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STOCHASTIC MODELLING OF GROUNDWATER FLOW AND SOLUTE TRANSPORT IN AQUIFERS

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ABSTRACT

This paper presents an introductory overview of recently developed stochastic theories for tackling spatial variability problems in predicting groundwater flow and solute transport. Advantages and limitations of the theories are discussed. Lastly, strategies based on the stochastic approaches to predict solute transport in aquifers are recommended.

KEY WORDS Spatial variability Stochastic modelling Groundwater flow Solute transport

INTRODUCTION

Predicting any natural process is a very difficult task. The complexity of natural systems often prohibits our understanding of governing principles of the systems. For some natural systems such as groundwater reservoirs, we seem to understand the governing principle of the system (i.e. many laboratory and small-scale field experiments have substantiated the validity of Darcy's law for flow through porous media). The principle, however, is often limited to a narrow range of scales. When applying the principle to field-scale problems, we encounter the problem of extrapolating the principle to large-scale systems, due to the spatial and temporal variability of system characteristics. Consequently, our predictive ability for flow and solute transport through large-scale geological reservoirs is hindered.

Spatial variability of hydrologic parameter values in field situations has long been recognized. Accurate predictions require a detailed characterization of the spatial distribution of hydrologic parameter values in an aquifer. In view of physical, time, and economic constraints, however, such an approach is currently not considered feasible for studying large-scale aquifers. Therefore, most analyses of groundwater flow and solute transport in the past had to assume the aquifer homogeneous or to characterize the aquifer with a limited number of samples. On the other hand, many methods of estimating hydrologic properties of aquifers (such as aquifer tests) have to rely on the homogeneity assumption because of mathematical difficulties in including the heterogeneity. Thus, logical questions to ask are: how accurate is the prediction based on the homogeneity or simplified assumptions of heterogeneity? Are the aquifer parameter values estimated by analyses using the homogeneity assumption useful for our predictive models?

The purpose of this paper is to address these problems and to provide an introductory overview of the stochastic approaches which have been developed recently to tackle these problems in field-scale aquifers. Finally, general strategies of predicting groundwater flow and contaminant transport in field-scale aquifers are recommended.

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CONCEPTS OF GROUNDWATER FLOW AND TRANSPORT MODELLING

Scales of heterogeneity, REV, dispersion and measurement scale

Predictions of solute transport in aquifers generally have to rely on mathematical models based on groundwater flow and convection-dispersion equations. For groundwater flow the governing equation is

$$\nabla \cdot (K \cdot \nabla h) = S_s \frac{\partial h}{\partial t} \tag{1}$$

where K is the hydraulic conductivity tensor, h is the hydraulic head, and S_s is the specific storage. For given boundary and initial conditions, and hydraulic parameter values, (1) can be solved for a hydraulic head distribution. Then, with the knowledge of head distribution, conductivity and porosity, the direction and magnitude of groundwater flow can be determined by using Darcy's law.

For simulating solute transport, a convection-dispersion equation often used is

$$\frac{\partial c}{\partial t} = \nabla \cdot (D \cdot \nabla c) - v \cdot \nabla c \tag{2}$$

where c is the concentration of the solute, D is the dispersion coefficient, and v is the groundwater velocity. The dispersion coefficient is generally defined as the product of velocity, v, and dispersivity, α (i.e. $D = \alpha v$) which is regarded as the transport property of a porous medium.

In order to apply such mathematical models to a field situation, hydrologic parameters such as hydraulic conductivity, storage coefficient, and dispersivity, reflecting physical properties of the site have to be specified. However, these parameter values commonly exhibit a high degree of spatial variability in large-scale aquifers. As an example, Figures 1a and b show hydraulic conductivity distributions in two cross-sections of the sandy aquifer at the Borden site in Canada. The cross-sectional profiles, resulting from a sampling effort which involves a total of 1279 hydraulic conductivity measurements, manifest randomly distributed and complex lenticular structures. Without such a detailed mapping, the aquifer would have been treated as a homogeneous aquifer with a uniform hydraulic conductivity, and effects of these complex structures on flow and solute transport, thus, would have been lost. Obviously, to delineate such complex features and to predict their effects would require an intensive sampling effort and a high-resolution numerical simulation.

In addition, the spatial variability also varies with the scale of the problem, as pointed out by many researchers (e.g. Dagan, 1986; Gelhar, 1986). For example, the size of the heterogeneity within a core sample is related to variations in pore size and geometry. Such variabilities are denoted as the laboratory-scale heterogeneity. On the other hand, heterogeneities due to geologic stratification or layering in a formation are classified as the field-scale heterogeneity. The regional-scale heterogeneity represents the variation of geologic formations or facies. Variations among sedimentary basins are, then, classified as the global-scale heterogeneity, and so on. Therefore, heterogeneity exists at all scales of observations. This scale-dependent heterogeneity further complicates the analysis of flow and solute transport in aquifers.

To resolve problems of heterogeneities at the laboratory scale, hydrologists rely on the concept of representative elementary volume (REV). For example, in a saturated core sample, flow takes place through a complex network of interconnected pores or openings. Obviously, it is practically impossible to describe in any exact mathematical manner the intricate pore structure which controls the flow through porous media. As a result, one has to abandon the basic equations governing fluid flow (such as the Navier–Stokes equations) at the pore-scale level. Similar to the continuum hypothesis in fluid mechanics, groundwater hydrologists have to overlook the microscopic or pore-scale flow patterns inside individual pores and consider some average flow over a certain volume of porous media. This volume over which the flow is averaged is defined as an REV (Bear, 1979). Using the REV concept, we essentially bypass both the microscopic level, at which we consider what happens to each fluid particle, and the pore level, at which we consider the flow pattern within each pore and between pores, and then move to the macroscopic level at

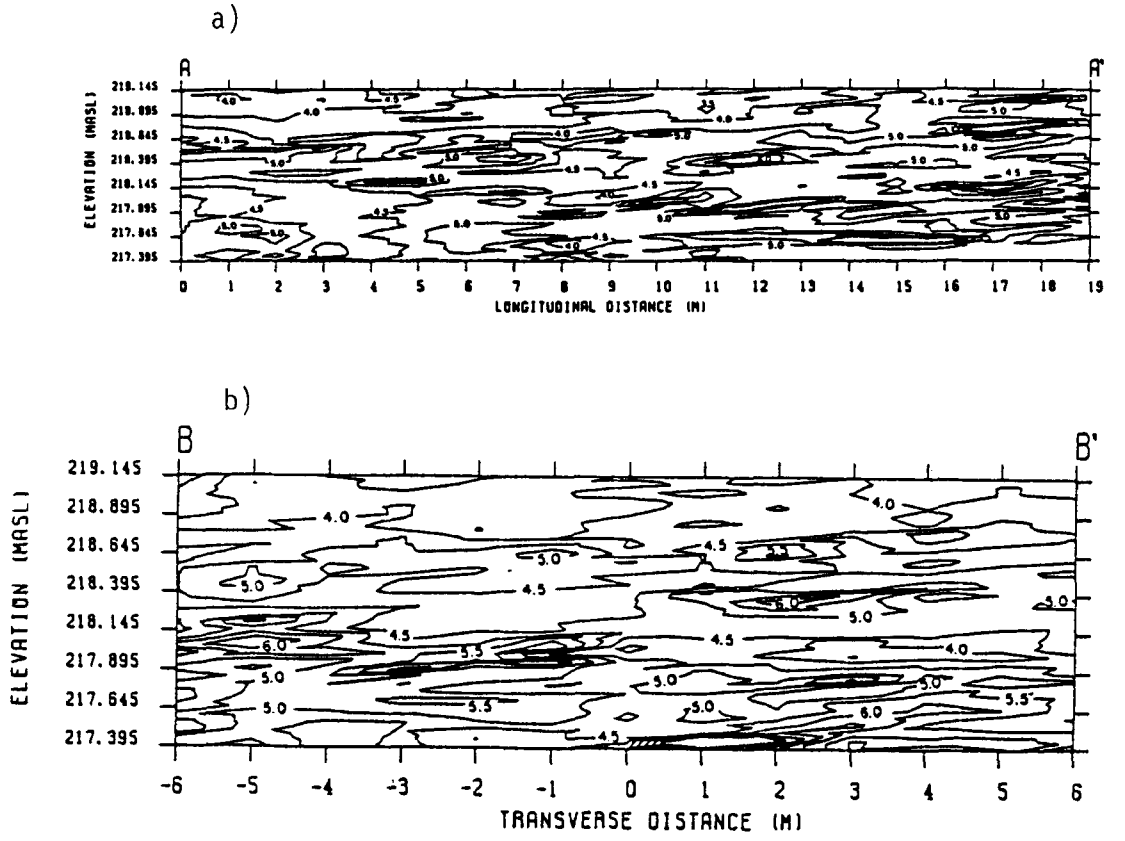

Figure 1. Cross-sectional view of the hydraulic conductivity distribution along a longitudinal and a transverse direction in the Borden Sandy aquifer (Sudicky, 1986)

which only average phenomena over the REV are considered. As a result, the properties we define represent averaged values, and the medium can be considered as a continuum over which our differential calculus applies.

Because the predicted flow behaviour based upon classic groundwater flow equations represents an average over the REV, flow behaviours deviating from the average due to the heterogeneity at scales smaller than the size of the REV are overlooked. Generally, neglecting the effect of small-scale variations has little impact on the assessment of groundwater quantity (e.g. average discharge, groundwater availability, etc.). Nevertheless, such small-scale variations can have profound impacts on transport of solute in porous media, because the small-scale variations represent fast or slow flow channels where solutes are likely to travel, thus resulting in the spread of solutes.

To include effects of small-scale variations in the analysis of solute transport in porous media, the concept of hydrodynamic dispersion is used. That is, concentration fluxes from the fast and slow flow channels are included in a transport equation via a dispersive flux, and furthermore Fick's law is assumed to be valid for this flux (dispersive flux is linearly proportional to the concentration gradient). Therefore, the classical solute transport equation includes a convective and a dispersive term, representing mass fluxes resulting from the average flow velocity and flow velocities deviating from the average, respectively. Equation 2 manifests this concept: the first term on the right-hand side represents the dispersive flux, and the second term represents the convective flux. This dispersion approach is similar to the molecular diffusion concept in chemistry, and hydrodynamic dispersion in surface water hydrology. However, the velocity variation in porous media under steady-state uniform flow conditions is mainly attributed to the heterogeneity of porous media, whereas in diffusion it is the random collision of molecules, and in surface water hydrology it is the channel roughness

and shear effects, etc. In addition, many laboratory experiments in the past also demonstrated that the effect of the small-scale heterogeneity on solute movement in porous media varies with the magnitude of the average groundwater velocity. It is generally agreed that the hydrodynamic dispersion coefficient is approximately linearly proportional to the average velocity. The constant of proportionality is defined as dispersivity, a parameter representing heterogeneities of porous media at scales smaller than the size of the REV (i.e. the average grain size in a uniformly packed soil column, Bear, 1972.)

