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Groundwater Quality Management Under Uncertainty: Stochastic Programming Approaches and the Value of Information

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A stochastic optimization model for containment of a plume of groundwater contamination through the installation and operation of pumping wells is developed. It considers explicitly uncertainty about hydraulic conductivity in the aquifer and seeks to minimize the expected total cost of operating the pumping wells plus the recourse cost incurred when containment of the contaminant plume is not achieved. Four different formulations of the model are examined, ranging from simply replacing all uncertain parameters by their expected values to a full stochastic programming with recourse model involving nonsymmetric linear quadratic penalty functions. The full stochastic programming with recourse model, which minimizes the expected total costs over a number of realizations of outcomes of the random parameters, is nonlinear and possibly nonconvex and is solved by an extension of the finite generation algorithm. The value of information about the uncertain parameters is defined through the differences between the values of the optimal solutions to the different formulations. A sample problem is solved using all four formulations. The results indicate that the explicit incorporation of uncertainty does make a difference in the solutions obtained. The work indicates that stochastic programming with recourse is a useful tool in management under uncertainty, and that it can be used with reasonable computational resources for problems of moderate size.

INTRODUCTION

The objective of managing groundwater in contaminated areas is to either remove the plume of polluted water, contain it within a specified zone, or control its flow away from wells, streams, and lakes in which water quality is to be protected. These objectives can be attained by inserting curtain walls into the aquifer between the plume and the zone to be protected, or by digging up and removing the polluted soil, but more usually by installing and operating pumping and/or recharge wells so as to control the flow field. Planning and operation of such remediation schemes is aided by simulation and optimization models. Simulation allows the investigation of "what if" questions, which allow the comparison of alternative schemes. Optimization models are designed to find the solution that is best according to a specified objective, usually economic, while satisfying a set of stated physical, technological, legal, and other constraints.

Any groundwater management scheme has to be planned, installed, and operated under many uncertainties. These uncertainties stem from incomplete information about the aquifer properties, its boundaries and boundary conditions, the location and intensity of the pollution sources, and the existing flow field in the aquifer before remediation has begun, as well as from economic, regulatory, and political factors.

In this paper we present an optimization model for (1) locating pumping and recharge wells within an aquifer and then (2) operating them, in steady state, so as to control groundwater gradients and thus keep a plume of polluted water from entering a protected zone. The primary innovation of the approach presented in this paper is that the optimal solution is sought under uncertainty about the hydraulic conductivities in the aquifer. The objective function includes the cost of operating the wells, as well as recourse costs resulting from the possible leakage of contaminated water into the protected zone. Neither the costs of operating the wells, nor the recourse costs due to leakage of the plume, are known with certainty in advance since they depend on the stochastic aquifer parameters.

In this paper we focus on the uncertainty about aquifer properties, for several reasons. First, aquifer properties (such as hydraulic conductivities) can never be known with certainty. Hydraulic conductivities are measured from pumping tests or by taking soil samples (cores) from the site and measuring these samples in the laboratory, but these methods provide only local or at best zonal data. In principle, other uncertain parameters such as boundary conditions and locations of contaminants could be determined without completely disrupting the site. Secondly, 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 conceptual difficulty.

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We use a stochastic optimization method, which incorporates the uncertainties and their economic consequences explicitly into the objective function and into the relevant constraints. In this model the decisions about location and sizing of wells are made "here and now." However to determine the exact cost of operating the wells and the amount to be paid in possible recourse costs we must "wait and see" how these pumping rates affect the head field across the site and how the contaminant plume reacts.

The equations that describe groundwater flow are incorporated into the optimization model as constraints. Even though some of the coefficients in these constraints are treated as random parameters, for any actual realized values of these parameters the equations must always hold, since they describe physical laws. The goal is to contain the plume by creating a groundwater gradient that will prevent flow into the protected zone, but this goal cannot be guaranteed to materialize for a given pumping/recharge scheme, due to the randomness of the aquifer parameters.

Some previous groundwater management models have incorporated this uncertainty by using chance-constrained linear programming. Chance-constrained models have the advantage that they are no larger than the corresponding deterministic models and thus are not too difficult to solve. However, they have the disadvantage that only the probability of violating a constraint is controlled, while the extent and consequences of a violation, when it does occur, are not taken into account. Thus, for example, if a constraint on some water quality standard can be violated no more than 2% of the time, then a solution which would allow this standard to be exceeded only slightly but with a somewhat higher probability, say, 2.5% of the time, would not be accepted. However, a solution with a very extreme violation of the standard which occurs, say, 1.9% of the time, would be accepted. To remedy this deficiency somewhat, several probabilistic constraints could be incorporated together into the same chance-constrained model (at the cost of expanding it) but even then the cost resulting from a violation cannot be taken into consideration.

In the method presented in this paper, stochastic programming with recourse, the form of the penalties will affect the frequency and the extent of constraint violations. Recourse models are often much larger than the corresponding deterministic models, and require different solution techniques. However, due to advances in both stochastic optimization methods and in computer technology, useful stochastic optimization problems can be formulated and solved without excessive computer resources.

This paper will discuss a number of formulations of a stochastic programming model for managing groundwater quality under uncertainty. The formulations vary in the degree of complexity; in general, the more complex formulations allow greater realism and modeling flexibility. We shall examine and compare the solutions from these different formulations, to determine the effect of uncertainty on the management process and to give insight into the value of obtaining information at various times in the planning and management process. We demonstrate these techniques on a sample problem involving the containment of a polluted plume. As evidence of the computational feasibility of these techniques, all calculations are carried out on a personal computer.

In the next section we provide a brief review of the literature relevant to this problem and to the background of stochastic programming. We then present the stochastic optimization model developed for this problem, analyze the value of information, and finally show results for a sample problem.

LITERATURE REVIEW

Deterministic optimization models for the containment of contamination by gradient control have been developed by *Molz and Bell* [1977], *Remson and Gorelick* [1980], *Colarullo et al.* [1984], *Atwood and Gorelick* [1985], and *Lefkoff and Gorelick* [1986]. In the following subsection, optimization models for groundwater management that include uncertainty are discussed, followed by a brief overview of methods for solving stochastic programming problems with recourse.

Groundwater Management Under Uncertainty

One traditional way of dealing with uncertainty in optimization models is to do postoptimality sensitivity analysis to determine the effect on the optimal solution of small changes in model data. *Aguado et al.* [1977] used sensitivity analysis to examine the effect of changes of hydraulic conductivity on the optimal solution of a model for site dewatering. They developed a model to minimize pumping while meeting specified head values by embedding the discretized equations for groundwater flow as constraints in the optimization model. After solving the model for an isotropic, homogeneous aquifer they then changed the hydraulic conductivity at each nodal point and solved the optimization model again to determine how the change in this parameter affected the optimal pumping plan. *Willis* [1979] also used embedding for a model to manage a site for both water supply and waste disposal. He used parametric methods to examine the allowable changes in waste concentrations as the water quality standards are relaxed. *Gorelick* [1982] used a concentration response matrix in an optimization model to determine the maximum waste disposal rates that still meet water quality standards over time. He also used parametric methods to examine the sensitivity of the total waste disposal capacity to changes in the disposal rate at individual wells.

Uncertainty can also be modeled using stochastic simulation. *Bredehoeft and Young* [1983] used a simulation model to investigate how variation in surface water supply affects investment in well capacity for an area where both groundwater and surface water are used for irrigation. The study investigated the extent to which well capacity is being used to avoid income fluctuation of farmers in the area.

