European Journal of Operational Research 77 (1994) 1-26
North-Holland

Theory and Methodology

Containing groundwater contamination: Planning models using stochastic programming with recourse

Janet M. Wagner
University of Massachusetts, Boston, MA, USA

Uri Shamir *Technion,*
Haifa, Israel

David H. Marks
Massachusetts Institute of Technology, Boston, MA, USA

Received January 1992; revised July 1992

Abstract: This paper examines the problem of operating pumping wells in order to contain an area of groundwater contamination when the aquifer properties of the area are uncertain. A stochastic program with simple recourse is formulated, involving a non-convex quadratic objective subject to linear constraints. This problem is solved using an extension to the Finite Generation Algorithm that will find an at least locally optimal solution to a problem involving a non-convex quadratic objective function. A numerical example is presented and analyzed.

Keywords: Programming; Probabilistic; Water; Management

1. Introduction

Increasingly, human activities such as leaks from underground storage tanks, landfills, and septic systems, and movement of contaminants such as road salt and pesticides from the surface are threatening the quality of groundwater supplies. Since most countries rely on these groundwater supplies for part or all of their drinking water, models for managing these supplies - and in particular models for managing the contamination of these supplies - are of considerable interest. Often, one of the first tasks undertaken when contamination in a groundwater supply is discovered is to contain the region of contamination in order to protect neighboring areas. This paper discusses models developed using the technique of stochastic programming with simple recourse that are intended to assist decision makers in placing and operating pumping wells so as to reduce or prevent the spread of' groundwater contamina-

Correspondence to: University of Massachusetts, Boston, MA, USA.

SSDI 0377-2217(92)00385-L

tion. In this study, the objective is to establish a 'capture curve' or 'interception envelope' around the area of contamination and then to install and operate wells in the region so as to ensure that no groundwater flows across the capture curve from the contaminated area into an uncontaminated area.

Many of the elements in groundwater systems are uncertain. Locations, quantities, and types of pollutants released are often not well known. The properties of the aquifer that govern groundwater flow and transport can vary widely over a small area, and these parameters are usually only known at a few discrete points. Boundaries of the flow field and conditions along these boundaries are also uncertain. Many existing groundwater models ignore these uncertainties. This work develops models and formulations that explicitly incorporate uncertainty.

The models discussed in this paper have the potential to incorporate a number of types of uncertainty. We will, however, concentrate on the uncertainties in the aquifer parameter of hydraulic conductivity, for several reasons. First, these aquifer properties can never be known with certainty. Hydraulic conductivities are measured by taking soil samples (cores) from the site and measuring these samples in the laboratory. Taking sufficient samples to completely characterize the hydraulic conductivities throughout the site would destroy it and would spread the contamination further. In principle, other uncertain parameters such as boundary conditions and locations of contaminants could be determined without completely disrupting the site. Second, once a problem has been formulated that includes the uncertainty in the aquifer parameters, many of the other sources of uncertainty can be considered without additional computational or theoretical difficulties.

The stochastic optimization models developed in this paper employ the concept of recourse. Recourse considerations are very natural for this application. It is desirable to place the barrier wells and put them into operation fairly quickly - leading to considerable 'here and now' costs. However, due to uncertainties about values of the aquifer parameters, once the wells are in place contamination of areas to be protected may still occur. Thus, 'wait and see' recourse costs may be incurred to deal with this additional contamination. These costs could occur, for example, because of changes in the pumping plan, because of the need to treat water pumped for supply, or due to the costs of obtaining water from alternate sources. In this application, we also include the possibility of obtaining benefits from the water pumped from the wells, such as selling the water to be used for industrial processes or agriculture where the quality requirements are not as stringent as for municipal water use.

Groundwater quality in this study is to be controlled by looking solely at the directions of groundwater flow (gradient control). The models developed in this paper involve as variables only well pumping rates and hydraulic heads. By not including variables related to water quality (such as contaminant concentrations), the problem becomes much more tractable. However, the eventual goal for this work is to directly control contaminant concentrations, which would require concentrations to be included as decision and/or state variables. With this addition, the equations describing water flow become non-linear and often non-convex (c.f. Gorelick, 1983). Thus, to allow the later expansion of these methods to include quality variables, the methods presented in this paper for the simpler containment problem were specifically designed to allow non-convex elements. The algorithm described in this paper allows a non-convex quadratic objective, Wagner (1988) contains a method that allows non-convex quadratic elements in *both* the objective and the constraint functions.

The model developed for this study, unlike previous models for groundwater quality management, is non-linear, non-convex, and stochastic. This model is solved using a new stochastic programming algorithm based on the Finite Generation Algorithm (FGA) (Rockafellar and Wets, 1986a,b) for stochastic programming with simple recourse for convex quadratic programs. The new algorithm has been extended to allow non-convex quadratic elements in the objective (only local optimal solutions are guaranteed).

The paper is organized as follows. Section 2 presents a brief literature review. Section 3 presents the formulation for the containment problem. Section 4 sketches the development of the stochastic programming algorithm used to solve the groundwater model. Computational details of its implementation are discussed in Section 5. Results are discussed in Section 6, followed by concluding remarks in Section 7.

2. Literature review

This study involves three elements: 1) models for groundwater management via contamination containment (gradient control), 2) representations of uncertainty of aquifer parameters, and 3) methods for stochastic programming with recourse. Work available in the literature for each of the above elements is discussed below.

2.1. Groundwater management via contamination containment

The problem considered in this work is based on one analyzed by Gorelick (1987) using a response matrix model. A response matrix model represents the groundwater system by a matrix which gives the (linear) response of the aquifer to a given set of pumping and recharge rates. This matrix is obtained by regression on the results of numerical simulations from a groundwater model that solves the partial differential equation representation of the aquifer. Gorelick did investigate the problem of aquifer parameter uncertainty, by finding a 'robust' solution to contain the contamination over 10 representative sets of aquifer parameters. Our model differs from Gorelick's in that it does not use a response matrix, and includes the concept of recourse. However, since the two models deal with similar problems, our test problem is taken to be as close as possible to the one examined by Gorelick.

Other studies with response matrix models focusing on gradient control include Colarullo et al. (1984), Atwood and Gorelick (1985), and Lefkoff and Gorelick (1986). These studies did not investigate the question of parameter uncertainty.

In contrast to the response matrix approach, the discretization of the partial differential equations of water (and contaminant) transport can be embedded in a linear or non-linear programming model. Molz and Bell (1977) and Remson and Gorelick (1980) used embedding in models for containing groundwater flows, again without considering uncertainty in the aquifer parameters.

Embedding and response matrix approaches have been used for a number of groundwater management problems, including 1) models only involving groundwater quantity, and 2) groundwater quality management via concentration control. Gorelick (1983) provides a comprehensive review of this work to that date.

Ranjithan et al. (1990) developed a method using neural networks to screen realizations of hydraulic conductivities (or transmissivities) to determine which realizations should be used in a subsequent contaminant containment optimization model. This neural network procedure can be used to identify the one or the few realizations of the random parameters that will most constrain the final design, for example those realizations that will require high volumes of pumping to contain a contaminant plume. Once the neural network has been trained, a large number of hydraulic conductivity realizations can be screened and considerable computational savings can be realized by using only these 'pessimistic' realizations in stochastic optimization methods.

Groundwater quality management models incorporating uncertainty have also been developed for models that explicitly incorporate concentration. These models include Wagner and Gorelick (1987, 1989), Andricevic (1990), and Andicevic and Kitandis (1991).

2.2. Stochastic analysis of groundwater systems

This paper focuses on the uncertainty regarding the properties of the soil governing groundwater flow, specifically hydraulic conductivity. Hydraulic conductivity can be measured for a small soil sample from the site, but it will vary greatly across a site. For any real life problem we have neither the time nor the money to measure the hydraulic conductivity for every element needed for the groundwater model, nor is it likely to be wise to disturb the site to that extent. Thus hydraulic conductivity is, to us, unknowable and must be treated as an uncertain parameter.

The stochastic nature of aquifer parameters has been a topic of considerable research for over a decade. Field data indicates that hydraulic conductivities *(K)* are log-normally distributed (e.g. Freeze,

1975) and spatially correlated (Hoeksema and Kitanidis, 1985). They are also usually assumed to be stationary, in the sense that the correlation between the values of K at two points is a function only of the distance between the points (and not, for example, a function of the location of the points themselves). Thus we treat the hydraulic conductivity as a spatially distributed random variable, also called a random field. Useful review articles on this subject are those by Dagan (1986) and Gelhar (1986).

2.3. Stochastic programming with recourse

Stochastic programming with recourse involves a two (or more) stage process. First a decision is made and implemented, usually involving some costs, then the world unfolds. At a later stage, as a consequence of the realization of some uncertain events, additional costs are incurred (possibly as a result of additional actions). Simple recourse refers to the situation where only costs are incurred at the second stage and no additional decisions are made. The cost of a decision then consists of 1) a deterministic cost incurred 'here and now' as the decision is put into effect, and 2) a stochastically distributed 'wait and see* penalty or recourse cost, which is incurred after the stochastic elements of nature are realized. In contrast with chance constraints, programming with recourse allows us to assign increasingly higher penalties for increasingly larger violations of standards.

In recent years, several methods have been developed for stochastic programming with recourse, for problems with stochastic variables which can be described with discrete distributions. Many of these methods rely on decomposition. Rockafellar and Wets (1976, 1983, 1986a,b) developed algorithms based on Dantzig-Wolfe (price-directed) decomposition, by exploiting the duality properties of general linear-quadratic stochastic programming problems with recourse. They developed a decomposition method called the Finite Generation Algorithm (FGA) for the two-stage convex quadratic problem which uses a linear-quadratic penalty recourse function. This method is shown to have linear convergence at every step.

The FGA was successfully applied to solve a problem involving the management of lake eutrophication (Somlyody and Wets, 1988). Eiger and Shamir (1991) used this method to model the optimal multi-period operation of a multi-reservoir system with uncertain inflows and water demands.

