FINAL REPORT
U.S. Department of Energy
**LEAST-COST GROUNDWATER
REMEDATION USING UNCERTAIN
HYDROGEOLOGICAL
INFORMATION**

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1 Executive Summary

The design of groundwater remediation pump-and-treat well networks under aquifer parameter measurement uncertainty can be addressed using an optimal-design strategy based upon the concept of robust optimization. The robust-optimization approach allows for the admission of design alternatives that do not satisfy all design constraints. However in the selection process the algorithm penalizes such selections based upon the number of constraints violated. The result is a design which balances the importance of reliability with overall project cost.

The robust-optimization method has been applied to the problem of groundwater-plume containment and risk-based groundwater remediation design. Designs dedicated to groundwater-plume containment assure that the contaminant plume will not extend beyond a prespecified perimeter. Inwardly directed groundwater velocity must be achieved along this perimeter. The outer-approximation optimization technique in combination with a groundwater flow model (PTC) is used to solve this optimal-design problem.

The risk-based groundwater-remediation design approach seeks to achieve prespecified water-quality goals at specified locations at specified times using, in this case, pump-and-treat technology. The modified tunneling optimization method in combination with a groundwater flow and transport model (PTC) is used to solve this optimal-design problem.

In a third design approach both the plume containment and the risk-based approaches are combined into one remediation strategy. The combined approach has also been addressed.

2 Research Objectives

The goal of the proposed research was to formally accommodate parameter uncertainty in the design and decision-making process associated with groundwater remediation. The individual objectives were:

1. develop the mathematical representation of a groundwater remediation optimization algorithm that includes uncertainty in hydraulic conductivity using the robust optimization approach;
2. prepare a FORTRAN computer program that will solve the equations obtained from objective 1;
3. test and verify the resulting FORTRAN program to assure that the formulation provided in 1 is being solved correctly;
4. employ the resulting software to a hypothetical problem;
5. evaluate the effectiveness of the resulting algorithm on solving the hypothetical problem.

3 Methods and Results

3.1 The Methodology

Many optimization models approach the problem of incorporating uncertainty into the model by using stochastic methods (Wagner [13],[14], Watkins [15],[16]). When this is done, all possible uncertain values are assumed to have equal probability of occurrence. This method often results in over-designed systems.

We applied a different optimization technique to incorporate uncertainty in our model. The method used in this work is called robust optimization (Mulvey [11]). Robust optimization is a multi-scenario approach to handling uncertainty in the optimization design. In this approach, each of the scenarios represents a possible realization of the uncertain parameter. In the groundwater remediation problem, we examine the uncertainty in the hydraulic conductivity. Each scenario represents one possible hydraulic conductivity field.

Once the possible realizations have been determined, they are used to obtain an optimal remediation design. There are a number of different interpretations of the robust optimization technique. In our setup, the objective function consists of two nested minimization problems. First we assume that each of the chosen scenarios represents the true hydraulic-conductivity field. Assuming that scenario x is the true scenario, we hold that the constraint values for scenario x must be satisfied, while violations of the constraints for all other scenarios will result in the amplification of the objective function. This amplification is represented in the objective function as a penalty cost associated with the violation of the constraint. The penalty cost in the robust optimization problem has three components. The first is the constraint violation. The second is the total

weight, which can be thought of as a risk aversion term. The third component is the weight associated with the frequency of occurrence of the scenario. For example, if the scenario has a low probability of occurrence, then in the event that the constraint is violated for that particular scenario, the penalty cost will be low due to the low probability of occurrence. This third component of the penalty term prevents the optimal design from being biased towards improbable scenarios. Assuming that each of the scenarios is the true scenario, the optimal solution is determined. This final solution is then the minimum over all of the solutions determined for each randomly selected scenario.

