Optimal location of monitoring wells for detection of groundwater contamination in three-dimensional heterogeneous aquifers

PASCAL STORCK
Department of Civil Engineering, University of Washington, Seattle, Washington, USA

ALBERT J. VALOCCHI & J. WAYLAND EHEART
Department of Civil Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois, USA

Abstract We present a multi-objective stochastic optimization method for the design of monitoring networks for the initial detection of groundwater contamination at waste disposal facilities. A Monte Carlo approach is used to generate a large number of equally likely realizations of a random hydraulic conductivity field and a leak location. A finite-difference groundwater flow model and a particle-tracking model is used to generate a contaminant plume for each realization. Information from the flow and transport simulations is passed to an optimization model based upon a facility location analogy. The optimization model is a large integer programming problem which is solved by the method of simulated annealing. Optimal trade-off curves among three conflicting objectives are obtained. These objectives are: (1) maximum detection probability, (2) minimum cost (i.e., minimum number of monitoring wells), and (3) minimum volume of contaminated groundwater at the time of detection. The model is applied to a hypothetical scenario in order to examine the sensitivity of the trade-off curves to various model parameters.

INTRODUCTION

The Resource Conservation and Recovery Act (RCRA) establishes regulations to be followed in the design of a groundwater monitoring well network to detect contaminant leaks from hazardous waste disposal facilities and municipal solid waste landfills. RCRA requires the installation of a sufficient number of wells that can detect a contaminant leak before it crosses the compliance boundary. The compliance boundary is defined as a vertical surface surrounding the landfill outside of which the concentration of contaminant must remain below regulatory limits. Unfortunately for the operator of the landfill, these regulations provide no clear guidance on the "best" place to put these wells in relation to the landfill and the compliance boundary. By placing the wells away from the landfill at the compliance boundary an unnecessarily large portion of the aquifer may be contaminated before the leak is detected. By placing the wells as close as possible to the landfill, the contaminant plume may initially pass
undetected through the well network only to be detected much later (if at all) after a large extent of the aquifer has been contaminated and the compliance boundary violated.

The problem of where to place these wells is further compounded by the uncertainty that is characteristic of groundwater problems. The main sources of uncertainty which influence the design of a monitoring well network are the hydrogeological uncertainty associated with groundwater flow and contaminant transport and the uncertainty about the exact location of the contaminant leak in the landfill. Furthermore, the issue of the "best" or optimal placement of the wells is confused by exactly what is meant by optimal. The main objectives typically considered when determining the performance of a monitoring well network are conflicting. These objectives are (1) to minimize the number of monitoring wells in the network, (2) to maximize the well network's probability of detecting a contaminant leak and (3) to minimize the extent of contamination when the leak is first detected by the well network. The conflicting nature of these objectives precludes the existence of one optimal solution and forces the landfill operator to consider a number of non-inferior networks. In this paper we present a multi-objective stochastic optimization framework for addressing the monitoring network design problem. Our method yields optimal trade-off curves among the three objectives noted above. By applying the method to a hypothetical problem we examine the sensitivity of the trade-off curves to various modeling assumptions.

**METHOD**

**Overview**

Our method is an extension of the work reported by Meyer (1992) and Meyer et al. (1994), which is restricted to two-dimensional groundwater systems. A conceptual model of the three-dimensional groundwater transport problem is illustrated in Fig. 1. The aquifer is assumed to have a rectangular-box geometry with dimensions (XL, YL, ZL); there is regional flow in the +x direction driven by the hydraulic gradient which is fixed by the assumed constant head values at the upstream (H1) and downstream (H0) faces (left and right) of the aquifer. The top boundary of the aquifer is a prescribed-flux type having one of three possible values: qr is the natural groundwater recharge flux which applies outside of the landfill area; ql is the landfill flux which applies within the landfill except at the location of the leak; and qs is the contaminant source flux which applies at the location of the leak. The other three faces of the aquifer (front, back, and bottom) are assumed to be zero-flux boundaries. Groundwater flow and contaminant transport are simulated by numerical models, which are described further below.

