Procedures for Uncertainty Analyses Applied to a Landfill Leachate Plume

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Abstract

Environmental data often have features that are distinct from data in other branches of science. These features include spatial and/or temporal auto-correlation, natural heterogeneity, measurement errors, small sample sizes, and simultaneous existence of different types and qualities of data. Realistic environmental modeling requires simulation procedures that account for all of these features. In this study, a model of uncertainty analysis, BUDA, is used to account for the noted features and provide a unified framework for quantification, propagation, and reduction of uncertainty. The BUDA model is used to analyze the development of a chloride plume around an old landfill to the year 2020. This article describes the different components of BUDA as they relate to the landfill application.

Introduction

Environmental protection is becoming an increasingly important social, political, and research issue. The past several decades have seen much effort directed toward the development of analytical and technological tools dealing with anticipated environmental problems ranging from ground water pollution to ozone layer depletion.

Environmental data have many characteristic features, including the following:

1. Most environmental data exhibit spatial and/or temporal auto-correlation. Ignoring this feature leads to inefficient use of the available information (e.g., Abbaspour et al. 1996).
2. Environmental data exhibit natural heterogeneity. Realistic spatial simulation programs should maintain this heterogeneity.
3. Most input parameters in environmental studies, including geostatistical parameters (i.e., mean, variance, range, nugget, and shape of the auto-correlation structure), are highly uncertain. Ignoring parameter uncertainty may lead to severe underdesigns in projects (e.g., Abbaspour et al. 1996).
4. Measured data usually contain non-negligible measurement errors. Ignoring measurement errors can have far-reaching consequences for data worth models and interpretation of modeling results.
5. Environmental data sets are generally very small and do not lend themselves easily to statistical analyses. This means studies must rely on subjective information.
6. Collected data are mostly used as inputs in sophisticated simulation programs where uncertainties and errors can further propagate. Neglecting to propagate the errors and uncertainties may give a false picture of modeling results.
7. Different types of data are often available. Special procedures are needed that can combine and use all available data.

The objective of this work is to demonstrate the use of a new methodology for dealing with environmental projects. The BUDA (Bayesian Uncertainty Development Algorithm) uncertainty analysis model is presented and applied to an example landfill problem. The important features of BUDA are: the special characteristics of environmental data are accounted for, and a number of different procedures dealing with quantification, propagation, and reduction of uncertainty are linked together and unified under one algorithm.

The landfill under consideration is located near Aaura in Switzerland and has been used as a toxic waste repository. Measures such as covering the surface with grass and installing drainage and pumps to remove and remediate the discharge have been taken to stop the spread of contaminants. In performing the landfill analysis, our goal was to establish whether these measures were enough to contain the landfill. To simulate the chloride plume, we used random field techniques to generate conditional hydraulic conductivity data, where the conditioning data included hard (measured) conductivity values as well as soft (estimated) conductivity values. The soft data were obtained from a relationship between hydraulic conductivity and borehole profile description. The invoked geostatistical model for the hydraulic conductivity had uncertain parameters which included the mean, sill, range, and nugget. Next, we propagated the uncertainties in the parameters to a goal function using a two-dimensional transport model. An inverse procedure was subsequently used to decrease the uncertainty in the initial estimates of the parameters, followed by a data worth analysis to show the effect of additional measurements of hydraulic conductivity on the confidence of the model prediction. In the inverse analysis, the initial estimates of the input parameters were conditioned on 70 measured chloride concentrations. The reduction in uncertainty

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of the input parameters obtained by inverse conditioning, which included the hydraulic conductivity parameters as well as the system porosity and dispersivity, was compared with the results of a data worth analysis which considered taking up to 50 more hydraulic conductivity measurements. Finally, we applied our model to predict the spatial distribution of the chloride around the landfill in the year 2020. This information was used to judge the efficiency and safety of the current measures implemented to stop the spread of contaminants from the immediate vicinity of the landfill boundaries.

Literature Review

In recent years, tremendous advances have been made in modeling and analyzing environmental projects. Here we discuss some of these advances as they relate to the fields of soil and water protection.

Modeling of Water and Contaminant Movement in Soil and Ground Water

In the past, flow and transport models were scarce and model users often had to develop their own models. This lack severely limited the use of modeling for practical applications. In recent years there has been a surge of user-friendly, general and specific purpose models. User-friendly programs equipped with automated mesh generators and graphical interfaces have made modeling a viable tool for practical applications in academia, engineering, and governmental research agencies (for a list and a summary of some of these programs see Abbaspour and Schulin [1996]).

Employment of Stochastic Simulations

Stochastic simulation is in recognition of parameter uncertainty inherently associated with environmental studies. Propagating input uncertainty gives rise to stochastic simulations, where, in Monte Carlo type simulations, instead of producing one scenario based on an unlikely set of average input values, one produces many scenarios to represent reality. Advances in random field analysis have provided more options to depict the environment in more realistic ways.

Advances in Geostatistical Estimation and Simulation Techniques

While geostatistical techniques are powerful estimation tools, their use in environmental studies have been limited due to large variability and small size of data sets. Recent development of techniques that make geostatistics more relevant to practical environmental applications include the introduction of co-kriging techniques (Myers 1982; Journel and Huijbergts 1978) that allow linear regression using data defined on different attributes; indicator kriging (Journel 1983), which allows reproduction of patterns of spatial connectivity by a least-square estimate of the conditional cumulative distribution function (ccdf) for a set of cutoff points; indicator principle component kriging (Suro-Perez and Journel 1991), which evaluates the ccdf of several categorical variables; and the Markov-Bayes model of soft kriging (Journel 1986; Zhu and Journel 1993) which uses soft or fuzzy data and generates posterior conditional distributions.

In addition to these estimation methods, a number of simulation techniques have also been developed. Stochastic simulation, in a geostatistical context, is defined as the process of building alternative, equally probable, high-resolution models of the spatial distribution for a random variable (Deutsch and Journel 1992). Simulation techniques, as opposed to estimation techniques, are better suited for environmental projects and risk assessment studies. These techniques are intended to produce a better picture of reality, and to eliminate unrealistic smoothing that is characteristic of spatial averaging methods.

Employment of Conditional Simulation Procedures

Conditional simulation techniques honor the measurement points at their measurement locations. They bring geostatistical techniques much closer to depicting the field data.

Use of Different Data Types (Qualities) in Simulations

It is typical for an engineering situation to have data of different types, with each having a relatively small sample size. An important achievement in geostatistical simulation programs is the ability to use data of different types and qualities. This allows use of all types of information, thus in effect increasing the sample size. Poeter and McKenna (1995) used soft geologic data and expert opinion to reduce uncertainty associated with flow and transport predictions in ground water. Some geostatistical techniques can now account for soft data types such as Markov-Bayes simulation technique (Alabert 1987; Zhu and Journel 1993), which uses soft or fuzzy data and generates posterior conditional distributions of a primary variable, and Co_Est algorithm (Abbaspour et al. 1998), which provides the possibility of using pedotransfer functions to obtain better estimates of a primary variable. Pedotransfer functions are regression equations or models which relate hard-to-measure field properties to more basic and easily measured properties.