In earlier formulations using the robust-optimization formulation to address the contaminated-groundwater containment problem, the values of the hydraulic conductivity fields were chosen randomly from a given probability density function (pdf) (Watkins[15],[16], Karatzas[8]). The scenario weight must be carefully considered when random sampling is done. If equal weights are assigned to each scenario, the advantages of the robust optimization are not maximized.

We have addressed the problems associated with scenario weighting via a new method of sampling that ensures that each of the scenarios has equal weight. This method is derived from the Latin hypercube method of sampling. In this approach, the probability-density function that describes the uncertainty in hydraulic conductivity is separated into equal areas. In the Latin hypercube method of sampling a sample is selected randomly from each of the separate areas (Figure 1).

Figure 1: Illustration of concept of equal-area sampling using a log-normal distribution of the hydraulic-conductivity field.

When equal-area sampling is used to determine the samples that are used to represent the uncertainty in the hydraulic conductivity, each of the scenarios analyzed in the robust optimization problem has an equal probability of occurrence. This simplifies the robust optimization problem because the weight associated with each scenario is equal. For simplicity, we set this weight to be equal to one over the total number of scenarios analyzed.

Equal area sampling also allows the modeler to observe convergence of the optimal solution to a reliable solution. This is done by observing the change in the optimal solution as the number of scenarios examined in the robust optimization problem increases. When the change in the optimal solution is small, a reliable representative optimization solution is achieved. It is observed that as the number of scenarios increases, the value of the optimal solution to the gradient constraint problem increases monotonically.

Historically a lognormal distribution curve has been used to describe the uncertainty in the hydraulic conductivity (Law [10], Csallany and Walton [3], Freeze and Cherry [5]). When examining a histogram of hydraulic conductivity data, the lognormal distribution does conform to the data. Hydraulic conductivity is never negative and the lognormal distribution has positive probability values only for positive values, so the lognormal distribution is a reasonable distribution for describing the uncertainty in the hydraulic conductivity.

Because the lognormal distribution has positive probabilities for all positive values of hydraulic conductivity, one may truncate the lognormal distribution function to attain a limited range of positive hydraulic conductivity values, and hence achieve convergence of the optimal remediation design with an increase in the number of scenarios examined. When the distribution is truncated at 95% and 65% two different optimal solutions are converged upon (Figure 2). When the distribution is truncated at 95% the value of the optimal solution is greater than when the distribution is truncated at 65%. This implies that the optimal solution converged upon is highly dependent upon the amount of truncation of the lognormal distribution. Because the amount of truncation is subjective, we examined an alternative to truncation of the lognormal distribution function by examining a pdf that can have a form similar to the lognormal distribution, but has positive probabilities for a limited range of values.

The beta distribution function has many different forms, the J form, the U form and the normal form, which can take a shape very similar to the appearance of a lognormal distribution (see Figure 2). The common attractive characteristic of all of these forms, however, is that positive probability values only occur for a limited range of hydraulic conductivity values. The modeler must specify what range of values the beta distribution will cover, and techniques can be used to fit a beta distribution to hydraulic conductivity data.

The ability of the beta distribution to accurately represent hydraulic-conductivity values observed in the field was tested. Data from the Dakota Sandstone was successfully fit with the beta distribution (see Figure 4).

Using a beta distribution to describe the uncertainty in the hydraulic conductivity, it is possible to observe convergence of the optimal remediation design

Figure 2: Cost estimates obtained using the entire lognormal distribution, the distribution truncated at 95% and the distribution truncated at 65%.

Figure 3: An illustration of the ability of the Beta distribution to fit a lognormal distribution.

Dakota Sandstone Data

Raw Data

RMS: Logn = 0.1839
Beta = 0.0531

Transformed Data

RMS: Normal = 0.0658
Beta = 0.0579

Figure 4: A comparison of the beta and lognormal distribution fits to the Dakota Sandstone data. RMS stands for root-mean-square fit error between the histogram and the continuous distribution.

with an increase in the number of scenarios examined in the robust optimization problem. Because the data determines the range of values covered by the beta distribution, this optimal solution is not dependent upon the discretion of the modeler. This solution is totally objective.

