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A REVIEW OF THE SCALE PROBLEM AND APPLICATIONS OF STOCHASTIC METHODS TO DETERMINE GROUNDWATER TRAVEL TIME AND PATH

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ABSTRACT

The groundwater travel time along the fastest path of likely radionuclide transport is a regulatory criterion used to assess the hydrogeologic quality of a high-level radioactive waste repository. Hydrologists and engineers are limited in their ability to define with confidence the fastest path, owing to the heterogeneous nature of geologic materials. Field measurements of hydraulic properties such as in test or observation wells, are inherently averages of properties at scales smaller than the scale of the field measurement. As a result of averaging, subscale information is lost and there is uncertainty in defining the fastest trajectory of groundwater. This scale problem is explained through a review of the continuum and REV concepts in groundwater hydrology. The application of hydrodynamic dispersion concepts is recommended as a means of incorporating the effect of subscale heterogeneity on the fastest groundwater travel time.

Sources of uncertainties in predicting groundwater travel time are discussed in the report. The uncertainties are mainly attributed to the heterogeneous nature of geologic formations. The heterogeneity of geologic materials can, however, be characterized quantitatively using geostatistical methods. Important statistical parameters include mean and variance, as well as the spatial correlation structures of the hydrologic properties within the hydrogeologic system. These parameters may be obtained from limited data base. Stochastic methods, reviewed and explained in this report, can take advantage of the geostatistical characterization to predict large-scale groundwater flow and solute transport. Several examples from recent scientific literature are provided to illustrate the application of stochastic methods to the groundwater travel time analysis.

Stochastic methods in subsurface hydrology have only recently been evaluated under field conditions for a few locations, and validation of the theories is

incomplete, especially in unsaturated fractured rocks. Nevertheless, research efforts should continue to improve the state-of-the art. Geostatistics and stochastic methods will be valuable tools in addressing the groundwater travel time objective.

1.0 INTRODUCTION

1.1 Purpose and Scope

Daniel B. Stephens & Associates, Inc. was requested by the U.S. Nuclear Regulatory Commission (NRC), through Nuclear Waste Consultants, to conduct a review of the literature pertaining to stochastic approaches for characterizing the uncertainty in predicting groundwater travel path and travel time in saturated media. Enclosed is the draft final report of this study. As directed by the NRC, the report addresses the following:

- -review of uncertainties in groundwater travel time and path which are attributed to hydrogeologic parameters
- -critical reviews of relevant scientific articles relevant to the analysis of uncertainties in prediction of groundwater travel time and path
- -a discussion of the significance of the findings to the NRC's waste management program
- -explanations and illustrations of the stochastic concept and methods of stochastic analysis
- -a glossary of terms relevant to stochastic analyses

In addition, the report discusses the concept of the representative elementary volume (REV). The report also attempts to clarify the relationships between the REV scale, the measurement scale of hydraulic properties and scale of modeling.

The proposed work is motivated in large part by federal regulations pertaining to the performance of high level waste repositories, in particular, the groundwater travel time (GWTT) objective. As stated in 10 CFR 60.113(a)(2), the GWTT performance objective is:

"The geologic repository shall be located so that pre-waste-emplacement groundwater travel time along the fastest path of likely

radionuclide travel from the disturbed zone to the accessible environment shall be at least 1,000 years or such other time as may be approved or specified by the Commission."

The NRC has drafted generic technical positions on groundwater travel time to help explain this phase, as well as the rest of the regulation (NRC, 1986, 1988). One of the key points requiring clarification is the definition of "the fastest path of likely radionuclide transport". Hydrogeologists are well aware that there are many possible pathways, but which one is the fastest and how fast does groundwater travel along it? Herein, enters the element of uncertainty. There is uncertainty not only in identifying the fastest path from limited subsurface data but also in travel time owing to the uncertainty in path length as well as in data or approaches used to compute travel time.

As our report will illustrate, stochastic methods are well-suited to deal with uncertainty in groundwater travel time and travel path analysis. However, they have only been developed for groundwater problems within the last decade. The mathematical complexities presented in theoretical articles in the scientific literature are not easily assimilated by most practitioners. Moreover, because field tests to validate stochastic models have not been completed, most hydrogeologists are still reluctant to apply these models. One of the underlying purposes of our review is to explain the principles of stochastic models without resorting to the mathematical details and give examples of how the stochastic methods may be applied in the analysis of groundwater travel time and travel path.

1.2 Background

Uncertainties in predicting groundwater travel times and paths arise primarily from heterogeneity of aquifer materials. Heterogeneity is a continuous phenomenon; it exists at all scales (from microscale to megascale). However, heterogeneous materials may be treated as homogeneous at one observation scale, and

heterogeneous at a different scale. That is, the definition of heterogeneity is a relative one, depending on the scale of observation. Thus, the heterogeneity observed is directly related to the scale of the problem.