Adaptation of Inverse Simulation for Parameter Identification

Inverse modeling is a process for conditioning the input parameters on the observed primary outputs. The inverse approach recognizes that most practical applications do not have enough input data to establish a credible modeling result. Reviews of this subject are given by Yeh (1986) and Kool et al. (1987). The procedure generally involves minimization of a squared difference function of some measured and simulated variable. A common problem with inverse procedures involving a least square minimization scheme is stability and convergence. Abbaspour et al. (1997a) introduced a general algorithm for parameter estimation which appears to be always stable and convergent.

Use of Bayesian Statistical Framework

Bayesian statistics have been shown to be particularly useful in applications with geologic (Einstein and Baecher 1983), hydrologic (Wood and Rodrigues-Iturbe 1975; Vicens et al. 1975), or hydrogeologic (Gates and Kisiel 1974; Grosser and Goodman 1985; Freeze et al. 1990) components. The main difference between the classical and Bayesian statistical approach is the use of a prior estimate of the form of the probability density function and its statistics. The prior estimate is largely subjective and could be based on limited early data from the site or similar sites, or on the engineer's expert opinion. When additional data become available, they are used to update the prior estimates of the statistics to posterior estimates using Bayes theorem. Use of subjective information based on experience is prevalent in engineering practices; invoking a Bayesian approach hence could be advantageous to a practicing engineer. The implication in adopting a Bayesian framework for an engineering project is that the project iterates among data analyses, field work, and decision making, while collection of data is commonly based on the results of a data worth model in preposterior analysis. Pre-posterior analysis is the exercise of sampling from the prior distributions of input data rather than field sampling.

Data worth analysis (Gates and Kisiel 1974; Ben-Zvi et al. 1988; James and Freeze 1993; Abbaspour et al. 1996) is probably the most important feature of a Bayesian framework. Collection of field data is expensive and time consuming, and particularly in engineering situations, assessment of the worth of data can be of paramount importance. By using a Bayesian framework, issues commonly sought by engineers can be addressed, such as the quantity of risk based on current information, the number of additional samples needed to decrease the risk to an acceptable level, the type of data that should be collected, and where they should be taken.

An important criticism of the Bayesian statistics deals with the use of subjective priors. This problem is alleviated in BUDA by the initial conditioning of the prior estimates of parameter uncertainties on a set of measured data such as concentration or hydraulic head.

An Overview of BUDA

The main components of the BUDA uncertainty model are schematically depicted in Figure 1. The statistical framework of BUDA is Bayesian in nature, reflecting the fact that unknown parameters are treated as random variables. The Bayesian framework of BUDA allows a unified treatment of natural and informational uncertainties. A detailed explanation of BUDA is given elsewhere (Abbaspour et al. 1996). The model has three main components: problem definition, uncertainty analysis, and failure and risk analysis. The objective of the problem definition phase is to obtain knowledge of the physical system and the underlying flow and transport processes, as well as to collect all existing information. A conceptual model of the physical system is subsequently developed to permit flow and transport simulations using a computer code. This stage should permit one to express the objectives of the project by means of a goal (objective) function. Identification of a goal function is an important task as this function will be used to define and determine in a quantitative fashion the best alternative design, the worth of further sampling, and ultimately the failure or risk of a project. The next set of procedures in BUDA deals with the quantification, propagation, and reduction of uncertainties. A first step in the uncertainty analysis involves probabilistic depiction of all uncertain input data; this depiction is based on all available information and experts' opinion. After quantification, uncertainties in the state parameters are propagated into the goal function by using a hydrologic simulation model. Finally, uncertainties in the state parameters, and subsequently in the goal function, are reduced by employing random field analyses, inverse analyses, and data worth analyses. Random field analyses are included as part of the uncertainty reduction since incorporation of soft data and generation of conditional hydraulic conductivity fields produce more accurate hydraulic conductivity input data which subsequently lead to more accurate output results.

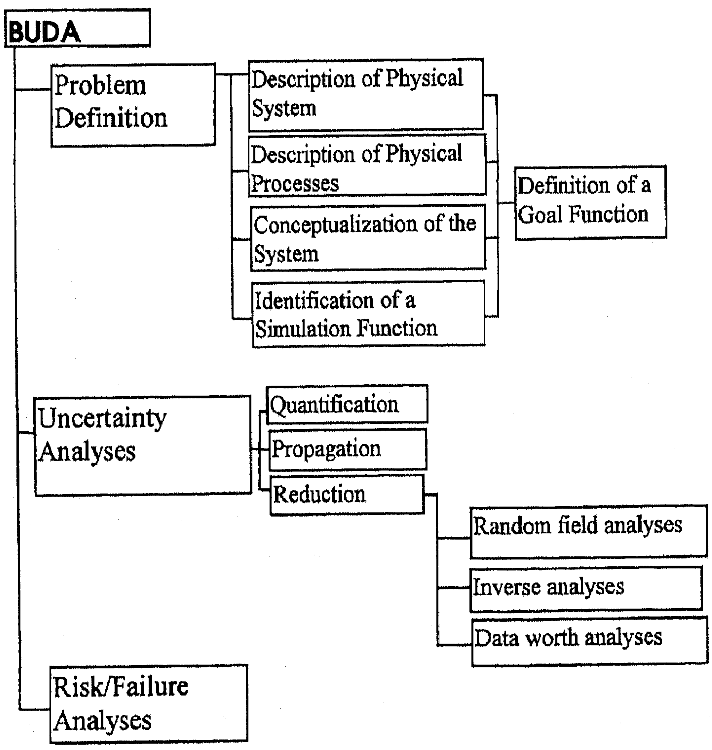

Figure 1. The main components of BUDA.

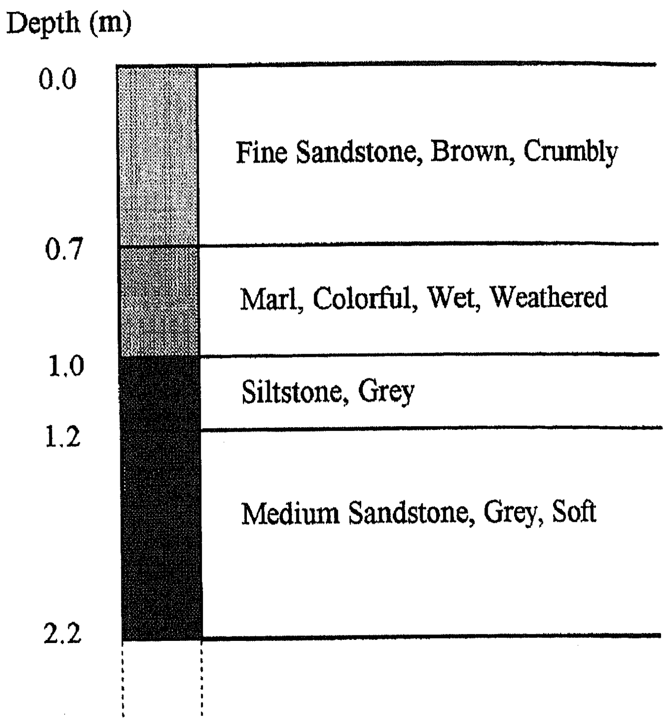

Figure 2. A typical segment of a chart used for the profile description of a borehole.

The final component of BUDA deals with risk analysis. One of the challenges of environmental projects is the assessment of risk which is closely related to that of failure. Risk is project dependent and must be defined separately for each project. Quantitatively, risk is usually expressed as the product of the probability of failure and the cost of failure. In BUDA, the probability of failure is derived from the marginal or Bayesian distribution of the goal function which must also embody the definition of failure.