It is observed that the optimal remediation design is converged upon using equal area sampling on the beta distribution in approximately 30 scenarios. If random sampling (not Latin-hypercube sampling) is used, one cannot know how many scenarios must be examined to attain a reliable optimal solution. The value of the optimal solution will sporadically increase as the number of scenarios examined increases. Convergence to an optimal solution cannot be assured when random sampling of a pdf is performed, and so a large number of scenarios must be employed to ensure that a reliable optimal solution has been attained using robust optimization. For this reason we prefer to use equal area sampling.

Included in the present work is an analysis of the spatial variability of the hydraulic conductivity in the model. Superimposed on each of the scenarios are 30 randomly correlated spatial variability matrices. The number of scenarios necessary to achieve a convergent solution was analyzed to be x . The spatial variability matrices were then superimposed, and the robust optimization problem was solved for x times 15 scenarios. The optimal solution does not vary significantly from the solution attained without the spatial variability. The value of the new optimal solution is slightly higher, but this is expected because the spatial variable term will increase the hydraulic conductivity in some loca-

tions, thereby increasing the contributions to the penalty term and the required pumping. Convergence occurs when the same number of scenarios is examined in the non-spatially variable case. This suggests that the convergence exercise should be completed using the simple case that examines the design uncertainty only. Once a solution is converged upon, the spatial variability should then be superimposed upon the scenarios required for convergence so that a more realistic model can be used in the final remediation design.

3.2 The Mathematics

The general form of an optimization problem consists of a set of equations that must be solved simultaneously. For each system, there is an objective that must be met. Further, there are constraints placed upon the system. Let us first formulate the optimization problem that will result in a least cost pump-and-treat groundwater remediation design that is not subject to uncertainty in the hydraulic conductivity. This design will have constraints such that the hydraulic gradients will contain a contaminated plume. The formulation of this problem is as follows:

$$\text{Objective : } \min \sum_i k_i q_i \quad (1)$$

$$\text{Subject to : } g - \sum_i (h_i^1 - h_i^2) \leq 0$$

$$0 \leq q_i \leq \max(q)$$

where

$k_i \equiv$ cost per unit pumping at well i

$q_i \equiv$ pumping rate at well i

$g \equiv$ required gradient necessary for containment

$h_i^1 - h_i^2 \equiv$ the gradient due to pumping at well i

$\max(q) \equiv$ maximum allowable pumping.

As noted in § 3.1, robust optimization is a method of optimization that incorporates the uncertainty of the hydraulic conductivity into the pump-and-treat optimization problem. It does this by examining multiple realizations of the hydraulic conductivity simultaneously. In our interpretation of robust optimization, two nested minimizations must be completed. The first minimization requires determining a least-cost remediation design assuming that one of the realizations is the true hydraulic conductivity field. All other realizations in this minimization problem represent the uncertainty in the hydraulic conductivity. For each of the true realizations, the gradient constraints must be satisfied. Violations of the constraints for the non-true realizations may occur, however, when a violation for one of these realizations does occur, a penalty cost is added to the cost of pumping. Once a least cost remediation design is determined for each realization representing the true realization, the designs with the minimum

cost is said to be the solution to the robust optimization problem. The robust-optimization formulation for the gradient-constrained groundwater remediation problem is as follows:

$$\begin{aligned}
\text{Objective} & : \min_{S^* \in \Omega} \left\{ \min_{q_i} \sum_i k_i q_i + \omega \frac{1}{|N|} \sum_{S \in \Omega, S \neq S^*} \max(0, \xi_S) \right\} \\
\text{subject to} & : g - \sum_i (h_i^1 - h_i^2) \leq 0 \text{ for } S^* \\
& 0 \leq q_i \leq \max(q) \forall S \text{ and } S^*
\end{aligned} \tag{2}$$

where

$\Omega \equiv$ the set of all possible scenarios

$S^* \equiv$ the true scenario.