Algorithms have also been developed based on Benders' (resource-directed) decomposition. Dantzig and Madansky (1961), Van Slyke and Wets (1969), and Birge and Louveaux (1985) have developed methods for stochastic linear two-stage problems with recourse based on this approach. Nested decomposition methods for linear multi-stage problems were developed by Birge (1982a) and Noel and Smeers (1985). Louveaux (1980) developed a nested decomposition method for multi-stage stochastic quadratic programming problems.

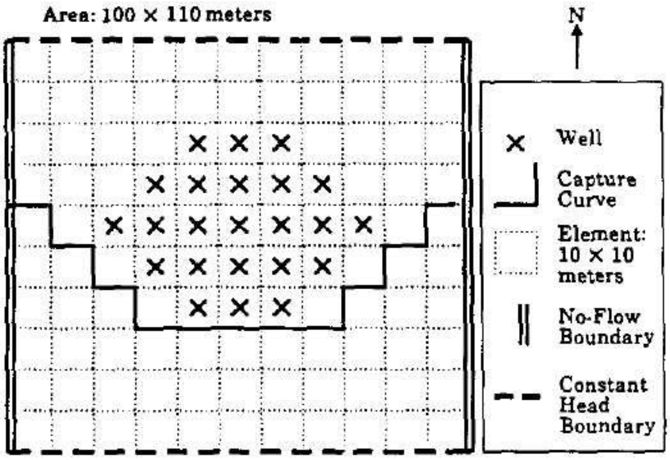
2.4. Model overview

The model and solution method discussed in this paper were developed after careful examination of the existing models, and include the following extensions:

* this model is, we believe, the first groundwater model to include the concept of recourse to account for costs due to unforeseen outcomes, and thus one of the first groundwater models to incorporate methods developed for stochastic programming with recourse.
* this method allows the use of a non-convex quadratic objective, and
* this fairly sophisticated method was implemented on a personal computer and uses existing, readily available codes to solve the subproblems.

3. Formulation of the groundwater contamination containment problem

This study was intended to develop and test the methodology for using stochastic programming with recourse for groundwater contamination containment problems, and was not developed to model a



Natural Mean Gradient = 1%

Figure 1. Plan view of aquifer with capture curve

specific site. Thus, as an initial effort, we have chosen to model a fairly uncomplicated problem but one which we feel to have sufficient detail to test the method. Below we start by formulating a problem for an area with known (deterministic) and constant hydraulic conductivity (homogeneous aquifer). We then extend this formulation to an area with unknown (stochastic) hydraulic conductivities that vary over the region (heterogeneous aquifer).

3.1. Initial deterministic formulation

We have chosen to model a confined aquifer, namely a groundwater bearing layer that is confined between two impermeable layers. The flow through the aquifer, with bottom at depth s and with thickness b, occurs due to differences in hydraulic heads throughout the aquifer. Viewing the aquifer from above, in plan (Figure 1), we use the standard approach of averaging all aquifer parameters over its depth, and so we model flow only in two dimensions. We will deal with steady-state flow only.

A numerical model of the site is based on a set of connected finite elements (Figure 1), with $n = l, 2, \ldots, N$ elements in the x direction, and $m = 1, 2, \ldots, M$ elements in the y direction. The capture curve (flow barrier) is established to be along the edges of these elements. We let / = 1, 2,..., L be the index of the edges along the capture curve.

Some of the finite elements may contain pumping wells; we assume these wells are at the center of the elements. The decision variables for this problem are the pumping rates $(w_{n\ m})$ at each well. Elements with no wells will have their pumping rates fixed at 0.

Additionally, the variables of hydraulic head (h_{nm}) must be included in this formulation. The head can be thought of as the level to which water would rise in a well built in the aquifer, measured from the bottom of the aquifer. Head variables appear in the objective, as well as in the constraints derived from the equations governing water flow.

Our objective function includes the energy costs of pumping and a term accounting for any benefit obtained from the pumped water. The energy cost of pumping is a function of the rate at which water is lifted times the distance it is lifted. The total energy cost of pumping is given by

$$\sum_{n} \sum_{m} C w_{n,m}(s - h_{n,m}) \tag{1}$$

where

C = Daily cost of pumping (\$/meter^3/meter of elevation X86400 seconds/day).
w_{nm} = Pumping rate (meters^3/second).
s = Height of the ground surface [measured from the bottom of the aquifer] (meters).
h_{nm} = Hydraulic head (meters).

The benefit term allows us to account for the fact that in some applications, the water that is removed from the barrier wells may be used (possibly after treatment) for such purposes as industry or irrigation. The benefit is assumed to be proportional to the total amount of water squared, and so is given by

$$B\left(\sum_n \sum_m w_{n,m}\right)^2 \tag{2}$$

where B = daily benefit (\$/[meters^3/ second]^2/ day).

This particular benefit term is used only for illustration. It was chosen to be non-convex since we wish to be able to handle non-convex elements in this method so as to eventually be able to explicitly include concentration variables in the model. Any convex or non-convex quadratic objective function could be accommodated by this method, including one with stochastic elements (i.e. stochastic cost or benefit coefficients).

The objective function is then

$$\min \sum_n \sum_n C w_{n,m}(s - h_{n,m}) - B\left(\sum_n \sum_m w_{n,m}\right)^2. \tag{3}$$

The groundwater system is modeled by embedding discretizations of the partial differential equations governing groundwater flow as constraints in the optimization problem. Other constraints in the problem involve the specification of the flow direction across the capture curve and pumping limits.

The flow in the aquifer is described by a set of finite difference equations. These equations can be expressed more concisely be reordering the matrices of pumping rates w_{nm} and heads h_{nm} as vectors w, and h_t, where i = 1, 2,...,/, and I = nXm. The flow equations can then be expressed in the following form:

$$\sum_j F_{i,j} h_j = w_i - f_i \quad \forall i \tag{4}$$

where

F_ij = Coefficients whose values depend on the geometry of the finite difference model and aquifer properties (conductivities). fi = Constants that depend on the boundary conditions.

The matrix F = $\{F_{ij}\}$ gives the response of the heads h_t to the pumping rates w_t and incorporates the hydraulic conductivities at a site as well as data about the site geometry. This matrix is derived in Appendix A.

Requiring flow to be inward along the capture curve gives the following constraints:

$$h_l^{\text{in}} - h_l^{\text{out}} \le 0 \quad \forall l \tag{5}$$

where

$h^l/^l$ = Head for an element just to the inside of the capture curve.

A$^{\text{out}}$ = The corresponding head for an element just to the outside of the capture curve.

For this application, we restrict the pumping rates to be non-negative and less than some specified maximum value w. Without substantially changing the solution method, we could allow recharge wells by allowing the pumping rates to be negative. Also, for simplicity in this application w is assumed to be the same for all elements.

Thus the deterministic optimization problem can be stated as

$$\text{Min} \sum_i C w_i (s - h_i) - B\left(\sum_i w_i\right)^2$$

$$\text{subject to} \quad \sum_j F_{i,j} h_j = w_i - f_i \quad \forall i \tag{6a}$$

$$h_l^{\text{in}} - h_l^{\text{out}} \le 0 \quad \forall l \tag{6b}$$

$$0 \le w_i \le \bar{w} \quad \forall i. \tag{6c}$$

This problem is a linear-quadratic program (a quadratic objective function subject to linear constraints).

3.2. Stochastic formulation

The major source of uncertainty in this problem is the uncertainty about the values of the hydraulic conductivities. We include this uncertainty in model parameters as follows. First since the hydraulic conductivities are not constant but vary from place to place within the region, instead of using constant K_x and K_y, we allow different values of K between each two adjacent nodal points. (Note, hydraulic conductivities do not refer to a point but instead to flow through a cross-section between two points.). Additionally, for a given site we assume that we do not know the exact values of the hydraulic conductivities, but instead we know only that they are log-normally distributed (with known mean and variance), and spatially correlated (with known correlation structure) (Dagan, 1986).

To use the extended FGA we need to obtain discrete values for the hydraulic conductivities that represent the joint probability distribution. One method that has been used to obtain this discrete distribution (Eiger and Shamir, 1991) involves discretizing the values for each conductivity into several levels and then looking at all possible combinations of these levels over the set of random variables. This approach is infeasible in this application, since to model any problem of interest requires many finite elements and thus many conductivity value combinations, resulting in a very large (deterministic) problem. Additionally, since the hydraulic conductivities are correlated, it is not clear just how to calculate the probability of each combination of conductivity levels.

We choose not to represent the Entire distribution, but instead to take a sample of possible realizations from this distribution. The details on how this sampling is done are discussed in a later section. For now we just assume that we have <*o* = 1, 2,..., *{I* realizations, with each realization giving us a set of hydraulic conductivity values for the entire site. Each realization has probability *ir^*. We wish to use as large a sampling as possible, so *O* is potentially quite large.

Each realization *o>* has a different matrix *F,* and a different set of constant /. Also, for a fixed pumping plan *w,* a different set of heads will result at each nodel point. Thus we substitute F_w, *f^*, h_w, *h*™, and /i^{out} into the deterministic formulation.

Since the problem is stochastic we cannot guarantee that a selected pumping plan will actually result in

$$h_l^{in} - h_l^{out} \le 0 \qquad (7)$$

ω

on all boundary points / = 1, 2,..., *L.* We define the degree to which this constraint is violated at any boundary / and for any realization by

$$v_{l,\omega} = h_{l,\omega}^{in} - h_{l,\omega}^{out}. \qquad (8)$$

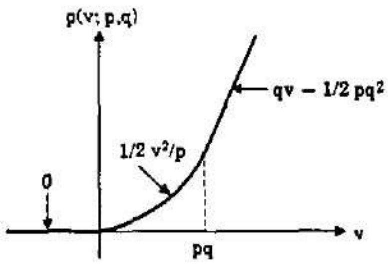


Figure 2. Linear-quadratic penalty function

The recourse cost is represented by a linear-quadratic penalty function for a violation v (Rockafellar and Wets, 1986a,b) as follows (see Figure 2):

$$\rho(v; p, q) = \begin{cases} 0, & v \leq 0, \\ \frac{1}{2}v^2/p, & 0 \leq v \leq pq, \\ qv - \frac{1}{2}pq^2, & v \geq pq. \end{cases} \tag{9}$$

The parameters p and q must be positive, and are specified by the decision maker. This method allows the use of different penalty parameters at different points (i.e. to penalize 'leaks' at one point more than another), and can even allow these parameters to be stochastic. For simplicity in this application, the same values of the penalty parameters were used for all boundary cells and for all realizations.