Application of BUDA to a Landfill Analysis

Problem Definition

The example selected for our analysis involves a landfill site near Aarau, Switzerland. For the interest of brevity we keep the problem definition to a minimum in this paper. For more details, interested readers are referred to the Sondermülldeponie Kölliken Annual Reports (1991, 1992, 1993, 1994).

Landfill Site and Data

The landfill site was used as a toxic waste repository and lies in a former clay pit excavated in an aquitanian fresh water molasse. The molasse is composed primarily of marls and variegated clays

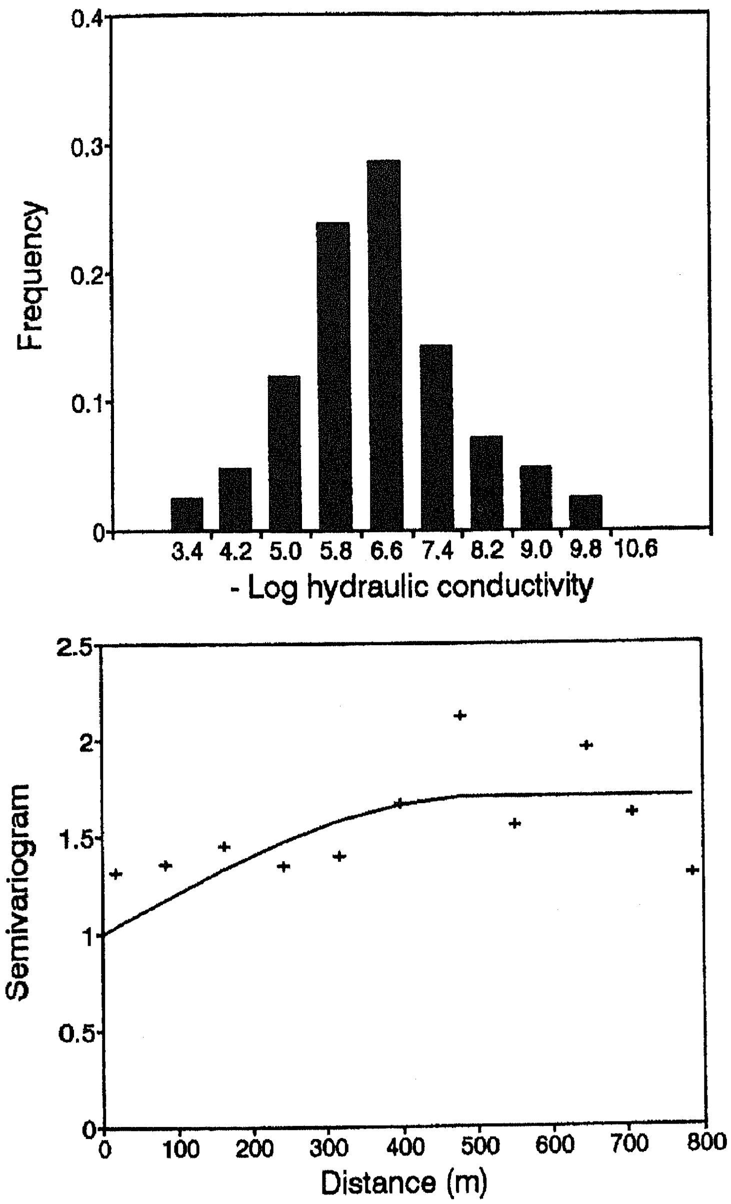

Figure 3. The frequency distribution of the variable z = –log K based on 42 measurements, and the semivariogram of z based on 298 data points (42 measured and 256 estimated).

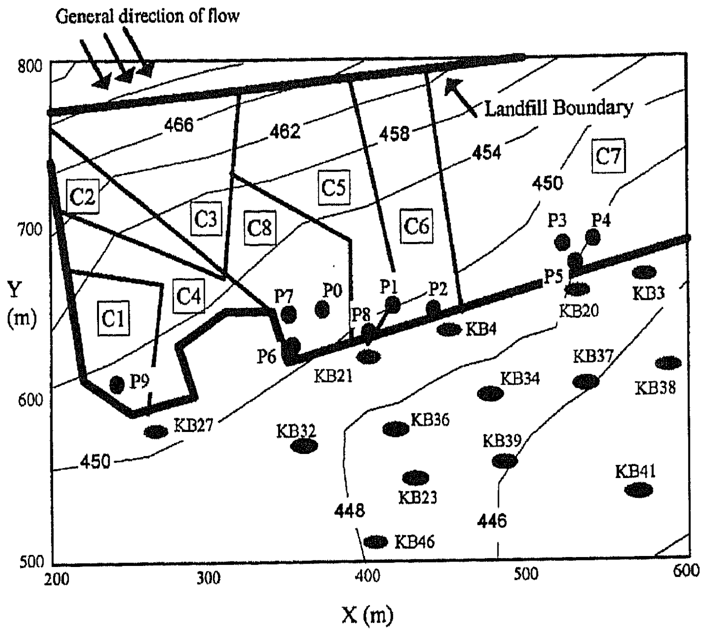

Figure 4. Some pertinent information concerning the modeling domain showing the landfill boundary, the isolines of the hydraulic head used as initial condition, the eight different landfill compartments, locations of the 10 pumps, locations of the seven boreholes (KB23, KB32, KB34, KB36, KB37, KB39, and KB41) where observed chloride concentrations were used for conditioning the parameters, and locations of the seven boreholes (KB3, KB4, KB20, KB21, KB27, KB38, and KB46) where chloride concentrations were used for model validation.

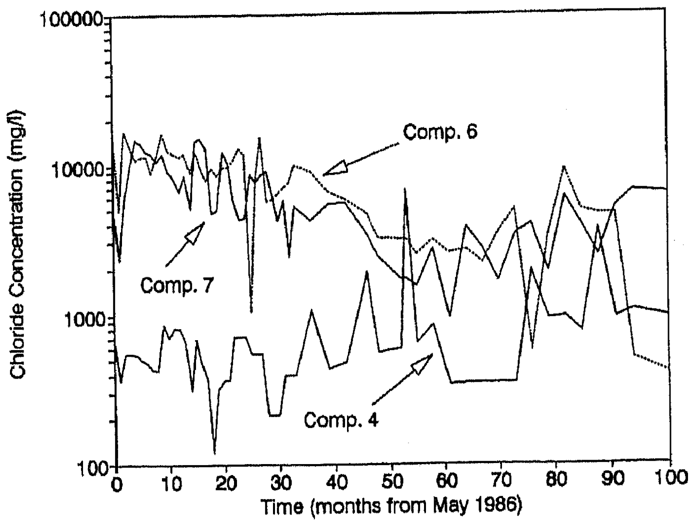

Figure 5. Concentration of chloride inputs into the system from three landfill compartments as a function of time.

interlayered with sandstone banks (Martinson 1994). The site contains approximately 60 boreholes which were drilled between 1970 and 1990 in a 800 m by 600 m area. Most of the boreholes were drilled to a depth of 30 m. Detailed lithologic descriptions were made for all boreholes, an example of which is shown in Figure 2. Hydraulic conductivities were measured at several different depths in 17 boreholes, giving a total of 42 hard data points. The measurements were made over average vertical distances of 3 m using a double packer technique. The average measurement error for this technique in a molasse geology is about one order of magnitude (Peck et al. 1988; and local expert estimates). A frequency distribution of the measured conductivity data is shown in Figure 3. Figure 4 shows additional details of the landfill area. Hydraulic head and concentration of chloride were measured several times between May 1986 and May 1994 in several boreholes. The location of some of the boreholes are shown in Figure 4 as KBs. The landfill itself consisted of eight compartments (C1 to C8). Chloride concentrations were measured regularly in each compartment from May 1986 to May 1994 in wells located at the south corner of each compartment. The sources of chloride are mostly salts dissolving from decomposing cinder and construction materials. Figure 5 shows the chloride concentrations measured in compartments C4, C6, and C7.