Such an approach based on the REV concept, using Equations 1 and 2, seems adequate for dealing with laboratory-scale heterogeneity. In fact, results of numerous laboratory experiments involving uniformly packed sandboxes or soil columns have confirmed the validity of the REV approach (Bear, 1972). The REV concept, thus, becomes the foundation of many principles of groundwater hydrology. However, when we apply these principles to large-scale aquifers, we somehow forget the basic assumption of the REV approach. That is, the flow behaviour predicted by a continuum-based REV model represents an average behaviour of the flow over the REV, and does not necessarily depict phenomena measured or observed at scales much smaller than the size of the REV. For example, the drawdown predicted by the Theis solution, which assumes that the aquifer is homogeneous, will be different from that observed in a well tapping a local clay lens. The drawdown at this observation well will reflect the response of the clay lens to the stress caused by pumping and will not necessarily represent the response of other parts of the aquifer, unless the aquifer is truly homogeneous. By the same token, one may not be able to obtain a meaningful transmissivity value estimated from hydrography at this well using methods that assume aquifer homogeneity. This problem can be attributed to the fact that the screen length over which the hydraulic head is averaged in a well may not agree with the size of the REV used in the classical continuum theory for homogenizing the heterogeneous aquifer. Hence, to be consistent with the continuum theory, the measurement scale (screen length in this case) should be the same as (or larger than) the REV which allows us to treat the aquifer as a homogeneous one.

Similarly, the concentration calculated from Equation 2 depicts the average concentration of a chemical species over the REV only. This implies that the predicted concentration based on Equation 2 may not be equivalent to that measured at a volume much smaller than the size of the REV. Again, to be consistent with the theory, the measurement scale for the concentration must be at least the same as the size of the REV. Generally, this scale requirement is met in a laboratory tracer experiment where a soil column is packed with a relatively uniform sand. In such a soil column, the variation in grain size and geometry contributes to the heterogeneity and the concentration of a tracer collected at the end of the column is often the average concentration over the cross-sectional area of the column which contains numerous grains or pores. Because of this average and the large contrast between the size of the heterogeneity and the cross-sectional area of the soil column, success in predicting tracer movement in soil columns has been widely reported.

On the other hand, an aquifer consists of heterogeneities of many different scales, such as variations in pore geometry and size, layers, facies, and sedimentary structures. Treating such an aquifer as a homogeneous one in mathematical analyses is tantamount to employing a large-size REV, many times the largest heterogeneity. However, our sampling devices (such as the screen length of an observation well) are generally much smaller than the size of the REV. Therefore, predictions based upon an assumption of homogeneity will likely deviate from our observations unless the sampling interval is much larger than the size of heterogeneity (e.g. Black and Freyberg, 1987).

APPROACHES FOR SPATIAL VARIABILITY

Deterministic approach

For decades, hydrologists have relied on deterministic approaches to predict flow and solute transport in many highly heterogeneous aquifers. The deterministic approach implies that parameter values in a mathematical model are known and specified at all points in the solution domain. The deterministic approach can be subdivided into an equivalent homogeneous and a heterogeneous approach. The equivalent homogeneous approach assumes that a heterogeneous aquifer can be treated as an equivalent homogeneous one whose hydraulic properties are constant in space. Such constant properties are called effective properties

and are generally obtained by employing large-scale hydraulic tests and inverse procedures, such as aquifer tests, or by averaging many small-scale tests (i.e. the arithmetic, geometric, or harmonic mean of conductivity values obtained from slug tests). These effective parameters are then used as input to mathematical models to predict groundwater flow or transport of contaminants in the aquifer in an average sense. The heterogeneous approach, on the other hand, utilizes all available field data to delineate heterogeneities of the aquifer. This approach is intended to characterize the behaviour of groundwater flow or transport of contaminants in aquifers at high resolutions.

Regardless of whether treating the aquifer as a homogeneous or heterogeneous one, the deterministic approaches suffer from many drawbacks. Firstly, there are no conclusive means to obtain effective parameters of the equivalent homogeneous aquifer using data from large-scale hydraulic tests. For example, one must determine how many observation wells are needed to employ Theis' solution properly to estimate the effective transmissivity. In other words, the question raised earlier on consistency between the scales of field data and model's REV is never answered. On the other hand, if one relies on small-scale hydraulic tests (e.g. slug tests and conductivity measurements using core samples), the hydraulic parameter values measured at various parts of the aquifer are likely to be different. Then, logical questions to ask are: how are the data to be averaged to obtain the effective hydraulic properties for the equivalent homogeneous aquifer? And provided that such an effective hydraulic conductivity can be defined, how can the predicted results be related to our observations? The heterogeneous approach is not immune from problems either: can we predict flow and transport in heterogeneous aquifers using only limited data collected from small-scale tests? How does one assign aquifer property values at locations where no measurements were made? What is the magnitude of uncertainty in our predictions if only a limited number of data are available? To answer these questions, a probabilistic approach is necessary, and a stochastic approach seems most appropriate.

Stochastic approach

Although the theories based on stochastic approaches to tackle spatial variability problems in groundwater hydrology have been developed only in the past decade, many recent field experiments in both saturated zones (Freyberg, 1986; Sudicky, 1986; Garabedian *et al.*, 1991) and unsaturated zones (Yeh *et al.*, 1986; Greenholtz *et al.*, 1988; McCord *et al.*, 1991) have already indicated that the stochastic theories are promising at least for geological formations with relatively mild heterogeneities, regardless of many simplifying assumptions used in their development. In the following sections, the stochastic approach is introduced by first discussing the concept of statistical representation of heterogeneity. Then, recently developed stochastic theories of flow and transport in groundwater systems are discussed. Finally, strategies for predicting flow and transport of contaminants in large-scale aquifers are suggested.

STATISTICAL REPRESENTATION OF HETEROGENEITY

Aquifers are inherently heterogeneous at various observation scales. Characterizing the heterogeneity at a scale of our interest generally requires information of hydrologic properties at every point in the aquifer. To delineate such a detailed hydraulic property distribution in aquifers of sizes of tens of kilometres obviously requires numerous measurements, considerable time, and great expense, and is generally considered impractical and infeasible. The alternative is to utilize a small number of samples to estimate the variability of parameters in a statistical framework. That is, the spatial variation of a property is characterized by its probability distribution estimated from samples. For instance, Law (1944) and Bennion and Griffiths (1966) reported that the distribution of porosity data in an aquifer is normal. Hoeksema and Kitanidis (1985) suggested that the spatial distribution of storage coefficient may be log-normal. Hydraulic conductivity distributions (Figure 2) are usually reported to be log-normal (Law, 1944; Bulness, 1946; Warren *et al.*, 1961; Bakr, 1976; Freeze, 1975; and Sudicky, 1986) or other (Jensen *et al.*, 1987).

Based on such a statistical approach, Freeze (1975) treated hydraulic conductivity as a random variable and analysed the uncertainty in groundwater flow modelling. However, recent analyses of hydraulic conductivity data (Bakr, 1976; Byers and Stephens, 1983; and Hoeksema and Kitanidis, 1985) showed that although the hydraulic conductivity values vary significantly in space, the variation is not entirely random,

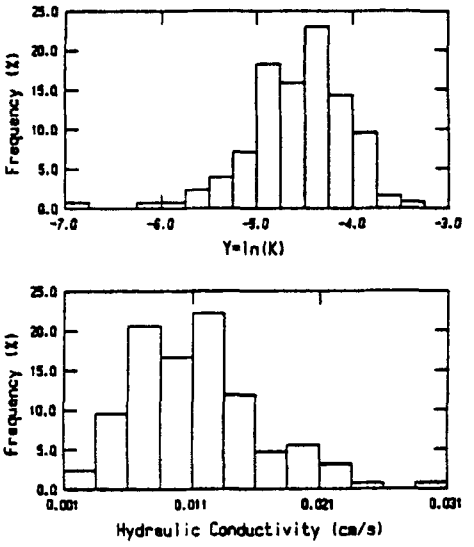

Figure 2. Frequency histograms for ln(K) and K at the Borden site

but correlated in space. Such a correlated nature implies that the parameter values are not statistically independent in space and they must be treated as a stochastic process, instead of a single random variable.

To explain the stochastic conceptualization of the spatial variability of hydrologic parameters, the hydraulic conductivity data measured along a vertical bore hole in a sandstone in Illinois (Bakr, 1976) are used as an example (see Figure 3). The value of hydraulic conductivity at a point, x_0, along the bore hole can be conceptualized as one of many possible geological materials that may have been deposited at that given point. Thus, the hydraulic conductivity at that point is a random variable, $K(x_0, \omega)$. The ω indicates that there are many possible values of K at x_0. Similarly, the hydraulic conductivity values at other locations along the bore hole are random variables. As a results, hydraulic conductivity values of the entire depth of the bore hole may be considered as a collection of many random variables in space. Namely, if conductivity is observed at locations $x_1, x_2, x_3 \ldots x_n$, then $K(x_1, \omega)$ is a random variable, $K(x_2, \omega)$ another random variable, and so on out to $K(x_n, \omega)$. Each has a probability distribution and furthermore, the probability distributions may be interrelated. The chance of finding a particular sequence of hydraulic conductivity values along the bore hole, $K(x, \omega_1)$, depends not only on the probability distribution of the hydraulic conductivity at one location but also on those at other locations. This implies that actual hydraulic conductivity values along the bore hole are one possible sequence of $K(x, \omega_1)$ out of all the possible sequences, $K(x, \omega)$. In the vocabulary

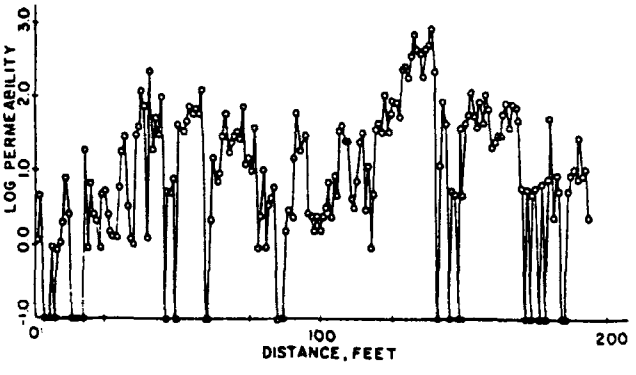

Figure 3. Log saturated conductivity values of Mt. Simon Sandstone, Illinois (Bakr, 1976)

of stochastic processes, the probability of finding of the sequence is then defined as the joint probability distribution or joint distribution. All these possible sequences are called an ensemble, and a realization refers to one of the possible sequences.

In order to determine the probability of occurrence of a particular sequence of random variables, a joint distribution of these random variables must be known. This joint distribution is completely defined only if the probabilities associated with all possible sequences of $K(x, \omega)$ values along a bore hole are known. Obviously, the joint distribution is not available in real-life situations because hydraulic conductivity values sampled along a bore hole represent only one realization out of the ensemble of the hydraulic conductivity values along the bore hole. Therefore, one must resort to simplified assumptions, namely, stationarity and ergodicity.

Stationarity (or strict stationarity) implies that any statistical property (joint distribution, mean, and variance) of a stochastic process remains stationary or constant in space. Ergodicity means that by observing the spatial variation of a single realization of a stochastic process, it is possible to determine the statistical property of the process for all realizations. Since in reality one always deals with a specific geologic formation (i.e., one realization) rather than an ensemble of such formations, one has no choice but to adopt the assumption of ergodicity as a working hypothesis for the stochastic approach. With this assumption in mind, the ensemble parameter, ω, will be dropped from our notations in subsequent discussions for convenience.

