Hydrogeological Decision Analysis:  
1. A Framework

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Abstract

This paper is the first in a four-part series that describes the application of decision analysis to engineering design for projects in which the hydrogeological environment plays an important role. The methodology is well-suited to the design of containment facilities at new waste-management facilities, purge-well networks in contaminant remediation applications, or drainage systems in geotechnical projects. It is based on a risk-based philosophy of engineering design. It involves the coupling of three separate models: a decision model based on a risk-cost-benefit objective function, a simulation model for ground-water flow and transport, and an uncertainty model that encompasses both geological uncertainty and parameter uncertainty. The approach can be used for the comparison of alternative engineered components of a system, for the design of monitoring systems, and for the assessment of data worth in the design of site investigation programs. This first paper lays the framework; the subsequent papers describe how the methods can be applied in geotechnical and waste-management applications.

1.0 Introduction

The process of engineering design is often described as a sequence of decisions between alternatives under conditions of uncertainty. This is a particularly apt definition for the types of engineering projects that arise in a hydrogeological context. Hydrogeologists and engineers are often asked to address alternatives: Can we dewater a site with five wells, or do we need ten? Can we attain waste containment with a single liner, or do we need two? Can we satisfy regulatory compliance with monitoring wells on 500-foot spacings, or does it have to be 100?

Moreover, in engineering projects that require a knowledge of the hydrogeological environment, uncertainty as to the system properties and expected conditions is far greater than in most traditional engineering practice. Not only do we have uncertainty as to the parameter values needed for our design calculations, we even have uncertainty about the very geometry of the system we are trying to analyze. The uncertainties of lithology, stratigraphy, and structure introduce a level of complexity to geotechnical and hydrogeological analysis that is completely unknown in other engineering disciplines.

Decision-makers base their decisions on an economic analysis of the alternatives. This analysis takes into account the costs and benefits of each alternative, but it must also give weight to the associated risks. Risks reflect uncertainty, and in many hydrogeological settings, the risks associated with decision-making are high.

This is the first of a series of articles that will describe the application of decision analysis in engineering projects that have a hydrogeological component. Decision analysis provides the link between the economic framework in which decisions are made and the results of the technical analyses on which decisions are based. The methodology is well-suited to systems with large uncertainties and high risks. It has proven itself in the design of large dams and in nuclear engineering applications. We believe that its application in hydrogeological projects has the potential to lead to cost savings in the design of dewatering systems, waste-containment facilities, and remedial projects involving the cleanup of contaminated ground water. It is well-suited to the design of site-investigation programs and monitoring

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Received July 1989, revised January 1990, accepted January 1990.

Discussion open until March 1, 1991.
networks, and it can be used to assess the potential worth of additional data from either source.

In this first paper of the series, we provide a complete outline of the method from beginning to end, but we do so at a conceptual level without detailed examples. The examples will follow in subsequent papers. We will show how an uncertainty model can be coupled with a hydrogeological simulation model and an economic decision model to provide a rational tool for decision-making. The methodology rests on a risk-based philosophy of engineering design, in which the risk of failing to meet design objectives reflects the uncertainty in the technical analysis. It is best carried out in a Bayesian framework in which prior uncertainties are reduced to lesser posterior uncertainties as additional field data are collected. It makes use of conditional and unconditional simulations, and it can be carried out in a direct or inverse mode.

We recognize that some or all of these concepts may be new to many practicing hydrogeologists. We believe that they have considerable value in practice, and it is for this reason that we believe a series of review articles on hydrogeological decision analysis is timely. The emphasis in the body of the papers will be on concepts and methodology. The necessary theoretical background will be presented in appendices. Detailed theoretical treatments will be referenced but not presented.

It is not necessary that the methodology presented in these papers be accepted in total, nor, we hope, will it be rejected outright. It is modular in nature, and there are many alternative approaches for each of the modules. We will try to draw attention to these alternatives by reference. In one sense, we are providing the reader with a set of analytical tools, but in a broader sense, we are trying to popularize a set of ideas. We believe that these ideas have a great potential to rationalize the decision-making procedures that are required in the current hydrogeological environment of technical, legal, economic, and political complexity.

1.1 Engineering Design: Objectives, Constraints, and Decision Variables

Most engineering projects have a single primary technical objective that drives the design. Many projects must try to meet their objective within a set of technical, legal, or political constraints.

When uncertainty arises, it is no longer possible to ensure that a particular engineering design will meet both the objective and the constraints with certainty. In these circumstances, the design problem is usually couched in one of two ways: either the objective is set up so that it will always be satisfied but there is some probability that the constraints will not be met; or the constraints are set up so that they will always be satisfied but there is some probability that the objective will not be met.

Engineering alternatives are differentiated from one another on the basis of their technical components. The variables that can be used to define and differentiate alternatives are known as decision variables. A better understanding of objectives, constraints, and decision variables is best gleaned by looking at some examples:

![Diagram of an aquifer development problem](image)

**Fig. 1. Aquifer development problem.**

1.1.1 Water-Supply Applications

Consider the simple aquifer development problem shown in Figure 1. The objective is to develop a groundwater supply that will deliver water to a private or municipal-water system at the demand rate $Q_d$. The project may be subject to a constraint whereby the drawdowns are limited to a value $\Delta h$. The constraint may apply at all points in the aquifer, or possibly at a single compliance point, B, where a regulatory monitoring well is to be established.

Assuming that the aquifer is a relatively thin one and that the wells are to be screened across the full thickness of the aquifer, the design questions at hand are: How many wells should be installed? Where should they be located? And, what should be their pumping rates? Those questions define the decision variables as the number of wells, N, the pumping rates, $Q_i(x_i, y_i), i = 1 \ldots N$, and the locations, $(x_i, y_i), i = 1 \ldots N$.

Decision analysis identifies the best alternative from a suite of specified alternatives. For example, in the case at hand, if the demand, $Q_d$, were 1000 gpm, one might examine 5-10 alternatives, each involving 1 to 4 wells, and each with various patterns, spacings, and pumping rates, such that $\Sigma Q_i \geq 1000$ and $\Delta h$ is not exceeded at point B.

The detailed discussion of how to determine which alternative is "best" is postponed until later in the paper, but it should be clear that the decision is based on economics. It will depend on the income that can be generated by producing the water (the benefits), the capital costs and operational costs of producing the water (the costs), and the probabilistic costs associated with failing to meet the objective or the constraint (the risk). The probability of failing to meet the objective or the constraint will be largely dependent on our estimates of the transmissivity and storativity of the aquifer. The probabilistic costs associated with producing excessive drawdowns would revolve around potential regulatory penalties imposed by a watermaster or water-management district, the cost of well deepening or well replacement for nearby residents, and/or the litigation costs associated with such penalties and claims. The probabilistic costs associated with failing to meet the demand would revolve around the
client's willingness to pay, possible litigation, and/or loss of reputation and goodwill.

The water-supply problem will not be discussed further in this sequence of papers. It has been treated in a coupled technical/economic context more so than any of the other hydrogeologic design problems raised in these papers (cf. Bredhoefit and Young, 1970), although it has not been treated in the specific manner recommended here.

1.1.2 Geotechnical Applications

Ground-water control has become a vital part of many modern geotechnical projects. Problems frequently encountered include stability of natural and excavated slopes and excessive seepage into excavations and underground openings. To achieve dewatering targets, the design engineer will typically introduce a ground-water control system that may include dewatering wells, horizontal drains, and/or drainage galleries. Dewatering schemes are expensive; in many cases it is difficult to establish the point at which additional dewatering costs are no longer justified by reductions in risk of failure. The design approach proposed in this paper lends itself naturally to the solution of such problems.

Consider the problem of designing the slope in a large open pit mine, portrayed in Figure 2. The design objective is to excavate the steepest possible pit wall because a slope increase of only one degree will reduce operating costs by several millions of dollars. However, deepening the pit wall also increases the risk of slope failure. By improving stability, ground-water control allows the mine operator to excavate at a steeper angle while maintaining an acceptable risk of failure. In this problem, the design variables include the pit wall angle, and the type, spacing, depth, and pumping rates of the dewatering wells or drains. The third paper in this series will examine how the risk-based design approach, coupled with an analysis of ground-water flow and slope stability, can be used to identify the best dewatering strategy and slope design.

1.1.3 Waste-Management Applications

One of the potential areas of greatest current interest for the application of risk-based design procedures lies in the siting and design of new waste-management facilities, and the design of remedial activities at facilities where groundwater contamination incidents have already occurred.

Consider the question of siting in Figure 3. Alternative sites along a rivershore are under consideration for a landfill. The decision variable here is the location of the landfill. The objective of the owner-operator will be to get the landfill sited and into profitable operation. A state or federal environmental agency will provide the constraints in the form of maximum concentration limits for a set of priority pollutants at compliance points such as B or C. Alternatively, siting regulations may focus on pre-waste-emplacement advective ground-water travel time from the source to a compliance point; this too would constitute a design constraint. The mechanism of failure would require leakage from the landfill and the migration of a plume past the compliance points. The probability of such an event would depend both on the engineered barriers at the landfill and on estimates of the hydraulic conductivity and porosity of the geological materials.

If a site has already been chosen, and alternative containment strategies are under assessment, the decision variables will reflect alternative answers to such questions as: How many liners should be used? Should liners be synthetic or natural materials? What should be the design specifications for the thickness and permeability of synthetic liners? Is a leachate collection system necessary? A cap? Drainage? And so on.

Suppose an existing facility requires remediation of an unacceptable contaminant plume as shown in Figure 4. The landfill has been closed by a regulatory agency and the objective of the owner-operator is to get his facility on-line again. The constraints are concentration limits at compliance point C. Preliminary assessment of alternatives has limited attention to pump-and-treat scenarios. The technical objective is to create a capture zone that prevents migration past AB and encompasses the entire plume and source area. The problem is an entirely different one from the water-supply problem or the excavation-dewatering problem presented earlier, but the decision variables are the same: the number, depth, location, and pumping schedules of the purge wells.
In the remainder of this paper, the conceptual framework will be presented in a general context. The methodology is equally applicable to any of the myriad engineering design problems that might be encountered in water-supply, geotechnical, or agricultural projects where there is a hydro-geological component. The second paper in this series will describe how the methodology might be applied in a waste-management context, both with respect to new-facility design, and remedial action. The third paper will provide a geotechnical example, in the form of risk-based design of dewatering systems in aid of slope stability. The final paper in the series will be addressed to questions of data worth and the design of site investigation programs.

1.2 The Design Process as an Integrated Sequence Involving Economic Tradeoffs

Consider as an example the design process at a new landfill. It involves a sequence of at least four steps: (1) site screening, (2) site investigation at the selected site, (3) design of the containment facility, and (4) design of the monitoring network. Each of these steps involves a decision process among alternatives. Which site should be selected? How many holes will be drilled during site investigation? How many liners are needed for containment? How many monitoring points are needed?

In the traditional approach, there has been a tendency to treat each of these decision processes independently. They are carried out sequentially, and decisions in the later steps are postponed until the results arising from the decisions made in earlier steps are available.

We espouse a more integrated decision process in which a set of alternatives are lined out in such a way that each alternative covers the entire design process. This allows the owner-operator to assess economic tradeoffs between the various steps. Once a site has been selected, for example, would it be better to use minimal site investigation and a conservative design, or on the contrary, would it be better to carry out a detailed site investigation in the hopes of buying reduced construction costs? The owner-operator would like to know how to partition his resources among the competing requirements of site investigation, containment, and monitoring.

Consider the three alternatives lined out in Table 1. Alternatives 1 and 2 utilize the same levels of site investigation and monitoring. Presumably, the specifications for each drillhole (e.g. geologic logging, geophysical logging, hydraulic conductivity testing, etc.), and for each monitoring well (e.g. depths to be sampled, frequency of sampling, etc.), are also the same. Alternative 2 differs from Alternative 1 only in the fact that it offers more conservative containment design. The question at hand: Is the addition of the direct cost of the second liner offset by an equivalent or greater reduction in the probabilistic cost associated with a reduced risk of failure? If Alternative 3 is compared with Alternative 2, it can be seen that the issue here is one of tradeoff. Does a reduced site investigation, coupled with a more conservative monitoring scheme, constitute a better design strategy?

It must be emphasized at this point that the integrated approach does not require that all decisions be reached at the beginning before site investigation results can be assessed. On the contrary, as will become clear later, we espouse a sequentially iterative decision process whereby decisions are constantly reassessed and updated as additional site information becomes available. But at each of these decision points, it is the fully integrated alternatives that are assessed.

1.3 The Complexity of the Design Environment

Engineering design in a hydrogeological context is carried out in a complex technical, economic, legal, and political environment.

The geological environment is often heterogeneous and complex. The hydrogeological conditions are usually uncertain. The engineering project, itself, involves many interdependent components. Decisions between alternative courses of action are based on economic decision-making. They are often subject to constraints that arise from the legal regulatory framework. The entire process is carried out in an adversarial environment in the political arena.