The problem of scale does not exist only in hydrology (Dooge, 1986), but poses many difficulties for every branch of science and every one of us living in the universe. It controls our perception of everything that we see and feel. The scale problem is best illustrated in the book entitled "Powers of Ten" by Morrison and Morrison (1982). The book contains visual images ranging from a scale of 10^{25} meters to 10^{-14} meters. At a scale of 10^{25} meters galaxies are seen as tiny clusters in empty space. At a scale of 10^{23} meters, the Milky Way appears as one of a number of bright spots in empty space. The spiral structure of the Milky Way becomes apparent at a scale of 10^{21} meters. A scale of 10^{13} meters encompasses the orbits and all the planets of the solar system. At the scale between 10^{-7} and 10^{-9} meters, we see the various structures of DNA molecules, and so on. Similarly, in groundwater hydrology, at a scale of 10^{6} meters one may observe variations among groundwater basins. Various geologic formations become noticeable at a scale of 10^{3} meters. A scale of 10 meters may encompass various layers of clay, sand, and gravel. We can no longer recognize the irregularity of layers, but we do recognize pore structures at a scale of 10^{-6} meters. Water molecules within pores are visible at a scale of 10^{-8} meters, and so on as the scale of observation decreases.

Heterogeneity exists in groundwater hydrology at all scales. However, once we select a scale of observation, we often neglect phenomena at subscales. This is exactly the way our formulas, equations, and laws are developed in all sciences, including groundwater hydrology. Subscale phenomena we ignored, however, may play vital roles in solving or studying the problems of interest. Furthermore, different laws and equations may be developed or discovered at different scales and may not be appropriate for studying problems at another scale. For instance, a

representative elementary volume as used in the study of flow through porous media would be different from that for flow through fractures or karsts. When predicting groundwater travel times and paths, we may face the difficulty of extrapolating equations and laws developed for a small scale to solve problems at a larger scale, for example over distances of 10 km or more.

In the following chapters, we will first discuss of the continuum hypothesis in fluid mechanics and groundwater hydrology, and then we will show the development of equations for groundwater flow at different scales. We will then discuss the uncertainties in predicting groundwater travel times and paths and finally review some recent advances in groundwater hydrology to tackle the scale related problems.

2.0 BASIC CONCEPTS IN GROUNDWATER HYDROLOGY

2.1 Continuum Assumption in Fluid Mechanics

The most fundamental assumption in fluid mechanics is the continuum assumption in which the fluid is assumed to behave as if it were continuous in space at the macroscopic scale, say 10^{-2} meters.

For example, at the macroscopic scale, one can see water in a garden hose, and the water is continuous throughout the hose. However, if we examine a fluid at the microscopic scale, say 10^{-8} meters, the mass of the material in a fluid is concentrated in the nuclei of the atoms composing a molecule and is not uniformly distributed over the column occupied by the liquid. Using the garden hose example, we can view the velocity of water moving through the hose in perhaps two ways, depending upon the scale of interest. In the first case, at the macroscopic scale, the velocity is simply the volumetric discharge rate per unit cross-sectional area. For steady-state conditions, the velocity is constant in space along the hose. In the second case, at the microscopic scale, the velocity of individual fluid molecules is highly variable along their path through the hose. This molecular velocity is virtually impossible to measure. However, we are normally concerned with the behavior of matter on a macroscopic scale which is much larger than the distance between molecules. Accordingly, the properties of a fluid defined in fluid mechanics have to represent the property values over such a macroscopic volume. The properties contained in this volume are thus regarded as the average values being spread uniformly over that volume instead of, as at the microscopic scale, being concentrated in a small fraction of it. This macroscopic representation of the fluid makes it possible to treat the fluid as a continuum in space. This approach in fluid mechanics is known as the continuum approach and the associated hypothesis that the

fluid can be so represented is called the continuum approach.

Indeed, the properties of the fluid at the macroscopic scale are continuous and smoothly varying, if observed with any of the conventional measuring devices. When a measuring device is inserted in a fluid, it responds in some way to a property of the fluid within some small neighboring volume, and provides a measure which is effectively an average of that property over the volume. The device, such as a pitometer for measuring velocity, is normally chosen so that the volume is small enough for the measurement to be a local one; that is, further reduction of the volume does not change the reading of the device. However, the volume is large enough to contain an enormous number of molecules so that the fluctuations arising from the different properties of molecules have no effect on the observed average. Therefore, we can define a reproducible property of the fluid. Of course, if the averaging volume is so small as to contain only a few molecules, the number and kind of molecules in the volume at the instant of observation will fluctuate from one observation to another, and the measurement will vary in an irregular way, with the size of the averaging volume corresponding to the measuring device. Figure 2.1 illustrates the way in which a measurement of velocity of the fluid would depend on the averaging volume of the device. We are able to regard the fluid as a continuum when, as shown in the figure, the measured fluid property is constant for volumes which are small on the macroscopic scale but large on the microscopic scale.