Because the stationarity is a very stringent assumption, and because in many cases important properties of a stochastic process can be assessed by moments, i.e. the mean (first moment) and covariance function (second moment), an assumption of weak or second-order stationarity is often invoked. The first moment (mean) of $K(x)$ is defined as:

$$\mu = E[K] = \int_0^\infty K f(K) dK \tag{3}$$

where $E[]$ stands for the expected value, i.e., the average over the entire ensemble, and $f(k)$ is the joint density distribution of K. The covariance function is defined as:

$$c(\xi) = \text{cov}[K(x + \xi), K(x)] = E[(K(x + \xi) - \mu)(K(x) - \mu)] \tag{4}$$

Second-order stationarity implies that the mean is a constant and the covariance function depends only on the separation distance, ξ. It is the distance that separates any two samples in the calculation of the covariance function. This assumption allows us to characterize the stochastic process by using only its mean and covariance function. If the separation distance is set to zero, the covariance function becomes the variance. If the separation distance is set to zero, the covariance function becomes the variance. An autocorrelation function is simply defined as the ratio of the covariance function to its variance, i.e.,

$$\rho(\xi) = \frac{c(\xi)}{\sigma^2} \tag{5}$$

The autocorrelation function represents the persistence of the value of a property in space.

Generally, the autocorrelation function value of the hydraulic conductivity data tends to drop rapidly as the separation distance increases. The decline of the correlation can be represented by many different autocorrelation models. The one commonly used is an exponential decay model (Bakr *et al.*, 1978; Gelhar and Axness, 1983; Yeh *et al.*, 1985a,b,c):

$$\rho(\xi) - \exp\left\{-\left[\left(\frac{\xi_1}{\lambda_1}\right)^2 + \left(\frac{\xi_2}{\lambda_2}\right)^2 + \left(\frac{\xi_3}{\lambda_3}\right)^2\right]\right\} \tag{6}$$

where ρ is the autocorrelation function, ξ is the separation vector, and the integral scales (or correlation scales) in the x, y, and z directions are λ_1, λ_2, and λ_3, respectively. The integral scale is defined as the area

under an autocorrelation function if the area is a positive and non-zero value (Lumley and Panofsky, 1964). For the exponential model, the integral scale is the separation distance at which the correlation drops to the $\exp(-1)$ level. At this level, the correlation between data points is considered insignificant. That is, data points separated by distances larger than the correlation scale are only weakly associated with each other. Furthermore, if the correlation scales of a random field are the same in all the directions, the random field is said to be statistically isotropic. On the other hand, statistical anisotropy implies that the correlation scales of the random field are different in all the directions; that is, the variability of the field has a preference for certain directions.

On an intuitive basis, the correlation scale may be interpreted as the average length of clay lenses or sedimentary structures (for example, cross-bedding, stratification, etc.). Hydraulic property values of samples taken within the clay lens tend to be similar; correlation between sample values is near unity. However, sample values are quite different if one sample is taken within the clay lens and the other outside the lens; the resulting correlation will be small. Thus, the autocorrelation function is a statistical measure of spatial stucture of hydrogeologic parameters. Table I presents a summary of correlation scales for hydraulic conductivity or transmissivity in a variety of geologic environments in which data were collected by methods ranging from cores to aquifer tests.

Using the stochastic representation, spatial variability of hydrogeologic properties thus can be characterized by the means and covariance functions of the properties. Notice that this approach does not provide information about the values of aquifer properties at any location in the aquifer but provides a way to quanitfy the spatial variability of the properties. That is, we only know where the mean value of the properties lies and how widely the property values spread around the mean value.

Table I. Variances and correlation scales for log hydraulic conductivity or log transmissivity (Gelhar, 1986)

Source	Medium	σ_f	Correlation scale, (m)	Overall scale, (m)
Bakr (1976)	Sandstone aquifer	1·5–2·2	0·3–1·0V	100
Smith (1978)	Outwash sand	0·8	0·4V	30
Delhomme (1979)	Limestone aquifer	2·3	6300H	30000
Binsariti (1980)	Basin fill aquifer	1·0	800H	20000
Russo and Bressler (1981)	Hamra Red Mediterranean soil	0·4–1·1	14–39H	100
Luxmoore *et al.* (1981)	Weathered shale subsoil	0·8	<2H	14
Sisson and Wierenga (1981)	Silty clay loam soil (alluvial)	0·6	0·1H	6
Viera *et al.* (1981)	Yolo soil (alluvial fan)	0·9	15H	100
Devary and Doctor (1982)	Alluvial aquifer (flood gravels)	0·8	820H	5000
Byers and Stephens (1983)	Fluvial sand	0·9	0·1V	5
			>3H	14
Hoeksema and Kitanidis (1985)	Sandstone aquifer	0·6	45000H	5×10^5
Hufschmied (1985)	Sand and gravel	1·9	0·5V	20
Sudicky (1985)	Outwash sand	0·6	0·1V	20

Correlation scales based on e^{-1} correlation distance: H, horizontal sampling, V, vertical sampling.

STOCHASTIC MODELLING OF FLOW AND SOLUTE TRANSPORT IN AQUIFERS

Employing the stochastic conceptualization of field heterogeneity, many stochastic methods for solving groundwater problems have been developed in the past decade. Similar to the deterministic approach, the stochastic methods can also be implemented as effective parameter (equivalent homogeneous) or heterogeneous approaches.

Effective parameter approach

The principle of this approach is identical to the equivalent homogeneity concept in the deterministic approach. As discussed in the deterministic approach, one of the major problems facing this approach is how to extrapolate small-scale measurements to large-scale effective parameters. Furthermore, since models based on the effective parameters predict the bulk behaviour of aquifers, the discrepancy between the bulk behaviour and the behaviour observed at scales much smaller the REV must be addressed. The stochastic perturbation-spectrum method to be discussed in the following paragraphs provides a means to resolve these problems although debate on the concept of the effective parameter continues (see Smith and Freeze, 1979; Anderson, 1989).

The perturbation-spectrum analyis is an analytical approach which has been used extensively by Gelhar and his coworkers (e.g. Gelhar, 1976; Bakr *et al.*, 1978; Gutjahr *et al.*, 1978; Mizell *et al.*, 1982; Gelhar *et al.*, 1979; and Gelhar and Axness, 1983; Yeh *et al.*, 1985a, b, c; Mantoglou and Gelhar, 1987a, b, c). To illustrate the approach, let us consider steady-state flow in a heterogeneous but locally isotropic aquifer (i.e., the hydraulic conductivity at the scale of core samples is isotropic) with infinite lateral extent. The governing flow equation is:

$$\frac{\partial}{\partial x_i}\left[K(x)\frac{\partial h}{\partial x_i}\right] = 0, i = 1, 2, 3 \tag{7}$$

where K is the isotropic hydraulic conductivity, and is a function of the spatial coordinates. The Einstein summation convention is used (i.e. repeated indices imply summing over the range of the indices). If $K \neq 0$, Equation 7 can be rewritten as:

$$\frac{\partial^2 h}{\partial x_i \partial x_i} + \frac{\partial \ln K}{\partial x_i}\frac{\partial h}{\partial x_i} = 0 \tag{8}$$

If the natural log of hydraulic conductivity, $\ln K$, and the hydraulic head, h, are assumed to be second-order stationary stochastic processes, Equation 8 becomes a stochastic partial differential equation. $\ln K$ and h can be decomposed into means and fluctuations of these values about their means, i.e.

$$\begin{aligned} h &= H + h',\ E[h] = H, \text{ and } E[h'] = 0. \\ \ln K &= F + f,\ E[\ln K] = F, \text{ and } E[f] = 0. \end{aligned} \tag{9}$$

where H and F are the means of h and $\ln K$, and h' and f are perturbations of h and $\ln K$, respectively. By substituting Equation 9 into Equation 8, and taking the expected value, we obtain a mean equation:

$$\frac{\partial^2 H}{\partial x_i \partial x_i} + \frac{\partial F}{\partial x_i} + \frac{\partial F}{\partial x_i}\frac{\partial H}{\partial x_i} + E\left[\frac{\partial f}{\partial x_i}\frac{\partial h'}{\partial x_i}\right] = 0 \tag{10}$$

Subtracting the mean Equation 10 from Equation 8 gives:

$$\frac{\partial^2 h'}{\partial x_i \partial x_i} + \frac{\partial f}{\partial x_i} + \frac{\partial F}{\partial x_i}\frac{\partial h'}{\partial x_i} - E\left[\frac{\partial f}{\partial x_i}\frac{\partial h'}{\partial x_i}\right] + \frac{\partial f}{\partial x_i}\frac{\partial h'}{\partial x_i} = 0 \tag{11}$$

If we assume that the log hydraulic conductivity perturbation f is small (aquifer is not highly heterogeneous), say, $\sigma_f^2 < 1{\cdot}5$ (Ababou *et al.*, 1988), it is logical to expect the head perturbation h will be small. Then, it is reasonable to neglect terms that involve products of perturbations so that the perturbation equation can be written as:

$$\frac{\partial f}{\partial x_i}\frac{\partial H}{\partial x_i} + \frac{\partial F}{\partial x_i}\frac{\partial h'}{\partial x_i} + \frac{\partial^2 h'}{\partial x_i \partial x_i} \approx 0 \tag{12}$$

This equation represents a first-order approximation of the relationship between the perturbations in $\ln K$ and h' in a steady-state flow with mean gradients, $\partial H/\partial x_i$.

The above mathematical procedures are equivalent to visualizing the heterogeneous aquifer as a collection of finite elements, and flow in each element is described by the governing flow equation with a constant hydraulic conductivity value. A collection of an infinite number of elements whose hydraulic conductivities are spatially correlated is then equivalent to an ensemble in the stochastic sense. Taking the expected value (ensemble average) of Equation 8 with stochastic parameters is tantamount to homogenizing the heterogeneous aquifer and to ignoring the details of the flow behaviour in each element but examining the average behaviour of the flow in all the interconnected elements. The perturbation equation thus depicts the deviation of the flow from the mean flow.

Using the perturbation-spectrum technique and assuming statistical isotropy in $\ln K$, Bakr *et al.* (1978) solved Equation 12 to analyse the effects of spatial variability on steady-state groundwater flow. Closed forms of head variance expressions (a statistic measure of the deviation of the head value at a point from the mean head) were derived for one- and three-dimensional flow fields in which hydraulic conductivity is a spatially-varying stochastic process. Several important conclusions about the effects of spatial variability were drawn from the results of the study. Hydraulic head distribution tends to be smooth due to the damping effect of the groundwater system. That is, the head values are correlated over a much longer distance than the hydraulic conductivity values, and variance in head is generally small. Moreover, the head values are anisotropic (i.e. correlated over a longer distance in the direction perpendicular to the mean flow than the direction parallel to the flow.), even if the hydraulic conductivity field is statistically isotropic. The head variance can be related to the variance of $\ln K$ by:

$$\sigma_{h'}^2 = \beta \sigma_f^2 J^2 \lambda^2 \tag{13}$$

where β is a constant having a value of 1 for one-dimensional flow, 1/3 for three-dimensional flow, J is the mean hydraulic gradient, σ_f^2 is the variance of the natural logarithm of hydraulic conductivity, and λ is the correlation scale. Equation 13 indicates that the variability in head will be small due to small J values in most aquifers (in the order of 10^{-3} or smaller.) In addition, the head variation predicted by a three-dimensional model is much smaller than that by a one-dimensional model. This means that a three-dimensional model would be much more appropriate for analysing flow and solute transport in field problems. It is also manifest from Equation 13 that the correlation scale is an important factor in the calculation of head variance or uncertainty in head prediction.

