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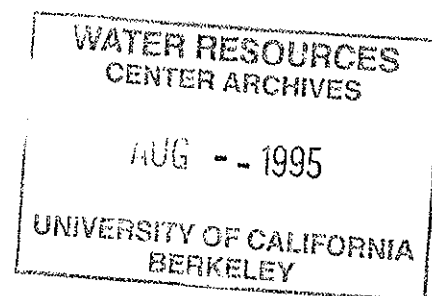
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OPTIMAL WELL NETWORK DESIGN FOR SUBSURFACE REMEDIATION AND POLLUTANT CONTAINMENT

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TECHNICAL COMPLETION REPORT

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OPTIMAL WELL NETWORK DESIGN FOR SUBSURFACE REMEDIATION AND POLLUTANT CONTAINMENT

ABSTRACT

A methodology for the restoration and cleanup of existing subsurface contaminated sites and for the containment of pollutants is developed. The remediation problem is posed as an optimization model where the rates and locations of pumping and injections are to be determined given the characteristics and extent of the contamination plume. The solution of the remediation problem is based on the econometric method of feedback control coupled with ground water flow and transport simulations. For site characterization and monitoring of the contaminant distribution and extent, an optimal sampling methodology is presented. The sampling design is based on geostatistical methods and yields optimal estimation of the subsurface parameters and pollutant concentrations, therefore providing informed decision-making for ground water remediation and contaminant removal. The remediation plan is optimized so as to lower the contamination level to a pre-specified level by the end of the remediation period while minimizing the cost of pumping and treatment. The objective function of the optimal feedback control model consists of a successive minimization of a weighted sum of squared deviations of the achieved cleanup level at each stage from the desired target level of ground water quality.

KEY WORDS: Ground Water Remediation, Optimization, Decision Models, Statistics, Contaminant Transport, Dynamic Programming, Water Quality Monitoring.

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NOTATION

A	global sorption matrix
$A^{(e)}$	element sorption matrix
A_t	econometric model coefficient matrix
\mathbf{a}_t	target value for the state variable
B	budget limit
B_t	econometric model coefficient matrix
C	solute concentration
$C^{(e)}$	finite element approximation for the solute concentration within element e
C_i	unknown solute concentration at node i
c_k	unit monitoring cost
\mathbf{c}_t	econometric model coefficient vector
\mathbf{C}_t	state variable vector containing pollutant concentrations
D	mechanical dispersion coefficient
$[D]$	global advection-dispersion matrix
$D^{(e)}$	element advection-dispersion matrix
D^*	molecular diffusion coefficient
D_h	hydrodynamic dispersion coefficient
D_m	solute molecular diffusion coefficient
F	global source/sink matrix
$F^{(e)}$	element source/sink matrix
F_t	econometric model coefficient matrix

G_t	feedback coefficient matrix
g_t	feedback coefficient matrix
h	piezometric head
Hg	total mercury concentration
I	identity matrix
Ig	grain size index
J	cost-to-go function
K	hydraulic conductivity
K_d	distribution coefficient
K_t	Ricatti matrix
M	solute source/sink
N	number of remediation time periods
n	porosity
N_m	number of monitoring nodes
p_t	econometric model coefficient vector
q	flow source/sink
q_{adv}	advective flux
q_{dif}	diffusive flux
q_{dis}	dispersive flux
q_T	total flux
r_0	efficiency criterion
R_i	finite element residual at node i

S	aquifer storativity
\mathbf{T}	aquifer transmissivity tensor
Tr	trace of a matrix
\mathbf{u}_t	control vector at stage t
\mathbf{V}	average ground water flow velocity
\mathbf{v}	ground water flow velocity
\mathbf{w}_t	econometric model coefficient vector
\mathbf{W}_t	penalty matrix
\mathbf{x}	space location
$\mathbf{Z}(\mathbf{x})$	value of a variable at space location \mathbf{x}
\mathbf{Z}^*	cokriging estimator for variable Z
α	dispersivity
α_L	longitudinal dispersivity
α_T	transversal dispersivity
Φ_t	feedback control model transition coefficient
ϕ	finite element basis function
Γ	matrix of cokriging coefficients
γ	variogram model
γ_{ij}	cross-variogram model
Ξ	econometric model coefficient matrix
Ψ_t	feedback control model transition matrix
Λ	feedback model coefficient matrix

λ	solute decay coefficient
λ_{ij}	cokriging coefficient
λ_t	econometric model coefficient vector
μ	Lagrange multiplier
μ_t	vector of random disturbances
η_t	feedback control model transition coefficient
ρ_b	bulk density of the porous medium
σ^2	variance of estimation
Θ	econometric model coefficient matrix
Θ_t	feedback control model transition coefficient
θ_t	feedback control model transition coefficient
τ	tortuosity of the porous medium

OPTIMAL WELL NETWORK DESIGN FOR SUBSURFACE REMEDIATION AND POLLUTANT CONTAINMENT

1. INTRODUCTION

1.1. Background:

Ground water remediation and aquifer restoration effectiveness is contingent upon the level of technical and technological expertise available. The extent and limits of remediation are, however, dependent additionally on the existing regulations, environmental protection goals, and economic factors such as the costs associated with the removal and treatment of pollutants. Given the high costs associated with remediation works due to the complexities of the subsurface conditions, high level of priority should be given to the design and planning of remediation strategies. Advances and progress in the domain of remediation design methodologies and accurate understanding of the phenomena governing subsurface flows and contaminant transport are as important as the enhancement of remediation techniques and practices. As the goal of ground water remediation is to restore the water quality to its pre-contamination condition, which is almost practically impossible, remediation efforts become a compromise given the existing regulations, the cost effectiveness of the cleanup, and the availability of information.

1.2. Statement Of The Problem:

Ground water contamination has become a serious problem in various parts of the state and the nation. A contaminated aquifer becomes a health hazard and a source of pollution that contributes to further degradation of the ground water quality in its vicinity.

Thus, rational and appropriate methods for aquifer remediation and pollutant containment are urgently needed to limit the progressive spreading of pollutants and prevent further contamination.

To correctly address the problem of subsurface pollution, it is essential to closely study the distribution and variability of the physical properties of the subsurface environment as well as understand the chemical and biological processes affecting the movement and fate of the contaminant. This project proposes a methodology for increasing the efficiency of remediation efforts using econometric methods.

1.3. Research Objectives:

The main objective of this research is to design an optimal plan to address the contamination problem in the subsurface environment. Toward the fulfillment of this objective, two main tasks are identified: (1) To develop an analytical method that systematically designs an optimal remediation network aiming to achieve a maximum, economically feasible, level of subsurface cleanup as well as prevent the migration and spreading of pollutants; and (2) to formulate a remediation strategy as a feedback control problem to determine optimal pumping and injection rates throughout the remediation horizon. This strategy is coupled with an optimal monitoring program so as to supply the control algorithm with accurate estimates of the state variables (e.g., pollutant concentrations and flow parameters) yielding a reliable description of the state of the ground water system.

2. MONITORING AND SITE CHARACTERIZATION

2.1. Introduction:

The success of any remediation technique depends highly on the site characterization, including the knowledge of the physical properties of the contaminated site, the phenomena affecting the movement and fate of the pollutants, and the accurate estimation of the parameters governing the contaminant transport and the ground water hydraulics. In this regard, monitoring constitutes the basic tool for acquiring information on different aspects of ground water flow and contaminant transport. The changes occurring within the ground water system, such as pollutant spreading and migration, are not obviously seen or detected given the aquifer physical structure. As a result, observation systems are needed for the purpose of increasing our knowledge about the subsurface environment and ameliorate our estimation of the governing parameters. Within the context of ground water remediation efforts, monitoring is considered as an essential tool for determining and analyzing the state of the quality of the ground water so as to obtain the necessary information for control decisions and management plans. Monitoring is also an important follow-up tool for assessing the effectiveness of remediation measures once they are applied.

2.2. Review of the Literature:

A number of studies have addressed the problem of monitoring network design. The design criteria and constraints are generally dictated by the specificities of the addressed problem as well as the pre-set objectives of the monitoring program. Showalter (1985) discussed how the objectives of a groundwater quality monitoring network are developed and how they are implemented in the design process. Hsueh and Rajagopal (1988) developed a model for groundwater quality sampling design with an emphasis on prevention of population exposure to contaminants. Most of the optimization techniques which have been employed to approach the problem of network design either maximize or minimize a given objective function while accounting for some other constraints. Among the proposed methodologies, a number of them consider the minimization of the variance of the monitored parameter estimates. Carrera *et al.* (1984) applied the kriging method to determine the optimal locations of sampling sites for the estimation of fluoride concentrations in groundwater. Rouhani (1985) proceeded by minimizing the variance of estimation using a variance-reduction algorithm; sampling sites which provide the maximum reduction in the variance of estimation are added to the monitoring network each at a time. Loaiciga (1989) defined the network optimization problem for the estimation of chloride concentrations in groundwater as a mixed-integer programming model. Woldt and Bogardi (1992) used a modified variance-reduction algorithm combined with a multi-criteria decision making using composite programming for designing ground water quality monitoring networks. McKinney and Loucks (1992) presented an algorithm for selecting

new monitoring locations so as to minimize the simulation model prediction variance. Loaiciga et al. (1992) reported a comprehensive literature review on groundwater quality monitoring network design, in which two main approaches were identified: the hydrogeological approach and the statistical approach. Unlike the latter, the former is fully based on qualitative and quantitative hydrogeological information (e.g., Everett, 1980). Quinlan et al. (1993) have examined the difficult problem of ground water monitoring in karstic aquifers.

The D-optimality approach, a parameter estimation criterion by which one minimizes the area of any $1-\alpha$ joint confidence region around the parameter estimates, has been frequently used in the domain of network design (Casman *et al.*, 1988; Nishikawa and Yeh, 1989; and Kettunen *et al.*, 1989). Knopman and Voss (1987, 1988b) examined the effect of change in solute concentration on parameter estimation and sampling design. They also addressed the problem of discrimination among solute transport models and how a sampling strategy affects model discrimination (Knopman and Voss, 1988a). Meyer and Brill (1988) used a Monte Carlo simulation of contaminant transport coupled with an optimization model for the design of a groundwater monitoring network with the goal of maximizing the probability of detection of a contaminant. Management and monitoring of ground water has been also treated as discrete time optimal control problems (Makinde-Odusola and Mariño, 1989; and Andricevic, 1990).

2.3. Procedure:

The sampling network design presented is based on the geostatistical method of cokriging which will be briefly outlined here. A more detailed theoretical development on the use of geostatistics in the domain of network design can be found in Ben-Jemaa *et al.* (1994). For a comprehensive description of the cokriging method the reader is referred to Journel and Huijbregts (1978), Myers (1982), and De Marsily (1986).

Geostatistics has been widely applied to hydrological problems. Aboufirassi and Mariño (1984) used cokriging to construct maps of aquifer transmissivity. Cokriging has been also used to assess stream water quality (Jager *et al.*, 1990; Seo *et al.*, 1990a, 1990b).

Ahmed and De Marsily (1987) compared a number of geostatistical methods for the estimation of aquifer transmissivity. Carrera *et al.* (1984) employed kriging for optimal sampling design of groundwater quality. Shamsi *et al.* (1988) used universal kriging for the design of a raingauging network.

Kriging and cokriging are estimation techniques via linear interpolation, providing best linear unbiased estimators known as "BLUE". The estimator consists of a linear combination of available observations. Equation (1) is the expression for the cokriging estimator; the kriging estimator is given by the special case in which a single variable is considered.

$$Z_j^*(x_0) = \sum_{i=1}^M \sum_{k=1}^{N_i} \lambda_{ij}^k Z_i(x_k) \quad j = 1, \dots, M \quad (1)$$

in which $Z_j^*(x_0)$ = the cokriging estimator of variable Z_j at space location x_0 ; λ_{ij}^k = the cokriging coefficient representing the contribution to the estimation of Z_j by the observation point of Z_i taken at location x_k ; M = the total number of regionalized variables used in cokriging; and N_i = the total number of observation points available for variable Z_i and used in the estimation. The above cokriging estimator Z^* could be a given contaminant concentration at location x_0 , while, if $M=2$, then Z_1 could represent the contaminant concentration and Z_2 could represent the hydraulic conductivity measured at N_1 and N_2 locations, respectively. The unbiasedness of the above estimator can be expressed in terms of the cokriging coefficients as:

$$\sum_{k=1}^{N_i} \lambda_{ii}^k = 1 \quad \text{for each } i \quad (2a)$$

and

$$\sum_{k=1}^{N_i} \lambda_{ij}^k = 0 \quad \text{for } i \neq j \quad (2b)$$

By minimizing the variance of the error of estimation:

$$\sigma^2 = E \left\{ [Z^*(x_0) - Z(x_0)]^2 \right\} \quad (3)$$

or, in the case of estimating the mean value over a block V , Z_V :

$$\sigma_V^2 = E \left\{ [Z_V^* - Z_V]^2 \right\} \quad (4)$$

and introducing the variogram and cross-variogram notation:

$$\gamma(h) = \frac{1}{2} E \left\{ [Z(x+h) - Z(x)]^2 \right\} \quad (5)$$

$$\gamma_{ij}(h) = \frac{1}{2} E \left\{ [Z_i(x+h) - Z_i(x)] [Z_j(x+h) - Z_j(x)] \right\} \quad (6)$$

a system of equations known as the cokriging equations is obtained (Myers 1982)

$$\sum_{k=1}^N \bar{\gamma}(x_k - x_{k'}) \Gamma_k + \bar{\mu} = \bar{\gamma}^{x_{k'}V}; \quad k' = 1, \dots, N \text{ (taking } N_i = N \text{ for all } i\text{'s)} \quad (7a)$$

and

$$\sum_{k=1}^N \Gamma_k = I \quad (7b)$$

in which

$$\bar{\gamma}(x - y) = \begin{pmatrix} \gamma_{11}(x - y) & \cdots & \gamma_{1M}(x - y) \\ \vdots & \ddots & \vdots \\ \gamma_{M1}(x - y) & \cdots & \gamma_{MM}(x - y) \end{pmatrix} \quad (8a)$$

$$\bar{\gamma}^{x_{k'}V} = \begin{pmatrix} \gamma_{11}^{x_{k'}V} & \cdots & \gamma_{1M}^{x_{k'}V} \\ \vdots & \ddots & \vdots \\ \gamma_{M1}^{x_{k'}V} & \cdots & \gamma_{MM}^{x_{k'}V} \end{pmatrix} \quad (8b)$$

are matrices of variogram and cross-variogram models;

$$\bar{\mu} = \begin{pmatrix} \mu_{11} & \cdots & \mu_{1M} \\ \vdots & \ddots & \vdots \\ \mu_{M1} & \cdots & \mu_{MM} \end{pmatrix} \quad (9)$$

is a matrix of Lagrange multipliers;

$$\Gamma_k = [\lambda_{ij}^k] = \begin{pmatrix} \lambda_{11}^k & \dots & \lambda_{1M}^k \\ \vdots & \ddots & \vdots \\ \lambda_{M1}^k & \dots & \lambda_{MM}^k \end{pmatrix} \quad (10)$$

is a matrix of cokriging coefficients, $\gamma_{ij}(\mathbf{x}-\mathbf{y})$ denotes the cross-variogram of variables Z_i and Z_j at space locations \mathbf{x} and \mathbf{y} , respectively, I is the identity matrix, and γ^{xv} denotes the mean value of $\gamma(\mathbf{h})$ when one extremity of the vector \mathbf{h} is fixed at point \mathbf{x} and the other extremity varies to describe the estimation block V . γ^{xv} can be written as:

$$\gamma^{xv} = \frac{I}{|V|} \int_V \gamma(\mathbf{x} - \mathbf{y}) d\mathbf{y} \quad (8)$$