In hydrogeological projects, approaches to engineering design that take into account only the technical factors are not suitable in this day and age. The design framework outlined in this paper provides the necessary integration of the technical and social aspects of the decision-making milieus.

The philosophy of design in a regulated environment is worthy of comment. In earlier decades, prior to the establishment of strict regulatory control over environmental protection, hydrogeologists and design engineers attempted...
to meet their technical and economic objectives within the self-imposed constraint that their designs protect the health and safety of the public and meet their aesthetic desires. In a regulated environment, protection of the health and safety of the public seems to have been taken over by the regulatory agencies, and most hydrogeologists and engineers would now feel that they have satisfied their ethical requirements if their designs meet the regulatory standards imposed by the regulatory agencies. Many engineers and hydrogeologists are seriously concerned about this development, and we share that concern, but it seems to now be a fact of life, and our design framework therefore reflects this reading of the current situation.

1.4 Approaches to Design

In this section, we review the classical safety factor approach to design, contrast it with the risk-balancing approach, and introduce the ideas behind a Bayesian design philosophy. In order to avoid confusion, we will first introduce and define some common terms.

The terms parameter and variable will be used in a threefold sense. We differentiate between: (1) hydrogeological parameters, (2) dependent variables, and (3) decision variables. Hydrogeological parameters include all media properties such as porosity, hydraulic conductivity, storativity, transmissivity, dispersivity, and the like. The dependent variables in ground-water contamination analyses are the hydraulic head (which is the dependent variable in the flow equation) and the concentration (which is the dependent variable in the transport equation). In direct simulations, the hydrogeological parameters are the input, and the dependent variables are the output. Secondary output variables, such as velocities, gradients, or travel times, are often calculated from the primary simulation output. Examples of decision variables have been given earlier. They are the engineering input variables used to define design alternatives. The decision variables for waste containment, for example, would include the number of liners, and the specifications for liner thickness and permeability.

Hydrogeological parameters are usually assumed to be time-invariant. They can be homogeneous or heterogeneous over space, and in either case, the parameter values may be viewed as certain or uncertain. The relationship between heterogeneity and uncertainty is explored more fully later in this paper.

The terms stochastic and deterministic are used in their usual sense. If a heterogeneous and/or uncertain input hydrogeological parameter is specified as having a distribution in probability, then so too will the output dependent variables. A stochastic analysis will be required to relate the two. If the hydrogeological parameters are known with certainty, or if most-likely representative values are used, then a deterministic analysis is possible. If the method of analysis involves a finite-difference or finite-element flow and/or transport model, then a deterministic analysis will require only one simulation, whereas a stochastic analysis using Monte Carlo simulation would require hundreds or thousands of runs.

1.4.1 Deterministic Safety-Factor Approach

In the traditional approach to engineering design, a safety factor, $F$, is defined as:

$$ F = \frac{C}{L} \tag{1} $$

where $C$ is the capacity, and $L$ is the load of the engineered system. The design approach typically involves calculating the capacity, $C$, and designing the project loads, $L$, such that the project satisfies a predetermined safety factor. In a slope stability context, where safety factors are widely used, the capacity, $C$, is calculated in terms of soil strength and the load, $L$, in terms of the soil stresses that are expected to develop under the proposed slope design.

In a regulated design environment, the capacity, $C$, often takes the form of a regulatory constraint that must be met. In a waste-management context, the safety factor might be specified in terms of contaminant concentration, with the capacity, $C$, defined as the allowable concentration, at a compliance point and the load, $L$, as the actual concentration that will develop there under the waste-management design.

If the safety factor is defined in terms of travel times, inverse values must be used because longer travel times are more desirable than shorter ones. As an example, consider liner design for a new landfill situated as in Figure 3. Let us assume that the only technical objective is to meet a regulatory constraint on pre-emplacement advective ground-water travel time from inside the engineered containment at $A$ to a regulatory compliance point at $B$. The capacity, $C$, would be defined as $1/T$, where $T$ is the allowable regulatory travel time, and the load, $L$, as $1/\tau_{AB}$, where $\tau_{AB}$ is the actual travel time. For a specified safety factor, $F$, it is therefore necessary that the liner design assure that $\tau_{AB} \geq FT$. The travel time, $\tau_{AB}$, is the sum of (1) the time until the liner breaches, $t^*$, and (2) the plume migration time, $t^{**}$. A deterministic analysis for $t^{**}$ would be carried out based on representative values of the hydraulic gradient, porosity, and hydraulic conductivity of the geologic materials at the site. The liner specifications would then be set so that $t^* = FT - t^{**}$.

1.4.2 Stochastic Risk-Balancing Approach

In recent years, it has been recognized (cf. Wu, 1974; Yen, 1978; Ang and Tang, 1984; Whitman, 1984) that a stochastic approach to design is more realistic. In this case, as shown in Figure 5(a), the load and the capacity are represented as probability density functions, and the probability of failure, $P_f$, is defined as the probability that $L$ exceeds $C$. A safety margin, $SM$, can be defined as the difference between capacity and load:

$$ SM = C - L \tag{2} $$

The probability of failure is equal to the probability that the safety margin is less than zero. In fact, if $L$ and $C$ are assumed to be normally distributed and independent, with means, $L$ and $C$, and standard deviations, $S_l$ and $S_C$, then it can be shown that the safety margin, $SM$, is also normally distributed [Figure 5(b)], with mean:
Fig. 5. (a) PDF's for load L and capacity C; (b) PDF for safety margin SM, showing probability of failure \( P_f \); (c) relation between SM and \( P_f \).

\[
\overline{SM} = \overline{C} - \overline{L}
\]  

and standard deviation:

\[
S_{SM} = \sqrt{S_C^2 + S_L^2}
\]

For any given suite of values of \( \overline{L}, \overline{C}, S_L, \) and \( S_C \), there is a fixed and calculable relationship between the mean safety margin, and the probability of failure, \( P_f \). Two such relationships are illustrated on Figure 5(c). In this figure, it has been assumed that the capacity, \( C \), is known with certainty (i.e., \( S_C = 0 \)). The curve for “high \( S_L \)” would apply to a case where there is considerable uncertainty in the load, \( L \). The curve for “low \( S_L \)” would apply to a case where there is less uncertainty. It can be seen from the diagram that a mean safety margin of 2.0 would imply a probability of failure of \( 10^{-4} \) in the more certain case but only \( 10^{-1} \) in the uncertain case. Even large values of SM have finite values of \( P_f \).

In the risk-balancing approach to design, it is common to use the probability of failure, \( P_f \), as the measure of design uncertainty. This probability of failure, when multiplied by the dollar consequences of failure constitutes the risk, which has units of dollars, and which can be included with the direct benefits and costs in a risk-cost-benefit objective function in an economic decision-making framework.

Perhaps to offset the negative connotations of the term probability of failure, some supporters of this approach (cf. Harr, 1987) prefer to work with the inverse, \( L - P_f \), which they term the reliability. They then refer to this approach to engineering design as the reliability-based approach. We do not avoid the loaded implication of announcing the existence of a probability of failure, preferring the more candid approach of educating the public to this reality.

### 1.4.3 Bayesian Design Philosophy

The methodology described in these papers is carried out within a Bayesian framework. This section is designed to provide the reader with some early appreciation of what this entails.

It is easiest to start from a statistical perspective, where there have always been two philosophical camps; those who espouse classical statistics, and those who espouse Bayesian statistics. Classical statistics require the development of a probability density function based on measured data. Estimates of the mean and variance of the data set, or the use of such statistics to test hypotheses, must await the existence of sufficient data to allow the form of the probability density function to be established, and to assure that the desired level of confidence in the estimates has been reached. When additional data become available, they are used to enlarge the data set, and the summary statistics are recalculated with a higher level of confidence.

With a Bayesian statistical approach, a prior estimate of the form of the probability density function and its summary statistics is made. This prior estimate may be based on limited early data, or it may be based on subjective information that is available in the form of experience and personal judgment, even before any measurements are taken. When additional data become available, they are used to update the prior estimates of the statistics to posterior estimates using Bayes theorem. The posterior estimates are influenced both by the new data and by the prior estimates. Under sparse data conditions, the Bayesian statistical estimates could be quite different from the classical statistical estimates for the same data set. As the data set becomes larger, the two sets of estimates converge.

In a hydrogeological context, data sets for porosity or hydraulic conductivity are commonly very sparse, and a classical statistical analysis may suggest that little has been learned from early measurement programs. It seems right and proper to allow the experience gained at other sites, or the implications that can be gleaned from “soft” data at the site, to play a role in reducing uncertainty. In a Bayesian context, this type of information provides the basis for the subjective prior estimates that may still exert considerable influence on posterior estimates following data collection.

In an engineering context, the Bayesian approach fits perfectly into the sequential design framework described earlier, whereby the design engineer iterates between analysis and measurements, as the project progresses. If the analysis takes the form of a hydrogeological simulation model, the Bayesian approach supports the establishment of a preliminary model early in the project, followed by continual updating as field data become available. This is an approach that will find favor with most modelers. It allows for ongoing interaction between the needs of the modeler and the design of a data collection network.

The application of Bayesian updating in a geostatistical context for data sets that represent heterogeneous, uncertain hydrogeological parameters is described later in the
paper. In a later paper it will be seen that Bayesian ideas are fundamental to assessing the value of information and the worth of additional data. For a more detailed introduction to Bayesian decision theory in an engineering context, the reader is directed to Benjamin and Cornell (1970).

1.5 Components of a Design Framework

As illustrated on Figure 6, our design framework has six components: a decision model, a hydrogeological simulation model, an engineering reliability model, a geological uncertainty model, a parameter uncertainty model, and a field investigation program.

The decision model allows for the comparison of alternative sites and/or engineering designs. It is an economic analysis based on a risk-cost-benefit objective function.

The engineering reliability model is used to represent the expected performance of engineered components of the system. The hydrogeological simulation model is used to represent the expected performance of the hydrogeological component of the system. It can be an analytical solution or a numerical model of the hydrogeological system at the site; most often it will probably be a finite-difference or finite-element model of flow and transport. The hydrogeological simulation model and the engineering reliability model are utilized in a stochastic mode; their purpose is to predict the probability of failure which is a component of the risk term in the decision model.

The simulation must be stochastic in order to take into account the uncertainty in the hydrogeological system that always exists in heterogeneous hydrogeological environments. The uncertainty in the geological boundaries is described by the geological uncertainty model and the uncertainty in parameter values is described by the parameter uncertainty model.

The form of the uncertainty models and the values of their parameters are determined from the data generated by the field investigation program. In this paper, the design of field investigation programs is not addressed. This issue is postponed to a later paper in the series which will deal specifically with data worth.

The remainder of this paper provides a more detailed description of the philosophy and concepts underlying the decision model, the simulation model, the reliability model, and the uncertainty models.

2.0 Decision Model

There are many decisions involved in the design of a decision model. Figure 7 provides an organized summary of the issues. Most of the boxes on Figure 7 could apply to any type of hydrogeological design project, but the lowermost box on "Decision Variables" is specific to a waste-management context. In the remainder of this section, we will utilize this context to provide a more detailed discussion of the issues.

2.1 Objective Function

It should be clear from earlier discussions that the technical objective of design in waste-management applications from an owner-operator’s perspective usually involves satisfying a constraint in the form of a regulatory standard. The economic objective of design must be to meet the technical objective in such a way as to maximize the profit (or minimize the loss) to the owner-operator. From his perspective, we can define an objective function as the net present value of the expected stream of benefits, costs, and risks, taken over an engineering time horizon, and discounted at the market interest rate (Crouch and Wilson, 1982). If an objective function, \( \Phi_j \), is defined for each \( j = 1 \ldots N \) alternatives, then the goal is to maximize \( \Phi_j \):

\[
\Phi_j = \sum_{t=0}^{T} \frac{1}{(1+i)^t} [B_j(t) - C_j(t) - R_j(t)]
\]

where \( \Phi_j \) = objective function for alternative \( j \) [\$]; \( B_j(t) \) = benefits of alternative \( j \) in year \( t \) [\$]; \( C_j(t) \) = costs of alternative \( j \) in year \( t \) [\$]; \( R_j(t) \) = risks of alternative \( j \) in year \( t \) [\$]; \( T \) = time horizon [years]; and \( i = \) discount rate [decimal fraction].

The risks \( R(t) \), in (5) are defined as the expected costs associated with the probability of failure:

\[
R(t) = P_f(t) C_f(t) \gamma(C_f)
\]

where \( P_f(t) \) = probability of failure in year \( t \) [decimal fraction]; \( C_f(t) \) = costs associated with failure in year \( t \) [\$]; and \( \gamma(C_f) \) = normalized utility function [decimal fraction, \( \gamma \geq 1 \)].

In equation (5), the \( C(t) \) term represents the costs to the decision-maker and the \( B(t) \) term represents the benefits. If the decision-maker is the owner-operator of a new waste-management facility at the design stage, and a set of alternative conceptual designs are under consideration, then the costs would be the capital costs and operational costs of constructing and operating the waste-management facility under each design, and the benefits would be the revenues for services provided. The probabilistic costs, \( C_f(t) \), that appear in the risk term are those costs that would be incurred only in the event of failure. The utility function, \( \gamma(C_f) \), in equation (6) allows one to take into account the
possible risk-averse tendencies of some decision-makers. It will be discussed more fully in the following subsection.

