selection shown in equation (12).

$$P_c \leq \frac{s-1}{s} \tag{12}$$

The parameter s represents the total number of individuals that compete in each tournament, which is two for binary tournament selection. Equation (12) is intended to protect pertinent building blocks from being lost in mating. Based on this equation, P_c was set to 0.5. The parameter settings for N and P_c were verified using equation (13) in conjunction with initial results from the management model.

$$N\ln(N) > -\ln\left(\frac{1}{n_{opt}}\right)\frac{2^{2K}\ln(s)2^{n_{opt}}}{P_c n_{opt}^{\frac{5}{2}}} \tag{13}$$

Equation (13) represents a "necessary condition for convergence" to an optimum composed of multiple building blocks [*Thierens and Goldberg*, 1993]. The condition requires that the time scale of convergence ($N \ln(N)$) must be greater than the time scale of innovation, which is represented by the right-hand side of equation (13), to prevent premature convergence. The time scale of innovation is the time required for the GA to create new building blocks to obtain the solution being sought. All of the parameters in equation (13) have been previously defined except $n_{opt,}$ which represents the total number of building blocks (or sampling points) required for an optimal solution. Preliminary results showed this value ranged from a minimum of 8 to a maximum of 12 points depending on the interpolation technique used to calculate mass estimates. The convergence condition of equation (13) is satisfied over the entire range of values for n_{opt} when N, P_c, and P_m are set to 100, 0.5, and 0.01, respectively.

4 Results and Discussion

The management model developed in this study combines numerical simulation, interpolation, and adaptive search to reduce long-term monitoring costs. Three methods were implemented for the case study discussed in Section 3. Initially, each potential sampling plan was judged based on inverse distance weighting mass estimations and cost. The inverse distance-based solution is a fast, lower accuracy method that could be used as a conservative screening tool to discern if more accurate methods are justified. The second method used kriging to attain low cost, highly accurate sampling plans. Kriging requires substantial modeling and analysis at an increased cost to the management model user, but the solutions based on kriging are more accurate and less costly than sampling designs found by inverse distance weighting. The final solution method combines the inverse distance and kriging solutions into a hybrid method. The hybrid method demonstrates how initial solutions found using inverse distance weighting can be refined using kriging to reduce the computational effort associated with kriging.

The GA is a stochastic optimization algorithm that is inherently based on random number generation, which causes slight variations in solutions with changes in the seed value used in the random number generator. All of the subsequent solutions used the same initial seed for the random number generator to maintain comparability among the three methods. Note that the solutions discussed in the subsequent sections are the least-cost and most accurate sampling plans found in the final converged populations of each method. Two conditions had to be satisfied before the GA was considered to be converged. The first condition required that a single subset of the potential monitoring points had to be sampled by approximately 90 percent of the individuals within the last generation. The second condition further stipulated that all of the

remaining monitoring points could not be sampled by more than 10 percent of individuals within the final generation. Figure 4 shows which wells were used in the least-cost, most accurate sampling designs found by all three methods. The locations of each well number are given in Figure 2. The management model found between 8 and 12 wells to sample in the final designs selected depending on the solution method. Note that the solutions found are not unique: the final converged populations for each of these methods consists of several potential designs that are effective in reducing costs and estimating contaminant mass. Identifying several effective monitoring plans allows regulators and other decisionmakers to consider other unmodeled objectives in selecting a final plan.

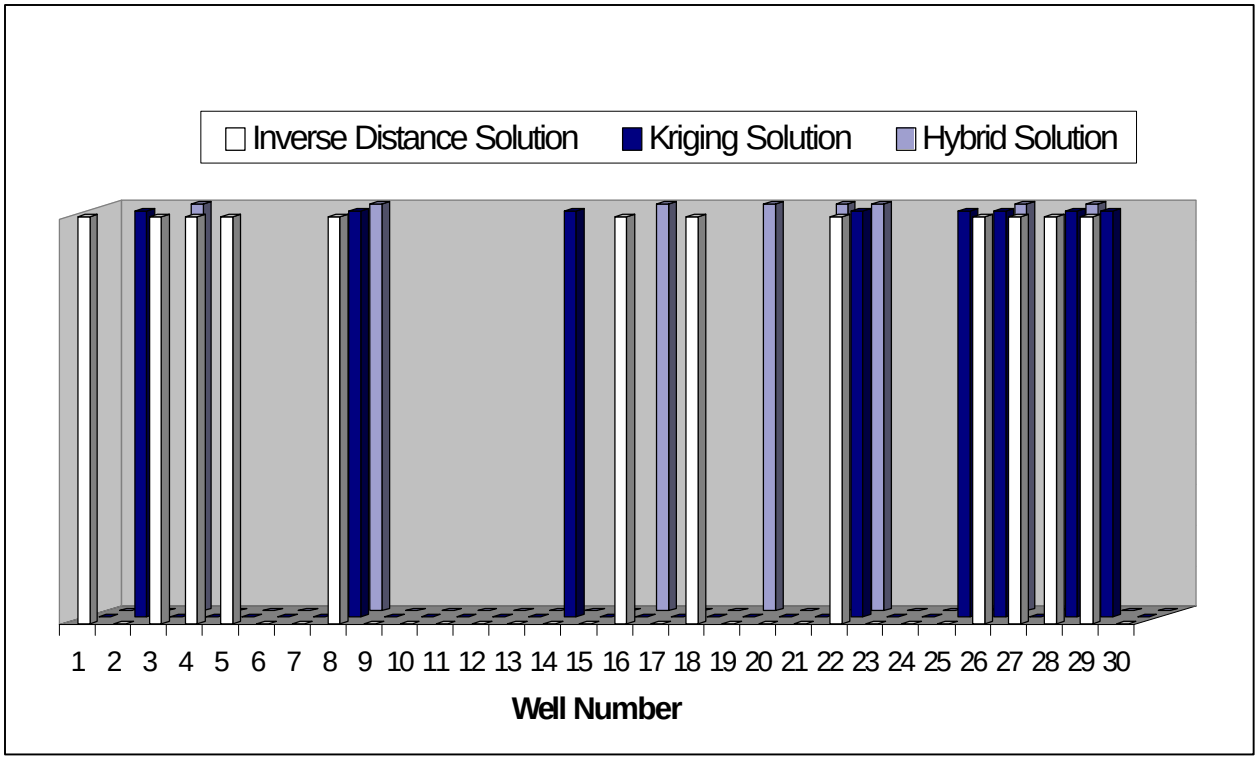

Figure 4. Least-cost, most accurate sampling designs

4.1 Inverse Distance Weighting-based Solution

Figure 5 shows a plan view of the least-cost, most accurate sampling design found using inverse distance weighting. The solution uses 12 sampling points to estimate the total mass of

BTEX dissolved in the groundwater within the two-dimensional sub-domain. The proposed sampling locations are highlighted along the full extent of the plume, indicating that the GA has converged to a sampling design that effectively delimits the full extent of the BTEX plume. The plume is sampled using two transects along its longitudinal axis. The spacing of these transects delimit the plume's extent in its transverse direction. Using inverse distance weighting, $Mass_{All}$ (the global mass estimate for the sub-domain using all of the 30 available sample locations) was found to be 47.4 kg. Recall that the actual mass of dissolved BTEX within the sub-domain is 37.6 kg, yielding an estimation error of 26 percent. The mass estimate based on sampling only the 12 locations shown in Figure 5 also equals 47.4 kg. Hence, the management model was able to reduce sampling costs by 60 percent without increasing the mass estimation error above 26 percent. Identifying this solution required 10,000 mass estimates, which required an average of 0.04 seconds per evaluation or a total computing time of 6.7 minutes.