By solving the cokriging system of equations (7), the cumulative variance of estimation, consisting of the sum of the individual estimation variances of all the cokriged variables (Myers, 1984), can be calculated by:

$$\sigma^2 = Tr \left(\sum_{k=1}^N \bar{\gamma}^{xkv} \Gamma_k \right) + Tr \left(\bar{\mu} - \bar{\gamma}^{vv} \right) \quad (9)$$

in which Tr denotes the trace of the matrix and γ^{vv} is given by:

$$\gamma^{vv} = \frac{I}{|V|^2} \int_V \int_V \gamma(\mathbf{x} - \mathbf{y}) d\mathbf{x} d\mathbf{y} \quad (10)$$

It is important to note that the cokriging system of equations as well as the estimation variance, expressed in terms of the variogram and cross-variogram models, depend only on the distances between sampling points, hence on the geometry of the

sampling network. This is an important feature that makes cokriging a suitable tool in the domain of network design where the goal is to find the best layout of the sampling network.

2.4. Monitoring Model Development

Given the fact that estimates of pollutant concentrations are very important inputs for remediation models, a plausible sampling network is one that provides accurate parameter estimates with low variance of the error of estimation. The total monitoring cost is also an important factor in the sampling network design. To increase monitoring efficiency, a network design yielding a low monitoring cost is preferred. The optimization of a sampling network is therefore a multiobjective problem. There exists a tradeoff between the two objectives described above, namely monitoring cost reduction and estimation variance minimization. To proceed with the network optimization, two optimization models are presented: the first model consists of minimizing the variance of estimation subject to a given budget constraint (Ben-Jemaa *et al.* 1994), and the second model consists of minimizing the total monitoring cost and assessing the significance of any decrease in the variance of estimation produced by additional monitoring expenditures.

In the case of the variance minimization approach (model one), a monitoring budget limit will be set as the model constraint and the optimization model will be written as:

$$\underset{\Gamma_k, \mu}{\text{Minimize}} \quad Tr \left(\sum_{k=1}^{N_m} \bar{\gamma}^{x_k V} \Gamma_k \right) + Tr \left(\bar{\mu} - \bar{\gamma}^{VV} \right) \quad (11)$$

subject to the unbiasedness of the estimation:

$$\sum_{k=1}^{N_m} \Gamma_k = I \quad (12)$$

and to the resource availability:

$$\sum_{k=1}^{N_m} c_k \leq B \quad (13)$$

in which N_m = the total number of sampling sites; c_k = the unit monitoring cost at space location k ; and B = the budget limit. From the cokriging equations (7), one can see that values of the cokriging coefficients depend on the estimation domain as well as the sampling locations (\mathbf{x}). Noting that variogram and cross-variogram models are also dependent on the sampling locations, the matrix product between Γ and γ in the objective function (11) makes the latter nonlinear.

When using the cost minimization approach (model two), a given value of the variance of estimation that could be considered as a reasonable limit for the estimation accuracy level, can be used as the model constraint. A more comprehensive approach would be to impose a constraint on the additional information gain per unit increase in monitoring cost. Thus, the model constraint will consist of a lower limit for the rate of decrease in the estimation variance per unit cost added so as to maintain an economically efficient design. The optimization model can then be formulated as:

$$\text{Minimize } \sum_{k=1}^{N_m} c_k \quad (14)$$

subject to the efficiency criterion:

$$\frac{\Delta \sigma^2}{|\Delta c|} \geq r_0 \quad (15)$$

and to the unbiasedness of the estimator:

$$\sum_{k=1}^{N_m} \Gamma_k = I \quad (16)$$

2.5. Monitoring Model Application

The presented sampling design is applied for the design of a monitoring network to assess the distribution and extent of mercury contamination in the sediments of Clear Lake, California (Ben-Jemaa *et al.*, 1995). Mercury contamination of the lake originated from the Sulphur Bank Mercury Mine located on the western shore of the lake. Observed data points from Suchanek *et al.* (1993) are used for variogram and cross-variogram calculations. Collected data points consist of observations of total mercury (Hg) in the sediments and the sediment grain size index (I_g). The grain size index describes the particle size distribution and is calculated by assigning a weighing factor for each particle size range as follows: 0 for clay range, 1 for silt range, 2 for sand range, and 3 for gravel range. The grain size index is obtained by multiplying each of the above weighting factors by the corresponding percentages found for each of the four particle size ranges. Figure 1 shows

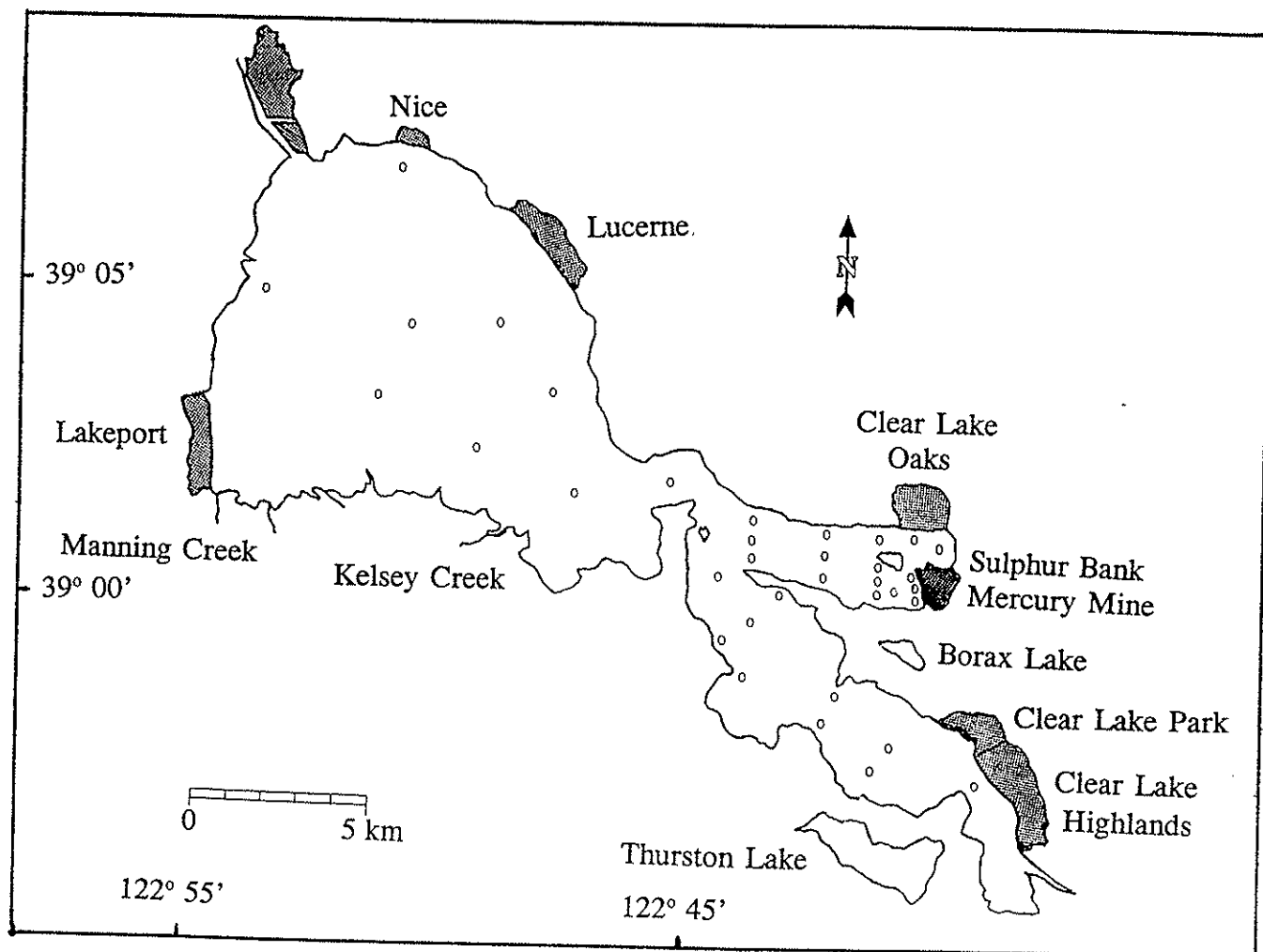


Figure 1. Map of Clear Lake, California

the locations of the observation points within the lake. The data set used in the analysis consists of 35 pairs of average values of Hg and I_g observations taken from several sample replicates. The study by Suchanek *et al.* (1993) shows a considerably low within-site variability (between replicates) as compared to the relatively high between-site variability (between samples taken at different sites).

Experimental variograms are calculated from observed data points using a discrete form of the variogram. Given that mercury data was found to be lognormal, its variogram analysis is carried out in terms of logHg. Analytical functions for the experimental models are then selected from among commonly used variogram models (Journel and Huijbregts, 1978) via a nonlinear least squares fitting technique (Yost *et al.*, 1989). Unlike regular fitting techniques, the variogram fitting technique has a weighting procedure which is proportional to the number of observations per distance class and inversely proportional to the mean class distance. A distance class consists of a group of data pairs which are separated by distances belonging to the same distance range interval *a priori* defined. The calculated experimental variograms for logHg and I_g and their corresponding spherical estimated variograms (γ_1 and γ_2) are shown in Figures 2 and 3, respectively, and expressed as:

$$\gamma_1(h) = 0.22 + 4.03 \times \left(1.5 \times \frac{h}{22} - 0.5 \times \left(\frac{h}{22} \right)^3 \right) \quad (17)$$

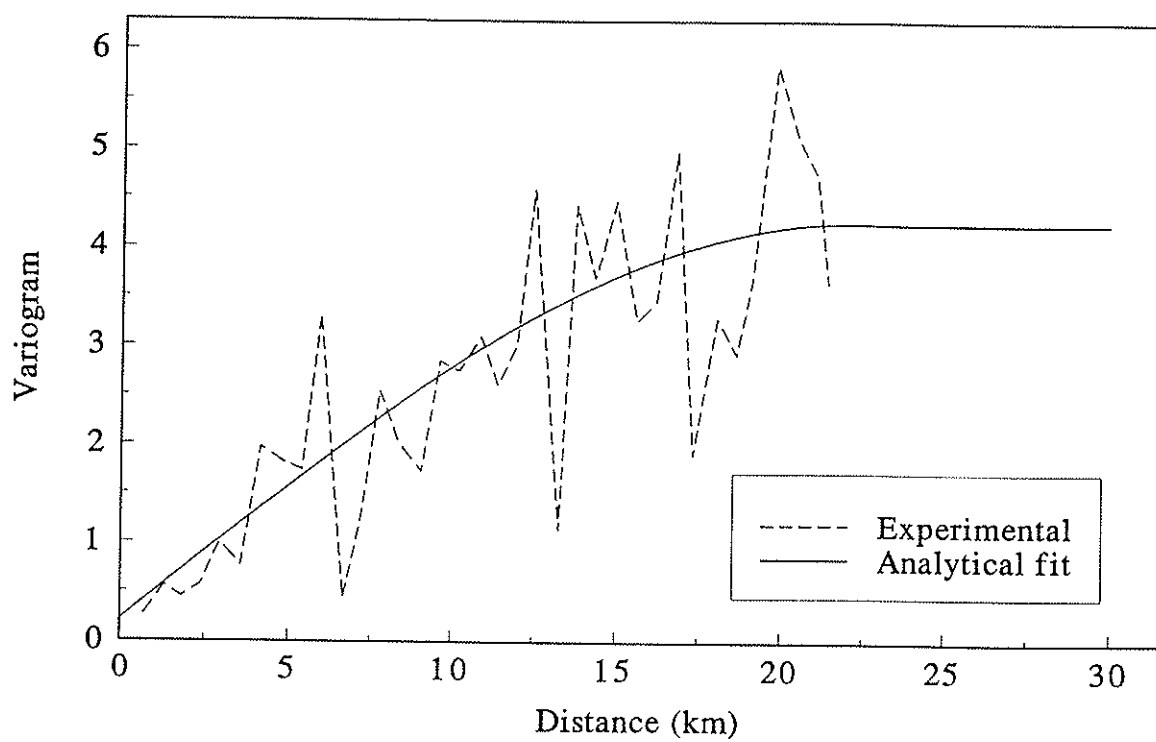


Figure 2. Variogram of logHg: Experimental (dashed line) and Spherical Fit (solid line)