The continuum assumption allows us to attach a precise meaning to the various physical properties at any point in space. The various fluid properties such as density, velocity, and temperature can thus be treated as continuous functions of time and position in the fluid which satisfy the requirements of differential calculus. On this basis, we shall be able to establish differential equations governing the motion of the fluid. The equations are macroscopic equations that are independent of the nature of the particle structure which is generally discontinuous in space and

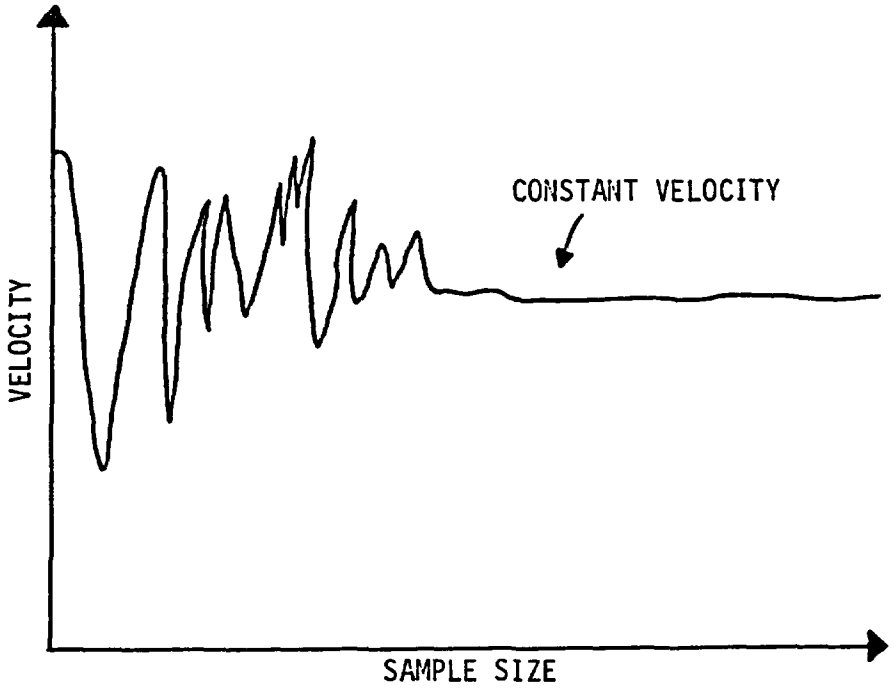


Figure 2.1. Dependence of velocity measurements upon sample size within a fluid.

time.

2.2 Continuum Assumption in Groundwater Hydrology

In saturated porous media (granular materials), flow takes place through a complex network of interconnected pores or openings. Although the fluid itself may be considered as a continuum by the continuum hypothesis used in fluid mechanics, the flow path may be discontinuous because of the complex nature of the pore geometry. 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. By doing so, they are employing the concept of a continuum, which is analogous to the concept used in fluid mechanics and other branches of sciences. The minimum volume over which the continuum assumption applies in flow through porous media, however, is much larger than the one defined in fluid mechanics (Figure 2.2). In groundwater hydrology, this volume is called the representative elementary volume (REV) (Bear, 1979). Using the REV concept, we essentially bypass both the microscopic level, at which we consider what happens to each molecule in the fluid, 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 which only averaged phenomena over the REV are considered. Thus, a REV is simply a volume over which we carry out the averaging process, as shown in Figure 2.2.

A more practical definition of the REV may be given as follows: an REV is a volume that is sufficiently large to contain a great number of pores so that a mean property exists, and it is sufficiently small so that the parameter variations at a scale

