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MULTICRITERIA MANAGEMENT OF GROUNDWATER QUALITY UNDER UNCERTAINTY

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ABSTRACT

The primary purpose of this research project is to incorporate parameter uncertainty into the development of multicriteria planning and management tools for groundwater quality problems. We have focused upon three criteria -- cost, water quality, and sensitivity. We have also focused upon a particular type of management strategy -- the use of injection and extraction wells to control and remove a contaminant plume.

Two different stochastic management tools have been developed in this project -- the Marginal Sensitivity Technique (MST), and the Parameter Configuration Technique (PCT). The former technique designs a "best" pumping scheme with respect to cost and parameter sensitivity and determines the tradeoff between these two criteria. The latter technique seeks to identify unfavorable (but physically plausible) spatial distributions of groundwater parameters. The MST uses an efficient method to compute the sensitivity of the hydraulic gradient along the plume boundary with respect to changes in transmissivity values throughout the flow domain. The maximum sensitivity is constrained to be less than or equal to a user-supplied parameter. A parametric linear programming algorithm is used to determine the tradeoff between cost and sensitivity. The PCT finds a "bad" set of spatially varying transmissivity values by solving a constrained optimization problem. The constraints, which guarantee that the transmissivity field is physically reasonable, are based upon geostatistical concepts.

The MST has been applied to a simple hypothetical problem involving uniform flow through a two-dimensional, homogeneous aquifer. The MST shows that it is possible to increase pumping (i.e., cost) in such a way so as to manipulate the groundwater system into states of low sensitivity to parameter changes. A hypothetical example problem was constructed to illustrate the use of the PCT. Two pumpout schemes were designed, under the assumption of uniform transmissivity; one scheme was based on one extraction well, the other on one extraction and one injection well. The least-cost design (pumping scheme) of each was then subjected to a PCT-generated transmissivity field. For the data set used, the least-cost one-well scheme captured 85% of the contaminant and the two-well design captured 86%.

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KEYWORDS -- groundwater pollution, groundwater management, mathematical models

INTRODUCTION

Contamination of a groundwater supply is a complex and formidable problem for state and local water authorities. Because of the wide range of technical options, managers of groundwater resources face a complex task in rationally devising practical programs to protect aquifers from contamination from waste disposal facilities. The practice of aquifer cleanup is still in its infancy; however, there are several restoration operations currently in progress. Such operations may consist of one or more of the following: isolation of the contaminated plume by the construction of an engineered barrier (e.g., a bentonite slurry wall), hydraulic control of plume migration by selective pumping from existing or new wells, installation of purge wells to extract and possibly treat the polluted groundwater, and removal of the pollutant source.

In this research, we have focused upon restoration of polluted aquifers by active hydraulic methods which usually involve control of plume migration by selective pumping/injection of new or existing wells and the installation of purge wells to extract and possibly treat the contaminated groundwater. Optimal design of a restoration strategy is an enormously complicated problem because: (1) the state of the groundwater system (i.e., the spatial distribution of pollutant concentration) is nonlinearly related to the decision variables (i.e., the well locations and pumping quantities), and (2) aquifer parameter values are inherently heterogeneous and uncertain. Cost and water quality are the two primary criteria in the design of an aquifer restoration system. However, since there are always insufficient data on the physical parameters associated with pollutant movement through aquifers, another major objective is to decrease the sensitivity of the system to unforseen changes in the ambient conditions or errors in the estimates of the physical parameters.

Although there have been numerous studies dealing with optimal design of aquifer restoration systems (e.g., Gorelick et al., 1984; Atwood and Gorelick, 1985; Colarullo et al., 1984), these investigations have all assumed that aquifer parameters are known with complete certainty. In light of the well-established uncertainty in groundwater flow parameters, the deterministic nature of these previous studies must be regarded as a serious deficiency.

The primary purpose of this research project is to incorporate parameter uncertainty into the development of multicriteria planning and management tools for groundwater quality problems. We have focused upon three criteria -- cost, water quality, and sensitivity. We have also focused upon a particular type of management strategy -- the use injection and extraction wells to control and remove a contaminant plume.

Two different stochastic management tools have been developed in this project -- the Marginal Sensitivity Technique (MST), and the Parameter Configuration Technique (PCT). The former technique designs a "best" pumping scheme with respect to cost and parameter sensitivity and determines the tradeoff between these two criteria. The latter technique seeks to identify unfavorable (but physically plausible) spatial distributions of groundwater parameters. The former is restricted to situations where the assumed transmissivity field is "close" to the actual one, but it is relatively simple computationally since linear programming techniques are used. However, the PCT is difficult computationally due to its inherent nonlinearity. These two techniques are described further in the following sections.

MARGINAL SENSITIVITY TECHNIQUE

If hydrodynamic dispersion is neglected, then groundwater flow simulation models can be used to predict the impact of a given pumping scheme upon contaminant plume migration. Despite their simplicity, such models serve as practical preliminary screening tools to evaluate proposed designs of purge well systems (Keely, 1984). Atwood and Gorelick (1985) and Colarullo et al. (1984) have recently shown how to combine groundwater flow models with optimization techniques in order to determine the least-cost pumping strategy that will achieve specified hydraulic control of the plume migration. These models are examples of the general class of groundwater optimization-simulation models reviewed by Gorelick (1983). Use of these models requires specification of the spatial distribution of all groundwater flow parameters (e.g., transmissivity), as well as the boundary conditions and the location of the contaminant plume and the injection/extraction wells. In light of the well-established uncertainty in hydraulic parameters, the deterministic nature of these models must be recognized as a serious deficiency. The least cost pumping strategy is of little utility if containment of the contaminant plume is highly sensitive to the assumed transmissivity field. Low sensitivity to changes in assumed parameter values is an equally important criterion in practice. For the purposes of this project, we define a "robust" strategy as one that exhibits small sensitivity to parameter changes.

The MST is a simple method for incorporating uncertainty into the design of hydraulic gradient control schemes. This method explicitly accounts for the tradeoff between cost and robustness in a multi-objective framework. We assume two-dimensional, steady flow in a horizontal aquifer and we restrict our attention to the case where transmissivity is the only uncertain parameter. The transmissivity field is heterogeneous and is assumed to consist of a certain number of homogeneous subdomains. Our formulation is based upon the use of sensitivity coefficients (Sykes et al., 1985; McElwee, 1982) to define a measure of robustness as the sensitivity of the performance of a given pumping strategy to transmissivity changes at certain critical locations. Model solution is computationally simple since it can be obtained with parametric linear programming techniques.

Traditional Formulation Without Parameter Uncertainty

In this section we briefly review the traditional management model formulation where parameter uncertainty is neglected. Atwood and Gorelick (1985) present this formulation in greater detail. Since hydrodynamic dispersion is neglected in this study, contaminants will migrate along the flow pathlines which are completely specified by the groundwater flow equation. For the case of steady, horizontal flow through an isotropic aquifer, the governing flow equation is

$$\frac{\partial}{\partial x}\left(T\frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(T\frac{\partial h}{\partial y}\right) = W \qquad (1)$$

where T is the transmissivity $[L^2T^{-1}]$; h is the piezometric head [L]; W is the volumetric inflow per unit area due to fluid sources and sinks $[LT^{-1}]$; and x,y are the cartesian space coordinates [L]. If the only sources and sinks are wells, then

$$W = -\sum_{j=1}^{NW} Q_j \, \delta(x - x_{w_j}, y - y_{w_j}) \tag{2}$$

where Q_j is the extraction (positive) or injection (negative) rate for well number j [L^3T^{-1}]; NW is the total number of wells; x_{w_j}, y_{w_j} is the location of well j [L]; and $\delta(x,y)$ is the Dirac delta function [L^{-2}].

The decision variables in the management model are the injection/extraction rates, Q_j, at a preselected set of well locations (x_{w_j}, y_{w_j}). The goal of contaminant plume containment can be expressed mathematically as a set of target hydraulic gradients at a series of check points located around the perimeter of the plume (see Atwood and Gorelick, 1985). Thus, h can be considered to be the state variable of the system, and the groundwater flow equation (1) provides the linear response function that relates the system state to the decision variables. The objective is to find the least cost pumping strategy that will achieve the desired hydraulic control of the plume. Instead of directly solving for the least cost strategy, we will find the solution that minimizes the sum of extraction and injection rates.

Following Atwood and Gorelick, the management model can be expressed as

Objective:

$$\text{Min} \sum_{j=1}^{NW} (u_j + v_j) \tag{3}$$

Constraints:

$$\sum_{j=1}^{NW} R_{ij}(u_j - v_j) \geq g_i \quad , \quad i = 1, 2, \ldots, NGP \tag{4}$$

$$\left.\begin{array}{l} 0 \leq u_j \leq Q_{max} \\ 0 \leq v_j \leq Q_{max} \end{array}\right. \quad , \; j = 1, 2, \ldots, NW \tag{5}$$

where u_j is the extraction rate at well j; v_j is the injection rate at well j; g_i is the target hydraulic gradient at location i; R_{ij} is the gradient response coefficient, which gives the impact of a unit extraction at well j upon the gradient at location i; NGP is the number of gradient check points; and Q_{max} is an upper bound on the maximum possible extraction/injection rate. Due to linearity, R_{ij} is constant with respect to u_j and v_j. It is simple to add an additional constraint restricting the total injection to be less than or equal to the total extraction, since this would be practical requirement for most pumping strategies. Linear programming can be used to find the optimal solution to the above management model. As discussed by Atwood and Gorelick, the use of (3) through (5) permits the linear program to decide automatically whether a particular well should be injecting or extracting.

For simple situations with a homogeneous transmissivity field and ideal domain geometry, the gradient response coefficients, R_{ij}, can be obtained from analytical solutions to equation (1) (Tung, 1986; Maddock, 1972). In the general case where numerical simulation models are used to solve (1), R_{ij} values can be obtained by executing the model once for each possible well location (Gorelick, 1983; Atwood and Gorelick, 1985). In this study, we use a finite element model with linear triangular basis functions to solve equation (1). As will be discussed further in the next section, the so-called adjoint sensitivity theory recently presented by Sykes et al. (1985) can also be utilized to obtain R_{ij} values.