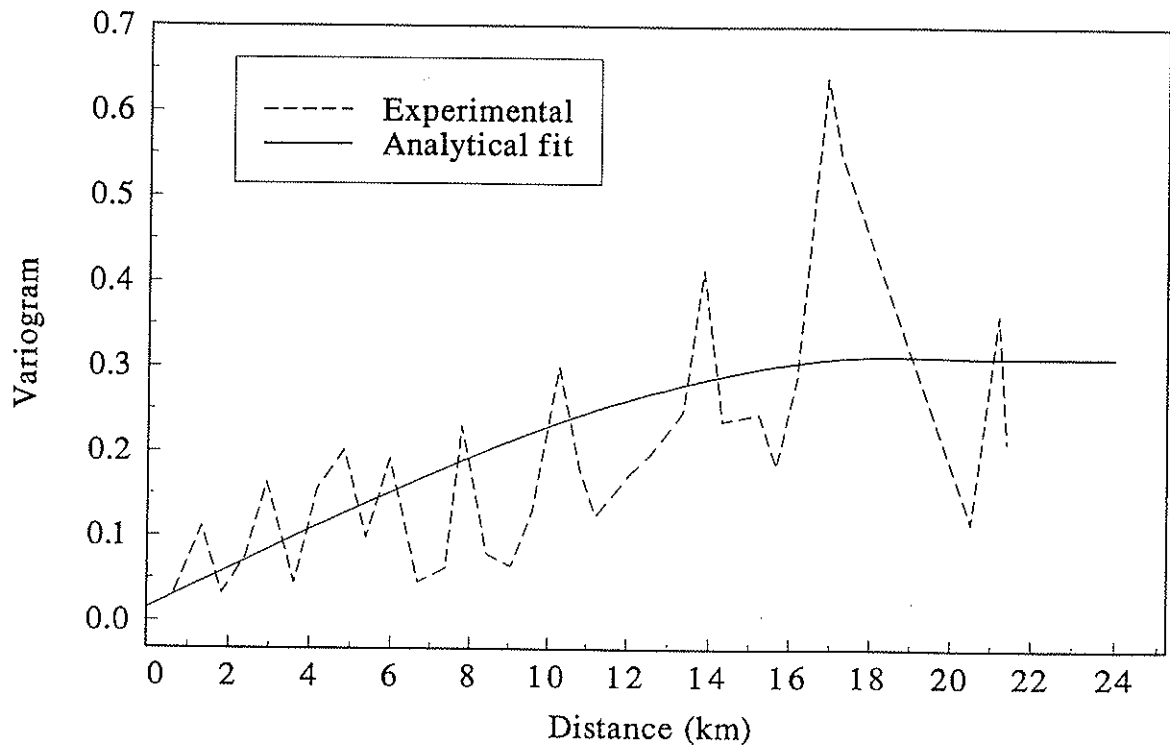


Figure 3. Variogram of I_g : Experimental (dashed line) and Spherical Fit (solid line)

$$\gamma_2(h) = 0.015 + 0.3 \times \left(1.5 \times \frac{h}{18} - 0.5 \times \left(\frac{h}{18} \right)^3 \right) \quad (18)$$

Figure 4 shows the experimental cross-variogram between the two variables and its spherical estimated cross-variogram (γ_{12}) given by:

$$\gamma_{12}(h) = 0.05 + 0.53 \times \left(1.5 \times \frac{h}{20} - 0.5 \times \left(\frac{h}{20} \right)^3 \right) \quad (19)$$

With the purpose of designing an optimal sampling network to observe the mercury contamination in the middle and lower sections of the lake, a grid of 41 nodes is superimposed on the considered region (Figure 5). The grid consists of square elements with a mesh size of 1 km. The considered region is taken as the estimation block (V) on which the cokriging variance of estimation has to be minimized.

By solving the nonlinear optimization model (Equations 14-16) with the above variogram models as inputs, the resulting optimal solution obtained using the variance minimization approach with a budget limit allowing 10 sampling sites yielded a variance of estimation of 1.89. To assess, however, the amount of additional information gained for each additional unit of sampling expenditure, the cost minimization approach (Equations 17-19) was used and a tradeoff curve relating the variance of estimation to the allocated monitoring budget is constructed (Figure 6). By setting an efficiency ratio (r_0), the network designer can optimize the sampling design while taking into account the level of economic efficiency desired. By examining the cost-variance minimization tradeoff curve (Figure 6),

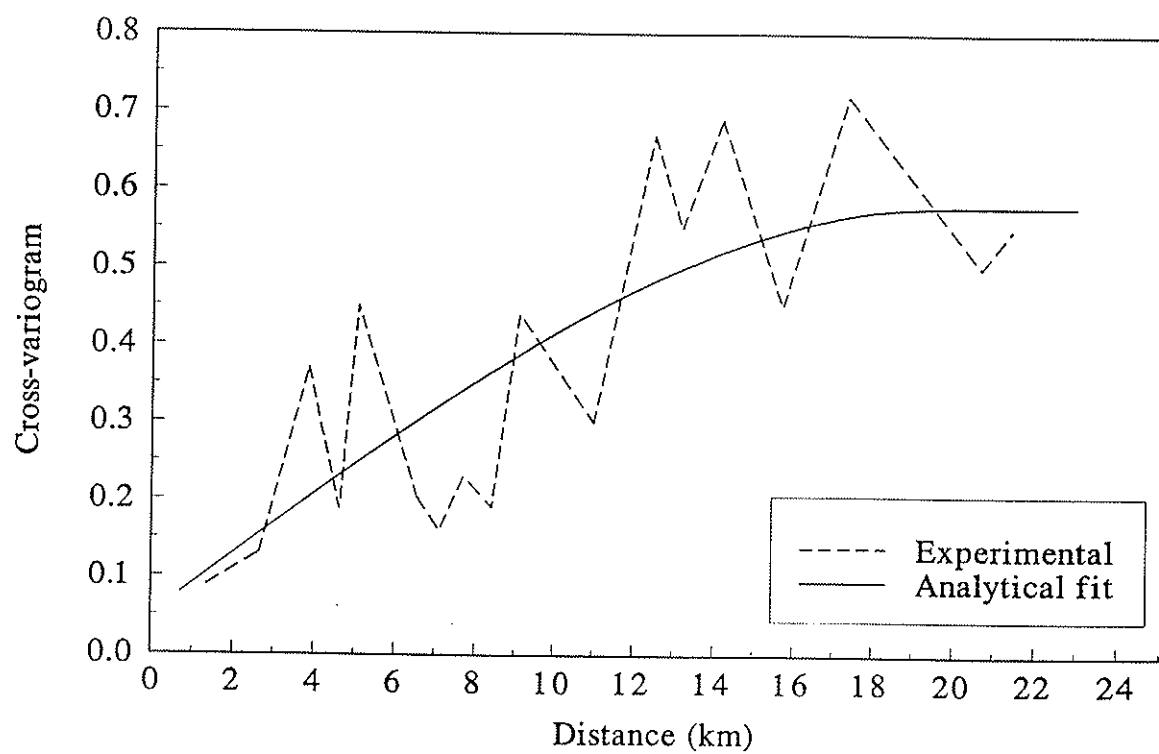


Figure 4. Cross-variogram of logHg-I_g: Experimental (dashed line) and Spherical Fit (solid line)

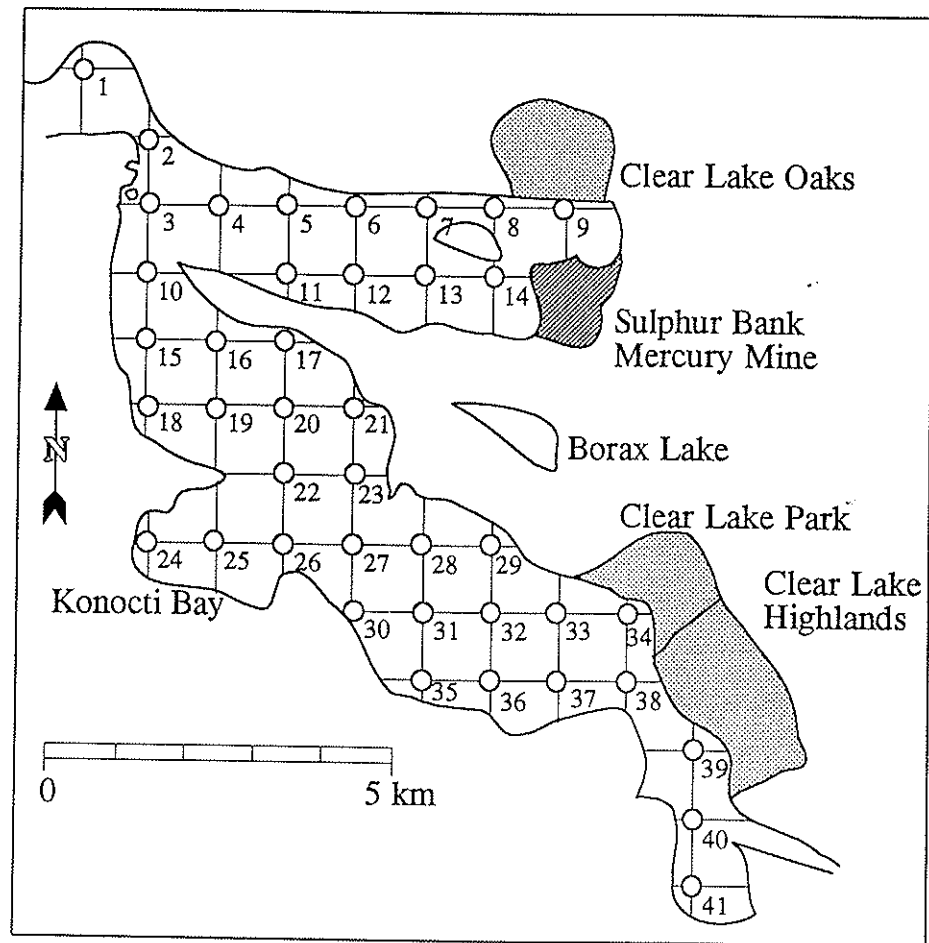


Figure 5. Candidate Sampling Sites within the Study Region (circles)

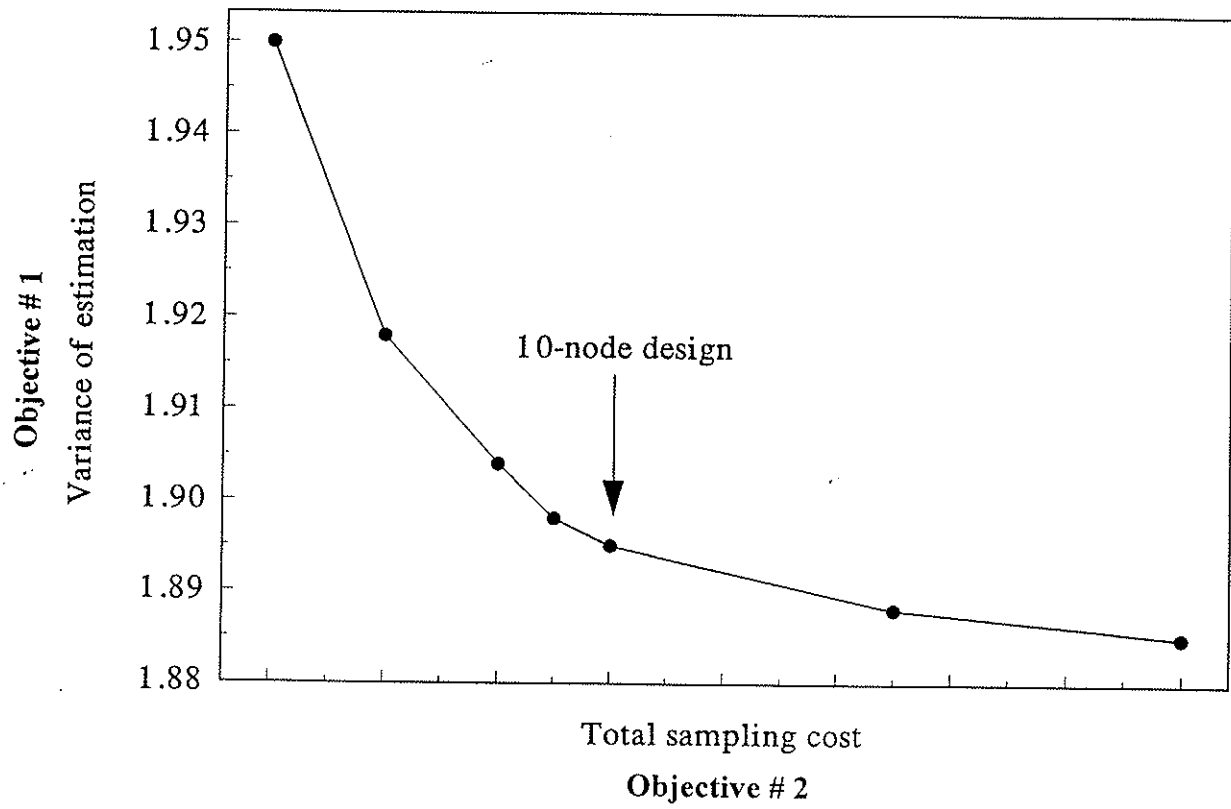


Figure 6. Cost-Variance Minimization Tradeoff Curve

one can see that the variance of estimation decreases substantially in the beginning. However, as the allocated monitoring budget becomes higher, the contribution of each additional sampling expenditure to the variance of estimation decrease becomes smaller, hence, the sampling network becomes less and less efficient. It is important to note that both models will yield exactly the same solution every time the budget limit is reached. However, in the case of a large budget, the cost minimization approach (model two) will yield a more efficient design, even though the first approach may give a lower variance of estimation by violating the efficiency criterion.