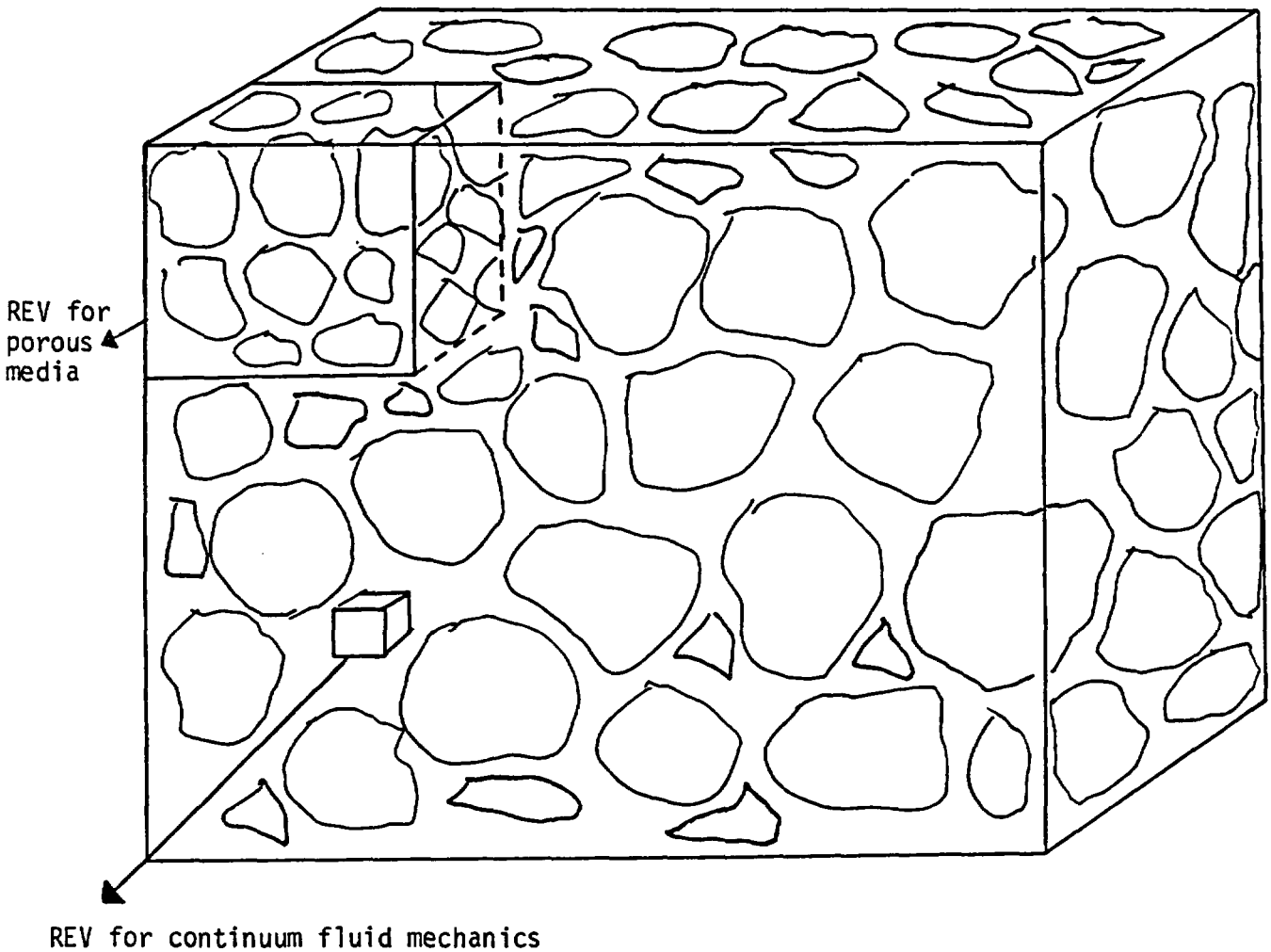


Figure 2.2. Different averaging volumes in fluid mechanics and porous media.

larger than the size of REV can be represented by continuous functions which satisfy the requirements of the classic differential calculus (De Marsily, 1986).

The REV concept is also defined through a rigorous mathematical expression suggested by Marle (1967). At pore-scale, the spatial distribution of pore openings could be highly erratic, analogous to electronic signals superimposed with random noises. Then, an REV is merely a noise filter similar to the one in electrical engineering that filters out the random noises and produces a smooth signal (Figure 2.3). Mathematically, this process can be formulated as:

$$H(x) = \int h(x + \eta)\, f(\eta)\, d\eta \qquad (2.2.1)$$

where H(x) is the smoothed, continuous, output signal, h(x) is the original, noisy, and erratic signal, and $f(\eta)$ is the filter or a weighting factor. Figure 2.3a shows a filter function which eliminates high frequency noises but retains the smooth sinusoidal signal. Some filter functions can smooth noises and signal as shown in Figure 2.3b. In groundwater hydrology, H(x) is the macroscopic property of porous media and $f(\eta)$ is the weighting function used within the volume or window over which the pore-scale properties are averaged, i.e., the REV. For example,

$$f(\eta) = \begin{cases} \frac{1}{V}, & \text{within the volume } V \\ 0, & \text{otherwise} \end{cases} \qquad (2.2.2)$$

2.3 Homogeneity, Heterogeneity, and Scale

The definitions of homogeneity and heterogeneity follow from the concept of the REV. From the previous discussion, it should be clear that as the size of the

window or the volume over which the averaging takes place increases, the noise level in the output will decrease (Figures 2.3). Therefore, if one properly chooses the size of the averaging volume, a material with a spatially-varying property may thus be treated as a material with a spatially-constant property. This material is then defined as homogeneous. This situation is analogous to that in Figure 2.3b. Now, consider a porosity distribution of a hypothetical porous medium. If one chooses a pin point as the sample size to define porosity, let us assume that Figure 2.4a would represent the porosity distribution along a transect of the porous medium. At a point, the void has a porosity value one, and the solid zero. If one averages the values of porosity over a window that is larger than a point, say, as large as one solid or void space, the "new" porosity distribution of the aquifer will look like that shown in Figure 2.4b where the sharp boundary between voids and solid is smeared out due to the averaging over the window. It should be evident that if a window slightly larger than one solid space is used, the porosity values of the aquifer will still vary in space but the variation will be relatively smooth and continuous. Therefore, the aquifer is heterogeneous and it can be described by our continuum mathematics. If one chooses a window which is equal to two void spaces to define the porosity values at every point within the medium, the medium should obviously have a constant porosity over the entire medium. In fact, the porosity will be 0.5 everywhere if the averaging window is equal to two void or solid spaces. Hence, the medium as far as porosity is concerned is a homogeneous medium (Figure 2.4c). This window can be considered as the minimum size of the REV for conceptualizing the medium as a homogeneous one. Suppose one applies this window to another porous medium which has a checkerboard porosity distribution but with larger void and solid sizes. The porosity distribution defined by the average porosity over the same window becomes nonuniform. In other words, the medium now is considered heterogeneous. But, if one again chooses a window that is equal to the size of the