Gutjahr *et al.* (1978) defined effective hydraulic conductivity for heterogeneous $\ln K$ fields as the mean Darcy flux divided by the mean hydraulic gradient. They concluded that the effective hydraulic conductivity in one-dimensional flow, perpendicular to layering, is the harmonic mean

$$K_e = K_g \exp[-\sigma_f^2/2] \tag{14}$$

where K_g is the geometric mean of K, and the arithmetic mean for flow parallel to bedding, i.e.:

$$K_e = K_g \exp[\sigma_f^2/2] \tag{15}$$

In the three-dimensional flow situation, the effective hydraulic conductivity is given by Gelhar and Axness (1983) as

$$K_e = K_g \exp[\sigma_f^2/6] \tag{16}$$

which is slightly greater than the geometric mean. They suggested that the geometric mean of K may be a good estimator for the effective hydraulic conductivity values for field situations.

Gelhar and Axness (1983) investigated the effective hydraulic conductivity of large-scale aquifers in which the hydraulic conductivity field is assumed to be statistically anisotropic. They showed that the effective hydraulic conductivity, in general, is a second-rank symmetric tensor whose principal components depend on the ratios, λ_1/λ_2 and λ_1/λ_3. Figure 4 shows the dependence of the principal hydraulic conductivities for the case with $\lambda_1 = \lambda_2 \neq \lambda_3$ on the degree of variability of log hydraulic conductivity as well as the geometry of the heterogeneity as characterized by the ratio of λ_1/λ_3.

These results provide a practical tool for predict flow and solute transport in large-scale aquifers. Hydrologic modellers always face the problem of insufficient data (for example, hydraulic conductivity measurements). As a first step towards solving such a problem, one may use these limited data to determine the variance of ln K and correlation scales and thus, the effective hydraulic conductivity can be estimated by using Equations 14, 15, 16, depending on the dimensionality of the model, or by using Figure 4. Consequently, the mean flow behaviour can thus be estimated. In fact, a successful application of this approach to the mean flow path of tracers in a field experiment was reported by Sudicky (1986). If there are no hydraulic conductivity data available, one may still approximate the effective conductivity by using the variances and correlation scales of similar kinds of materials reported in the literature (see Table I). Once the mean flow is determined, the head variance can be evaluated and can then be used as a measure of the error in the effective parameter model as a result of unmodelled aquifer heterogeneity. Therefore, the head variance is an appropriate model calibration target for defining the detailed hydraulic conductivity distribution,

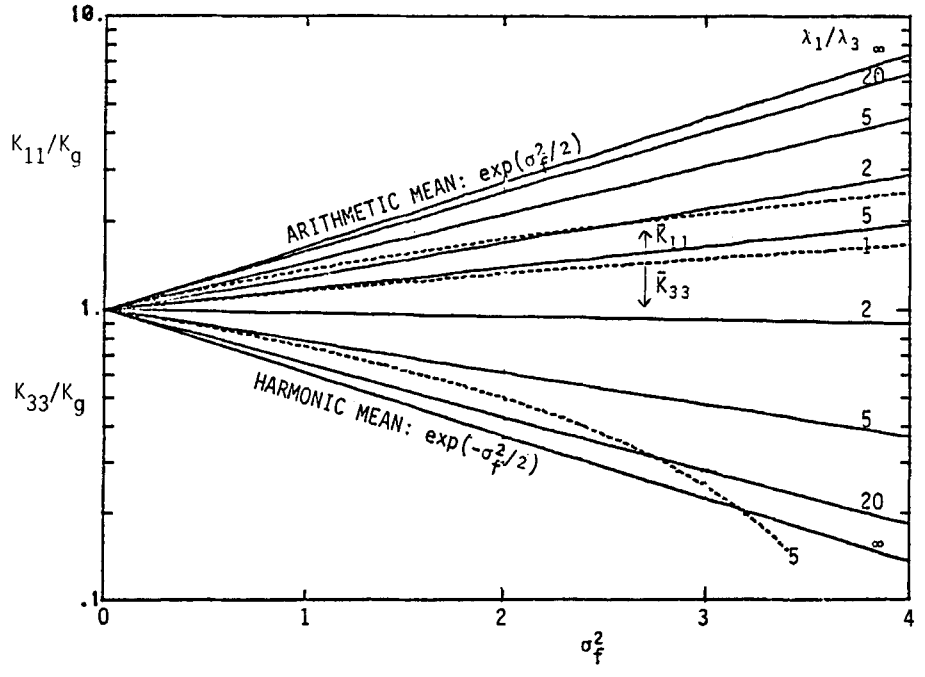

Figure 4. Effective hydraulic conductivities parallel ($\bar{K}_{11}$) and perpendicular ($\bar{K}_{33}$) to bedding: the solid lines are the generalization (60) and the dashed lines are the first order results (59): $\lambda 1 = \lambda 2$

provided that other sources of error are also considered. The hydraulic conductivity field obtained from the calibration may, then, be used to approximate the movement of solutes in aquifers. Application of such an approach to field problems was illustrated in the paper by Gelhar (1986).

An alternative approach is to use the estimated effective hydraulic conductivity to predict the migration of a contaminant plume resulting from the average flow. Since flow predicted based on the effective hydraulic conductivity ignores the fast or/and slow moving solute particles due to subscale velocity variations which can cause the spread of the plume, the hydrodynamic dispersion concept must be employed. Generally speaking, the REV involved in this case is large. Thus, the dispersion due to the variation in hydraulic conductivity values at scales smaller than this REV is typically called macrodispersion and the dispersivity the macrodispersivity. To relate macrodispersivities to the spatial variability of hydraulic conductivity measurements. Gelhar and Axness (1983) derived mathematical expressions by the perturbation-spectrum technique. One of their results is

$$A_{11} = \sigma_f^2 \lambda / \gamma^2 \tag{17}$$

where A_{11} is the longitudinal macrodispersivity at large time, σ_f^2 is the variance of f, λ is the correlation scale of the statistically isotropic porous medium, and γ is the flow correlation factor which depends on the direction of the mean flow and the orientation of the heterogeneity. Equation 17 implies that the macrodispersivity values can be estimated from the knowledge of the variation of local-scale hydraulic conductivity values without conducting a large-scale field tracer experiment. Although conducting a large-scale field tracer experiment is most appropriate for determining solute movement in aquifers, it is impractical in terms of time and expense required for such an experiment. On the other hand, local-scale hydraulic conductivity values have commonly been measured in many aquifers. These data are generally not quite adequate for any detailed numerical simulations, but may be suitable for estimating the statistical parameters required for the macrodispersivity determination. Hence, the macrodispersivity approach is a practical tool for solving many groundwater pollution problems without resorting to extensive site characterization.

It should be pointed out that the macrodispersivity is also an effective parameter (i.e. an ensemble averaged parameter). It represents the subscale velocity variation averaged over many possible aquifers of similar heterogeneity, or the variation averaged over many parts of an aquifer. Thus, the macrodispersivity approach produces the mean concentration distribution only. However, the actual concentration distribution observed in an aquifer may be quite different from the mean. For example, Figure 5 shows the differences between an observed concentration distribution in the Borden sandy aquifer and a mean concentration distribution calculated from the classic convection-dispersion equation with macrodispersivity values. A measure of the difference between the two distributions (concentration variance) becomes necessary. Vomvoris and Gelhar (1990) developed an expression for the concentration variance and found that the concentration variance is proportional to the mean concentration gradient and to the variance and correlation scales of log-hydraulic conductivity; it is inversely proportional to local dispersivity values. They concluded that the concentration variance could be large, depending on the magnitude of the parameters. Since Equation 17 is valid only for large times, or after the plume has been displaced for a large distance, when the mean concentration gradient is small, the macrodispersion approach will produce satisfactory results.

Similar research on macrodispersion has been presented by many other researchers (e.g. Dagan, 1984, 1986, 1987). Dagan (1987) derived the spatial statistics of the Eulerian velocity field in heterogeneous aquifers, converted the velocity statistics to the Lagrangian displacement variances, and derived analytical expressions for the time-dependent macrodispersivities in two-dimensional planes and three-dimensional aquifers. His approach is based on Taylor's theorem of diffusion (1922) but in Dagan's analysis the spatial statistics of the velocity field are related to the heterogeneity structure of the hydraulic conductivity field through the governing groundwater flow equation. If the hydraulic conductivity field is considered to be statistically isotropic, for early time periods (i.e. $t << \lambda/v$), the spatial displacement variances are given by:

$$\sigma_{11}^2(t) = \frac{8}{15} \sigma_y^2 v^2 t^2 + 2D_L t \tag{18}$$

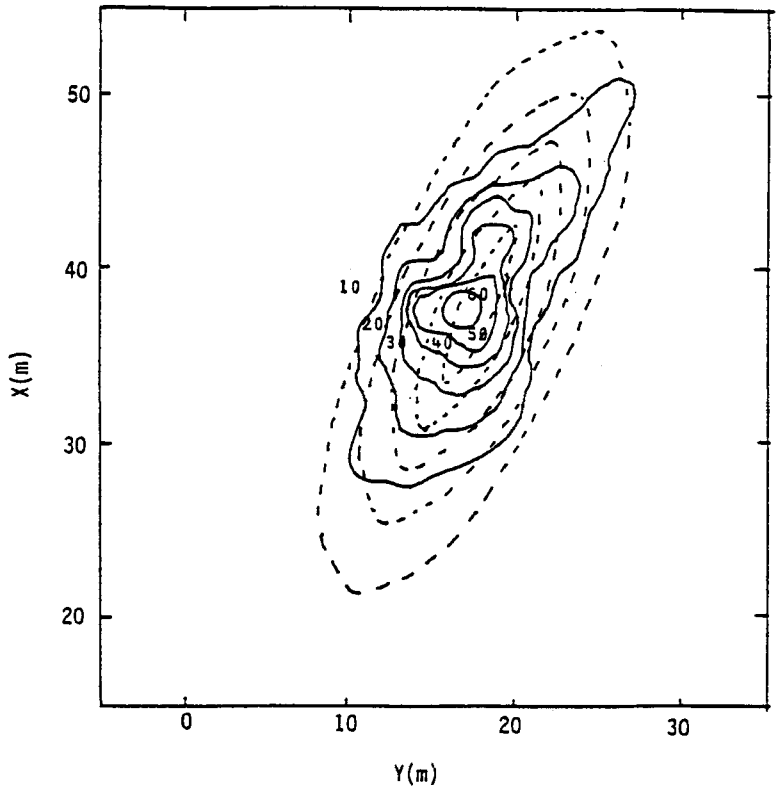

Figure 5. Schematic illustration of an observed depth-averaged concentration profile (solid) and a mean profile (dash), calculated from the macrodispersion equation (modified from Sudicky, 1986)