In equation (5), the $C(t)$ term represents an actual cost to the owner-operator whereas the $R(t)$ term represents a probabilistic cost. One might ask why the actual benefits, $B(t)$, are not balanced by a term for probabilistic benefits. Although we have not seen such a term in the literature, there is value in employing such a term for cases involving remedial action. In this case, we are starting from a failed position and we wish to assess alternative remedial schemes in terms of their probability of success in meeting some performance standard associated with cleanup. Let us define a term of the form:

$$V(t) = P_r(t) B_e(t) \gamma(B_a)$$

(7)

where $P_r(t) = \text{probability of success in year } t \text{ [decimal fraction]}$; $B_e(t) = \text{benefits associated with success in year } t \text{ [S]}$; and $\gamma(B_a) = \text{normalized utility function [decimal fraction]}$. If the $V(t)$ term is incorporated, the objective function becomes:

$$\Phi_j = \frac{1}{(1+i)^t} \sum_{t=0}^{T} \frac{B_j(t) - C_j(t) + V_j(t) - R_j(t)}{\text{for all } j}$$

(8)

It is worth noting in equations (5)-(8) that almost all the terms are economic. The technical input to the objective function comes only in the two probability terms, $P_r(t)$ and $P_p(t)$. This identifies more clearly that the role of the simulation model in the decision-making process is to predict the probabilities of failure or success of the design alternatives under assessment.

### 2.2 Utility, Risk-Aversion, and Risk-Perception

The risk-analysis literature (cf. Lindley, 1971; Fischhoff et al., 1981; Crouch and Wilson, 1982) has always touted the concept of utility for use in the risk term of a decision analysis.

The concept of utility encompasses the second and third terms on the right-hand side of equation (6). Utilities are numerical measures used to quantify the relative desirability of consequences or outcomes. Utility theory holds that decision-makers often do not make decisions on the basis of the expected cost associated with failure. Rather, they exhibit their risk-averseness by multiplying these expected costs by a factor which is thought to depend on the level of expected failure costs relative to the net worth of the decision-maker.

The role of the normalized utility function, $\gamma(C_j)$, used in (6) is to incorporate risk-averseness into the objective function. For risk-averse behaviour, $\gamma > 1$, and for risk-neutral behaviour, $\gamma = 1$. Small owner-operators who do not have a large net worth are the most likely to use a risk-averse utility function. Larger companies are more likely to take a risk-neutral approach. Risk-aversion is also influenced by the availability of liability insurance.

Risk-aversion should not be confused with risk-perception. People usually do not have a realistic estimate of their risk due to actual or perceived threats. This causes them to overestimate the expected value of $C_j$. From the

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Fig. 7. Components of a decision model.
point of view of the owner-operator, his perceived risk is the one he should apply in a risk-cost-benefit analysis; he is the decision-maker and he has the right to take into account his perceptions as well as his aversions. The more experienced a company is in the waste-management industry, the more likely they are to have accurate risk-perceptions.

Having raised the issues of risk-aversion and risk-perception, we now propose to dismiss them, at least for the remainder of this lead article. We will assume from here on that our decision-makers come from large experienced companies with a realistic view of the $C_f$ terms, and that they are willing to set the $\gamma$-terms in equations (6) and (7) equal to unity for all $C_f$.

### 2.3 Failure and Success

The calculation of the probability of failure, $P_f(t)$, or the probability of success, $P_s(t)$, requires definitions of failure and success. We define **failure** with respect to a new waste-management facility, as a ground-water contamination incident that violates a performance standard at a regulatory compliance point. We define **success** with respect to a remedial program at a contaminated facility, as a cleanup program that satisfies a performance standard at a regulatory compliance point.

Among the possible compliance points or compliance surfaces where performance standards might be invoked for a new facility (Cartwright et al., 1981; Domenico and Palciauskas, 1982; LeGrand, 1982) are: (1) the zone between the liners at a multilinear installation, (2) the outside boundary of the containment facility, (3) the boundary of the physical plant of the waste-management facility, (4) the property boundary, or (5) a downstream well-field, aquifer, stream, or lake. For remedial programs, compliance might be required: (1) inside the plume, (2) at the plume boundaries, or (3) at a downstream well-field, aquifer, stream, or lake.

For new landfills, performance standards usually take the form of maximum concentration limits for particular chemical species in a regulatory monitoring well. Similar performance standards are commonly established for remedial programs. In the siting of a high-level nuclear-waste repository, one of the primary performance standards involves the pre-waste-emplacement advective ground-water travel time from the repository to a compliance point. The methodology described in this paper is equally applicable to either of these types of performance standard.

Before closing this section we want to draw the reader’s attention to the fact that in the earlier section that introduced the stochastic risk-balancing approach to design, the probability of failure, $P_f$, was treated as a time-independent parameter, whereas in equation (6) it appears as a time-dependent parameter, $P_f(t)$. The concepts are unchanged. We have simply recognized the more realistic situation where the capacities and/or loads are time-dependent and so too, therefore, is the probability of failure.

In the extended objective function represented by equation (8), it is our intention that either the failure term, $R_f(t)$, or the success term, $V_s(t)$, be used, but not both. We anticipate that the $R_f(t)$ term will be used for decision analyses involving new facilities, and the $V_s(t)$ term will be used for decision analyses involving remedial actions. For any particular analysis, it could be argued that $P_s = 1 - P_f$, in which case the two terms are not independent and there is no need for both. In this case, the "probability of success" is equivalent to the "reliability" as defined earlier.

In this section, we have placed the emphasis on regulatory performance standards. It is also possible for regulatory agencies to set design standards in the form of liner specifications, monitoring-well requirements, and the like. The risk-cost-benefit framework can easily include the impact of design standards on the decision analysis.

### 2.4 Probabilistic Costs and Benefits

The probabilistic costs, $C_f(t)$, that appear in the risk term associated with the probability of failure are those that would be incurred only in the event of failure. They would include any fines, taxes, or charges that might be levied by the regulatory agency for failure to meet the performance standards; the costs of litigation should any arise; the costs of remedial action; and the value of any revenues foregone if operations must be curtailed or stopped. It is also becoming clear that there is often considerable loss of goodwill in the community associated with ground-water contamination incidents.

In some regulatory jurisdictions it is becoming common to require the posting of a performance bond before construction of a waste-management facility. A failure would result in a withholding of the return of the performance bond.

The probabilistic benefits, $B_s(t)$, associated with success in a remedial cleanup could include permission to reopen a waste-management facility, the removal of legal liability, and the return of community goodwill.

### 2.5 Perspective of the Decision-Maker, Time Horizon, Discount Rate, and Decision Variables

Throughout this article, we have tended to present the decision analysis framework from the perspective of the owner-operator of a waste-management facility. From this perspective, the pertinent time horizon for decision-making is a relatively short one, on the order of 20-50 years, and the pertinent discount rate is the market interest rate on borrowed money. The decision variables that he will have under consideration are those listed on Figure 7. Figure 8 is a schematic plot of the cost-flow situation faced by a new facility (after Dieter, 1983).

The discount rate and the time horizon are not really independent in a net-present-value economic analysis. It can be shown (cf. Dieter, 1983) that for a discount rate of 10%, the net present value of future dollars approaches zero for periods more than about 50 years into the future. A rational decision-maker will not use a time horizon longer than the economic period indicated by the time value of money.

The siting, licensing, and construction of a waste-management facility usually takes place in an adversarial political environment. There are many other players in the game; among them are regulatory agencies, host communities, insurance companies, and environmental lobby groups.
Each has their own perspective and each can define their own benefits, costs, and risks. The regulatory agency, for example, which presumably works in the public interest, would define societal benefits in terms of the value of clean ground water, and societal risks in terms of human health and environmental protection. Their time horizon would be longer and their discount rate lower than that used by an owner-operator. In principle, the decision-analysis framework described in this paper could be applied by any of these decision-makers, although as Massmann and Freeze (1987a, 1987b) point out, there are real difficulties in assigning dollar values to resource commodities and to human health and life. Societal decision-making, in the context of groundwater contamination, is addressed more fully in the works of Raucher (1983, 1984); Sharefkin, Schacter, and Kneese (1984); Schacter (1985); and Kaunas and Haines (1985).

2.6 Optimal Risk and Acceptable Risk

For the purposes of this discussion, let us separate out the three terms of the objective function (5), so that:

\[
\Sigma B = \sum_{t=0}^{T} \frac{1}{(1+i)^t} [B(t)]
\]

(9a)

\[
\Sigma C = \sum_{t=0}^{T} \frac{1}{(1+i)^t} [C(t)]
\]

(9b)

\[
\Sigma R = \sum_{t=0}^{T} \frac{1}{(1+i)^t} [R(t)]
\]

(9c)

Let us assume that we are involved in a project with no direct revenues, so that \(\Sigma B = 0\), and the decision analysis reduces to a risk-cost minimization. Let us further assume that a set of alternatives have been analyzed and \(\Sigma C, \Sigma R\), and the objective function, \(\Phi\), have been calculated for each. These values could be plotted as in Figure 9. This figure illustrates the tradeoff that exists between the actual costs of design and operation, \(\Sigma C\), and the probabilistic costs associated with failure, \(\Sigma R\). The optimal alternative is the one that maximizes \(\Phi\) (i.e., the one that minimizes \(-\Phi\)), and the risk associated with this alternative constitutes the optimal risk from the owner-operator's perspective.

Acceptable risk is a societal concept. It is indirectly set on behalf of society by the regulatory agencies. If it is their perception that the optimal risk from the owner-operator's perspective is greater than the acceptable risk, then they should increase the regulatory penalties in such a way that they drive the owner-operator's optimal risk closer to that which society considers acceptable.

2.7 Decision Analysis and Optimization

Engineering systems analysis can be carried out in either a decision-analysis framework or an optimization framework. Optimization involves the determination of optimal values for a set of decision variables in an engineering system. Optimality is defined with respect to a specified objective function and is subject to a set of constraints. Decision analysis involves the determination of the best alternative from a discrete set of specific alternatives. Preference is based on a specified objective function. Optimization is a more general approach than decision analysis in that it provides the optimal alternative from the set of all possible alternatives, whereas decision analysis provides only the best alternative from a specified set of alternatives. Gorelick (1983) provides a review of available optimization techniques in a hydrogeological context. Lefkoff and Gorelick (1987) provide a user's manual to their linear optimization program, AQMAN, which can be applied to many of the engineering design problems discussed in this paper.

However, there are two types of limitation that can constrain the applicability of currently available optimization models. First, most methods are based on a linear programming approach, and this approach requires a linear objective function, linear constraints, and linear flow equations in the simulation model (if such a model is part of the
optimization system). The latter part of this limitation obviates application to unconfined surficial aquifers, unless simplifying assumptions can be invoked to linearize the flow equations. Second, it has been traditional to apply optimization techniques in a deterministic framework, so that such methods are not suitable for risk analysis or other probabilistic approaches to making decisions.

Both these limitations are currently being removed by researchers in the field. On the linearity front, Gorelick et al. (1984) provide a deterministic, nonlinear programming solution to a plume capture problem. On the stochastic front, Wagner and Gorelick (1987) present a chance-constrained optimization solution to the plume capture problem, and Tung (1986) describes a chance-constrained model in a ground-water management context. In a chance-constrained optimization scheme, the probability of failing to meet a constraint is allowed, but is not usually coupled with the cost of failure to produce a risk. If it were, the benefits and costs would appear in the objective function, and the risks in the constraints. The structure of a decision analysis, on the other hand, puts the costs, benefits, and risks all into dollar terms, and all into the objective function. The objectives and constraints are thus treated in an integrated consistent fashion.

In summary, decision analysis is less general than optimization, but it suffers no limitations with respect to linearity or stochastic application, and it is well-suited to the risk-based philosophy of engineering design.

### 2.8 Alternative Objective Functions

The risk-cost-benefit objective function defined by equations (5) or (8) is suited to a decision-maker who wishes to maximize the net present value of his expected stream of benefits, costs, and risks. While this decision criterion is rational and widely used, it is not the only available criterion. Alternative objective functions are discussed in Appendix I.

The risk-cost-benefit approach is based on calculation of the probability of failure, $P_f$, or the reliability, $1 - P_f$. Hashimoto et al. (1982a, 1982b) have suggested that reliability does not provide a complete measure of technical performance. They introduce the concept of robustness in engineering design. A design is robust if it has the flexibility to permit adaptation to a wide range of potential conditions at little cost. When there is large uncertainty in future loads, robustness is very desirable. There may be economic tradeoffs available between reliability and robustness.

Figure 10 (adapted from Crouch and Wilson, 1982) summarizes the application of a decision model to a set of alternatives. Our methodology uses the classical net-present-value approach with a risk-cost-benefit objective function. We do not consider robustness in our decision criterion, although there is no reason why such a concept could not be incorporated if desired.