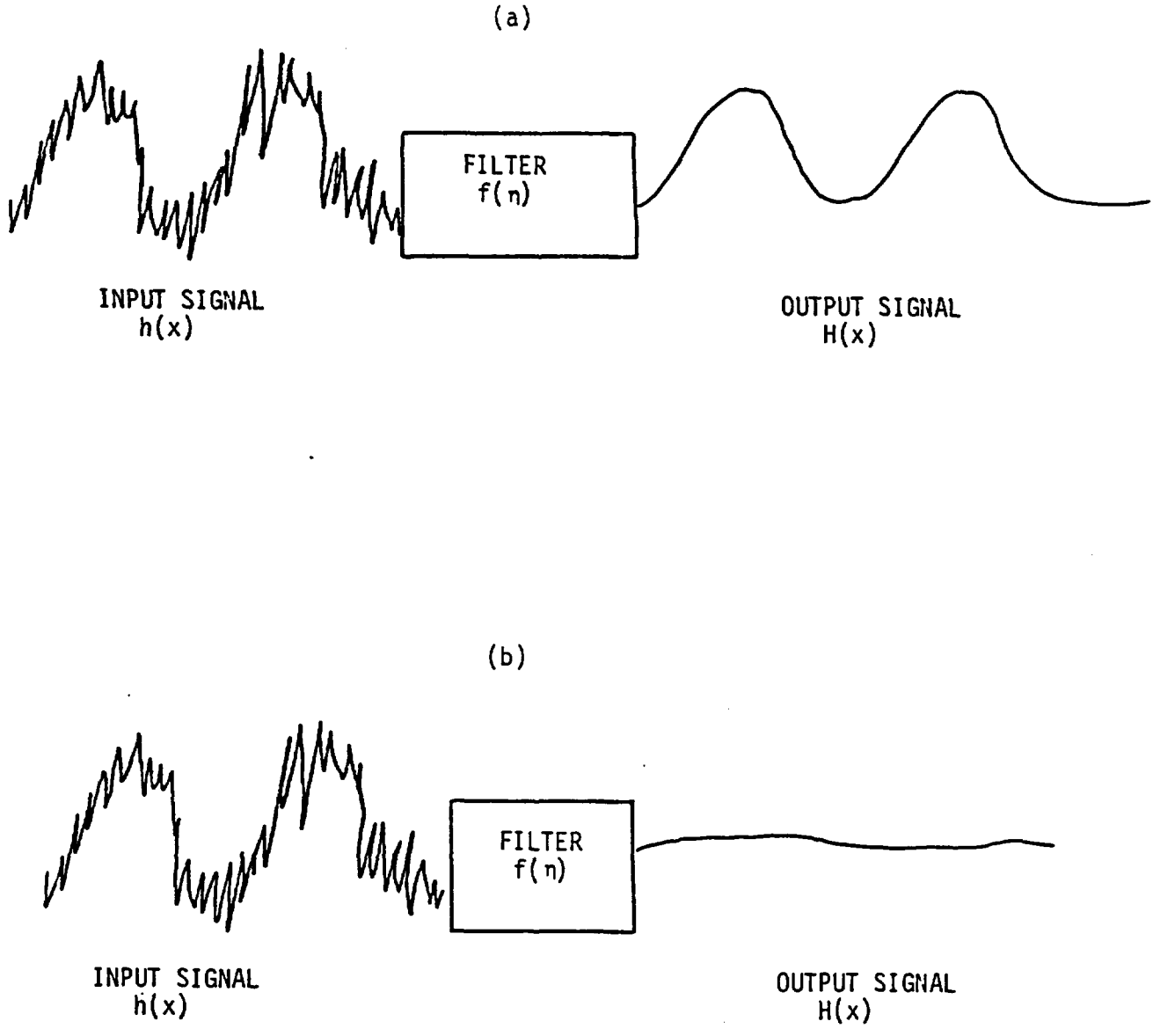


Figure 2.3. Effects of filters on noisy signals.
a) Filter affects noise only, and b) filter affects noise and most of signal.