We consider only two sources of uncertainty—groundwater transport, as modeled by the assumption of a randomly heterogeneous hydraulic conductivity field, and source location, as modeled by the assumption of a randomly located localized source within the landfill area. The source concentration is assumed to be constant in time. Other parameters, in particular the recharge rates qr, ql, and qs, are assumed to be known and steady.
It should be noted that our methodology is in no way restricted to the simplified domain illustrated in Fig. 1. A problem having a more realistic irregular geometry could be accommodated, but would require the use of more complicated and flexible simulation models instead of the ones we have implemented which are restricted to simple box-type aquifers. It is also possible to extend our methodology to incorporate additional uncertain parameters (e.g. the recharge rates), although this would entail increased computational effort.

In addition to specifying the domain geometry shown in Fig. 1, we assume candidate locations for the monitoring wells. A potential monitoring well is defined by the $x,y,z$ coordinates of the top of the well screen and the screen length. While the model is restricted to considering only one screened interval per monitoring well, the screened length for each well need not be the same. We adopt a Monte Carlo approach and generate a large number of equally-likely plumes resulting from failure of the landfill. A single Monte Carlo realization consists of the following three steps: (1) generation of a realization of a random $K_s(x,y,z)$ field, where $K_s(x,y,z)$ is the saturated hydraulic conductivity, (2) solution of the steady-state groundwater flow model to obtain the velocity field for the given realization of hydraulic conductivity, a random leak location, and assumed values of the vertical aquifer recharge rates, and (3) simulation of the transport of the resultant contaminant plume until it reaches a compliance boundary. A list of the screened intervals of the potential monitoring wells that detect each plume, and the plume volume at initial detection for each well is then recorded and passed to the optimization model.
Transport simulation

Details about the computational aspects of the method can be found in Storck (1994). Here we just provide a brief summary. We use the turning bands model of Tompson et al. (1989) to generate the stationary random $K_s$ fields required in step (1). This model assumes $K_s$ is lognormally distributed with a given mean, variance, and exponential correlation structure. For step (2) we use a three-dimensional steady-state finite difference model based upon that developed by Meyer et al. (1989). Step (3) requires the lion’s share of the computational effort. We found that solution of the three-dimensional advection-dispersion equation was too expensive computationally, even if we implemented highly efficient codes like the Laplace-Transform-Galerkin method (see Sudicky, 1989) which performed ideally in our two-dimensional analysis (Meyer et al., 1994). Due to these limitations, a particle tracking method has been implemented that models only the advective transport of the contaminant plume. (See Kinzelbach (1988) and Tompson & Gelhar (1990) for a discussion on the development and implementation of the particle tracking equations). Since dispersion acts to increase the volume that a plume contaminates, ignoring the effect of dispersion results in smaller plumes that are more difficult to detect. Thus ignoring dispersion is a conservative assumption that agrees with pessimistic (worst-case) design philosophy.

Particles are spread uniformly throughout the randomly chosen leak node, and these particles are simply advected until they exit the problem domain. The contaminant plume is traced out by recording the grid cells in the model domain through which at least one of the particles passes. These cells are then considered to be fully contaminated with a concentration equal to the source concentration. In general, a monitoring well screen will include both contaminated and uncontaminated grid cells. Determination of if and when a plume is detected by a monitoring well is carried out by comparing the flux-averaged concentration in the monitoring well with a specified threshold detection limit. If the flux-averaged concentration in the well is greater than the detection threshold, the plume is assumed to be detected by that well. Details about the computation of the flux-averaged concentration are given by Storck (1994).