Modeling of Chloride Transport

The landfill site was analyzed using a two-dimensional horizontal flow and transport model, SWMS_2D (Simunek et al. 1994). Analyses of hydraulic head measurements and water fluxes at the northern landfill boundary indicated that there were only small temporal fluctuations in the system, and that the response to rainfall events were minimal. Initial hydraulic heads and chloride concentrations were estimated by kriging using measured values from 70 boreholes in April 1986. The hydraulic head isolines are shown in Figure 4. All four boundaries of the system were assumed to be constant head boundaries. There were 10 pumping stations (P0 to P9) at the southern boundary of the landfill. We assumed pumping had occurred at constant rates and obtained average values for each pump from available records. Chloride concentrations were simulated and values were recorded at seven observation points (KB23, KB32, KB34, KB36, KB37, KB39, and KB41 in Figure 4) for which we had simultaneous observations at 10 different times for a total of 70 observed data points. The 70 observations were used as conditioning data in an inverse procedure, with the goal function being formulated as:

$$g = \sqrt{\frac{1}{70}\sum_{i=1}^{i=70}(C_s - C_m)_i^2} \tag{1}$$

where C_s is simulated chloride concentration, and C_m the measured chloride concentration. We emphasize that a project may have more than one goal function depending on the type of analysis being performed. The choice of the goal function in Equation 1 was based on the objectives of the inverse analysis. For failure and risk analysis, the difference between actual and risk-based critical concentration at a monitoring point would probably be more suitable.

Uncertainty Analysis

Quantification of Uncertainty in Input Parameters

We decided to treat hydraulic conductivity, porosity, and longitudinal dispersivity as random variables. Along with the boundary conditions, these parameters were thought to have the most important effects on the nonreactive transport modeling results. Based on preliminary analyses, we were relatively confident about the accuracy of the imposed constant head boundary conditions, but quite uncertain about the values of hydraulic conductivity, porosity, and dispersivity. The hydraulic conductivity was treated as a spatially random variable requiring four parameters for its characterization: mean, sill, range, and nugget. Based on our preliminary analysis, the shape of the semivariogram for the hydraulic conductivity was assumed to be spherical. Due to the lack of more detailed information, and on the basis of the local expert opinion, we assumed porosity and dispersivity to have univariate uniform distributions within [0.10, 0.30] and [10, 30] m, respectively. Transverse dispersivity was assumed to be two tenths of the longitudinal dispersivity.

To improve the hydraulic conductivity data set, we developed a pedotransfer function relating measured hydraulic conductivities to borehole profile descriptions. Descriptive qualifiers representing borehole profiles, such as the example in Figure 2, were transformed into dummy variables (see Abbaspour and Moon [1992] for more details) and correlated with measured conductivities in a backwards stepwise multiple regression analysis (Zar 1984). Pedotransfer functions (PTFs) are regression equations or models which relate hard-to-measure field properties to more basic, and generally more easily measured, properties. Literature abounds with such equations that have been derived for different properties (e.g., Batjes 1996; Salchow et al. 1996; Wösten et al. 1995; Abbaspour and Moon 1992). The local pedotransfer function obtained in this study to estimate saturated hydraulic conductivity (K) was expressed as:

$$\begin{aligned} -\log K = 6.59 + 1.48\,FS - 1.30\,MS + 1.35\,SN - 1.36\,CC \\ - 1.43\,CR1 + 1.16\,CY1 - 0.79\,CR2 \end{aligned} \tag{2}$$

in which the variables are defined as:

FS = 1 if texture is fine sandstone, = 0 otherwise
MS = 1 if texture is medium sandstone, = 0 otherwise
SN = 1 if texture is siltstone, = 0 otherwise
CC = 1 if sandstone contains carbonate, = −1 if it does not, = 0 if texture is not sandstone
CR1 = 1 if fine sandstone is crumbly, = 0 otherwise
CY1 = 1 if fine sandstone is clayey, = 0 otherwise
CR2 = 1 if medium sandstone is crumbly, = 0 otherwise

Equation 2 yielded a model correlation coefficient of 0.82, a standard error of estimation of 0.82, and a cross validation correlation coefficient of 0.73. This equation was then used to estimate 256 values of soft hydraulic conductivity data.

Using the program Co_Est (Abbaspour et al. 1998), we generated hydraulic conductivity random fields. The advantage of Co_Est over co-kriging is that Co_Est (1) combines measured and estimated hydraulic conductivity data to form a larger data set and, hence, requires only one semivariogram; (2) accounts for both measurement and estimation errors in the input data; and (3) can directly use one or several pedotransfer functions to obtain estimates of the primary variable. In our example, using a set of 298 values of hydraulic conductivities (42 measured plus 256 estimated), we calculated the experimental semivariogram shown in Figure 3. The mean, sill, nugget, and range of the semivariogram were in turn treated as random variables. The uncertainty in these parameters arises from measurement and estimation errors, as well as from having a limited number of data points. Based on our preliminary analyses, a hydraulic conductivity probabilistic model was chosen. The mean and sill of the logarithm of hydraulic conductivity were considered to have a joint normal gamma distribution represented by three parameters: the mean, the sill, and an equivalent prior sample size (Benjamin and Cornell 1970). The marginal distribution of the sill is proportional to Chi-squared, while the conditional distribution of the mean given the sill is normally distributed. It is often possible to find for a particular problem a normal gamma distribution which closely approximates an experimenter's estimated actual prior distribution of the mean and sill (DeGroot 1975). The probability model for the shape of the semivariogram, the nugget, and the range cannot, in most practical situations, be fully inferred from the available data, and hence may ultimately have to rely heavily on the judgment and experience of a geologist or engineer. In our example, we assumed that the spatial parameters were independent of the mean and sill, that the nugget was uniformly distributed within [0.6, 1.1], and that the range was also uniformly distributed within [0, 500]. Note that this model was chosen on the basis of our preliminary analyses and could be replaced by any other probabilistic model.

In this analysis, the flow/transport model consists of six random variables: mean, sill, nugget, and range of the logarithm of hydraulic conductivity, as well as system porosity and dispersivity. It should be noted that the hydraulic conductivity random fields directly honor the 42 measured data and, indirectly through the soft data, the system geology at 256 locations. We also emphasize that one only needs to assign some reasonable values to the parameters for expressing the prior uncertainties of the input state parameters. In the next step, as the inverse analysis is invoked, the uncertainties will be conditioned on the observed values and hence adjusted to a more reasonable range as dictated by the goal function.