4.2 Kriging-based Solution

The results from the kriging method showed significant potential for further reducing monitoring costs. Figure 6 shows a plan view of the least-cost, most accurate kriging solution, which used 8 sampling locations. This solution decreases monitoring costs by an additional 13 percent relative to inverse-distance weighting. Using kriging with all 30 monitoring locations, $Mass_{All}$ was calculated to be 35 kg with an estimation error of 7 percent relative to the "true" mass of BTEX in the sub-domain. The global mass estimate for BTEX based on the 8 sampled locations shown in Figure 6 is equal to 34 kg, with an estimation error of 10 percent. The mass estimation error was increased by 3 percent while the sampling costs were reduced by 70 percent relative to sampling at all available locations. Figures 5 and 6 show that the solutions based on both kriging and inverse-distance weighting are similar in form. The kriging solution uses 3

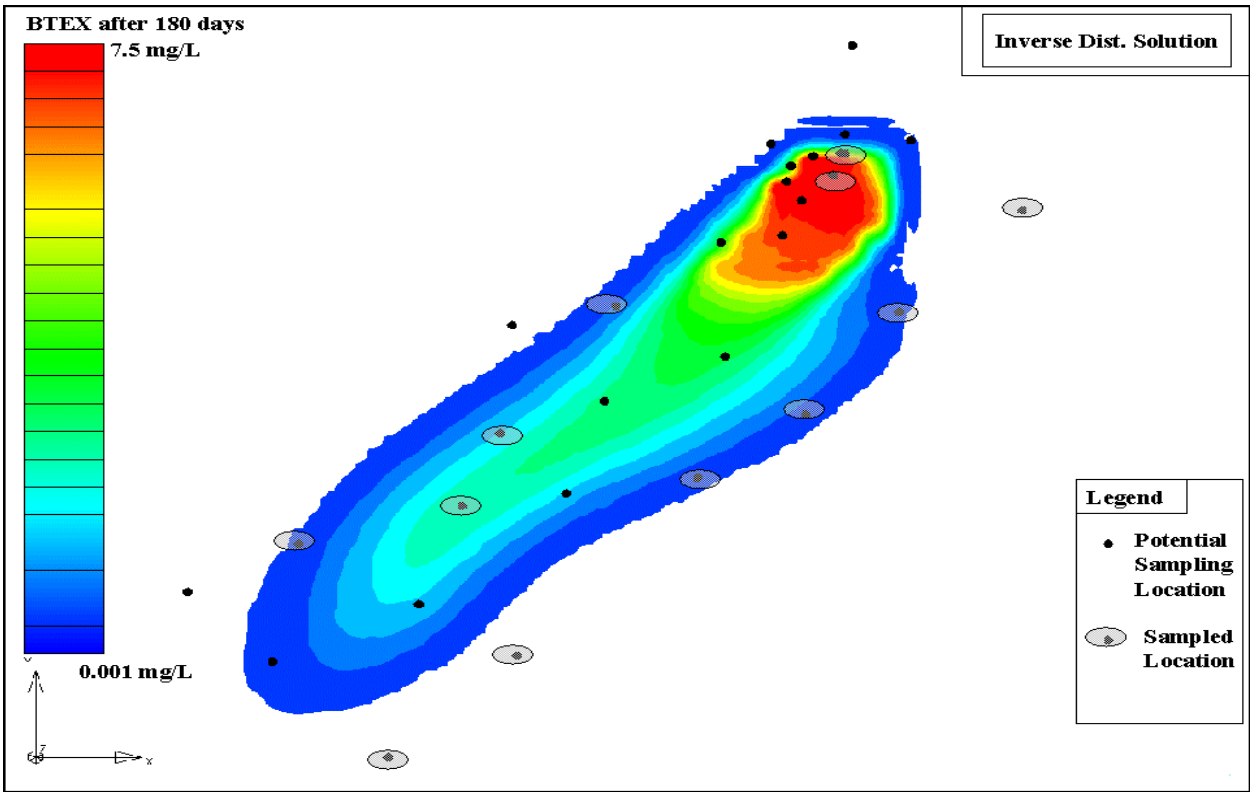

Figure 5. Inverse distance solution

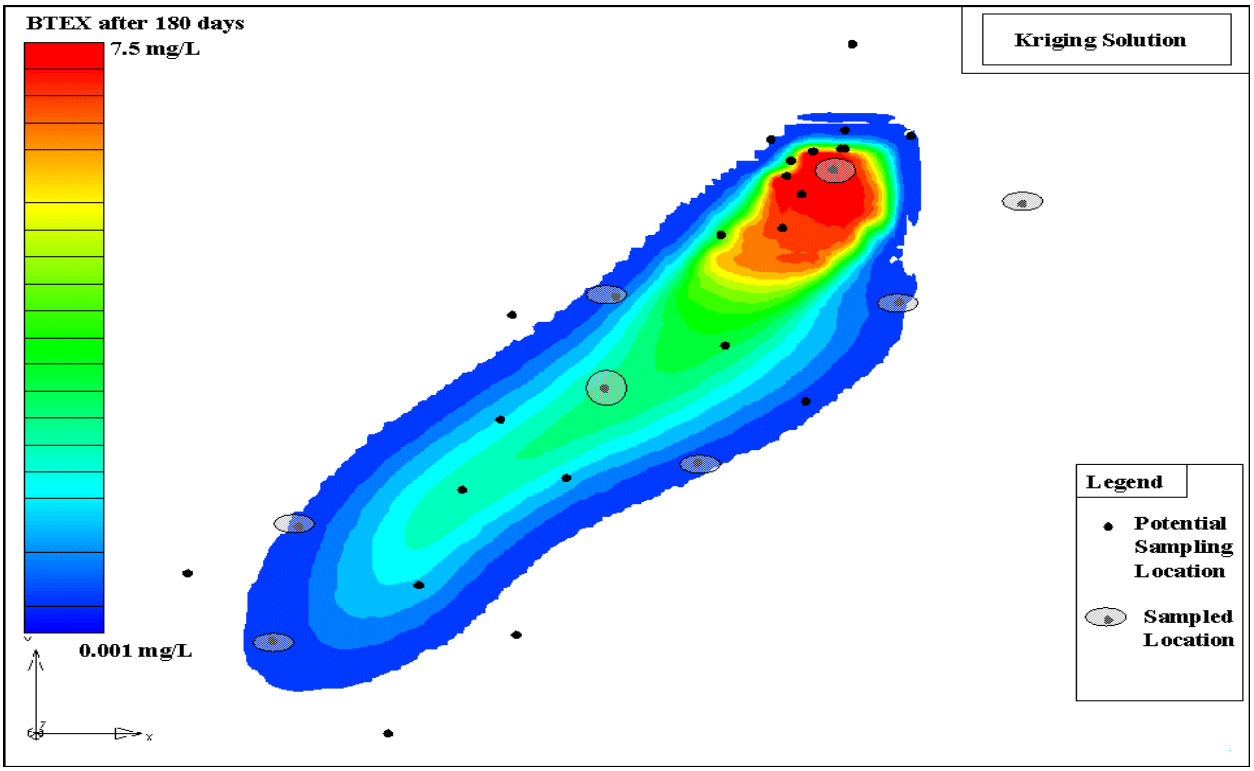

Figure 6. Kriging solution

points along the longitudinal axis of the plume and the 5 remaining points to delimit the plume in its transverse direction. The solution was attained after 75 generations or 7500 function evaluations (requiring an average of 1.4 seconds per evaluation, for a total computing time of 3 hours).

4.3 Hybrid Solution

Each function evaluation using inverse distance weighting required only 2.9 percent of the computational time required by kriging. The purpose of the hybrid method is to reduce the total computational time required to attain a more accurate kriging-based solution. During the first step of the hybrid method, inverse-distance weighting is used to evolve the population for 100 generations. In the second step of the hybrid method, a kriging-based search further refines