### 3.0 Engineering Reliability Model

In the design of engineering projects using an objective function like equation (5), it is necessary to calculate the probability of failure in any year $t$, $P_f(t)$. For engineering projects in a hydrogeological context, there are usually two components to the potential failure mechanisms, one component that involves the engineered portion of the facility, and one component that reflects the hydrogeological environment.

In a new waste-management facility, for example, failure would require both that the containment structure be breached, and that the contaminant plume resulting from the breach migrate to a compliance point. If the regulatory criteria are couched in terms of travel time, we require estimates of both the time until breach of containment, $t^*$, and the travel time through the hydrogeological environment, $t^{**}$. Both will be uncertain, the first because of uncertainties in the breach mechanisms, and the second because of uncertainties in the hydrogeological system. Calculation of $P_f(t)$ will require the generation of a probability density function (PDF) for both $t^*$ and $t^{**}$.

In this study, our emphasis is on the hydrogeological component of uncertainty. Consideration of the hydrogeological uncertainties can be handled by a geological uncertainty model and a parameter uncertainty model, and a PDF for $t^{**}$ can be developed by the stochastic application of a hydrogeological simulation model. All three of these model components of our decision framework are described later in this paper.

Consideration of the expected life and potential mortality of the engineered components of the design system, as would be required to estimate a PDF for $t^*$ in the above example, are often handled with a form of engineering reliability theory. Mortality curves usually reflect the potential for early failure caused by faulty manufacture or installation, and the potential for later failure caused by old age or wear. The details will not be presented here. The interested reader is directed to one of the many available reliability textbooks for further information (cf. Ang and Tang, 1984; Harr, 1987). Suffice it to say here that our framework for hydrogeological decision analysis, as outlined on Figure 6, envisages the coupled application of an engineering reliability model to treat the engineered components of the system and a hydrogeological simulation model to treat the hydrogeological components.
4.0 Hydrogeological Simulation Model

The purpose of the simulation model is to provide an estimate of the probability of failure, Pr, for use in the decision model. The simulation model may take the form of an analytical solution, or it may take the form of a numerical model. In either case, it provides a predictive analysis of ground-water flow and/or contaminant transport in the hydrogeological environment. We assume that the readers of this journal have considerable familiarity with this component of the design framework, so our discussion is largely limited to a summary of the available options.

For the purposes of the discussion presented in this paper, we have selected a specific set of options that are representative of a relatively simple hydrogeological environment: steady-state, saturated flow with advective contaminant transport. Under the first heading in this section, we discuss the reasons for this selection, and note some of the ramifications of this emphasis.

The decision framework described in this paper is a modular one. The simulation model need not be the one used in our discussion. Rather, it should be designed to suit the needs of the project at hand. As summarized in the boxes on Figure 11, these needs revolve around: (1) the nature of the project, (2) the geological environment at the site, (3) the hydrogeological environment at the site, (4) the contaminant properties and expected transport mechanisms, and (5) the mode of simulation.

The first four of these boxes are self-explanatory. They allow us to define the appropriate boundary-value problem that lies at the core of the simulation model. The last box, the simulation mode, requires more discussion, and separate subsections follow to differentiate between deterministic and stochastic simulation, conditional and unconditional simulation, and direct and inverse simulation.

4.1 Emphasis on Steady, Saturated Flow with Advective Transport

The framework presented in this paper can, in principle, be applied to any combination of options from Figure 11. For the purposes of this paper, however, we will limit ourselves to a very simple hydrogeological environment: steady, saturated flow with advective transport. Under these conditions, where dispersion and retardation are unimportant, most plumes that develop will be long and thin, with a width that is roughly equal to the width of the source. The concentration of the contaminant species as a function of time at any location in the path of the plume will be a step function in which the concentration instantaneously changes from the ambient concentration, C0, to the contaminated concentration, C1. The advective rate of migration depends on the pattern of hydraulic heads, h(x, y), obtained as a solution to the flow equation:

\[ \frac{\partial}{\partial x} [K(x, y) \frac{\partial h}{\partial x}] + \frac{\partial}{\partial y} [K(x, y) \frac{\partial h}{\partial y}] = 0 \]  \hspace{1cm} (10)

with suitable boundary conditions prescribed. Given the hydraulic gradients, [\(\partial h/\partial x(x, y)\)], from the simulation results, together with the pattern of hydraulic conductivity,
\( K(x, y) \), and effective porosity, \( n(x, y) \), one can calculate the velocity field, \( V(x, y) \):

\[
V(x, y) = \frac{K(x, y)}{n(x, y)} \frac{\partial h}{\partial l}(x, y) \quad (11)
\]

Given the velocity field, \( V(x, y) \), it is a simple matter to calculate the travel time, \( t^* \), from the source to a specified compliance point.

This simple transport environment has been selected for three reasons. The first is that it simplifies the parameter uncertainty analysis and allows us to present the main thrust of our methodology in a simple and straightforward manner, unencumbered by the complications of dispersivities, retardation factors, and decay constants. Second, we note that advectively controlled contaminant migration is a common feature in high-permeability sand-and-gravel deposits of the type that have figured prominently in many published contamination incidents (cf. National Research Council, 1984; Wood, 1984). Third, most current capture-zone analyses for the design of pump-and-treat remedial action are based on steady-state, advective transport.

Table 2 summarizes the input and output for a steady, saturated, advective model. Input requirements include: (1) the boundaries of the flow domain; (2) the boundary conditions; (3) the location of boundaries between geological layers, units, or zones; (4) the spatial distribution of hydraulic conductivity, \( K(x, y) \), and porosity, \( n(x, y) \), within each layer, unit, or zone; and (5) the location of the source. For remedial analysis, the locations of the plume boundaries are also required. The strength of the source, or the pattern of concentrations within the plume, are not required for an advective analysis, as long as it is assumed that the performance standard for the contaminant under analysis, \( C^* \), is greater than the ambient concentration, \( C_0 \), and less than the plume concentration, \( C_1 \).

The output from the advective analysis is the head distribution, \( h(x, y) \), from which the gradients, the plume-front migration velocities, and the plume-front travel times can be determined. Such output can be programmed for delivery as equipotential output, stream-function output, particle-tracking output, or travel-time output.

### 4.2 Deterministic and Stochastic Simulation

All of the input parameters listed in Table 2 are subject to uncertainties. The methods of addressing these uncertainties are described in Section 5.0. Here, we consider only how such uncertainties can be taken into account in predictive simulation. One can distinguish two approaches: (1) deterministic simulation with sensitivity analysis, and (2) stochastic simulations.

With deterministic analysis, a base-case simulation is undertaken using the modeler's best estimates of the parameter values, and a sensitivity analysis is then carried out to investigate the impact on the output of variations in the input. Aguado et al. (1977) and McElwae (1984) describe the application of sensitivity analysis to ground-water models. Sykes et al. (1985) and Wilson and Metcalf (1985) describe an improved approach using adjoint sensitivity operators that can lead to considerable savings in computer time.

In stochastic analysis, uncertainty in the input parameters is specified in the form of a probability density function, or by the mean and the variance of such a distribution. There are three basic approaches used to propagate these uncertainties through the hydrogeological simulation model to estimate uncertainties of output variables: (1) first-order analysis, (2) perturbation analysis, and (3) Monte-Carlo analysis.

First-order analysis is a simple and direct means of propagating uncertainty. It can be employed with either analytical or numerical solutions of the governing equations, but it is limited to linear or nearly linear systems, for which the coefficient of variation of model parameters is much less than one (Peck et al., 1988). It requires only the first two moments (the mean and the variance) of the input parameters, and it provides only the first two moments of the predicted output variables. The approach has been used in ground-water applications by Dietischer and Wilson (1981), Townley and Wilson (1985), and Sitar et al. (1987). The structure of the algorithms is such that it makes use of a coefficient matrix similar to that used in sensitivity analysis, so that much of the theory originally developed there, including that of adjoint operators, is of value in first-order uncertainty analysis. The approach is unsuitable for the estimation of failure probabilities unless some assumptions can be made about the form of the PDF of the output variable.

The method of perturbation analysis has been fully developed for ground-water applications by Gelhar and his coworkers (cf. Bakr et al., 1978; Gutjahr et al., 1978; Gutjahr and Gelhar, 1981; and two recent review articles, Gelhar, 1984; Gelhar, 1986). With this approach, both the output variable and the input parameters are defined in terms of a mean plus a perturbation about the mean. The relationship between input and output uncertainties can be developed using two general techniques. One technique involves developing relationships in the spectral domain using the theory

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**Table 2. Summary of Input and Output for Two-Dimensional, Steady, Saturated, Advective Transport Simulations**

<table>
<thead>
<tr>
<th>Input</th>
<th>Output</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boundaries of flow domain</td>
<td>Hydraulic head distribution, ( h(x, y) )</td>
</tr>
<tr>
<td>Boundary conditions on boundaries of flow domain</td>
<td>Hydraulic gradients</td>
</tr>
<tr>
<td>Boundaries between geological layers, units, or zones</td>
<td>Plume-front migration velocities</td>
</tr>
<tr>
<td>Hydraulic conductivity ( K(x, y) ) in layers, units, or zones</td>
<td>Plume-front travel times</td>
</tr>
<tr>
<td>Porosity distribution, ( n(x, y) ) in layers, units or zones</td>
<td></td>
</tr>
<tr>
<td>Source location</td>
<td></td>
</tr>
<tr>
<td>Plume boundaries</td>
<td></td>
</tr>
</tbody>
</table>

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750
of Fourier-Stieljes integrals and an inverse Fourier transform. The mathematics are difficult but elegant. The approach is best suited to analytical solutions, an infinite flow domain, and a small coefficient of variation in input uncertainty. Spectral solutions may be most useful in the early stages of a decision analysis in that they provide relatively straightforward expressions to calculate initial estimates of uncertainty in the output variables.

A second technique for relating input and output uncertainties using perturbation analyses is to solve the perturbation equations using numerical techniques such as finite-element and finite-difference methods (e.g., Tang and Pinder, 1977; Sagar, 1978; Graham and McLaughlin, 1989).

Monte Carlo simulation provides the most general approach to uncertainty propagation. With this approach, a large number of equally likely realizations of each parameter field are generated, and the hydrogeological simulation model is run for each realization. The method requires that the full PDF be known for each input parameter. The PDF of the output variables is obtained from a statistical analysis of the output from the Monte Carlo runs. Peck et al. (1988) discuss some of the issues involved in Monte Carlo analysis of ground-water systems. The method is widely used because of its generality and simplicity. It can be used with analytical or numerical solutions, in infinite or bounded domains, and for any level of input uncertainty. Its Achilles heel lies in the computer-intensive nature of the endeavor. For complex transport problems in large heterogeneous domains, Monte Carlo analysis may be computationally infeasible. However, for steady, saturated, advective transport in two-dimensional systems on the scale of an engineering site, Monte Carlo simulation is a feasible proposition. It is the method that we have used in the examples presented in this series of papers.

In most advective transport analyses, the input parameter with the largest uncertainty is the hydraulic conductivity, K. As we will show in section 5.2, K must be treated as an autocorrelated spatial stochastic process. The need for this approach, and the available tools for the generation of the necessary hydraulic conductivity realizations in a two-dimensional domain are discussed at that time.

4.3 Conditional and Unconditional Simulation

Stochastic simulations identify uncertainty in predicted output variables due to uncertainty in input parameters. This uncertainty can be reduced by measurements of the input parameters.

Unconditional simulations are simulations that are not conditioned on any measured input. In the Bayesian framework, they are usually simulations designed to produce prior estimates of output uncertainty based on subjective estimates of input values made before measured data become available.

Conditional simulations are simulations that are conditioned on the values of measured input parameters, and on the specific locations of those measurements. At the points of measurement of K, for example, uncertainty in K is reduced to zero (or to the level of measurement error). Between the points of measurement, uncertainty in K remains. Stochastic conditional simulation provides the transfer function that predicts the uncertainty in hydraulic heads, and therefore in travel time, t**. The framework presented in the later sections of this report utilizes both conditional and unconditional simulation.

The available tools for updating uncertainties under the influence of additional input measurements are discussed later in the paper. One of these tools is kriging, and applications of conditional simulation are often associated with discussions of kriging (cf. Clifton and Neuman, 1982; Dagan, 1982).

4.4 Direct and Inverse Simulation

In a direct simulation, knowledge of the hydraulic conductivity (or transmissivity) is used to make predictions about the pattern of hydraulic head. In an inverse simulation, knowledge of the hydraulic head is used to draw inferences about the pattern of hydraulic conductivity.

It is in an inverse simulation that concepts of model calibration are introduced into our decision model. Uncertainty predictions using conditional simulations that preserve only the values of the measured input parameters are based on an uncalibrated flow model. By adopting the procedures of inverse simulation, we can condition upon both hydraulic conductivity and hydraulic head data.