This shape for the penalty function was chosen for a number of reasons. First, it allows the decision maker great flexibility. By choosing the parameters p and q appropriately the penalty can be made to look almost linear, almost quadratic, or a mixture of the two. The parameter values also determine the magnitude of the penalty. The form of the penalty function has a number of desirable theoretical properties, including the fact that it is differentiable everywhere, and that is has an easily expressed conjugate function (Rockafellar and Wets, 1986a,b).

For a given pumping plan w, the cost of this plan will consist of the energy cost of pumping minus the benefit obtained from water pumped *plus* the recourse cost. This cost will vary for each realization of the hydraulic conductivities. The objective is to minimize the *expected* cost. The stochastic optimization problem can be stated as

$$\text{Min} \sum_{\omega} \pi_{\omega} \Big[\sum_i C w_i (s - h_{i,\omega}) + \sum_l \rho(v_{l,\omega}) \Big] - B \Big(\sum_i w_i \Big)^2$$

$$\text{subject to} \quad \sum_j F_{i,j,\omega} h_{j,\omega} = w_i - f_{i,\omega} \quad \forall i \forall \omega, \tag{10a}$$

$$v_{l,\omega} = h^{\text{in}}_{l,\omega} - h^{\text{out}}_{l,\omega} \quad \forall l \forall \omega, \tag{10b}$$

$$0 \leq w_i \leq \overline{w} \quad \forall i. \tag{10c}$$

The violation terms $p(v_{llo})$ can be expressed as the minimum value of a quadratic objective function subject to linear constraints (Rockafellar and Wets, 1986a), as follows:

$$\rho(v) = \min_{v', v''} \tfrac{1}{2}(v')^2/p + qv''$$

$$\text{subject to} \quad v' + v'' \geq v \tag{1la}$$

$$v'' \geq 0. \tag{1ib}$$

Thus the stochastic optimization problem (10) can be rewritten without the explicit penalty function simply as a quadratic objective function subject to linear constraints. However, potentially the number of realizations fl could be very large, so this optimization problem could involve a very large number of both constraints and variables.

We can reduce the number of variables and the number of constraints in this problem considerably by exploiting the fact that the values of h_{ioi} are completely determined from the flow constraints, once the values of $w_($ have been set. In Appendix B, we show that —F_u is positive definite. Thus we can remove the variables h from the problem by rearranging the head constraints to obtain

$$\boldsymbol{h}_{\omega} = F_{\omega}^{-1}(\boldsymbol{w} - \boldsymbol{f}_{\omega}). \tag{12}$$

Substituting (12) into (10) we obtain the following optimization problem:

$$\operatorname{Min} \sum_{\omega} \pi_{\omega} \left[\sum_{i} C w_i \left(s - \sum_{j} F^{-1}_{i,j,\omega} \{ w_j - f_{j,\omega} \} \right) + \sum_{l} \rho(\upsilon_{l,\omega}) \right] - B \left(\sum_{i} w_i \right)^2$$

$$\text{subject to} \quad \upsilon_{l,\omega} = \sum_{j} G_{l,j,\omega} \{ w_j - f_{j,\omega} \} \quad \forall l \forall \omega, \tag{13a}$$

$$0 \le w_i \le \overline{w} \quad \forall i, \tag{13b}$$

where

$$G_{l,j,w} = \left[F^{-1}_{l,j,\omega} \right]^{\text{in}} - \left[F^{-1}_{l,j,\omega} \right]^{\text{out}}. \tag{14}$$

Notational note: the violations concern only the / heads along the boundary, namely *h*™$_w$ and *h*^. Thus to calculate the violations in (13) we need only certain rows of matrix *F*~^{l}, which we denote as [fj^1]^1" *and[F~^{l}]^{om}*. If we have /elements and calculate gradients at *L* points, *F*~^{l} is of size *IX I,* and *[F-^{l}]^* and *IF'^{l}]*™^{l} are *L xl.*

Again, using (11) the penalty function can be rewritten. Also, in the development of the original finite difference equations we included a term w_t for each element, even those with no wells. For elements *i* with no wells we restrict w_t = 0. Further reduction of this problem is possible by eliminating these decision variables. This straightforward reduction was made in the final implementation, but will not be explicitly discussed here.

Removal of these head variables and constraints, and elimination of the pumping levels for finite elements with no wells, leaves the problem in a form that can be exploited by an extension of the Finite Generation Algorithm. (Rockafellar and Wets, 1986a,b) The inversion of these matrices F_M is done once in a 'preprocessing' step before the optimization problem is solved, resulting in considerable computational savings.

4. Stochastic programming algorithm

To provide a good representation of the range of possible conductivity fields it is necessary to use a large number of scenarios. Discretizing the possible conductivity values and then constructing every possible scenario is impractical. (For example, in the sample problem discussed in the next section, even if each finite element could take on only two possible conductivity values, the full set would require 2^{110} realizations!) Even with the sample of 100 realizations used in the following sample problems, the full primal problem would have over 1700 decision variables and over 1700 constraints. This optimization problem is also non-convex. Using commercial non-linear optimization codes for even the sample problem would require at least a workstation environment, if not a mainframe. The extended Finite Generation Algorithm, developed to solve this problem, exploits its special structure using decomposition. The subproblem that is solved in this method is independent of the number of realizations, resulting in great computational savings and, in fact, the ability to solve this problem using only personal computers.

The extension of the FGA (Rockafellar and Wets, 1986a,b) developed for this work, uses decomposition to solve a dual problem developed from a Lagrangian function for the primal problem (13). The original FGA for convex quadratic problems was extended to handle the non-convex quadratic objective by using a proximal point term to convexify the problem. This sections sketches the development of the extended FGA. For additional details of this algorithm see Wagner (1988).

4.1. Lagrangian function and dual problem

We rewrite (13) by defining

$$R_{i,j} = -2C\sum_{\omega}\pi_\omega F^{-1}_{i,j,\omega} - 2BE_{i,j} \quad \forall i\ \forall j,$$

$$r_i = Cs + C\sum_{\omega}\pi_\omega \sum_j F^{-1}_{i,j,\omega} f_{j,\omega} \quad \forall i,$$

where $E = \{E_{ij}\}$ is a matrix of all 1's.

Then the stochastic optimization problem (13) becomes

$$\text{Min} \sum_i \sum_j \tfrac{1}{2} w_i R_{i,j} w_j + \sum_i r_i w_i + \sum_\omega \pi_\omega \sum_l \rho(v_{l,\omega})$$

$$\text{subject to} \quad v_{l,\omega} = \sum_i G_{l,i,\omega}(w_i - f_{i,\omega}) \quad \forall l\ \forall\omega \tag{15a}$$

$$0 \le w_i \le \bar{w} \quad \forall i. \tag{15b}$$

(Again, by using (11) these penalty terms can be rewritten in minimization form.)

Consider the following Lagrangian function:

$$L(w,z) = \sum_i \sum_j \tfrac{1}{2} w_i R_{i,j} w_j + \sum_i r_i w_i + \sum_\omega \pi_\omega \sum_l \left(z_{l,\omega}\left[\sum_i G_{l,i,\omega}(w_i - f_{i,\omega})\right] - \tfrac{1}{2} p z^2_{l,\omega}\right),$$
$$0 \le w_i \le \bar{w} \quad \forall i,$$
$$0 \le z_{l,\omega} \le q \quad \forall l\ \forall \omega. \tag{16}$$

This Lagrangian function $L(w, z)$ is concave with respect to z when $p > 0$. It would be convex with respect to w if the matrix $R = \{R_{ij}\}$ was positive definite, but since $-E$ is not positive definite neither is R.

We can add the following positive definite proximal point term to $L(w, z)$ so as to force the function to be convex with respect to w:

$$\tfrac{1}{2}\theta \sum_i \sum_j (w^*_i - w_i) D_{i,j} (w^*_j - w_j) \tag{17}$$

where

θ = A (large) positive number.

D_{ij} = Any positive definite matrix.

w^* = The optimal solution to (13) (obviously unknown in advance).

The augmented Lagrangian function is then

$$L'(w,z) = \sum_i \sum_j \tfrac{1}{2} w_i R_{i,j} w_j + \sum_i r_i w_i + \sum_\omega \pi_\omega \sum_l \left(z_{l,\omega}\left[\sum_i G_{l,i,\omega}(w_i - f_{i,\omega})\right] - \tfrac{1}{2} p z^2_{l,\omega}\right)$$
$$+ \tfrac{1}{2}\theta \sum_i \sum_j (w^*_i - w_i) D_{i,j} (w^*_j - w_j),$$
$$0 \le w_i \le \bar{w} \quad \forall i,$$
$$0 \le z_{l,\omega} \le q \quad \forall l\ \forall \omega. \tag{18}$$

For θ sufficiently large, $L'(w, z)$ is convex with respect to w. It is also still concave with respect to z when $p \ge 0$.

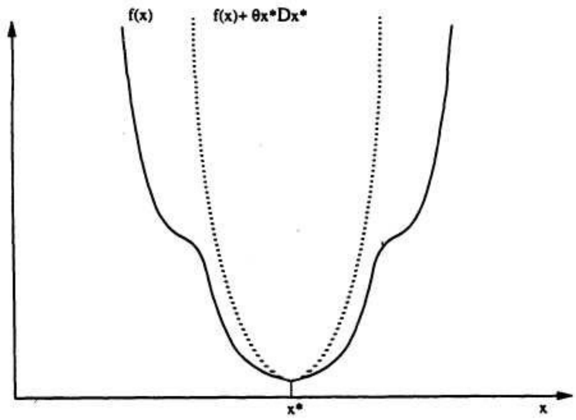


Figure 3. Non-convex and augmented (convex) function

Define the primal and dual augmented problems as follows:

$$P_{\text{aug}} = \inf_{w} \sup_{z} L'(w, z) \tag{19}$$

$$D_{\text{aug}} = \sup_{z} \inf_{w} L'(w, z). \tag{20}$$

and

Figure 3 illustrates the relationship of an augmented and an unaugmented objective function. The augmented primal problem is equivalent to the stochastic optimization problem in (13), since at optimality the value of the proximal point equals zero.