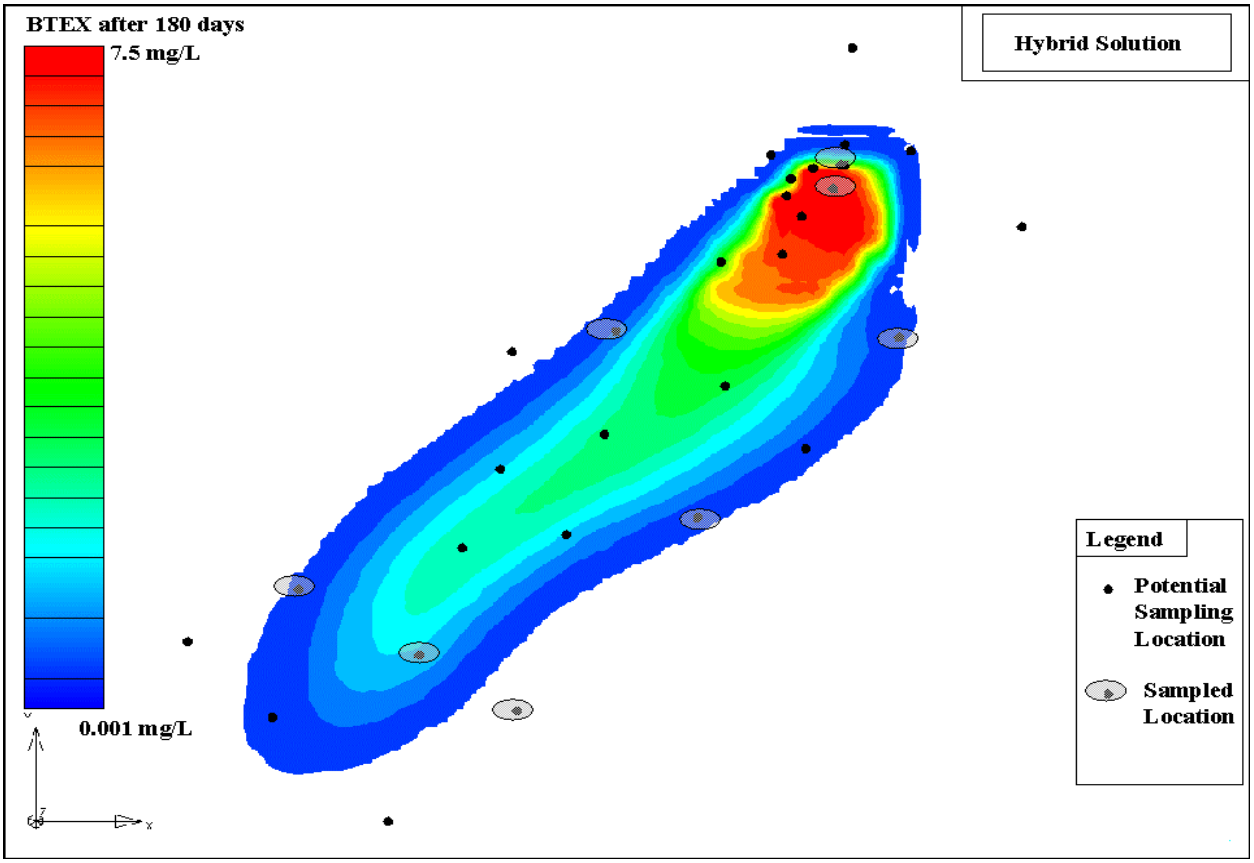

Figure 7. Hybrid solution

the 100^{th} generation attained from inverse-distance weighting by simultaneously reducing sampling costs and identifying higher accuracy solutions. Figure 7 shows the plan view of the hybrid solution with the sampled locations highlighted. The eight monitoring locations again delimit the plume in both its longitudinal and transverse directions. Note that the hybrid method and the pure kriging-based solutions in Figures 6 and 7 both use 8 sampling locations, many of which are the same. The hybrid solution yielded a mass estimate of 34.5 kg with an estimation error of 7.4 percent. It was attained in only 41 generations or 4100 kriging mass estimates, reducing the total time of computation by more than 40 percent relative to using kriging alone.

5 Conclusions and Further Extensions

The management model developed in this study has significant potential for reducing long-term monitoring costs. The combination of numerical fate-and-transport simulation, interpolation, and adaptive search has resulted in a method that could be applied to numerous sites undergoing long-term monitoring. The methodology is general and could be easily modified to use historical data analysis instead of numerical simulation or to change from a global mass approach to a local concentration approach. This study has also demonstrated the use of several tools for guiding a competent search of the vast decision spaces encountered in long-term monitoring problems and other water resources applications. Population sizing and time scale analysis can be used in the implementation of a simple GA to prevent premature convergence and ensure that optimal or near optimal sampling designs are found.

The management model can be applied using a tiered approach. Initially, a solution based solely on inverse-distance weighting interpolation can be used as a screening tool to determine if a site satisfies the implicit assumption of data redundancy and could benefit from a more comprehensive analysis using geostatistical modeling. Spatial modeling using the GA in combination with kriging-based mass estimation greatly improved the solutions found. The management model application showed that kriging-based solutions reduced the mass estimation errors by nearly 70 percent relative to solutions found using inverse distance weighting. The kriging-based method also reduced sampling costs by an additional 13 percent over the more conservative inverse distance weighting method. The hybrid solution combined both methods to reduce the computational time by more than 40 percent relative to using kriging alone, with little or no loss in accuracy. The hybrid method shows great promise for reducing computational effort and future research will investigate other types of hybrid methods.

Given the potential rapid growth of the decision space of this problem, the computational efficiency of the method used to search the decision space must be considered. When compared with other optimization techniques, GAs have the advantage of being able to solve discrete, non-convex, discontinuous problems without differentiation [*Goldberg*, 1989]. *Goldberg and Deb* [1991] show that the rate of convergence for a simple GA under binary tournament selection is proportional to $N \log (N)$ function evaluations, where N is the total population size. The population size, N, required to insure near optimal solutions is proportional to the total number of building blocks, as shown in equation (11) of this study [*Harik et al.*, 1996]. Since a single building block is equal to a single binary value, there are a total of n building blocks in each of the N binary strings that compose the overall population where n is again the total number of potential sampling locations. Using these relationships, the theoretical time required to find near optimal solutions for the binary coded GA used in this study is then proportional to $n \log (n)$ [see *Goldberg*, 1993]. The decision space of this study grows as a function of 2^n, while the computational complexity of using a simple GA to solve this problem grows only as a sub-quadratic function of n. Hence, the simple GA is quite efficient at solving this problem.

Future research will investigate the uncertainties in the management model so that monitoring plans can be developed that are robust for the range of possible conditions existing in the subsurface. Monitoring frequency will also be investigated. Other plume interpolation methods will also be explored for their effect on monitoring designs. Finally, the necessity of measuring costly constituents versus inexpensive constituents will be explored based on existing historical data, particularly within the context of monitoring natural attenuation, which can require decades of costly sampling.

Appendix A. Genetic Algorithm Parameter Analysis

A simple GA with a population size of 100 was used to investigate how the fitness of the best individual varies as a function of the crossover and mutation probabilities over the span of 100 generations. The test case used in this study consisted of a hypothetical site with a 60-meter by 20-meter homogeneous and isotropic sandy aquifer contaminated with BTEX. Figure 8 is a plan view schematic of the modeled domain. The figure shows the hydraulic flow and contaminant transport boundary conditions used in this study.