A method that has been used to incorporate uncertainty in the optimization model itself is to use chance constraints, so that certain constraints are not met exactly under all conditions, but instead are only met with a specified level of reliability. *Tung* [1986] used a response function in a model to maximize the yield from a confined, homogeneous, and nonuniform aquifer without violating head limits specified at various points in the aquifer. He treated the transmissivity (T) and storativity (S) as random variables, formulated the head restrictions as chance constraints, and used first-order analysis and quasi-linearization to develop the linear deterministic equivalents of the chance constraints. Tung also used stochastic simulation to investigate the validity of his model. *Wagner and Gorelick* [1987] developed a nonlinear chance constraint model to find optimal remediation plans (either pumping for contaminant removal or recharge for in-ground dilution) so as to meet water quality standards at specified points in the aquifer. This procedure coupled parameter estimation and response matrix methods to first- and second-order moment analysis to transform parameter uncertainty into chance constraints on concentration levels. This study also used simulation to validate the assumptions made in the first-order moment analysis. *Hantush and Marino* [1989] developed a model to maximize the pumping from an aquifer linked to a stream, while maintaining limits on heads in the aquifer and depletion from the stream over time with a specified level of reliability. This model considered variation in hydraulic conductivity and specific yield due to measurement error, spatial averaging and the "inherent stochastic description" of porous media. This model used an analytical approximation to link drawdowns and stream depletion rates due to pumping, and formulated the chance constraints analytically (using lognormal distributions). In all of these chance constraint models, sensitivity analysis was also performed to assess the effect of the reliability levels used for the chance constraints.

Maddock [1974] developed an optimization model for the management of the conjunctive use of surface water and groundwater, which included uncertainty by using statistical analysis. The aquifer was modeled with a distributed parameter model. The demands imposed on the sources were modeled as being stochastic. The objective was to minimize the discounted expected energy cost of pumping. This expected cost was derived by including the statistics of the water demand so that the operating decisions are based on the variance and correlation of these demands, as well as on their expected values. The constraints included meeting expected water demand and on average meeting downstream water rights.

Gorelick [1987] and *Wagner and Gorelick* [1989] developed optimization models that incorporate uncertainty by finding solutions that are optimal over a number of possible realizations of uncertain parameters. *Gorelick* [1987] developed a model based on a response matrix to minimize the pumping required to keep contaminated groundwater from flowing out across a capture curve in an aquifer with spatially variable hydraulic conductivity. He generated 130 possible realizations, and then selected 10 representative realizations. The constraints for all 10 realizations were incorporated into the optimization model, and a minimum pumping solution was found such that the contaminant would be contained within the capture curve for all 10 realizations. *Wagner and Gorelick* [1989] developed a nonlinear model also based on a response matrix for remediation of a contaminated aquifer. The objective was to minimize pumping while meeting water quality standards. The uncertainty in this problem is due to spatial variability in the hydraulic conductivities. One formulation developed a plan with minimum pumping to meet standards over 30 realizations of hydraulic conductivity. A second formulation found the optimal pumping rate for a single well for each of 1000 realizations. The results of these 1000 realizations were then used to characterize the probability distribution of pumping rates.

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 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.

Andricevic [1990] and *Andricevic and Kitanidis* [1990] developed methods using stochastic differential dynamic programming to develop pumping plans for groundwater management and monitoring. In the work by *Andricevic* [1990] the objective was to minimize the expected value of a weighted sum of the deviations from both specified pumping levels at each pumping well and specified head levels at each control point. In the work by *Andricevic and Kitanidis* [1990] the objective was to minimize the expected value of a weighted sum of pumping and exceedance of a specified concentration standard. In both of these methods, uncertainty about hydraulic conductivity is included in the model by treating the hydraulic conductivity values as a random field. These models are dynamic, meaning that the pumping strategies are revised over time, as the effects of the pumping plan and additional monitoring data become known. Both models allow management plans and monitoring plans to be developed concurrently.

Risk analysis methods are also used to deal with uncertainty. In risk analyses the uncertainties in model inputs (such as timing and sizes of spills and leaks) are translated into uncertainties in outputs (such as probability of exceeding standards or the probability of contamination of a well). Risk analyses specifically dealing with groundwater include *Kaunas and Haimes* [1985], *Hobbs et al.* [1988], and *Lichtenberg et al.* [1989].

Stochastic Programming With Recourse

Stochastic programming with recourse involves a two (or more) stage decision process. First a decision is made and implemented; then the world unfolds. At a later stage recourse actions are taken, usually at some cost. 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, stochastic programming with recourse allows increasingly higher penalties to be incurred 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, 1986*a*, *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.

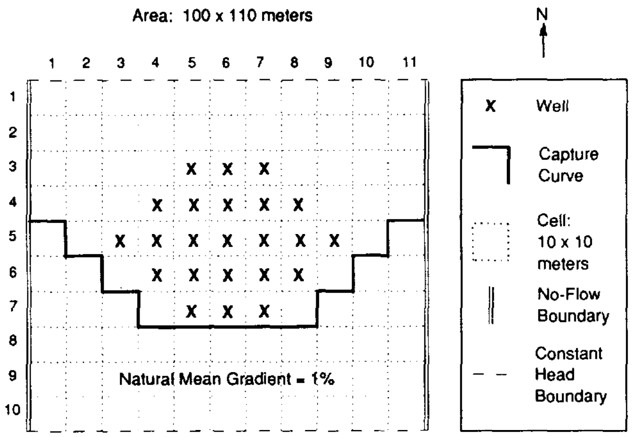

Fig. 1. Plan view of aquifer with capture curve.

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 multiperiod operation of a multireservoir 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 multistage problems were developed by *Birge* [1982*a*] and *Noel and Smeers* [1985]. *Louveaux* [1980] developed a nested decomposition method for multistage stochastic quadratic programming problems.

FORMULATION OF A STOCHASTIC PROGRAM WITH RECOURSE

As an example of a stochastic program with recourse for managing groundwater quality, we will look at the problem of containing an area of groundwater contamination by maintaining hydraulic gradients across a "capture curve" or "interception envelope." Although many elements in this problem could be uncertain, we focus on the uncertainty in the values of the hydraulic conductivity. In this problem, the recourse costs are modeled as a penalty that depends on the degree of "leakage" across the capture curve. This formulation is one of simple recourse, since the penalties are simply assessed, and are not a result of "second-stage" decisions made in order to minimize the recourse costs.

We start by formulating a problem for an area with homogeneous soil of known hydraulic conductivity. We then extend this formulation to an area with heterogeneous soil with imperfectly known conductivity. Note, the term hydraulic conductivity is used throughout this paper for generality. However, for the aquifer modeled in this paper the aquifer thickness is constant so we could also describe this model as incorporating uncertain transmissivity.

Deterministic Optimization Problem

We consider a confined aquifer with uniform thickness b, which is modeled as $i = 1, \cdots, I$ connected finite elements. (See for example, Figure 1.) The aquifer contains an area of contamination, which we wish to prevent from crossing a "capture curve," which is prescribed along certain edges of these elements. In order to contain the contamination it is necessary to create a gradient into the capture zone across the capture curve by pumping one or more possible control wells. The pumping will lower water levels inside the capture zone and create the desired gradients.