The augmented dual problem is developed as follows. We define

$$T_{i,j} = R_{i,j} + \theta D = -2C \sum_{\omega} \pi_{\omega} F^{-1}_{i,j,\omega} - 2BE_{i,j} + \theta D_{i,j} \quad \forall i \forall j, \tag{21a}$$

$$t_i = r_i + \sum_{\omega} \pi_{\omega} \sum_{l} z_{l,\omega} G_{l,i,\omega} - \theta \sum_{j} D_{i,j} w^*_j$$

$$= Cs + \sum_{\omega} \pi_{\omega} \Big(C \sum_{j} F^{-1}_{i,j,\omega} f_{j,\omega} + \sum_{l} z_{l,\omega} G_{l,i,\omega} \Big) - \theta \sum_{j} D_{i,j} w^*_j \quad \forall i. \tag{21b}$$

Then from (18) and (20) and by rearranging we obtain

$$D_{\text{aug}} = \sup_{0 \le z_{l,\omega} \le q} \inf_{0 \le w_i \le \overline{w}} L'(w, z) = \sup_{0 \le z_{l,\omega} \le q} \sum_{\omega} \pi_{\omega} \sum_{l} \Big(-z_{l,\omega} \sum_{i} G_{l,i,\omega} f_{i,\omega} - \tfrac{1}{2} p z^2_{l,\omega} \Big)$$
$$+ \tfrac{1}{2} \theta \sum_{i} \sum_{j} w^*_i D_{i,j} w^*_j + \inf_{0 \le w_i \le \overline{w}} \sum_{i} \sum_{j} \tfrac{1}{2} w_i T_{i,j} w_j + \sum_{i} t_i w_i \tag{22}$$

The inf above involves a concave function so its optimal value is equal to its Lagrangian dual. Using variables u\ on constraints 0 < w_t and variables u'' on constraints $w_t < w$, we can rewrite the latter part above as

$$\sup_{u', u'' \ge 0} \inf_{0 \le w_i \le \overline{w}} \sum_{i} \sum_{j} \tfrac{1}{2} w_i T_{i,j} w_j + \sum_{i} t_i w_i + \sum_{i} u'_i w_i + \sum_{i} u''_i (w_i - \overline{w}_i). \tag{23}$$

A point will provide this inf if and only if the gradient of the objective function at this point (with respect to x) is equal to zero, namely when

$$\sum_{j} T_{i,j} w_j + t_i - u'_i + u''_i = 0 \quad \forall i. \tag{24}$$

So we can add this constraint and ignore the inf in (23). We can also substitute (24) in the objective function in (22). Finally, by this substitution and by rearranging, the approximate augmented dual is

$$D_{\text{aug}} = \sup_{z,u',u''} \sum_{\omega} \pi_\omega \left(-\sum_l z_{l,\omega} \left[\sum_i G_{l,i,\omega} f_{i,\omega} \right] - \tfrac{1}{2} p z_{l,\omega}^2 \right) - \sum_i \sum_j \tfrac{1}{2} w_i T_{i,j} w_j + \tfrac{1}{2}\theta \sum_i \sum_j w_i^* D_{i,j} w_j^* - \sum_i u_i'' \overline{w}$$

subject to $u_j', u_j'' \geq 0 \quad \forall j,$ (25a) (25b)

$$\sum_j T_{i,j} w_j + t_i - u_i' + u_i'' = 0 \quad \forall i, \tag{25c}$$

$$0 \leq z_{l,\omega} \leq q \quad \forall l \ \forall \omega.$$

In the augmented dual problem, the decision variables are $z_{l(O}$, $u^f j$, uj and w_t. This problem has« objective function which is concave with respect to z, subject to linear constraints.

4.2. Solution of dual problem using the finite generation algorithm

The augmented dual problem has relatively few constraints, but since there is a variable for evei] realization *co,* this problem potentially has a very large number of variables. Thus in its full form augmented dual is also potentially much too large to be solved directly. Thus a decomposition approa to solving this problem was developed as follows.

Instead of looking at the entire decision space (dimension = L X17 X /), we look only at a subset i the space. At each step in the algorithm we have a small set of a = 1,... A feasible dual points (for eacl /, *co,* and *a,* 0 <$z_{l(oa}$<q). The current set of feasible dual points at iteration v is denoted $\{z$^:$a = l,\dots,A\}$. The dual feasible region of the full problem is approximated by the convex combination of these A points. The augmented dual problem is then solved over this reduced space (*not* over th much larger full dual feasible space). In the extended FGA a sequence of these reduced problems il solved, with each iteration updating the set of points *{zj.* In fact, for the extended FGA this feasible*i* need only contain two points at any iteration. Thus even though this decomposition approach requin the solution of several problems (instead of a single problem) the reduced problems are so small that th total computational requirements are considerably reduced.

To develop the reduced dual problem, we first replace $z_{l(O}$ in the augmented dual problem by j convex combination of the approximating points as follows:

$$z_{l,\omega} = \sum_\alpha \lambda_{l,\alpha} z_{l,\omega,\alpha} \tag{26}$$

and we add the following constraints:

$$\sum_\alpha \lambda_{l,\alpha} \leq 1 \quad \forall l, \qquad \lambda_{l,\alpha} \geq 0 \quad \forall l \ \forall \alpha. \tag{27}$$

Next, we define the following expected value terms:

$$\overline{zGf}^{\nu}_{l,\alpha} = \sum_\omega \sum_j \pi_\omega z_{l,\omega,\alpha} G_{l,j,\omega} f_{j,\omega},$$

$$\overline{zz}^{\nu}_{l,\alpha,\beta} = \sum_\omega \pi_\omega \tfrac{1}{2} p z_{l,\omega,\alpha} z_{l,\omega,\beta},$$

$$\overline{zG}^{\nu}_{l,j,\alpha} = \sum_\omega \pi_\omega z_{l,\omega,\alpha} G_{l,j,\omega}. \tag{28}$$

The approximate augmented dual can then be written as

$$D_{\text{aug}}^{\nu} = \sup \sum_{l} \sum_{\alpha} -\overline{zGf}^{\nu}_{l,\alpha}\lambda_{l,\alpha} - \sum_{l} \sum_{\alpha} \sum_{\beta} \overline{zz}^{\nu}_{l,\alpha,\beta}\lambda_{l,\alpha}\lambda_{l,\beta} - \sum_{i} \sum_{j} \tfrac{1}{2} w_i T_{i,j} w_j + \tfrac{1}{2}\theta \sum_{i} \sum_{j} w_i^* D_{i,j} w_j^*$$

$$- \sum_{i} u_i'' \overline{w}$$

$$\text{subject to} \quad u_j', u_j'' \geq 0 \quad \forall \psi, \tag{29a}$$

$$\sum_{j} T_{i,j} w_j + t_i^{\nu} - u_i' + u_i'' = 0 \quad \forall i, \tag{29b}$$

$$t_i^{\nu} = Cs + \sum_{\omega} \pi_{\omega}\left(C \sum_{j} F^{-1}_{i,j,\omega} f_{j,\omega}\right) + \sum_{l} \sum_{\alpha} \overline{zG}^{\nu}_{l,i,\alpha} - \theta \sum_{j} D_{i,j} w_j^* \quad \forall i, \tag{29c}$$

$$\sum_{\alpha} \lambda_{l,\alpha} \leq 1 \quad \forall l, \tag{29d}$$

$$\lambda_{l,\alpha} \geq 0 \quad \forall l \ \forall \alpha. \tag{29e}$$

This approximate problem involves decision variables A/a, A^, u'p uj, and w,. It is a quadratic program. None of these variables are indexed by o>. If the number of points chosen (^4) is small, the problem involves only a moderate number of variables and constraints, and can be easily solved, on a personal computer, by existing non-linear optimization codes.

The FGA is similar to price directed decomposition for linear programming, and generalized linear programming for non-linear programming. The algorithm starts with a small arbitrary set of feasible points. A step in the algorithm proceeds as follows.

At each iteration the approximate problem is solved and optimal values obtained for \/a, A^, u'*, **and** w"*. We obtain new approximate dual points as follows:

$$z^{*\nu}_{l,\omega} = \sum_{\alpha} \lambda^*_{l,\alpha} z^{\nu}_{l,\omega,\alpha}. \tag{30}$$

We also obtain dependent dual variables w'' which are feasible in the augmented dual problem, so we can also find the current violations v^{ν} and value of the augmented primal problem as follows:

$$v^{\nu}_{l,\omega} = \sum_{i} G_{l,i,\omega}(w_i^{\nu} - f_{i,\omega}) \quad \forall l \forall \omega \tag{31}$$

and

$$P_{\text{aug}} = \sum_{i} \sum_{j} \tfrac{1}{2} w_i^{\nu} R_{i,j} w_j^{\nu} + \sum_{i} r_i w_i^{\nu} + \tfrac{1}{2}\theta \sum_{i} \sum_{j} (w_i^* - w_i^{\nu}) D_{i,j} (w_j^* - w_j^{\nu}) + \sum_{\omega} \pi_{\omega} \sum_{l} \rho(v^{\nu}_{l,\omega}). \tag{32}$$