$S \equiv$ the scenarios that are not considered to be the true scenario.

$\omega \equiv$ total weight for the penalty term.

$N \equiv$ the total number of scenarios.

$\frac{1}{|N|} \equiv$ individual weight of each scenario.

$\xi_S \equiv$ the constraint violation for the scenario ($S \neq S^*$)

The values of the hydraulic conductivity for each scenario are determined by using equal area sampling of the probability density function that represents the uncertainty in the hydraulic conductivity as described in § 3.1. Consider first the equation that describes the lognormal distribution function (Gelhar[6]):

$$P(x) = \frac{1}{\sigma x \sqrt{2\pi}} \exp \left(\frac{-(\ln(x) - \mu)^2}{2\sigma^2} \right)$$

where

$\mu \equiv$ mean of $\ln(x)$

$\sigma \equiv$ standard deviation of $\ln(x)$.

The equal-area sample values, x_i , for a lognormal distribution curve can be determined by solving the following equation for x_i :

$$\frac{i}{n+1} = \int_0^{x_i} P(x) dx$$

where

$P(x) \equiv$ the lognormal distribution function.

$n \equiv$ the total number of equal-area samples desired.

$x_i \equiv$ the i^{th} sample.

The solutions for the equal area samples for the lognormal distribution function are given by:

$$x_i = \exp \left(\sqrt{2}\sigma \text{ inver } f \left(\frac{2i}{n} - 1 \right) + \mu \right)$$

If the truncated lognormal distribution is used the equal area sample values are expressed as follows:

$$x_i = \exp \left(\sqrt{2}\sigma \text{ inver } f \left(\frac{2i\tau}{n} - 1 \right) + \mu \right)$$

where

$\tau \equiv$ the amount of truncation expressed as a decimal.

The functional form of the beta distribution is:

$$P(y) = \frac{1}{\beta(p, q)} \frac{(y-a)^{p-1}(b-y)^{q-1}}{(b-a)^{p+q-1}}$$

The function $\beta(p, q)$ is the beta function. The values a and b define the lower and upper bounds of the range of possible hydraulic conductivities, and p and q are parameters that describe the shape of the beta function. (Johnson [7]).

In this analysis the beta distribution that best approximates the lognormal distribution function is used. The values of the four parameters were determined that best represented the lognormal distribution. First the range of hydraulic conductivity values is set between zero and one, so $a = 0$ and $b = 1$. Based upon the shape of the lognormal distribution curve, this is not a bad approximation for this problem. In a non-theoretical problem, the true data would determine the range of values chosen. As mentioned earlier, this was indeed considered.

Second, the highest frequency in the lognormal distribution and the beta distribution are required to occur at the same hydraulic conductivity value. This ensures that the beta distribution has a shape similar to a lognormal distribution. The final parameter is determined by conducting a linear search such that the difference between the theoretical lognormal distribution curve and the beta distribution curve is minimized.

The beta distribution function is not integrable, so an analytic expression for the equal area points cannot be derived for this distribution. The area under the curve from 0 to a given hydraulic conductivity value is determined by examining the incomplete beta function:

$$I_{y_i}(p, q) = \frac{1}{\beta(p, q)} \int_0^{y_i} \frac{(y-a)^{p-1}(b-y)^{q-1}}{(b-a)^{p+q-1}} dy$$

The incomplete beta function has a series expansion and so the value of y_i can be numerically determined by evaluating a continued fraction routine using a modified version of Lentz's method (Press [12]). Using these numerical approximations it is possible to conduct a linear search for each of the equal area samples.

