Design of Optimal, Reliable Plume Capture Schemes: Application to the Gloucester Landfill Ground-Water Contamination Problem

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Abstract

A ground-water quality management model is applied to the Gloucester Landfill site, located near Ottawa, Canada, to examine the effectiveness of various single-well pumping schemes for the capture of dissolved contaminants. Deterministic and stochastic design analyses are conducted through ground-water solute transport modeling of the site. The purpose of the modeling analysis is to develop contaminant capture designs that both require minimum pumping rates and possess high probabilities of success.

Optimization based upon deterministic simulation indicates that a well located at the front of the plume would effect plume capture and require the lowest pumping rate. However, a smaller total volume of water could be pumped and still effect plume capture if the well were located at the center of the plume and pumped at a higher rate for a shorter time. Stochastic optimization analyses are used to overdesign the pumping rates so that possible design error is overcome. The analyses indicate that design reliability may be increased from 50 to 90 percent by pumping an additional 18 percent at the front or 27 percent at the center of the plume. These pumping overdesign factors are the first such values calculated using the stochastic optimization approach applied to a field site.

1.0 Introduction

For a small-scale aquifer reclamation project, simple calculations may be performed to design a ground-water pumping system required to initiate cleanup activities (i.e., Keely and Tsang, 1983; or Javandel and Tsang, 1986). However, such an approach may not provide the optimal or most reliable design for addressing a contamination problem. This is because physical complexities, like spatial variability of hydraulic conductivity and recharge, and incomplete knowledge of the flow and transport systems often exist but are not accounted for with simple calculations. A non-optimal design requires more project resources than necessary, while an unreliable design possesses a low probability of achieving project goals. The consequences of employing a design that is questionably adequate, instead of one that is both optimal and reliable, increase in significance with the scope and duration of the project.

Some of the questions that may be considered during design of a large-scale aquifer reclamation project are:

- What are the well locations and pumping rates that will achieve plume capture for a minimum cost?
- What is the level of confidence that a particular pumping design will succeed in capturing the plume?
- What is the appropriate level of pumping overdesign to achieve a desired reliability of plume capture?

The ground-water quality management technique developed by Wagner and Gorelick (1987) is a design tool that addresses the above-mentioned questions. Work presented here demonstrates the first application of that technique to design of a pumping system for ground-water contaminant capture at a field site. The purposes of this demonstration are to: (1) convey the usefulness of the method for ground-water remediation planning, and (2) provide information on overdesign requirements for reliable plume capture at field sites.

2.0 The Gloucester Landfill: Contamination History, Hydrogeologic Setting, and Ground-Water Simulation

2.1 Contamination History

Between 1969 and 1980, the Canadian government operated a Special Waste Compound for the disposal of hazardous liquid wastes within the Gloucester Municipal Landfill, located just south of Ottawa, Ontario, Canada (Figure 1). During this time approximately 100 m^3 of solvents, wood preservatives, pesticides, acids, toxic metal compounds, and oils were placed into shallow trenches and subsequently combusted through the detonation of explosive charges (Jackson et al., 1985). The extent of ground-water contamination resulting from this disposal practice was recognized in 1981 when a preliminary hydrogeologic

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Received July 1991, revised July 1992, accepted August 1992. Discussion open until July 1, 1993.

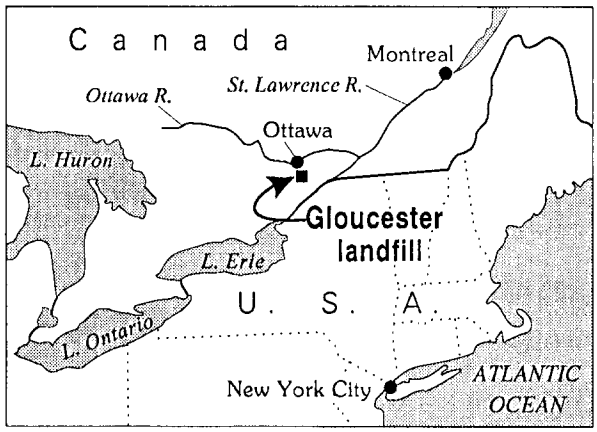

Fig. 1. Site location map.