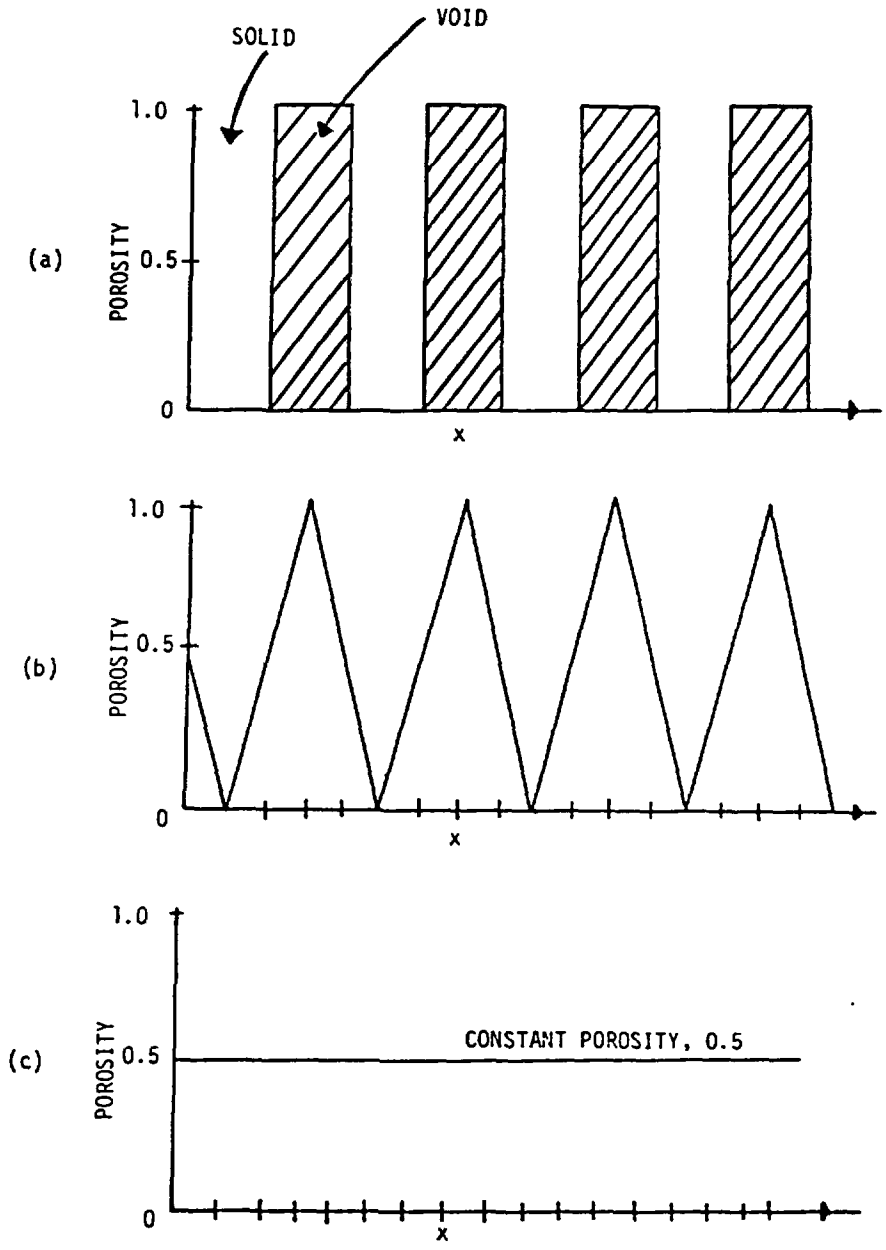


Figure 2.4. Effects of averaging volume on porosity distribution. (a) A hypothetical solid and void distribution. (b) Size of averaging volume equals one void volume. (c) Size of averaging volume equals two void volumes.

two void or solid spaces of this checkerboard, one can define this medium as a homogeneous porous medium. From this simple example, it can be seen that in order to obtain the homogeneity, the size or the REV has to be much larger than the size of heterogeneity.

The size of the REV varies with the size of the blocks in the examples or the size of heterogeneity in reality. The size of heterogeneity depends on the scale of the problem that we encounter. For instance, the heterogeneity within core samples is likely due to the variation in grain size. We may call this variability the laboratory-scale heterogeneity. Heterogeneity due to geologic stratification or layering in a formation may be classified as the field-scale heterogeneity. The regional-scale heterogeneity then represents the variation of geologic formations or facies. Furthermore, variations among sedimentary basins may be classified as the global-scale heterogeneity, and so on. Similar definitions of the scale of heterogeneity were given by Dagan (1986) and Gelhar (1986). Regardless of the definition of the scale of heterogeneity, one has to recognize that the heterogeneity is a continuous phenomenon which exists at all scales.