The objective is to minimize the total daily cost of the remediation strategy. The deterministic objective function is

$$\min \sum_i A_1 w_i(s - h_i) - A_2\left(\sum_i w_i\right)^2 \qquad (1)$$

where

A_1 daily cost of pumping, (dollars m^{-3} (m of elevation)$^{-1}$)(86,400 s d^{-1});

w_i pumping rate in cell i, m^3/s;

s height of the ground surface (measured from the bottom of the aquifer), m;

h_i head in cell i, m;

A_2 daily benefit, (dollars (m^3)$^{-2}$) (86,400 s d^{-1}).

The first term represents the cost of pumping. The second term represents the payoff or benefit from the use of the water that is removed from the aquifer. Water pumped from the site may be used (possibly after treatment) for industry or irrigation. This benefit term could be any linear or quadratic function of the pumping rates (w_i). For illustration, we assume the benefit of water to be proportional to the square of the total amount of pumped water.

The groundwater system is modeled by embedding the discretizations of the partial differential equations governing groundwater flow as constraints in the optimization problem. These constraints (developed in Appendix A) are

$$\sum_j F_{i,j} h_j = w_i - f_i \qquad \forall\, i \qquad (2)$$

where $F_{i,j}$ are coefficients determining flow between cells i and j whose values depend on the geometry of the finite difference model and the hydraulic conductivities ($K_{x,y}$), and f_i are constants for cell i that depend on the boundary conditions.

Constraints are added to require that the head gradients (and thus the water flow) be inward across the capture curve, as follows:

$$h_l^{\text{in}} - h_l^{\text{out}} \leq 0 \qquad \forall\, l \qquad (3)$$

where h_l^{in} are the head values on the inside of the capture curve, h_l^{out} are the head values of the outside of the capture curve, and l is the index of cell pairs that form the boundary.

Lastly, in this model we allow only pumping (no recharge), so the pumping rates are restricted to be nonnegative. They are also restricted to be below some maximum value:

$$0 \leq w_i \leq \overline{w} \qquad \forall\, i. \qquad (4)$$

Thus this deterministic optimization problem has a nonlinear objective function subject to linear constraints.

Stochastic Optimization Problem

The uncertainty in this problem is assumed to come from the stochastic nature of the hydraulic conductivities (K).

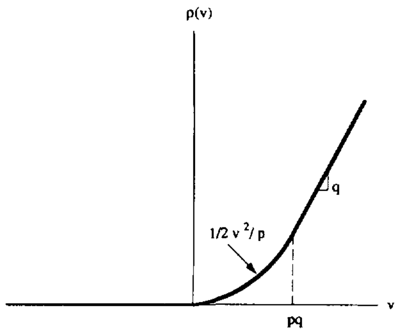

Fig. 2. Linear-quadratic penalty function.

First we assume that these hydraulic conductivities can vary from place to place within the region. 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 lognormally distributed, with known mean and variance, and spatially correlated with a known correlation structure.

Uncertainty is included in the optimization formulation by sampling the stochastic field of continuous hydraulic conductivity values. This sampling is done by obtaining a (possibly quite large) set of realizations of this distribution, with each realization consisting of a distinct value for the hydraulic conductivity of each cell. These realizations are indexed by ω ($\omega = 1, 2, \cdots, \Omega$). Each realization is assumed to occur with probability π_ω.

Each realization ω will result in a different matrix F and, for a fixed pumping plan $\mathbf{w}$, a different set of heads for each realization. Thus we write F_ω, $\mathbf{h}_\omega$, $\mathbf{h}_\omega^{\text{in}}$, and $\mathbf{h}_\omega^{\text{out}}$ in the stochastic formulation.

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

$$h_{l,\omega}^{\text{in}} - h_{l,\omega}^{\text{out}} \le 0 \qquad \forall\, l\, \forall\, \omega. \tag{5}$$

We define the amount to which this constraint is violated at any boundary l and for any realization ω by

$$v_{l,\omega} = h_{l,\omega}^{\text{in}} - h_{l,\omega}^{\text{out}}. \tag{6}$$

A positive value for this violation term means that there is some leakage of contaminated water into the protected zone, past the planned capture curve. This leakage is assumed to result in a recourse cost, such as treatment costs for water pumped at the supply wells or costs for some other remedial action required to counteract the contamination of the protected zone. This recourse cost is represented by a linear-quadratic penalty function for a violation v as follows (see Figure 2):

$$\begin{aligned} \rho(v; p, q) &= 0 & v &\le 0 \\ \rho(v; p, q) &= \tfrac{1}{2}v^2/p & 0 \le v &\le pq \\ \rho(v; p, q) &= qv - \tfrac{1}{2}pq^2 & v &\ge pq. \end{aligned} \tag{7}$$

The parameters p and q must be positive, and are specified by the decision maker.

The shape of this penalty function was chosen for a number of reasons. First, it allows the decision maker great flexibility. The slope of the linear portion, the point of transition from the quadratic to the linear portion, and thus the shape of the entire function can be controlled through choice of the parameters p and q. This function also has a number of desirable theoretical properties, including the fact that it is differentiable everywhere, and that it has an easily expressed conjugate function [*Rockafellar and Wets*, 1986*a*, *b*].

Now, for a given pumping plan $\mathbf{w}$, the cost will consist of the energy cost of pumping plus the recourse cost minus the benefit obtained from the pumped water. This cost will vary for each realization of the hydraulic conductivities. The objective is to minimize the expected cost. The stochastic optimization problem is then

$$\min \sum_\omega \pi_\omega \left[\sum_i A_1 w_i (s - h_{i,\omega}) + \sum_l \rho(v_{l,\omega}) \right] - A_2 \left(\sum_i w_i \right)^2$$

subject to

$$\begin{aligned} &\sum_j F_{i,j,\omega} h_{j,\omega} = w_i - f_i && \forall\, i\, \forall\, \omega \\ &v_{l,\omega} = h_{l,\omega}^{\text{in}} - h_{l,\omega}^{\text{out}} && \forall\, l\, \forall\, \omega \\ &0 \le w_i \le \bar{w} && \forall\, i. \end{aligned} \tag{8}$$

For simplicity in this application, the same values of the penalty parameters p and q are used for all locations along the boundary cells and for all realizations. It would be possible to use different parameters, for example, to penalize violations at one location more than at another.

This formulation involves simple recourse, since the penalties are uniquely determined once the "here and now" decision variables are set. More generally, the recourse costs themselves may be found from an optimization problem that is solved after the "here and now" plan has been implemented and after the uncertain values have become known.

The penalty function $\rho(v)$ can be expressed as a quadratic function subject to linear constraints [*Rockafellar and Wets*, 1986*a*], as follows:

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

subject to

$$v' + v'' \ge v \qquad v'' \ge 0. \tag{9}$$

Thus, by replacing $\rho(v_{l,\omega})$ in (8) by the objective of (9) and by adding in the constraints from (9), the stochastic program can be rewritten as a quadratic objective function subject to linear constraints. This form of the problem was used to develop the solution method; however, for clarity, we will continue to write $\rho(v_{l,\omega})$ in the formulations presented in this paper.

To use (8) as a management tool, sufficient discrete realizations should be generated to characterize the continuous distribution. For a problem with a small number of random variables, where each variable can be represented by a small number of values, the complete distribution could be represented by generating a realization for every possible combination of random outcomes. However, due to the number of random variables and extent of variation, in this problem it is not computationally feasible to generate a complete set of realizations to completely characterize the distribution. Also, even if we did generate a complete set of realizations of the discretized distribution, the resulting optimization problem would be too large to solve. Thus we used a Monte Carlo approach to obtain samples from this distribution, and used this set of Monte Carlo–generated realizations to represent the distribution in the optimization problem.