and

$$\sigma_{22}^2(t) = \sigma_{33}^2(t) = \frac{1}{15}\sigma_y^2 v^2 t^2 + 2D_T t \tag{19}$$

for three-dimensional flow, where σ_{11}^2, σ_{22}^2, and σ_{33}^2 are the displacement variances in the direction of flow, and in lateral directions, respectively. Local-scale dispersion coefficients in the longitudinal and the transverse directions are D_L and D_T, respectively, v is the mean velocity, t is time, and λ is the correlation scale of the hydraulic conductivity field. The parameter σ_y^2 represents the variance of the natural log hydraulic conductivity in three-dimensional flow and the variance of the natural log of transmissivity in two-dimensional flow. The results of the two-dimensional flow analysis are:

$$\sigma_{11}^2(t) = \frac{3}{8}\sigma_y^2 v^2 t^2 \tag{20}$$

$$\sigma_{22}^2(t) = \frac{1}{8}\sigma_y^2 v^2 t^2 \tag{21}$$

For large time periods (i.e. $t > > \lambda/v$), the three-dimensional results are:

$$\sigma_{11}^2(t) \approx 2\sigma_y^2 v\lambda t + 2D_L t \tag{22}$$

$$\sigma_{22}^2(t) = \sigma_{33}^2(t) \approx \frac{2}{3}\sigma_y^2 \lambda^2 t \tag{23}$$

and the two-dimensional results,

$$\sigma_{11}^2(t) \approx 2\sigma_y^2 \lambda vt\left[1 - \frac{3\ln(vt/\lambda)}{2vt/\lambda}\right] \tag{24}$$

$$\sigma_{22}^2(t) \approx \sigma_y^2 \lambda^2[\ln(vt/\lambda) - 0{\cdot}933] \tag{25}$$

Note that the displacement variance is the spatial variance of a tracer plume, representing the size of the plume at a relative concentration equal to the $\exp(-1)$ level if the plume is assumed to have a normal distribution. Macrodispersion coefficients can be determined by taking the time derivative of the displacement variances. Since the spatial displacement variances (Equations 18 to 21) for early time periods depend on t^2, the macrodispersion coefficient grows with time or mean travel distance (this is the so called scale-dependent dispersion). For late time periods, the concentration variances (Equations 22, 23, 24 and 25) are a function of t only, and the macrodispersion coefficients or macrodispersivities are constant over time. Note that Equations 18–25 evaluate the spatial displacement variance (or the second moment of a plume) and do not predict the shape of the concentration plume but its 'size' (Yeh, 1987). Thus, the classic convection-dispersion equation, which assumes the validity of Fick's law, is avoided. Similar expressions for the displacement variances in statistically anisotropic media were reported by Dagan (1988), Neuman and Zhang (1990), and Zhang and Neuman (1990).

In general, these results seem to compare favourably with those obtained from a field tracer experiment (Freyberg, 1986; Sudicky, 1986) conducted in a sand aquifer in Canada (see Figure 6). Analysis of a recent field tracer experiment by Garabedian *et al.* (1991) in a glacial outwash aquifer also indicated that the stochastic results (i.e. Gelhar and Axness, 1983; Dagan, 1987) are robust, regardless of many assumptions used in the development. However, such a statement may be premature at this time since many disputes on the use of Dagan's two-dimensional model for the Borden site continue (see Kemblowski, 1988; and White, 1988). Moreover, Naff *et al.* (1988) developed a three-dimensional macrodispersion model for perfectly stratified aquifers and attempted to reproduce the field experimental results at the site. However, they found that the three-dimensional model, which is more realistic than the two-dimensional model developed by Dagan (1987), does not reproduce the tracer concentration distribution as well as the two-dimensional model. Naff *et al.* (1989) attributed the discrepancy to temporal variation in flow patterns which is not considered in all the stochastic models. Daga (1989) defended the two-dimensional approach with the conjecture that there exists a clay lens of large lateral extent, prohibiting vertical spreading of the tracer plume. This conjecture, however, has not been verified. Clearly, the robustness of the macrodispersion approach still remains to be tested.

Overall, the major advantage of the analytical approaches by Gelhar and Axness (1983), Dagan (1987), and others is that they provide an explicit expression relating the variability of local hydraulic conductivity measurements to the macrodispersivity and the spatial variance of the mean concentration distribution. Thus, one can estimate the effective hydraulic conductivity and the macrodispersivity values of large-scale aquifers if the statistical parameters characterizing the variability of the small-scale hydraulic conductivity values are known. The major drawback of the method is that the solution (or the formula) may be valid only for small values of variations in hydraulic conductivity because of the omission of perturbation product terms in the analysis. Several studies have shown the results to be valid for the variance of $f = 1$ (Gelhar, 1986). For cases where a large variance in f is expected (such as in fracture rocks where in one case the variance of $\ln K$ has been reported to be about 8·7, (Neuman, 1987)), the accuracy of the perturbation-spectrum approach seems doubtful. One should also keep in mind that the macrodispersion model predicts the mean (or ensemble averaged) concentration distribution. Even if the macrodispersion model is valid for large variance of f or other parameters, the actual distribution may be significantly different from the mean concentration distribution. Thus, the usefulness of the macrodispersivity approach is limited.

Further, the perturbation-spectrum approach assumes stationarity. In a basin-scale aquifer, the hydraulic conductivity field is likely to be non-stationary because of changes in depositional environments which may contain heterogeneities of a variety of scales (e.g. Gelhar, 1986; Anderson, 1989). How to incorporate such a

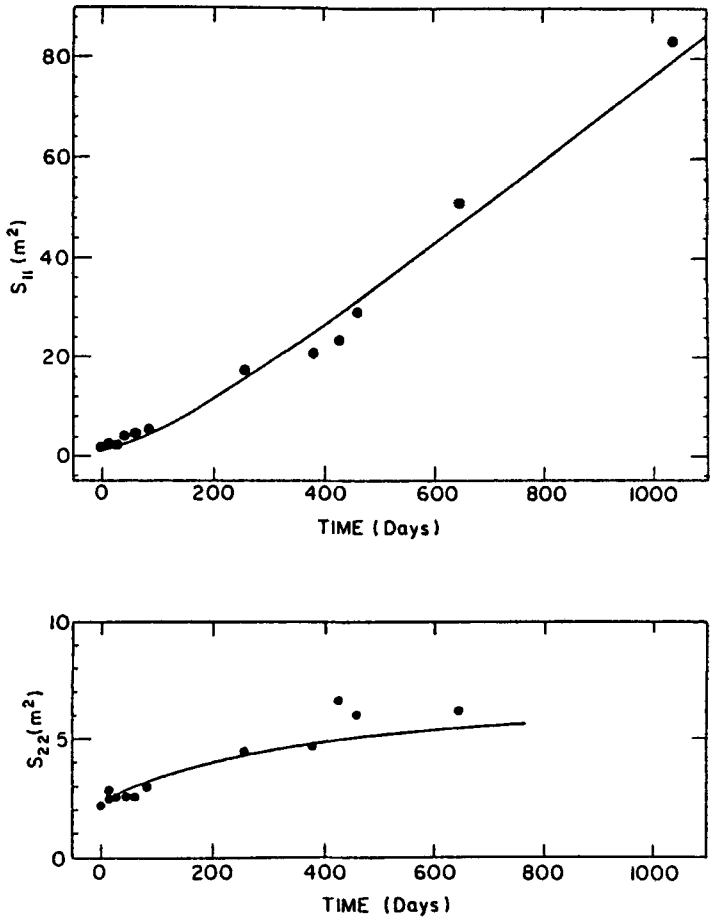

Figure 6. A comparison of observed (dots) and theoretical (line) spatial concentration variance in the longitudinal and transverse directions (Dagan, 1987)

feature in the approach remains to be explored. Finally, the validity of using the classic convection-dispersion equation for predicting solute concentration distribution in a large-scale aquifer is still under debate (e.g. Gelhar *et al.*, 1979; Yeh, 1987, and others), even if macrodispersivities can be determined.

Heterogeneous approach

Several methods including geostatistics, Monte Carlo simulations, and conditional simulations can be considered as the heterogeneous approach in the stochastic modelling of flow and solute transport in aquifers.

Geostatistics. To illustrate the theory and utility of geostatistics in predicting flow and solute transport in groundwater systems, we will consider one of the common problems facing groundwater modellers when dealing with simulations of flow and solute transport in field problems: how to estimate the value of an aquifer property at locations where there are no data available. For example, if one assumes that local-scale dispersion is negligible, and movements of solutes are mainly controlled by the major flow pattern, one may attempt to use a two-dimensional, depth-average, finite difference, groundwater flow and solute transport model (say, a particle tracking model) to simulate solute movements in a groundwater basin. For accuracy or other reasons, one may design a 2000-node mesh for the entire basin. However, only 50 measured transmissivity values scattered around the entire basin may be available. To assign transmissivity values

objectively to the remaining nodes, one may have to resort to use of mathematical tools. Geostatistics is one of the possible tools. Geostatistics is a statistical method used to estimate or interpolate the parameter values at points in space where no samples are available. The technique has been widely used for decades in the mining industry to estimate ore grades (Journell and Huijbregts, 1978). Recently, this technique has been applied to groundwater hydrology to address spatial variability problems. In principle, geostatistics concepts are similar to stochastic concepts. They both are used to analyse variables distributed in space. However, some of the terminology is different. For example, the term 'random function' is used in geostatistics to define a collection of correlated random variables. That is, at a point x_1, the function $F(x_1)$ is a random variable and the random variables at x_1 and $x_1 + \xi$ are not independent but correlated. According to this definition, it is clear that the random function is equivalent to the stochastic process defined earlier. Similarly, a 'regionalized variable' is used in geostatistics to define a function $f(x)$ which takes a value at every point x of coordinates (x_1, x_2, x_3) in three-dimensional space (Journel and Huijbregts, 1978). In other words, a regionalized variable is simply a particular realization of a certain random function of stochastic process.

Two important parts of geostatistics are (1) identification of the spatial structure of the variable (variogram estimation, trend estimation, etc.) and (2) interpolation or estimation of the value of a spatially distributed variable from neighbouring values taking into account the spatial structure of the variable (kriging, co-kriging, etc., de Marsily, 1986).