Since we are using a discrete numerical model to solve (1), we follow Atwood and Gorelick and express the gradient at a particular location on the plume boundary as the difference between the piezometric head at two nodes on opposite sides of the plume boundary. Therefore, for successful plume containment,

$$h_{A_i} - h_{B_i} \geq \Delta h_{target_i} \tag{6}$$

where points A and B are typically located just outside and inside, respectively, of the plume boundary, and Δh_{target} is set equal to zero (a flat gradient) or to some desired inward gradient. The adjacent points A and B are called a gradient check pair. If we define the response coefficient, R_{ij}, as the impact of a unit extraction at well j upon the difference $h_{A_i} - h_{B_i}$, then we can use superposition to write

$$h_{A_i} - h_{B_i} = h_{A_i}^{reg} - h_{B_i}^{reg} + \sum_{j=1}^{NW} R_{ij}(u_j - v_j) \tag{7}$$

where the reg superscript signifies a regional flow field which may be present in the absence of any pumping. Letting $\Delta h_i^{reg} = h_{A_i}^{reg} - h_{B_i}^{reg}$, we can combine (6) and (7) to give the constraint equation (4), where g_i is expressed as

$$g_i = \Delta h_{target_i} - \Delta h_i^{reg} \tag{8}$$

Formulation With Parameter Uncertainty

Once the gradient response coefficients (R_{ij}) are specified, the deterministic management model presented in equations (3), (4), and (5) can be solved by standard linear programming algorithms. In order to determine R_{ij}, the numerical solution of (1) is used; however, this numerical solution requires specification of the spatial distribution of the transmissivity. In practical applications, there will always be considerable uncertainty about the transmissivity field. Hence, the response coefficients appearing in (4) must be regarded as uncertain quantities, and the management model must be recast as a stochastic optimization problem. In this section we present a simple formulation using linear deterministic mathematical programming tools that accounts for uncertainty in the gradient response coefficients appearing in (4).

The idea behind our method is based upon the concept of sensitivity coefficients, which can be defined as

$$\frac{\partial P}{\partial \alpha}$$

where P is some performance measure that is a scalar function of system state and α is any system parameter. Sensitivity coefficients are discussed further by Gillham and Farvolden (1974), McElwee and Yukler (1978), and Sykes et al. (1985); they have been used mostly in the context of the groundwater inverse problem (McElwee, 1982; Neuman, 1980) and first-order analysis of stochastic groundwater models (Townley and Wilson, 1985). We assume that the deterministic management model, (3) through (5), has been solved using a "best estimate" of the transmissivity field. However, in some specific regions the transmissivity values are uncertain; in these regions, sensitivity coefficients are used to measure the impact of a small change in transmissivity upon contaminant plume containment. Sensitivity coefficients defined in such a way provide a qualitative measure of the robustness of a decision strategy. For the purposes of this investigation, we define a robust decision strategy as one that is capable of successfully containing the contaminant plume if actual transmissivities differ slightly from their assumed values. Minimization of the overall sensitivity of a pumping strategy to transmissivity changes then becomes a second objective which we append to equations (3) through (5).

Management Model Formulation:

As discussed previously, contaminant plume migration is evaluated mathematically in terms of hydraulic gradients at specified locations on the plume boundary. A sensitivity coefficient that expresses the impact of transmissivity changes upon the performance of a given pumping strategy can be defined as

$$s_{ik} = \frac{\partial P_i}{\partial T_k} \tag{9}$$

where

$$P_i = h_{A_i} - h_{B_i} \tag{10}$$

is the hydraulic gradient at check pair i and T_k is the transmissivity in region k. (In this study, we assume that the aquifer's transmissivity field is comprised of a finite number of homogeneous subdomains.) The absolute value of s_{ik} is a measure of the robustness of any particular management strategy; strategies with small values of $|s_{ik}|$ will still successfully contain the contaminant plume even if the transmissivity differs slightly from its assumed value.

We can use the sensitivity coefficients to formulate a "sensitivity" criterion, J_s, to be minimized along with the "cost" criterion given by (3). Many choices for J_s are possible, such as a weighted sum of $|s_{ik}|$ or $(s_{ik})^2$. However, to maintain a linear formulation, we use a minimax criterion

$$\text{Min } J_s \qquad (11)$$

$$J_s = \max_{\substack{k \in K^* \\ i \in I^*}} |s_{ik}|$$

where K^* is a subset of the total number of transmissivity zones containing the uncertain transmissivity values and I^* is a subset of the total number of gradient check pair locations containing the points where the gradient control constraints (4) are binding. The groundwater flow equation (1) provides the required coupling between s_{ik} and the decision variables (u_j and v_j); the details are presented in the next section.

The new management model is obtained by adding the sensitivity criterion (11) to the deterministic formulation (3) through (5). Thus, the new model is

Objectives:

$$\text{Min } \sum_{j=1}^{NW} (u_j + v_j)$$

$$\text{Min } J_s$$

where J_s is given by (11) with the constraints are given by (4) and (5). In order to solve the multiobjective management problem, we use the so-called constraint method where the sensitivity criterion is placed into the constraint set (Loucks et al., 1981; Neuman, 1973).

Objective:

$$\text{Min} \sum_{j=1}^{NW} (u_j + v_j) \tag{12}$$

Constraints:

$$\sum_{j=1}^{NW} R_{ij}(u_j - v_j) \geq g_i \qquad i = 1, 2, \ldots, NGP \tag{13}$$

$$|s_{ik}| \leq s_{max} \qquad i \in I^*, \quad k \in K^* \tag{14}$$

$$\begin{aligned} 0 \leq u_j \leq Q_{max} \\ \qquad\qquad j = 1, 2, \ldots, NW \\ 0 \leq v_j \leq Q_{max} \end{aligned} \tag{15}$$

where s_{max} is the maximum allowable absolute sensitivity value. Parametric linear programming techniques can be used to solve (12) through (15) for various values of s_{max} thus allowing examination of the tradeoff between cost (as measured by the sum of injection and extraction rates) and robustness (as measured by s_{max}).

Calculation of the Sensitivity Coefficients:

The relationship between s_{ik} and the pumping rates is obtained when (7) is substituted into (9). The result is

$$s_{ik} = s_{ik}^{reg} + \sum_{j=1}^{NW} S_{ij}^{k}(u_j - v_j) \tag{16}$$

where

$$s_{ik}^{reg} = \frac{\partial \, \Delta h_i^{reg}}{\partial T_k} \tag{17}$$

$$S_{ij}^{k} = \frac{\partial R_{ij}}{\partial T_k} \tag{18}$$

S_{ij}^{k} can be regarded as a sensitivity response coefficient since it measures the impact of a unit extraction at well j upon s_{ik}. The sensitivity of the regional flow field to transmissivity changes is defined by s_{ij}^{reg} in (17).

We use the discrete adjoint sensitivity theory as presented by Sykes et al. (1985) in order to calculate S_{ij}^k efficiently. The discrete finite element approximation to (1) can be expressed as

$$[A(\{T\})]\{h\} = \{B_h\} \tag{19}$$

where $[A(\{T\})]$ is the global stiffness matrix which is a function of $\{T\}$, the vector containing the transmissivity value in each homogeneous subdomain, $\{h\}$ represents the vector of unknown nodal head values, and $\{B_h\}$ is the load vector which accounts for well pumping (equation 2) and boundary conditions. Because the governing groundwater flow equation (1) (subject to Dirchlet and Neumann boundary conditions) is self-adjoint, the matrix $[A]$ is symmetric. According to Sykes et al., if a performance measure P_i is defined as in (10), then the adjoint sensitivity method gives

$$\frac{\partial P_i}{\partial T_k} = \{\Psi^*\}_i^T \{B_\psi\} \tag{20}$$

where

$$\{B_\psi\} = \frac{\partial\{B_h\}}{\partial T_k} - \frac{\partial[A]}{\partial T_k}\{h\} \tag{21}$$

and $\{\Psi^*\}_i$ is called the adjoint state and satisfies

$$[A]\{\Psi^*\}_i = \frac{\partial P_i}{\partial\{h\}} \tag{22}$$

The matrix $[A]$ appearing in (21) and (22) is the global stiffness matrix from the finite element model (19); hence, if a direct matrix solver is utilized only one factorization of $[A]$ is necessary to find both $\{h\}$ and $\{\Psi^*\}$. Since P_i is the simple linear function defined by (10), the right hand side of (22) is a vector with +1 in the location corresponding to point A, −1 in that corresponding to B, and zero elsewhere. All terms in (21) are readily obtainable; further details regarding the solution of (20) through (22) are given in the paper by Sykes et al.

The solution of (20) gives the contribution of the regional flow field to the overall sensitivity (s_{ik}^{reg} in equation 16) when $\{h\}$ in (21) is the finite element solution to (19) for the case of zero pumping. Recall that S_{ij}^k is defined by (18) and that R_{ij} is equal to $(\partial P_i/\partial Q_j)$ where P_i is given by (10) and Q_j is the extraction rate at well j. Therefore, S_{ij}^k can be obtained by differentiating (20) with respect to Q_j. Thus

$$S_{ij}^k = \{\Psi^*\}_i^T \frac{\partial}{\partial Q_j}\{B_\psi\} \tag{23}$$

where

$$\frac{\partial\{B_\psi\}}{\partial Q_j} = - \frac{\partial[A]}{\partial T_k} \frac{\partial\{h\}}{\partial Q_j} \tag{24}$$

The vector $\partial\{h\}/\partial Q_j$ appearing in (24) above can be found by solving a modified form of (19).

$$[A] \frac{\partial\{h\}}{\partial Q_j} = \frac{\partial\{B_h\}}{\partial Q_j} \tag{25}$$

where the right hand side vector has −1 in the location corresponding to node j and zero elsewhere (if well locations are coincident with nodal points).

Equation (25) represents the standard technique for finding the gradient response coefficients. Since R_{ij} is defined as $\partial(h_{A_i} - h_{B_i})/\partial Q_j$, R_{ij} is equal to the difference between elements of the vector $\partial\{h\}/\partial Q_j$ corresponding to nodes A and B. Also, since Sykes et al. note that adjoint state physically represents the change in the performance measure caused by a unit volume influx of water at a particular location, R_{ij} is alternately given by the element of the vector $\{\psi^*\}_i$ in (22) corresponding to node j.