Optimization problem

The output from the above described three dimensional Monte Carlo simulation procedure is a list of the monitoring wells that detect each contaminant plume and the contaminated volume of the aquifer at the time of initial detection at each well. This information is given to a separate optimization model which has three objectives: (1) maximization of the fraction of plumes detected by the network, (2) minimization of the average contaminated volume at the time of detection, and (3) minimization of the total number of required monitoring wells. This multi-objective problem is treated by using the so-called weighting and constraint methods. That is, the formal objective function used in the model is a weighted sum of the first two objectives, while the third objective above is treated as a constraint. The optimization model is a large integer programming problem based upon a facility location analogy; it is solved approximately using the simulated annealing technique. Details are given by Meyer (1992) and Meyer et al. (1994).
RESULTS FOR A HYPOTHETICAL PROBLEM

Description and base case results

The network design method was applied to a simple hypothetical problem similar to that shown schematically in Fig. 1. The model domain was chosen to represent one unit of length (L) in the direction of regional flow (x-axis) and 0.5 units of length (0.5L) along the width and depth (y and z axis) respectively. The number of grid cells in each direction was chosen as 50 along the x-axis and 25 along the y and z axis. This choice of grid spacing results in all model domain cells having uniform cubic dimensions (0.02L x 0.02L x 0.02L). Once the model domain was chosen and discretized, the landfill area could be incorporated as some subset of the model domain cells. The landfill was chosen to include 180 potential leak nodes all with dimensions equal to one model cell. This landfill was positioned on the top of the model domain (z=0.5L) and extended from x=0.25L to x=0.5L along the x-axis and from y=0.1L to y=0.4L along the y-axis. The potential monitoring wells are also specified as some subset of the model domain cells. Each potential monitoring well corresponds to a vertical column of model domain cells. The top of this column corresponds to the top of the well’s screened portion. The depth of the column (counted in units of model cells) represents the screen length of the well. For this application three rows of monitoring wells along the x-axis were considered (x=0.6L, 0.75L, 0.9L). Each row consisted of 12 locations along the y-axis where a well could be positioned. Furthermore, at each (x, y) location up to 20 different monitoring well screen starting depths could be chosen; there is a total of 720 potential monitoring wells in the network.

Storck (1994) applies the network design model to this hypothetical site in order to test the sensitivity of the resulting non-inferior performance trade-off curves for the following model parameters: (1) the number of Monte Carlo Realizations (plumes), (2) the variance of the ln K_s (hydraulic conductivity), (3) the correlation length, (4) the regional recharge, (5) the leak recharge, (6) the screen length, (7) the detection limit, (8) the number of particles used in particle tracking, and (9) the areal extent of the leak. Here we report only the impact of variance of the ln K_s field.

Before examining the sensitivity of the design results to model parameters, it is useful to develop an understanding of the behavior of these trade-off curves in both objective (well network performance) and decision (well number and location) space for the three dimensional hypothetical model with base parameters. The base parameters used for this application are given in Table 1. Figure 2 shows the non-inferior performance trade-off curves obtained for a number of different well networks sizes when the three dimensional model is applied to the hypothetical site with base parameters. These trade-off curves represent the best monitoring well networks with a given number of monitoring wells for the two performance attributes; percentage of simulated plumes detected and average contaminated volume of the detected plumes. The percentage detection attribute is simply the percentage of the simulated plumes (usually 500) that the given monitoring well network was able to detect. Therefore, when the network performance is given as X% detected, that statement means that 500X (as % X) where detected by the network. (Assuming that 500 plumes were simulated.) However, due to the finite sample size, the reported X% detected value is only a point estimator of the actual percentage of plumes that would be detected by the
network. This fact implies that a confidence region exists around the point estimator in which the actual percent of plumes detected by a given network is expected to occur.

The average contaminated aquifer volume of the detected plumes is calculated by averaging the total number of model cells contaminated when each plume is first detected over all plumes that are detected. This average is then normalized with respect to an arbitrarily chosen “large” plume. This normalized sum is then divided by the total number of plumes detected by that network. For this paper the normalization parameter was selected to be 550 grid cells. Although the average volume of detection was used as an estimator of the “volume” objective in this project, any other statistical estimator could be used (e.g. the 95th percentile). Furthermore, due to the finite sample size, any method used to evaluate the contaminated volume objective is only a point estimator of the true value. Therefore, a confidence region exists around this point estimator in which the true value lies.