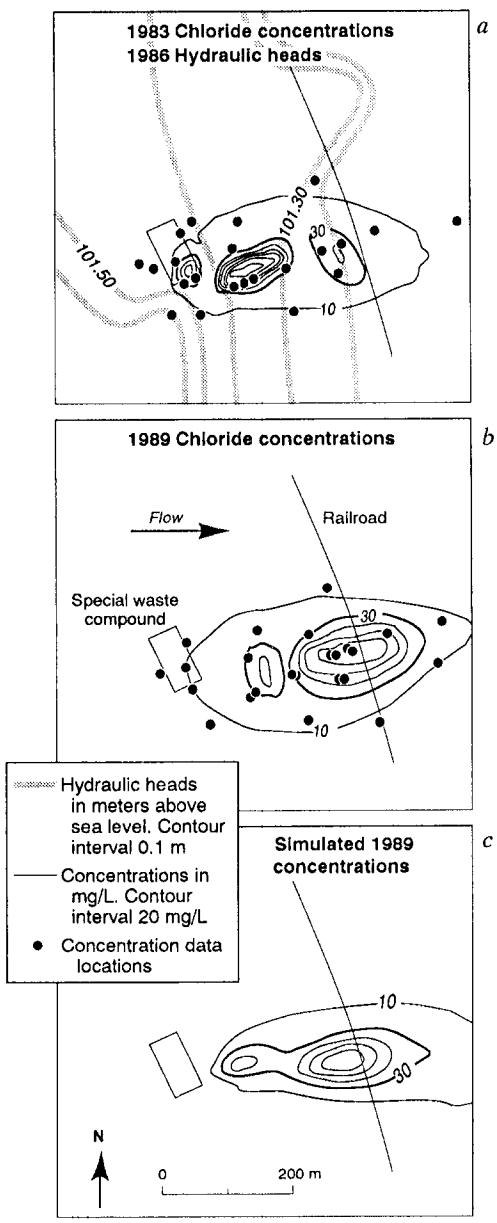

Fig. 2. a: 1986 hydraulic heads and depth-averaged 1983 chloride concentrations. b: Depth-averaged 1989 chloride concentrations. c: Simulated 1989 chloride concentrations. (Adapted from Gailey et al., 1991).

investigation of the site was completed. The investigation indicated that contaminated ground water had emanated from the disposal site in a multilayered aquifer system and was migrating towards a light-industrial area supplied by ground water.

2.2 Hydrogeologic Setting

The National Water Research Institute (NWRI) of Environment Canada, formerly with the National Hydrology Research Institute, began to study the contamination problem in 1979 to determine contaminant migration and fate. The ultimate goal is aquifer reclamation. The investigation has produced a significant amount of information about the aquifer system at the Gloucester Landfill (Jackson et al., 1985; and Jackson and Patterson, 1989).

Ground-water flow at the site is semiconfined, passing through unconsolidated deposits that comprise a sequence of interlayered gravels, sands, silts, and clays underlain by a glacial till. These sediments were deposited primarily as outwash in a periglacial environment during retreat of the Wisconsin ice sheet some 12,000 years ago (Rust, 1977). Figure 2a presents an interpretation of the October 1986 hydraulic head data for the outwash aquifer. Flow is northeasterly across the site.

NWRI has regularly collected concentration data from multilevel piezometers installed in the portion of the outwash aquifer where confined flow occurs. In addition to organic contaminants at the site, chloride was monitored. Figures 2a and 2b respectively present depth-averaged interpretations of that chloride concentration data for 1983 and 1989. The plume peaks shown are consistent with both the concentration data, and the results of episodic waste disposal and seasonal ground-water recharge.

2.3 Ground-Water Simulation

Simulation models of the ground-water system at the Gloucester Landfill site were previously developed for flow by Bahr (1984) and for flow and transport by Crowe and Shikaze (1989). Neither of these works included a complete assessment of model prediction error. Such an assessment is desirable when predictive modeling is performed since some degree of prediction error always results from the combined effects of: (1) use of simplifying assumptions in model application, and (2) errors in measurement of data used for model calibration. Without an assessment of prediction error, there is not basis for assessing confidence in a model-based aquifer reclamation design prior to field testing.

The most recent modeling of the Gloucester site (Gailey et al., 1991) was performed specifically to assess model prediction uncertainty for both ground-water flow and solute transport. The model created in that work is used here to develop pumping design options for contaminant capture. A brief review of the model is presented in the remainder of this section; additional details about model construction, calibration, and justification of modeling assumptions is presented in Gailey et al. (1991).