We can reduce the number of variables in this problem by exploiting the fact that the values of $h_{i,\omega}$ are completely determined from the flow constraints, once the values of w_i have been set. (We say that the values $h_{i,\omega}$ are dependent stochastic variables.) The matrix $-F_\omega$ is positive definite (Appendix B). Thus we can remove the dependent variables $h_{i,\omega}$ from the problem by rearranging the head constraints to obtain

$$h_{i,\omega} = \sum_j F_{i,j,\omega}^{-1}(w_j - f_j). \tag{10}$$

Substituting (10) into (8), we obtain the following optimization problem:

$$\min \sum_\omega \pi_\omega \left[\sum_i A_1 w_i \left(s - \sum_j F_{i,j,\omega}^{-1}\{w_j - f_j\} \right) + \sum_l \rho(v_{l,\omega}) \right] - A_2 \left(\sum_i w_i \right)^2$$

subject to

$$v_{l,\omega} = \sum_j G_{l,j,\omega}\{w_j - f_j\} \qquad \forall\, l\, \forall\, \omega$$

$$0 \le w_i \le \bar{w} \qquad \forall\, i \tag{11}$$

where

$$G_{l,j,\omega} = [F_{l,j,\omega}^{-1}]^{\text{in}} - [F_{l,j,\omega}^{-1}]^{\text{out}}. \tag{12}$$

(Regarding notation, note that the violations concern only the l heads along the boundary, namely, $h_{l,\omega}^{\text{in}}$ and $h_{l,\omega}^{\text{out}}$. Thus to calculate the violations $v_{l,\omega}$ we need only certain rows of matrix F_ω^{-1}, which we denote as $[F_\omega^{-1}]^{\text{in}}$ and $[F_\omega^{-1}]^{\text{out}}$. If we have I elements and calculate gradients at L points, F_ω^{-1} is of size $I \times I$, and G_ω, $[F_\omega^{-1}]^{\text{in}}$, and $[F_\omega^{-1}]^{\text{out}}$ are of size $L \times I$.)

In the development of the original finite difference equations we included a term w_i for each element, even for those elements with no wells. For elements i with no wells we restrict $w_i = 0$. Further reduction of the size 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 in the formulations given in this paper.

Method of Solution

By using the optimization form of the penalties from (9) the optimization problem (11) can be written as an optimization problem with a nonlinear and possibly nonconvex objective function subject to linear constraints. In this problem, the decision variables are the pumping rates (w_j). The violations ($v_{l,\omega}$) are completely specified by these pumping rates, and can be thought of as dependent variables. Thus the problem actually involves only a moderate number of decision variables. However, there remains the necessity of having a set of violation constraints for each realization included in the problem, leading to an extremely large number of constraints. Thus due to its size, this full optimization problem could not be solved easily.

Rockafellar and Wets [1986*a*, *b*] have developed the finite generation algorithm (FGA) for solving convex linear-quadratic stochastic optimization programming problems with recourse. The FGA solves the dual problem, which has a large number of decision variables but a moderate number of constraints, by using decomposition in the dual space to obtain an approximation to the dual problem that is much smaller than the original. Each iteration of the FGA involves the solution of this small dual approximation and updating of the approximated terms.

When the objective function (of the primal) is convex, the FGA is guaranteed to converge to the global optimum. The extended FGA used in this work [*Wagner*, 1988] allows for the inclusion of nonconvex quadratic elements in the objective or constraints. The nonconvexity is included by the addition of a proximal point term to the original problem large enough to convexify the problem and allow the formulation of the dual problem. This proximal point term is also updated at every iteration. For a nonconvex problem the final solution may only be a local optimum.

In the implementation of the extended FGA used in this paper, in each iteration a convex nonlinear optimization subproblem is solved using GAMS (version 2.02)/MINOS (version 5) [*Brooke et al.*, 1988]. Solution of the largest optimization problem considered in this paper could be solved in about 1 hour on a PC clone.

Representation of the Hydraulic Conductivities

The hydraulic conductivities for each realization were obtained by using a turning bands program to generate a realization of the random hydraulic conductivity field [*Tompson et al.*, 1987]. This turning band program generates spatially correlated variables from a normal distribution with mean of 0 and standard deviation of 1. The program can produce output from a normal distribution with user-specified mean and standard deviation by linear transformation of the variables, as well as from a lognormal distribution by taking the log of the normally distributed variables.

These variables are spatially correlated in two dimensions according to the stationary exponential correlation function:

$$C(\xi) = \sigma^2 \exp\left\{ -\left[\left(\frac{\xi_1}{\lambda_1}\right)^2 + \left(\frac{\xi_2}{\lambda_2}\right)^2 \right]^{1/2} \right\} \tag{13}$$

where

$C(\xi)$ stationary anisotropic covariance for two points separated by vector ξ;
σ^2 variance of the random field;
ξ_i separation along dimension i ($i = 1, 2$);
λ_i correlation scale along dimension i.

(Note that the turning bands program actually generates hydraulic conductivities over three dimensions, and we have used one plane from this space.)

Each run of the turning bands program produces a realization of the hydraulic conductivities for each cell; realizations from separate runs are independent. Thus each realization is equally likely, so $\pi_\omega = 1/\Omega$.

One additional step is needed to use the hydraulic conductivity values in the finite difference equations. The hydraulic conductivities generated by the turning bands program are for cell centers. However, in the finite difference equations, we require the hydraulic conductivity that will give the correct flow between the centers of the two elements. To find the "average" or effective hydraulic conductivity between the two elements, we employed the common approach of using the harmonic average:

$$K_{\mathrm{eff}} = \frac{2(K_i K_j)}{K_i + K_j}. \tag{14}$$

These hydraulic conductivities are incorporated into the F matrices, as described in Appendix A. These matrices were inverted before they were incorporated in the optimization programs, using a FORTRAN program for LU decomposition [*Press et al.*, 1986].

THE VALUE OF INFORMATION IN THE DECISION-MAKING PROCESS

The value of the information about the hydraulic conductivities depends on when in the decision-making process the information is obtained and to what extent this information can affect further decisions. To examine the value of information, we will develop a number of different stochastic optimization formulations based on the framework developed above, and use their solutions to define measures of the value of information.

The best case for a decision maker is when there is no uncertainty at all, and the problem is deterministic. We examine this case by solving the deterministic problem of (1) subject to (2)–(4), with all hydraulic conductivities set to their expected value. In our case, the site is then homogeneous, since the hydraulic conductivity distributions are all assumed to have the same mean.

In the next case examined, the gradient constraints across the capture curve are treated, not as hard constraints, but as constraints which may be violated at some cost. This penalty cost for constraint violations is included in the objective function. This case is the closest to the following formulations of the stochastic problems, and is therefore used for comparison. We define EV as the value of the optimal solution to the problem with all data set to their expected values.