Propagation of Uncertainty

To propagate the uncertainties in the parameters of our transport model, we used the BUSIM program of Abbaspour (1997b). The use of this program is schematically depicted in Figure 6. Each parameter was divided into a number of strata. For the sill and mean, which were characterized by distributions, the cumulative scale ranges (0 to 1) were divided into a number of strata, and the

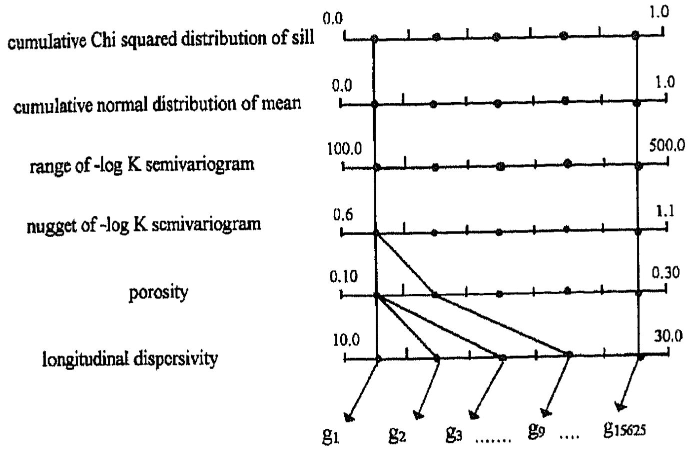

Figure 6. A schematic representative of uncertainty propagation in a stratified sampling setup. The values of the goal functions obtained are used to build a cumulative frequency distribution of the goal.

first moment of each stratum was taken to represent that stratum. Then, depending upon the speed of the simulation program, we followed one of two different sampling strategies: exhaustive stratified sampling, or random stratified sampling. In the exhaustive sampling approach, the goal function is calculated for all possible combinations of the parameter strata. This means that for our six parameters, each divided into five strata, the transport simulation program must be run $5^6 = 15{,}625$ times and the goal function calculated for each run. The resulting frequency distribution of the goal immediately yields the marginal Bayesian distribution of the goal function for use in a model of risk analysis. If the transport simulation program takes too long to run, then an alternative random sampling can be invoked where only a random subsample of the exhaustive case is used to run the simulation program. The marginal Bayesian distribution of the goal function is then calculated using the random subsample. For the example in this study, we used a random stratified sampling technique which simulated about 10% of the exhaustive 15,625 runs.

The Bayesian distribution is expressed as:

$$f_X(x) = \int_{\mathbf{b}} f_X(x|\mathbf{b})\, f_B(\mathbf{b})d\mathbf{b} \tag{3}$$

where bold characters are vectors, X is a random variable expressing the model output such as the goal function or, in our case, also the chloride concentration, and **b** is the vector of random input parameters. The distribution given by Equation 3 can be interpreted as a weighted average of all possible distributions which are associated with different values of the input parameters (Benjamin and Cornell 1970). Also, the Bayesian distribution $f_x(x)$ is a marginal distribution in the sense that $f_x(x)$ does not depend on the unknown parameters which, through the integrals, have been removed from the equation. We also note that as the distribution of input parameters, **b**, becomes more and more concentrated about the true values of the parameters, the Bayesian distribution will approach the true distribution of X. A higher precision in the distribution of input parameters can be obtained by random field analyses, inverse analyses, and collection of more data. One should generally expect the Bayesian distribution to have a larger variance than the true distribution, as the former incorporates both inherent and statistical uncertainty (Benjamin and Cornell 1970).

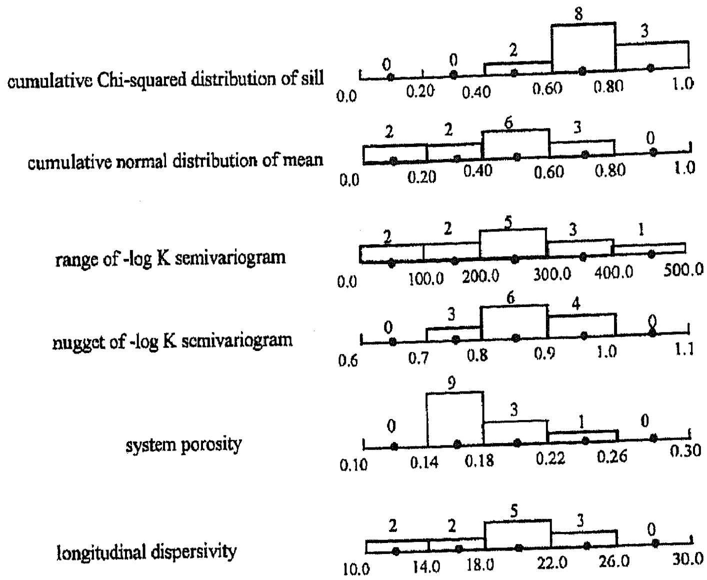

Figure 7. Frequency distribution of the scores in each stratum. The strata with the largest scores are most likely to contain the desired estimates.

Reduction of Uncertainty

Inverse Analysis

To reduce our prior estimates of the parameter uncertainties, and subsequently the variance of the Bayesian distribution of the goal function, using an inverse procedure, we invoked the SUFI program of Abbaspour et al. (1997a). In SUFI, the runs already performed in the propagation step are used to score the strata combinations of the parameters. Initially, all strata in Figure 6 are assigned a score of zero. Then, for every combination of the parameter strata for which the value of the goal function is less than a critical value, each stratum receives a score of one. Performing this step for each run leads to a score distribution for the parameter strata as shown in Figure 7. The high score areas are more likely to contain the minimum value of the goal function. Therefore, the strata at each end of the parameters that receive no or relatively small scores are eliminated, thereby reducing the uncertainty domain of each input parameter. If the initial estimate of the uncertainty for a parameter was set too small and the desired parameter value was located to the right of the interval, then the right-most stratum would typically receive a high score with most or all other strata scoring zeros. In this case, one would update the parameter by extending the interval to the right. A few iterations are generally required before reaching a final minimum. We emphasize that this procedure can be used to obtain different degrees of conditioning. A "strongly conditioned," or "fitted," parameter set is obtained by reaching the absolute minimum of the goal function, whereas a "mildly conditioned" parameter set results when the absolute minimum of the goal function is not yet reached. The absolute minimum of the goal is reached when successive iterations result in the same value. As will be shown later, a mildly conditioned parameter set generally gives better results for prediction at other points.

The effect of the parameter uncertainty propagation on the simulated chloride concentrations, and the subsequent reduction using inverse procedures, are illustrated in Figure 8. This graph shows the 95% confidence intervals of the Bayesian distribution of the simulated values based on the prior parameter estimates and after conditioning, the expected value of the simulated concentrations after conditioning, and the observed concentrations at a particular location and time. The prior average expected value of the goal function, E(g), was in excess of 2400 mg l^{-1} with a variance in excess of 1,500,000, whereas after conditioning E(g) reduced to about 250 mg l^{-1} with a variance of about 150,000.