In summary, the management model is given by (12) through (15). Required input to the management model includes the gradient response coefficients R_{ij}, the sensitivity response coefficients S^k_{ij}, and the regional flow contribution to the overall sensitivity s^{reg}_{ik}. These parameters are calculated as follows:

1. Equation (19) is solved to find the regional flow field.
2. For each gradient check point (or the subset I^* of binding check points) (22) is solved for the adjoint state $\{\psi^*\}_i$.
3. Equation (20) is evaluated with $\{B_\psi\}$ given by (21) and $\{h\}$ as the regional flow field. This yields s^{reg}_{ik}.
4. For each possible well location, (25) is solved for $\partial\{h\}/\partial Q_j$. R_{ij} is evaluated as described above by taking the difference between appropriate elements of $\partial\{h\}/\partial Q_j$.
5. Equation (23) is evaluated to find S^k_{ij}.

As discussed by Sykes et al., the computational burden of the adjoint sensitivity analysis performed in steps 1-5 above is not excessive. We use a direct matrix solver for the finite element system solved in step 1 and thus the same matrix decomposition is used in steps 2 and 4. The matrices $\partial[A]/\partial T_k$ in (21) and (24) are very sparse and are easily evaluated during the element assembly process used to generate the global stiffness matrix [A].

Application to a Hypothetical Problem

In this study we have based our implementation of the MST upon a linear triangular finite element model of groundwater flow. The transmissivity is constant within a finite element but varies among different elements; that is, the total number of discrete transmissivity zones (the dimension of {T} in eqn. 19) equals the number of elements. A direct banded matrix solver is used in (19), (22), and (25). The linear programming problem is solved using the optimization package XMP (Department of Management Information Systems, University of Arizona, Tucson, Arizona).

In order to illustrate the utility of our method, we consider the simple case of uniform regional flow through a homogeneous aquifer. Figure 1 shows the location of the contaminant plume, the gradient check pairs, and the wells. A uniform finite element mesh is used, as also shown in Fig. 1. The regional hydraulic gradient is 0.01, and the transmissivity field is assumed homogeneous with a value of 100 m^2/day.

We first apply the traditional management model (3) - (5) to this problem. In all of the results reported here, Δh_{target_i} in (8) is equal to zero (a flat target gradient at the check pair locations) and Q_{max} in (5) is equal to a very large number so that there is essentially no upper bound on the pumping rates. The gradient response coefficients R_{ij} in (4) are obtained using the adjoint state method described previously and the linear programming problem was solved using XMP. As expected, the optimal solution to this problem involves extraction at a rate of 820 m^3/day from well 1 (the central well within the plume) with all other wells inactive. Also as expected, the hydraulic gradient at check pair 1 is the binding constraint (see Table 1).

The optimal strategy noted above will fail if the transmissivity in certain locations differs from its assumed value of 100 m^2/day. The adjoint state technique can be used to calculate the effect of changes in the assumed transmissivity values upon the gradient at check pair 1. That is, eqn. (20) can be utilized to calculate $s_{1k} = \partial P_1/\partial T_k$ for each k. The results for $|s_{1k}|$ are illustrated in Figure 2. It should be noted that $s_{1k} \approx s_{1k}^{reg}$ (see eqn. 16) for elements located far from well 1. Likewise, the value of s_{ik} for an element far from all potential well locations is dominated by the regional flow contribution (s_{ik}^{reg}) and hence it is impossible for any pumping strategy to decrease that value of $|s_{ik}|$ unless new potential well locations are introduced.

The results in Fig. 2 show that elements 90 and 91 (see Fig. 1 for element locations) possess the largest values of $|s_{ik}|$. The region occupied by these elements can be thought of as a high sensitivity or "critical" zone. Hence, apart from the optimization model developed in this paper, the adjoint state method itself is a valuable aid in identifying regions where additional parameter measurements are most needed. For the sake of illustration, we consider that the only uncertain values of transmissivity are those of elements 90 and 91; all other elements have their transmissivity fixed at the assumed value of 100 m^2/day. In this situation, a tradeoff between cost and robustness can be determined by solving the optimization model (12) through (15) for various values of the parameter s_{max}. In (14), I^* contains all three gradient check pairs, and K^* contains elements 90 and 91; hence, there are six sensitivity constraints. Optimal pumping strategies for selected values of s_{max} are listed in Table 1. Positive values in Table 1 signify extraction and negative values, injection. The last column is the sum of the extraction and injection rates and thus represents the overall cost of a particular optimal strategy. Figure 3 is a plot showing the tradeoff between cost (as measured by the total pumping) and robustness (as measured by s_{max}). Also shown in

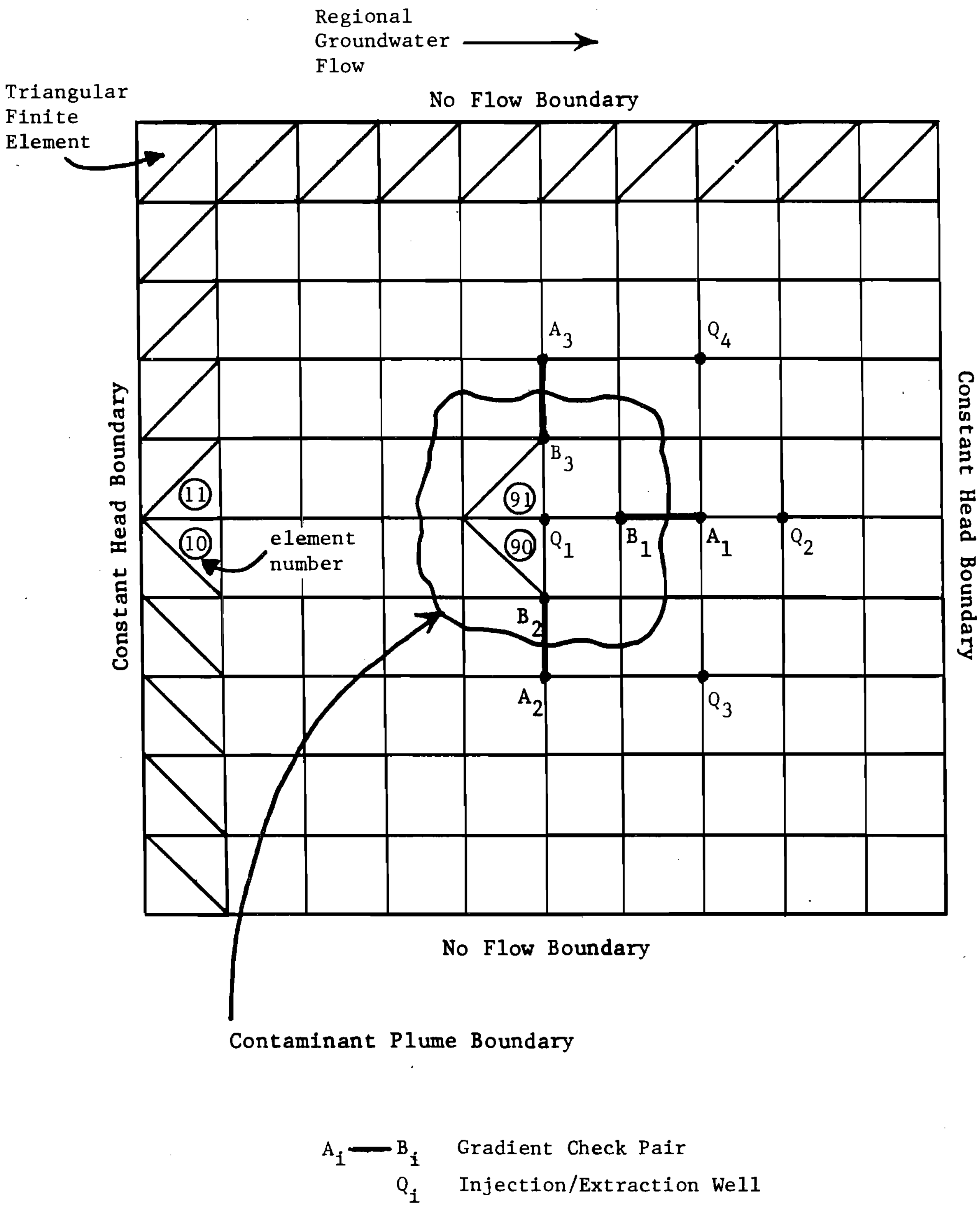

Figure 1. Hypothetical Example Problem Showing Finite Element Discretization and the Contaminant Plume Location