2.6. Network Design Sensitivity:

The sampling design model is mainly expressed in terms of the adopted variogram models. Thus, the goal of this section is to assess the sensitivity of the sampling network design solution to the type of variogram model used in the simulation. As the cokriging system of equations involves two variogram models, one for each variable, and a cross-variogram, it is more convenient for conducting this sensitivity analysis to consider a univariate case involving only one variogram model and study its effect on the sampling design solution. For this reason, the special univariate case of the optimization model (Equations 14-16) is used. The optimization model can then be rewritten as:

$$\text{Minimize}_{\lambda_k, \mu} \quad \sum_{k=1}^{N_m} \lambda_k \gamma^{x_k V} + \mu - \gamma^{VV} \quad (20)$$

subject to the unbiasedness condition:

$$\sum_{k=1}^{N_m} \lambda_k = I \quad (21)$$

and to the budget constraint:

$$\sum_{k=1}^{N_m} c_k \leq B \quad (22)$$

To study the effect of the adopted analytical variogram model, the experimental variogram for logHg is fitted with three different analytical models (Figure 7): a spherical model γ_s , as given in Equation 20, an exponential model γ_E , and a linear model γ_L , given respectively by:

$$\gamma_E(h) = 5.45 - 5.51 \times e^{(-0.074 \times h)} \quad (23)$$

$$\gamma_L(h) = 0.63 + 0.19 \times h \quad (24)$$

By solving the sampling design problem using each of the above variogram models, the resulting sampling designs are shown in Table 1. The obtained sampling networks corresponding to the different variogram models show very little difference in their layouts. This result is in accordance with the argument presented by Rouhani and Fiering (1986) that the ultimate estimation of variogram has little effect on the network design. Even though a large number of the optimal monitoring sites are common for the three cases, the variance of estimation changes considerably with the adopted model. It is also important to note that lower values of the variance of estimation are not necessarily

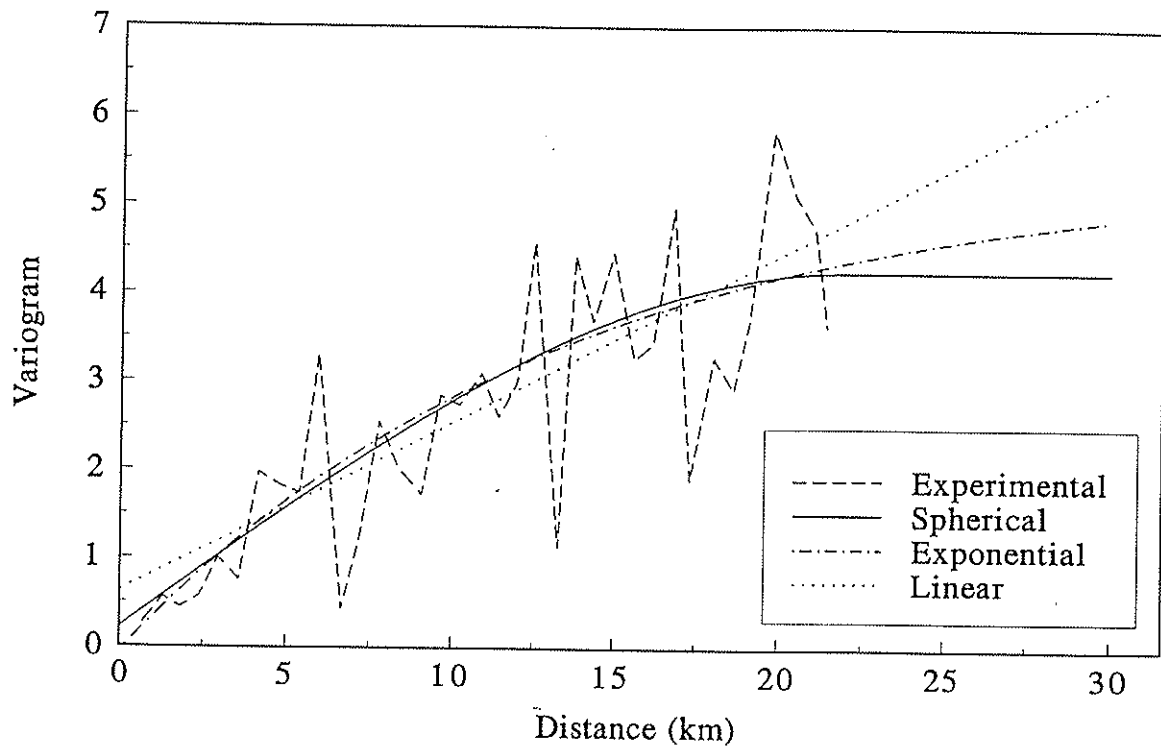


Figure 7. Different Analytical Variogram Fits for the logHg Experimental Variogram

TABLE 1. Effect of the Analytical Variogram Model on the Sampling Design

Solution

Analytical variogram model (1)	Mean square of residuals (2)	Optimal sampling sites (3)	Variance of estimation (4)
Spherical	20.3	1, 3, 5, 7, 9, 19, 24, 32, 37, 40	2.089
Exponential	20.6	1, 3, 7, 9, 16, 24, 35, 37, 39, 40	0.024
Linear	22.3	1, 3, 7, 9, 16, 24, 32, 34, 39, 41	0.069

associated with variogram models having lower mean square of residuals in the variogram estimation. Thus, a design yielding a lower variance of estimation is not necessarily one in which the selected variogram is the best fit to data, and therefore might be questionable.

To study the effect of different variogram parameters on the network design solution, a spherical variogram is used and the sampling design problem is solved for different values of each parameter while keeping the others constant. The parameters in question are: the range, the nugget variance, and the spatial variance. Table 2 shows the resulting sampling design results for different values of the range (a) using the following spherical variogram model with a nugget variance and a spatial variance of 0.22 and 4.03, respectively:

$$\gamma(h) = 0.22 + 4.03 \times \left(1.5 \times \frac{h}{a} - 0.5 \times \left(\frac{h}{a} \right)^3 \right) \quad (25)$$

The obtained results show a slight variability in the final network layout as the range is changed. However, one can clearly see the effect of the range on the variance of estimation. As the range increases, the variance of estimation decreases. At small range values, the variance of estimation decreases slowly. However, as the range becomes larger, the variance of estimation decreases at a faster rate and then tends to stabilize for very large values of the range (Figure 8). The above result can be explained by the fact that for larger values of the range, the correlation between observations persists for longer distances,

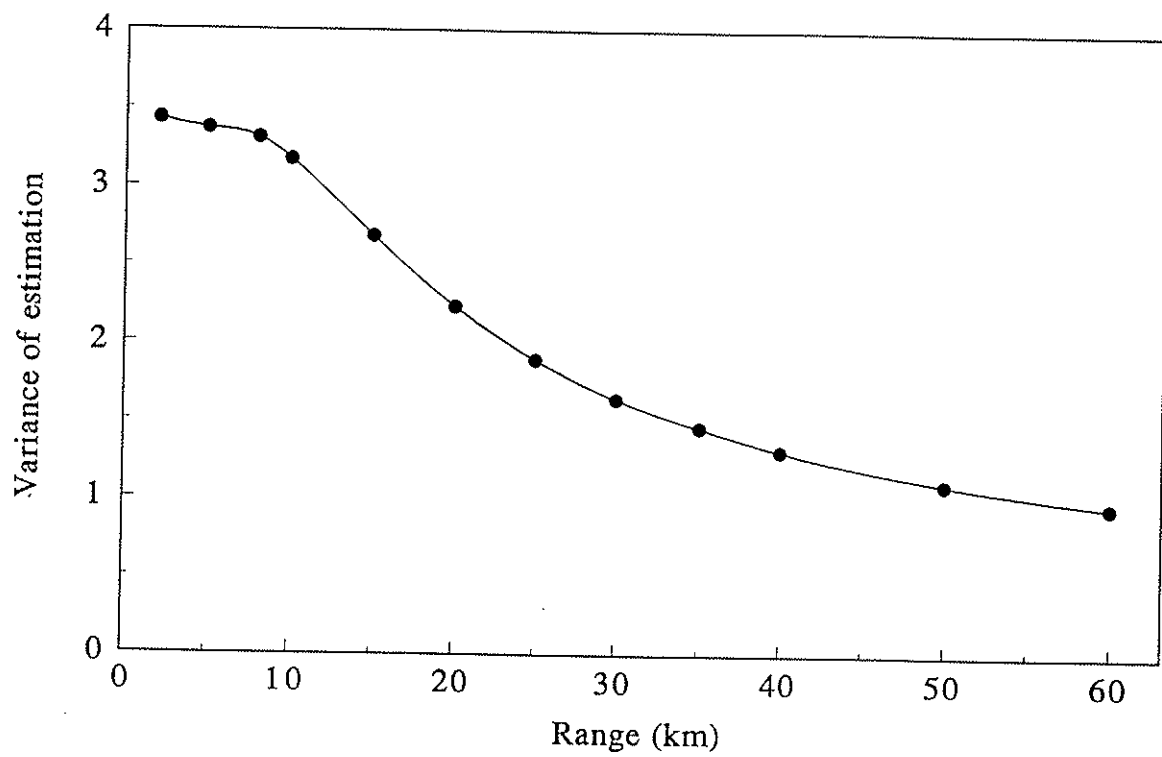


Figure 8. Effect of the Variogram Range

TABLE 2. Effect of the Range on the Sampling Design Solution

Range (km) (1)	Optimal sampling sites (2)	Variance of estimation (3)
1	1, 3, 7, 9, 11, 14, 22, 24, 34, 40	3.52
5	2, 5, 7, 9, 14, 19, 25, 34, 36, 41	3.37
10	1, 3, 5, 7, 9, 19, 24, 32, 37, 40	3.17
15	1, 3, 5, 7, 9, 19, 24, 32, 37, 40	2.68
20	1, 3, 5, 7, 9, 19, 24, 32, 37, 40	2.23
30	1, 3, 5, 7, 9, 19, 24, 32, 37, 40	1.64
40	1, 3, 5, 7, 9, 19, 24, 32, 37, 40	1.31
50	1, 3, 5, 7, 9, 19, 24, 32, 37, 40	1.10
60	1, 3, 5, 7, 9, 19, 24, 32, 37, 40	0.96

whereas, for the case of smaller values of the range the correlation approaches zero very fast.

The sill of a variogram is the sum of the spatial variance and the nugget variance. The spatial variance represents the variance of the variable in question and the nugget variance is the discontinuity occurring at the origin which is mainly caused by measurement errors and system micro-variabilities. Unlike the range, the variance of estimation is found to increase proportionally with the nugget variance as well as the spatial variance (Figures 9 and 10). The sampling network layout is again almost unaffected by varying the nugget and spatial variances (Tables 3 and 4); however, their impact on the variance of estimation is expected since they describe the variability of the variable in question.

2.7. Summary and Conclusions:

The problem of selecting a sampling design is a multicriterion problem given its contradicting objectives, namely: minimizing the sampling cost and increasing the estimation accuracy or minimizing the variance of estimation. To deal with an optimization problem of this nature, an efficiency criterion is introduced to assess the cost effectiveness of additional resource allocations as compared to the additional information gain. The obtained sampling network results show a clear tradeoff between minimizing the allocated sampling budget and the information gain or variance reduction. As the total sampling cost increases, the contribution of each additional cost unit to the estimation variance reduction becomes smaller.

TABLE 3. Effect of the Nugget Variance on the Sampling Design Solution

Nugget variance (1)	Optimal sampling sites (2)	Variance of estimation (3)
0.00	1, 3, 5, 7, 9, 11, 14, 19, 34, 41	1.87
0.05	1, 3, 5, 7, 9, 11, 14, 19, 34, 41	1.92
0.10	1, 3, 5, 7, 9, 19, 24, 32, 37, 40	1.97
0.20	1, 3, 5, 7, 9, 19, 24, 32, 37, 40	2.07
0.30	1, 3, 5, 7, 9, 19, 24, 32, 37, 40	2.17
0.40	1, 3, 5, 7, 9, 19, 24, 32, 37, 40	2.27
0.60	1, 3, 5, 7, 9, 19, 24, 32, 37, 40	2.47
1.00	1, 3, 5, 7, 9, 19, 24, 32, 37, 40	2.87
1.50	1, 3, 5, 7, 9, 19, 24, 32, 37, 40	3.37

TABLE 4. Effect of the Spatial Variance on the Sampling Design Solution

Spatial variance (1)	Optimal sampling sites (2)	Variance of estimation (3)
0.5	1, 3, 5, 7, 9, 19, 24, 32, 37, 40	0.45
1.0	1, 3, 5, 7, 9, 19, 24, 32, 37, 40	0.68
1.5	1, 3, 5, 7, 9, 19, 24, 32, 37, 40	0.92
2.0	1, 3, 5, 7, 9, 19, 24, 32, 37, 40	1.14
3.0	1, 3, 5, 7, 9, 19, 24, 32, 37, 40	1.61
5.0	1, 3, 5, 7, 9, 19, 24, 32, 37, 40	2.54
10.0	1, 3, 5, 7, 9, 19, 24, 32, 37, 40	4.85
15.0	1, 3, 5, 7, 9, 19, 24, 32, 37, 40	7.17