Data Worth Model

To compare uncertainty reduction in the goal function using inverse analysis versus uncertainty reduction based on taking more hydraulic conductivity samples, we invoked the data worth model routine in BUDA. In this routine, an expected conditional hydraulic conductivity field is estimated by propagating the uncertainties in the four hydraulic conductivity parameters through a set of linear measurement equations (Bryson and Ho 1975; Abbaspour et al. 1998), and calculating the mean of the Bayesian distribution of the hydraulic conductivity at each node of the finite-element mesh representing the region of study. Then a desired sample, in terms of the number of sampling points and/or locations, is taken from the expected hydraulic conductivity field. Here we should make a distinction between decision analysis framework and optimization framework (Freeze et al. 1990) with respect to the choice of a sampling strategy. Optimization involves the determination of the best sampling strategy with respect to a given goal function. Decision analysis involves selection of the best sampling strategy from a limited number of given strategies. Within the framework of BUDA, optimization would be difficult to achieve, mainly due to the large number of data points–sampling location possibilities. Decision analysis, however, is easily implemented. We selected 11 different sampling strategies consisting of different numbers of hydraulic conductivity samples, i.e., 2, 4, 8, 12, 16, 20, 24, 28, 36, 40, and 50. For each sampling strategy we calculated average E(g) values, with the results illustrated in Figure 9. This figure shows that E(g) decreases as the number of samples increases. For 50 hydraulic conductivity samples, E(g) decreases to about 430 mg l^{-1} (variance = 500,000) from an initial value of about 2400 mg l^{-1} (variance = 1,500,000). The expected goal obtained by the inverse analysis (i.e., 250 mg l^{-1} [variance = 150,000]) is still substantially smaller than 430 mg l^{-1} obtained by sampling 50 hydraulic conductivities. Hence, the inverse analysis using 70 conditioning chloride concentration data was worth more than 50 additional hydraulic conductivity samples in terms of reducing the uncertainty in E(g). One reason for the effectiveness of the inverse procedure is that usually the uncertainty in all state parameters are modified instead of only one parameter, as in the case for the addition of more data.

In fairness to the data worth analysis, however, one is not likely to collect 50 hydraulic conductivity samples to reduce uncertainty in the goal functions. The expected values in Figure 9 of the goal function, E(g), and the value of sample information, EVSI, which is the mirror image of the E(g), show that the value of additional samples lessens increasingly. Differentiating the EVSI curve with respect to the number of samples yields a utility curve. The maximum point of the utility curve reveals the best sampling strategy. Because of a large initial goal value and large errors in the hydraulic conductivity samples, we are advised to use only four samples during the initial round of sampling in this example. After taking the four samples in the field, we should update the parameters and repeat the analysis again.

Figure 8 shows that, although the expected value of the goal function after conditioning is relatively small (i.e., 250 mg l^{-1}), the confidence intervals around the simulated concentrations are still very large. Inverse modeling is a procedure of conditioning input parameters on the basis of observed concentrations; hence, the small values of the expected goal function are to be expected.

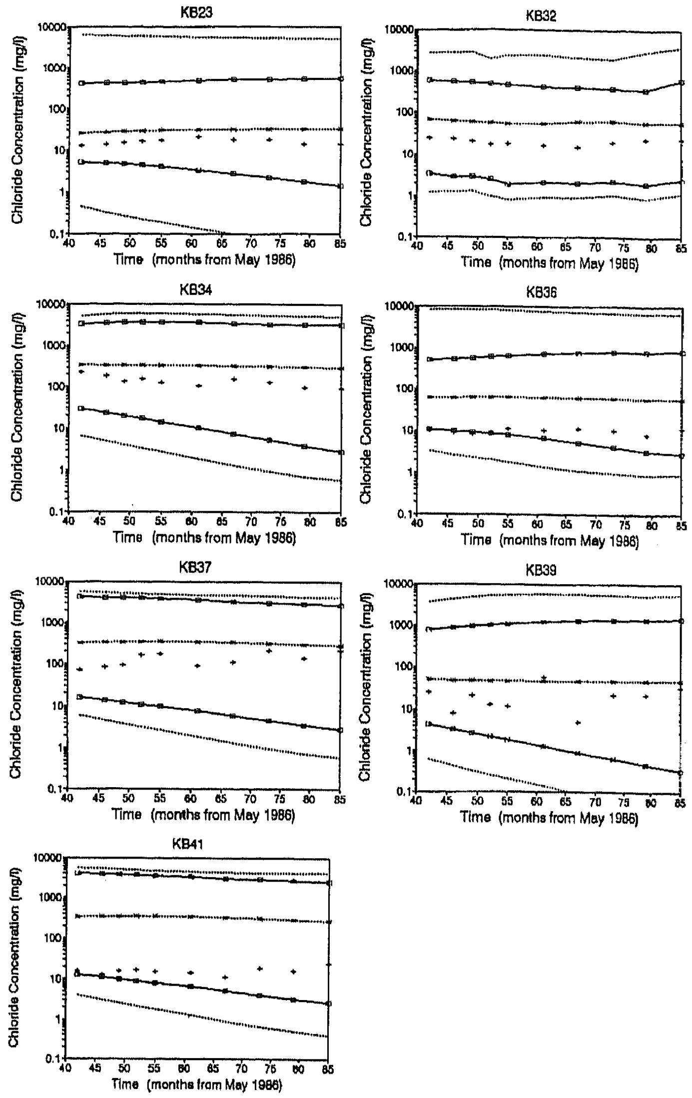

Figure 8. Chloride concentration of the seven boreholes used in inverse analysis as a function of time. The plus signs are the observed values, the outer dashed lines are the 95% confidence interval of the Bayesian distribution for simulated concentrations with the prior parameter uncertainties, the inner symbolized solid lines are same as the latter but with parameter domains mildly conditioned to chloride observations, and the inner symbolized dashed line is the expected value of the simulated concentrations based on the conditioned parameter domains.

However, reduction in the goal function may not also result in locations for which we have not conditioned, or have no observations. The goodness of the prediction at those points is reflected by the variance (about 150,000) of the goal function after the inverse analysis. To reduce this variance, we invoked the data worth analysis again, using this time the conditioned parameters obtained by inverse analysis, and produced curves similar to those in Figure 9. The results again suggested taking four additional hydraulic conductivity samples which would improve the variance of the goal to about 120,000. Hence, in BUDA, we used inverse procedure to decrease uncertainty in the prior estimates of the state parameters, followed by a data worth analysis to improve the confidence in the predictions. Depending on the outcome of a risk analysis model, taking the suggested four hydraulic conductivity samples may not be justified within the current example, given the small improvement to be expected.

Validation Analysis

In light of the preceding discussion, and as a validation run, we used the parameter set obtained by the inverse analysis and simu-

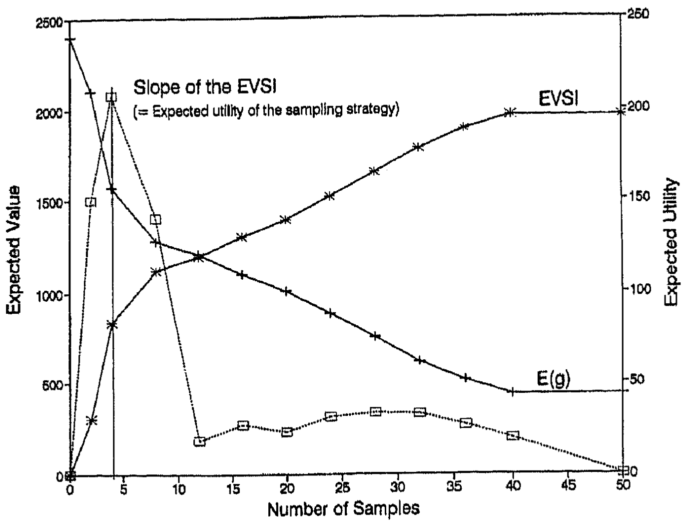

Figure 9. Expected values of the goal and the sample information, and expected utility of the sampling strategies vs. the number of samples. The optimum sampling strategy is where the maximum utility occurs.