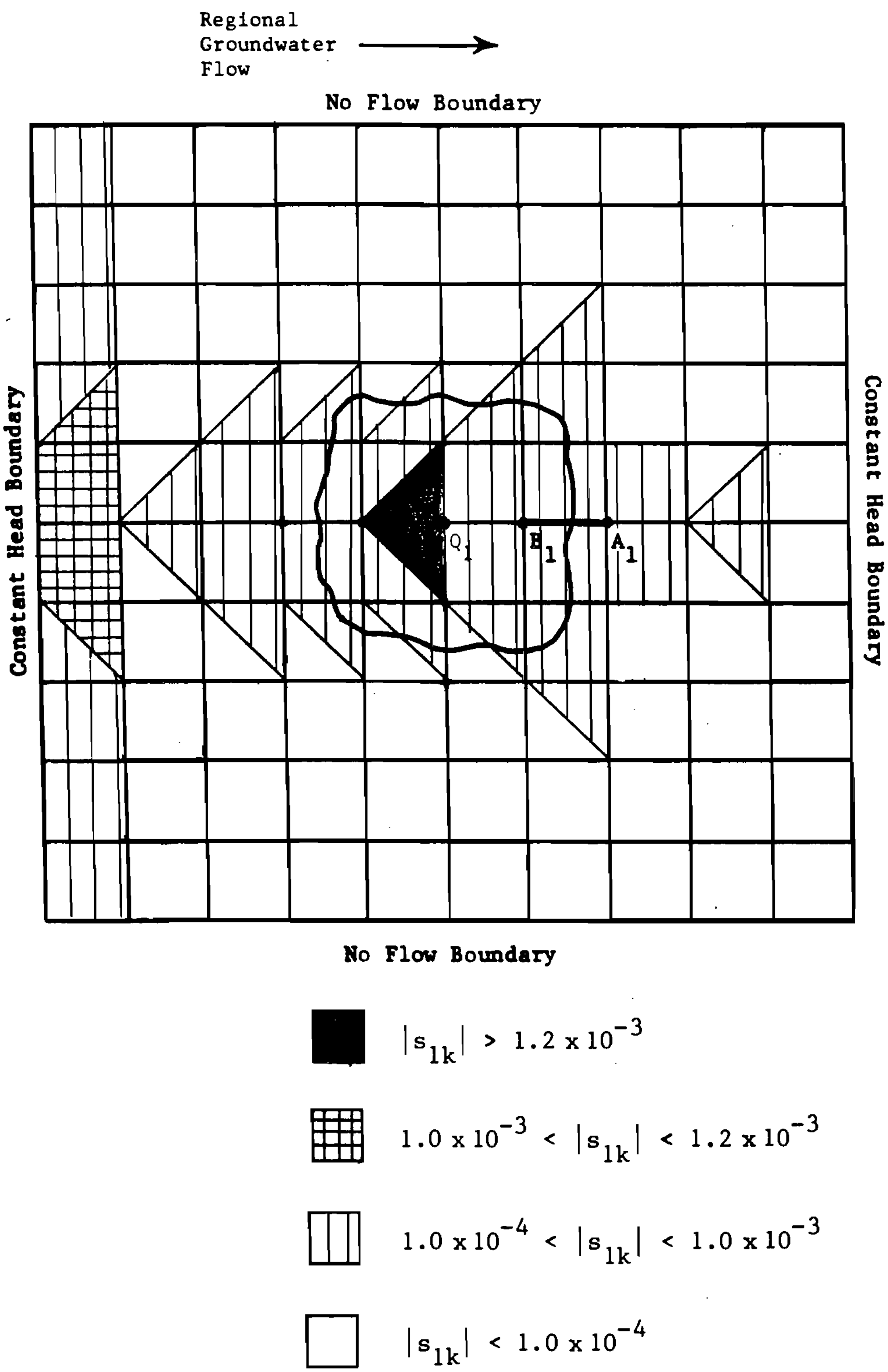

Figure 2. $|s_{1k}|$ Values Corresponding to the Optimal Pumping Scheme Without Consideration of Parameter Uncertainty

Table 1 are the binding gradient check pair (13) and sensitivity (14) constraints; for example when $s_{max} = 1.5 \times 10^{-4}$ all three gradient check pair constraints are binding as are the sensitivity constraints for check pair 1 and elements 90 and 91.

TABLE 1. Optimal Solutions for Hypothetical Problem

s_{max}	Optimal Pumping Rates* Q_1	Q_2	Q_3	Q_4	Binding† Constraints	Total Pumping
no uncertainty	820	0	0	0	GP1	820
1.2×10^{-3}	781	-54	0	0	GP1 $s_{1,90}$ $s_{1,91}$	835
1.0×10^{-3}	634	-259	0	0	GP1 $s_{1,90}$ $s_{1,91}$	893
5×10^{-4}	264	-774	0	0	GP1 $s_{1,90}$ $s_{1,91}$	1030
1.5×10^{-4}	84	-926	-775	-775	GP 1,2,3 $s_{1,90}$ $s_{1,91}$	2560

* All pumping rates are m^3/day; positive values signify extraction and negative values signify injection

† The top line shows the binding gradient check pair constraint; the bottom line shows the binding sensitivity constraints.

The results shown in Table 1 and Figure 3 demonstrate that it is possible to use selective withdrawal and injection to manipulate the groundwater system into states of low sensitivity to parameter changes. Given the assumed configuration of well locations, it is generally possible to identify least cost pumping strategies that meet the dual goals of plume containment and sensitivity diminishment. Detail examination of the solution on the boundary of the feasible space (s_{max}=6.8x10^{-5}) reveals that the sensitivity constraints for check pairs 2 and 3 are almost binding. Due to the signs of the various s_{ik}^{reg} and S_{ij}^{k} values, any additional change in the pumping rates that will effect a decrease in the check pair 1 sensitivity will cause an increase in the check pair 2-3 sensitivity. New wells would need to be introduced to expand the feasible space.

In order to test the solutions listed in Table 1, we have performed groundwater flow simulations where the transmissivities for elements 90 and 91

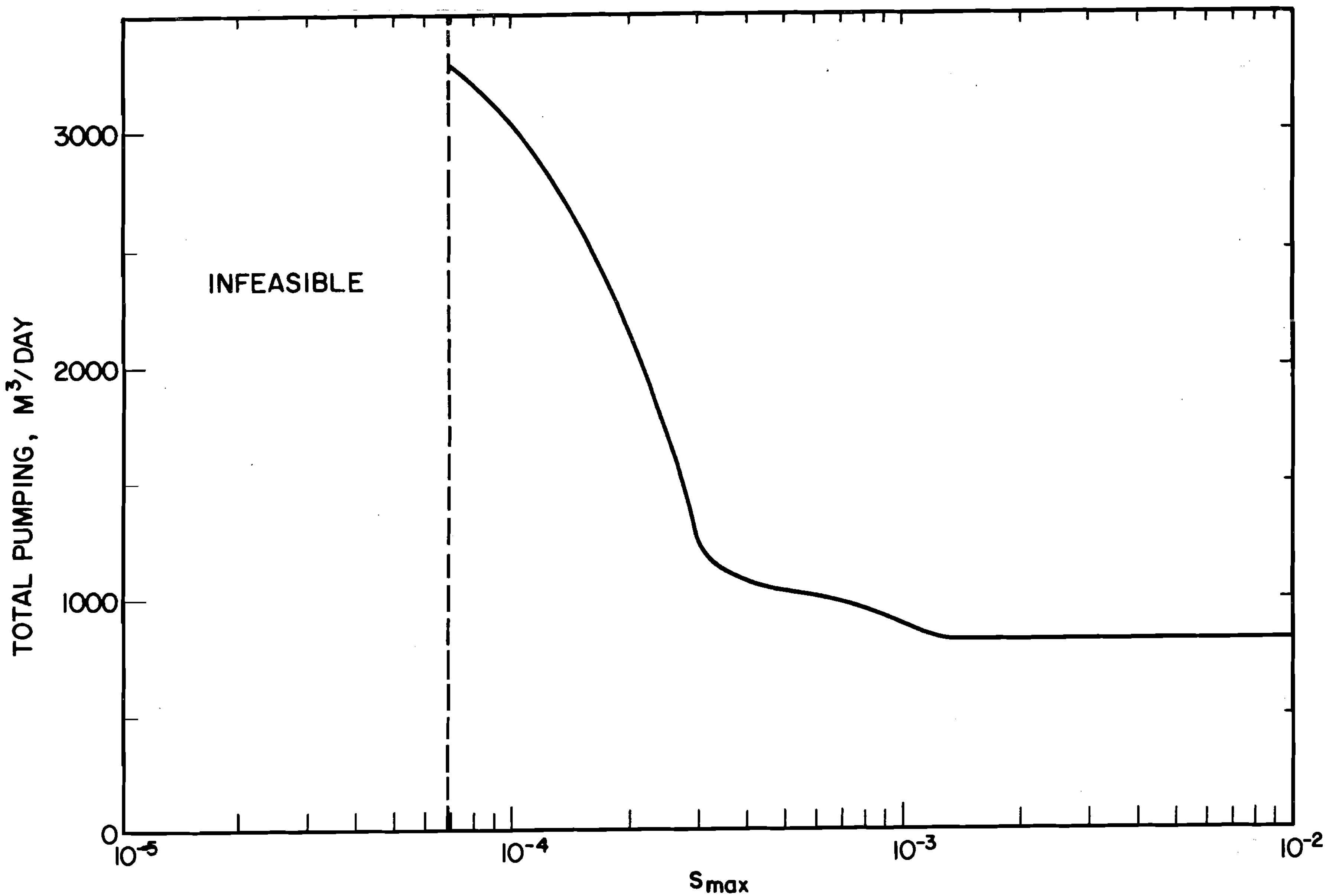

Figure 3. The Tradeoff Between Total Pumping and Sensitivity for the Hypothetical Example Problem

are changed from their assumed value of 100 m^2/day. We would expect that pumping schemes corresponding to high s_{max} values would fail to contain the plume whereas schemes corresponding to low s_{max} values would still successfully achieve plume control. Since the hydraulic gradient at check pair 1 is most sensitive to transmissivity changes, the value of P_1 (see eqn. 10) indicates the status of plume containment -- positive values (inward directed gradient) indicate success and negative values, failure. Table 2 shows the results of these simulations for several different pumping schemes and parameter value changes. It can be seen that the most robust (lowest s_{max}) scheme successfully contains the plume even for a 50% change in the element transmissivity values. It is interesting that the traditional approach (without uncertainty) yields an optimal pumping scheme that fails when the critical element transmissivity values change by only 10%. The results listed in Table 2 generally verify the validity of our formulation. Given the assumptions and definitions built into our model, solutions identified as being more "robust" do indeed successfully control the plume even when transmissivities differ from their assumed values.

TABLE 2. Effect of Transmissivity Changes Upon Plume Containment for Selecting Pumping Schemes

Pumping Scheme s_{max}	Q_1	Q_2	Q_3	Q_4	$T_{90}, T_{91}^*=110$ P_1†	$T_{90}, T_{91}=125$ P_1	$T_{90}, T_{91}=150$ P_1
no uncertainty	820	0	0	0	-0.024	-0.050	-0.082
5×10^{-4}	264	-774	0	0	-0.006	-0.012	-0.020
1.5×10^{-4}	84	-926	-775	-775	+0.002	+0.005	+0.008

* transmissivity (m^2/day) in elements 90 and 91
† value of hydraulic gradient at check pair 1

Our method can in principle be utilized if more elements are considered to have uncertain transmissivity values (i.e., increasing the size of the set K^* in eqn. 14). However, in this case the feasible region will be greatly reduced given the problem definition in Figure 1. For example, when every element in the domain is included in K^*, the check pair 1 - elements 10 and 11 ($s_{1,10}$ and $s_{1,11}$) sensitivity constraint becomes binding for s_{max} values slightly less than 1.2×10^{-3}. As mentioned previously, sensitivity coefficients for elements 10 and 11 are dominated by the regional flow contribution and hence it is not generally possible for any pumping scheme to decrease $s_{1,10}$ and $s_{1,11}$ significantly. Due to the signs of the various s_{ik}^{reg} and s_{ij}^{k} coefficients, there is a conflict between decreasing the sensitivity for elements 90-91 and elements 10-11. Hence, the optimization problem has no feasible solution for s_{max} values below approximately 1.0×10^{-3} and no reasonably robust pumping strategy can be determined.