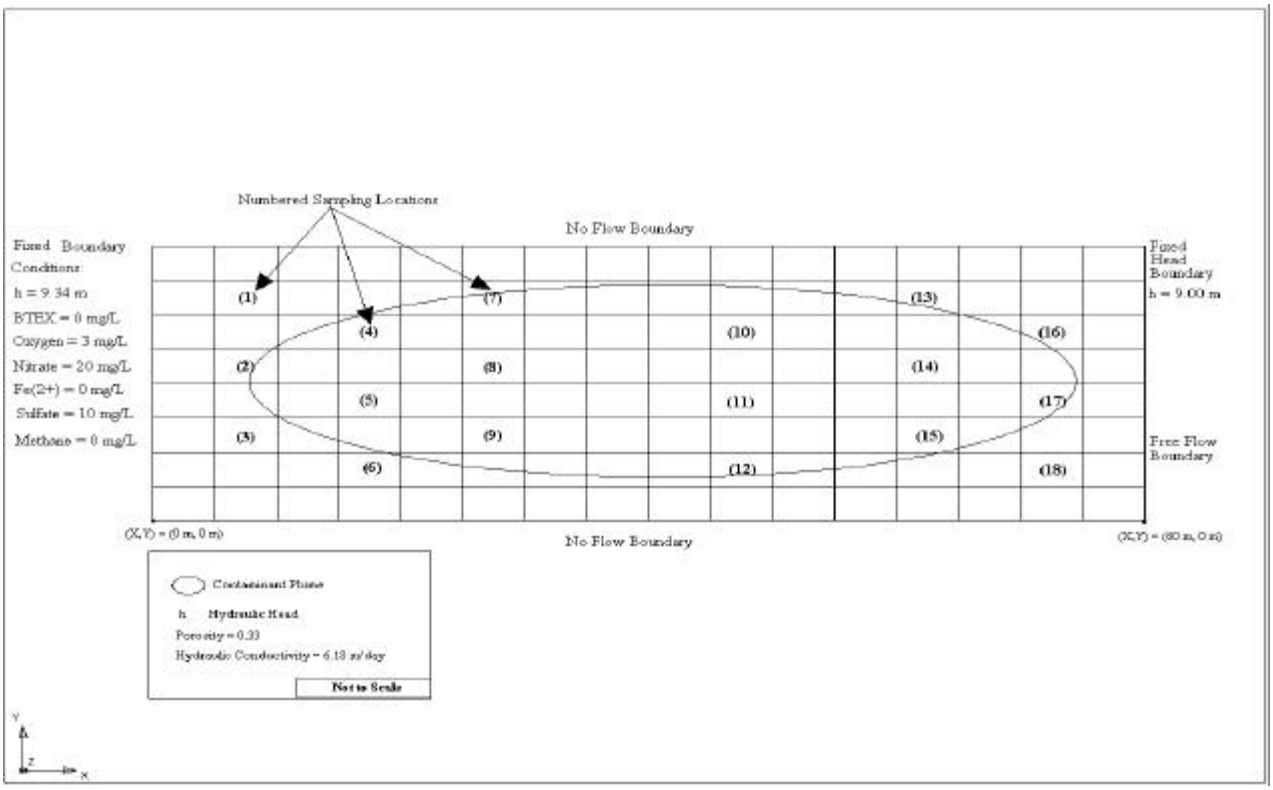

Figure 8. Numerical domain for GA parameter analysis

The domain was discretized into a 16 by 8 grid using a grid spacing of 3.8 meters and 2.5 meters in the X and Y directions, respectively. A 1-day time step was used in the transient simulation of BTEX fate-and-transport. Monitoring well locations and numbers are displayed on the figure. The decision space searched by the GA for this case has 2^{18} possible solutions.

Potential sampling plans were evaluated using global mass estimates attained from kriging. The same spatial modeling methodology used in the management model application was followed in this GA parameter analysis. Improving the sampled data's fit to the normal distribution found used the fitting parameter *A* of equation (7) with a value equal to 39.6. Structural analysis found that the spatial correlation of the contaminant data from RT3D was best described using the Gaussian model shown in equation (14) from *Deutsch and Journel* [1992].

$$g(h) = c\left[1 - \exp(-\frac{h^2}{a^2})\right] \tag{14}$$

The range (*a*) and sill variance (*c*) fitting parameters were found to equal 19.4 and 2.5, respectively. Lastly, the plume's length along its longitudinal axis was 60 meters, which was the value used to specify r_k (the maximum search radius) defined in equation (9).

Crossover probabilities were varied from 0 to 1 with a step size equal to 0.1. Mutation probabilities were varied from 0 to 0.1 using a step size of 0.01. Figure 9 shows the objective function values of the best individuals found by the GA as a function of these probabilities.

Note that the best individual sampling plans shown in Figure 9 minimize the objective function value (cost and the mass estimation error penalty) on the z-axis. The results shown in Figure 9 illustrate that a majority of the solutions found in the runs had objective function values less than or equal to 1400. These solutions used 8 monitoring wells and had mass estimation errors less than 1 percent. All of these solutions would be acceptable in satisfying the objective of this study. However, note in Figure 9 that problems arose when the probability of mutation ranged between 0 and 0.02. The figure shows that using a mutation probability in this range in conjunction with crossover probabilities either less than 0.2 or above 0.6 could cause the GA to fail to reach acceptable solutions. An explanation of the GA's failure can be found by solving equation (13) in Section 3.4 for a theoretical minimum P_c as shown in equation (15) [*Thierens*

and Goldberg, 1993]. The theoretical minimum for this case study was found to equal 0.15, which agrees well with the results shown in Figure 11.

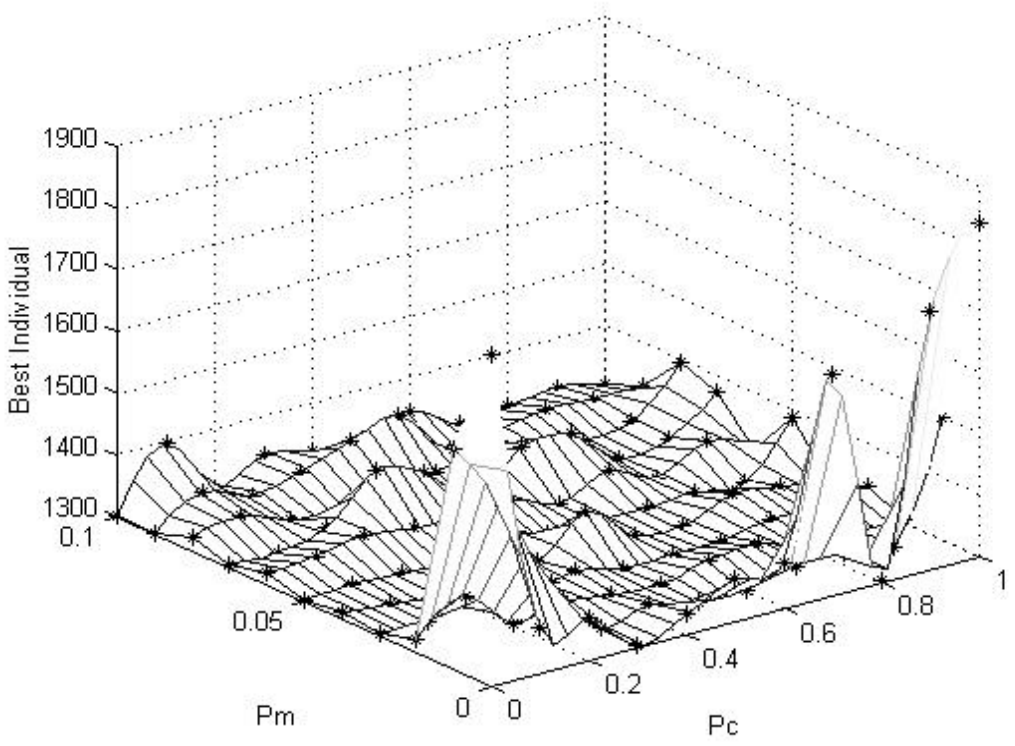

Figure 9. Map of best individual sampling plans

$$P_c > -\ln\left(\frac{1}{n_{opt}}\right)\frac{2^{2K}\ln(s)2^{n_{opt}}}{N\ln(N)n_{opt}^{\frac{5}{2}}} \tag{15}$$

Where

Pc = minimum crossover probability

n_{opt} = the number of building blocks needed for an optimal solution, set equal to 8 for this problem

K = order of the building blocks, set equal to 1 for this problem

s = selection pressure, set equal to 2 for binary tournament selection

N = population size, set equal to 100 for this problem

The GA's failure for some of the crossover probabilities above 0.6 can be explained when high rates of crossover cause pertinent building blocks to be lost as the decision space is searched [*Thierens*, 1995]. Equation (12) in Section 3.4 gives a limit intended to minimize the disruption of building block processing, which is a critical component of the GA. The theoretical maximum crossover probability was found to be 0.5, which also agrees with the data shown in Figure 9. It should be noted that as the probability of mutation increased above 0.02 the upper bound on the probability of crossover in equation (12) no longer applied. This result is expected because the performance theory for simple GAs generally uses a probability of mutation equal to the inverse of the population size in accordance with *De Jong* [1975], as previously discussed in Section 3.4. The results of this parameter analysis show that the theoretical relationships shown in equations (10) and (11) serve as effective guides in setting both P_c and P_m for the simple binary coding used in this analysis. A similar finding would also be expected when the equations are used to set P_c and N for a fixed P_m, as discussed in Section 3.4.