The next best case for the decision maker is when there is uncertainty in the data, but this uncertainty is resolved before the decision has to be made. Since we are conducting an a priori analysis, before the outcomes are known, we must consider all possible outcomes. In other words, it is as if the same decision problem were posed repeatedly, but each time with a different realization of the random variables. We therefore have to solve many deterministic optimization problems, each of which may have a different optimal solution with a different optimal value. We are interested in the distribution of the optimal value of these "wait and see" problems. In reality, for this problem, we do not have the option of "waiting" to "see" the hydraulic conductivity values before we make a decision. However, the expected value of these optimal solutions is a lower bound on the optimal value of the actual recourse problem [*Madansky*, 1960], and we may gain insight by looking at the ensemble of these optimal "wait and see" values and solutions. We define WS as the expected value of optimal solutions to the wait and see problems.

When the uncertainty cannot be resolved before the decision has to be made, we have the recourse problem (11). The solution to this problem provides the "here and now" pumping scheme, which is to be implemented immediately. We then "wait and see" what the added cost is, including the recourse cost. The optimal solution minimizes the expected total cost (pumping cost − benefit from water + recourse cost). We define RP as the value of the optimal solution to the recourse problem.

Finally, we can also calculate the value, over all realizations of the hydraulic conductivities, of implementing the pumping plan resulting from the solution of the problem with all variables set at their expected values, while including the recourse costs for each realization. We can then calculate the expected value of these values. We define EEV as the expected value of the optimal solution of the expected value problem, with recourse costs included, implemented over the ensemble of Ω realizations.

Madansky [1960] has shown that for a linear program with uncertain right-hand sides the following inequalities hold:

$$\mathrm{EV} \le \mathrm{WS} \le \mathrm{RP} \le \mathrm{EEV}. \tag{15}$$

We shall examine the actual values obtained in our example to see whether these inequalities hold for our nonlinear convex and nonlinear nonconvex sample problem.

Birge [1982*b*] has defined the value of the stochastic solution (VSS) as

$$\mathrm{VSS} = \mathrm{EEV} - \mathrm{RP} \tag{16}$$

which is the difference between the expected total costs (including recourse) for the solution from the model not explicitly considering uncertainty (the expected value model), and the model that did explicitly consider uncertainty (the full recourse model).

RESULTS

In this section, a sample problem of determining a pumping plan to contain an area of groundwater contamination is described. This problem is then solved using the above stochastic programming formulations, and the results of the different formulations are compared.

Description of the Sample Problem

The sample contaminant containment problem used in this paper (Figure 1), is a smaller version (10 × 11 cells) of a sample problem examined by *Gorelick* [1987]. Measuring from the bottom of the aquifer, the confining layer is at 100 m and the surface at 150 m. A 1% gradient is imposed by constant head boundaries of 110 m to the north and 100 m to the south. To the east and west are no-flow boundaries. The capture curve (shown in the figure) has 17 "edges," and there are 23 possible pumping wells.

The daily cost of pumping (A_1) was set to \$13.824 m^{-3} m^{-1} d^{-1}. This figure is based on 0.0032 kWh of energy to lift 1 m^3 of water a height of 1 m and \$0.05 kWh^{-1} for electricity. In all formulations, two sets of problems were run, one set including no benefit of water ($A_2 = 0$) and the other set with the benefit $A_2 = 500\ (m^3)^{-2}\ d^{-1}$.

The maximum pumping rate ($\bar{w}$) was set to 0.1 $m^3\ s^{-1}$ for all wells. This maximum rate is quite high, and was rarely an active constraint.

The mean hydraulic conductivity was taken from *Gorelick* [1987] to be 0.0004 m s^{-1}, giving a transmissivity of 0.04 m^2 s^{-1}. To generate realizations of heterogeneous hydraulic conductivities, the turning bands program requires the (geometric) mean hydraulic conductivity value of the lognormal hydraulic conductivity distribution and the standard deviation of the underlying normal distribution. A standard deviation of 1 was used. Thus 95% of the ln K values should fall between -8.82 and -6.82, corresponding to a range of K values of 0.000147 to 0.00108 m s^{-1}. For all cases, the hydraulic conductivities were assumed to be isotropic and exponentially correlated with the correlation scale equal to 10 m.

One hundred realizations of the hydraulic conductivities were generated ($\Omega = 100$). Ideally, a different set of realizations would be run for each formulation, but due to the time involved in inverting the F matrices, both the "wait and see" and the recourse formulations were run with the same 100 realizations.

For all cases, the parameter values were $p = 0.1$ and $q = 10$.

Problems with a single realization such as the expected value problem and the individual "wait and see" problems were solved directly using GAMS (version 2.02)/MINOS (version 5) [*Brooke et al.*, 1988]. The recourse problem was solved using the extended finite generation algorithm [*Wagner*, 1988].

Expected Value Problem Results

If we set all the hydraulic conductivities to their expected values (0.0004 m s^{-1}), we obtain a deterministic problem with homogeneous soil. We can model this problem two ways: (1) with the gradient restrictions as "hard" constraints, or (2) with violations of the gradient restrictions allowed but penalized in the objective function.

The nonlinear program with the gradient restrictions as "hard" constraints is

$$\min \sum_i A_1 w_i \left(s - \sum_j \bar{F}^{-1}_{i,j}\{w_j - f_j\} \right) - A_2 \left(\sum_i w_i \right)^2$$

subject to

$$\sum_j \bar{G}_{l,j}\{w_j - f_j\} \le 0 \qquad \forall\, l$$

$$0 \le w_i \le \bar{w} \qquad \forall\, i \tag{17}$$

where $\bar{F}^{-1}$ and $\bar{G}$ contain the expected values of the F^{-1} and G matrices.

The nonlinear program with the gradient restrictions as "soft" constraints is

$$\mathrm{EV} = \min \sum_i A_1 w_i \left(s - \sum_j \bar{F}^{-1}_{i,j}\{w_j - f_j\} \right) + \sum_l \rho(v_l) - A_2 \left(\sum_i w_i \right)^2$$

subject to

$$v_l = \sum_j \bar{G}_{l,j}\{w_j - f_j\} \qquad \forall\, l$$

$$0 \le w_i \le \bar{w} \qquad \forall\, i. \tag{18}$$

Table 1 presents the results for both of these models for two problems. The first problem involves no benefit of water ($A_2 = 0$) and so is convex. The second problem does involve a benefit of water ($A_2 = 500$) and is not a convex problem. As expected, the cost is lower and the optimal pumping rates are higher for the case when benefit is obtained from the water. When the gradient restrictions are treated as "soft" constraints the total cost is less, again as expected. All results show symmetry, also as expected.

The expected value problem with the penalized gradient constraints is the closest formulation to the subsequent problems, and can best be used for comparison. Thus from these runs EV = \$169.71 for the no-benefit case and EV = \$131.71 for the benefit case.