If the values of the primal and dual problems are equal ($P_{\text{aug}} = D^{\nu}_{\text{aug}}$), we stop because we have found the optimal solution. Otherwise, we find a new point $z^{\nu+1}$, which is the point that gives the maximum value of L'(H-", z), by solving

$$\sup_{z} \sum_{i} \sum_{j} \tfrac{1}{2} w_i^{\nu} R_{i,j} w_j^{\nu} + \sum_{i} r_i w_i^{\nu} + \sum_{\omega} \pi_{\omega} \sum_{l} \left(z_{l,\omega}\left[\sum_{i} G_{l,i,\omega}(w_i^{\nu} - f_{i,\omega})\right] - \tfrac{1}{2} p z^2_{l,\omega} \right)$$

$$+ \tfrac{1}{2}\theta \sum_{i} \sum_{j} (w_i^* - w_i^{\nu}) D_{i,j} (w_j^* - w_j^{\nu}),$$

$$0 \leq z_{l,\omega} \leq q \quad \forall l \ \forall \omega. \tag{33}$$

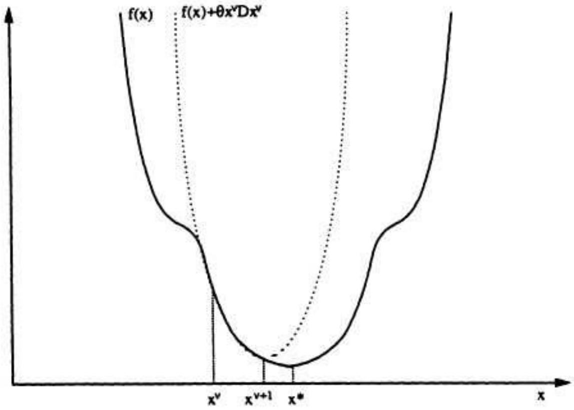


Figure 4. Non-convex and augmented (convex) functions with estimated proximal point

We do not, however, have to explicitly solve (33), since the optimal values of $z_{lo)}$ can be given in closed form as follows (Wagner, 1988):

$$z_{l,\omega} = \begin{cases} 0 & \text{for } v_{l,\omega} \le 0, \\ v_{l,\omega}/p & \text{for } 0 \le v_{l,\omega} \le pq, \\ q & \text{for } v_{l,\omega} \ge pq. \end{cases} \quad (34)$$

Note, this is the piecewise derivative of *p(v ; p, q).* I

For the next iteration, a new set of feasible dual points $\{z^{v}{}_{a}{}^{+1}\}$ must be constructed. This set must! contain z^{*v} and z^{v+1} and may contain additional points if desired. Eiger and Shamir (1991) performed! some numerical experiments on the original FGA, and found that keeping additional points did not seeml to significantly decrease the running time of the algorithm. Thus in this study, to keep the size of the! approximate augmented dual problem to a minimum, only these two points were kept at each iteration.!

There is one additional difficulty. The proximal point w^* was chosen as the optimal solution to thel primal problem which we don't know in advance. Thus, we obtain w * iteratively as follows:

* make an initial estimate of w^*, called w^{*v};
* use w^{*v} in the approximate augmented dual problem (29) as the proximal point, and solve using thel FGA;
* use w^v from the approximate augmented dual solution as the estimated proximal point w^{*p+1} in I the next iteration.

Figure 4 shows an example of one step of this process. We perform successive solutions of the I approximate augmented dual problem to obtain better and better estimates of w^*. Unfortunately, with I only an estimate of w* this process may be attracted to local, not global optima, and may provide al solution that is only locally optimal (Figure 5).

In summary, the steps of the extended Finite Generation Algorithm with proximal points are asl follows:

Step 0. (Outer loop initialization) Choose initial proximal point w*[1], and any positive definite matrix

Step 1. (Inner loop initialization) Set v = \. Choose set of initial points (z^). Select 0.

Step 2. (Subproblem) Calculate the expected value terms (28). Solve the approximate dual problem (29), making sure at each iteration that *0* is sufficiently large to maintain convexity. Obtain z^{*v} and w^v, calculate v^v and $P_a"_{ug}$. If $PZ_{ug} = D"$ go to Step 5.

Step 3. (Generation of new point). Define z from (34).

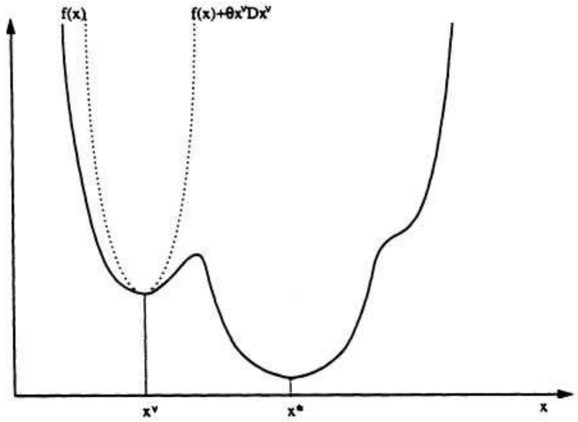


Figure 5. Non-convex and augmented (convex) functions with proximal point at local optima

Step 4. (Modification of polytope). Choose from $\{z^v_a\}$, z^{*v}, and z^{v+1} a subset of points to be included in set $\{z^{v+1}_a\}$, which includes at least the points z^{*v} and z^{v+1}. Set $v = v + 1$. Return to Step 2.

Step 5. (Update proximal point) If w^v is sufficiently close to w^{*v}, *stop,* we accept w^v as being sufficiently close to the (possibly only locally) optimal solution. Otherwise, set $H>^{*v+1} = w^v$, set $v = v + 1$, and return to Step 1.

4.3. Implementation notes

Due to the possibility of being attracted to a local optima, this initial estimate of w * can have a large effect on the solution obtained. One obvious choice for the initial w* is to use the optimal values of the decision variables attained from solving the optimization problem when all uncertain values are set to their expected values. This approach was used for the sample problem examined in this paper since this 'expected value' initial point has the natural interpretation of being the optimal plan for a homogeneous aquifer with known hydraulic conductivity. Another possibility would be to solve the primal problem separately for a small number of possible realizations of the uncertain parameters, and then to average (or in some other way combine) these separate solutions.

In this study, the set of initial feasible dual points {z^} was chosen as $z_1 = 0$ and z_2 = the values obtained from (34) using the initial proximal point w^{*1}.

The algorithm will work with *any* positive definite matrix *D.* For the implementation discussed in this paper the easiest possible positive definite matrix, the identity matrix /, was used.

We want to choose 0 to be just large enough to allow the problem to remain convex. If the value chosen for 0 is too small, the solution of the subproblem will be unbounded and will 'blow up'. Large values of 0 will cause slow improvement in the estimates of w*. In the implementation for this paper, values for 0 were determined by trial and error, by starting with a value of 0 = 10 and increasing it each trial by a factor of 10 until a solution to the subproblem was obtained. Usually a value of 0 = 10 was sufficient, although for a few problems values as high as 0 = 1000 were needed to obtain a solution for the first few subproblems. This 'trial and error' approach should work in other applications as well.

In the implementation of the extended FGA, one additional change was made. In the algorithm given above, the approximate augmented dual problem is solved to optimality in an inner loop, *before* the proximal point is updated in an outer loop. In numerical experiments (Wagner, 1988) on related problems, it was found that the algorithm still converged, and the solution was obtained more quickly, when the approximate dual was not solved to optimality. Thus in each iteration, at Step 4 the polytope is set to include the two points z^{*v} and z^{v+1}, *and* the proximal point was updated to be $w^{*v} = w^v$. The control of the algorithm is then simplified, since the inner loop and the outer loops are merged into one.

One of the advantages of this decomposition based method is that although the size of the full primall problem (13) grows linearly with the number of realizations of the random variables considered, the size of the FGA subproblem is *independent* of the number of realizations used. Thus, fairly complicate distributions and fairly fine discretizations of these distributions could be modeled with this method without great increases in the computer resources being required. However, as the number of realiza-f tions used increases, the work required for preprocessing of input data would increase, and probably the[number of subproblems required to be solved would increase as well.

5. Computational details

The extended FGA, as described in the previous section, was implemented on a PC Limited (Dell)l 286 (12 MHz) personal computer. The modeling language and optimization package GAMS (2.02 AT/XT)/MINOS(5) (an earlier version of Brooke et al., 1988) was used to solve the approximat* augmented dual problems. Computational details of this implementation are discussed in the followin subsections.

5.1. Modeling uncertainty in hydraulic conductivities

The hydraulic conductivities for each realization were obtained by using a turning bands program 1 generate a realization of the random field (Tompson et al., 1987). This program generates spatia correlated variables from a normal distribution with mean = 0 and standard deviation = 1. The progra can also produce output from a normal distribution with user-specified mean and standard deviation (b linear transformation of the variables), as well as according to a log-normal distribution (by taking the lo of the normally distributed variables).

The turning band program is a computer based simulation of 2- and 3-dimensional random fields.' turning bands algorithm involves the generation of a series of 1-dimensional processes along linei radiating from the coordinate origin and their subsequent projection and combination at arbitrary point^ in space, yielding discrete values of realizations of the field. The line processes were generated using *i* Fourier integration method. For more details see Tompson et al. (1987).

For each realization these variables are also spatially correlated in three dimensions according to stationary exponential correlation function

$$C(\xi) = \sigma^2 \exp\left[-\left\{(\xi_1/\lambda_1)^2 + (\xi_2/\lambda_2)^2 + (\xi_3/\lambda_3)^2\right\}^{1/2}\right] \quad (35)$$

where

C(£) = The stationary anisotropic covariance for two points separated by vector £.
cr^2 = The variance of the random field.
g; = The separation along dimension / (/ = 1, 2, 3).
A, = The correlation scale along dimension i.

Each run of the turning bands program produces a realization of the hydraulic conductivities for ea element in the site; realizations from separate runs are independent. Thus each realization is equallj likely, so ir_w = *I/O.* The turning bands program generates hydraulic conductivities over a three-dimen sional rectangle, and numerical problems can occur if the rectangle is too 'flat'. Thus one plane from 1 three-dimensional rectangle was used for the two-dimensional groundwater containment problem.

One additional step is needed to use the conductivity values in the finite difference equations. For i finite element, the conductivity generated by the turning bands program is the proportionality constanl that will give the correct flow for a given gradient *across the element.* However, in the finite differeno equations, we require the conductivity that will give the correct flow *between the centers* of the elements. To find the 'average' or effective conductivity between the two elements, we employed thel common approach of using the harmonic average:

$$K_{\text{eff}} = 2(K_i K_j)/(K_i + K_j). \quad (36$$

5.2. Implementation of the extended finite generation algorithm

For this implementation 20 iterations were run per problem, which gave a maximum difference between $P£_{as}$ and $D\%_{ug}$ of $0,114. The expected costs for these problems were mostly in the hundreds of dollars, so this gap was judged to be acceptable. The maximum change in dual problem from the 19th to the 20th iteration was $0,027.