There are two classes of inverse simulation in general use: (1) the indirect approach, and (2) the geostatistical approach. In the indirect approach, the model conductivities are iteratively updated until the model heads are "sufficiently close" to the observed heads. This is the approach that is widely applied in a deterministic trial-and-error style throughout the ground-water modeling community. At the research level, it has been recognized for some years now that indirect solutions to the inverse problem should be based on a statistical framework. Peck et al. (1988) group the available methods into three categories: (1) weighted least-squares estimation (cf. Cooley, 1982); (2) Bayesian estimation (cf. Neuman and Yakowitz, 1979), and (3) maximum likelihood estimation (cf. Carrera and Neuman, 1986). Loaiciga and Marino (1987) provide an assessment of these various techniques in terms of their impact on management decisions.

While these last three methods use a statistical framework, they do not use a geostatistical approach. The geostatistical approach differs from them in that it considers the hydraulic conductivity to be a spatial stochastic process. Because conductivity and head are coupled through the governing flow equation, the head is also a spatial stochastic process, and is jointly distributed with the conductivity. Measurements of either conductivity or head therefore contain information which can be used to estimate the conductivity field. Kitanidis and Vonvoris (1983), Hoeksema and Kitanidis (1984), and Dagan (1985) pioneered the geostatistical approach to the inverse problem.

Some aspects of inverse theory are incorporated in a later paper in this series in order to examine the joint worth of hydraulic head measurements and conductivity measurements in site investigation programs using the risk-cost-benefit decision model described earlier.
5.0 Uncertainty Models

5.1 Geological Uncertainty and Parameter Uncertainty

Predictions of hydraulic-head patterns or plume-front travel times at field sites are subject to large uncertainties because of the uncertainty in input parameters. Figure 12 provides schematic emphasis of the uncertainties that may be present in the input parameters summarized back in Table 2. There may be uncertainty in the geological configuration, the hydrogeological parameters, the boundaries, and the source or plume location. For the purposes of analysis, one can classify the uncertainties highlighted in Figure 12 into two groups: (1) those that involve uncertainty in the location of boundaries, and (2) those that involve uncertainty in parameter values. Table 3 identifies the two groups. Most of the boundary uncertainties are geological in nature. We therefore identify the need for two uncertainty models: a geological uncertainty model to address the geological boundary uncertainties, and a parameter uncertainty model to address uncertainty in hydrogeological parameters. This need was highlighted earlier on Figure 6, and the organization of this section of the paper is based on a differentiation of these two types of uncertainty. Source-area and plume boundary uncertainty can be handled in a similar manner to geological boundary uncertainty.

5.2 Parameter Uncertainty Model

The parameter uncertainty model (see Figure 6) provides the tools for quantifying the uncertainty in the spatially distributed values of input hydrogeological parameters within a hydrogeological unit. It also includes the methodology for calculating the reduction in uncertainty that can be achieved by a specific proposed measurement program. It is differentiated from the geological uncertainty model treated in a later subsection which addresses uncertainties in the location of boundaries between hydrogeological units.

In this section, we first clarify the relationship between heterogeneity and uncertainty. We then present a description of the elements of stochastic process theory, and a comparison of the classical methods of updating uncertainty based on kriging, with the Bayesian updating procedures we espouse. Finally, we discuss the variance reduction issues that arise because of differences between measurement scales and simulation scales. The presentation in the body of the paper is descriptive; the mathematics are presented in the Appendices.

Table 3 identified the hydraulic conductivity \( K(x, y, z) \) and the porosity, \( n(x, y, z) \) as the hydrogeological parameters of interest for steady saturated advective transport. For the purposes of discussion in this section, we have selected the hydraulic conductivity as the uncertain parameter. The same conceptual framework would hold for porosity, or for any of the other hydrogeological parameters that might arise from more complex transport formulations. However, consideration of the joint uncertainties of more than one parameter at a time, while conceptually straightforward, would add considerable complexity to our presentation.

For the purposes of explanation, we have constrained our limited mathematical presentation to a one-dimensional stochastic process, and our qualitative graphical presentation to two-dimensional fields. The methods are equally applicable to three-dimensional domains. Neuman (1982) and Peck et al. (1988) provide excellent reviews of the concepts and issues underlying the treatment of parameter uncertainty in hydrogeology.

5.2.1 Description of Heterogeneity: Stochastic Process Theory

Most data sets that have been gathered for hydraulic conductivity display a skewed statistical distribution. This is not surprising in view of the fact that conductivities can vary over several orders of magnitude, but must all be positive. Most workers have found that a lognormal distribution fits the data well (cf. Freeze, 1975). Although it is not a requirement of our methodology, we too will assume a lognormal distribution, and present our material in terms of the log hydraulic conductivity, \( Y \), defined as:

\[
Y_i = \ln K_i
\]  

(12)

The parameter \( Y \) is normally distributed. The population of \( Y \) has a mean \( \mu_Y \), and a variance, \( \sigma_Y^2 \). (In shorthand,
function can be expressed either in terms of distance, \( \rho_Y(h) \), or in terms of lag, \( \rho_Y(k) \). The autocorrelation function may take a number of forms; two of the most commonly used functions are the exponential and spherical models. If it is found to be exponential:

\[
\rho_Y(h) = \exp\left[-|h|/\lambda_Y\right]
\]

(13)

where \( \lambda_Y \) is an exponential decay parameter, known as the correlation length. It is a measure of the distance over which the \( Y \)-value is correlated; specifically, it is the distance over which \( \rho_Y(h) \) decays to a value of \( e^{-1} \). The area under the curve is called the integral scale, \( \epsilon_Y \), where:

\[
\epsilon_Y = \int_0^\infty \rho_Y(h) \, dh
\]

(14)

Both the correlation length and the integral scale are one-parameter descriptions of the correlation structure. It is reasonable to anticipate a direct relationship between the magnitude of the correlation length and the average dimension of bedding structures within a sedimentary deposit. Hoeksema and Kitanidis (1985) summarize the autocorrelation properties of a large suite of selected aquifers.

The integral scale or the correlation length form a part of the description of heterogeneity. A full geostatistical description of the heterogeneity of \( Y \) is given by the three-parameter stochastic process defined by the autocorrelated normal distribution, \( Y : N[\mu_Y, \sigma_Y, \epsilon_Y] \) or \( Y : N[\mu_Y, \sigma_Y, \lambda_Y] \). It is assumed for the purposes of our ongoing discussions that the stochastic process is stationary, that is, that the values of \( \mu_Y, \sigma_Y, \) and \( \lambda_Y \) are constant over space in the domain of interest. If trends in these parameters are present, it is assumed that such trends are first removed, and that the residuals are stationary.

#### 5.2.2 Heterogeneity, Uncertainty, and Ergodicity

Uncertainty as to the exact spatial distribution of hydraulic conductivity values arises because of our knowledge that conductivity values tend to exhibit heterogeneity, even within individual hydrogeological units. Heterogeneity and uncertainty are thus related, but they are not the same thing. Heterogeneity is in the geology, whereas uncertainty is in the mind of the analyst (Figure 14). The concept that allows us to integrate these issues, through the description of the \( K(x, y, z) \) field as a random realization of a stochastic process, is known as ergodicity.

Consider a two-dimensional region of a horizontal confined aquifer (Figure 15) within which \( n \) measurements of \( Y \) are available: \( Y_1, Y_2, \ldots, Y_n \). Now suppose that we wish to estimate the value of \( Y_j \) at some position \( j \) that lies between (and well away from) any of the measured \( Y_i \). If we assume that the most likely estimate of \( Y_j \) is \( \bar{Y} \) (the mean value of the measured \( Y_i \)), and if we assume that our uncertainty about the value of \( Y_j \) is normally distributed with standard deviation, \( \sigma_Y \) (the standard deviation of the measured \( Y_i \)), then we are accepting the ergodic hypothesis. It is far from the only hypothesis we could use to state our uncertainty, but it is logical and commonly used. It is basically a philosophical judgment; there is no science to back it.
up. What we are saying, again from elementary statistics, is that we think there is an 84% chance that the value of $Y_i$ is greater than $\bar{Y} - S_Y$ (or $\mu_Y - \sigma_Y$), a 50% chance that it is greater than $\bar{Y}$ (or $\sigma_Y$), and a 16% chance that it is greater than $\bar{Y} + S_Y$ (or $\mu_Y + \sigma_Y$).

Acceptance of the ergodic hypothesis is a required step if we are to apply the stochastic process theory that follows. It allows us to reduce the statistical requirements for analysis from that of a multivariate statistical distribution involving all of the individual unknown $Y_i$ values, to that of a univariate distribution in $Y$ over the hydrogeologic domain of interest.

5.2.3 Prior Uncertainty and Unconditional Simulation

Given the above framework for the description of heterogeneity, and given an acceptance of the ergodic hypothesis, we now turn to the question of the uncertainty in $K$ at unmeasured points.

Our uncertainty is greatest before we take any measurements at all, but in a classical statistical framework, we would have no way of estimating the values of $\mu_Y, \sigma_Y, \epsilon_Y$, or $\lambda_Y$, prior to taking measurements. In a Bayesian framework, however, we may make subjective prior estimates of these parameters. We do so by using our knowledge of the geological environment at the site, our interpretation of any available “soft” data at the site, our past experience with respect to available data at similar sites, precedent, and common sense.

Consider now a one-dimensional field of $Y$ values: $\{Y_1, Y_2, \ldots, Y_n\}$ as in Figure 13(a), where the locations of the $Y_i$ now represent points at which we wish to estimate the expected value and uncertainty of $Y_i$ prior to the taking of measurements. Let $\{\mu_i\}$ be the vector of expected values, and let $\{\tau_{ij}\}$ be the vector of variances that describes our uncertainty. Prior to taking measurements, and under the ergodic hypothesis, all the expected values, $\{\mu_1, \mu_2, \ldots, \mu_n\}$ in the $\{\mu_i\}$ vector will be equal to $\mu_Y$, our subjective prior estimate of the mean of the stochastic process that describes the log hydraulic conductivity field, and all the uncertainty values $\{\tau_{11}, \tau_{22}, \ldots, \tau_{nn}\}$ will be equal to $\sigma_Y^2$, the subjective prior estimate of the variance of the stochastic process that describes the log hydraulic conductivity field.

Given $\{\mu_i\}$ and $\{\tau_{ij}\}$ and an autocorrelation function like (13), it is possible to generate an infinite number of equally likely realizations of the log hydraulic conductivity field. There are several methods for doing so. The two most popular are Cholesky decomposition (cf. Clifton and Neuman, 1982), and the turning bands approach (Mantoglou and Wilson, 1982). Smith and Freeze (1979a) used a nearest-neighbour algorithm that is conceptually straightforward, but has operational disadvantages in comparison with the other two methods. Freeze (1980) used a spectral technique. The interested reader is directed to these references for details. The infinite set of equally likely realizations defines an ensemble. The actual pattern of hydraulic conductivity variations at a field site is considered to be one member of this ensemble.

Prior realizations are not conditioned on any measured $Y$ values; they are unconditional realizations suited to unconditional simulation. Figure 16 (after Smith and Freeze, 1979b) displays the output uncertainty in hydraulic head for a steady, saturated flow system in a dimensionless two-dimensional vertical section based on unconditional Monte Carlo simulations with a finite-element model. Figure 16(a) shows the expected value of the hydraulic head field, $h(x, z)$, and Figure 16(b) shows the uncertainty in head, $S_h(x, z)$, where uncertainty is defined as one standard deviation about the mean. The maximum uncertainty exceeds 15%.

For each realization of the unconditional simulation, one can calculate a travel time for flow through the system, and taken together, these produce a prior travel-time PDF like that shown on Figure 16(c). The probability of failure, $P_f$, might be defined as the probability that the travel time is less than some regulatory standard.

In the above description, the uncertainty vector $\{\tau_{ij}\}$ has been given a double subscript because in reality it consists of the diagonal terms of the autocovariance matrix $\{\tau_{ij}\}$. This matrix figures prominently in the mathematical presentation of stochastic process theory in Appendix IV.
5.2.4 Posterior Uncertainty: Bayesian Updating and Conditional Simulation

Assume that some measurements of log hydraulic conductivity now become available at one or more points in the aquifer. For the purpose of explanation, we return to our one-dimensional sequence of points, \( \{ Y_1, Y_2, \ldots, Y_n \} \), and assume that the measurement \( Y_4 \) has become available. This measurement allows us to update our prior vector of expected values, \( \{ \mu_i \} \), to a posterior vector, \( \{ \mu_i' \} \), and our prior vector of uncertainties, \( \{ \tau_{ii} \} \), to a posterior vector, \( \{ \tau_{ii}' \} \), where the term posterior refers to the situation after the measurement becomes available. At \( i = 4 \), the posterior expected value, \( \mu_4' \), will equal \( Y_4 \), and if there is no measurement error, the posterior uncertainty, \( \tau_4' \), will be equal to zero. Because of the autocorrelation properties of the log hydraulic conductivity field, the influence of this measurement will propagate through the vector of expected values and the vector of uncertainties, changing the expected values and reducing the uncertainty in a region around the point of measurement, the size of which depends on the correlation length. The quantitative posterior values can be calculated using the Bayesian updating procedures outlined by Hachich and Vanmarcke (1983) and Massmann and Freeze (1987a). The mathematics are presented in Appendix IV.