Like the autocorrelation function described previously, the variogram is simply a way of defining the spatial structure of a random field. Variogram analysis is based on the intrinsic hypothesis which is less stringent than the second-order stationarity assumption. Recall that second-order stationarity requires that the data have a constant mean and that the covariance function depends on the separation distance only. However, the intrinsic hypothesis requires only that the mean of the differences between two data points is constant or depends on the separation distance, ξ, and the variance of the difference depends on the separation distance. For example, if we consider the hydraulic conductivity, $K(x)$, as a random field, under the intrinsic hypothesis, it must satisfy the following two conditions:

$$E[K(x + \xi) - K(x)] = m(\xi)$$
$$1/2\ var[K(x - \xi) - K(x)] = \gamma(\xi) \tag{26}$$

where m and γ are mean and variogram, respectively, and are functions of ξ, and not of x. Figure 7 shows the general behaviour of a variogram. As indicated in the figure, when the variance of the variable is finite, the variogram tends towards an asymptotic value equal to this variance, $var[K(x)]$. This is called the sill of the

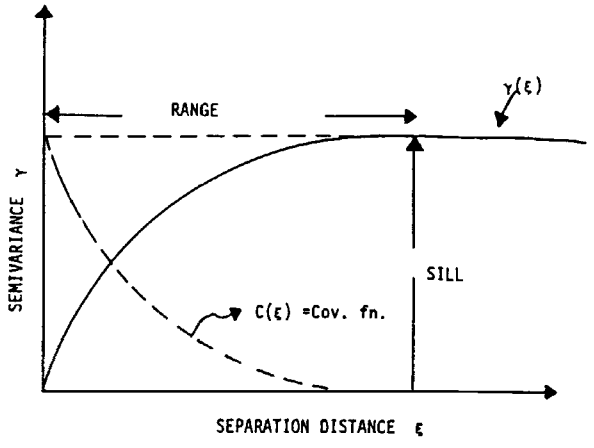

Figure 7. General behaviour of a variogram

variogram, and the distance at which the variogram reaches its asymptotic value is called the range, λ. The range is analogous to the correlation scale discussed earlier: beyond the range, the regionalized variables $K(x)$ and $K(x + \xi)$ are no longer correlated. In fact, the variogram is a mirror image of the covariance function if the data represent a second-order stationary process.

The other principal tool of geostatistics is kriging, which is an estimation technique. To illustrate the principle behind kriging, let us suppose that we are studying the transmissivity distribution in an aquifer, $T(x)$, and having measurements of its values at a number of locations, $x_1, x_2, \ldots, x_n$, we wish to predict its value at the location x_0. Intuitively, we would use the transmissivity values measured at sample locations x_1, $x_2, \ldots, x_n$, in predicting the unknown transmissivity value $T(x_0)$. In fact, this is, at least conceptually, identical to the way a contour map of transmissivity is manually drawn by geohydrologists. If we express this concept in a mathematical formula, we would write

$$\bar{T}(x_0) = F(T(x_1), T(x_2), \ldots, T(x_n)) \tag{27}$$

where $\bar{T}(x_0)$ represents the transmissivity estimate. In other words, the unknown $\bar{T}(x_0)$ is a function of the known transmissivity values. The question now is how do we choose the function F? To answer this we must first decide on the 'criterion' which we will use to measure the accuracy of $\bar{T}(x_0)$ as a predictor of $T(x_0)$. The simplest and most widely used measure of accuracy is the 'mean square error' (MSE),

$$MSE = E[\bar{T}(x_0) - T(x_0)]^2 \tag{28}$$

If we adopt this as our criterion, then the problem is to find that form of F which minimizes the MSE. If we do not restrict the form of F in any way, then the solution is the conditional expectation of $T(x_0)$, given $T(x_1)$, $T(x_2) \ldots, T(x_n)$, i.e.

$$\bar{T}(x_0) = E[T(x_0) | T(x_1), T(x_2), \ldots, T(x_n)] \tag{29}$$

The intuitive interpretation of the conditional expectation, as explained by Priestley (1981), may be seen as follows. Suppose we consider all the possible realizations of the process $T(x)$. Within this ensemble, we would expect that there must be a subset of all the realizations which consists of the values of T's at our sample locations, $x_1, x_2, \ldots X_n$ (Figure 8). The condition imposed on the expectation simply means that we will only consider this subset and discard the realizations which do not agree with the measured T values at x_1, $x_2, \ldots, x_n$ when we take the expectation. Since the subset will have different values for T at the unsampled location, x_0, the way to make our 'best' prediction of the value at x_0 is to take the expected value or the average of the different values of T in the subset at location x_0. The average value of T at x_0 over this subset

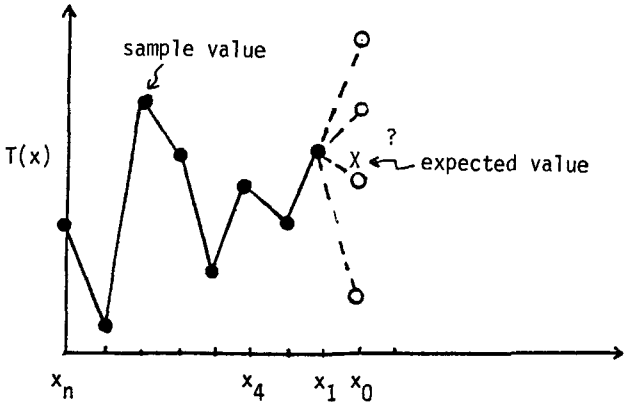

Figure 8. Schematic illustration of the conditional expectation concept

is precisely what we mean when we refer to the conditional expectation of $T(x_0)$, given $T(x_1)$, $T(x_2), \ldots, T(x_n)$.

However, the conditional expectation requires the joint distribution of $T(x_1)$, $T(x_2), \ldots, T(x_n)$, which we hardly ever know. The nearest we can approach this problem is to argue that in many cases we would expect such joint distributions to be approximately multivariate normal. If the joint distributions were normal, then the conditional expectation is a linear function of $T(x_1)$, $T(x_2), \ldots, T(x_n)$ in which case we can write the predictor of $T(x_0)$ more explicitly as

$$\bar{T}(x_0) = a_{01} T(x_1) + a_{02} T(x_2) + \cdots + a_{0n} T(x_n) \tag{30}$$

where $a_{01}, a_{02}, \ldots, a_{0n}$ are constants; a_{01} denotes the weight associated with the measurement at the location x_1 and the estimate at location x_0, and so on up to a_{0n}. The remaining step is to determine the values of the coefficients, $a_{01}, a_{02}, \ldots, a_{0n}$, which minimize the MSE. Since the MSE is a quadratic function of the $T(x)$, the values of these coefficients may be determined from a knowledge only of the autocovariance function (or variogram in the case of intrinsic random fields) of the process. Of course, we can decide to consider only linear predictors, even if the process is not multivariate normal. The argument being that if the process is jointly normal then the linear predictor is optimal, whereas if the process is not jointly normal then, in general, we would be unable to evaluate the conditional expectation and so we might as well seek the best linear predictor.

Now, we will briefly examine the theory of kriging. The most general form of kriging is termed 'Universal Kriging,' in which the values of points in space may be estimated from irregularly distributed samples in the presence of trends (or non-stationarity). If the data set is stationary, a less involved operation can be used to estimate the values of the points. This technique is referred to simply as 'Ordinary Kriging' or 'Kriging' (see Journel and Huijbregts, 1978).

Again, we will use the estimation of transmissivity values at unsampled locations in between test wells as an example. To find the transmissivity estimate $\bar{T}(x_0)$ of the unknown quantity $T(x_0)$, kriging uses a weighted linear sum of all the available sample values (measured transmissivity values):

$$\bar{T}(x_0) = \sum_{i=1}^{n} a_{0i} T(x_i) \tag{31}$$

where the a_{0i} are called the kriging weights, and $T(x_i)$ are sample values. In order to limit the choice of the kriging weights, we will impose two conditions. The first condition is that the expected value of the estimate of $T(x_0)$ should be the same as the expected value of $T(x_0)$, i.e.,

$$E[\bar{T}(x_0)] = E[T(x_0)] \tag{32}$$

This condition implies that the kriging estimator has to be unbiased. It then follows that in the constant mean case the sum of the weighting factors must be unity.

$$\sum_{i=1}^{n} a_{0i} = a_{01} + a_{02} + \cdots + a_{0n} = 1 \tag{33}$$

The second condition is that the error of estimation should be minimal:

$$E[(\bar{T}(x_0) - T(x_0))^2] = \text{minimum} \tag{34}$$

This latter condition, along with (11) leads to a system of equations of the form:

$$\sum_{j=1}^{n} a_{0j} \gamma(x_i - x_j) + \varepsilon = \gamma(x_i - x_0) \tag{35}$$

where $\gamma(x_i - x_j)$ represents the variogram corresponding to a separation distance, ξ, equal to the distance between points x_i and x_j. Similarly, $\gamma(x_i - x_0)$ represents the variogram over a distance equal to that beween the point x_0 to be estimated and the point x_j. ε is a Lagrange multiplier. Combining the constraint that the kriging weights must sum to one, the system of equations can be solved to obtain optimal a_{0i} values which can then be input to Equation 31 to obtain the estimate of $T(x_0)$. The estimator, $\bar{T}(x_0)$, is a linear combination of the n data values. The n weights a_{0i} are calculated to ensure that the estimator is unbiased and that the estimation variance is minimal. Thus, kriging is a best linear unbiased estimator (BLUE). If the random field is multivariate normal, then kriging is equivalent to the conditional expectation which is an optimal estimator (in the mean square error sense).

The kriged estimate $\bar{T}(x_0)$ is based on samples located a distance away from the estimated point. The values at these distant points are only partially related to the value at the kriged point, the degree of relationship being expressed by the variogram. Therefore, we do not expect our estimate, $\bar{T}(x_0)$, to be exact. This point should be clear if we reexamine the conditional expectation discussed previously. That is, in the case where the T is a multivariate normal random process, the estimate, $\bar{T}(x_0)$, is simply the average of T valuesat the location x_0 from a subset of $T(x)$ which agree with the sample values at the sample locations. The spread of all the T values at x_0 around the average is then determined by the kriging variance, σ_T^2, which is

$$\sigma_T^2(x_0) = \sum_{j=1}^{n} a_{0j}\gamma(x_i - x_0) + \varepsilon \tag{36}$$

Notice that the variance is not a measure of the deviation of the estimate from the true T value at x_0. However, the smaller the variance, the greater the reliability of the estimate $\bar{T}(x_0)$. Conversely, an estimate with a large associated variance must be utilized with caution. In practice, the kriging variance can be used to determine the optimal location for additional field tests. For example, hypothetical locations can be added to the actual data base to calculate the reduction in the kriging variance. Thus, kriging is considered as a valuable tool in quantifying uncertainty in interpolated data and in assessing the value of additional data during any site characterization.

Kriging is different from other interpolation or extrapolation techniques because it considers the spatial structure (variogram) of the variable. It also provides a measure of the probable error associated with estimates of the unknown values. However, for many cases, kriging may have no advantages over polynomial trend surface and may even perform poorly by comparison (Davis, 1973). Unlike some regression models that fit a surface to the data base, kriging preserves the values at points of measurement. Note that the model and objectives behind polynomial or surface fitting differ from those in kriging. For that reason a comparison between the methods may not be appropriate. In trend surfaces the objective is to fit the mean value, while in kriging reconstructing the actual surface is the goal. In this sense kriging includes a kind of conditioning without using the normality assumption.