The full implementation involved FORTRAN programs for data generation and manipulation, five GAMS files containing problem and solution data, MINOS to solve the non-linear optimization files, and DOS batch files to control the calculations. A brief description of the full implementation is given below. Realizations of hydraulic conductivities between each adjoining pair of finite elements in the site were generated by repeatedly using the turning bands program (Tompson et al., 1987). A FORTRAN program was used to combine these realizations with boundary data to obtain the matrices F_a (see Appendix A) and then to invert these matrices. Other FORTRAN programs were used to calculate the vector $/_w$ and generate the matrices G_w. Once the data were generated, the extended FGA was run iteratively using five GAMS files, which were combined using the GAMS/MINOS 'restart' capability.

In practice, the inversion of the F_u matrices turned out to be the most time consuming step in the entire implementation, requiring approximately 6 minutes per matrix (for a 110 X 110 matrix), or about 10 hours for 100 inversions. For this initial implementation these matrices were inverted using, for simplicity, a straightforward implementation of Gaussian elimination. A more sophisticated inversion routine, taking advantage of the banded structure of this matrix, could easily be developed and should reduce this data preprocessing time considerably. Nonetheless, by 'preprocessing' these matrices once and for all greatly reduces the size of the optimization problem. Thus, this inversion step results in great savings in the computational work required to solve the optimization problems and thus allows these multi-scenario problems to be solved using only personal computers.

For the groundwater containment problems, twenty iterations were used. One problem did converge exactly in this number of iterations, the rest had primal and dual optimal values which were quite close. Again, these solutions may only be locally optimal.

6. Results

AU model runs were done for a problem on a 100 X 110 meter site, which was modeled with 10 X 11 finite elements (Figure 1). Each element is 10 meters square *(Ax* = Ay = 10 meters). Measuring from the bottom of the aquifer, the confining layer is at 100 meters and the surface at 150 meters. To the north is a constant head boundary of 110 meters, to the south is a constant head boundary of 109 meters (gradient = 0.01). To the east and west are no-flow boundaries. The contamination is contained to the north of the capture curve shown in the figure. In all, the capture curve has 17 'edges'. There are 23 possible pumping wells, all within the capture curve.

The daily cost of pumping (C) was set to $13.824/meters^3/meter X 86400 seconds/day. This figure is based on 0.0032 kilowatthours of energy to lift one cubic meter of water a height of one meter, and $0.05/kilowatthour for electricity.

The maximum pumping rate *(w)* was set to 0.1 meters^3/second. This value was considerably higher than was obtained in any run, except for one run in which the benefit of water was set to a high value so as to force the maximum amount of pumping.

The mean conductivity was taken from Gorelick (1987) to be 0.0004 meters/second for all runs, with standard deviation of the underlying normal distribution = 1. Thus 95% of the In ^-values should fall between -8.82 and -6.82, corresponding to a range of lvalues of 0.000147 to 0.00108. For all cases the conductivities were assumed to be isotropic, so $A_{:} = A_2 = (A_3)$.

A maximum of 100 realizations of the hydraulic conductivities were used per run *(fl* = 100). Ideally, a different set of realizations would be run for each problem, but due to the time involved in inverting the *F* matrices, for all runs discussed in this paper the realizations were taken from the *same* set of 100 used in run 5. For runs requiring less than all 100 realizations, the first 10 or 50 realizations were used.

Table 1
Capture curve model parameters

Run	Number of outcomes (w)	Penalty parameter P	Penalty parameter q	Correlation scale A (meters)	Standard deviation **Q**	Benefit of pumping $w ($/[m³/s]²)
1	1	0.1	10	10	0	0
2	2	0.1	10	10	1	0
3	10	0.	10	10	1	0
4	50	0.	10	10	1	0
5	100	0.	10	10	1	0
6	1	0.	10	10	0	500
7	2	0.	10	10	1	500
8	10	0.	10	10	1	500
9	50	0.	10	10	1	500
10	100	0.1	10	10	1	500
11	100	10	10	10	1	0
12	100	100	10	10	1	0
13	100	0.1	10	10	1	750
14	100	0.1	10	10	1	1000

Fourteen problems were solved. Parameters varied over the runs are p and q of the penalty parameters, benefit of water B, the convexifying constant 0, the standard deviation of the hydraulic conductivities Q, and the correlation scale A. The values for these parameters are given in Table 1.

As an example of these results, runs 1, 6, and 10 will be examined in detail. Following the results from these three runs, patterns observed by looking at various series of runs will be examined.

6.1. Effect of heterogeneous and stochastic soil parameters

Run 1 is the simplest case with no uncertainty in the hydraulic conductivities, a homogeneous aquifer) and no benefit of water (thus a convex problem). *(K*= 0.0004 meters/second in *all* elements.)

For run 1 the expected cost of pumping was $169.71 per day, with $9.28 in penalties (5.5%). optimal pumping plan (presented in a pattern to match the well configuration in Figure 1) is

```
                     x  x  x
           0.063 x   x  x  x      0.063
0.071        x       x  x  x        x x     0.071
                     x  x  x
                     x  x  x
```

where x indicates no pumping at all at this well (all values in meters³/second). (As a reminder, thel capture curve is below the well array.) The maximum outward gradient was 0.93, which occurred running north to south at both edges (columns 1 and 11).

Run 6 still has deterministic hydraulic conductivities and a homogeneous aquifer, but includes thel benefit of water (non-convex problem). *(B* = $500/[meters³/second]²/day.) The expected cost for run(was $131.71 per day, with $2.78 in penalties (2.1%). The optimal pumping plan is

```
                     x  x  x
           0.070     x  x  x      0.070
0.071        x       x  x  x        x x     0.071
             x       x  x  x
                     x  x  x
```

The maximum outward gradient was 0.51, which occurred running north to south at both edges (columns 1 and 11).

Since the sites are homogeneous, the pumping plan is perfectly symmetrical since there would be no reason to pump one side more than the other. In both cases the wells used are along the upper edge of the well array, not near the capture curve. Only 4 of the possible 23 wells are employed. Since some benefit can be derived from the pumped water, in comparison to the deterministic no benefit case in this optimal plan more water is pumped but the cost decreases due to the money recovered from the use of this water. In both deterministic cases, only a small percentage of the expected costs is to be used for penalties.

Run 10 included stochasticity (100 realizations), heterogeneous hydraulic conductivities (a = 1), and benefit of water. The optimal pumping plan for this run was quite different from that for the deterministic homogeneous sites. The expected cost for run 10 was \$196.96 per day, with \$95.30 in penalties (48.4%). The optimal pumping plan is

```
               x   x   x
      0.072  x    x    x         0.086 x
0.036     x     x    x    x       0.022
        x     x    x    x
               x   x   x
```

The maximum outward gradient over all realizations was 2.64, which occurred running west to east between columns 8 and 9. The distribution of costs over the 100 realizations for this plan is given in Figure 6. If this plan was implemented, over the 100 realizations the actual cost would range from \$103.07 (0% penalties) to \$436.18 (77.2% penalties).

Note that because of the heterogeneity this pumping plan is no longer perfectly symmetrical. Still the same 4 of the 23 possible wells are employed. The total volumes pumped are quite similar in the deterministic stochastic cases. The expected cost is considerably higher in the stochastic heterogeneous case, with a considerably higher percentage of this cost being reserved to pay possible penalties. The plan for the deterministic case will be much less costly on average since it can be optimized for the one set of known conductivity values, unlike the plan for the stochastic case where the plan which is best 'on average' may be, in fact, quite costly for a particular realization of hydraulic conductivities.

6.2. Effect of the number of realizations

Runs 1-5 all examine the convex problem, with no benefit of water, and increasing number of conductivity realizations (from 1 to 100). Run 1 included only one homogeneous realization, runs 2-5 included 2, 10, 50, and 100 heterogeneous realizations, respectively. The results are as follows presentated in Table 2.

The distribution of actual costs over the 100 realizations for the optimal solution from run 5 is shown in Figure 6.

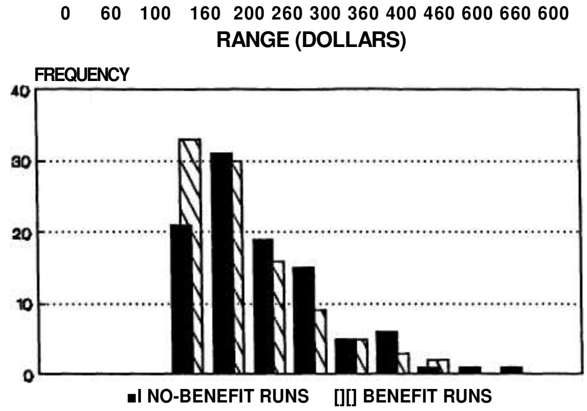


Figure 6. Distribution of optimal solution over 100 realizations

Table 2

Run	Number of realizations	Expected total cost ($)	% of expected cost in penalties (%)	Total pumping (meters/second)
1	1	169.71	5.5	0.268
2	2	143.56	43.9	0.140
3	10	207.00	46.3	0.191
4	50	213.60	47.6	0.190
5	100	217.51	50.7	0.181

The optimal pumping plan for all 5 runs used at least the same 4 wells as in run 1. Runs 4 and 5 also used one additional well in the center of the bottom row of the well array, at a very low rate (0.006 meters/ second or less).

The pumping for the deterministic homogeneous case is higher than for the stochastic heterogeneous cases, since in the deterministic case the pumping can be optimized for the one realization. In the stochastic case, no one plan will be good for all realizations, so less money is spent on pumping and more reserved for penalties.

The expected costs increase as the number of realizations increase. The percent of expected costs accounted for by the penalties also increases slightly with the increasing number of realizations. It is interesting that the cost for the problem including two heterogeneous realizations is actually less than for the deterministic homogeneous case.