The authors simulated ground-water flow and solute transport at the site using the model SUTRA (Voss, 1984). Two-dimensional steady-state flow under isotropic, con-

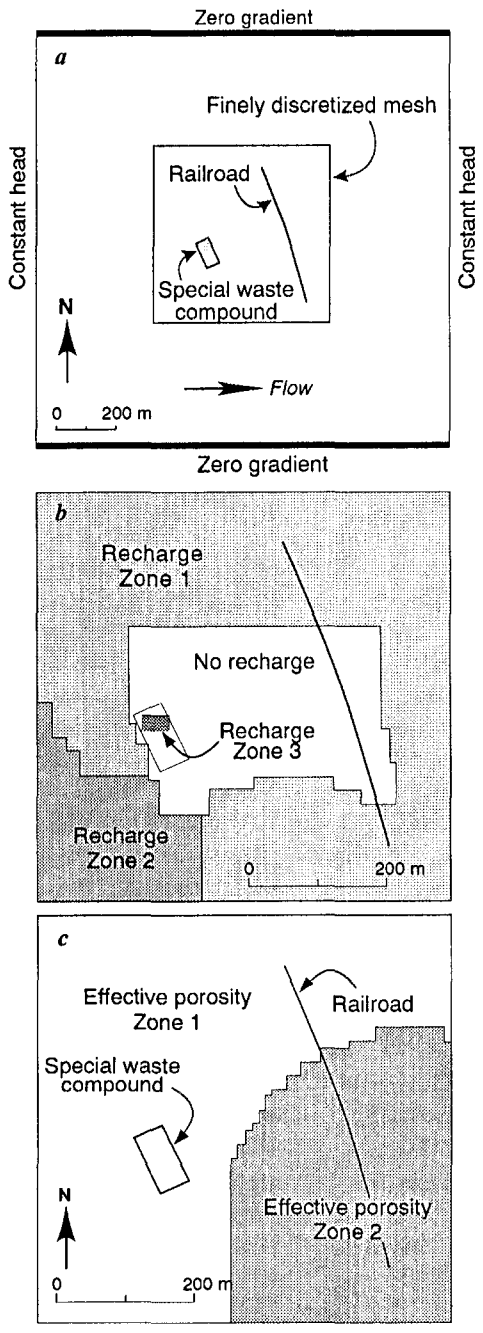

Fig. 3. a: Model area showing types of boundary conditions and site landmarks. b: Recharge parameter zonation. c: Effective porosity parameter zonation where Zone 1 was fixed at 0.30 based upon prior information. Figures 3b and 3c show only the fine mesh zone indicated in Figure 3a. (Adapted from Gailey et al., 1991).

fined conditions was simulated with a combination of constant-head and zero-gradient boundaries that were consistent with regional ground-water flow information (Figure 3a). Initial conditions for transient transport simulation consisted of depth-averaged chloride concentrations for June 1983 (Figure 2a). Chloride was chosen as the best candidate for transport modeling for three reasons: (1) the chloride concentration data set was larger, both spatially and temporally, than that of the contaminants monitored at the site; (2) no consideration of chemical reactions was necessary since chloride is likely transported as a conservative solute; and (3) the chloride plume extended further from the source area than that of any other contaminant and, therefore, design based upon chloride concentrations was sufficient to capture all contaminants at the site. Discretization requirements for modeling solute transport involved use of variably sized finite-element mesh with the finest mesh located in the center of the model domain (Figure 3a).

Many parameter values for the model were determined directly from field data. The parameters left to be estimated were hydraulic conductivity, recharge rate, and effective porosity. Estimation of a single hydraulic conductivity value for the site in terms of its natural logarithm allowed adequate simulation of the ground-water system. It was necessary to consider the recharge and effective porosity as spatially variable. This variation was accounted for by dividing the model domain into zones and assigning a different parameter value to each (Figures 3b and 3c). The location and geometry of each zone was based upon site topography and sediment stratigraphy, as well as the observed spatial distributions of hydraulic head and contaminant concentration.

Estimates of the parameter values and their associated covariances were obtained through multiple nonlinear simulation-regression. During this procedure, heads from October 1986 (Figure 2a) and chloride concentrations from both May 1988 and May 1989 (Figure 2b) were matched simultaneously in a coupled-process inverse procedure. The 1989 chloride concentrations simulated with the estimated parameters are shown on Figure 2c.