PARAMETER CONFIGURATION TECHNIQUE

The design of a pumping system to contain and remove a plume of contaminant requires that some basic information about the aquifer be known, such as aquifer thickness, hydraulic conductivity, storativity, permeability of overlying and underlying strata, the hydraulic head, effects of evapotranspiration and infiltration, and perhaps porosity. Quite often these parameters are not adequately known throughout the region of interest to predict the aquifer response to pumping with a sufficient degree of accuracy. Due to the heterogeneous nature of most aquifers, the uncertainties involved in predictions of aquifer behavior and solute transport can be considerable.

Several kinds of uncertainty are present in predicting the behavior of aquifers. These include: (a) intrinsic uncertainty, which defines a natural variability of aquifer properties such as transmissivity; (b) information uncertainty, which includes measurement error or information insufficient to define an aquifer parameter adequately, and which can be reduced through additional measurements; and (c) conceptual uncertainty, where the general framework for the modeling process is an inappropriate descriptor of the true system. This report will focus on the effects of the first two categories, viz. parameter uncertainty and information uncertainty; conceptual uncertainty is assumed not to exist.

The presence of variability, coupled with incomplete information for its specification, has recently led many researchers to describe aquifer behavior in probabilistic terms where prediction uncertainty is a consequence of parameter uncertainty. Dettinger and Wilson (1981) used first and second order analyses of numerical models to study prediction uncertainty. This approach presumes that the first two moments of the random variable in question are sufficient to characterize its distribution. Work by Freeze (1975) indicated that such a method is appropriate when applied to systems with parameters having relatively small variance and where the boundary conditions are well known. This implies that the system must be fairly well defined to begin with, a condition that does not often occur in aquifer modeling.

Monte Carlo simulation as a tool for analyzing parameter uncertainty has been explored by Freeze (1975), Smith and Freeze (1979), Pettyjohn et al. (1984) and Smith & Schwartz (1980). In this approach numerous solute transport simulations are performed with the uncertain parameter inputs of each simulation being generated at random from given probability distributions. The results of these simulations are combined to establish some probability relationship for solute movement. This method can easily be applied to aquifer systems of high variability which may be difficult to examine in terms of analytical formulae. Unfortunately, this brute force approach yields results which can be interpreted only in terms of the specific system being modeled. Although it is generally more expensive than other analysis techniques, it is not limited by restrictions such as the small variance assumption of first order analysis discussed above.

Work by Smith and Schwartz (1981) exemplifies quasi-stochastic modeling to account for spatial uncertainty. In their study an aquifer parameter, hydraulic conductivity, is treated as a random variable having a log-normal probability distribution, but the values of hydraulic conductivity for each point are statistically correlated with the values at neighboring points.

Wang and Williams (1984) discuss the risk associated with assumptions on transmissivity values used in designing hydraulic barrier methods. They make an assessment of these risks by determining best and worst case conditions from limits set on the values of permeability (K) and storativity (S) in a homogeneous aquifer. The best condition occurs for a high K and low S, while the worst condition occurs for low K and high S. This approach could be used to design purge systems for a homogeneous aquifer, but cannot be used for an aquifer known to exhibit spatial heterogeneity. A system designed in a robust fashion under this method could easily fail if the aquifer were in fact heterogeneous.

Uber et al. (1985), Sykes et al. (1985), and the work reported above in this document addresses uncertainty in water quality management planning by considering the change in a performance measure (i.e., its sensitivity) due to small deviations in the uncertain parameter from its expected value. The sensitivity can be used as an inverse measure of the robustness of a management plan. The parameter configuration technique contrasts with these marginal sensitivity approaches by considering the influence of large perturbations of the uncertain parameters on the management plan.

The aforementioned works quantify parameter uncertainty in order to describe aquifer behavior in probabilistic terms. The methods they present could be valuable in exploring the possible outcomes of a given remedial action plan. None of these techniques, however, addresses the problem of determining a robust design for a heterogeneous aquifer whose parameters are not known accurately. The Parameter Configuration Technique selects the values of a spatially varying parameter whose pattern of variation, rather than whose absolute magnitude, is chosen to represent a pessimistic (but realistic) set of design conditions.

All spatially varying parameters governing mass transport are assumed known except one, e.g., transmissivity, porosity, or storativity. The task of finding the "worst" set of parameter values is cast as a constrained optimization problem that is solved by a packaged mathematical algorithm. The statistical information about the uncertain parameters is expressed as a set of constraints representing statistical limits on their individual and relative values. The objective function is chosen such that, when optimized, a worst-case spatial distribution of the uncertain parameter will result which will provide the most severe test of the remedial action design.

Formulating an objective function to represent the worst-case distribution is not always a straightforward matter. For example, it is not clear what conditions will maximize the transfer of contaminant mass from a plume to regions beyond the influence of a remedial action design. The nature of the worst-case condition created by the optimization program depends to a large extent on how the user formulates the objective function. The ultimate objective is to select the values of transmissivity throughout the aquifer in a manner which could cause a proposed pumping scheme to fail most severely.

Feasibility constraints, defined by statistical information, restrict the optimal choice of parameter distribution to those combinations that are statistically consistent with other observations of the parameter under similar conditions. In this study, these constraints express limits on the variogram of the transmissivity. In addition, the mean transmissivity is presumed to be known within statistical limits.

Once an "optimal" transmissivity field has been generated, it can subsequently be used as input data to either a design optimization model (such as the marginal sensitivity technique) or a simulation model wherein pumping decisions are entered as input. It might be used iteratively with the former to produce a robust design or to assess the tradeoff between cost and robustness.

Hypothetical Example Problem

A hypothetical example problem is constructed to illustrate the use of the PCT. Two pumpout schemes are designed to contain and remove a contaminant plume, using standard analytical design techniques and assuming uniform transmissivity. One scheme is based on one extraction well, the other on one extraction and one injection well. The least-cost design (pumping scheme) of each is subjected to a PCT-generated transmissivity field that assumes certain limits on the variogram and mean transmissivity, the same value for the mean as the transmissivity value for the uniform transmissivity field, and a set of objective function weights chosen to maximize the transmissivity in a band cutting through the polluted region and minimize it in the vicinity of the well(s).

It is assumed that a confined aquifer has been contaminated by a plume of hazardous substance. The plume location has been estimated from several monitoring wells, and well locations and pumping rates must be selected to contain the plume and purge the contaminant before it moves downgradient into regions where the aquifer serves as a water supply source. The system should be both cost-efficient and effective, but the transmissivity field is not well-known.

An expensive testing study could be conducted to define the transmissivity throughout the aquifer more accurately, but it is decided first to analyze a basic pumping system design for a pattern of transmissivities that will severely test the performance of the pumping system, in effect, measuring the sensitivity of the design to spatial variability. A diagram representing the contaminated region and proposed well sites is presented in Figure 4.

Data available on the aquifer for the study region are limited. Several core samples have been taken in the study region to establish the aquifer media composition, thickness, and porosity. These samples suggest a seam of high transmissivity material roughly corresponding to the zone indicated in Figure 4, but the transmissivity in this region is unknown. The PCT is set up to maximize transmissivity in this region and to minimize it around one of the wells. Figure 5 shows the objective function weights used for a 10 x 10 array of transmissivity values.