Figure 17 provides a hypothetical example that shows a two-dimensional mapping of the updating of \( \{ \mu_i \} \) to \( \{ \mu_i' \} \) and \( \{ \tau_{ii} \} \) to \( \{ \tau_{ii}' \} \). A comparison of Figures 17(b) and 17(d) shows a decrease in the uncertainty associated with estimates of \( Y_i \) over most of the flow field due to the influence of three measurements of \( Y \). An example with a smaller correlation length would show a smaller region of uncertainty reduction.

Thus far we have described the Bayesian updating procedure as taking place from an unconditional prior to a conditional posterior, but the method can be used to go from any prior to any posterior, regardless of whether the prior is conditioned on measurements or not. If one envisages a staged site investigation, one would envisage updating the uncertainty matrix from \( \{ \tau_{ii} \} \) to \( \{ \tau_{ii}' \} \) to \( \{ \tau_{ii}'' \} \), and so on. In each instance, the new data further constrains the possible range of variations in the ensemble of realizations defined by the stochastic model.

At each stage it is possible to generate a set of equally likely conditional realizations using similar programs and procedures to those used to generate unconditional realizations. One can then apply Monte Carlo simulation on the conditional realizations to produce estimates of the output hydraulic head field and its uncertainty. Measurements will reduce the uncertainty in the predicted head values and the travel times. Figure 16(c) displayed both a prior and posterior travel-time PDF that schematically indicates how uncertainty reduction through measurements could lead to a reduction in the probability of failure associated with 1000-year travel time.
5.2.5 Bayesian Updating and Kriging

The parameter uncertainty model using Bayesian updating as described thus far could easily be replaced by a parameter uncertainty model based on kriging.

Kriging provides an alternate way to address the interpolation problem outlined in Figure 15, where we wish to estimate the expected value, \( Y_i \), and the uncertainty associated with the estimate, at points between a set of measurement points, \( \{Y_1, Y_2, \ldots, Y_n\} \). Kriging can be used with conditional simulation in the same way as Bayesian updating to predict uncertainties in output hydraulic head fields.

Kriging is closely related to Bayesian updating, both in spirit and in the nature of the calculations. However, there are differences in the jargon, and in the assumptions and philosophy that underlie the methods. These differences are summarized and explained in Appendix V. Our emphasis is on the Bayesian approach rather than the classical kriging approach because we feel it is better suited to the style and needs of engineering design.

5.2.6 From Measurement Scale to Simulation Scale: Variance Reduction

If the aquifer volume represented by a measurement, \( Y_i \), at one point in an aquifer is the same as the volume associated with the estimated uncertain value, \( Y'_i \), at some other point in an aquifer, then the kriging or Bayesian updating methods can be applied in the manner described thus far. Commonly, however, the measurements are obtained with single-well slug tests on a scale of, say, 0.1 to 1 m, or multiple-well pump tests on a scale of 10-100 m, while the uncertain estimates are required for the elements of a finite-element model with block sizes on the order of 100-1000 m. The statistics of the measured values are not immediately compatible with one another or with the needs of the model due to the fact that they are averaged over different volumes of a stochastic field. It is necessary to adapt the parameter statistics to the scale of interest.

This step can be accomplished by a straightforward spatial integration (cf. de Marsily, 1984, 1986). Vanmarcke (1983) provides a series of formulae that evaluate the integrals for simple geometric configurations, such as squares and rectangles, that are pertinent for a finite-element grid. Journel and Huijbregts (1978) also provide formulae and type curves for this purpose. One of Vanmarcke’s variance reduction formulae is presented in Appendix VI. Dagan (1986) provides an elegant theoretical discussion of the scale issue in ground-water flow and transport.

Figure 18 provides a summary of the possible features that might be included in a parameter uncertainty model for a given application at a given site.

5.3 Geological Uncertainty Model

The parameter uncertainty model described in the previous section allows the decision-maker to take into account his uncertainty with respect to hydrogeological parameter values within a particular geological unit, layer, or zone. In many cases, however, there is a more fundamental uncertainty: the location of the boundaries between the geological units, layers, or zones. In this section we provide some examples of the types of geological boundary uncertainty that may be encountered. For one representative case we discuss two approaches to the reduction of this uncertainty.

5.3.1 Types of Geological Uncertainty

There are an infinite number of potential geological environments. However, one can try to simplify the situation by idealizing the subsurface into a set of rectilinear geological blocks of various volumes separated from one another by horizontal and vertical planar boundaries. Horizontal boundaries might reflect the overburden-bedrock surface or the boundaries between stratigraphic units in a horizontally layered sedimentary sequence. Vertical boundaries might reflect the lateral extent of alluvial aquifers or structural boundaries controlled by steeply dipping faults. In any case, the usual approach in the development of a hydrogeological model is to try to identify those units that can be classified as aquifers and those that can be classified as aquitards with emphasis on their continuity and connectivity.

The first step in developing the geological model is to decide on a classification criterion that can be used to differentiate aquifers and aquitards. The classification would be a relative one, suited to the hydrogeological environment at hand. The criterion would usually be the hydraulic conductivity or some analog to it such as grain-size distribution, geophysical response, or borehole-log descriptions. Some techniques that might be used in cases where classification is
not straightforward include factor analysis, cluster analysis, pattern recognition, and image analysis (Baecher, 1972; Wu, 1988).

In this paper, we will use a simple but realistic geological environment to advance our ideas about geological uncertainty. Consider the question of aquitard continuity, first introduced in the cross-sectional view on Figure 12. If the horizontal aquitard shown on the figure is continuous, then any contaminant plume that might develop from a waste-management facility on surface will probably be constrained to the upper aquifer horizon. If it is not continuous, and particularly if there is pumping in the lower aquifer, the plume may be drawn through the holes in the aquitard. The probability of this occurrence could have a large impact on the probability of failure and the risk term associated with specific alternative designs for a new facility, a remedial cleanup, or a monitoring network. In some cases it might control the identification of the best alternative with the risk-cost-benefit decision model.

Uncertainty as to the presence of holes in the aquitard would be reduced by the drilling and logging of boreholes. We will look at two methods by which the geological data obtained from such boreholes could be used to assess the reduction in uncertainty: search theory, and indicator kriging.

5.3.2 Reduction of Geological Uncertainty with Search Theory

Search theory treats the drillhole intersection with the aquitard as a yes-no situation. Either the aquitard is present at the location of the drillhole, or it is absent, in which case a hole of some dimension exists. The first applications of search theory in a geological context were in the mineral exploration field for the design of drilling patterns in search of ore bodies. Drew (1979), for example, provides an analysis of the optimum drilling pattern and hole spacing for elliptical targets of various sizes. Savinskii (1965), and Singer and Wickman (1969), provide probability tables for locating elliptical targets with a rectilinear grid of drillholes. These analyses and tables are relevant for hydrogeological exploration.

Consider a circular target of diameter, a, and a square drillhole grid of spacing, d [Figure 19(a)]. The tables referenced above provide the probability that the target will be missed by the grid even though such a target exists. As the grid spacing is reduced [Figure 19(b)], this probability decreases for all target diameters. If the target is an aquitard hole, pattern drilling can be used to reduce the probability of its existence (i.e., to reduce the uncertainty associated with its possible presence).

If a hole is encountered, its size may be pertinent. Marshall (1964) describes an optimal sequential search method for locating drillholes to determine target size, once the target is encountered in a single hole. (In our case, the target, being a hole, is “encountered” when the aquitard is absent.)

Search theory can be perceived as a geostatistical model just as is stochastic process theory. One can have a subjective Bayesian prior; one can generate an infinite number of equally likely aquitard-continuity/hole-location scenarios; one can generate conditional and unconditional Monte Carlo simulations; and one can use the results with the decision model to select the best alternative design for a new facility or a remedial program.

Finally, we note that the concepts of search theory are also pertinent to uncertainty reduction with respect to plume boundaries in the design of remedial programs where ground water has become contaminated. Capture-zone analysis is quite sensitive to plume extent, and it may be worth comparing the cost-effectiveness of further exploratory drilling relative to the cost of a more conservative purge-well network as a means to reducing risk.

5.3.3 Reduction of Geological Uncertainty with Indicator Kriging

Indicator kriging is a particular type of kriging (Journel, 1984, 1986a) based on the same principles and methods noted earlier with respect to the kriging of hydraulic conductivity fields. It differs from ordinary kriging (Appendix V) in that instead of a parameter being kriged directly, its probability of exceeding a threshold value is kriged. For this reason the approach is also called probability kriging.

For the aquitard continuity problem, one might define a hole as an area in which the aquitard thickness is less than one meter. Drilling logs would provide the aquitard-thickness data that could be indicator kriged with respect to the one-meter threshold. The result would be a map of the probability that the aquitard has a thickness greater than the threshold value.

![Fig. 19. (a) A circular target of diameter a and a square drilling pattern with spacing d; (b) results of search theory analysis (based on Savinskii, 1965).](image-url)
If containment-failure scenarios at a waste-management site are based on advection or matrix diffusion of contaminants across an aquitard, one might want to use indicator kriging on an integrated parameter involving some combination of gradient, thickness, conductivity, and diffusion coefficient.

Figure 20 summarizes the potential features of a geological uncertainty model.

5.3.4 Reduction of Geological Uncertainty with Hydraulic Head Data

Inverse simulation is of potential use in reducing uncertainty in the geologic model as well as in providing estimates of the spatial variability in medium properties. The influence on the hydraulic head distribution of a stratified aquifer/aquitard sequence, or the presence of a window through an aquitard, may be reflected in a set of hydraulic head measurements. Research within our group is currently directed toward issues of discriminating between different geologic models within the framework of an inverse simulation.

5.3.5 Joint Application of Parameter Uncertainty Model and Geological Uncertainty Model

There is no reason why the search-theory model (or indicator-kriging model) for geological uncertainty (Figure 20) and the stochastic-process model for parameter uncertainty (Figure 18) could not be run in tandem, but to date this has not been done by the research community. Where stochastic process models have been applied in a decision framework (cf. Feinerman et al., 1985; Massmann and Freeze, 1987b), it has been for a single hydrogeological unit with certain boundary locations. Geological uncertainty models are just now being introduced to the hydrogeological community.

One possibility that falls short of a full integration of the two types of uncertainty, but which has appeal as a practical tool in a layered system, would involve a geological uncertainty model for layer boundaries and an uncertain representative log-hydraulic-conductivity value for each layer. These representative values are best viewed as being $\bar{Y}$ values; that is, they would be determined as the arithmetic mean of a set of point $Y$-measurements (the geometric mean of a set of point $K$-measurements), were such measurements available. The uncertainty in these representative values would be reflected by the variance of $\bar{Y}$, not the variance of $Y$ itself. The variance in $\bar{Y}$ is much less than that for $Y$ (Benjamin and Cornell, 1970). One can therefore view the representative values as $N: [\mu, \sigma]$ and Bayesian prior estimates of $\sigma$ should reflect the lesser uncertainties associated with $\bar{Y}$ than those commonly used for $Y$. As an aside, it should be noted that the very existence of an equivalent hydraulic conductivity value requires some implicit assumptions with respect to the orientation of the hydraulic gradient and the dimensionality of the analysis (Dagan, 1986).

6.0 Summary and Limitations of Decision Framework

Figure 21 provides a summary of the decision framework presented in this paper. It involves an iterative process

Fig. 20. Components of a geological uncertainty model.

Fig. 21. Summary of decision framework presented in this paper.
between analysis and field measurement. A subjective prior interpretation of the hydrogeological environment is first analyzed with an unconditional stochastic simulation. The level of uncertainty reduction that can be achieved by field measurements is assessed with posterior conditional stochastic simulation. After each phase of field measurements, the available engineering alternatives are compared with an economic decision model. Before each new phase of field measurements, a data worth assessment is carried out to determine whether further measurements are economically justified. When the point is reached where they are not, the best alternative is selected as the design decision.

6.1 Data Worth

One of the most valuable features of this decision framework is its ability to assess the worth of a proposed site-investigation program prior to actually taking the measurements. This is possible because the uncertainty reduction that can be attained by a measurement program depends only on the number and location of the measurements, not on their measured values. The uncertainty reduction feeds into the risk term in the risk-cost-benefit objective function. A proposed site-investigation program should only be carried out if the risk reduction it will achieve is greater than the cost of carrying it out.

A full treatment of the data worth issue is postponed until a later paper in this series, as is the debt owed to earlier hydrogeological researchers in this field (Baecher, 1972; Maddock, 1973; Gates and Kiesel, 1974).

6.2 Limitations

Some of the limitations associated with Bayesian stochastic process theory are outlined by Freeze et al. (1988). They identify four issues of special significance. These issues revolve around: (1) the appropriateness of the Bayesian approach, (2) the application of inverse simulation, (3) identification of trends and zonations in hydraulic conductivity, and (4) problems associated with small-sample statistics.