Table 1 contains the parameter values and covariances estimated by Gailey et al. (1991). The covariances for the estimated parameter values, which indicate the levels of estimation uncertainty, were generally small. This high confidence in the calibrated model was achieved because concentration history-matching in the model calibration process provided information about ground-water flux across the site. Without this flux information, a wide range of estimated parameter values would have provided equally reasonable matches to the head data, and the model calibra-

Table 1. Parameters Estimated by Simultaneously Matching Concentration and Head Data

	Parameter Estimates and Standard Deviations				
	Ln(K)	*R_1 (m/s)*	*R_2 (m/s)*	*R_3 (m/s)*	*θ_2 (—)*
Mean	-8.77 (K = 1.55E-04 m/s)	4.68E-09	3.60E-08	5.32E-08	0.17
Standard deviation	1.36E-01	8.27E-10	2.86E-09	6.70E-08	3.01E-02
	Covariance Matrix				
Ln(K)	1.85E-02	1.05E-10	1.24E-10	5.47E-09	2.46E-03
R_1	1.05E-10	6.84E-19	1.39E-19	1.12E-17	1.27E-11
R_2	1.24E-10	1.39E-19	8.16E-18	7.36E-17	3.37E-11
R_3	5.47E-09	1.12E-17	7.36E-17	4.49E-15	8.11E-10
θ_2	2.46E-03	1.27E-11	3.37E-11	8.11E-10	9.08E-04

Notes: (1) Parameter zonations are indicated on Figure 3.
(2) Based upon field data, θ was set equal to 0.30.

tion would have been uncertain (Neuman, 1973). Given a range of parameter values, there would be a range of pumping rates for any plume capture design, and selection of a single pumping rate would not be possible.

3.0 Deterministic Ground-Water Quality Management for Plume Capture

The model developed by Gailey et al. (1991) was used to investigate plume capture designs for the Gloucester Landfill site. Design development involved selection of a single well location and pumping rate that would effect contaminant capture with a minimal pumping rate. This was performed by intially formulating a deterministic optimization problem where the model predictions are assumed to be without error.

3.1 Formulation of the Deterministic Design Problem

Pumping strategies were developed for capture of the chloride plume observed at the Gloucester site. Optimization analyses were performed for five different well locations spaced 100 meters apart along the plume (Figure 4). Each analysis identified the minimum pumping rate required to remove all water having solute concentrations greater than or equal to a chosen level (10 mg/l) within a specified period. Minimization of pumping rate, which may be considered as a surrogate for minimizing a portion of project cost, was the objective.

Two types of concentration constraints were used in each optimization analysis to develop time-constrained plume capture designs. First, cleanup-time constraints were specified to insure that no concentrations would be greater than 10 mg/l at the end of the cleanup period. There were 743 cleanup-time constraints; one for each finite-element node in the model where the plume was present (Figure 4). Second, migration-control constraints were specified along a boundary oriented transverse to the direction of solute transport (Figure 4). Use of those constraints ensured that the designs would control plume migration regardless of any cleanup-time requirements. There were 24 finite-element nodes located along the migration control boundary. Concentrations at these nodes were evaluated throughout the simulated cleanup (eight times per year). For cleanup times of 6, 12, and 18 years, there were 1152, 2304, and 3456 migration-control constraints, respectively.

The deterministic optimization formulation for this design problem is expressed as:

$$\text{Minimize } Q \tag{1}$$

Subject to

$$c_i \leq 10 \text{ mg/l}, \quad i = 1, n \tag{2}$$

$$c_j \leq 10 \text{ mg/l}, \quad j = 1, m \tag{3}$$

$$Q \geq 0 \tag{4}$$

where Q is the discharge rate at the well location considered; c_i are simulated concentrations for the cleanup-time constraints; c_j are simulated concentrations for the migration-control constraints; n is the number of cleanup-time constraints; and m is the number of migration-control constraints. The above formulation is a nonlinear optimization problem (Gorelick et al., 1984) and was solved by linking the simulation model for the site to a nonlinear optimization code (NPSOL, Gill et al., 1986) as in the work of Wagner and Gorelick (1987) and Wagner (1988). The simulation-optimization method may be applied using any finite-difference or finite-element solute transport model. Predicted chloride concentrations for June 1991 were used as initial concentration conditions for the simulation model.