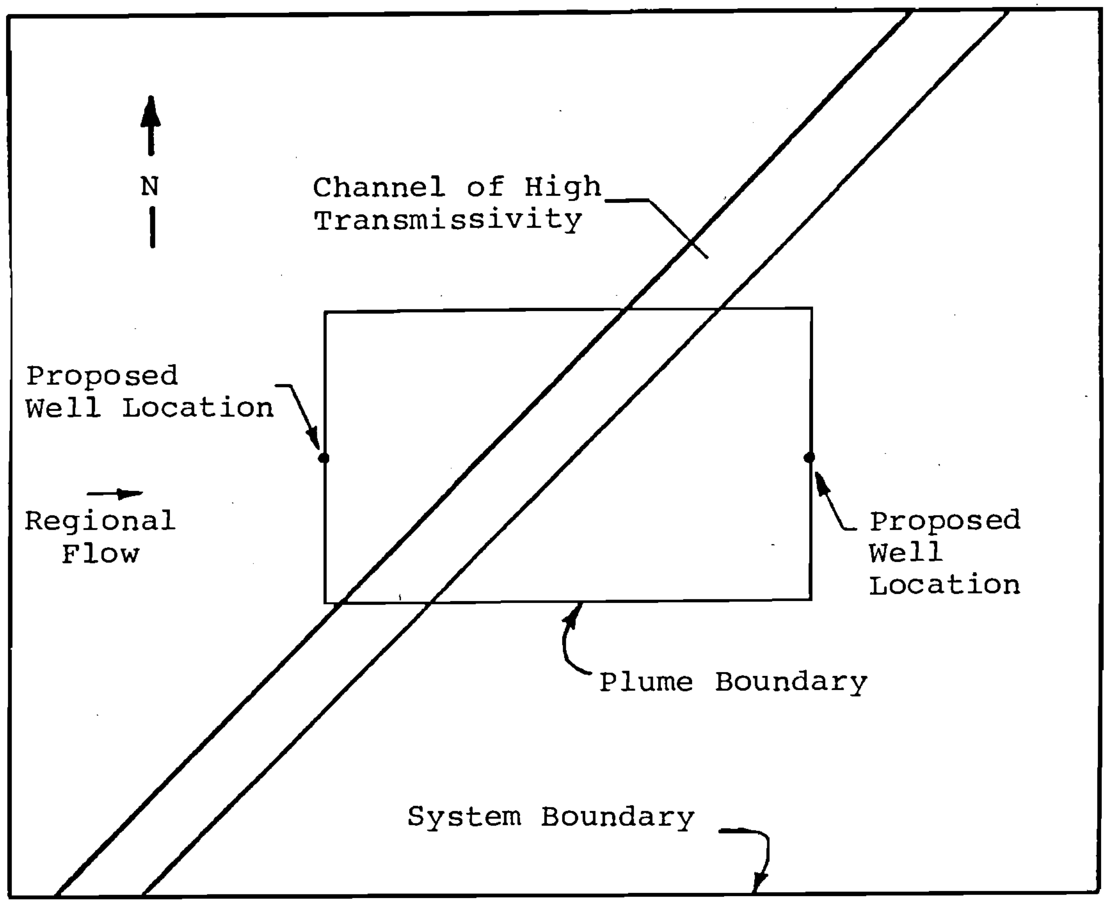

Figure 4. Diagram of Contaminated Aquifer

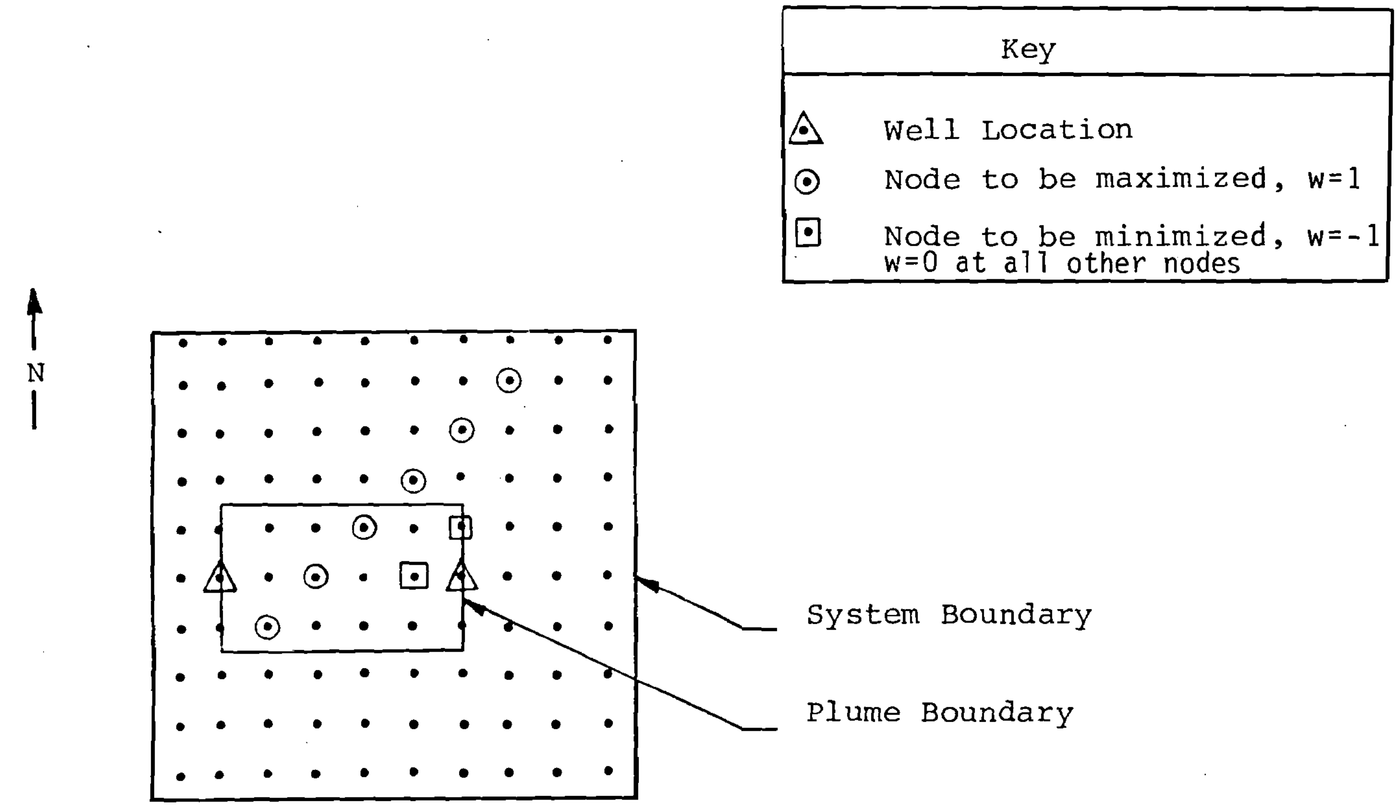

Figure 5. Objective Function Values

These weights are chosen to maximize the transmissivity in a "channel" slicing through the contamination zone and directed away from the wells, and to minimize it around the extraction well. Such a configuration was thought most likely to cause the remedial action pumping scheme to fail to contain the entire plume. An alternative choice of W_j's might be a weighted sum of the optimal s_{ik}'s from the marginal sensitivity technique. (This was not used in this research because the results of the marginal sensitivity technique were not available at the time.)

Point transmissivity measures are assumed to have been taken at the two potential well locations using slug test procedures; the transmissivity values for these points are included in the PCT formulation as very narrow bounds on the transmissivity at these points.

For the 10x10 grid of transmissivities used in this study, the parameter configuration approach is thus formulated as the following constrained optimization problem:

Maximize: $$\sum_j W_j T_j$$

Subject to:

$$LBV_k \leq \sum_{j \varepsilon j_k} (T_j - T_{j-k})^2 \leq UBV_k \ , \quad k = 1, 2, 3$$

$$LBV_k \leq \sum_{j \varepsilon j_k} (T_j - T_{j-k})^2 \leq UBV_k \ , \quad k = 10, 20, 30$$

$$LBM \leq \sum_j T_j \leq UBM$$

$$LBT \leq T_j \leq UBT \quad , \forall j$$

where T_j is the transmissivity at point j, W_j is the objective function weight assigned to T_j, the UB's, and LB's represent upper and lower bounds on the east-west variogram, the north-south variogram, the mean transmissivity, and each individual transmissivity for the four constraints, respectively. (For the 10 x 10 grid, the points are numbered 1 through 10 for the first east-west row, 11 through 20 for the second, etc., so that the north-south variogram is calculated as the sum of squares of differences of transmissivities whose indices differ by an integer multiple of 10.) These bounds may in general be based on statistical confidence intervals for these parameters or the designer's judgment of their likely range.

In practice it is difficult to establish such statistical confidence intervals for the variogram constraints. A grid of readings of the regionalized variable is often used to calculate the variogram, and these observations are spatially correlated. In this research it is assumed that a number of independent, spatially uncorrelated, sets of transmissivity readings exogenous to the contaminated aquifer but within the same geological system have been used to establish confidence intervals for the mean and variogram of the transmissivity of the formation, In accordance with the observations of many other investigators, transmissivity is assumed lognormally distributed. The difference of adjacent transmissivities, since it is expected to be symmetric about zero, is assumed normally distributed, allowing the variogram confidence interval to be based on the standard chi-square statistic. The mean and variogram for the contaminated aquifer are then assumed bounded by the confidence intervals for the mean and variogram for the formation. An arbitrary choice of 50 degrees of freedom, implying 51 exogenous independent observations, is assumed. The geological strata at all 51 separate locations are assumed to have undergone the same geophysical processes that led to the formation of the high-conductivity seam. The 90 percent confidence intervals for the mean value of transmissivity and for the variogram values are listed in Table 3. The variogram constraints are developed more thoroughly in the Appendix.

TABLE 3. Ninety Percent Confidence Intervals

Transmissivity Parameter	Lower Bound	Upper	Units
Mean:	32.1	50.0	m^2/hr
Variogram:			
γ(100')=Lag 1	650	1,260	m^4/hr^2
γ(200')=Lag 2	1,190	2,260	"
γ(300')=Lag 3	1,510	2,930	"

Although the objective function is linear, the geostatistical constraints are quadratic and thus a nonlinear solution algorithm is required. The generalized reduced gradient (GRG) algorithm developed by Lasdon et al. (1976) is used in this study.

Since the constraint set includes quadratic upper and lower bounds, it is generally non-convex. This was confirmed by difficulties encountered in this study in obtaining identical optimal solutions from different starting conditions. Furthermore, the problem as formulated in this study may have a large number of alternative optima. It is clear, for example, that if weights of unity (1.0) are assigned certain transmissivities in the objective function then the objective function contours will parallel the mean constraints.

Although the global maximum is not easily obtained using reduced gradient techniques, it is believed that this algorithm is adequate to generate solutions which are useful. Results indicate that although solutions obtained using different starting points are different from one another, they are not radically different in either objective or decision space.

A transmissivity field was generated using the parameter configuration technique with the objective function weights indicated in Figure 5. The upper and lower bounds for the transmissivities were set at 300 and 5 m^2/hr, respectively, except at the two nodes where they were assumed known. The nodes to be maximized were initialized at a value of 275 m^2/hr, and the other nodes were initialized at 25 m^2/hr. The transmissivity results are indicated on Figure 6.

Aquifer Restoration Designs:

Two pumping schemes designed under the assumption of transmissivity homogeneity are considered. The first consists of a single extraction well at the downstream edge of the plume pumping at a rate sufficient to create a no-flow boundary (stagnation line) around the plume area. The analytical relationship between the pumping rate and the distance y indicated in Figure 7 is given by (Vennard and Street, 1982):

$$y = \frac{q}{4\nu}$$

where q is the pumping rate per unit aquifer thickness and ν is the regional flow velocity. As shown in the figure the stagnation line "A" circumscribes the plume and theoretically should allow for no convective transport across this boundary in a homogeneous aquifer. It is clear, that should some heterogeneity exist, e.g., in the region of the upper right hand corner of the plume, then it would be quite possible that pumping rate "A" will be inadequate to contain all of the plume.

Another practical pumping scheme which has been employed to extract and treat contaminated groundwater is the pumping and recharge well pair, where the extraction well is located near the downgradient edge of the plume and the injection well is located near the upgradient edge of the plume. Groundwater extracted by the downgradient well is treated prior to reinjection at the upgradient well. Both of the wells pump at the same rate, creating a bounded region of the aquifer whose water is continuously being treated and recycled until a sufficient amount of contaminant has been purged. For a homogeneous aquifer with regional flow the bounded region is described analytically by (Vennard and Street, 1982):

$$0 = \nu y + \frac{q}{2\pi}\left(\arctan\frac{y}{x+a} - \arctan\frac{y}{x-a}\right)$$

where ν is the regional flow velocity, q is the pumping rate per unit aquifer thickness, and y, x and a are defined in Figure 8, which illustrates the no-flow boundaries for several pumping rates.