Once the equal-area sample values have been determined, the scenarios are defined assuming perfectly homogeneous, but uncertain aquifer properties, each

with the different sample values determined. Spatial variability (mentioned in § 3.1) is introduced into the problem by superimposing 15 spatially correlated randomly distributed fields upon each of the scenario values. These fields were generated using the subroutine SGSIM that is part of the GSLIB package developed by the Stanford Center for Reservoir Forecasting (Deutsch [4]). The extension of the approach to correlated random hydraulic conductivity fields is theoretically possible, but the required computational effort is such that it was not considered within the scope of this project.

Hydraulic head response is linear with respect to pumping. For this reason the gradient constraints are also linear. In the example problem considered in this work, the pumping wells used for containment are located in the interior of the desired capture zone. Each of the gradient-constraint surfaces is influenced in a similar manner by pumping at either of the wells because they are in the interior of the capture zone. The contributions of the penalty term to the objective function for this robust optimization problem are such that the global solution to this optimization problem occurs on the boundary of the feasible region. For this reason it is possible to use the method of outer approximation to solve this optimization problem (Karatzas [9]).

The objective function cannot be expressed analytically as a function of pumping rates from each of the wells. Rather, for each combination of pumping, the objective function is determined numerically by solving the finite-element groundwater flow model known as the Princeton Transport Code (PTC)(Babu [1]). The groundwater flow equation is as follows:

$$\nabla \cdot \mathbf{K} \cdot \nabla h(\mathbf{x}, t) - S \frac{\partial h(\mathbf{x}, t)}{\partial t} - Q_i = 0 \quad (3)$$

where

$S \equiv$ specific storage coefficient.

$h \equiv$ hydraulic head.

$\mathbf{K} \equiv$ the hydraulic conductivity of the aquifer.

$Q_i \equiv$ source/sink flow from well i

3.3 Sample Problem for the Gradient-constrained Case

For this investigation a groundwater flow model consisting of a 30 nodes by 30 nodes equally spaced mesh is employed. The finite-element model represents an area that is 870 meters by 870 meters (see Figure 5). The boundary conditions on this model are such that there is no groundwater flow out of the northern and southern boundaries of this model and there are constant head conditions of 25 and 5 meters on the western and eastern boundaries respectively. These conditions create an ambient uniform hydraulic gradient across the model. This is a single layer model with a uniform thickness of 30 meters. The two possible well locations are noted by the asterisks on Figure 5. These locations are interior to the desired capture zone. The capture zone is realized by placing gradient constraints on pairs of nodes located along the line defining the maximum extent

of the desired capture zone. The gradient constraints are such that the flow of groundwater must be towards the wells after three years of pumping.

Figure 5: Definition sketch for the example containment model. The well locations are represented by the asterisks. The aquifer thickness is defined as $b=30\text{m}$.

The hydraulic conductivity is determined for each scenario by either sampling a representative lognormal distribution, a truncated lognormal distribution function, or a beta-distribution function. The lognormal distribution function used in this study is generated by setting the mean, μ , equal to 0.01 meters per hour and a standard deviation of the related normal distribution, σ , equal to 1.0 meters per hour.

As was the case earlier, the lognormal distribution function is truncated at the 95th percentile and at the 65th percentile (see Figure 1). Analyses are also conducted on these truncated distributions.

The beta distribution that best fits the representative lognormal distribution is one where the beta distribution parameters are given by $a=0$, $b=1$, $p=1.299$ and $q=81.037$.

The spatial distribution matrices that are used in this model are generated, as noted earlier, using the SGSIM subroutine of the GSLIB package. The matrices have a correlation length of 120 meters, which equates with a correlation

over a maximum of four nodes in the model. The lognormal distribution for the spatial distribution is one tenth of the distribution used for the design uncertainty.