Runs 6-10 all examine the non-convex problem, with benefit of water included, and increasing number of conductivity realizations (from 1 to 100). For all of these runs B = \$500/ [meters^3/ second]^2/day. Run 6 included only one homogeneous realization, runs 7-10 included 2, 10, 50, and 100 heterogeneous realizations, respectively. The results are given in Table 3.

The optimal pumping plan for all runs 6, 8, 9, and 10 used at least the same 4 wells as used in run 1, Run 7 did not use the left most well. Runs 9 also used one additional well to the left of the center on the bottom row of the well array, at a very low level (0.002 meters/second).

Again, compared to cases with no benefit of water, the expected costs are lower and the total pumping higher. Again, as the number of realizations increases the expected cost increases. For the stochastic cases the percentage of expected costs in penalties is in the same 45-50% range as in the no-benefit for water case.

6.3. Effect of penalty parameter

Runs 5, 11, and 12 examine the convex problem, with no benefit of water included, as the penalties are relaxed. In all of these runs the slope of the linear part of the penalty was unchanged (q = 10). The other parameter p was changed from 0.1 to 1 to 10 (Figure 7). One-hundred realizations were used for all runs. The results are given in Table 4.

The optimal pumping plans for all these runs used a maximum of 4 wells, although different wells were chosen for each run. For all runs the wells in columns 3 and 9 do the bulk of the pumping.

Table 3

Run	Number of realizations	Expected cost ($)	% of expected cost in penalties (%)	Total pumping (meters/second)
6	1	131.71	2.1	0.282
7	2	132.64	41.8	0.148
8	10	187.45	47.8	0.203
9	50	192.06	46.1	0.217
10	100	196.96	48.4	0.216

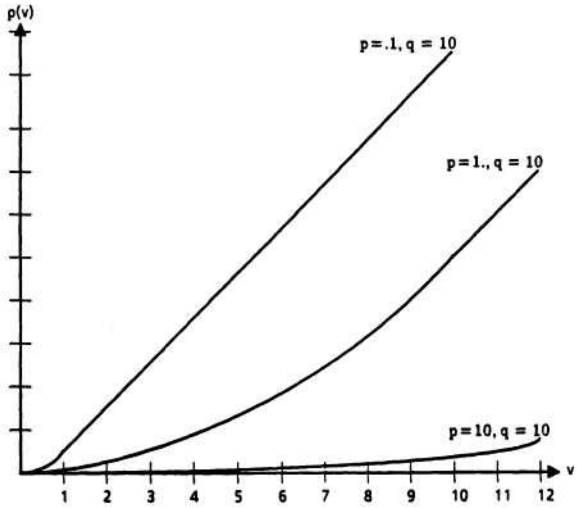


Figure 7. Decreasingly severe penalty functions

As might be expected, the expected costs go down as the penalties are relaxed, as does the total amount of pumping. It is interesting to note that the percentage of the cost accounted for by the penalties is still in the range of 45-50%, regardless of the severity of the penalties.

6.4. *Effect of benefit of water*

Runs 10, 13, and 14 examine the non-convex problem, with increasing benefit of water included. One-hundred realizations were used for all runs. The results are presented in Table 5.

The optimal pumping plans for runs 10 and 13 use the same 4 wells, with run 13 using two additional wells. Run 14 has all wells pumping at their maximum values.

As expected, the amount of pumping increases as the benefit of water increases, and the costs decrease. At B = 1000 the benefit of water overwhelms all other considerations, and the maximum amount of water is pumped out. In this case the pumping rates are unrealistically high and the gradients are also unrealistic high.

Table 4

Run	P	q	Expected cost ($)	% of expected cost in penalties (%)	Total pumping (meters/second)
5	0.1 1	10	217.51	50.7	0.181
11	10	10	140.92	48.6	0.126
12		10	53.37	48.3	0.049

Table 5

Run	Benefit of water $/[meters^3/second]^2	Expected cost ($)	% of expected cost in penalties (%)	Total pumping (meters/second)
10	500	196.96	48.4	0.216
13	750	183.58 -	47.8	0.236
14	1000	3284.66		2.300

6.5. Value of the stochastic solutions

We can calculate the value of the stochastic solution (VSS) as defined by Birge (1982b) as follows. Tha problems solved in runs 1 and 6, with an aquifer with known conductivities, are also the stochastiij problems with all unknown values replaced by their expected values. The optimal pumping plans given I these runs are then the plans that would be given by a deterministic model that ignored the uncertaint in the problem. The cost for this 'expected value plan', *including* recourse cost can then be calculated fo each realization. The average cost over the 100 realizations will then give an estimate of the expected cost of the 'expected value' plan. The difference between the expected cost of the 'expected value **planf** and the expected cost of the plan from the full recourse model is the value of the stochastic solution

For the case when no benefit of water is considered, the expected value including recourse of deterministic solution is $262.71 with 40.4% of this cost due to recourse costs. The expected cost fron the full stochastic model (run 5) was $217.51. Thus, ignoring uncertainty in the no-benefit case wouli) increase the expected costs about 21%.

For the case when benefit of water is considered, the expected value including recourse of deterministic solution is $230.45 with *45.9%* of this cost due to recourse costs. The expected cost fron the full stochastic model (run 10) was $196.96. Thus, ignoring uncertainty in the case including benef would increase the expected costs about 17%. In both cases, the savings in expected costs due tij explicitly incorporating uncertainty are substantial.

7. Conclusions

A model was formulated to examine the management of groundwater quality that explicitly incoi rates uncertainty about the aquifer parameters at the site. The model incorporates recourse costs anJ allows a non-convex objective. This stochastic optimization problem was solved on a personal compute^ using an extension to the FGA that allows a non-convex quadratic objective function, by using a proxiraa point term to convexify the problem. This extended algorithm was used to solve several sample probler involving the containment of groundwater contamination under uncertainty about hydraulic conductivij ties. For all of the problems examined, convex and non-convex, the algorithm converged withoi difficulty. The results of the various runs are consistent with one another, and in general are consisten with our intuition about the physical system.

Solutions obtained from the stochastic recourse model including heterogeneity differ substantially from solutions obtained from deterministic models for homogeneous sites. In general the solutions tha optimize over an ensemble of realizations of hydraulic conductivities have less pumping than the determined for the homogeneous case. We can characterize these stochastic programming solutions 'wait and see' strategies, where initially a low cost plan is implemented with the intent of having mone set aside to pay possible later recourse costs. Interestingly, in these examples the expected cost due penalties was almost always in the 45-50% range, even over a fairly wide range of penalty parameter number of realizations, cost parameters, and expected total costs.

This work can be extended in a number of ways. In this paper, the constraints are assumed to linear. The FGA has also been extended to allow non-convex quadratic constraints (Wagner, 1988). important extension of this method would be to allow the solution of multi-stage recourse problems.

Since this work was primarily developmental in nature, considerable improvement in the implementaj tion of this algorithm is possible. Current work is involved in improving the inversion routines, antj streamlining the solution process. Implementation improvements will allow us to model sites with greater number of finite elements and thus eliminate possible boundary effects from these analyses.

There are also a number of direct extensions of this method for the groundwater containment problem to other related problems of managing groundwater quality. The model described in this papq looks only at controlling flow as a means of managing groundwater quality. We would like to include more detailed description of contaminant flow by directly including the variables of contaminantl concentrations. Thus management options could include diluting the contamination to allowable levels, and/or diverting contaminant flow away from water supply wells, and would also allow for modeling of phenomena such as dispersion and diffusion against a gradient.

Appendix A

The following partial-differential equation is used to describe two-dimensional steady-state flow in an anisotropic confined aquifer:

$$\frac{\partial}{\partial x}\left(K_x b \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y b \frac{\partial h}{\partial y}\right) \pm \delta = 0 \tag{A.1}$$

where
x, y = Length, width (meters).
K_t = Hydraulic conductivity in the direction / (meters/ second). *b*
= Aquifer thickness (meters), and *h* = Head (meters).
8 = Point input/output of water (meters/second). We discretize this equation
to obtain the following finite difference equation:

$$-K_x\frac{(h_{n,m}-h_{n-1,m})}{\Delta x}b\Delta y - K_x\frac{(h_{n,m}-h_{n+1,m})}{\Delta x}b\Delta y - K_y\frac{(h_{n,m}-h_{n,m-1})}{\Delta y}b\Delta x$$

$$-K_y\frac{(h_{n,m}-h_{n,m+1})}{\Delta y}b\Delta x = w_{n,m}. \tag{A.2}$$

where
$\Delta x, \Delta y$ = Length and width of element (meters).
$w_{n,m}$ = $\delta \Delta x \Delta y$.

Using the above equation for each element, with the appropriate set of boundary conditions, we obtain a system of linear equations that describes the response of the heads in each element to the imposed pumping rates.

We choose these boundary conditions to be as follows. We model a rectangular site. We assume that impermeable boundaries exist along the east and west site boundaries. We assume that the site is bordered on the north and south by regions of known, constant heads. These constants head values are substituted into the finite difference equation for elements along the north and south boundaries, thereby introducing constant terms. In addition, these boundary heads are measured, at the boundary of the cell so the corresponding denominator in the flow terms is \&y, not *Ay.*

The finite difference equations are linear in *h* and *w.* By rearranging the / finite difference equations we obtain a linear system which can be represented (in vector notation) as

$$\boldsymbol{Fh} = \boldsymbol{w} - \boldsymbol{f} \tag{A3}$$

1	2	3
4	5	6
7	8	9

Figure A.l. Numbering for nine element system

where
F = An (/ X /)-matrix of the head coefficients.
$\boldsymbol{h}$ = An /-vector of head variables.
w = An JV-vector of pumping variables.
/ = An /-vector of constants (from the boundary conditions).