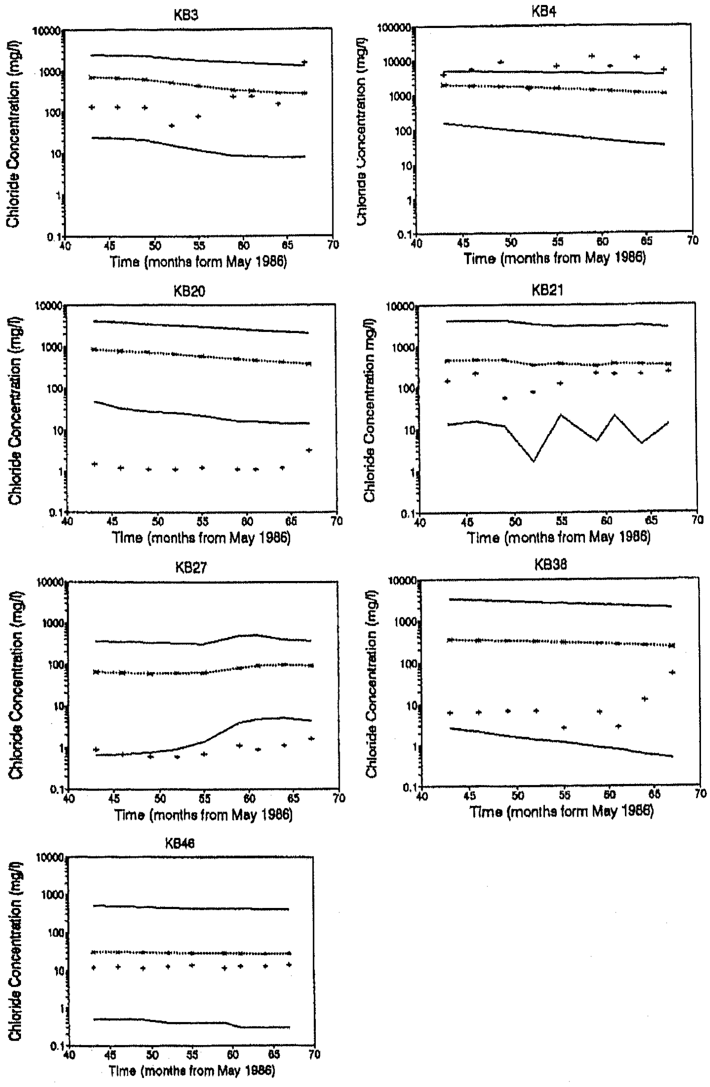

Figure 10. Chloride concentration of the seven boreholes used in model validation as a function of time. The simulations are based on the conditioned parameters. The plus signs are the observed values, the solid lines are the 95% confidence interval of the Bayesian distribution for simulated concentrations, and the symbolized dashed line is the expected value of the simulated concentrations.

lated chloride concentrations at boreholes KB3, KB4, KB20, KB21, KB27, KB38, and KB46 (Figure 4). Note that these observation stations were not used in the inverse analysis. Observations were available for each borehole at nine different times during May 1986 to November 1991. We considered a validation run to be successful if the observed concentrations fell within the simulated 95% confidence interval of the Bayesian distribution. Unsuccessful validation could arise for different reasons, such as incorrect parameterization of the system, underestimation of initial parameter uncertainties, too strongly conditioning parameters on the set of conditioning data, and nonideal system behavior such as preferential flow not considered in the governing flow or transport equations. The first three cases could be remedied by considering different parameterizations; for example, by treating the boundary conditions also as random variables, by increasing the initial parameter uncertainty, or by invoking a milder conditioning of the parameters, respectively. The case of nonuniform system behavior, however, is more difficult to remedy since this problem requires hydrologic simulation programs capable of simulating nonuniform flow phenomena. Few if any programs of this type may be really applicable to such problems.

The results of the validation run are illustrated in Figure 10 for a set of mildly conditioned parameters. The observations in locations KB3, KB21, KB27, KB38, and KB46 were roughly within the acceptable ranges, whereas KB20 was severely overestimated, and KB4 underestimated by the model. The very high and the very low concentrations observed at KB20 and KB4 suggest the presence of preferential flow in the system. Large increases in the parameter uncertainties could not capture the high concentrations observed at KB4, or the low concentrations at KB20. This situation shows the difficulty inherent in validating continuum models for systems that behave in a nonuniform manner. It should be noted that for a set of strongly conditioned parameters (results not shown further), the chloride concentrations observed at most of the other validation boreholes would also fall outside of the 95% confidence interval. The degree of conditioning, therefore, may be chosen on the basis of the performance of the validation analysis.

Prediction

Using the parameter set obtained by inverse analysis, we predicted the chloride distribution for the year 2020. The expected chloride distribution and associated standard deviation are shown in Figures 11 and 12, respectively. The calculations required estimates of the amounts of chloride released from the different landfill compartments. Figure 5 shows three typical behaviors from May 1986 to October 1994. Inputs from compartments 6 and 7 show a general downward trend, while the input from compartment 4 somewhat increases, at least until t = 50 months. We acknowledge that future chloride inputs into the system (to the year 2020) will be difficult to quantify. The release of leachate from a landfill, in any real situation, is probably one of the most difficult and uncertain variables to quantify. In our example we assumed that the chloride input from each compartment followed an exponentially decaying function, plus a random fluctuation. The random fluctuation was further assumed to have a normal distribution with a mean of zero and a known variance. The variance was calculated by removing the trends and obtaining the average of the running variances from May 1986 to October 1994.

We emphasize that the Bayesian distributions of the chloride concentration at a given point were not normal but exhibited a long

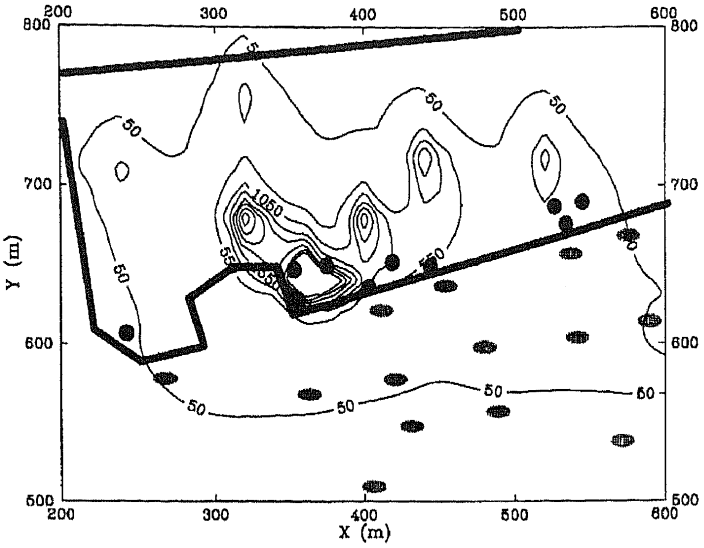

Figure 11. Predicted distribution of the expected value of the chloride concentration around the landfill area in the year 2020. Also shown are the locations of the pumps and the observation boreholes.