A two-dimensional solute transport model developed by Prickett et al. (1981) was used to simulate the aquifer response to pumping and contaminant movement. It is assumed that the pollutant evenly dispersed in the vertical direction, dispersion has been excluded as a transport process, and constant heads at the boundaries create the regional gradient. The values for specific parameters used in the simulation model are listed in Table 4.

27.4	29.9	33.8	42.1	48.4	58.5	67.0	45.0	39.9	33.2
29.5	32.7	43.2	52.4	63.3	94.6	68.8	176.7	67.7	67.5
30.9	37.0	48.0	56.8	80.2	60.1	179.9	56.1	52.3	32.8
35.4	42.7	53.0	78.1	63.3	131.9	58.8	82.8	39.8	40.2
38.0	38.4	71.7	61.4	129.9	58.7	5.0	52.0	34.2	36.4
32.4	44.0 ****	54.5	126.2	54.0	5.0	33.0 ****	35.9	33.5	29.9
50.3	51.5	121.8	60.6	75.8	51.9	34.0	40.1	30.4	28.8
32.7	38.9	43.5	61.1	54.5	31.8	28.2	31.6	28.0	26.9
37.5	41.9	63.5	57.1	46.2	32.4	30.4	29.2	26.8	25.9
32.3	33.8	48.3	39.0	38.8	31.6	28.3	27.3	25.8	25.4

(Transmissivities in m^2/hr)

000.0 : node to be maximized

000.0
**** : node assigned fixed value

000.0 : node to be minimized

Figure 6. Transmissivity Field

TABLE 4. Values of Parameters in Simulation Model

Aquifer Thickness:	50 feet
Porosity:	0.2
Grid Cell Dimensions:	50 x 50 feet
Grid Discretization:	20 x 20
Overall Aquifer Dimensions:	1000 x 1000 feet
Number of Particles Released:	1,000

Two sets of simulations are performed using this transmissivity field. The first set assumes the single (downgradient) well pumping system described above using the values of pumping rates shown in Figure 7. The resulting capture efficiency for each pumping system is presented in Table 5. From the table it can be seen that pumping rates greater than 400 m^2/day are predicted to capture all of the particles. Note that the pumping rate that is adequate to capture all the contaminant under the assumption of homogeneity (230.5 m^2/day) only captures 85.2% of it for this pessimistic configuration.

TABLE 5. Capture Efficiency for Single Well Pumping Scheme

Pumping Rate (m^2/day)*	Stagnation Line, Fig. 7	Number of Particles Captured	%
230.5	A	852	85.2
274.0	B	922	92.2
397.4	C	1,000	100.0

*well delivery rate (m^3/day) divided by aquifer thickness.

The second series of simulations uses the same field with the two well (injection/extraction) system depicted in Figure 8, using the pumping rates indicated on the figure. The resulting capture efficiency for each set of pumping rates is presented in Table 6. It is interesting to note that the single well scheme is more effective than the two well design for intermediate pumping rates. Located at the edge of the plume, the injection well is expected to move contaminant away from it in a somewhat radial direction from it, but the spreading is more pronounced in the region of high transmissivity. The high transmissivity region exacerbates the spreading of the contaminant away from the downgradient well, resulting in a lower capture efficiency compared to the single well scheme. For other transmissivity fields, the two well scheme may outperform the single well scheme.

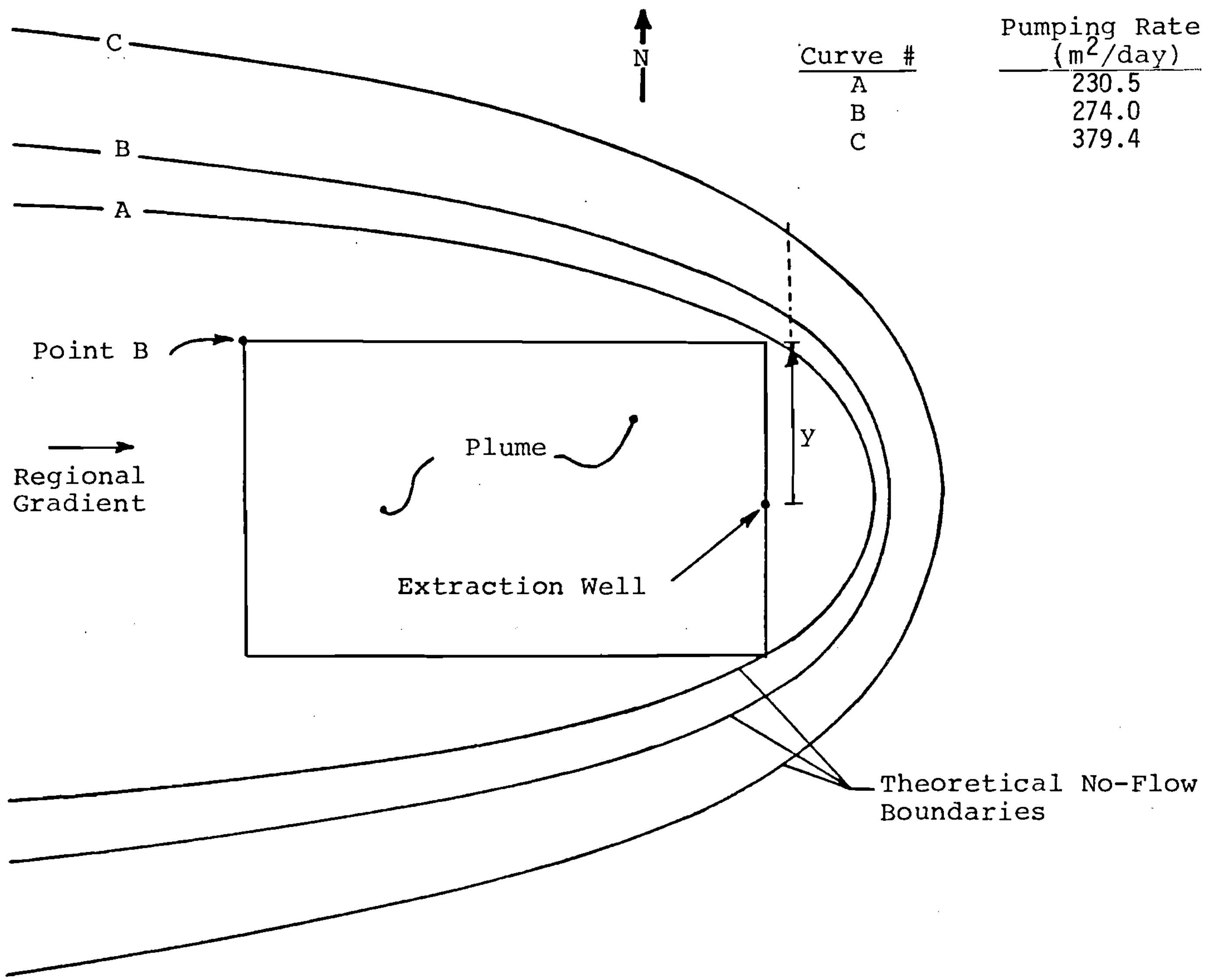

Figure 7. Single Well Pumping Scheme

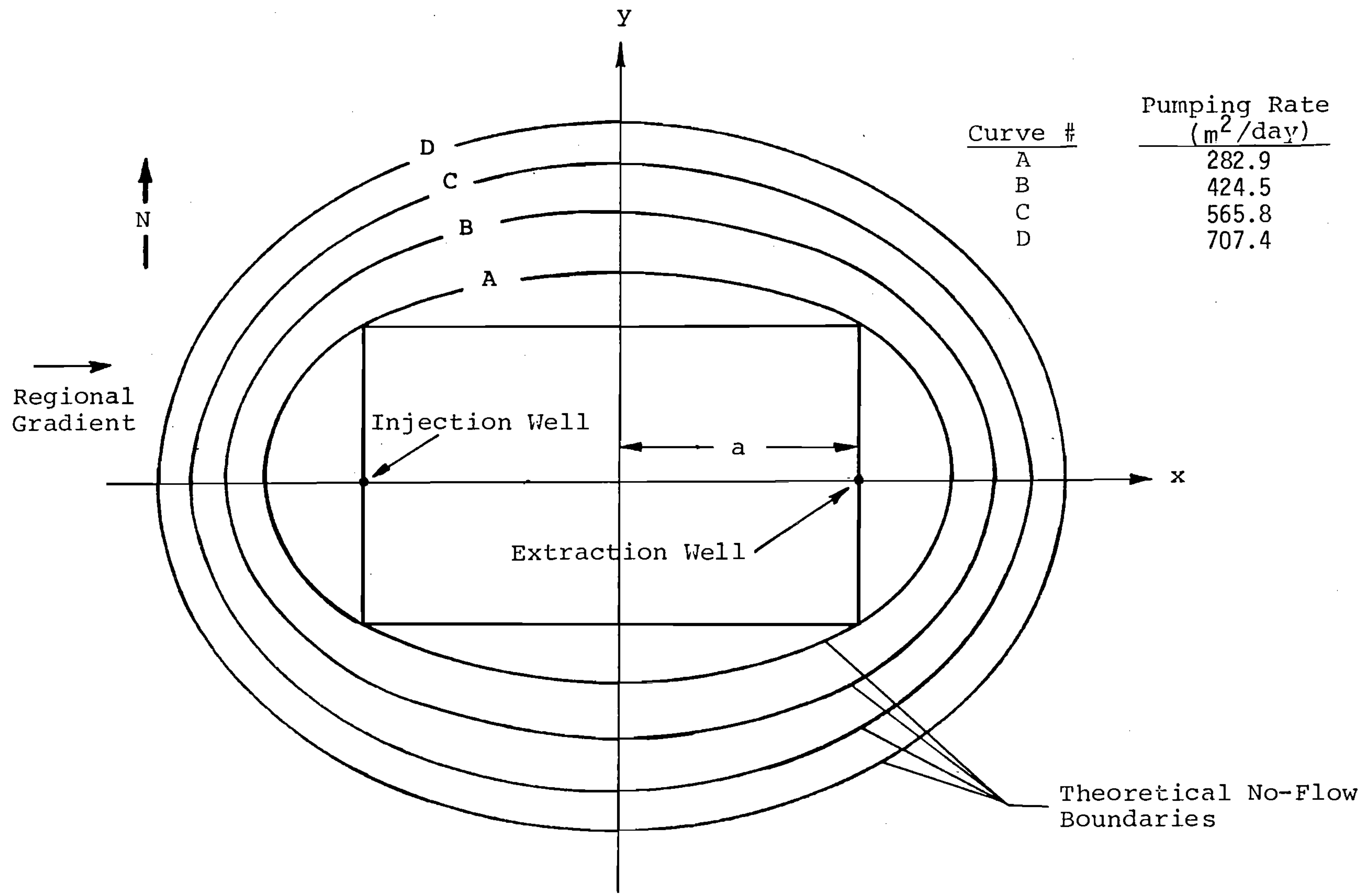

Figure 8. Two Well Pumping Scheme

TABLE 6. Capture Efficiency for Two Well Pumping Scheme

Pumping Rate (m^2/day)*	Stagnation Line, Fig. 8	Number of Particles Captured	%
282.9	A	857	85.7
424.5	B	959	95.9
565.8	C	987	98.7
707.4	D	1,000	100.0

*well delivery rate (m^3/day) divided by aquifer thickness.