We believe that engineering decision-making is best carried out in a Bayesian framework in which subjective data are used in the analyses on which decisions are based. We hold that such data are included one way or another in all analyses, but that Bayesian analysis incorporates data in an open and objective way. Nevertheless, it is clear that the subjectivity of the prior estimates can lead to bias (cf. Merkhofer and Runnchal, 1988), and that the process could easily be abused. Some scientists and engineers may feel that using subjective priors is unscientific or unprofessional, and there is question as to public and political acceptance.

The decision framework outlined in this paper is currently undergoing extension to include inverse simulation. It is clear that hydraulic-head data, used in conjunction with hydraulic-conductivity data, have considerable data worth, but the assessment of that worth requires an inverse formulation. A modeler introduces his personal judgments in an inverse simulation in the design of the interpretation model, specification of upper and lower bounds on parameter values, and in assigning measurement error at data points. It is still unclear to what extent subjective prior information can be used to obtain meaningful results from the inverse approach. A related question concerns the relationship between the scale at which the heterogeneity of K is described and that which is required for hydrogeologic calibration.

The identification of boundaries between hydrologic units and trends within hydrogeologic units may prove difficult, especially in fractured rocks involving complex, discontinuous, structural features that may exert considerable influence on flow and transport. Current geostatistical methods do not sufficiently emphasize the uncertainty spawned by potential geological misinterpretations.

The potential Achilles heel for the application of uncertainty models at engineering sites lies with the problems that arise when data networks are sparse and sample sizes small (cf. Eslinger and Sagar, 1988). Among the steps where limitations due to small-sample statistics may arise are the following: (1) testing the hypothesis of a lognormal distribution for hydraulic conductivity, (2) testing for stationarity of the hydraulic-conductivity field, (3) determining the most appropriate form of the autocorrelation function and estimating the values of its parameters, (4) obtaining significant uncertainty reduction in the Bayesian updating step, and (5) application of the inverse procedures. It must be emphasized that the stochastic approach is not a substitute for an inadequate data base.

Having noted these small-sample weaknesses, we emphasize again that they are common to all types of decision analysis. Our approach highlights the weakness of sparse data networks by identifying the existence of a large risk. It also identifies the best decision given the level of data available, regardless of whether that level is sparse or full.

Decision analysis can be questioned on an even more fundamental level than that raised above. The risk-analysis literature abounds with articles addressing the issue of whether a risk-cost-benefit framework is philosophically sound and politically acceptable for decisions that affect the public interest (cf. Howard, 1981). The discussions revolve around the appropriateness of large discount rates and short time horizons, and the questions of ethics and equity associated with the concept of acceptable risk. We have avoided these issues in this paper by taking the perspective of the owner-operator of a waste-management facility and not the perspective of a regulatory agency protecting the public interest. For further discussion of these issues, see Freeze (1988).

Acknowledgments

The work reported in this article was supported by grants to Allan Freeze and Leslie Smith from the Natural Sciences and Engineering Research Council of Canada. This work was partially supported by National Science Foundation Grant CES-8858526 to Joel Massmann.

The authors benefited greatly from discussions over the past few years with Ghislain de Marsily, Gedeon Dagan, Tom Maddock, and Steve Gorelick.
Table 4. Decision Matrices and Alternative Objective Functions

<table>
<thead>
<tr>
<th>Decision variable</th>
<th>State of nature</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>S1</td>
</tr>
<tr>
<td>a1</td>
<td>C11</td>
</tr>
<tr>
<td>a2</td>
<td>C21</td>
</tr>
<tr>
<td>a3</td>
<td>C31</td>
</tr>
</tbody>
</table>

Table 4b. Water-Supply Example:

<table>
<thead>
<tr>
<th></th>
<th>T &lt; 500</th>
<th>500 &lt; T &lt; 1000</th>
<th>T &gt; 1000</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pr = 0.1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pr = 0.1</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Pr = 0.8</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>a1 — 1 well</td>
<td>$3 m.</td>
<td>$2 m.</td>
<td>$16 m.</td>
</tr>
<tr>
<td>a2 — 2 wells</td>
<td>$4 m.</td>
<td>$10 m.</td>
<td>$13 m.</td>
</tr>
<tr>
<td>a3 — 4 wells</td>
<td>$6 m.</td>
<td>$7 m.</td>
<td>$8 m.</td>
</tr>
</tbody>
</table>

Table 4c. Regrets for Water-Supply Example:

<table>
<thead>
<tr>
<th></th>
<th>T &lt; 500</th>
<th>500 &lt; T &lt; 1000</th>
<th>T &gt; 1000</th>
</tr>
</thead>
<tbody>
<tr>
<td>a1 — 1 well</td>
<td>$9 m.</td>
<td>$8 m.</td>
<td>$0 m.</td>
</tr>
<tr>
<td>a2 — 2 wells</td>
<td>$2 m.</td>
<td>$0 m.</td>
<td>$3 m.</td>
</tr>
<tr>
<td>a3 — 4 wells</td>
<td>$0 m.</td>
<td>$3 m.</td>
<td>$8 m.</td>
</tr>
</tbody>
</table>

Appendix I. Alternative Objective Functions and Design Criteria

The objective function used in the body of the text is based on expected utility. The alternative that maximizes the decision-maker’s expected utility is selected as the preferred alternative. Although this criterion is used most often in decision analysis approaches, other objective functions and decision criteria have been proposed. Two common alternatives to the expected utility criterion are the maximin criterion and the minimax regret criterion. These two criteria can be described by referring to the decision matrix presented in Table 4a. The rows of this matrix correspond to alternative decision variables available to the decisionmaker and the columns correspond to various states of nature that may be relevant to the decision problem. A consequence can be assigned to each pair of decision variables and states of nature.

As an example, consider the water-supply decision summarized in Table 4b. The owner-operator of this water supply is considering three alternative pumping strategies for developing a supply of 1000 gpm. Alternative a1 is to use one well, alternative a2 is to use two wells, and alternative a3 is to use four wells. The consequence for each alternative is defined as the net present value of future benefits and costs. If we assume the sole source of uncertainty in this system is the transmissivity of the aquifer, then this transmissivity is the state of nature. The consequence depends only upon the number of wells that are selected and on the aquifer transmissivity. Probabilities have been assigned to each of the three transmissivity values listed in Table 4b. These probabilities may have been determined subjectively or may be based on hydraulic head or hydraulic-conductivity data.

The expected utility decision criterion or objective function requires that utilities be assigned to each consequence included in the decision matrix. However, if a risk-neutral approach is adopted, then the consequences can be directly expressed in terms of dollars without assigning utilities. The alternative that gives the maximum expected utility is selected. For the water-supply example included in Table 4a, the one-well alternative, a1, would be chosen using a risk-neutral expected value objective function because the expected value of this alternative, $12.7 million, is largest.

The maximin decision criterion requires selecting the alternative whose minimum consequence is largest. The procedure is to identify the least desirable consequence for each alternative under consideration and to then select the alternative that gives the best of these least desirable consequences. For the example presented in Table 4b, the four-well strategy, alternative a3, would be selected using the maximum criteria because its minimum consequence, $6 million, is the maximum for all three alternatives.

The minimax regret criterion requires that consequences first be converted into regrets. The regret that a decision-maker experiences after selecting an alternative is the difference between the consequence associated with the alternative that was selected and the consequence associated with the alternative that would have been selected if the actual state of nature were known. For the example presented in Table 4b, the regret associated with alternative a1 if the transmissivity is less than 500 ft/day is $2 million. If the decision-maker had known the transmissivity was less than 500 ft/day, he would have selected alternative a1 because it gives the maximum consequence, $6 million. The decision-maker’s regret at selecting alternative a2 when the transmissivity is less than 500 ft/day is the difference between $4 million and $6 million. Regrets for other pairs of pumping strategies and transmissivities are presented in Table 4c. The procedure of minimax regret criteria is to select that alternative whose maximum regret is smallest. For the water-supply decision described in Table 4c, alternative a2 would be selected using the minimax regret criterion because its maximum regret, $3 million, is the smallest for the three alternatives.

Decisions may also be based, either wholly or in part, on robustness. An alternative is more robust if the consequences associated with that alternative are less sensitive to uncertainties and states of nature. For the water-supply decision, alternative a1 is most robust because it is least sensitive to the transmissivity of the aquifer.

Persuasive arguments can be made in favor of the maximum expected utility criterion. These arguments are based on the assertion that the criterion or objective function based on utility is most “rational.” The example included in Table 4 is somewhat contrived in that the “best” alternative depends upon the decision-maker’s objective function or decision criterion. There are many instances in which the same alternative would be chosen using any of the criteria. These instances correspond to robust decisions in the same sense as the robust alternatives described in the previous paragraph.
Appendix II. Stochastic Process Theory:
Definition of Terms

Table 5 provides a summary of the notation that appears in the stochastic process theory described in the main body of the text and developed more fully in Appendix IV.

Given a set of measurements of log hydraulic conductivity, \([Y_1, Y_2, Y_3, \ldots, Y_n]\), the mean, \(\bar{Y}\), the variance, \(S_y^2\), the autocovariance, \(c_{Yk}\), and the autocorrelation, \(r_{Yk}\), are defined as follows:

\[
\bar{Y} = \frac{1}{n} \sum_{i=1}^{n} Y_i
\]

\[
S_y^2 = \frac{1}{n} \sum_{i=1}^{n} (Y_i - \bar{Y})(Y_i - \bar{Y})
\]

\[
c_{Yk} = \frac{1}{n} \sum_{i=1}^{n} (Y_i - \bar{Y})(Y_{i-k} - \bar{Y}) = c_{Yk}/S_y^2
\]

where \(k\) is the lag. If the measurement, \(Y_i\), is made at position, \(X_i\), and the measurement \(Y_{i-k}\) at \(X_{i-k}\), then the separation, \(h\), is defined as \(|X_i - X_{i-k}|\).

The correlation length, \(\lambda_Y\), and the integral scale, \(\epsilon_Y\), are defined as equations (13) and (14) in the main body of the text.

Appendix III. Stochastic Process Theory:
Relationships Between Y and K

The development of the stochastic process theory in the main body of the report and in Appendix IV is carried out with respect to log hydraulic conductivity, \(Y\), because the development is more straightforward in that light. The results of a decision analysis would probably be presented with respect to hydraulic conductivity, \(K\), directly, because the results are more easily grasped in that light. The two sets of statistical parameters are easily related (Vanmarcke, 1983). If \(Y = \ln K\), with \(Y\) normally distributed, and the mean, variance, and autocorrelation function with respect to \(Y\) are given by \(\mu_Y, \sigma_Y^2\), and \(\rho_Y\), then \(K\) is lognormally distributed, and the mean, variance, and autocorrelation function with respect to \(K\) are given by:

\[
\mu_K = \exp[\mu_Y + (1/2)\sigma_Y^2]
\]

\[
\sigma_K^2 = \{\exp[\sigma_Y^2] - 1\}\{\exp[2\mu_Y + \sigma_Y^2] - 1\}
\]

\[
\rho_K = \{\exp[\rho_Y \sigma_Y^2] - 1\}/\{\exp[\sigma_Y^2] - 1\}
\]

If we accept the ergodic hypothesis and consider the uncertainty in the value of \(Y\) at some unmeasured point, we can say that there is a 16% chance \(Y\) exceeds \(Y_{16}\), a 50% chance \(Y\) exceeds \(Y_{50}\), and an 84% chance \(Y\) exceeds \(Y_{84}\), where \(Y_{16} = \mu_Y + \sigma_Y, Y_{50} = \mu_Y, \) and \(Y_{84} = \mu_Y - \sigma_Y\). For these exceedance probabilities, \(K_{16} = \exp[Y_{16}], K_{50} = \exp[Y_{50}],\) and \(K_{84} = \exp[Y_{84}].\) Note that \(Y_{50}\) is both the median and the mean of the \(Y\)-distribution, whereas \(K_{50}\) is the median, but not the mean, of the \(K\)-distribution. In particular, note that \(K_{16} \neq \mu_K + \sigma_K\), nor is there any simple relationship between them.

Appendix IV. Stochastic Process Theory:
Autocovariance Matrix and Bayesian Updating

In this appendix, we present the necessary mathematical background to carry out the prior and posterior uncertainty calculations described in Sections 5.2.3 and 5.2.4.

Consider, as we did there, a one-dimensional field of \(Y\) values: \([Y_1, Y_2, \ldots, Y_n]\), where the locations of the \(Y_i\) represent points at which we wish to estimate the expected value and uncertainty of \(Y_i\) before and after taking a set of measurements. The most compact notation is that of a vector of expected values, \([\mu_i]\), and an autocovariance matrix, \([\tau_{ij}]\) (Figure 22).