Distribution Problem Results

If we were able to repeatedly "wait and see" what the hydraulic conductivities were and subsequently solve the optimization problem, we would obtain a distribution of optimal pumping costs. In order to approximate the "wait and see" distribution we solved 100 deterministic problems (one for each realization of the hydraulic conductivities) and then analyzed the statistics of the outcomes. The "wait and see" problem is

$$\mathrm{WS}_k = \min \sum_i A_1 w_i \left(s - \sum_j F^{-1}_{i,j,k}\{w_j - f_j\} \right) + \sum_l \rho(v_{l,k}) - A_2 \left(\sum_i w_i \right)^2$$

subject to

$$v_{l,k} = \sum_j G_{l,j,k}\{w_j - f_j\} \qquad \forall\, l$$

$$0 \le w_i \le \bar{w} \qquad \forall\, i. \tag{19}$$

We then estimate the expected value of the distribution by taking the mean of these solutions:

$$\overline{\mathrm{WS}} = \sum_{k=1}^{\Omega} \pi_k \mathrm{WS}_k. \tag{20}$$

TABLE 1. Results of Expected Value Problems

Well Location*		Pumping Rates, m^3 s^{-1}			
		Hard Constraints		Penalized Gradient Restrictions	
Row	Column	No Benefit	With Benefit	No Benefit	With Benefit
3	5	0	0	0	0
	6	0	0	0	0
	7	0	0	0	0
4	4	0.063	0.078	0.063	0.070
	5	0	0	0	0
	6	0	0	0	0
	7	0	0	0	0
	8	0.063	0.078	0.063	0.070
5	3	0.072	0.072	0.071	0.071
	4	0	0	0	0
	5	0	0	0	0
	6	0	0	0	0
	7	0	0	0	0
	8	0	0	0	0
	9	0.072	0.072	0.071	0.071
6	4	0	0	0	0
	5	0	0	0	0
	6	0	0	0	0
	7	0	0	0	0
	8	0	0	0	0
7	5	0	0	0	0
	6	0	0	0	0
	7	0	0	0	0
Total		0.270	0.300	0.268	0.282

	Costs, dollars			
	Hard Constraints		Penalized Gradient Restrictions	
	No Benefit	With Benefit	No Benefit	With Benefit
Pumping	179.09	179.39	160.43	168.68
Benefit	0.00	−45.00	0.00	−39.76
Penalty	0.00	0.00	9.28	2.79
Total	179.09	134.39	169.71	131.71

*Well location refers to Figure 1.

The first set of runs was intended to examine the convex problem, where no benefit is derived from the water that is pumped from the site. One hundred scenarios were run, producing a minimum cost ranging from \$46.90 to \$437.53, with an average of \$171.54. A histogram of the results is shown in Figure 3. About 83% of the total costs were between \$150 and \$250. The penalty cost ranged from \$2.73 to \$302.85. These penalty costs represent between 6% and 70% of the total cost with an average of 44% over all 100 outcomes. The optimal number of wells used for these scenarios ranged from a minimum of two to a maximum of five wells, with 93% of the outcomes using two, three, or four wells. The 11 interior wells were never used. Of the remaining 12 wells, the wells at the beginning and the end of the fifth row were used 79% and 77% of the time, respectively.

In the second set of runs we included benefit obtained from the water pumped from the site ($A_2 = 500$). Minimum total cost ranged from −\$6914.45 to \$409.25. (Only two outcomes had negative costs, indicating that enough benefit could be obtained from the pumped water so as to make a profit. For these two cases, the optimal pumping plan included some of the wells' being pumped at their maximum rates, leading to unrealistic head gradients. Thus these two pumping plans are neglected in the subsequent calculations.) About 78% of the outcomes had minimum total cost of between \$100 and \$200. The average minimum total cost of

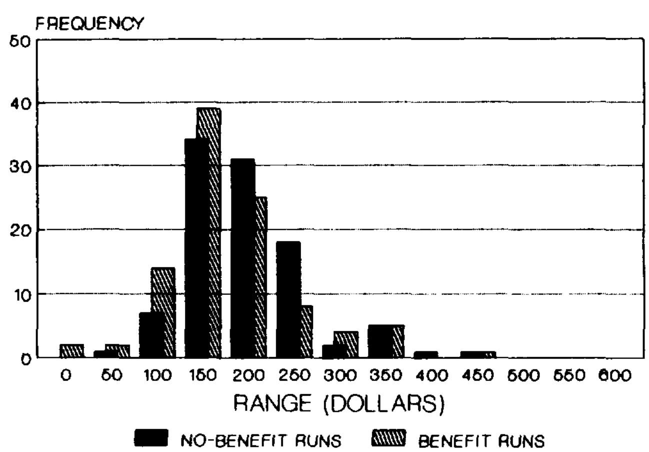

Fig. 3. Cost distribution of "wait and see" problem.

the plans with positive cost was \$152.55. This average cost is less than the no-benefit case (\$171.54) since the revenues from the water pumped out can be used to reduce the total cost of operation. The percent of total cost of operation that is due to the penalty cost had a range of between 0% and 73% with an average of 34%. The number of wells used ranged from a minimum of two to a maximum of 12, with 92% of the outcomes using two, three, or four wells. As in the runs with no benefit from the water, the 11 interior wells were never used. Again the wells at the beginning and the end of the fifth row were the most widely used, 72% and 65% respectively.

From these runs, WS = \$171.54 for the no-benefit case and WS = \$152.55 for the benefit case.

Recourse Problem Results

The recourse problem includes a number of realizations of the hydraulic conductivities. The solution to the recourse problem provides the pumping plan that minimizes the expected total cost (including recourse cost) over these realizations. For these problems, 100 sets of hydraulic conductivity realizations were used. This problem (developed previously) can be stated as

$$\text{RP} = \min \sum_{\omega} \pi_{\omega} \left[\sum_{i} A_1 w_i \left(s - \sum_{j} F^{-1}_{i,j,\omega}\{w_j - f_j\} \right) + \sum_{l} p(v_{l,\omega}) \right] - A_2 \left(\sum_{i} w_i \right)^2$$

subject to

$$v_{l,\omega} = \sum_{j} G_{l,j,\omega}\{w_j - f_j\} \qquad \forall\, l\, \forall\, \omega$$

$$0 \le w_i \le \bar{w} \qquad \forall\, i \tag{21}$$

Table 2 presents the recourse problem solutions. Again, two cases were run, one with and one without benefit of water. The expected total cost for the case with no benefit of water was \$217.51, which included 51% for expected recourse costs. The total costs over the 100 outcomes ranged from \$108.34 to \$508.33. A histogram of the results is shown in Figure 4. The total pumping in this case was 0.181 $m^3\ s^{-1}$. The expected total cost for the case including benefit of water was \$196.96, which included 48% for expected recourse costs. The total costs over the 100 outcomes ranged from \$103.07 to \$436.18. The total pumping in this case was 0.216 $m^3\ s^{-1}$.

In both of these solutions only four or five wells, out of a possible 23, are to be used. These wells are on the "edges" of the pumping area. We also note that the pumping pattern is no longer symmetrical. Over one realization with heterogeneous soil we would, in fact, not necessarily expect the pumping plan to be symmetrical; however over enough realizations we might expect the plan would be symmetrical. Thus this asymmetry may indicate that more than 100 realizations should be used in the model. *Gorelick* [1987] also obtained asymmetric optimal pumping plans.

From these runs, RP = \$217.51 for the no-benefit case and RP = \$196.96 for the benefit case.

The problem for the case without benefit of water is convex, so the finite generation algorithm will converge [*Rockafellar and Wets*, 1986*a*, *b*] and it will converge to the global minimum. For the nonconvex case (with benefit of water) we have no such assurances. To test the convergence of the solution and the robustness of this solution, the optimal solution obtained from the recourse problem was perturbed by first adding and then subtracting a small value to each possible pumping well in turn. The expected costs of these perturbed solutions were then computed. For very small perturbations (±0.001) some perturbed solutions did

TABLE 2. Results of Recourse Problems

Well Location*		Pumping Rates, $m^3\ s^{-1}$	
Row	Column	No Benefit	With Benefit
3	5	0	0
	6	0	0
	7	0	0
4	4	0.045	0.072
	5	0	0
	6	0	0
	7	0	0
	8	0.058	0.086
5	3	0.045	0.036
	4	0	0
	5	0	0
	6	0	0
	7	0	0
	8	0	0
	9	0.033	0.022
6	4	0	0
	5	0	0
	6	0	0
	7	0	0
	8	0	0
7	5	0	0
	6	0.006	0
	7	0	0
Total		0.187	0.216
		Costs, dollars	
		No Benefit	With Benefit
Pumping		107.28	124.99
Benefit		0.00	−23.33
Penalty		110.23	95.30
Total		217.51	196.96

*Well location refers to Figure 1.