2.4 Darcy's Law

With the concept of the REV in mind, one should recognize that every property defined in groundwater hydrology (such as volumetric flow rate, hydraulic head, porosity, hydraulic conductivity, and storativity, etc.) involves measurement over a certain volume. The same is true for the principles and laws used in groundwater hydrology. The most important example would be Darcy's law, which states that groundwater specific discharge is linearly proportional to the hydraulic gradient with a constant of proportionality:

$$q = \frac{Q}{A} = KI \qquad (2.4.1)$$

where q is the specific discharge with dimensions of (LT^{-1}), Q is the volumetric flow rate (L^3T^{-1}), I is the gradient (LL^{-1}), A is the cross-sectional area perpendicular to the direction of flow (L^2), and K is a constant of proportionality which is usually called hydraulic conductivity (LT^{-1}). Darcy's law is an empirical equation, although one can prove the validity of the equation using rigorous mathematics and physics (Hubbert, 1940). Nevertheless, it is simply a linear regression equation showing the relationship between gradient and specific discharge through a column of soil of a certain volume. Therefore, Darcy's law is a macroscopic law because the volume where the law applies is obviously much larger than many pores.

2.4.1 Hydraulic conductivity. In the laboratory, hydraulic conductivity is generally determined from a column test which uses either a constant head permeameter or a falling head permeameter. Regardless of whether one uses a constant or falling head permeameter, the measured hydraulic conductivity is an average value over the length of the column. To illustrate this point, we will examine the case where the column consists of a single homogeneous soil. If a constant head permeameter is used, then steady-state flow will be established. The flow rate through the column is, according to Darcy's law:

$$Q = KAI = KA \frac{h_1 - h_2}{L} \tag{2.4.2}$$

where h_1 and h_2 are the hydraulic heads measured at points 1 and 2, and L is the distance between the two points (Figure 2.5). If we measure Q, A, and I, we certainly can determine the K value, the hydraulic conductivity. Obviously, in a core sample, the calculated hydraulic conductivity, K, represents some average small-scale hydraulic conductivity variations within the core. To illustrate the concept of an average K, we consider a second case where the porous medium contains layered

heterogeneity (Figure 2.5). Again, if a constant head permeameter is used, steady flow exists. This implies that the flow rates across any cross-section of the column must be equal. That is:

$$Q_1 = Q_2$$

$$K_1 \; A \; \frac{h_1 - h}{L_1} = K_2 \; A \; \frac{h - h_2}{L_2} \qquad (2.4.3)$$

where K_1 and K_2 are the hydraulic conductivity values of soils 1 and 2, respectively; h_1 is the water level at reservoir 1, and h_2 is the water level at reservoir 2; h is the head value at the interface between the two soils; and L_1 and L_2 are the thicknesses of layer 1 and layer 2, respectively. If the head at the interface is not measure, one can solve Equation (2.4.3) for h at the interface by knowing the hydraulic conductivities and thickness of the individual layers:

$$h = \frac{L_1 L_2}{K_1 L_2 + K_2 L_1} \; \frac{(K_1/L_1)\, h_1 + (K_2/L_2)\, h_2}{L} \qquad (2.4.4)$$

where L is $L_1 + L_2$. If this expression for h is substituted into the left-hand side of equation (2.4.3), one obtains:

$$Q = A \; \frac{K_1 K_2 L}{K_1 L_2 + K_2 L_1} \; \frac{h_1 - h_2}{L} \qquad (2.4.5)$$