Appendix B. Initial Conditions for Electron Acceptors

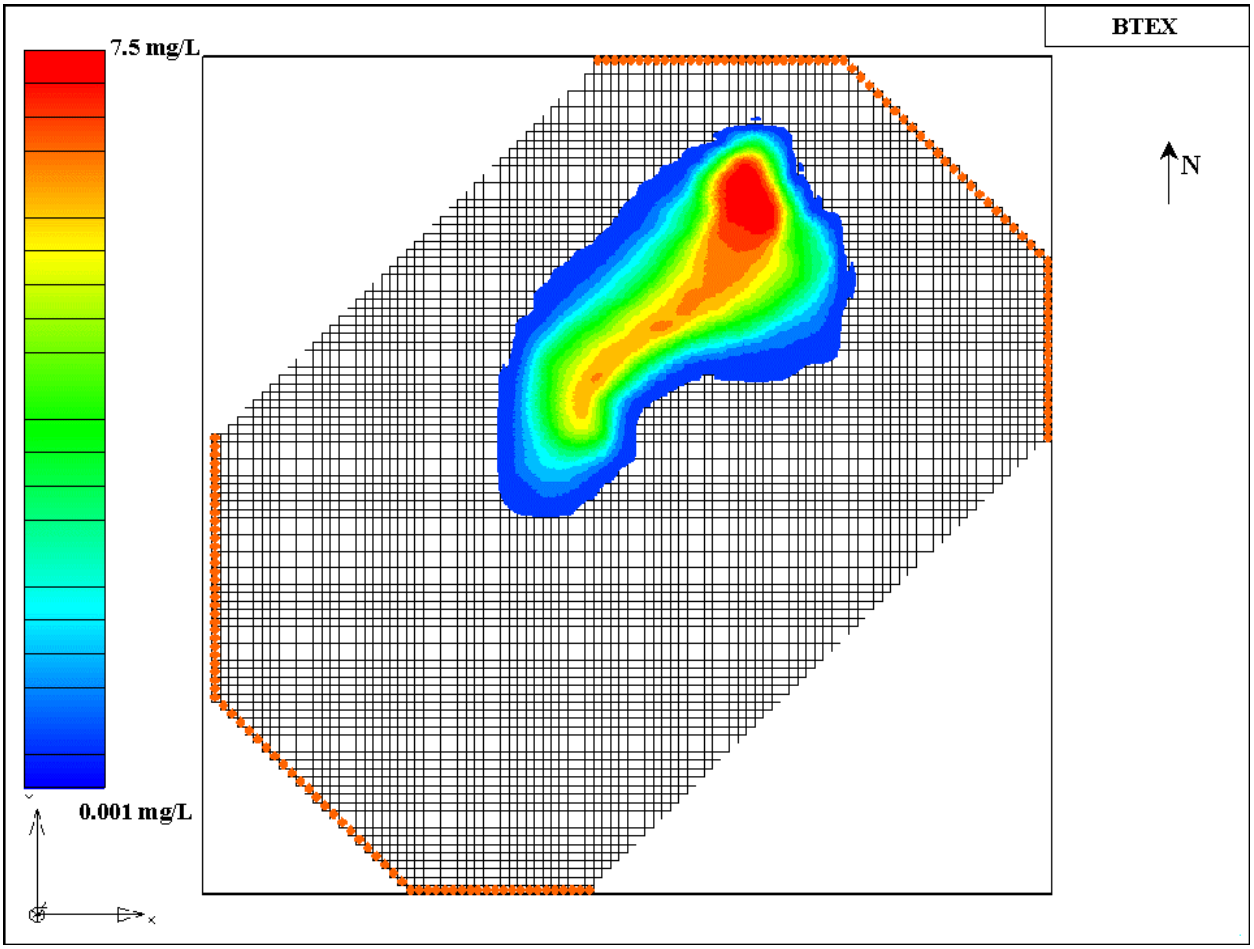

Figure 10. Contoured map of the initial BTEX concentrations

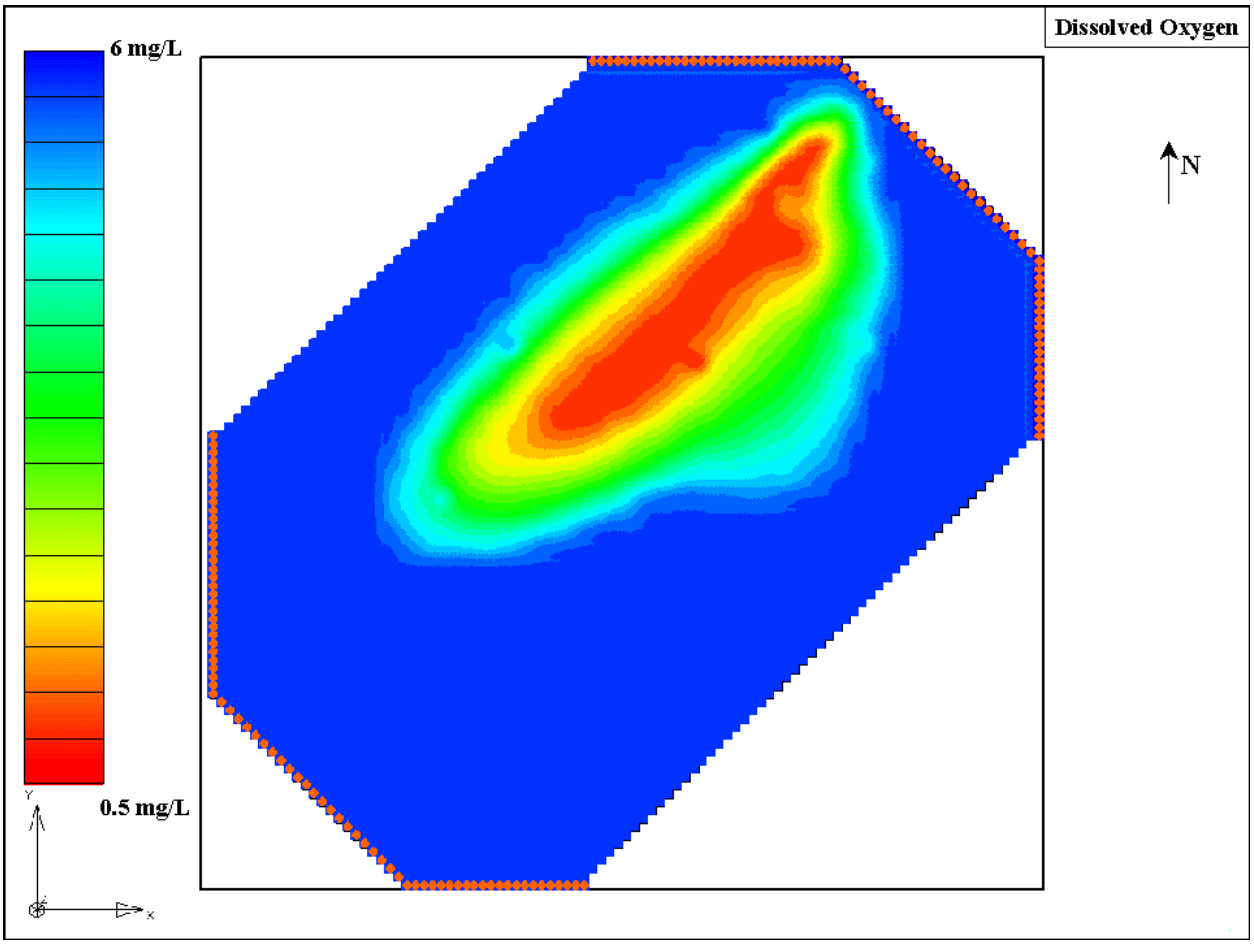

Figure 11. Contoured map of the initial dissolved oxygen concentrations

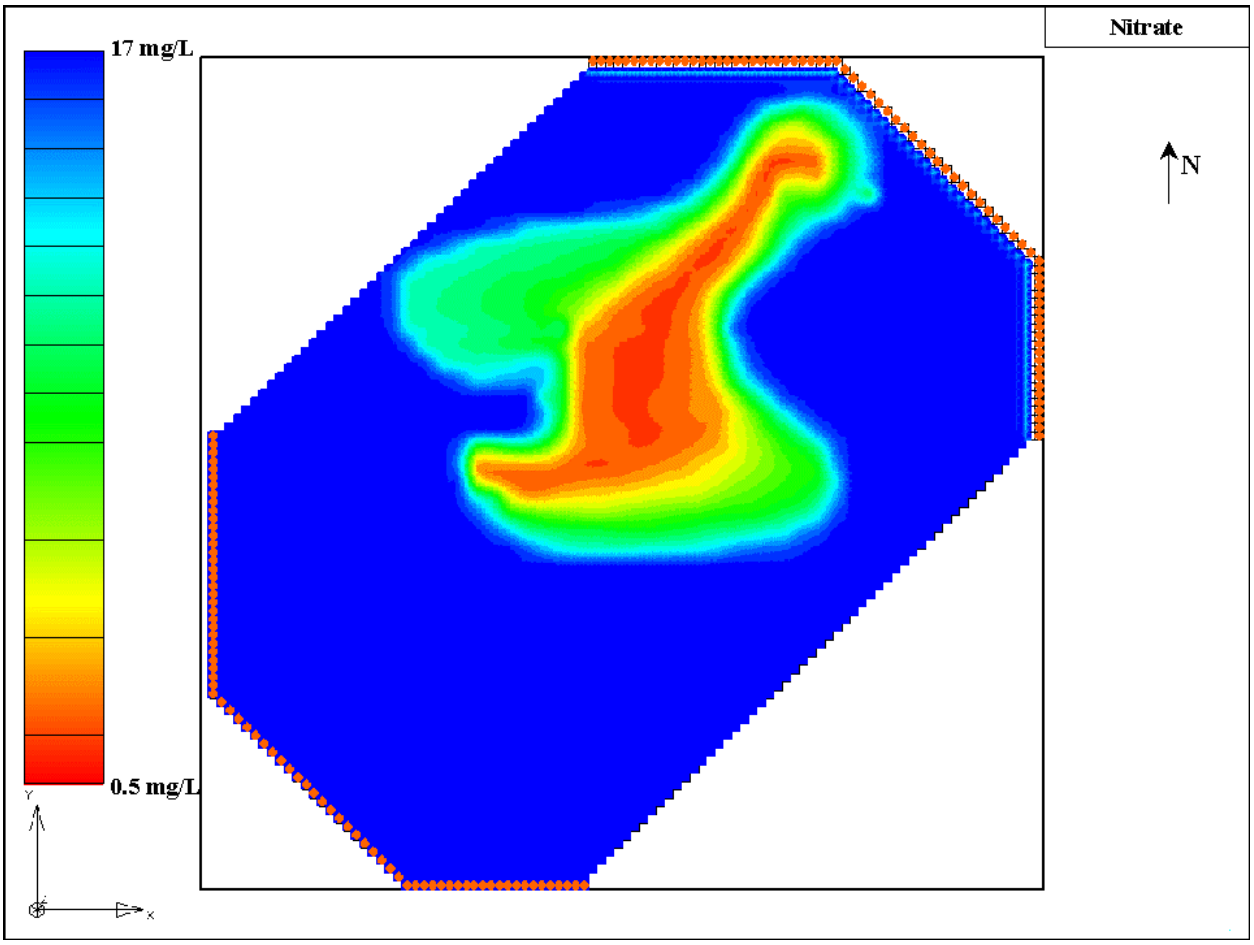

Figure 12. Contoured map of the initial nitrate concentrations

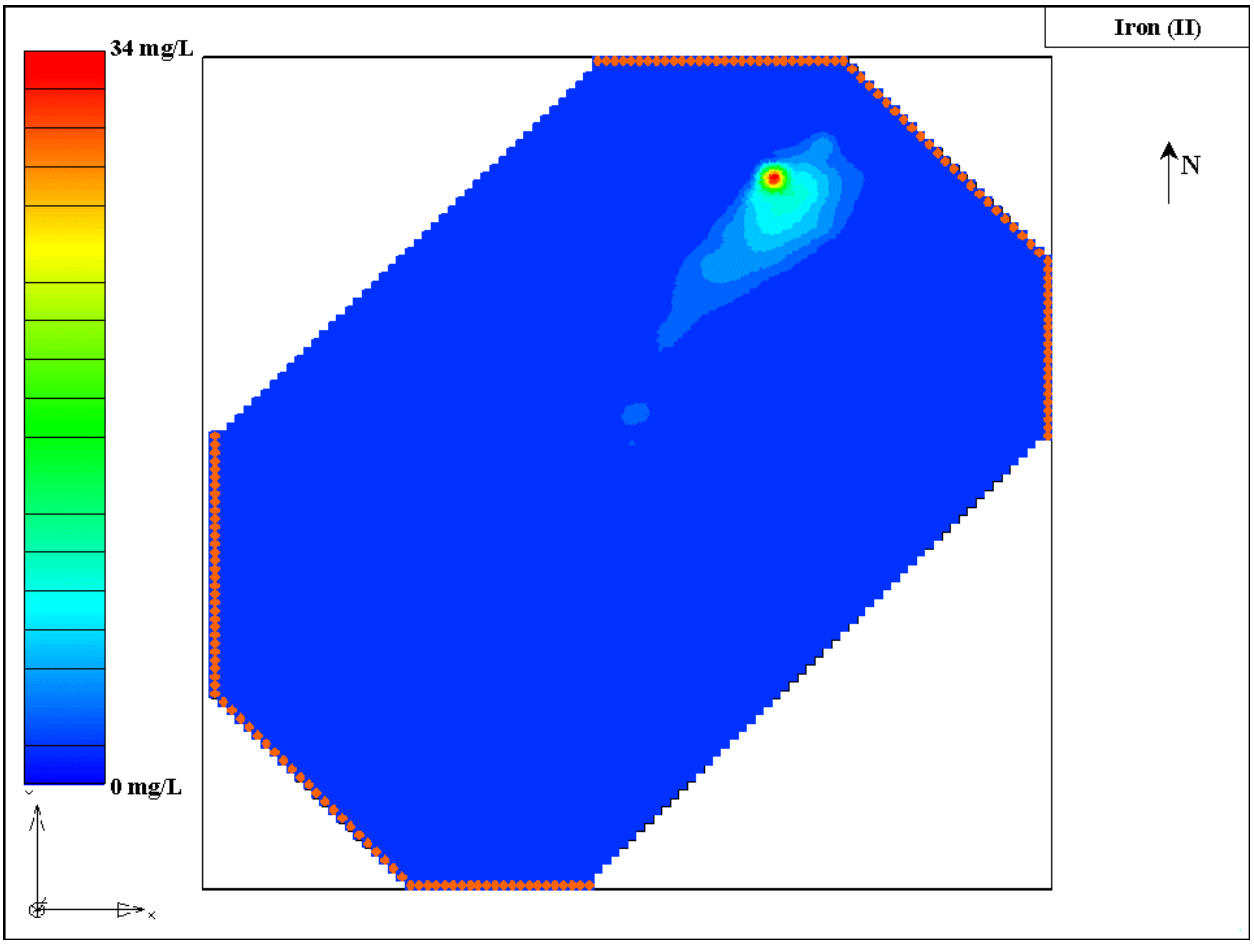

Figure 13. Contoured map of the initial iron (II) concentrations

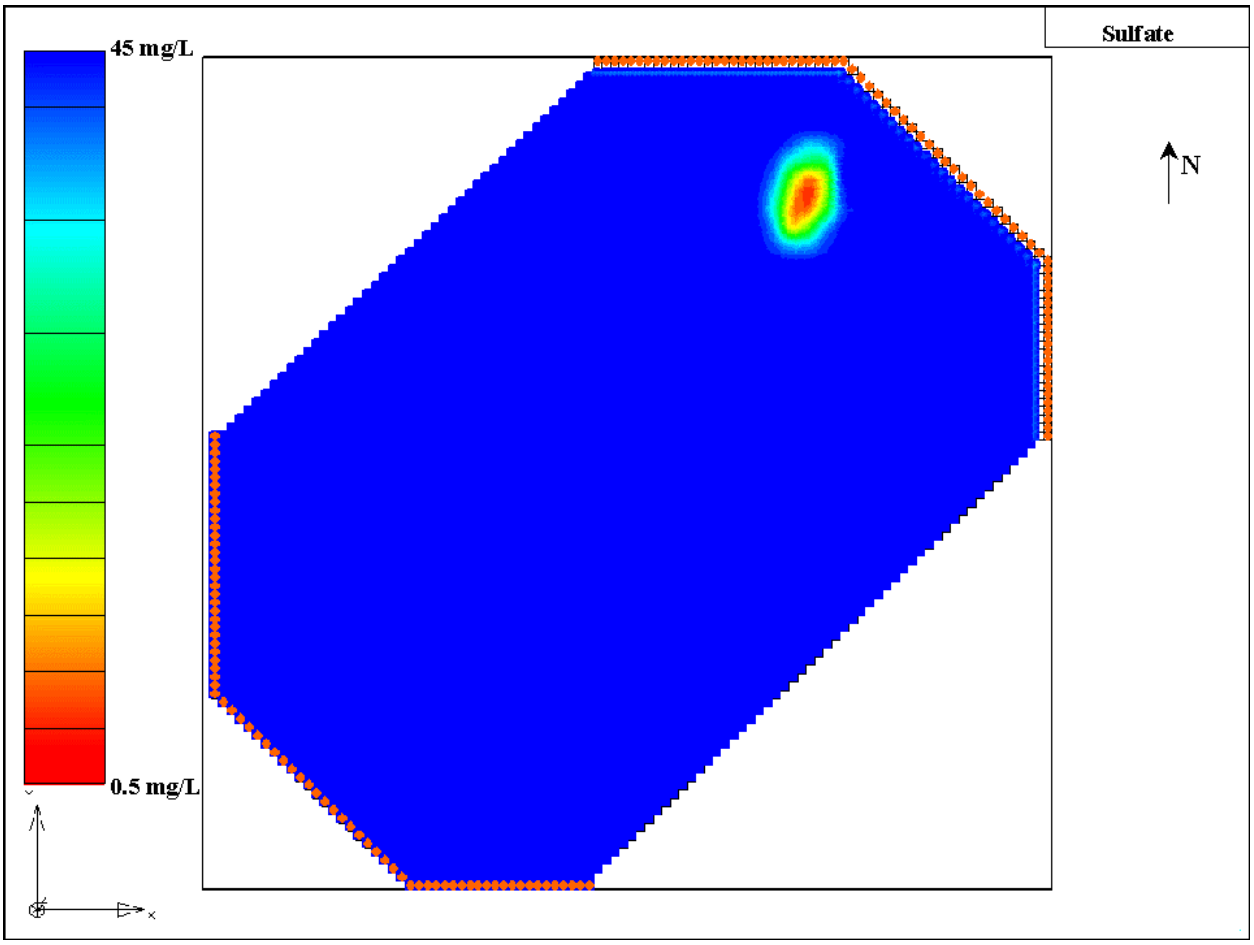

Figure 14. Contoured map of the initial sulfate concentrations

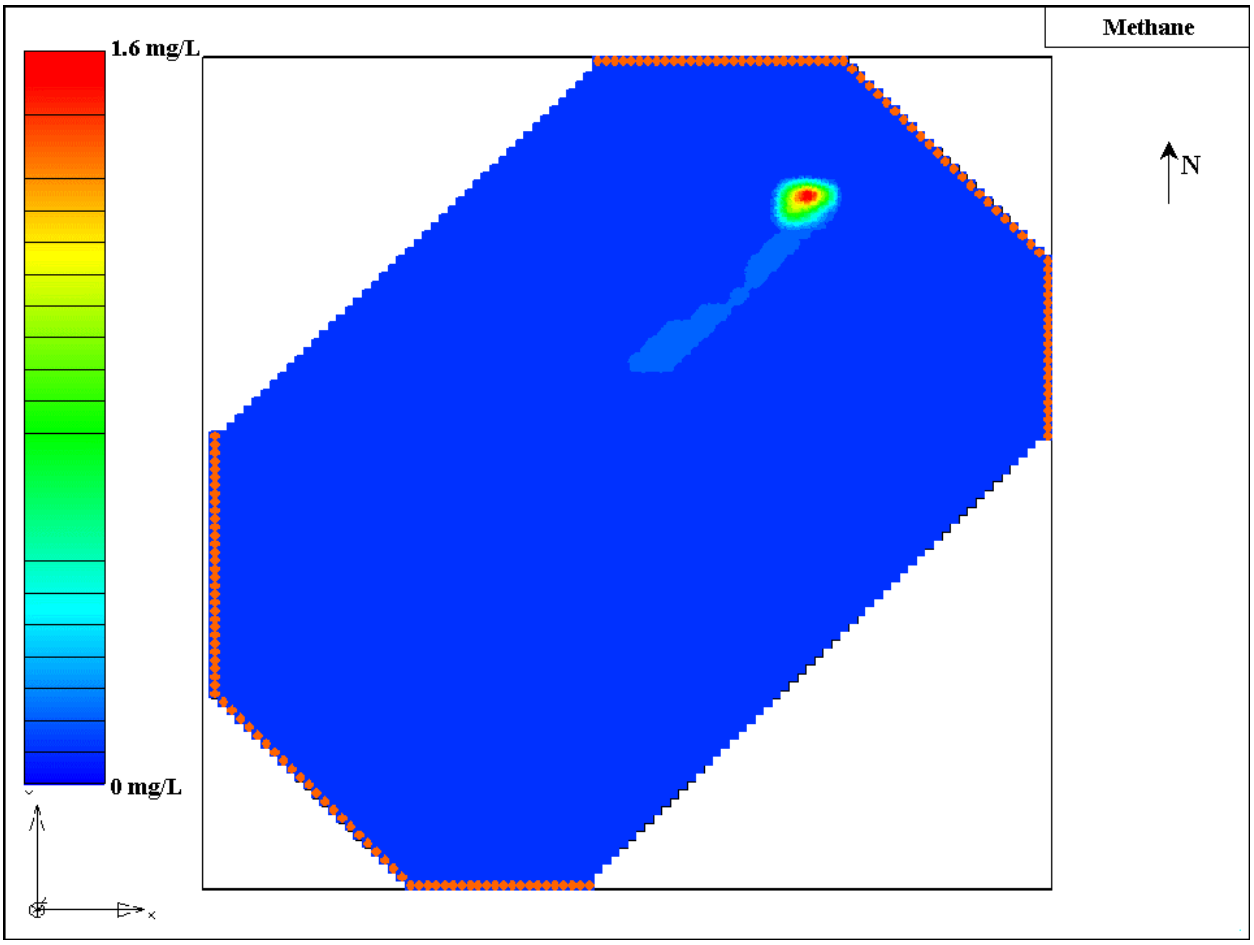

Figure 15. Contoured map of the initial methane concentrations

Bibliography

ASCE Task Committee on Geostatistical Techniques, Review of Geostatistics in Geohydrology I: Basic Concepts, *Journal of Hydraulic Engineering*, 116(5), 612-632, 1990a.

ASCE Task Committee on Geostatistical Techniques, Review of Geostatistics in Geohydrology II: Applications, *Journal of Hydraulic Engineering*, 116(5), 633-658, 1990b.

ASTM, *Standard Guide for Risk-Based Corrective Action Applied at Petroleum Release Sites* (E1739-95), American Society for Testing and Materials, West Conshohocken, PA, 1995.