Since non-zero coefficients appear only on terms linking neighboring elements, the matrix F **hasl** special banded structure. For example, numbering the finite elements as in Figure A.1 matrix F has thel following structure:

$$F = \left|\begin{array}{ccccccccc} \bullet & \bullet & 0 & \bullet & 0 & 0 & 0 & 0 & 0 \\ & & & 0 & & 0 & 0 & 0 & 0 \\ 0 & & & & 0 & . & 0 & 0 & 0 \\ . & 0 & \bullet & \bullet & & 0 & . & 0 & 0 \\ 0 & \bullet & 0 & & \bullet & & 0 & . & 0 \\ 0 & 0 & . & 0 & & & & 0 & \bullet \\ 0 & 0 & 0 & \bullet & 0 & \bullet & & & 0 \\ 0 & 0 & 0 & 0 & \bullet & 0 & \bullet & \bullet & \bullet \\ 0 & 0 & 0 & 0 & 0 & & 0 & & \bullet \end{array}\right| \qquad \text{(A.4)}$$

Appendix B

Statement A.l. *The matrix* $-F_{\omega}$ *is positive definite.*

Proof. We start with the following example (Figure B.I). Let $\Delta x = \Delta y = b = 1$. The matrix F for this system is

$$F = \begin{bmatrix} -K_{n,m} - 4K_n & K_{n,m} \\ K_{n,m} & -K_{n,m} - 4K_m \end{bmatrix}. \qquad \textbf{(5)}$$

The value of $-\boldsymbol{w}^{\mathrm{t}}\boldsymbol{F}\boldsymbol{w}$ is then

$$-\boldsymbol{w}^{\mathrm{t}}\boldsymbol{F}\boldsymbol{w} = (K_{n,m} + 4K_n)w_n^2 - 2K_{n,m}w_n w_m + (K_{n,m} + 4K_m)w_m^2. \qquad (6)1$$

Rearranging,

$$-\boldsymbol{w}^{\mathrm{t}}\boldsymbol{F}\boldsymbol{w} = K_{n,m}(w_n - w_m)^2 + 4K_n w_n^2 + 4K_m^2 w_m^2 > 0 \quad \text{unless } w_n = w_m = 0. \qquad (7)1$$

So $-w^l Fw > 0$ for all w, and $-F$ is positive definite for this example.

In general for an *NxN* system with heterogeneous soil, for each realization <*o* we generate a distind value of K for each pair of adjacent nodes. We show that the sum — $w^l F_{a)} w$ can be broken up into a sun of positive terms, each involving only one of the distinct X-values.

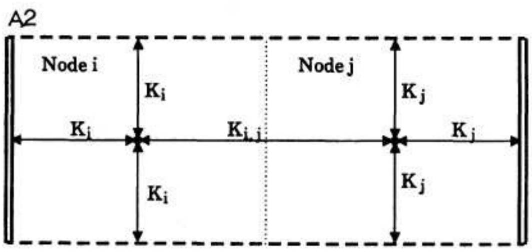


Figure B.I. Hydraulic conductivities for two element system

For any two nodes *n* and *m,* we have K_{nm}, which appears in *F^* only at position *(n, n),* (m, m), *(n,* m) and (m, *n).* Pre- and post-multiplying — F_w by *w,* the only terms involving K_{nm} will be

$$c\left[K_{n,m}w_n^2 - 2K_{n,m}w_nw_m + K_{n,m}w_m^2\right] = c\left[K_{n,m}(w_n - w_m)^2\right] \geq 0 \quad \forall w_n \text{ and } w_m \tag{8}$$

where *c* = the positive constant *biAx/Ay)* for north-south flow and *b(Ay/Ax)* for east-west flow.

For nodes *n* along the no-flow boundaries, the term for horizontal flow across the boundary is set to zero, so the corresponding ^-values for these terms do not appear in F_m.

For nodes *n* along the constant head boundaries, K_n will appear only in one term, with value *$1cK_nwl$* > 0 for w_n ¥= 0. (In the example the values were *$4cK_nw$%* because these nodes were along *two* constant head boundaries.)

Thus all conductivity values, whether on the boundaries or not, can be grouped into non-negative terms, with some terms strictly positive. Thus *-w'F^w* > 0 (for all *w* ¥= 0), and *-F*™ is positive definite. D

Acknowledgements

The authors would like to thank Professor Stephen Graves for his advice and review of this work, and Professor Steve Gorelick of Stanford and the USGS for advice. This project was supported by NSF grant CEE 84-8369.

References

Andricevic, R. (1990), "A real-time approach to management and monitoring of groundwater hydraulics", *Water Resources Research* 26/11, 2747-2755. Andricevic, R., and Kitanidis, P.K. (1990), "Optimization of the pumping schedule in aquifer remediation under uncertainty",

Water Resources Research 26/5, 875-885. Atwood, D.F., and Gorelick, S.M. (1985), "Hydraulic gradient control for ground water contaminant removal", *Journal of*

Hydrology 76, 85-108. **Birge, J.R.** (1982a), "Decomposition and partitioning methods for multistage stochastic linear programs", Department of Industrial

and Operations Engineering Technical Report 82-6, University of Michigan, Ann Arbor, MI. **Bilge,** J.R. (1982b), "The value of the stochastic solution in stochastic linear programs with fixed recourse", *Mathematical*

Programming 24, 314-325. **Birge,** J.R., and Louveaux, F.V. (1985), "A multicut algorithm for two-stage stochastic linear programs", Department of Industrial

and Operations Engineering Technical Report 85-15, University of Michigan, Ann Arbor, MI. **Brooke,** A., Kendrick, D., and Meeraus, A. (1988), *GAMS: A User's Guide,* Scientific Press. **Colarullo,** S.J., Heidari, M., and Maddock, III, T. (1984), "Identification of an optimal ground water strategy in a contaminated

aquifer", *Water Resources Research* 20/5, 747-760. **Dagan,** G. (1986), "Statistical theory of groundwater flow and transport: Pore to laboratory, laboratory to formation, and formation

to regional scale", *Water Resources Research* 22, 102S-134S. **Dantzig,** G., and Madansky, A. (1961), "On the solution of two-stage linear programs under uncertainty", in: J. Neyman (ed.),

Proceedings of the Fourth Berkeley Symposium on Mathematical Statistics and Probability, Vol. 1, University of California Press, Berkeley, CA, 165-176. **Eiger,** G-, and Shamir, U. (1991), "Optimal operation of reservoirs by stochastic programming", *Engineering Optimization* 17,

293-312. Freeze, R.A. (1975), "A stochastic-conceptual analysis of one-dimensional groundwater flow in nonuniform homogeneous media",

Water Resources Research 11, 725-741.

Gelhar, LJ. (1986), "Stochastic subsurface hydrology from theory to applications", *Water Resources Research* 22, 135S-145S.

Gorelick, S.M. (1983), "A review of distributed parameter groundwater management modeling methods", *Water Resources Research* 19, 305-319. **Gorelick,** S.M. (1987), "Sensitivity analysis of optimal groundwater contaminant capture curves: Spatial variability and robust

solutions", in: *Proceedings of the NWWA Conference on Solving Groundwater Problems with Models,* National Well Water Association, Dublin, OH. Hoeksema, R.J., and Kitanidis, P.K. (1985), "Analysis of spatial structure of properties of selected aquifers", *Water Resources*

Research 21, 563-572.

Lefkoff, L.J., and Gorelick, S.M. (1986), "Design and cost analysis of rapid aquifer restoration systems using flow simulation and) quadratic programming", *Ground Water* 24/6, 777-790. Louveaux, F.V. (1980), "A solution method for multistage stochastic programs with recourse with application to an energyl investment program", *Operations Research* 28, 889-902. Molz, F.J., and Bell, L.C. (1977), "Head gradient control in aquifers used for fluid storage", *Water Resources Research* 13/4,l 795-798. Noel, M.C., and Smeers, Y. (1985), "Nested decomposition of multistage nonlinear programming with recourse", Discussion Paperl 8505, CORE, Louvain, Belgium. Ranjithan, $., Eheart, J.W., and Garrett, Jr., J.H. (1990), "Application of a neural network in groundwater remdiation under! conditions of uncertainty", in: *International Workshop on New Uncertainty Concepts in Hydrology and Water Resources,}* presented at Madralin, Poland. Remson, I., and Gorelick, S.M. (1980), "Management models incorporating groundwater variables", in: D. Yaron and C.S. Tapierol (eds.), *Operations Research in Agriculture and Water Resources,* North-Holland, Amsterdam, 333-355. Rockafellar, R.T., and Wets, RJ.-B. (1976), "Stochastic convex programming: Relatively complete recourse and inducedl feasibility", *SIAM Journal on Control* 14, 574-589. Rockafellar, R.T., and Wets, RJ.-B. (1983), "A dual solution procedure for quadratic stochastic programs with simple recourse",! in: V. Pereyra and A. Reinoza (eds.), *Numerical Methods (Lecture Notes in Mathematics 1005),* Springer-Verlag, BerlinJ 574-589. Rockafellar, R.T., and Wets, R.J.-B. (1986a), "Linear-quadratic programming problems with stochastic penalties: The finitel generation algorithm", in: V.I. Arkin, A. Sniraev and RJ.-B. Wets, (eds.), *Stochastic Optimization,* Springer-Verlag, Berlin. Rockafellar, R.T., and Wets, RJ.-B. (1986b), "A lagrangian finite generation technique for solving linear-quadratic problems inl stochastic programming", *Mathematical Programming Studies* 28, 63-93. Somlyody, L., and Wets, RJ.-B. (1988), "Stochastic optimization models for lake eutrophication management", *Operations\ Research* 36,660-681. Tompson, A.F.B., Ababou, R., and Gelhar, L.W. (1987), "Application and use of the three-dimensional turning bands random fieldl generator: Simple realization problems", Parsons Laboratory Report 313, Massachusetts Institute of Technology, Cambridge,! MA. Van Slyke, R., and Wets, R.J.-B. (1969), "L-shaped linear programs with applications to optimal control and stochasticl programming", *SIAM Journal on applied Mathematics* 17, 638-663. Wagner, B.J., and Gorelick, S.M. (1987), "Optimal groundwater quality management under parameter uncertainty", *Wate< Resources Research* 23/7, 1162-1174. Wagner, B.J., and Gorelick, S.M. (1989), "Reliable aquifer remediaion in the presence of spatially variable hydraulic conductivity! From data to design", *Water Resources Research* 25/10, 2211-2225. Wagner, J.M. (1988), "Stochastic programming with recourse applied to groundwater quality management", Ph.D. Thesis,] Massachusetts Institute of Technology, Boston, MA.