3.4 Extension to the Concentration-constrained Case

In the preceding, we considered the case of a gradient-constrained problem. While the concentration, or risk-based constrained problem is conceptually a natural extension of the gradient-constrained problem, from an operations-research perspective it is very different. The mathematical statement of the risk-based constrained problems is

$$\begin{aligned}
& \min \sum_i c_i q_i + \omega \frac{1}{|N|} \sum_{S \in \Omega} \max(0, \xi_S) \\
\text{subject to} \quad & g - \sum_i (h_i^1 - h_i^2) \leq 0 \\
& \bar{c} - c_j \leq 0 \\
& 0 \leq q_i \leq \max q \quad \forall S
\end{aligned} \tag{4}$$

where the variables are as defined in equation 2 but for c_j , which is the concentration and $\bar{c}$ which is the target concentration. Note that in equation 4 the gradient-constrained problem is a subset of the more general problem. The concentration-constrained case includes the gradient-constrained case.

The equation needed, in addition to equation 3, to represent the concentration constraints in term of the decision variable q_i is the groundwater-transport equation which is written

$$\frac{\partial c(\mathbf{x}, t)}{\partial t} + \nabla \cdot (\mathbf{v}c)(\mathbf{x}, t) - \nabla \cdot \mathbf{D} \cdot \nabla c(\mathbf{x}, t) - Q_i \bar{c}_i = 0 \tag{5}$$

where

$\mathbf{v}(\mathbf{x}, t)$ is the groundwater velocity

$\mathbf{D}$ is the dispersion coefficient and

$c(\mathbf{x}, t)$ is the concentration of the designated species.

Equation 5 can be extended to include chemical reactions and retardation without substantially changing the general concepts presented herein. The velocity appearing in equation 5 is obtained using the solution from equation 3 via Darcy's Law

$$\mathbf{v}(\mathbf{x}, t) = -\mathbf{K} \cdot \nabla h(\mathbf{x}, t)$$

The methodology needed to solve the resulting optimization problem is much more complex than that required to solve equation 1. A new formulation based upon the 'tunneling method' was developed for this task. The tunneling approach is especially effective when dealing with problems exhibiting multiple minima on the interior of an otherwise differentiable objective function surface.

3.5 Sample Problem for the Concentration-constrained Case

The example problem is presented in Figure 6. A contaminant source is located to the left of the figure in a left-to-right flowing field. Two pumping wells and one injection well are located as indicated along with three observation wells where the specified-concentration constraint of 0.005 ppb must be satisfied.

Figure 6: Definition figure for the concentration-constrained sample problem .

The concentration-constrained problem generates an objective-function surface with multiple minima as shown in Figure 7. The tunneling method, as modified, provides an effective tool to solve this optimization problem. Generally the objective-function surface is not known, but it was computed herein for illustration in the case of this simple example problem.

4 Results

The robust optimization problem is solved for incrementally larger numbers of samples determined through equal-area sampling. Initially no spatial distribution is considered. Each distribution is examined independently for convergence to an optimal solution with increasing numbers of samples. Random sampling of the lognormal distribution is also examined. And finally, the spatial distribution is added to the problem to examine the affects it will have on convergence.

The number of scenarios examined is plotted versus the solution to the robust optimization problem. When random sampling is employed, the solutions to the

Figure 7: Objective function obtained for the concentration-constrained problem.

robust-optimization problem do not appear to converge to a stable optimum. While there is an increase in the value of the optimal solution as the number of scenarios examined increases, the increases occur as sporadic jumps, and convergence cannot be observed by using the random method of sampling. To ensure equal probability, however, those values that delineate the area under the pdf are used as our sample values. We call this method of sampling ‘equal-area sampling.’

When equal-area sampling is used, the values of the solutions to the robust optimization problem steadily increase as the number of scenarios examined increases. As the number of scenarios increases, the increase in the value of the solutions to the robust optimization problem can be examined, and convergence can be observed. Equal area sampling is a reliable way to determine the number of representative samples one needs in a robust optimization problem to determine a reliable optimal that is representative of the uncertainty in the hydraulic conductivity.

Further observations, however, indicate that the type of distribution used to describe the variability in the hydraulic conductivity plays an equal part in determining a reliable optimal solution.