Borden, R. C., R. A. Daniel, L. E. LeBrun IV, and C. W. Davis, Intrinsic biodegradation of MTBE and BTEX in a gasoline-contaminated aquifer, *Water Resources Research*, 33(5), 1105-1115, 1997.

Chapelle, Francis, H., Bioremediation of Petroleum Hydrocarbon-Contaminated Ground Water: The Perspectives of History and Hydrology, *Ground Water*, 37(1), 122-132, 1999.

Chiang, C. Y., J. P. Salanitro, E. Y. Chai, J. D. Colthart, and C. L. Klein, Aerobic Biodegradation of Benzene, Toluene, and Xylene in a Sandy Aquifer-Data Analysis and Computer Modeling, *Ground Water*, 27(6), 823-834, 1989.

Christakos, G. and Olea, R. A., A multiple-objective optimal exploration strategy, *Mathematical and Computer Modeling*, 11, 413-418, 1988.

Cieniawski, Scott, E., J. Wayland Eheart, and S. Ranjithan, Using genetic algorithms to solve a multiobjective groundwater monitoring problem, *Water Resources Research*, 31(2), 399-409, 1995.

Clement, T. P., Y. Sun, B. S. Hooker, and J. N. Petersen, Modeling Multispecies Reactive Transport in Ground Water, *Ground Water Monitoring and Remediation*, 18(2), 79-92, 1998.

Cooper, R. M., and J. D. Istok, Geostatistics applied to groundwater contamination I: Methodology, *Journal of Environmental Engineering*, 114(2), 270-285, 1988a.