Kriging provides estimates of aquifer properties at points in space. In a numerical model the aquifer is discretized into grids, within which hydraulic properties are assumed to be uniform. However, measurements of transmissivity or hydraulic conductivity, for example, typically represent a much smaller scale than the grid blocks of the model. In contrast to ordinary kriging, block kriging can be used to obtain average properties for the grid block (de Marsily, 1986). That is, the spatial correlation structure obtained from local measurements can be used to interpolate on a point or a real basis. De Marsily *et al.* (1984) described a method that combines kriging and numerical simulation to identify hydraulic characteristics of a reservoir from aquifer tests. The approach allows one to utilize a variety of available hydrogeologic information at different scales. Kriging was also used by Devary and Doctor (1982) to estimate uncertainties in pore velocity at the Hanford site from estimated fields of hydraulic conductivity, effective porosity, and hydraulic conductivity. A similar approach to estimating pore velocity was described by Neuman (1984).

In most field problems, groundwater hydrologists are likely to have both transmissivity and hydraulic head, or specific capacity data. Hydraulic head and specific capacity are generally correlated with transmissivity. It may be desirable to estimate transmissivity values at unsampled locations, using both

measured transmissivity and hydraulic head values or specific capacity data, instead of using transmissivity only. This type of technique using the kriging concept is called co-kriging. Detailed discussion on this subject is available in de Marsily (1986), and Kitanidis and Vomvoris (1983). Neuman (1984), Williams (1987), and Hoeksema and Kitanidis (1984) applied this approach to groundwater flow simulations.

Monte Carlo simulation

The most intuitive approach to dealing with spatial variability in a stochastic sense is Monte Carlo simulation. Although it is classified as one of the heterogeneous approaches in the sense that the hydraulic property values at every point in the aquifer are specified, it is, in principle, equivalent to the effective parameter approach based on the stochastic concept. They both derive the mean and variance of the head and/or concentration, but Monte Carlo simulation provides numerical results and requires fewer assumptions than the stochastic effective parameter approach. The principle of the method is straightforward; it assumes that the probability distribution of the parameter (for example, hydraulic conductivity) and its covariance function are available from measured field data. However, the probability distribution and covariance function do not provide information about the parameter value at a particular point in space. In order to obtain the spatial distribution of the parameter values, many possible realizations of hydraulic conductivity values that conform to the assumed probability distribution and the covariance function are then generated by using a pseudo-random number generator with special techniques (Gutjahr, 1989; Smith and Freeze, 1979; Mantoglou and Wilson, 1982). Each realization of the parameter values is subsequently input to flow and transport equations which are then solved by standard numerical or analytical methods. In most cases, numerical methods are used. Thus, a solution is obtained for each realization of the input parameters. If there are N realizations of input parameters used, then N realizations of output are obtained from solving the governing equations. It is then possible to analyse the output for each realization to obtain the expected value, variance, covariance, and distribution of the output. The principle is illustrated in Figure 9.

This method has been used by many researchers to investigate effects of heterogeneity on flow and solute transport in groundwater systems. For example, it was applied by Clifton *et al.* (1985) to analyse the uncertainty in predicting groundwater travel times and paths. Smith and Schwartz (1980, 1981a, b) used Monte Carlo simulation to determine uncertainties in solute transport predictions. Ababou *et al.* (1988) and Tompson and Gelhar (1990) conducted three-dimensional Monte Carlo simulations of flow and solute transport in heterogeneous geologic formations.

Although the Monte Carlo simulation is not restricted to small variances of input parameters and stationary assumptions, there are difficulties associated with the simulation method. First, a large number of realizations is necessary in order to obtain meaningful statistics from the output. This implies that extensive computer CPU time is required. Second, a groundwater basin must be discretized into many elements or blocks in numerical simulations. Using a direct numerical solver (such as Gaussian elimination) to solve such a large system of equations in numerical models is generally not feasible because of memory storage limitations of computers. Often, the solution technique has to rely on interative methods (such as ADI, SIP, SOR, or PCG). Iterative techniques may reduce the memory storage problems but may not result in the convergence of the solutions to the true ones for highly variable input parameter values. In variably saturated flow situations or other highly non-linear flow and transport systems, the governing equation must be solved by iterative methods, and one is often unable to obtain a solution even for homogeneous properties. The difficulties in obtaining solutions for flow and transport in such non-linear systems with stochastic parameters are tremendous. In addition to these grave difficulties, one major drawback of the approach is that no clear relationship between the statistics of input parameters and output parameters can be easily derived.

Conditional simulation

Generally speaking, hydraulic data for an aquifer are limited. To best utilize the data, conditional simulation is more appropriate than the standard Monte Carlo simulation. Conditional simulation is a special kind of Monte Carlo simulation technique. Unlike standard Monte Carlo simulation, it imposes

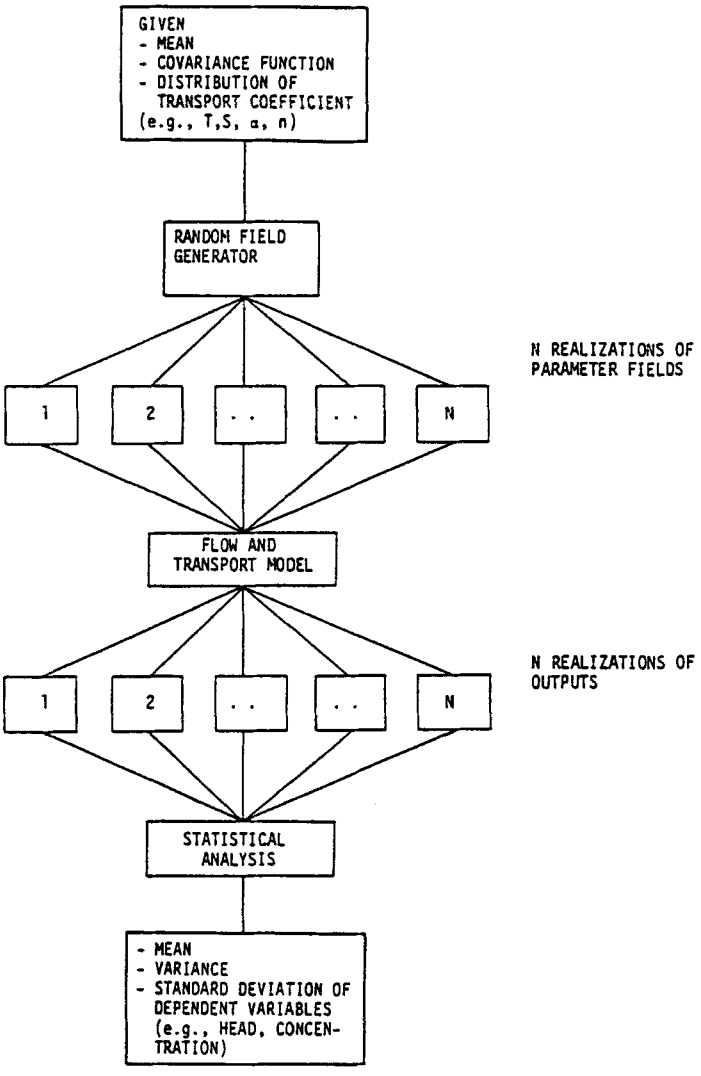

Figure 9. Schematic illustration of Monte Carlo simulation concept

sample values at the sample points. That is, in each realization, parameter values are kept constant and equal to the measured values at observation locations. Thus, there will be no uncertainty in the parameter values at measurement points, other than measurement errors. Consequently, we essentially eliminate many possible realizations of the hydraulic parameter value which do not agree with data at sample locations. As a result, we expect that the variance of output from the conditional simulation should be smaller than that from the Monte Carlo simulation. This concept is similar to the conditional expectation and kriging technique. The complete theory of a conditional simulation procedure based on kriging is given by Matheron (1973) and Journel and Huijbregts (1978). A schematic illustration of the conditional simulation concept is shown in Figure 10. Briefly, the procedures of the conditional simulation are: (1) to generate non-conditional simulations, that is, to synthesize different realizations of the random field of hydraulic properties which maintain the actual covariance function that has been inferred from the data, and (2) to condition the simulations obtained in the first step by making the realizations consistent with the measured sample values. The first step is identical to the standard Monte Carlo simulation. For the second step, one can employ kriging. From the actual sample values, kriging yields a transmissivity estimate, $\bar{T}(x)$, at the unsampled

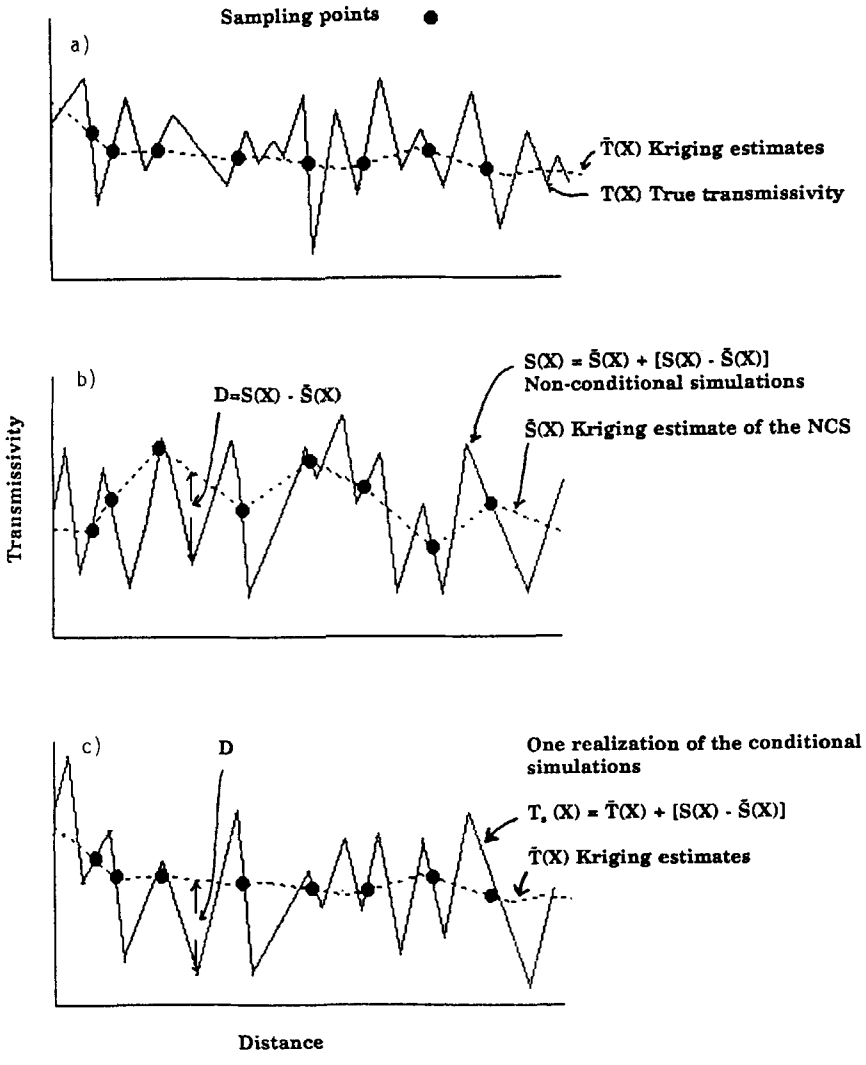

Figure 10. Schematic illustration of the conditional simulation

location which is simply the average of all possible values at a point x of the conditioned subset (Figure 10). The true value, $T(x)$, however, equals the estimate plus the error in the estimate, $[T(x) - \bar{T}(x)]$. That is,