**Table 5. Summary of Notation for Stochastic Process Theory**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Population statistic (stochastic process)</th>
<th>Population estimate</th>
<th>Sample estimate (realization)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mean</td>
<td>(\mu)</td>
<td>(\hat{\mu})</td>
<td>(\bar{Y})</td>
</tr>
<tr>
<td>Variance</td>
<td>(\sigma^2)</td>
<td>(\hat{\sigma}^2)</td>
<td>(S_y^2)</td>
</tr>
<tr>
<td>Autocovariance</td>
<td>(r_{Yk}) or (r_Y(h)) (\hat{r}_{Yk}) or (\hat{r}_Y(h))</td>
<td>(c_{Yk}) or (c_Y(h))</td>
<td></td>
</tr>
<tr>
<td>Autocorrelation</td>
<td>(\rho_{Yk}) or (\rho_Y(h)) (\hat{\rho}_{Yk}) or (\hat{\rho}_Y(h))</td>
<td>(r_{Yk}) or (r_Y(h))</td>
<td></td>
</tr>
<tr>
<td>Correlation length</td>
<td>(\lambda_Y)</td>
<td>(\hat{\lambda}_Y)</td>
<td></td>
</tr>
<tr>
<td>Integral scale</td>
<td>(\epsilon_Y)</td>
<td>(\hat{\epsilon}_Y)</td>
<td></td>
</tr>
</tbody>
</table>

![Fig. 22. Prior and posterior autocovariance matrix for a one-dimensional sequence of Y-values: \([Y_1, Y_2, \ldots, Y_n]\).](image-url)
Prior to taking measurements, and under the ergodic hypothesis, all the expected values, \([\mu_1, \mu_2, \ldots, \mu_n]\) in the \([\mu_i]\) vector will be equal to \(\mu_Y\), our subjective prior estimate of the mean of the stochastic process that describes the log hydraulic-conductivity field.

The autocovariances, \([\tau_{ij}, \tau_{i2}, \ldots, \tau_{in}]\) associated with each \(Y_i\) estimate are defined in Appendix II. It can be seen there that the autocorrelation function defined in equation (13) and displayed on Figure 13(c) is simply a normalized autocovariance function, so that the autocovariances in the \([\tau_{ij}]\) matrix in Figure 22 also reflect the decrease in autocorrelation of \(Y_i\) values with distance. The diagonal \(\tau_{ii}\) values of the autocovariance matrix form a vector: \([\tau_{ii}] = [\tau_{i1}, \tau_{i2}, \ldots, \tau_{in}]\), which is the vector of uncertainties in the expected values of \(Y_i\). Under the ergodic hypothesis, all the values \([\tau_{ij}, \tau_{i2}, \ldots, \tau_{in}]\) will be equal to \(\sigma_Y^2\), the subjective prior estimate of the variance of the stochastic process that describes the log hydraulic-conductivity field.

The taking of measurements allows us to update our prior estimate of \([\mu_i]\) and \([\tau_{ij}]\) to posterior estimates \([\mu_i]'\) and \([\tau_{ij}]'\) as schematically indicated on Figure 22. Actually, the measurements may have two separate effects on the prior estimates. In the first instance, the measurements may lead us to revise our estimates of the moments of the controlling stochastic process, \(\nu_Y, \sigma_Y, \) and \(\lambda_Y\) (Kitanidis and Vomvoris, 1983; Feinerman et al., 1986). In the second instance, the measurement locations lead to a reduction in uncertainty at these locations and in a region around the points of measurement as described in Section 5.2.4. A two-step Bayesian updating procedure is thus proposed (Massmann and Freeze, 1989). In the first step, one uses the data in an unconditional sense to calculate updated estimates, \(\nu_Y', \sigma_Y', \) and \(\lambda_Y'\) given the prior estimates, \(\nu_Y, \sigma_Y, \) and \(\lambda_Y\). These can be obtained from a straightforward application of Bayes theorem (Benjamin and Cornell, 1970). In this first step, then, the prior estimates of \([\mu_i]\) and \([\tau_{ij}]\) are unconditionally updated to produce \([\mu_i]'\) and \([\tau_{ij}]'\). In the second step, the data are used in a conditional sense, taking into account measurement locations, so that the unconditional posterior estimates, \([\mu_i]'\) and \([\tau_{ij}]'\), are conditionally updated to produce \([\mu_i]'\) and \([\tau_{ij}]'\). We now provide the math for these steps.

We assume \(Y\) is normally distributed and exponentially or linearly autocorrelated [so that knowledge of \(\rho_Y(h)\), and vice versa]. Given subjective prior estimates of \(\hat{\nu}_Y, \hat{\sigma}_Y, \) and \(\hat{\lambda}_Y\), and accepting the ergodic hypothesis, we can fill the terms of the prior vector of means, \([\mu_i]\), by:

\[
\mu_i = \hat{\mu}_Y \quad \text{for all } i
\]

The diagonal terms of the autocovariance matrix, \([\tau_{ii}]\), are given by:

\[
\tau_{ii} = \hat{\sigma}_Y^2 \quad \text{for all } i
\]

and the off-diagonal terms by:

\[
\tau_{ij} = \tau_{ii} \hat{\rho}_Y(h)
\]

where \(h = |X_i - X_j|\), \(X_i\) being the location of \(Y_i\), and \(X_j\) the location of \(Y_j\).

Assume that the \(Y_i\) represent log hydraulic-conductivity values in a set of finite-element blocks in a discretized flow field. Measurements are now made at \(p\) of the \(n\) blocks. The first step in the two-step process utilizes Bayes theorem (Massmann and Freeze, 1989) to estimate \(\hat{\mu}_Y', \hat{\sigma}_Y', \) and \(\hat{\lambda}_Y'\), given \(\mu_Y, \hat{\sigma}_Y, \) and \(\hat{\lambda}_Y\). The unconditionally updated terms of \([\mu_i]'\) and \([\tau_{ij}]'\) are then given by:

\[
\mu_i = \hat{\mu}_Y' \quad \text{for all } i
\]

\[
\tau_{ii} = \hat{\sigma}_Y'^2 \quad \text{for all } i
\]

\[
\tau_{ij} = \tau_{ii} \hat{\rho}_Y(h)
\]

where \(h = |X_i - X_j|\).

The second step makes use of the concept of a measurement equation (Hachich and Vanmarcke, 1983):

\[
[\mathbf{A}] = [\mathbf{B}] [\mathbf{Y}] + [\mathbf{e}]
\]

where \([\mathbf{A}] = p \times 1\) vector of measured values; \([\mathbf{Y}] = n \times 1\) vector of actual values; \([\mathbf{B}] = p \times n\) matrix of regression coefficients; and \([\mathbf{e}] = p \times 1\) vector of zero-mean measurement errors. The conditionally updated terms of \([\mu_1]'\) and \([\tau_{ij}]'\) are then given by:

\[
[\mu_1]' = [\mu_1]' + [\tau_{ij}]' [\mathbf{B}] [\tau_{ij}]' [\mathbf{B}]' + [E] \cdot (\mathbf{A} - [\mathbf{B}] [\mu_1]'_0)
\]

\[
[\tau_{ij}]' = [\tau_{ij}]' - [\tau_{ij}]' [\mathbf{B}]' [(\mathbf{B})' [\tau_{ij}]'] [\mathbf{B}] [\tau_{ij}]'_u
\]

where \([E]\) is the covariance matrix of \([e]\).

Figure 23 provides a 12-node one-dimensional example. Error-free measurements of \(Y_i\) and \(Y_j\) are used to update the prior \([\mu_i]\) and \([\tau_{ij}]\) given in Figure 23(a). The calculated \([\mu_i]'\) and \([\tau_{ij}]'\) of Figure 23(d) are the unconditionally updated first-step values, and the \([\mu_1]'\) and \([\tau_{ij}]'\) of Figure 23(e) are the conditionally updated second-step values. Figure 23(f) will be explained in Appendix V.

All the concepts and equations presented here for a one-dimensional system apply equally well in two and three dimensions, if a single-subscript node- or element-numbering system is used for the discretized field of \(Y\)-values. The matrices \([\tau_{ij}], [\mathbf{B}],\) and \([E]\) will, of course, be much larger, and much more regular than in the one-dimensional case.

**Appendix V. A Comparison of Bayesian Updating and Kriging**

The purpose of this appendix is to summarize the differences between Bayesian updating and kriging, as raised in Section 5.2.5. We do not present a full summary of the kriging methodology. Such a summary can be found in one of the many excellent review articles on kriging in hydrogeology (Delhomme, 1978; de Marsily, 1984, 1986; Journel, 1986b; American Society of Civil Engineers, in press). The comparison of the two approaches will focus on three issues: (1) the use of the variogram rather than an autocorrelation function, (2) the nature of the underlying assumptions about the stochastic process, and (3) the use of subjective prior estimates.
Fig. 23. A 12-node, one-dimensional example of Bayesian updating of a log hydraulic conductivity field: (a) prior vector of expected values and autocovariance matrix; (b) measurement locations; (c) calculated values for vector \([A]\) and matrices \([B]\) and \([E]\); (d) unconditionally updated posterior vectors of expected values and uncertainties; (e) conditionally updated posterior vectors of expected values and uncertainties; (f) conditionally updated posterior vectors of expected values and uncertainties determined from classical kriging package rather than Bayesian updating.

Readers familiar with the kriging literature will recognize the autocorrelation function of Figure 13(c) as an upside-down variogram. In kriging, the statistic that is used to represent the autocorrelation properties of the stochastic process is the variogram function, \(\gamma_Y(h)\), rather than the autocorrelation function, \(\rho_Y(h)\). The two are related by:

\[
\gamma_Y(h) = \rho_Y(0) - \rho_Y(h) = \rho_Y^2 - \rho_Y(h)
\]

The variogram usually plots upward from the origin to the right like a Theis curve. The variogram plays a role similar to the autocorrelation function in uncertainty reduction.

Assumptions regarding the form of the stochastic process are required for both kriging and Bayesian updating. With Bayesian updating, it is generally assumed that the stochastic process is second-order stationary; that is, both the mean, \(\mu_Y\), and the variance, \(\sigma_Y^2\), of the stochastic process must be constant over the flow domain under analysis. Kriging resorts to a weaker stationarity assumption known as the intrinsic hypothesis, which postulates a stationary mean, but requires stationarity only in the difference between paired values, \((Y_i - Y_j)\), rather than in the values themselves. The intrinsic hypothesis is appealing because it allows for the determination of the statistical structure even if the mean and variance of the stochastic process are not known. In such cases, it is still possible to define a variogram and that is all that is needed.

Actually, it is possible to differentiate between three types of kriging: (1) simple kriging, in which the mean is stationary and known, (2) ordinary kriging, in which the mean is stationary but unknown, and (3) universal kriging, in which the mean can be nonstationary (i.e., it may exhibit a trend or drift). The Bayesian updating equations outlined in Appendix IV are identical to the simple kriging equations.

In Appendix III we emphasized the need for a two-step updating procedure, in which the parameters, \(\mu_Y\) and \(\sigma_Y\), of the stochastic process are first updated in an unconditional sense (taking account of the measured values, but not their locations) and then in a conditional sense (taking account of the locations). It is in the first step that Bayesian updating differs from kriging, and the difference is philosophically and quantitatively important. Kriging is based on classical statistics, whereas Bayesian updating is based on Bayesian statistics. Classical statistics do not have a place for subjective prior estimates of the population statistics before taking measurements; the first estimates of these values must await the results of the first phase of measurements. Then, when a second phase of measurements becomes available, the new measurements are simply added to the earlier ones to create a larger sample. Bayesian updating invokes Bayes' rule to convert prior estimates to posterior estimates. For sparse data networks, the subjective prior will continue to play a role in the later estimates. The Bayesian posterior estimates of \(\mu_Y\) and \(\sigma_Y\) will be quantitatively different from the classical posterior estimates, and these differences will be propagated into the second step of the process, the conditional updating step, which is mathematically identical for the two approaches. Figure 23(f) displays conditionally updated expected values and uncertainties for the one-dimensional 12-node example introduced in Appendix IV, as determined from a kriging package that uses classical statistics. Comparison with Figure 23(e) emphasizes the fact that quite different values are obtained with Bayesian updating and classical kriging.

Appendix VI. Variance Reduction Formulæ

As an example of the variance reduction formulæ described in Section 5.2.6, consider the following expression for the prior estimates of the moments of the stochastic process describing log hydraulic conductivity in two dimensions (after Vanmarcke, 1983).

If \(\mu_1\), \(\sigma_1\), and \(\lambda_1\) represent the moments at the smaller of two scales, then \(\mu_2\) and \(\sigma_2^2\) at the larger scale are given by:

\[
\mu_2 = \mu_1
\]

\[
\sigma_2^2 = \frac{\Pi (\lambda_1)^2}{A_2} \sigma_1^2
\]

where \(A_2\) is the representative area of the larger scale. Vanmarcke also provides formulæ for \(\lambda_2\), and he provides
formulae for one-dimensional and three-dimensional systems, as well as two-dimensional. Note that the representative area at the smaller scale, \( A_1 \), does not appear in the equations, so variance estimates for blocks can be obtained even from measurements at points. For most realistic values of \( A_1 \) and \( A_2 \), the variance at block scale is much reduced from the variance of measurement scale.

References

Soc. Civil Engrs. v. 109, pp. 373-385.


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