Cooper, R. M., and J. D. Istok, Geostatistics applied to groundwater contamination II: Application, *Journal of Environmental Engineering*, 114(2), 287-299, 1988b.

Cooper, R. M., and J. D. Istok, Geostatistics applied to groundwater pollution III: Global Estimates, *Journal of Environmental Engineering*, 114(4), 915-928, 1988c.

De Jong, K. A., An analysis of the behavior of a class of genetic adaptive systems, Ph.D. dissertation, University of Michigan, Ann Arbor, MI, 1975.

Deutsch, Clayton V., and Andre G. Journel, *GSLIB: Geostatistical Software Library and User's Guide*, Oxford University Press, New York, NY, 1992.

Everitt, L. G., L. G. Wilson, and L. G. McMillon, Vadose zone monitoring concepts for hazardous waste sites, *Ground Water*, 20(3), 312-324, 1982.

Goovaerts, Pierre, *Geostatistics for Natural Resource Evaluation*, Oxford University Press, New York, NY, 1997.

Goldberg, David E., *Genetic Algorithms in Search, Optimization, and Machine Learning*, Addison-Wesley, New York, NY, 1989.

Goldberg, D. E., and K. Deb, A comparative analysis of selection schemes used in genetic algorithms, in *Foundations of Genetic Algorithms*, pp. 69-93, Morgan Kaufman, San Mateo, CA, 1991.