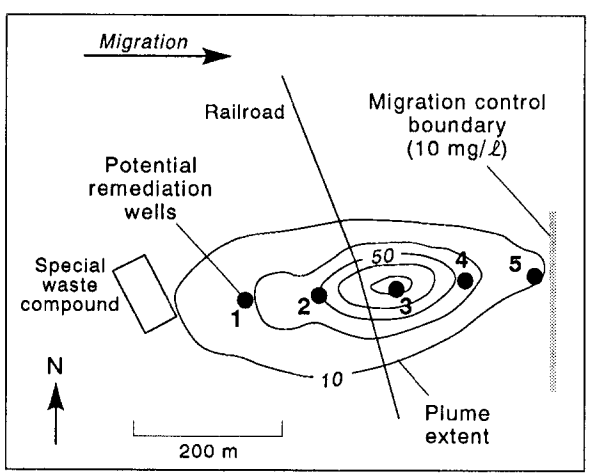

Fig. 4. Optimization formulation showing each of the five potential well locations, the migration control boundary, and the cleanup-time constraint locations as the area within the plume extent.

3.2 Results for Deterministic Design Analysis

Assessment of the deterministic design results is presented here. The designs are first considered with respect to the minimum pumping rate design criterion. Application of the designs to the field site and the potential for design modification are then discussed. Finally, other potentially important design selection criteria are used to assess the design results.

3.2.1 Optimal Pumping Rates and Well Locations for a Range of Cleanup Times

Optimal pumping rates for each of the five well locations considered (Figure 4) were determined for 6-, 12-, and 18-year cleanup times. Throughout this paper, the term optimal will be used to denote the minimum pumping rate. Figure 5 and Table 2 summarize the results of the analyses. For the 6-year cleanup time, the optimal design entails pumping at 3.60 l/s from well location #3 (Table 2). The steady-state head field and the resulting migration of chloride towards the well for this design are shown on Figure 6. The 6-year pumping rates for locations #1 and #2 are greater than that for location #3 (Figure 5) since higher ground-water velocities are necessary to draw the front of the plume to the well against the regional flow. The pumping rates for locations #4 and #5 are higher than that for location #3 because higher ground-water velocities are necessary to draw the back of the plume to the well within 6 years.

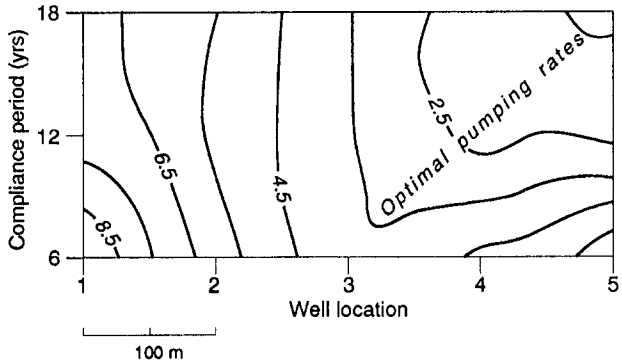

Fig. 5. Optimal pumping rate plotted as a function of both well location and cleanup time. Contour interval is 1.0 l/s. Well locations referenced on the horizontal axis are shown on Figure 4.

For the optimal 12-year cleanup design, enough time is available for the back of the plume to be drawn to a well location closer toward the plume front (well location #4). Because there is a longer cleanup period and the distance between the well and plume front is shorter, the pumping rate is less than for the 6-year design. Moving the well away from the optimal location requires higher pumping rates (Figure 5) for reasons presented abvove. For the optimal 18-year design, there is enough time for the back of the plume to be drawn to a well located at the plume front (well location #5). Since the plume front need not be drawn to the well, the lowest pumping rate is required (Table 2). This is the most desirable design.

It should be noted that the pumping rates for each cleanup period are within the range of values attained at the site during field tests. Also, the predicted drawdowns are small compared to the aquifer thickness. These are indications that the designs are reasonable for implementation at the site.