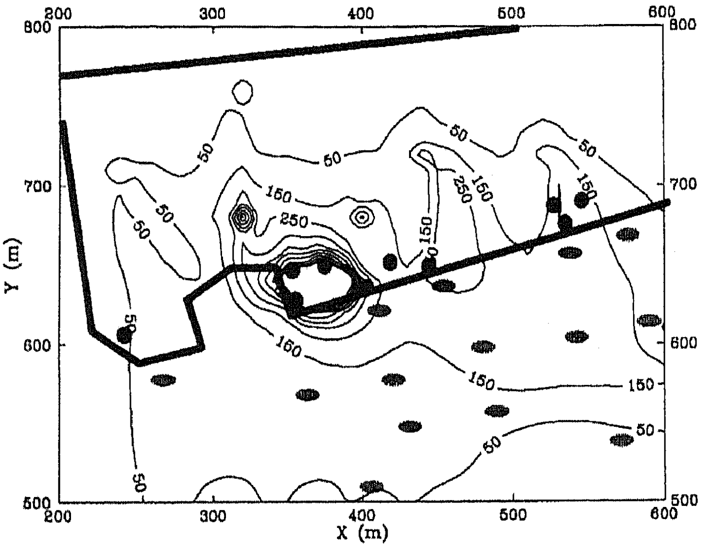

Figure 12. Standard deviation of the predicted chloride distribution in Figure 11.

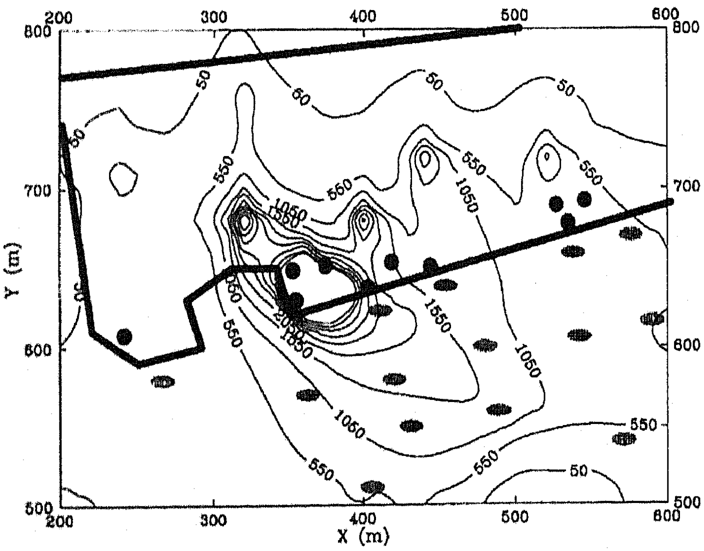

Figure 13. Predicted distribution of the chloride concentration at the upper 95% confidence interval of the Bayesian distribution in the year 2020.

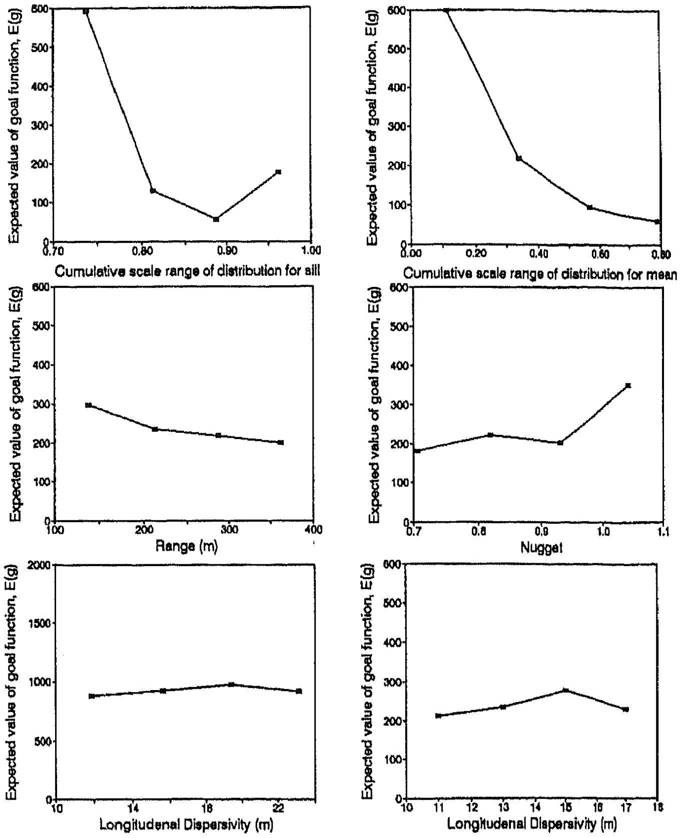

Figure 14. Sensitivity of the expected goal to the six state parameters. The graphs are based on the conditioned parameters.

upper tail. To demonstrate this feature, we plotted the chloride distribution associated with the upper 95% confidence interval in Figure 13. Figure 11 shows that the expected chloride plume will stay in the landfill vicinity until the year 2020. The distribution of the standard deviation of the chloride concentration in Figure 12, while suggesting the formation of a plume in the general direction of ground water flow, further confirms that the plume will stay within or in the immediate vicinity of the landfill. The distribution of the chloride concentration at the 5% significant level in Figure 13, however, revealed the formation of a distinct plume in the direction of flow, with a large amount of chloride moving far away from the landfill. This observation underlines the importance of obtaining a Bayesian distribution of the output, rather than only the first two moments. Based on the proposed uncertainty analysis, therefore, we would conclude that the present measures taken to contain the landfill are inadequate.

Sensitivity Analysis

Finally, we show the sensitivity of the goal function to the six parameters in Figure 14. In this analysis we kept the value of the parameter under consideration constant, while propagating the uncertainty of the other parameters as before and then calculating the expected value of the goal function. These steps were repeated for several values of the parameter under consideration. The results in Figure 14 were obtained with the mildly conditioned parameters. The plots in Figure 14 clearly show that the sill and the mean of the hydraulic conductivity probability model are the most sensitive parameters to the goal, and the dispersivity and porosity are the least sensitive.

Summary and Conclusions

In this paper we demonstrate the applicability of the BUDA uncertainty assessment program to analysis of a landfill problem. After selecting the state parameters, we quantified their uncertainty based on the available knowledge, propagated the uncertainties through a transport simulation program to a goal function, decreased the initial estimates of the uncertainty in the state parameters and, subsequently, in the goal function by means of an inverse procedure, and finally increased the prediction accuracy by taking four more hydraulic conductivity data as suggested by a data worth analysis. The procedures employed in BUDA are suitable for analyses of environmental projects as they take into account the natural uncertainty of most or all environmental data. Our analyses indicate that propagation of input uncertainty can lead to a large estimation variance. We also noticed that model validation can be difficult in the presence of nonuniform system behavior such as preferential flow. Furthermore, the importance of obtaining the entire Bayesian distribution of the output was demonstrated by plotting the chloride distribution at the 5% significance level. We conclude by stating that the procedures in BUDA, while respecting the special features of information available in environmental studies, provide a rational and unified framework for analyses of system uncertainty and risk.

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