Goldberg, D. E., K. Deb, and James H. Clark, Genetic algorithms, Noise, and the Sizing of Populations, *Complex Systems*, 6, 333-362, 1992.

Goldberg, D. E., Making Genetic Algorithms Fly: A Lesson from the Wright Brothers, in *Advanced Technology for Developers*, 2, 1-8, 1993.

Harik, G.R., E. Cantú-Paz, D. E. Goldberg, and B. L. Miller, The gambler's ruin problem, genetic algorithms, and the sizing of populations, *Proceedings of the 1997 IEEE Conference on Evolutionary Computation*, pp. 7-12, IEEE Press, New York, NY, 1997.

Holland, J. H., *Adaptation in Natural and Artificial Systems*, University of Michigan, Ann Arbor, Michigan, 1975.

Hsueh, Y. W., and R. Rajagopal, Modeling ground-water quality decisions, *Ground-Water Monitoring Review*, 8(4), 121-134, 1988.

Hudak, P. F., and H. A. Loaiciga, A location modeling approach for groundwater monitoring network augmentation, Water Resources Research, 28(3), 643-649, 1992.

Hudak, P.F., and H. A. Loaiciga, An optimization method for monitoring network design in multilayered groundwater flow systems, *Water Resources Research*, 29(8), 2835-2845, 1993.

James, Bruce, R., and Steven M. Gorelick, When enough is enough: The worth of monitoring data in aquifer remediation design, *Water Resources Research*, 30(12), 3499-3513, 1994.

Kelley, Mark, V. Magar, S. Brauning, J. Shahan, and G. B. Wickramanayake, *Intrinsic Bioremediation of Petroleum Hydrocarbons*, Naval Facilities Engineering Service Center, Technical Report TM-2185-ENV, Port Hueneme, CA, 1996.

Kitanidis, Peter K., *Introduction to Geostatistics with Applications in Hydrogeology*, Cambridge University Press, New York, NY, 1997.

Loaiciga, Hugo, A., An optimization approach for groundwater quality monitoring network design, Water Resources Research, 25(8), 1771-1780, 1989.

Loaiciga, Hugo, A., R. J. Charbeneau, L. G. Everett, G. E. Fogg, B. F. Hobbs, S. Rouhani, Review of Ground-Water Quality Monitoring Network Design, *Journal of Hydraulic Engineering*, 118(1), 11-37, 1992.

Lu, G., C. Zheng, and T. P. Clement, Simulating Natural Attenuation of BTEX at the Hill Air Force Base in Utah, *Ground Water,* In Press, 1999.

Massmann, J., and R. A. Freeze, Groundwater contamination from waste management sites: The interaction between risk-based engineering design and regulatory policy, 1, Methodology, *Water Resources Research*, 23(2), 351-367, 1987a.

Massmann, J., and R. A. Freeze, Groundwater contamination from waste management sites: The interaction between risk-based engineering design and regulatory policy, 2, Results, *Water Resources Research*, 23(2), 368-380, 1987b.

McDonald, Michael, G., and Arlen W. Harbaugh, *Techniques of Waster Resources Investigations of the United States Geological Survey: A Modular Three-Dimensional Finite-Difference Ground-Water Flow Model*, United States Geological Survey, Washington, D.C., 1988.

Meyer, P. D., and E. D. Brill, A method for locating wells in a groundwater monitoring under conditions of uncertainty, *Water Resources Research*, 24(8), 1277-1282, 1988.

Meyer, P.D., Albert J. Valocchi, and J. Wayland Eheart, Monitoring network design to provide initial detection of groundwater contamination, Water Resources Research, 30(9), 2647-2659, 1994.

McAllister, P.M., and C. Y. Chiang, A practical approach to evaluating natural attenuation of contaminants in ground water, *Ground Water Monitoring and Remediation,* 14(2), 161-173, 1994.

McKinney, D. C., and M. D. Lin, Genetic algorithm solution of groundwater management models, *Water Resources Research*, 30(6), 1897-1906, 1994.

National Research Council, *In Situ Bioremediation: When Does It Work?,* National Academy Press, Washington, D.C., 1993.

National Research Council, *Environmental Cleanup at Navy Facilities: Risk-Based Methods*, National Academy Press, Washington, D.C., 1999.

Nyer, Evan, Polly Mayfield, and Joseph Hughes, Beyond the AFCEE Protocol for Natural Attenuation, *Ground Water Monitoring and Remediation*, 18(3), 70–77, 1998.

Olea, R. A., Sampling design optimization for spatial functions, *Mathematical Geology*, 16(4), 365-391, 1984.

Rast, R., ed., *Environmental Restoration: Assemblies Cost Book*, R. S. Means Company, Kingston, MA, 1997a.

Rast, R., ed., *Environmental Restoration: Unit Cost Book*, R. S. Means Company, Kingston, MA, 1997b.

Ritzel, Brian J., J. Wayland Eheart, and S. Ranjithan, Using genetic algorithms to solve a multiple objective groundwater pollution containment problem, *Water Resources Research*, 30(5), 1589-1603, 1994.

Rouhani, S., Variance reduction analysis, *Water Resources Research*, 21(6), 837-846, 1985.

Rouhani, S., and T. J. Hall, Geostatistical schemes for groundwater sampling, *Journal of Hydrology*, 103, 85-102, 1988.

Smalley, J. B., *Risk-Based In-Situ Bioremediation Design,* M.S. Thesis, University of Illinois, Department of Civil and Environmental Engineering, Urbana, IL, 1998.

Smalley, J. B., and B. Minsker, Risk-based in situ bioremediation design using a noisy genetic algorithm, *Water Resources Research*, submitted 1999.

Storck, Pascal, J. Wayland Eheart, and Albert J. Valocchi, A method for the optimal location of monitoring wells for detection of groundwater contamination in three-dimensional aquifers, *Water Resources Research*, 33(9), 2081-2088, 1997.

Thierens, Dirk, and David E. Goldberg, Mixing in Genetic Algorithms, *Proceedings of the Fifth International Conference on Genetic Algorithms*, edited by S. Forrest, pp.38-45, Morgan Kaufmann Publishers, San Mateo, CA, 1993.

Thierens, D., *Analysis and design of genetic algorithms*, Doctoral dissertation, Katholieke Universiteit Leuven, Leuven, Belgium, 1995.

U. S. Environmental Protection Agency, *RCRA groundwater monitoring technical enforcement guidance document*, Office of Solid Waste and Emergency Response, (OSWER 9950.1), 1986.

U. S. Environmental Protection Agency, *Cleaning Up the Nation's Waste Sites: Markets and Technology Trends*, Office of Solid Waste and Emergency Response, (EPA 542-R-96-005), Washington, D.C., 1996.

U. S. Environmental Protection Agency, *Use of Monitored Natural Attenuation at Superfund, RCRA Corrective Action, and Underground Storage Tank Sites,* Office of Solid Waste and Emergency Response, (OSWER Directive 9200.4-17), 1997.

Wang, Q. J., The genetic algorithm and its application to calibration conceptual rainfall-runoff models, *Water Resources Research*, 27(9), 2467-2471, 1991.

Wiedemeier, T., J. T. Wilson, D. H. Kampbell, R. N. Miller, and J. E. Hansen, *Technical Protocol for Implementing Intrinsic Remediation with Long-Term Monitoring for Natural Attenuation of Fuel Contamination Dissolved in Groundwater,* Volume I, Air Force Center for Environmental Excellence Technology Transfer Division, San Antonio, TX, 1995a.

Wiedemeier, T., J. T. Wilson, D. H. Kampbell, R. N. Miller, and J. E. Hansen, *Technical Protocol for Implementing Intrinsic Remediation with Long-Term Monitoring for Natural Attenuation of Fuel Contamination Dissolved in Groundwater,* Volume II, Air Force Center for Environmental Excellence Technology Transfer Division, San Antonio, TX, 1995b.

Wiedemeier, T., M. A. Swanson, D. E. Moutoux, and E. K. Gordon, *Technical Protocol for evaluating Natural Attenuation of Chlorinated Solvents in Groundwater,* Air Force Center for Environmental Excellence Technology Transfer Division, San Antonio, TX, 1996.

Yfantis, E. A., G. T. Flatman, and J. V. Behar, Efficiency of kriging estimation for square, triangular, and hexagonal grids, *Mathematical Geology*, 19(3), 183-205, 1987.