The solutions to the robust optimization problem using equal-area sampling on the lognormal distribution curve do not converge to an optimal solution as the number of samples increases (Figure 8). This is due to the influence of the highest hydraulic conductivity value on the robust optimization problem. As

the number of samples increases in equal-area sampling, the highest hydraulic-conductivity value will increase without bound when a lognormal distribution curve is used to represent the hydraulic-conductivity variability.

When the truncated lognormal distribution curve is used to represent the hydraulic conductivity variability, convergence of the optimal solution does occur as an increasing number of samples is examined. The value to which the robust optimization problem converges is dependent upon the chosen degree of truncation. Determining the degree of truncation is not always clear. The truncated lognormal distribution should only be used when the modeler is sure that the truncation value is one where the sense of the uncertainty in the hydraulic conductivity value is not lost.

Figure 8: Rate of convergence of several approaches to solution of the gradient-constrained problem.

Convergence is also observed using equal area sampling applied to the beta distribution function. As noted in § 3.1 the advantage to using the beta distribution function over the truncated lognormal distribution function is that the range of hydraulic conductivity values spanned by the beta distribution function are determined by the variation in the hydraulic conductivity. The range of values is not determined by the modeler, and manipulation of the optimal solution is not an issue.

When the spatial variability is included, the value of the optimal solution increases. This is expected. The introduction of spatial variability increases slightly the highest hydraulic-conductivity value examined. This is reflected in a slightly higher value for the optimal solution. The introduction of the spatial

variability, however, does not negatively affect the convergence to a reliable optimal solution.

Because robust optimization is a multi-scenario approach, an effort has been made to decrease the number of scenarios necessary to represent the uncertainty in the hydraulic conductivity. Convergence of the robust optimization solution with an increasing number of scenarios is observed when applying equal area sampling to the truncated lognormal distribution and to the beta distribution. Because the beta distribution is determined purely by the hydraulic-conductivity distribution, this is the preferred distribution to use. Convergence is observed after approximately thirty scenarios.

The results of the concentration-constrained example problem are shown in Figure 9. The charts show the amount of pumping from the two wells (shown in Figure 6) that is required to satisfy the concentration constraints. Note that as the analyst demands that the solution satisfy more of the constraints (the weights increase), the costs also increase.

Weight indicates measure of risk aversion to system failure

Figure 9: Comparison of the costs obtained for the concentration-constrained problem using different weighting coefficients ω that reflect the importance of risk aversion to the analyst.

5 Relevance, Impact and Technology Transfer

5.1 Relevance

The above-described research can be used at once to minimize the costs of groundwater remediation using pump-and-treat technologies. Not only can the technology provide more cost-effective remedial designs, but also it can be used to redesign existing pump-and-treat facilities to make them more cost effective and less risky. The concepts and mathematical tools provided as a result of this research can be readily extended to more complex groundwater remediation systems. Reactive walls and biologically enhanced remediation systems can, for

example, be addressed using the strategies developed in this work.

5.2 Impact

The impact of the technology developed during the course of this research is twofold. Its utilization can result directly and immediately in a reduction in cost of new and existing groundwater remediation facilities. Application of the technology results in a reduction in cost that may be realized either via a savings in fixed costs or a decrease in operation and maintenance costs or a decrease in fines due to violations of government regulations because the uncertainty in hydraulic conductivity was not considered in the model. In addition, the trade-off between increased design reliability and increased cost is explicitly presented. An example of this trade-off is presented in Figure 9. As the aversion to potential system failure increases, so also do the costs.

5.3 Technology Transfer

The methodology generated via this research will be transferred using three approaches;

1. the conceptualization, formulation, testing and evaluation of the methodology has been and continues to be presented via publication in conference proceedings and professional journals, as well as in oral presentations at universities, research centers and professional meetings;
2. the methodology is presented as one element of professional short courses given by the principle investigators, and
3. the methodology is to be taught in graduate-level courses on optimal groundwater remediation design given at the University of Vermont.