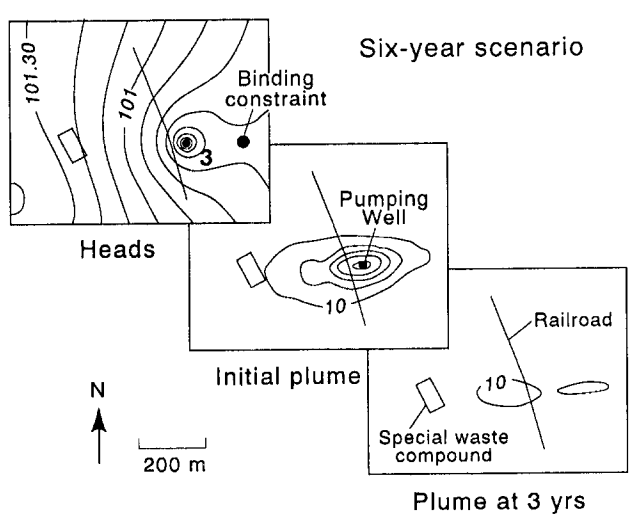

Fig. 6. a: Steady-state hydraulic heads for optimal 6-year cleanup design (pumping rate of 3.60 l/s at well location #3). The location for the binding constraint is shown. b: Concentrations in 1991 at the start of pumping. c: Concentrations predicted after 3 years of pumping.

Table 2. Optimal Pumping Rates and Locations for Variable Cleanup Time: Deterministic Design

Cleanup time (yrs)	*Well location*	*Pumping rate (l/s)*	*Total volume pumped (l)*	*Binding constraint*	*Lagrange multiplier*
6	3	3.60	6.81E + 08	Time	-0.16
12	4	1.98	7.48E + 08	Capture	-0.26
18	5	1.41	8.03E + 08	Capture	-0.06

3.2.2 Design Application

The most significant assumption required for applying the designs to site cleanup is that simulating transport of a conservative solute (chloride) is sufficient for development of aquifer reclamation designs for dissolved organic contaminants. This assumption is only valid if the contaminants are highly mobile. For contaminants that adsorb strongly to the aquifer material, plume migration control, rather than rapid cleanup, is all that may be achieved.

Pumping rates for performing rapid cleanup will be greater than those for performing plume migration control. Therefore, it would be wasteful to apply a design for rapid cleanup when the contaminants are highly retarded and only plume migration control is possible. Each optimization analysis indicates whether the optimal design is for rapid cleanup or plume migration control through the binding constraint. The binding constraint is that constraint equal to the cleanup level (10 mg/l) for a given optimal pumping rate. For single-well designs, all other constraint values will necessarily meet the cleanup level (be less than 10 mg/l).

The binding constraint for the optimal 6-year cleanup design is a cleanup-time constraint (Table 2). A higher pumping rate is necessary to satisfy the 6-year cleanup-time requirement than to establish plume migration control. Because the 6-year design is based upon cleanup time, it should be applied only to the remediation of mobile organic contaminants. The migration of less mobile contaminants would be controlled with this pumping design, but operation of the recovery system for longer than 6 years would be required, and the pumping rate would be higher than necessary for plume migration control.

The binding constraints for the optimal 12- and 18-year cleanup designs are from the set of migration-control constraints (Table 2). For each design, the allotted time is sufficient for the plume to migrate to the extraction well under flow conditions created by establishing a capture zone. These designs may be applied to the capture of all organic contaminants at the site. However, pumping from well location #5 (the 18-year design) is the most desirable because a lower pumping rate is required.

3.2.3 Design Sensitivity to Cleanup Level

Initially selected cleanup levels may not be the levels ultimately chosen for an aquifer reclamation project. For instance, levels based upon an assessment of risk to human health and the environment may be changed as new information is discovered about the toxicity of various contaminants. The cleanup levels may be made more stringent for

specific contaminants, while standards for other contaminants may be relaxed. Moreover, it has become evident during the past several years that predetermined cleanup levels are not always attainable because the efficiency of pump-and-treat technology depends upon site-specific conditions (Haley et al., 1991; U.S. EPA, 1989). It is possible that the level of cleanup attainable in the field may not be determined until after a design is developed and pumping has been conducted at a site for some time (U.S. EPA, 1992).

Altering the cleanup level after remedial action has begun may necessitate modification of the pumping design. For aquifer reclamation involving a single well, pumping rate modification can be performed through analysis of the Lagrange multiplier generated as part of the optimization analysis. No additional modeling analysis is required unless new well locations are to be considered.

Values of the Lagrange multipliers for the optimal designs are also presented in Table 2. Each value is associated with the binding constraint for the optimization solution and represents the sensitivity of the pumping rate to a unit change in the constraint value (Gill et al., 1981). For example, an increase in the cleanup constraint value from 10 to 11 mg/l would result in a 0.16 liter per second decrease in the optimal 6-year pumping rate. This lower pumping rate would be sufficient since the less stringent water quality standard would allow additional solute to: (1) remain in the aquifer when cleanup was complete, and (2) pass the migration control boundary during the remedial operation.