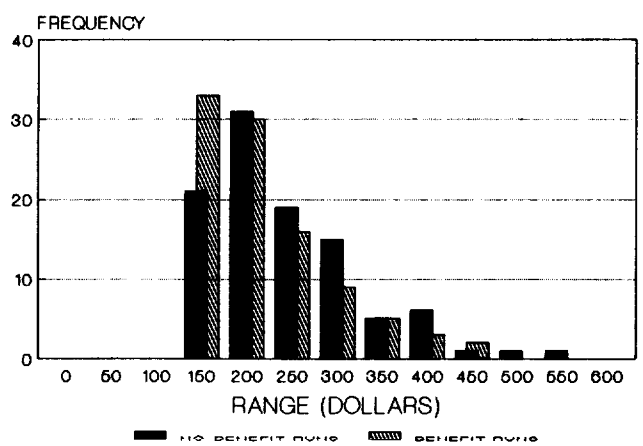

Fig. 4. Cost distribution of recourse problem.

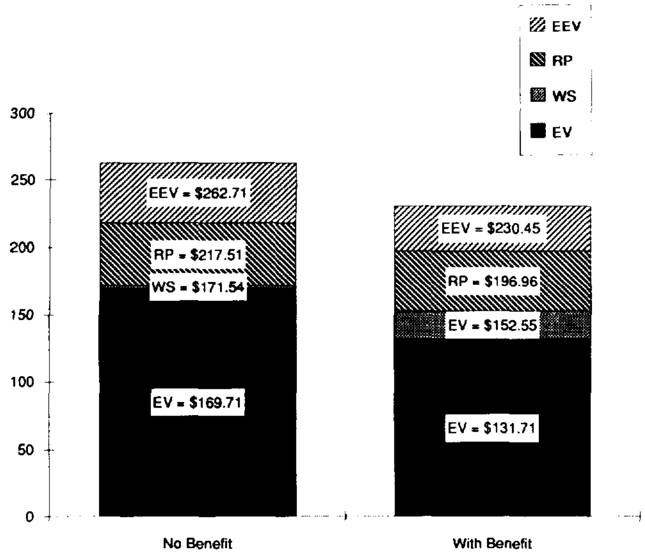

Fig. 5. Comparison of total costs.

have slightly lower expected costs than the reported "optimal" solution, indicating that the algorithm had not quite converged. However, perturbing the solutions by (±0.05) did result in all expected costs from the perturbed solutions being higher than the unperturbed solution, indicating that the reported solution is indeed quite close to an actual (at least) local minima.

Expected Value of Using the Expected Value Solution in the Recourse Problem Results

Finally, we can find the expected value of using the expected value solution in the full recourse problem (EEV). For this example we find that the EEV for the no-benefit case has an expected cost (including recourse) of $262.71, with 40% of this cost due to recourse costs. For the case including benefit, EEV is $230.45, with 46% due to recourse costs.

We also see that the form of the solutions is somewhat different when uncertainty is explicitly included. The recourse solutions call for less pumping than the expected value solutions. In a sense, the solutions from the recourse formulations can be thought of as reserving some of the budget available "here and now" to pay the "wait and see" recourse costs.

In summary, for the no benefit of water case,

$$(EV = \$169.71) \le (WS = \$171.54) \le (RP = \$217.51) \le (EEV = \$262.71) \quad (22)$$

and for the case when benefit of water is included,

$$(EV = \$131.71) \le (WS = \$152.55) \le (RP = \$196.96) \le (EEV = \$230.45). \quad (23)$$

These values are represented graphically in Figure 5. We see that Madansky's inequalities do hold for these nonlinear problems. The value of the stochastic solution (EEV − RP) is $45.20 for the no benefit case and $33.49 for the benefit case. Thus, ignoring the uncertainty in the model formulations (by using the EV solutions and then paying recourse) increases the expected costs by 21% in the no-benefit case and 17% in the benefit case. Aquifer remediation programs are often extremely expensive; thus savings in the range of 20% could be quite significant.

It is also interesting to compare the expected costs of the recourse solution with the expected "wait and see" cost. The "wait and see" expected cost is 21% less than the expected recourse cost for the no-benefit case and 23% less in the benefit case. Thus we estimate that we are paying a penalty of about 20% due to the fact that we must determine a pumping plan without knowing the heterogeneous hydraulic conductivities.

We also tried using the average of the "wait and see" solutions as a pumping plan in the recourse problem. This averaged plan is given in Table 3. The expected cost was $296.28 in the no-benefit case and $220.86 in the benefit case. These solutions represent a 36% and 12% increase over the cost of the optimal solution to the recourse problem. One problem with simply averaging these solutions is that the three to five wells that were used in each solution were often different wells, so that this averaged plan involves many wells pumping at low levels, a plan which is unlikely to be optimal.

TABLE 3. Averaged "Wait and See" Results

Well Location*		Pumping Rates, $m^3\ s^{-1}$	
Row	Column	No Benefit	With Benefit
3	5	0.009	0.009
	6	0	0.004
	7	0.019	0.028
4	4	0.077	0.058
	5	0	0
	6	0	0
	7	0	0
	8	0.082	0.057
5	3	0.056	0.055
	4	0	0
	5	0	0
	6	0	0
	7	0	0
	8	0	0
	9	0.059	0.044
6	4	0.009	0.004
	5	0	0
	6	0	0
	7	0	0
	8	0.010	0.006
7	5	0.006	0.008
	6	0.008	0.005
	7	0.008	0.010
Total		0.343	0.288

	Costs, dollars	
	No Benefit	With Benefit
Average "WS" Costs	171.54	152.55†
Pumping	201.04	167.17
Benefit	0.00	−41.47
Penalty	95.25	95.16
Total of pumping, benefit and penalty	296.29	220.86

*Well location refers to Figure 1.
†Does not include two realizations with negative costs.

CONCLUSIONS

Uncertainty in aquifer parameters affects the management of groundwater quality. Solutions from models that explicitly incorporate uncertainty are different from those that only use the expected values of uncertain parameters, and models that incorporate uncertainty can lead to savings, at least in the expected value sense.

Stochastic optimization can be used to explicitly incorporate uncertainty in management models. These techniques, although sophisticated, can be used without extensive computer resources. Small problems can be solved using PCs; larger problems could be solved on workstations.

The simple recourse formulation is useful for incorporating uncertainty and can, we believe, be used to model fairly realistic situations. The extended finite generation algorithm is available to solve nonlinear and nonconvex problems (with possibly only locally optimal solutions). This model allows considerable flexibility to the decision maker in the representation of and managerial response to uncertainty.

There are a number of possibilities for extensions of this work. Larger and more realistic containment problems could be solved using this technique. Presently the most time-consuming step, and the step requiring the most computer resources, is the inverting of the **F** matrices. The current inversions were done using a fairly time-efficient algorithm, but no attempt was made to save space by exploiting the special banded structure of the F matrix. More sophisticated matrix storage and inversion routines would allow faster preprocessing of the data to the extended finite generation algorithm and so would allow considerably larger problems to be solved. In the actual optimization step, the size of the problem is determined only by the number of possible pumping wells, not by the number of finite elements considered, so the size of the area studied need not be of great concern.