$$T(x) = \bar{T}(x) + [T(x) - \bar{T}(x)] \tag{37}$$

Since the kriging error $[\bar{T}(x) - T(x)]$ is unknown we can not evaluate this expression exactly. However, we may approximate it by the use of kriging and non-conditional simulation. In other words, in a given non-conditional simulation (one realization), kriging can be performed using the measured values at the actual sample locations as data to derive the kriging estimate, $\bar{S}$ (Figure 10b). The transmissivity value of the given non-conditional simulation $S(x)$ thus can be decomposed as the sum of the kriging estimate $\bar{S}(x)$ and the kriging error, i.e.,

$$S(x) = \bar{S} + [S(x) - \bar{S}(x)] \tag{38}$$

Since this value is derived from the non-conditional simulation, all terms are known. Note that $[S(x) - \bar{S}(x)] = 0$ at the sample locations. By substituting $[S(x) - \bar{S}(x)]$ for $[T(x) - \bar{T}(x)]$ in (37), the $T_s(x)$ for the conditional simulation is thus defined as:

$$T_s(x) = \bar{T}(x) + [S(x) - \bar{S}(x)] \tag{39}$$

Therefore, $T_s(x)$ is consistent with the measured values at the sample points; $T_s(x)$ and $T(x)$ have the same covariance functions. At unsampled locations, $[S(x) - \bar{S}(x)]$ does not equal zero and is different among realizations (or non-conditional simulation). Thus, conditional simulations create a conditioned subset of the ensemble, which agrees the measured value at sample locations. The average of many conditional simulations at a given point x is the kriging estimate, and its variance is the kriging variance. Generally speaking, hydraulic property fields resulting from conditional simulation are (1) smoother than unconditioned fields because they are conditioned subsets of the ensemble, but (2) more variable than kriged fields which essentially represent the conditional expected values (or average).

Although conditional simulation is subject to the same difficulties as those in the Monte Carlo simulation, it incorporates the data value at sample locations and is generally regarded as a more realistic approach. Applications of such conditional simulations using conductivity measurements to groundwater flow and solute transport problems by Delhomme (1979) and Smith and Schwartz (1981a, b) found that such conditioning does not reduce uncertainty significantly even when measurements are spaced as close as two log hydraulic conductivity correlation lengths.

A more elaborate conditional approach for simulating solute transport was employed by Wagner and Gorelick (1989). The approach was based on the inverse method developed by Kitanidis and Vomvoris (1983) and Hoeksema and Kitanidis (1985) which involves estimating the average, yet spatially variable, hydraulic conductivity field using both hydraulic conductivity and head measurements. Then, conditional realizations with the same degree of variability as the observed hydraulic conductivity fields are generated and used as input to a solute transport model to obtain solute distributions. The advantage of this type of conditional simulation is that the conductivity field is closer to the reality due to additional head measurements.

Graham and McLaughlin (1989) presented a novel approach to conditional simulation. Instead of computing the mean and variance of the concentration distribution from many simulations with conditioned random parameter fields as input, the mean and the covariance of the concentration distribution are solved directly from approximated moment propagation equations with a numerical method. The Kalman filter is used to update the moments when new measurements of the head, log conductivity, and concentration fields become available. Through two synthetic problems, the authors demonstrate that reasonably good estimates of the solute concentration distributions can be obtained by conditioning the ensemble moments on a small number of measurements located in regions of high concentration uncertainty.

Although the methodology is appealing, it requires concentration measurements which generally are not available at many proposed landfill sites. It is an attractive method for delineating existing plumes but it does not serve as a good predictive tool. In the case that concentration measurements are not available, their approach should yield results similar to those by the classical conditional simulation method using conductivity and head measurements. Furthermore, their moment propagation equations are first-order approximations which imply that the method is also limited to relatively homogeneous aquifers. From the computational efficiency point of view, the method may be inferior to the classical Monte Carlo and conditional simulations for a fully three-dimensional analysis due to the cumbersomeness of the Kalman filter. Regardless of these drawbacks, their methodology may provide a valuable tool for developing a sampling strategy to reduce uncertainties in characterizing existing contaminant plumes.

SUMMARY AND CONCLUSION

Predicting solute transport in a large-scale aquifer based on the current monitoring and modelling techniques is a difficult task. There are large uncertainties in predictions. These uncertainties arise mainly

from our inability to depict detailed spatial distributions of hydrologic parameters in large-scale aquifers. Although geological information is useful for defining large structures, some means of acquiring more detailed knowledge of the parameter distributions is necessary to improve our predictive capability. However, such techniques may not exist in the foreseeable future unless there are some technological breakthroughs in field testing. Until then, we may have to rely on stochastic approaches to obtain probabilistic results. Many of these approaches are available including the geostatistics method, the effective parameter approach, the Monte Carlo approach, and the conditional simulation. Each of these methods has limitations. Nevertheless, these approaches may at least provide us with some estimates of uncertainties in the predictions which may be crucial for regulatory and decision-making purposes. One should, however, bear in mind that the uncertainty estimates afforded by the stochastic models are themselves uncertain (e.g. Smith and Freeze, 1979; de Marsily, 1986.)

The approach using effective parameters with the macrodispersion concept may be attractive for relatively simple hydrogeologic systems. Recent field experiments (Sudicky, 1986; Freyberg, 1986; Garabedian *et al.*, 1991) show that mean travel times and paths of plumes in sandy and glacial outwash aquifers can be adequately predicted by the effective hydraulic conductivity formula developed by Gelhar and Axness (1983). The spatial displacement variances of the observed plumes are also in reasonable agreement with the stochastic results by Dagan (1987) and Naff *et al.* (1988).

However, the major technical concern with this effective parameter approach is its validity in the analysis of flow and solute transport in highly heterogeneous aquifers when the variance of the log saturated hydraulic conductivity is large. The omission of higher order terms in the perturbation-spectrum analysis may introduce large errors. On the other hand, in relatively homogeneous aquifers the existing analytical solutions to stochastic differential equations are only useful for simple flow fields, e.g. steady, uniform flow in an aquifer. Although the transient effect (Gomez-Hernandez and Gorelick, 1989) may be dissipated at large times after the stress moves through many parts of the heterogeneous aquifer, the stress may encounter heterogeneities of different scales.

Whereas the spatial displacement variance formulas in the stochastic results (Equations 18 to 25) provide a way to predict the relative size of the plume, the shape of the concentration distribution still remains unknown. That is, the macrodispersivity derived from the stochastic analysis does not warrant the use of the classical convection-dispersion equation based on Fick's law to predict the mean concentration distribution of a plume. In addition, the number of samples required to obtain accurate estimates of the parameters (such as correlation scales and covariance functions) for the macrodispersion models still needs to be investigated.

Nevertheless, one should look at the bright side of the approach and recognize the essence of any stochastic theory: a stochastic predictor will do better than others on the average in many trials under uncertainties. The effective parameter approach may, thus, serve as a practical tool for preliminary analyses (e.g. Gelhar, 1986), especially for cases where little information on aquifer properties is available.

Finally, one should bear in mind that the discrepancy between the mean concentration distribution derived from the effective approach and the one observed in reality increases with the degree of heterogeneity, even if the effective approach is technically flawless. Then, key questions we should ask ourselves are: are we interested in predicting the mean concentration distribution in highly heterogeneous aquifers, such as alluvial and fractured aquifers? Can we accept predictions with large degrees of uncertainties, say more than 50 per cent? In other words, under what degree of heterogeneity can the effective parameter approach be used to make predictions that provide us with an acceptable degree of uncertainty? The formula for the concentration variance estimate developed by Vomvoris and Gelhar (1990) may furnish a quick answer to this question. Indeed, this is the major advantage of the stochastic effective parameter approach.

Although the Monte Carlo simulation techniques may be superior to the stochastic effective parameter approach for predicting concentration distributions in aquifers since it involves fewer assumptions, it suffers the same difficulty as the effective approach. It also only produces means and variances of all the possible concentration distributions. Again, we are facing the same question as in the effective parameter approach. Do we need to conduct the Monte Carlo simulation if the aquifer is highly heterogeneous? Unfortunately, one has to conduct many tedious and time consuming simulations in order to answer this question if the effective parameter approach is not used.

Conditional simulations, which use available information at sample locations and eliminate many possible realizations which disagree with observations, will enhance our ability to model reality. Although the results of conditional simulations by Delhomme (1979) indicated that using the known transmissivity values at sample locations may not reduce the uncertainties in the prediction of groundwater heads significantly, using both head information and transmissivity values as constraints for the simulation may be useful. In addition, the results of the conditional simulations by Smith and Schwartz (1981b) showed that locations of sample data used in the conditional simulation may have important impacts on the reduction of uncertainties. The effects of sample locations and conditioning the simulations by hydraulic conductivity, hydraulic head, and porosity values on predicting solute transport in aquifers certainly deserves further investigation. Regardless of the amount of uncertainty that conditional simulations (using concentration, conductivity, and head values) can reduce, it is rational to include all the available parameter values in the prediction. It is clear that the uncertainty in the simulation will be gradually reduced as more and more data become available. Thus, the conditional simulation approach seems to be a promising mathematical tool that can bring us a step closer to reality.

As one approach to the problem of quantifying uncertainty in solute transport in porous media using stochastic methods, I suggest the following steps (1) groundwater hydrologists should utilize the principles of stratigraphy, sedimentology, and structural geology to delineate large-scale geologic units or structures which may contain the likely paths along which groundwater travels (Williams, 1988; Anderson, 1989). (2) 'Enough' data should be collected to characterize the hydrologic properties of as many geologic units as possible so that the general flow regime in those units can be defined. (3) An 'intensive' sampling program should be carried out to collect hydraulic conductivity, dispersivity, and porosity data from the geological units identified in step (1) using many small-scale tests (such as core samples from boreholes, or small-scale aquifer and tracer tests). (4) Groundwater hydrology modellers should characterize the spatial variability of the hydrologic parameters in the likely fast flow units by the stochastic concept (i.e., statistical distributions, spatial covariance functions, etc.). (5) With the calculated statistics for the hydrological parameters, one should use the effective parameter approaches (such as Gelhar and Axness, 1983; and Dagan, 1987) for a preliminary analysis to define the mean behaviour of the flow system or to calibrate flow models (see the example in Gelhar, 1986). It is important that the scale of samples be consistent. That is, if one decides to model the system at a certain scale, the entire field characterization program should use that scale. In this way, the results of the model calibration will provide a better estimate of the statistical parameters required for conditional simulations. (6) To complement the effective parameter approach, the inverse procedure developed by Kitanidis and Vomvoris (1983), and Hoeksema and Kitanidis (1984) which uses both hydraulic conductivity and head data to estimate the spatial covariance function of the hydraulic conductivity field should be used. The results of the inverse procedure will provide the proper input parameter values for the conditional simulation (7) Finally, with the available statistical parameters obtained from either the effective parameter approach or the inverse procedure, one should carry out conditional simulations using solute transport equations to determine the uncertainty in predicted solute concentration distributions. The same procedures should be repeated as additional data become available. Such an iterative conditional simulation will bring our predictions closer to reality.

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