CONCLUSIONS AND RECOMMENDATIONS

This report has presented the results of two new methods for the design of aquifer restoration systems in the face of parameter uncertainty. The MST produces a restoration system design and the PCT produces an extreme set of transmissivities to test that design. Project resources were inadequate to allow the very obvious next step of coupling the two techniques. For example, the optimal sensitivities from one run of the MST might be taken as weights in the next PCT run, which would produce a transmissivity field for the MST, which would, in turn, produce a new set of weights for the PCT, etc., until the designer is satisfied with the result. It would be appropriate to allow intervention on the designer's part, in order to incorporate his or her intuitive judgement, at each point in this process. For example, an "unrealistic" transmissivity set might be altered or a set of well locations and pumping rates that the designer felt would be "effective" might be included as the starting solution for the MST.

The MST is a simple method for incorporating parameter uncertainty into the design of hydraulic gradient control schemes. Although the formulation developed here is restricted to two-dimensional horizontal flow, in principle, the MST could be extended to more realistic (and computationally expensive) three-dimensional problems. However, since linear programming is utilized, the MST is restricted to situations where the governing groundwater flow equation is linear. Another consequence of the linearity requirement is that the sensitivity coefficients must be defined for small changes in transmissivity.

A major conclusion of this work is that it is possible to use selective injection and extraction to manipulate the groundwater system into states of low sensitivity to transmissivity changes. Thus, in general, it is possible to identify least-cost pumping strategies that meet the dual goals of plume containment and low sensitivity. However, as demonstrated in the mst example problem, no reasonably robust strategy can be found when the number of uncertain transmissivity zones is large relative to the number of wells.

The MST essentially consists of two components -- the optimization problem which is solved by linear programming and the response coefficient calculation which is accomplished by the adjoint state sensitivity method. Apart from the optimization component, the adjoint state method provides valuable information regarding the sensitivity of any proposed pumping scheme. Identification of the high sensitivity zones indicates the regions where additional soil borings and pump tests would be most cost-effective. It is also possible to identify robust pumping strategies by iterating between the traditional optimization problem (without uncertainty) and the adjoint state sensitivity method. The adjoint state method would be used to identify high sensitivity zones for a particular optimal pumping solution; the analyst would then modify the transmissivity in the critical zones in accord with engineering and geological judgment. Then the optimization problem would be solved for the new transmissivity field. This approach would be much more expensive computationally than the MST.

Since the adjoint state method computes the gradient response coefficient (R_{ij}) and the sensitivity response coefficient (S^k_{ij}), this information could be utilized to determine the best locations for additional pumping wells. This points to the exciting possibility of developing a simple mathematical programming technique to assist managers in the selection of well locations. The development of such a technique is a promising topic of future research.

The parameter configuration technique may be a useful method for assessing the robustness of simple pumping systems designed to contain and purge contaminant plumes from aquifers. The transmissivity fields generated using this technique may not represent the unique worst-case solutions. This is because of 1) the somewhat and necessarily arbitrary choice of an optimization criterion to represent the worst case, and 2) the problems of constraint set concavity and alternative optima for the formulation used in this research. From a practical perspective, however, the non-uniqueness of the solution is not expected to be a serious drawback as long as the objective function is well chosen.

Two interpretations of the PCT results is that they point to needs 1) for better statistical analytical techniques for geologic formations and 2) to incorporate the designer's intuitive judgement into the selection of a design strategy or a design parameter set. Intuitive judgment is of paramount importance as the designer views the results of different starting points and objective functions to work toward a parameter set that will lead to an acceptable restoration strategy. He or she must decide whether or not the extreme field, even though feasible according to the problem constraints, appears to be realistic and should feel at liberty to change the parameter values if it does not. For example, large or oscillatory fluctuations in transmissivity over small distances may be realistic for a glacial outwash aquifer but not for a sandstone aquifer. The variogram constraints would not preclude such fluctuations, and the inclusion of additional constraints to curtail them might be appropriate. For example, "smoothness" constraints that restrict the absolute difference between adjacent parameter values might be added for a sandstone aquifer. Of course, the inclusion of such constraints, which involve fourth-order statistics, might very well add to the difficulty of solution.

The notion of adding more constraints to the PCT to make use of available information could readily be extended to the incorporation of data on the heads at many points in the aquifer, if they are known. This amounts to including constraints for what has been called the "inverse problem" where one tries to solve for values of parameters governing flow, e.g., transmissivity, given data on hydraulic head throughout the system (see, e.g., Bear, 1979). This approach would require the inclusion of flow balance constraints for each node in a finite element formulation. The success of this method has been limited to cases where the head distribution exhibits a significant amount of contouring.

The objective function of the PCT, like that of many other systems-optimization techniques, must be somewhat arbitrarily chosen. The illustrative examples above used a fairly simple objective function to represent the "worst-case" condition. In general, the choice of a mathematical objective function to represent such conditions depends to a large extent on the personal judgment of the user, as well as prior qualitative information about the aquifer. Recall that prior knowledge of the existence of the high-transmissivity region was drawn upon in setting the objective function weights. Another possible choice for the weights might be the optimal sensitivities from the robust-design method discussed above. For such an objective function, those transmissivities whose increase would most adversely affect the performance function would be the ones the algorithm would attempt most to maximize.

Several assumptions made in the work reported here could greatly influence the results and are worthy of further discussion. One major assumption is that the variogram for the study region is known a priori. Little research has been done with transmissivity (or permeability) variograms and so it remains for future research to determine the conditions under which this assumption can be made.

The lower and upper bounds on the mean and variogram constraints were based upon the assumptions of 50 degrees of freedom, i.e., 51 independent observations. As explained above, the assumption of independence (if not of 51 observations) is unrealistic. No work has been done to date on deriving a variogram confidence interval for parameter observations at a single site in light of the particular dependence of variogram observations. Such work would be of value in further development of parameter configuration techniques.

The results of this study also point to a need for better characterization of geologic parameters. One type of study that would be helpful would combine detailed empirical scrutiny of aquifer transmissivity (through closely-spaced pumping tests) with a thorough analysis of such results using advanced statistical techniques. A follow-up study might also be conducted to assess the validity of applying such statistical techniques to other geologic formations or the same formation in a different location.

APPENDIX

DEVELOPMENT OF GEOSTATISTICAL CONSTRAINTS

The basic geostatistical concepts utilized in this paper were developed largely through work by Matheron (1965) and Delhomme (1978). Matheron forwarded the idea of the regionalized variable, i.e., a variable whose value is somehow related to its position. Delhomme developed the notion of the "intrinsic hypothesis", where the statistical distribution of the difference in the value of the regionalized variable between two points is the same at all points throughout the spatial domain and depends only upon the distance between, and the spatial orientation of, the two points.

An important geostatistical concept is the variogram, the variance of this distribution. This parameter can be used to describe the spatial variability of a regionalized variable, e.g., transmissivity (T). For example, if the mean difference in T between a pair of points separated by a distance h is symbolized as $T_m(h)$, where h is the magnitude of the vector describing the distance and direction between the point pair, then the value of $T_m(h)$ is

$$T_m(h) = \frac{1}{n} \sum_{i=1}^{n} (T(x_i) - T(x_i+h)$$

where x_i denotes the position of one sample point in the pair and x_i+h the position of the other, and n the number of pairs of samples. The expression for the variance of the differences in T is given by

$$\gamma(h) = \frac{1}{n} \sum_{i=1}^{n} [T[x_i] - T[x_i+h] - T_m(h)]^2$$

and if the expected value of the difference in T does not change throughout the region of interest, i.e., no regional trend, then this expression becomes

$$\gamma(h) = \frac{1}{n} \sum_{i=1}^{n} [(T[x_i] - T[x_i+h])]^2$$

since $T_m(h)$ is zero. This expression is referred to in geostatistical literature as the variogram, and has the units that the variance of the variable would have (e.g., for transmissivity the units are $length^4/time^2$).

An empirically determined variogram may serve as the basis for inferences about the (unknown) values of T throughout the rest of the aquifer. This is usually done by fitting the observed variogram to a variogram model. The intent of this action is to establish a smooth curve from which estimation of $\gamma(h)$ can be made for unsampled locations in the aquifer. Variogram models are also important in kriging procedures where ready-made tables are available for common models.

Two commonly used models are the spherical and exponential models. In both models the value of the variogram, $\gamma(h)$, gradually increases as h increases, eventually leveling off at a constant value referred to as the sill. The value for h where $\gamma(h)$ reaches the sill is referred to as the range. A discontinuity in the variogram at the origin is called the nugget effect and is attributed to both measurement error and micro-regionalization on a scale much smaller than the spacing of the points.

Confidence limits were set on these values. The 90 percent confidence interval for the mean value of T was calculated using the method described by Koch and Link (1970) for a lognormally distributed random variable. The 90 percent confidence interval for the variogram was determined using the chi-squared distribution method (Journel & Huijbregts, 1978). This range is given by:

$$\frac{(n-1)\Gamma(h)}{\chi^2_{95\%}} \geq \gamma(h) \geq \frac{(n-1)\Gamma(h)}{\chi^2_{5\%}}$$

where χ^2 is the chi-square statistic, n is the number of samples, $\gamma(h)$ is the sample variogram, and $\Gamma(h)$ is the population variogram. A population variogram is assumed for each of three values of h, viz., 100, 200, and 300 ft.

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