![Graph](image)

Fig. 2 Non-inferior performance trade-off curves for the hypothetical problem with base parameters listed in Table 1.
Figure 2 shows a clearly defined trade-off between the percentage of the simulated plumes a network can detect and the average contaminated volume of those detected plumes. There is also a steady improvement in the performance of the monitoring well networks as the number of monitoring wells in the network increases. This increase is most evident when more wells are added to small networks. When additional wells are added to large networks, there is a diminishing marginal return.

The reason for the trade-off in the performance attributes is most clearly seen by analyzing the networks from Figure 2 in decision space. These results are not shown here for the sake of brevity, but they are presented by Storck (1994). The trend shown in these results is that as the percentage of plumes detected increases the wells are optimally positioned further downgradient from the landfill. By moving further away, however, the wells allow more of the aquifer to be contaminated before they detect the plumes. Therefore, for a given number of wells, as the percentage of plumes detected increases, the average contaminated volume also tends to increase. Since the objectives are to maximize the percent detection and minimize the average volume, a trade-off must occur between the two attributes. A similar relationship was seen between the well locations and the network performance for the two dimensional model (Meyer et al. 1994).

Effect of the hydraulic conductivity variance

The level of heterogeneity of the hydraulic conductivity is one of the important factors that controls contaminant transport and therefore influences the final monitoring network. Variance of the In $K_s$ ($\sigma^2$) is one of the parameters that determines the degree of heterogeneity in the three dimensional method: a high variance will produce highly heterogeneous realizations with hydraulic conductivity values spanning a wide range, whereas, a low variance will produce more homogenous fields. The effect of the variance on the outcome of the three dimensional monitoring network design procedure was evaluated by performing several numerical experiments with varying values of $\sigma^2$. The $\sigma^2$ values used were 0.5, 0.75, 1.0 and 1.5 which represent increasing levels of heterogeneity. A list of the other model parameters used is given in Table 1.

The results of this analysis are shown in Fig. 3 for both 5 and 10 active wells in the network. These results indicate that the performance of the network decreases significantly with increasing variance of the hydraulic conductivity field. Aquifers with a large $\sigma^2$ will tend to form contaminant plumes with irregular shapes, which are more difficult to detect. Furthermore, a larger $\sigma^2$ implies more variation from one $K_s$ realization to another, implying greater uncertainty in the direction the plume travels. For both reasons the percentage of plumes detected is expected to decrease as $\sigma^2$ increases. In a more homogenous aquifer, the contaminant plumes take more uniform shapes and follow more predictable paths which are more easily detected. As $\sigma^2$ increases, the plumes also tend to become larger. This increase in plume volume results in an increase in the average contaminated volume per detected plume of the optimal networks (see Fig. 3) as the variance becomes larger. This increase in average volume is especially noticeable when $\sigma^2$ equals 1.5. At this high variance, a much larger amount of the aquifer is allowed to become contaminated in order to achieve the
highest detection percentage compared to the networks for the lower variances. Examination of the optimal networks in decision space reveals that the wells are located further from the landfill and tend to be more spread out perpendicular to the regional gradient as the value of $\sigma^2$ increases.

Finally, we note that our additional results which are not reported here suggest that the common practice of placing at least one monitoring well upgradient and three downgradient of the waste area is not a sufficiently large minimum. The extensive applications of the method reported by Storck (1994) show that even under the best
conditions for the statistical parameters, which are typical of relatively uniform alluvial aquifers, three optimally located downgradient wells have an expected probability of detection of less than 50% while five optimally located downgradient wells can achieve a maximum detection probability of approximately 80%. Over 10 optimally located wells were typically required to achieve detection probabilities of over 95%. Since these networks represent the optimal well placements for the given number of wells, networks designed by rules-of-thumb or professional judgement may lead to significantly worse reliability.

Acknowledgment We thank Phil Meyer and Ranji Ranjithan for their key contributions to this work. This paper is based upon research supported by the U.S. Environmental Protection Agency’s Environmental Monitoring Systems Laboratory. This paper has not been subject to the U.S. EPA’s peer and policy review and therefore does not necessarily reflect the views of the agency and no official endorsement should be inferred.

REFERENCES