5.4 Project Productivity

All elements of the proposed research were complete successfully.

5.5 Personnel Supported

George F. Pinder - Faculty
George P. Karatzas - Research Faculty
Karen Ricciardi - Graduate Student

5.6 Publications

K.L. Ricciardi and George F. Pinder "Risk based groundwater remediation design using a tunneling optimization algorithm," in Computational Methods in Water Resources, XIII, Calgary, Canada, 519-523, 2000

Two additional papers prepared for publication in peer-reviewed journals are in the internal review process and another is in preparation.

References

- [1] Babu D. K., G.F. Pinder and A. Niemi “Chemical transport by three-dimensional groundwater flows,” Report 84-WR-3, Water Resources Program, Department of Civil Engineering and Operations Research, Princeton University, 1987.
- [2] Belitz, K and J. D. Bredehoeft “Hydrodynamics of Denver Basin: Explanation of Subnormal Fluid Pressures,” AAPG Bulletin, 72(11), 1334-1359, 1988.
- [3] Csallany, S and W.C. Walton “Yields of Shallow Dolomite Wells in Northern Illinois, Illinois State Water Survey,” Report of Investigation 46, State of Illinois, Department of Registration and Education, Urbana, 1963.
- [4] Deutsch, C.V. and A.G. Journel “GSLIB: Geostatistical Software Library and User’s Guide,” Stanford Center for Reservoir Forecasting, Oxford University Press, New York, 1992.
- [5] Freeze, R. A. and J. A. Cherry “Groundwater,” Prentice-Hall: Englewood Cliffs, New Jersey, 1979.
- [6] Gelhar, L. W. “Stochastic Subsurface Hydrology,” Prentice Hall, Inc.: Englewood Cliffs, New Jersey, 1993.
- [7] Johnson, N. L. Samuel Kotz and N. Balakrishnan “Continuous Univariate Distributions,” Vol. 2, Ed. 2, John Wiley and Sons: New York, New York, 1995.
- [8] Karatzas, G. P. and G. F. Pinder “Groundwater contamination problems, Water pollution IV,” International Conference on Water Pollution: Modelling, Measurement, and Prediction, Computational Mechanics Publications, Southampton, United Kingdom, 4, 231-237, 1997.
- [9] Karatzas, G. P. and G. F. Pinder “Groundwater Management Using Numerical Simulation and the Outer Approximation Method for Global Optimization,” Water Resources Research, 29(10), 3371-3378, 1993.
- [10] Law, J. “A Statistical Approach to the Interstitial Heterogeneity of Sand Reservoirs,” Trans. AIME, 155, 202-222, 1944.
- [11] Mulvey, J.M. and R.J. Vanderbei “Robust optimization of large-scale systems,” Operations Research, 43(2), 264-281, 1995.
- [12] Press, W. H. et al. “Numerical Recipes in Fortran 77,” The Art of Scientific Computing, Vol. 1, Ed. 2, Cambridge University Press: New York, New York, 1992.
- [13] Wagner, B. J. and S. M. Gorelick “Optimal Groundwater Quality Management Under Parameter Uncertainty,” Water Resources Res., 23(7), 1162-1174, 1987.

- [14] Wagner, J. M., U. Shamir and H. R. Nematı “Groundwater Quality Management Under Uncertainty: Stochastic Programming Approaches and the Value of Information,” *Water Resources Res.*, 28(5), 1233-1246, 1992.
- [15] Watkins, D. W. and D. C. McKinney “Comparison of Stochastic Programming and Robust Optimization Models for Groundwater Plume Containment,” *North American Water and Environment Congress*, ASCE, 1996.
- [16] Watkins, D. W. and D. C. McKinney “Finding Robust Solutions to Water Resources Problems,” *Journal of Water Resources Planning and Management*, Jan/Feb, 49-58, 1997.