Chance constraints could also be included in the finite generation algorithm, with no additional work, by including the deterministic equivalents as "hard" constraints in the recourse model. This approach was used with the finite generation algorithm for convex problems by *Eiger and Shamir* [1991] for a problem of managing reservoir operations. Additionally, measurements of hydraulic conductivities taken at the site can be incorporated into this procedure, and thus reduce the uncertainty in these values. Using a method developed by *Wagner and Gorelick* [1989] the realizations of the hydraulic conductivities generated for use in the optimization problem could be made conditional upon available measurements.

The solution methods could also be extended in a number of ways. Some preliminary work has been done in including concentration variables so as to directly manage the water quality [*Wagner*, 1988]. It would also be interesting to see if the model could be extended to a dynamic case, in order to examine the transient behavior of gradients and contaminants under possible containment and remediation plans.

APPENDIX A

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

$$\frac{\partial}{\partial x}\left(K_x b \frac{\partial h}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y b \frac{\partial h}{\partial y}\right) \pm \delta = 0 \qquad \text{(A1)}$$

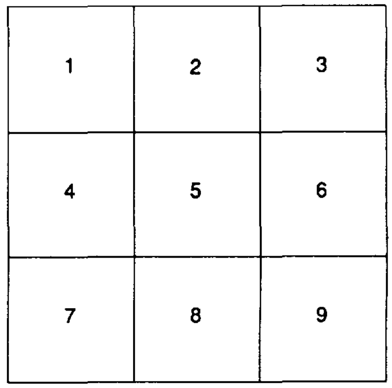

Fig. A1. Nine-element system.

where

- x, y length, width, m;
- K_i hydraulic conductivity in the direction i, m s^{-1};
- b aquifer thickness, m;
- h head, m;
- δ point input/output of water, m s^{-1}.

We discretize this equation to obtain the following finite difference equation:

$$-K_x \frac{(h_{n,m} - h_{n-1,m})}{\Delta x} b\Delta y - K_x \frac{(h_{n,m} - h_{n+1,m})}{\Delta x} b\Delta y - K_y \frac{(h_{n,m} - h_{n,m-1})}{\Delta y} b\Delta x - K_y \frac{(h_{n,m} - h_{n,m+1})}{\Delta y} b\Delta x = w_{n,m}. \qquad \text{(A2)}$$

where Δx, Δy are the length and width of the element (meters), and $w_{n,m} = \delta\Delta x\Delta y$.

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.

This model is applied to the site shown in Figure 1, which has fixed head boundaries to the north and south, and impervious boundaries to the east and west. The fixed heads are applied at the boundary of the site (thus at the boundary of the cells), so the corresponding denominator in the flow terms is $\Delta y/2$, not Δy.

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

$$F\mathbf{h} = \mathbf{w} - \mathbf{f} \qquad \text{(A3)}$$

where

- F $I \times I$ matrix of the head coefficients;
- $\mathbf{h}$ I vector of head variables;
- $\mathbf{w}$ N vector of pumping variables;
- $\mathbf{f}$ I vector of constants (from the boundary conditions).

Since nonzero coefficients appear only on terms linking neighboring elements, the matrix F has special banded structure. For example, numbering the finite elements as in Figure A1, matrix F has the following structure:

$$F = \begin{pmatrix} \cdot & \cdot & 0 & \cdot & 0 & 0 & 0 & 0 & 0 \\ \cdot & \cdot & \cdot & 0 & \cdot & 0 & 0 & 0 & 0 \\ 0 & \cdot & \cdot & \cdot & 0 & \cdot & 0 & 0 & 0 \\ \cdot & 0 & \cdot & \cdot & \cdot & 0 & \cdot & 0 & 0 \\ 0 & \cdot & 0 & \cdot & \cdot & \cdot & 0 & \cdot & 0 \\ 0 & 0 & \cdot & 0 & \cdot & \cdot & \cdot & 0 & \cdot \\ 0 & 0 & 0 & \cdot & 0 & \cdot & \cdot & \cdot & 0 \\ 0 & 0 & 0 & 0 & \cdot & 0 & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & 0 & 0 & \cdot & 0 & \cdot & \cdot \end{pmatrix} \quad \text{(A4)}$$

where the boldface dots represent nonzero elements.

APPENDIX B

Statement. The matrix $-F_\omega$ is positive definite.

Proof. We start with the following example (Figure A2). Let $\Delta x = \Delta y = b = 1$. The matrix F for this system is

$$F = \begin{bmatrix} -K_{n,m} - 4K_n & K_{n,m} \\ K_{n,m} & -K_{n,m} - 4K_m \end{bmatrix}. \quad \text{(B1)}$$

The value of $-\mathbf{w}'F\mathbf{w}$ is then

$$-\mathbf{w}'F\mathbf{w} = (K_{n,m} + 4K_n)w_n^2 - 2K_{n,m}w_nw_m + (K_{n,m} + 4K_m)w_m^2. \quad \text{(B2)}$$

Rearranging,

$$-\mathbf{w}'F\mathbf{w} = K_{n,m}(w_n - w_m)^2 + 4K_nw_n^2 + 4K_m^2w_m^2 > 0 \quad \text{(B3)}$$

unless $w_n = w_m = 0$. So $-\mathbf{w}'F\mathbf{w} > 0$ for all $\mathbf{w}$, and $-F$ is positive definite for this example.

In general for an $N \times N$ system with heterogeneous soil, for each realization ω we generate a distinct value of K for each pair of adjacent nodes. We show that the sum $-\mathbf{w}'F_\omega\mathbf{w}$ can be broken up into a sum of positive terms, each involving only one of the distinct K values.

For any two nodes n and m, we have $K_{n,m}$, which appears in F_ω only at positions (n, n), (m, m), (n, m) and (m, n). Premultiplying and postmultiplying $-F_\omega$ by $\mathbf{w}$, the only terms involving $K_{n,m}$ will be

$$c[K_{n,m}w_n^2 - 2K_{n,m}w_nw_m + K_{n,m}w_m^2] = c[K_{n,m}(w_n - w_m)^2] \geq 0 \qquad \forall\, w_n \text{ and } w_m \quad \text{(B4)}$$

where c is the positive constant $b(\Delta x/\Delta y)$ for north-south flow and $b(\Delta y/\Delta x)$ 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 K_n values for these terms do not appear in F_ω.

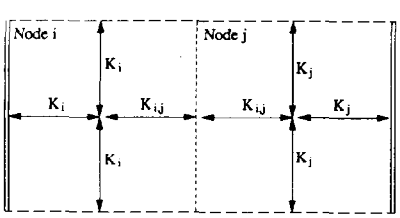

Fig. A2. Two-element system.

For nodes n along the constant head boundaries, K_n will appear only in one term, with value $2cK_nw_n^2 > 0$ for $w_n \neq 0$. (In the example the values were $4cK_nw_n^2$ because these nodes were along two constant head boundaries.)

Thus all conductivity values, whether on the boundaries or not, can be grouped into nonnegative terms, with some terms strictly positive. Thus $-\mathbf{w}'F_\omega\mathbf{w} > 0$ for all $\mathbf{w} \neq 0$, and $-F^\omega$ is positive definite.

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