3.2.4 Other Considerations for Design Selection

Factors other than pumping rate, such as cleanup duration and volume of ground water treated, will also affect the cost of a remedial operation. Although the 18-year optimal design requires the minimum pumping rate, the optimal 6-year design requires a minimum total volume of ground water to be pumped during the remedial operation (Table 2). If only mobile contaminants are of concern, the most cost-effective design may involve minimizing both the volume of ground water treated and the cleanup duration by applying the 6-year design.

4.0 Stochastic Ground-Water Quality Management for Reliable Plume Capture Pumping Schemes

Use of optimization to design contaminant capture requires that accurate models of ground-water processes be incorporated into the optimization procedure. However, models contain errors that result from several sources including model misspecification and parameter inaccuracy caused by data mismeasurement. Prediction error, which stems from these modeling errors, must be accounted for so that model-based designs do not fail when applied in the field. Design failure for this particular example would result in concentrations exceeding the cleanup level.

Consideration of prediction error in the design process generally requires pumping overdesign since increasing the pumping rate will decrease concentrations. Throughout this paper, the term pumping overdesign will be used to denote an increase in pumping rate to increase the probability of design success. Arbitrary pumping overdesign counteracts the economic benefits gained from using an optimal design (minimal pumping rate). Incorporating a statistically based pumping overdesign procedure into the optimization satisfies the need to increase design reliability while maintaining optimality of the design.

4.1 Formulation of the Stochastic Design Problem

Methods to account for model prediction error in optimal design include sensitivity analysis, Monte Carlo analysis, and stochastic programming. Stochastic programming entails an explicit incorporation of the effects of prediction error into the optimization procedure. Wagner and Gorelick (1987) developed such a method for hypothetical aquifer reclamation design in which model prediction error was evaluated in terms of uncertainty in estimated model parameters. That method is applied in this work.

The overdesign method is briefly presented in the following sections. Additional explanation may be found in Wagner and Gorelick (1986 and 1987). A two-step procedure is used to account for model prediction error in the design process. First is translation of model parameter uncertainty into prediction uncertainty. Second is overdesign by incorporating prediction uncertainty into the ground-water quality management formulation.

4.1.1 Prediction Uncertainty

Probabilistic interpretation of model predictions used in the design process acknowledges the possibility of constraint violation (design failure):

$$\text{Prob}\ (c \leq 10\ \text{mg/l}) \geq r \tag{5}$$

Designs developed with probabilistic constraints (expression 5) must meet the cleanup level with a reliability of r that is specified for the design (Figure 7).

For cases where concentration prediction error is normally distributed as a function of parameter uncertainty, the probabilistic constraint may be transformed into its deterministic equivalent:

$$\underbrace{E[c]}_{\text{DETERMINISTIC COMPONENT}} + \underbrace{F^{-1}(r)\ SD[c]}_{\text{PROBABILISTIC COMPONENT}} \leq 10\ \text{mg/l} \tag{6a}$$

or

$$c^* \leq 10\ \text{mg/l} \tag{6b}$$

where E [c] is the expected value of the predicted concentration; $F^{-1}(r)$ is the standard normal cumulative distribution value corresponding to the design reliability, r; r is the specified design reliability; SD [c] is the standard deviation of the predicted concentration; and c* is the probabilistically defined concentration prediction. The deterministic component of expression (6a) is derived through model prediction with the estimated parameter values. The probabilistic component is an expression of model prediction uncertainty that results from imprecise knowledge of the model parameter values. It is a scaled value of the concentration standard deviation, which is calculated with a first-order method. The

scaling factor $F^{-1}(r)$ is a function of the specified design reliability.

For a reliability of 50 percent, $F^{-1}(r)$ equals zero and the transformed probabilistic constraint [expression (6a) or (6b)] reduces to a deterministic constraint [expression (2) or (3)]. Therefore, there is a 50 percent probability that deterministic model predictions will underestimate field concentrations and designs based upon those predictions will fail. The magnitude of prediction error and the severity of design failure depend upon the amount of uncertainty associated with the model parameters. This uncertainty is indicated by the value of the probabilistic component.

4.1.2 The Overdesign Method

Addition of the probabilistic component to the concentration predictions ($r > 0.50$) requires an increase in the optimal pumping rate to account for higher predicted constraint concentrations. The probability that the model-based design will succeed in the field increases as a result of the higher pumping rate.