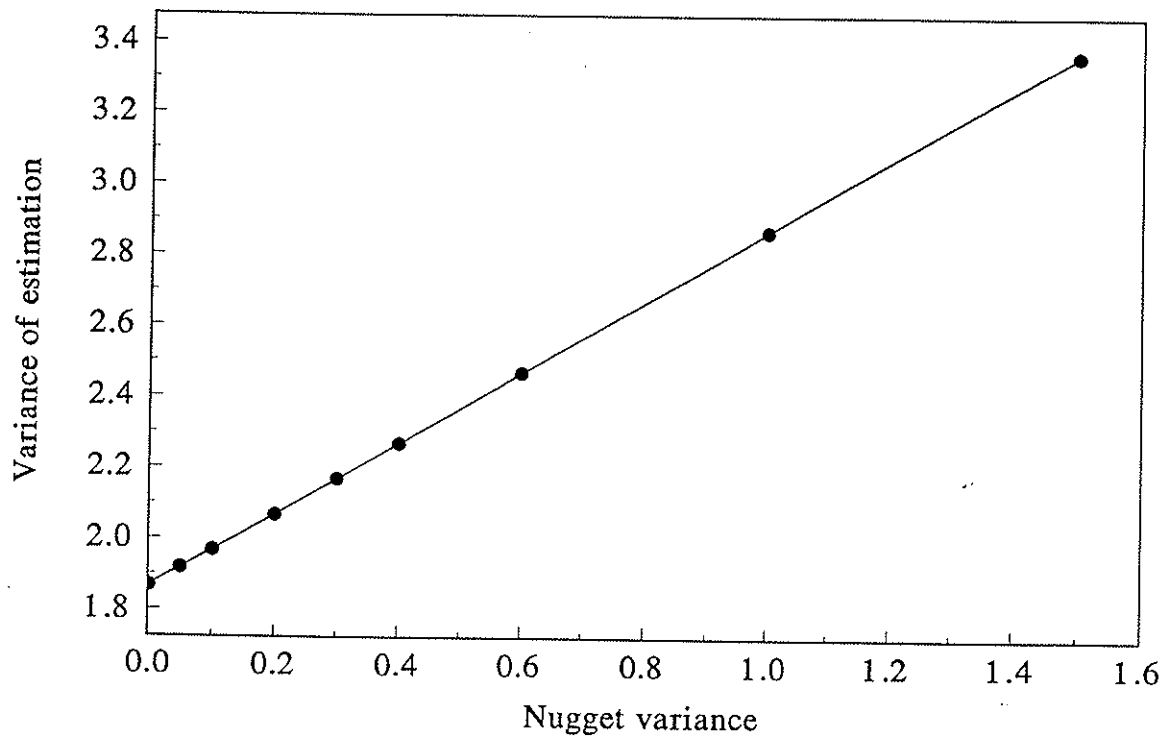


Figure 9. Effect of the Nugget Variance

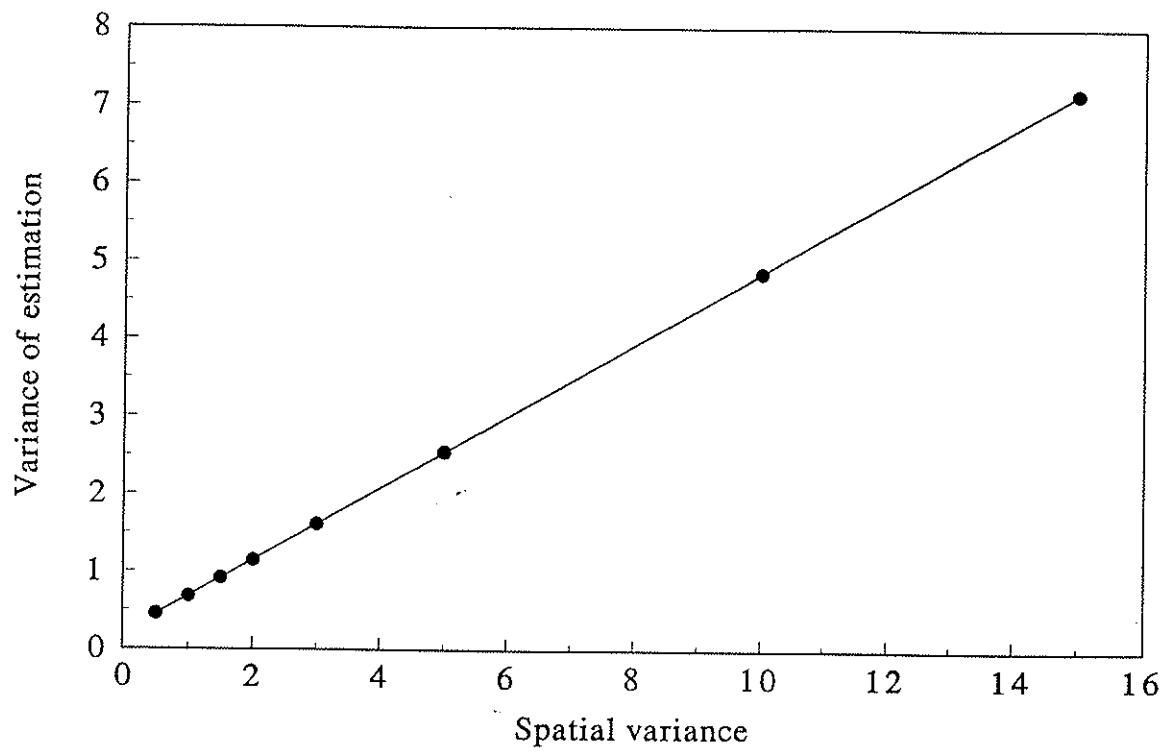


Figure 10. Effect of the Spatial Variance

The formulated sampling design methodology shows a minor sensitivity to the variations in the model inputs, mainly the selected variogram models and their parameters, when it comes to locating the sampling sites. The designer, however, should not be deceived by this apparent advantage of the methodology and great care should be taken in the variogram selection phase in order to adequately estimate the covariance structure of the parameters in question. Unlike the stability of the method in assigning the locations of the sampling sites, the resulting variance of estimation varies considerably with the input parameters. The sensitivity of the variance of estimation is especially critical in the case where the selected variogram models are used for estimation purposes.

3. GROUND WATER REMEDIATION AND POLLUTANT CONTAINMENT

3.1. Introduction:

The goal of ground water remediation techniques is to remove contaminants from the ground water. How well this objective is fulfilled by different techniques depends on numerous factors, mainly, the technical and technological expertise, site characterization and contaminant identification, and remediation and treatment costs. The determination of an effective remediation technique may be somewhat subjective and depends on the objectives as well as the physical and economical constraints. Besides the adopted remediation technology, the effectiveness of any remedial action also depends on the remediation plan and strategy.

3.2. Review of the Literature:

The problem of aquifer remediation and water quality management has been the focus of numerous studies. As the general aim in any remediation effort is to improve the ground water quality and decrease the contamination level, a number of proposed remediation models consist of minimizing the pollutant concentrations and/or the cost of the removal and treatment of the contaminated ground water.

Burn and McBean (1985) presented an optimization model for water quality planning in an uncertain environment. The methodology aims to enhance information gain from a screening model while considering the presence of uncertainties. Chance

constrained programming was used with the objective of reflecting the probabilistic violations of the water quality standards. Ranjithan *et al.* (1993) applied a neural network-based screening approach to a ground water reclamation via pump and treat. Cardwell and Ellis (1993) used a stochastic dynamic programming model for waste load allocation from multiple point sources. Tiedman and Gorelick (1993) presented a methodology to contain a contaminant plume migrating within an unconfined aquifer. The problem was formulated using stochastic nonlinear programming to determine the optimal minimum-pumping strategies for steady state hydraulic capture of the plume. Chang *et al.* (1992) used constrained optimal control using differential dynamic programming to determine optimal time-varying pumping rates in a ground water remediation problem. Similarly, Culver and Shoemaker (1993) employed differential dynamic programming combined with a quasi-Newton approximation for a pump and treat ground water remediation problem. Morgan *et al.* (1993) presented a mixed integer chance constrained programming technique for aquifer remediation design. By varying the degree of reliability, a trade-off curve between maximum reliability and minimum pumping is sought.

Gorelick and Remson (1982) used a linear programming superposition technique to manage several ground water pollutant sources so as to maximize waste disposal rates and not violate the ground water quality standards. Gorelick *et al.* (1984) combined ground water flow and contaminant transport simulations with nonlinear optimization to determine optimal pumping and injection rates for ground water quality control. Wagner and Gorelick (1989) examined the effect of uncertainty of the hydraulic conductivity on aquifer

remediation strategies. Andricevic and Kitanidis (1990) used a discrete time optimal control methodology for finding optimal pumping rates for aquifer remediation; the methodology used accounts for and reduces parameter uncertainty. Optimal pumping rates were sought via minimization of a performance index which encompasses the sum of the remediation costs. Such costs include the costs of pumping and treatment plus a terminal cost represented by a penalty for non-compliance with water quality standards. The performance index, or cost function, was treated as a random variable and the minimization of its expected value was adopted as the model's objective function. Ahlfeld *et al.* (1988a, 1988b) presented two optimization formulations for aquifer cleanup, a first approach aiming to extract a maximum amount of pollutant over the remediation period, and a second approach aiming to lower the contaminant concentration to a specified level. The objective functions adopted consist of: first, minimizing the sum of pollutant concentration at a specified set of nodes within the contaminated region, and second, minimizing the total cost of pumping. Jones *et al.* (1987) presented an optimal control model for ground water management using differential dynamic programming. Murray and Yakowitz (1979) applied a modified differential dynamic programming to a multi-reservoir control problem. Makinde-Odusola and Mariño (1989) used the feedback method of control to determine optimal pumping rates necessary to maintain the piezometric surface below a desired level. Andricevic (1990) used optimal control methods to determine withdrawal rates so as to satisfy a given water demand while keeping the piezometric heads close to some pre-specified levels.

This report presents a ground water remediation approach based on the econometric method of feedback control coupled with finite-element flow and contaminant transport simulations. The approach aims to determine the optimal control rules on the locations and rates of pumping and injection so as to lower the contamination below some pre-specified target level. The feedback control model used consists of a successive minimization of a loss function describing the deviation of the state variables (pollutant concentrations) from their targets.

3.3. Technical Methods For Ground Water Quality Control:

Analyzing different technical methods for controlling the ground water quality, two broad categories can be identified: Source control methods, and ground water control methods.

3.3.1. Source Control Methods: A natural course of action to minimize the pollution of ground water is to control the source of the contamination. Any reduction in the number of contamination sources and the amount of contaminant disposed, will result in less ground water contamination. Hence, source control methods are preventive methods (before the fact action) as compared to ground water control methods which are remedial measures (after the fact action).

In order to have a successful source control strategy, thorough identification of the sources, causes, and types of ground water pollutants should be made. Techniques for the control of ground water pollution sources are site and pollutant specific. These control

techniques are based on proper citing, design, construction, operation, and monitoring.

Ground water pollution sources are generally man-made or man-induced causes. Some of the man-made sources are:

- (a) Industrial pollution: caused by the dumping and disposal of industrial waste, production residuals, leaks from pipelines and underground tanks, and accidental spills of chemicals.
- (b) Agricultural pollution: caused by the application to agricultural fields of plant nutrients, fertilizers, pesticides, and animal waste. Unlike other types of pollution sources, agricultural pollution of ground water is generally distributed on a wide area and referred to as non-point source of pollution.
- (c) Urban pollution: caused by municipal waste water effluents as well as dumping of solid waste (landfills).

Other types of ground water pollution can be man-induced such as saltwater intrusions due to over-exploitation of aquifers and artificial ground water recharge by contaminated surface waters.

Controlling ground water pollution sources is a task that depends on the contamination source in question and may range from sanitary landfills for waste disposal to treatment plants for municipal and industrial wastewater. Point sources of pollution are relatively easier and more practical to control and contain; in contrast, non-point sources, mainly pollution from agricultural fields, are much more difficult to control. Nevertheless, a number of methods are available for controlling and reducing the contamination from

non-point sources such as the reduction of chemical leaching and deep percolation through drainage and collection systems, efficient irrigation scheduling, improved agricultural practices, and crop rotation.

3.3.2. Ground Water Control Methods: As mentioned earlier, groundwater control methods are needed as corrective measures in the case of an already contaminated aquifer. Groundwater control methods aiming to control and contain pollution can be divided into two main categories:

- (a) Restoration methods which proceed by a cleanup and removal of the contaminant from the aquifer such as pump and treat techniques, in situ bioremediation, and air stripping in the case of volatile compounds.
- (b) Containment or isolation methods: Such techniques aim at the isolation of the contaminated region in order to prevent further contamination due to the migration and spreading of the pollutants into adjacent regions.

Most of the ground water control techniques proceed by controlling the hydraulics and movement of water within the subsurface. Controlling the flow patterns can be achieved by modifying the pumping or recharge rates and patterns. Techniques based on the control of groundwater hydraulics are effective and practical as well as economical. In contrast, other contaminant isolation methods using underground physical barriers can be very costly to implement.

3.4. Governing Equations:

The equations used to describe the ground water system and to predict its evolution under the proposed remediation strategy are the basic ground water flow and transport equations:

$$\nabla \bullet (T \nabla h) = S \frac{\partial h}{\partial t} - q \quad (25)$$

$$v = -K \bullet \nabla h \quad (26)$$

$$\nabla \bullet (D \bullet \nabla c) - v \bullet (\nabla c) - M = \frac{\partial c}{\partial t} \quad (27)$$

where T is the transmissivity tensor, h is the piezometric head, S is the storativity, q is a flow source/sink term, v is the Darcy flow velocity, K is the hydraulic conductivity, D is the hydrodynamic dispersion, M is a solute source/sink term, and c is the contaminant concentration.

In the case of an isotropic medium, the four components of the hydrodynamic dispersion coefficient tensor can be expressed as (Bear, 1979)

$$D_{xx} = \alpha_L \frac{v_x^2}{v} + \alpha_T \frac{v_y^2}{v} + D^* \quad (28a)$$

$$D_{yy} = \alpha_T \frac{v_x^2}{v} + \alpha_L \frac{v_y^2}{v} + D^* \quad (28b)$$

$$D_{xy} = D_{yx} = (\alpha_L - \alpha_T) \frac{v_x v_y}{v} \quad (28c)$$

in which

v_x = the flow velocity component in the x-direction

v_y = the flow velocity component in the y-direction

$$v = \left[v_x^2 + v_y^2 \right]^{\frac{1}{2}} \equiv |\bar{v}| \quad (29)$$

α_L = the longitudinal dispersivity of the porous medium

α_T = the transversal dispersivity of the porous medium

D^* = the molecular diffusion coefficient which can be expressed in terms of the molecular diffusion and the tortuosity of the porous medium as

$$(D^* = D_m \tau) \quad (30)$$

where

D_m = the solute molecular diffusion

τ = the tortuosity of the porous medium

The equation for solute transport in saturated porous medium (Equation 27) expressed in Cartesian coordinates can be written as

$$\begin{aligned} \frac{\partial C}{\partial t} = & D_x \frac{\partial^2 C}{\partial x^2} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} - \frac{\partial}{\partial x} \left(\frac{v_x C}{n} \right) - \frac{\partial}{\partial t} \left(\frac{\rho_b K_d C}{n} \right) \\ & - \lambda \left(C + \frac{\rho_b K_d C}{n} \right) - \frac{q}{n} \end{aligned} \quad (31)$$

in which

v_x = the apparent ground water velocity

ρ_b = the bulk density of the porous medium

K_d = the distribution coefficient

λ = the solute decay coefficient (constant)

3.5. Phenomena Governing Contaminant Fate And Transport:

Spreading and migration of pollutants within the subsurface can be caused by a number of phenomena. Solute movement and spreading in a porous medium is a complex phenomenon and cannot be fully explained by water movement (spreading by advection). By analyzing the solute transport at the microscopic level, it was found that contaminant spreading within the ground water is also caused by the random movement of molecules, such phenomenon is known as molecular diffusion. Molecular diffusion enhances the spreading of pollutants both in the longitudinal and transversal directions to the average ground water flow. The physical characteristics of the porous medium force the flow to follow random and tortuous paths around the soil particles depicting velocity variations at the microscopic level. This phenomenon is known as mechanical dispersion. Mechanical dispersion coupled with molecular diffusion give the entity known as hydrodynamic dispersion.

The advective component of the solute flux is given by

$$q_{adv} = CV \quad (32)$$

in which

C = the pollutant concentration

V = the average flow velocity

The dispersive flux is given by

$$q_{dis} = -D \bullet \nabla C \quad (33)$$

in which

D = the coefficient of mechanical dispersion

The flux due to molecular diffusion is given by

$$q_{dif} = -D_d \tau \bullet \nabla C = D_d^* \bullet \nabla C \quad (34)$$

in which

D_d = the coefficient of molecular diffusion

τ = the tortuosity of the porous medium.

The pollutant flux due to the sum of dispersion and diffusion phenomena can then be written as

$$\begin{aligned} q_d &= -(D + D_d^*) \bullet \nabla C \\ &= -D_h \bullet \nabla C \end{aligned} \quad (35)$$

where

D_h = the coefficient of hydrodynamic dispersion.

The total flux of pollutant by advection, dispersion, and diffusion combined can be written as

$$q_T = n (-D_h \bullet \nabla C + CV) \quad (36)$$

with n representing the porosity of the porous medium.

In addition to advection, molecular diffusion, and mechanical dispersion, other important phenomena can affect the fate and transport of pollutant in ground water such as adsorption, solute decay, biodegradation, and other chemical reactions. Adsorption is the adhesion of the pollutant to the solid particles at the fluid-solid interface. This adhesion or adsorption is often caused by molecular forces and electrical attraction between the solid surface and the chemical molecules. Therefore, adsorption is a function not only of the pollutant characteristics but also of those of the aquifer solid matrix. Other factors can affect the chemical reactions between the pollutant components and the soil particles such as the temperature and the pH of the ground water.

4. AQUIFER REMEDIATION AS A CONTROL PROBLEM

4.1. Introduction:

The aim of this section is to transform the governing equation for solute transport and express it in the form of a system equation for an econometric model in order to formulate the remediation problem as a feedback control problem. Using a finite element formulation, the solute transport equation has to be transformed to conform to the following form:

$$C_t = A_{t-1} C_{t-1} + B_{t-1} u_{t-1} + c_{t-1} + \mu_{t-1} \quad (37)$$

The above equation is a standard form for a state equation of econometric models in which C_t is the state variable giving the pollutant concentration at stage t , u_t is a control vector, A_t and B_t are coefficient matrices of known elements, c_t is a coefficient vector, and μ_t is a vector of random disturbances. An econometric system could be fully controllable, and the method of feedback control can be applied (Figure 11), where the controls (inputs) are derived at each optimization stage depending on the current states of the system and the level of control achieved (outputs) toward reaching the target states.

In the case of ground water remediation problems, the situation is more complex and the ground water system cannot be fully controllable due to the natural random disturbances and other uncontrollable inputs. Instead, the econometric system can be treated as a partially controllable system, where in addition to the regular feedback

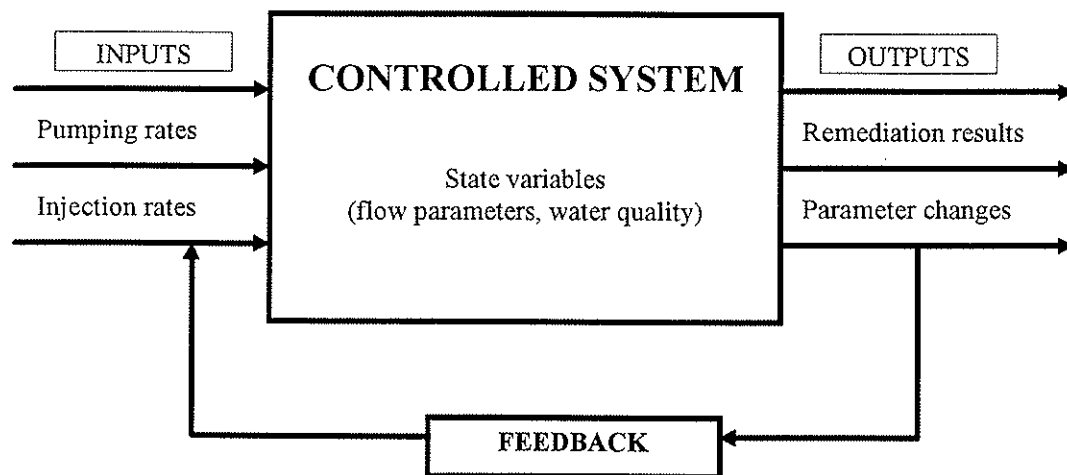


Figure 11. Feedback Model Diagram

inputs (controls) we have a set of random disturbances which act upon the system as well. As a result, the system outputs will show some undesirable components, which given will be taken into account at the next optimization stage through the feedback controllability (Figure 12).

4.2. Galerkin-Finite Elements Representation:

The Galerkin-finite element method, as a weighted residuals technique, uses an approximate integral formulation to replace the original governing partial differential equation for solute transport. To solve the transport equation, the method assumes a trial solution (\hat{C}) expressed as a linear combination of some shape functions ($\phi_i^{(e)}$)

$$\hat{C}^{(e)}(x, y, t) = \sum_{i=1}^n \{C_i(t)\phi_i^{(e)}(t)\} \quad (38)$$

in which

$\hat{C}^{(e)}$ = the approximate solution within the element e

$\phi_i^{(e)}$ = the basis functions for each node i within element e

C_i = the unknown solute concentrations at each node i within element e.

The above approximate solution \hat{C} approaches the actual solution C as the number of nodal points used in the finite element mesh (n) approaches infinity.

By substituting the approximate solution (Equation 38) in Equation 31, the solute transport partial differential equation will not be satisfied exactly, and an error (residual) occurs at every node in the problem domain. The contribution of element e to the residual at node i is:

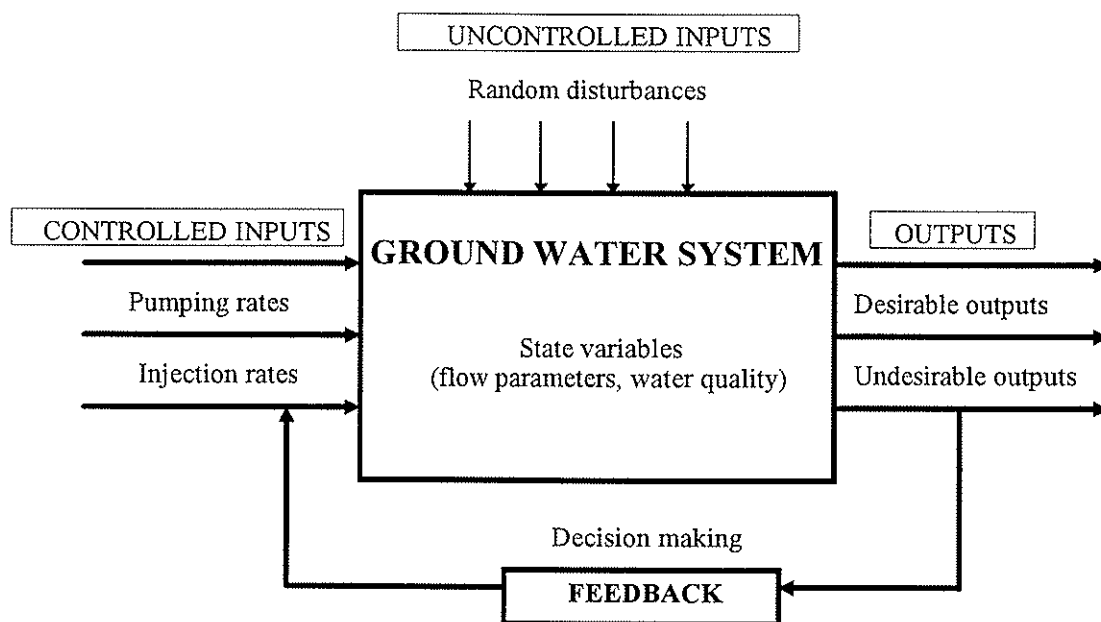


Figure 12. Aquifer Remediation as a Control Model

$$\begin{aligned}
R_i^{(e)} = & - \iiint_{V^{(e)}} \phi_i^{(e)}(x, y, z) \left\{ D_x^{(e)} \frac{\partial \hat{C}^{(e)}}{\partial x^2} + D_y^{(e)} \frac{\partial \hat{C}^{(e)}}{\partial y^2} + D_z^{(e)} \frac{\partial \hat{C}^{(e)}}{\partial z^2} \right. \\
& - \frac{v_x^{(e)}}{n} \frac{\partial \hat{C}^{(e)}}{\partial x} - \frac{\rho_b^{(e)} K_d^{(e)}}{n} \frac{\partial \hat{C}^{(e)}}{\partial t} - \lambda \left(\hat{C}^{(e)} + \frac{\rho_b^{(e)} K_d^{(e)}}{n} \hat{C}^{(e)} \right) \\
& \left. - \frac{\partial \hat{C}^{(e)}}{\partial t} - \frac{q^{(e)}}{n} \right\} dx dy dz
\end{aligned} \tag{39}$$

Expressing the approximate solution in terms of the basis functions in the above equation and rearranging terms gives:

$$\begin{aligned}
R_i^{(e)} = & - \iiint_{V^{(e)}} \phi_i^{(e)} \left\{ D_x^{(e)} \frac{\partial \hat{C}^{(e)}}{\partial x^2} + D_y^{(e)} \frac{\partial \hat{C}^{(e)}}{\partial y^2} + D_z^{(e)} \frac{\partial \hat{C}^{(e)}}{\partial z^2} \right\} dx dy dz \\
& + \iiint_{V^{(e)}} \phi_i^{(e)} \left\{ \frac{v_x^{(e)}}{n} \frac{\partial \hat{C}^{(e)}}{\partial x} \right\} dx dy dz \\
& + \iiint_{V^{(e)}} \phi_i^{(e)} \left\{ \frac{\rho_b^{(e)} K_d^{(e)}}{n} \frac{\partial \hat{C}^{(e)}}{\partial t} \right\} dx dy dz \\
& + \iiint_{V^{(e)}} \phi_i^{(e)} \left\{ \lambda \left(\hat{C}^{(e)} + \frac{\rho_b^{(e)} K_d^{(e)}}{n} \hat{C}^{(e)} \right) \right\} dx dy dz \\
& + \iiint_{V^{(e)}} \phi_i^{(e)} \left\{ \frac{\partial \hat{C}^{(e)}}{\partial t} \right\} dx dy dz \\
& + \iiint_{V^{(e)}} \phi_i^{(e)} \left\{ \frac{q^{(e)}}{n} \right\} dx dy dz
\end{aligned} \tag{40}$$

Using matrix notation, the above equation can be written as

$$\begin{pmatrix} R_1^{(e)} \\ \vdots \\ R_n^{(e)} \end{pmatrix} = [D^{(e)}] \begin{pmatrix} C_1 \\ \vdots \\ C_n \end{pmatrix} + [A^{(e)}] \begin{pmatrix} \frac{\partial C_1}{\partial t} \\ \vdots \\ \frac{\partial C_n}{\partial t} \end{pmatrix} + \begin{pmatrix} F_1^{(e)} \\ \vdots \\ F_n^{(e)} \end{pmatrix} \quad (41)$$

in which:

$$\begin{aligned} [D^{(e)}] = & \iiint_{V^{(e)}} \begin{bmatrix} \frac{\partial \phi_1^{(e)}}{\partial x} & \frac{\partial \phi_1^{(e)}}{\partial y} & \frac{\partial \phi_1^{(e)}}{\partial z} \\ \vdots & \vdots & \vdots \\ \frac{\partial \phi_n^{(e)}}{\partial x} & \frac{\partial \phi_n^{(e)}}{\partial y} & \frac{\partial \phi_n^{(e)}}{\partial z} \end{bmatrix} \begin{bmatrix} D_x^{(e)} & 0 & 0 \\ 0 & D_y^{(e)} & 0 \\ 0 & 0 & D_z^{(e)} \end{bmatrix} \begin{bmatrix} \frac{\partial \phi_1^{(e)}}{\partial x} & \dots & \frac{\partial \phi_n^{(e)}}{\partial x} \\ \frac{\partial \phi_1^{(e)}}{\partial y} & \dots & \frac{\partial \phi_n^{(e)}}{\partial y} \\ \frac{\partial \phi_1^{(e)}}{\partial z} & \dots & \frac{\partial \phi_n^{(e)}}{\partial z} \end{bmatrix} dx dy dz \\ & + \iiint_{V^{(e)}} \begin{bmatrix} \phi_1^{(e)} \\ \vdots \\ \phi_n^{(e)} \end{bmatrix} \frac{v_x^{(e)}}{n^{(e)}} \begin{bmatrix} \frac{\partial \phi_1^{(e)}}{\partial x} & \dots & \frac{\partial \phi_n^{(e)}}{\partial x} \end{bmatrix} dx dy dz \\ & + \iiint_{V^{(e)}} \begin{bmatrix} \phi_1^{(e)} \\ \vdots \\ \phi_n^{(e)} \end{bmatrix} \left[\lambda \left(1 + \frac{\rho_b^{(e)} K_d^{(e)}}{n^{(e)}} \right) \right] \begin{bmatrix} \phi_1^{(e)} & \dots & \phi_n^{(e)} \end{bmatrix} dx dy dz \end{aligned} \quad (42)$$

is an $n \times n$ element advection-dispersion matrix;

$$[A^{(e)}] = \iiint_{V^{(e)}} \begin{bmatrix} \phi_1^{(e)} \\ \vdots \\ \phi_n^{(e)} \end{bmatrix} \left[1 + \frac{\rho_b^{(e)} K_d^{(e)}}{n^{(e)}} \right] \begin{bmatrix} \phi_1^{(e)} & \dots & \phi_n^{(e)} \end{bmatrix} dx dy dz \quad (43)$$

is an $n \times n$ element sorption matrix; and

$$F_i^{(e)} = \iiint_{V^{(e)}} \phi_i^{(e)} \left\{ \lambda \left(\hat{C}^{(e)} + \frac{\rho_b^{(e)} K_d^{(e)}}{n} \hat{C}^{(e)} \right) \right\} dx dy dz \quad (44)$$

is an $n \times 1$ element source/sink matrix.