The stochastic optimization formulation is expressed as:

$$\text{Minimize } Q \tag{7}$$

Subject to

$$c_i^* \leq 10 \text{ mg/l}, \quad i = 1, n \tag{8}$$

$$c_j^* \leq 10 \text{ mg/l}, \quad j = 1, m \tag{9}$$

$$Q \geq 0 \tag{10}$$

All terms are defined previously. The locations of the cleanup time and migration-control constraints remain as in the deterministic formulation (Figure 4).

4.2 Results for the Stochastic Design Analysis

Portions of the deterministic design analysis were repeated as stochastic optimization problems in order to determine pumping overdesign requirements. Only a few stochastic optimization problems were considered since each analysis required large amounts of computer time. Optimal pumping rates for the 6- and 18-year designs were obtained for the deterministically derived optimal well locations (well locations #3 and #5, respectively). A reliability of 90 percent was used.

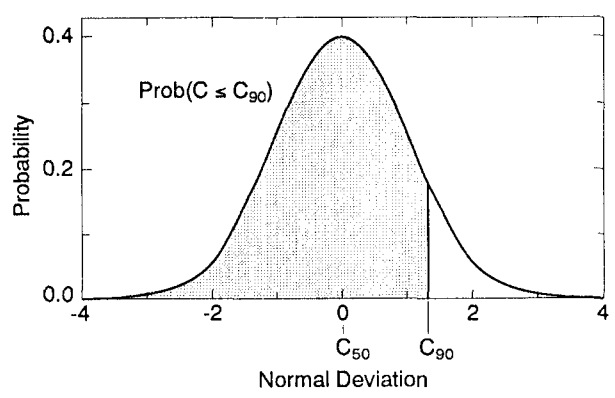

Fig. 7. The probability that field concentrations will be less than or equal to the water quality standard with a reliability of 90% (shown for a normal distribution).

Table 3. Optimal Pumping Rates for Variable Cleanup Time Stochastic Design (90% Reliability)

Cleanup time (yrs)	*Well location*	*Pumping rate (l/s)*	*Total volume pumped (l)*	*Overdesign factor*
6	3	4.57	8.66E + 08	27%
18	5	1.67	9.46E + 08	18%

Note: Well locations chosen on the basis of deterministic designs.

Table 3 summarizes the results of the analyses. Overdesign factors of 27 and 18 percent are required for the 6-and 18-year cleanups, respectively. These results indicate that the effect of model prediction uncertainty upon the optimal design is more significant for higher pumping rates. As for the deterministic results, the minimum pumping rate is associated with the 18-year cleanup, and the minimum volume of ground water pumped is associated with the 6-year design.

5.0 Conclusions

The use of models as planning tools is essential when ground-water remediation design must be conducted. No other method exists for assessing the effects of potential remedial actions prior to field implementation. Even with the assistance of a model, however, selection of the best design is often not a simple task since consideration of numerous design requirements complicate the selection process. Use of optimization techniques can aid production of model-based designs.

While optimization techniques may require considerable computational resources, the amount of professional time required to produce a design can be significantly reduced. Moreover, optimization results provide information pertinent to design implementation through identification of binding constraints and calculation of Lagrange multipliers.

The example presented here demonstrates application of an optimization technique to the design of a pumping system for contaminant capture in the saturated zone. As discussed, design selection depends upon both the intended application and the overall cost of remediation. An evaluation of pumping overdesign requirements for reliable aquifer reclamation was performed to complete the design process. To the best of our knowledge, these overdesign results are the first produced for a field site using the stochastic simulation-optimization approach. Although the results apply only to the Gloucester Landfill site, they provide some indication of the overdesign necessary to increase reliability of plume capture when a ground-water system is well-characterized.

Acknowledgments

Data from the Gloucester Landfill site were furnished by the National Water Research Institute of Environment Canada. The authors are grateful for the opportunity to have worked with this data set. We thank Allan Crowe of the National Water Research Institute for providing additional information based upon his field and modeling experience on the Gloucester Landfill project.

Funding for this study was provided by the Office of Research and Development, U.S. Environmental Protection Agency, under agreement R-815738-01 through the Western Region Hazardous Substance Research Center. The content of this study does not necessarily represent the views of the agency. Additional funding was provided by the Switzer Foundation. Computing facilities were provided by a grant from the Hewlett-Packard Company.

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