The quantity $\left[1 + \frac{\rho_b^{(e)} K_d^{(e)}}{n^{(e)}} \right]$ represents the retardation factor.

In the case of a lumped element formulation, where the Dirac Delta function is substituted for the shape functions, the sorption matrix above will become:

$$[A^{(e)}] = \left[1 + \frac{\rho_b^{(e)} K_d^{(e)}}{n^{(e)}} \right] \frac{V^{(e)}}{n} \begin{bmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{bmatrix} \quad (45)$$

By combining the element matrices above, global matrices can be obtained as

$$[D]_{\substack{\text{global} \\ (p \times p)}} = \sum_{e=1}^m [D^{(e)}]_{\substack{\text{expanded} \\ (n \times n)}} \quad (46)$$

$$[A]_{\substack{\text{global} \\ (p \times p)}} = \sum_{e=1}^m [A^{(e)}]_{\substack{\text{expanded} \\ (n \times n)}} \quad (47)$$

$$\{F\}_{\substack{\text{global} \\ (p \times 1)}} = \sum_{e=1}^m \{F^{(e)}\}_{\substack{\text{expanded} \\ (n \times 1)}} \quad (48)$$

Therefore, the weighted residual formulation for the solute transport equation can be written as

$$[D]_{(p \times p)} \begin{pmatrix} C_1 \\ \vdots \\ C_p \end{pmatrix} + [A]_{(p \times p)} \begin{pmatrix} \frac{\partial C_1}{\partial t} \\ \vdots \\ \frac{\partial C_p}{\partial t} \end{pmatrix} = \{F\}_{(p \times 1)} \quad (49)$$

or

$$[A] \{\dot{C}\} + [D] \{C\} = \{F\} \quad (50)$$

4.3. Econometric Model Development:

In order to write the transformed transport equation above in the form of an econometric model system equation, additional transformations are needed. For this purpose, the following finite difference formulations are used:

$$\dot{C} = \frac{\partial C}{\partial t} = \frac{C_{t+\Delta t} - C_t}{\Delta t} \quad (51)$$

$$C = (1 - w)C_t + wC_{t+\Delta t} \quad (52)$$

Depending on the choice of the parameter w in the above formulation, different cases can be identified:

$w = 0$ forward difference

$w = 0.5$ central difference (also known as Crank-Nicolson formulation)

$w = 1$ backward difference

By adopting the transformations (51) and (52), Equation (50) becomes

$$\begin{aligned} ([A] + w\Delta t[D])\{C\}_t &= ([A] + (1-w)\Delta t[D])\{C\}_{t-1} \\ &+ \Delta t \left((1-w)\{F\}_{t-1} + w\{F\}_t \right) \end{aligned} \quad (53)$$

Using a forward difference formulation ($w=0$) for the source/sink term, we get

$$([A] + w\Delta t[D])\{C\}_t = ([A] + (1-w)\Delta t[D])\{C\}_{t-1} + \Delta t\{F\}_{t-1} \quad (54)$$

Re-arranging terms in the above equation gives

$$\begin{aligned} \{C\}_t &= ([A] + w\Delta t[D])^{-1} ([A] + (1-w)\Delta t[D])\{C\}_{t-1} \\ &+ \Delta t ([A] + w\Delta t[D])^{-1} \{F\}_{t-1} \end{aligned} \quad (55)$$

The above form of the transport equation can now be written in the form of a system equation for an econometric model as

$$\{C\}_t = \Theta \{C\}_{t-1} + \Xi \{F\}_{t-1} \quad (56)$$

in which

$$\Theta = ([A] + w \Delta t [D])^{-1} ([A] + (1 - w) \Delta t [D]) \quad (57)$$

$$\Xi = \Delta t ([A] + w \Delta t [D])^{-1} \quad (58)$$

Posed in the form of a system equation for an econometric model, the transport equation can be solved using econometric methods. At each stage in time, the current states of the system (the pollutant concentration levels), $\{C\}_t$, are expressed as a function of the previous states, $\{C\}_{t-1}$, and the controls (pumping or injections) undertaken at the previous stage, $\{F\}_{t-1}$. The feedback method of control will be adopted to determine the optimal controls at each time step. The solution algorithm is detailed in subsequent sections.

4.4. Feedback Control Model

Using the above modified form (Equation 56) of the solute transport equation, the ground water remediation problem can be posed as a feedback control problem (Chow, 1981; and Kendrick, 1981). The objective function consists of a successive minimization of a loss function containing the squared deviations of the state variables from their prescribed target values to be reached by the end of the control process, and can be written as

$$J = \frac{1}{2} \sum_{t=1}^N \left(\hat{C}_t - a_t \right)' K_t \left(\hat{C}_t - a_t \right) \quad (59)$$

in which N is the number of time periods, \hat{C}_t is a vector containing the state variables (i.e., the pollutant concentrations at time t), a_t is a vector containing the target values of the state variables, and K_t is a penalty matrix for deviating from the target a_t . The minimization of the objective function in a feedback control problem is subject to a constraint of the form (56), where the state variable is expressed as a function of its previous value and of a control vector containing the undertaken decisions. In the case of groundwater remediation problems, the state variable can be taken as the pollutant concentration, whereas the control vector will contain information on the pumping and recharge rates and their locations. It is obvious that the contamination level at each stage will be directly dependent on the remedial decisions embedded in the control vector and on the state of the system on the previous stage. The optimization model can be written as

$$\underset{u_t}{\text{Minimize}} \quad J = \sum_{t=1}^N \left(\hat{C}_t - a_t \right)' K_t \left(\hat{C}_t - a_t \right) \quad (60)$$

subject to the state equation:

$$\hat{C}_t = A_{t-1} \hat{C}_{t-1} + B_{t-1} u_{t-1} + c_{t-1} + \mu_{t-1} \quad (61)$$

For notation ease, the difference term between the states and their desired targets will be represented by

$$C_t \equiv \hat{C}_t - a_t \quad (62)$$

The remediation problem expressed as an optimization model and posed in its above form (Equations 60-61) can be solved using the econometric method of feedback control. The solution process consists of a stage by stage optimization as described in the solution algorithm below. The solution process starts at the end period ($t = N$) by using the terminal conditions

$$K_N = W_N \quad (63)$$

$$p_N = w_N \quad (64)$$

and proceeds backwards in time in a stage by stage optimization using a dynamic programming approach. Equations (63) and (64) provide the terminal values at the end period for a set of difference equations known as the Ricatti equation, to be defined in the following section. These difference equations are used to transmit the cost or price information from the last period backward in time; at the terminal period, they provide information about the economic value (i.e., cost) of having the economic system at the terminal state C_N .

4.5. Feedback Control Solution Algorithm:

The feedback control problem as presented above is solved via a dynamic programming algorithm as a successive minimization of the objective function, also called the cost-to-go, at each stage. The basic idea of the algorithm is that at each given point in time one needs to minimize the cost-to-go from that point to the end. This is called the optimal cost-to-go noted as $J^*(C_t)$, where C_t is the state vector at time

period k and $J^*(C_t)$ is the cost of going from the state C_t to the desired target for the state at the terminal period of the remediation horizon.

The optimal control problem consists of finding the set of control vectors from the start to the terminal period so as to minimize the cost-to-go function. The problem can therefore be formulated as:

$$\text{Find } (u_t)_{t=1}^N \quad (65)$$

to minimize the cost-to-go:

$$\begin{aligned} J(C_t) = & \frac{1}{2} C_N' \hat{W}_N C_N + w_N' C_N \\ & + \sum_{t=0}^{N-1} \left(\frac{1}{2} C_t' W_t C_t + w_t' C_t + C_t' F_t u_t + \frac{1}{2} u_t' \Lambda_t u_t + \lambda_t' u_t \right) \end{aligned} \quad (66)$$

subject to the system equation

$$C_t = A_{t-1} C_{t-1} + B_{t-1} u_{t-1} + c_{t-1} + \mu_{t-1} \quad (67)$$

and the initial conditions

$$C_0 \quad (68)$$

where

C_t = the state vector ($n \times 1$) at time period t

u_t = the control vector ($m \times 1$) at time period t

W_t = $n \times n$ penalty matrix

w_t = $n \times 1$ vector

F_t = $n \times m$ matrix

$\Lambda = m \times m$ matrix

$\lambda_t = m \times 1$ vector

$A_t = n \times n$ coefficient matrix

$B_t = n \times m$ coefficient matrix

$c_t = n \times 1$ vector

The cost-to-go function as shown above (Equation 66) is written in its general quadratic form which, in addition to the term expressing the deviation of the states from their desired values, contains a similar term expressing the deviation of the controls from their desired values and a cross term. Both of these additional terms can be omitted, especially in a case where the controls which have to be determined are not required to follow a pre-specified path. Nevertheless, these terms are of special importance in the case of feedback control problems requiring the controls to match some given desired values.

The quadratic cost-to-go function at any time period t can be rewritten as

$$J^*(C_t) = J^*(t) = \frac{1}{2} C_t' K_t C_t + p_t' C_t \quad (69)$$

in which

$K_t = n \times n$ matrix known as the Ricatti matrix

$p_t = n \times 1$ vector

In order to derive the optimal feedback rules (i.e., find the optimal control vector), the solution algorithm starts at the terminal time period (N) and works backward toward the initial time period. The optimal cost-to-go at the terminal period can be written as

$$\begin{aligned}
J^*(N) &= \frac{1}{2} C_N' K_N C_N + p_N' C_N \\
&= \frac{1}{2} C_N' W_N C_N + w_N' C_N
\end{aligned} \tag{70}$$

working backward in time, the optimal cost-to-go in period N-1 can be written as

$$\begin{aligned}
J^*(N-1) &= \min_{u_{N-1}} \left\{ J^*(N) + \frac{1}{2} C_{N-1}' W_{N-1} C_{N-1} + w_{N-1}' C_{N-1} + C_{N-1}' F_{N-1} u_{N-1} \right. \\
&\quad \left. + \frac{1}{2} u_{N-1}' \Lambda_{N-1} u_{N-1} + \lambda_{N-1}' u_{N-1} \right\}
\end{aligned} \tag{71}$$

using the system equation

$$C_N = A_{N-1} C_{N-1} + B_{N-1} u_{N-1} + c_{N-1} + \mu_{N-1} \tag{72}$$

and substituting the terminal cost-to-go by its value, the cost-to-go for period N-1 can be rewritten as

$$\begin{aligned}
J^*(N-1) &= \min_{u_{N-1}} \left\{ \frac{1}{2} C_{N-1}' \Phi_{N-1} C_{N-1} + \frac{1}{2} u_{N-1}' \Theta_{N-1} u_{N-1} \right. \\
&\quad \left. + C_{N-1}' \Psi_{N-1} u_{N-1} + \phi_{N-1}' C_{N-1} + \theta_{N-1}' u_{N-1} + \eta_{N-1} \right\}
\end{aligned} \tag{73}$$

in which

$$\Phi_{N-1} = A_{N-1}' K_N A_{N-1} + W_{N-1} \tag{74}$$

$$\Theta_{N-1} = B_{N-1}' K_N B_{N-1} + \Lambda_{N-1} \tag{75}$$

$$\Psi_{N-1} = A_{N-1}' K_N B_{N-1} + F_{N-1} \tag{76}$$

$$\phi_{N-1} = A_{N-1}' (K_N c_{N-1} + p_N) + w_{N-1} \tag{77}$$

$$\theta_{N-1} = B_{N-1}' (K_N c_{N-1} + p_N) + \lambda_{N-1} \tag{78}$$

$$\eta_{N-1} = c'_{N-1} K_N c_{N-1} + p'_N c_{N-1} \quad (79)$$

Minimizing for u_{N-1} in the cost-to-go equation (73), yields

$$u'_{N-1} \Theta_{N-1} + C'_{N-1} \Psi_{N-1} + \theta'_{N-1} = 0 \quad (80)$$

solving for u_{N-1} in the above equation gives what is called the feedback rules for time period N-1

$$u_{N-1} = G_{N-1} C_{N-1} + g_{N-1} \quad (81)$$

with

$$G_{N-1} = -(\Theta'_{N-1})^{-1} \Psi'_{N-1} \quad (82)$$

$$g_{N-1} = -(\Theta'_{N-1})^{-1} \theta_{N-1} \quad (83)$$

The above matrices, G and g , are called the feedback matrices.

The cost-to-go for the period N-1 is a function of the states (C_{N-1}) as well as the controls (u_{N-1}), it can be expressed exclusively as a function of the states by substituting out the controls using the feedback rule (Equation 81). The cost-to-go will then be

$$J^*(N-1) = \frac{1}{2} C'_{N-1} K_{N-1} C_{N-1} + p'_{N-1} C_{N-1} \quad (84)$$

where

$$K_{N-1} = \Phi_{N-1} + G'_{N-1} \Theta_{N-1} G_{N-1} + 2\Psi_{N-1} G_{N-1} \quad (85)$$

$$p_{N-1} = (\Psi_{N-1} + G'_{N-1} \Theta'_{N-1}) g_{N-1} + G'_{N-1} \theta_{N-1} + \phi_{N-1} \quad (86)$$

The above two equations (85-86) are known as the Ricatti equations.

Similarly, the above results can be generalized and the feedback rules can be written for any time period t as

$$u_t = G_t C_t + g_t \quad (87)$$

with

$$G_t = - \left(\Theta_t' \right)^{-1} \Psi_t' \quad (88)$$

$$g_t = - \left(\Theta_t' \right)^{-1} \theta_t \quad (89)$$

and the cost-to-go as

$$J^*(t) = \frac{1}{2} C_t' K_t C_t + p_t' C_t \quad (90)$$

with the Ricatti equations

$$K_t = \Phi_t + G_t' \Theta_t G_t + 2 \Psi_t' G_t \quad (91)$$

$$p_t = \left(\Psi_t + G_t' \Theta_t' \right) g_t + G_t' \theta_t + \phi_t \quad (92)$$

where

$$\Phi_t = A_t' K_{t+1} A_t + W_t \quad (93)$$

$$\Theta_t = B_t' K_{t+1} B_t + \Lambda_t \quad (94)$$

$$\Psi_t = A_t' K_{t+1} B_t + F_t \quad (95)$$

$$\phi_t = A_t' \left(K_{t+1}' c_t + p_{t+1} \right) + w_t \quad (96)$$

$$\theta_t = B_t' \left(K_{t+1}' c_t + p_{t+1} \right) + \lambda_t \quad (97)$$

$$\eta_t = c_t' K_{t+1} c_t + p_{t+1}' c_t \quad (98)$$

It is important to express the feedback matrices and the Ricatti equations in terms of the original matrices of the feedback control problems (i.e., A , B , and c) instead of the intermediate matrices above. This can be achieved by substituting the

intermediate expressions (Equations 93-98) into the feedback matrices and the Ricatti equations (91-92), yielding the following form of the feedback rule

$$u_t = G_t C_t + g_t \quad (99)$$

with the feedback matrices

$$G_t = - \left[B_t' K_{t+1} B_t + \Lambda_t \right]^{-1} \left[F_t' + B_t' K_{t+1} A_t \right] \quad (100)$$

$$g_t = - \left[B_t' K_{t+1} B_t + \Lambda_t \right]^{-1} \left[B_t' (K_{t+1} c_t + p_{t+1}) + \lambda_t \right] \quad (101)$$

and the Ricatti equations

$$K_t = A_t' K_{t+1} A_t + W_t \quad (102)$$

$$- \left[A_t' K_{t+1} B_t + F_t \right] \left[B_t' K_{t+1} B_t + \Lambda_t \right]^{-1} \left[F_t' + B_t' K_{t+1} A_t \right]$$

$$p_t = A_t' (K_{t+1} c_t + p_{t+1}) + w_t \quad (103)$$

$$- \left[A_t' K_{t+1} B_t + F_t \right] \left[B_t' K_{t+1} B_t + \Lambda_t \right]^{-1} \left[B_t' (K_{t+1} c_t + p_{t+1}) + \lambda_t \right]$$

4.6. Solution Summary:

In summary, the feedback control problem is solved by following the steps below:

1. Start at the terminal period using the terminal conditions K_N and p_N .
2. Integrate the Ricatti equations back in time and compute K_t and p_t for all time periods.
3. With K_t and p_t known, calculate the feedback matrices G_t and g_t .

4. Substitute the feedback matrices in the feedback rule with the initial values of the states (C_0) to calculate the controls u_0 .
 5. Substitute u_0 and C_0 in the state equation to calculate the states for the next period (C_1).
 6. Use the calculated values of the states C_1 in the feedback rule to compute u_1 .
- Similarly, the computations continue until all the values of the states and control are determined.

REFERENCES

- Aboufirassi, M., and Mariño, M. A. 1984. "Cokriging of aquifer transmissivities from field measurements of transmissivity and specific capacity." *Mathematical Geology*, 16(1), 19-35.
- Ahlfeld, D. P., J. M. Mulvey, G. F. Pinder, and E. F. Wood. 1988a. Contaminated groundwater remediation design using simulation, optimization, and sensitivity theory: 1. Model development, *Water Resources Research*, 24(3), 431-441.
- Ahlfeld, D. P., J. M. Mulvey, G. F. Pinder, and E. F. Wood. 1988b. Contaminated groundwater remediation design using simulation, optimization, and sensitivity theory: 2. Analysis of a field site, *Water Resources Research*, 24(3), 443-452.
- Ahmed, S. and De Marsily, G. 1987. "Comparison of geostatistical methods for estimating transmissivity using data on transmissivity and specific capacity." *Water Resources Research*, 23(9), 1717-1737.
- Andricevic, R. and P. K. Kitanidis. 1990. Optimization of pumping schedule in aquifer remediation under uncertainty, *Water Resources Research*, 26(5), 875-885.

- Andricevic, R. 1990. "A real-time approach to management and monitoring of groundwater hydraulics." *Water Resources Research*, 26(11), 2747-2755.
- Bear, J. 1979. "*Hydraulics of Groudwater*." McGraw-Hill, New York.
- Ben-Jemaa, F., Mariño, M. A. and Loaiciga, H. A. 1994. "Multivariate geostatistical design of groundwater monitoring networks." *Journal of Water Resources Planning and Management, ASCE*, 120(4), 505-522.
- Ben-Jemaa, F., Mariño, M. A. and Loaiciga, H. A. 1994. "Sampling design for contaminant distribution in lake sediments." *Journal of Water Resources Planning and Management, ASCE*, 121(1), 71-79.
- Burn, D. H., and McBean, E. A. 1985. "Optimization modeling of water quality in an uncertain environment." *Water Resources Research*, 21(7), 934-940.
- Cardwell, H. and Ellis, H. 1993. "Stochastic dynamic programming Models for water quality management." *Water Resources Research*, 29(4), 803-813.
- Carrera, J., Usunoff, E. and Szidarovszky, F. 1984. "A method for optimal observation network design for groundwater management." *J. of Hydrol.*, 73, 147-163.
- Casman, E. A., Naiman, D. Q. and Chamberlin, C. E. 1988. "Confronting the ironies of optimal design: Nonoptimal sampling designs with desirable properties." *Water Resources Research*, 24(3), 409-415.
- Chang, L.-C., Shoemaker, C. A., and Liu, P. L.-F. 1992. "Optimal time-varying pumping rates for groundwater remediation: Application of constrained optimal control algorithm." *Water Resources Research*, 28(12), 3157-3173.

- Chow, G. C. 1981. *Econometric Analysis by Control Methods*, John Wiley, New York.
- Culver, T. and Shoemaker, C.-A. 1993. "Optimal control for groundwater remediation by differential dynamic programming with quasi-Newton approximations." *Water Resources Research*, 29(4), 823-831.
- DeMarsily, G. 1986. *Quantitative Hydrogeology*. Academic Press, San Diego, California.
- Everett, L. G. 1980. *Groundwater monitoring*. General Electric Company, Shenectady, N.Y.
- Gorelick, S. M. and I. Remson. 1982. Optimal dynamic management of groundwater pollutant sources. *Water Resources Research*, 18(1), 71-76.
- Gorelick, S. M., C. I. Voss, P. E. Gill, W. Murray, M. A. Saunders, and M. M. Wright. 1984. Aquifer reclamation design: the use of contaminant transport simulation combined with nonlinear programming, *Water Resources Research*, 20(4), 415-427.
- Hsueh, Y-W. and Rajagopal, R. 1988. "Modeling groundwater quality sampling decisions." *Groundwater Monitoring Review*, Fall, 121-134.
- Hudak, P. F., Loaiciga, H. A. and Mariño, M. A. 1993. "Regional scale ground water quality monitoring methods and case study." *Water Resources Center, Contribution 203*, University of California, Riverside, Calif., 74 p.

- Jager, H. I., Sale, M. J., and Schmoyer, R. L. 1990. "Cokriging to assess regional stream quality in the southern Blue Ridge Province." *Water Resources Research*, 26(7), 1401-1412.
- Jones, L., R. Willis, and W. W-G. Yeh. 1987. Optimal control of nonlinear groundwater hydraulics using differential dynamic programming, *Water Resources Research*, 23(11), 2097-2106.
- Journel, A. G., and Huijbregts, J. C. 1978. *Mining Geostatistics*, Academic Press, New York.
- Kendrick, D. 1981. "*Stochastic Control for Economic Models*." McGraw-Hill, New York.
- Kettunen, J., Siviö, H. and Varis, O. 1989. "An analysis of a sampling design, a case study of lake eutrophication." *Computational Statistics and Data Analysis*, (8), 81-91.
- Knopman, D. S. and Voss, C. I. 1987. "Behavior of sensitivities in one-dimensional advection-dispersion equation: Implication for parameter estimation and sampling design." *Water Resources Research*, 23(2), 253-272.
- Knopman, D. S. and Voss, C. I. 1988a. "Further comments on sensitivities, parameter estimation, and sampling design in one-dimensional analysis of solute transport in porous media." *Water Resources Research*, 24(2), 225-238.

- Knopman, D. S. and Voss, C. I. 1988b. "Discrimination among one-dimensional models of solute transport in porous media: Implications for sampling design." *Water Resources Research*, 24(11), 1859-1876.
- Loaiciga, H. A. 1989. "An optimization approach for groundwater quality monitoring network design." *Water Resources Research*, 23, 351-367.
- Loaiciga, H. A., Charbeneau, R. J., Everett, L. G., Fogg, G. E., Hobbs, B. F., and Rouhani, S. 1992. "Review of Ground-water quality monitoring network design." *J. Hydraul. Engr.*, 118(1), 11-37.
- Makinde-Odusola, B. A. and M. A. Mariño. 1989. Optimal control of groundwater by the feedback method of control, *Water Resources Research*, 25(6), 1341-1352.
- McKinney, D. C. and Loucks, D. P. 1992. "Network design for predicting groundwater contamination." *Water Resources Research*, 28(1), 133-147.
- Meyer, P. D., and Brill Jr., E. D. 1988. "A method for locating wells in a groundwater monitoring network under conditions of uncertainty." *Water Resources Research*, 24(8), 1277-1282.
- Morgan, D. R., Eheart, J. W., and Valocchi, A. J. 1993. "Aquifer remediation design under uncertainty using a new chance constrained programming technique." *Water Resources Research*, 29(3), 551-561.
- Murray, D. M. and S. J. Yakowitz. 1979. Constrained differential dynamic programming and its application to multireservoir control, *Water Resources Research*, 15(5), 1017-1027.

- Myers, D. E. 1982. "Matrix formulation of co-kriging." *Mathematical Geology*, 14(3), 249-257.
- Nishikawa, T. and Yeh, W. W-G. 1989. "Optimal pumping test design for the parameter identification for groundwater systems." *Water Resources Research*, 25(7), 1737-1747.
- Quinlan, J. F., Davies, G. J., and Worthington, S. R. H. 1993. "Review of groundwater quality monitoring network design," *J. Hydr. Engrg.*, ASCE, 119(12), 1436-1441.
- Ranjithan, S., Eheart, J. W., and Garrett, J. H., Jr. "Neural network-based sceerning for groundwater reclamation under uncertainty." *Water Resources Research*, 29(3), 563-574.
- Rouhani, S. 1985. "Variance reduction analysis." *Water Resources Research*, 21(6), 837-846.
- Rouhani, S. and Fiering, M. B. 1986. "Resilience of statistical sampling scheme." *Journal of Hydrology*, 7(1), 1-11.
- Seo, D-J., Krajewski, W. F., and Bowles, D. S. 1990a. "Stochastic interpolation of rainfall data from rain gages and radar using cokriging: 1. Design of experiments." *Water Resources Research*, 26(3), 469-477.
- Seo, D-J., Krajewski, W. F., Azimi-Zonooz, A., and Bowles, D. S. 1990b. "Stochastic interpolation of rainfall data from rain gages and radar using cokriging: 2. Results." *Water Resources Research*, 26(5), 915-924.

- Shamsi, U. M., Quimpo, R. G., and Yoganarasimhan, G. N. 1988. "An application of kriging to rainfall network design." *Nordic Hydrol.*, (19), 137-152.
- Showalter, P. 1985. "Developing objectives for the groundwater quality monitoring network of the Salinas river drainage basin." *Groundwater Monitoring Review* (Spring) 37-45.
- Suchanek, T. H., Richerson, P. J., Woodward, L.A., Slotton, D.G., Holts, L.J. and Woodmansee, C. E. E. 1993. "A survey and evaluation of mercury in sediment, water, plankton, periphyton, benthic invertebrates and fishes within the aquatic ecosystem of Clear Lake, California." Institute of Ecology, Division of Environmental Studies, University of California, Davis, California.
- Tiedman, C. and Gorelick S. 1993. "Analysis of uncertainty in optimal groundwater contaminant capture design." *Water Resources Research*, 29(7), 2139-2153.
- Wagner, B. J. and S. M. Gorelick 1989. Reliable aquifer remediation in the presence of spatially variable hydraulic conductivity: From data to design, *Water Resources Research*, 25(10), 2211-2225.
- Woldt, W. and Bogardi, I. 1992. "Ground water monitoring network design using multiple criteria decision making and geostatistics." *Water Resour. Bull.*, 28(1), 45-62.
- Yost, R. S., Trangmar, B. B., Ndiaye, J. P., and Yoshida, N. S. 1989. *Geostatistical Software for PC-DOS and MS-DOS, I. Semivariograms*, University of Hawaii, Department of Agronomy, Honolulu, Hawaii.