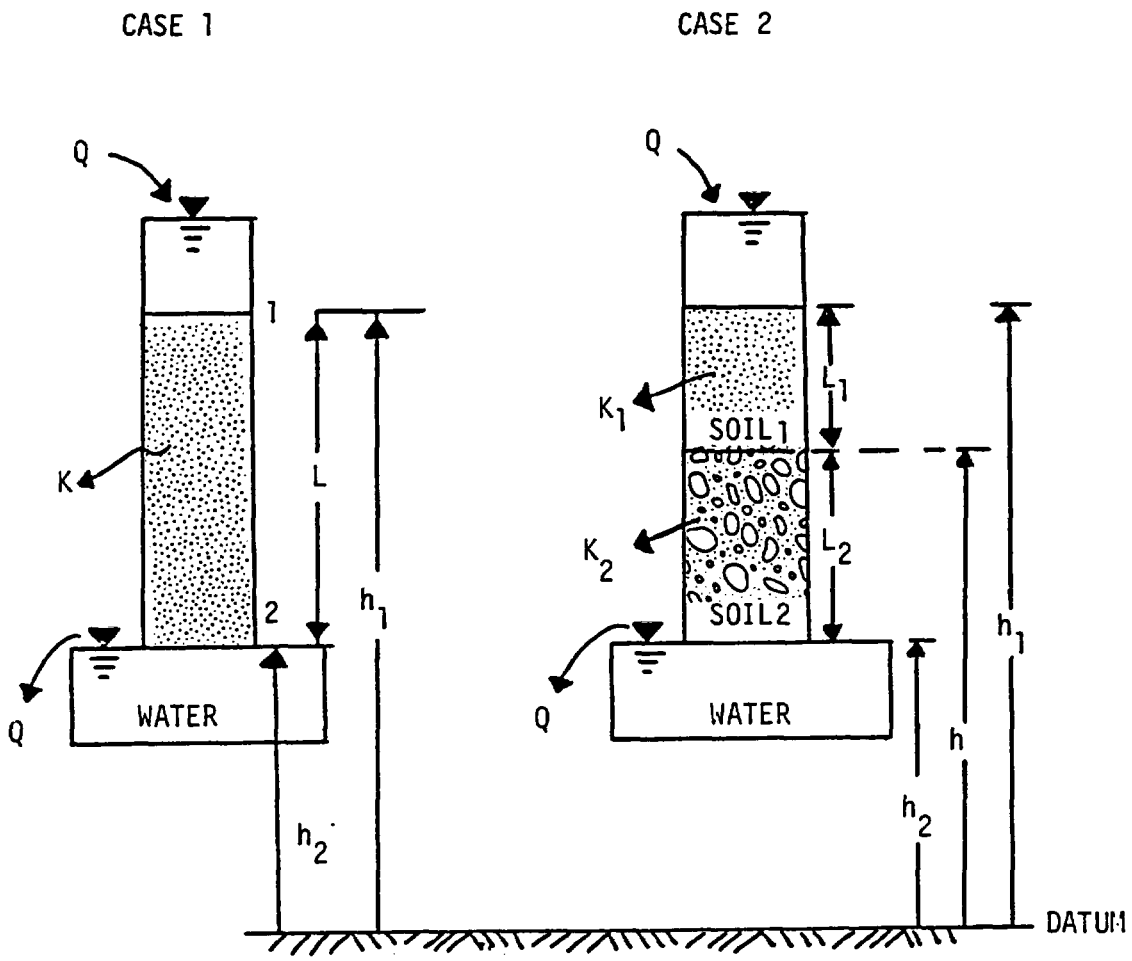


Figure 2.5. Hydraulic conductivity measurements using soil columns. Case 1 is a homogeneous(or equivalent homogeneous) soil column, and Case 2 is a two layer soil column.

This is the formula to determine the flow rate through the core sample from the permeameter. Let us attempt to determine the average hydraulic conductivity of this two-layer soil column. If a constant head permeameter is used, we can measure heads at the two ends of the column and the discharge from the column. Using the measured heads and discharge rate, from Darcy's law (2.4.2), the hydraulic conductivity can be easily determined by:

$$K_{ave} = \frac{QL}{A(h_1 - h_2)} \tag{2.4.6}$$

When equation (2.4.6) is used, we evidently assume that there is an equivalent homogeneous soil which should transmit the same amount of discharge as the layered soil column under the same head drop. Therefore, the K_{ave} value obtained from this calculation represents the K value of the equivalent homogeneous soil column and ignores the K values of each layer.

So, how is the K_{ave} value related to the K values of each individual soil? From a comparison of equation (2.4.2) and (2.4.5), one can see that:

$$K_{ave} = \frac{L}{L_1/K_1 + L_2/K_2} \tag{2.4.7}$$

As indicated in equation (2.4.7), the K value of the equivalent homogeneous soil column is the harmonic mean of the K's of individual soil layers. A similar analysis can be done where flow is parallel to the layers in the soil column. In this case, the average K obtained from the soil column will correspond to the arithmetic mean of the K's of the individual layers. That is:

$$K_{ave} = \frac{K_1 L_1 + K_2 L_2}{L} \qquad (2.4.8)$$

Based on the above discussion, one can see that the K values measured from a soil column test may vary with the size of the soil column. For instance, if the soil column is small enough to contain one soil layer, the value of K estimated is certainly the hydraulic conductivity of the layer. If the column contains more than one layer of soil, the estimated value of K is an average of the K for the individual layers. Furthermore, the average hydraulic conductivity depends on the direction of layering and the direction of flow. The average hydraulic conductivity should be the harmonic mean if the flow is perpendicular to the bedding, and the arithmetic mean if the flow is parallel to the bedding (Bear, 1979). Thus, we can draw a few conclusions about the hydraulic conductivity of a material, namely; it is an average over many small-scale values, it depends on the size of averaging volume (i.e., the total length of the soil column), the heterogeneity (i.e., the K values of individual layers), the size of the heterogeneity (i.e., the thickness of each layer), and the flow direction.

The average hydraulic conductivity can be easily determined from a soil column test. However, one should recognize two important facts in the column test. First, the heads at the ends of the soil column are kept constant over the cross section of the soil column, so the heads represent averages over the cross sections. Second, the discharge is measured with respect to the entire cross-sectional area of the soil column, including voids and solids. In essence, to calculate hydraulic conductivity, one needs to know the average hydraulic head over the cross-sectional area of porous media through which flow rate is measured. Without measurements of head and flow rate at the same scale, one may not be able to define an average or effective hydraulic conductivity. This is especially problematic for a large-scale

field site. Inasmuch as in the field problem analogous to the column in figure 2.5, the hydraulic head measured by a piezometer is generally regarded as a "point" measurement, and we usually do not have an instrument to measure the total discharge from a large aquifer. Hence the limitations of the measuring capacity of our instruments may restrain us from using the averaging rules discussed above, or at least from using Darcy's equation directly to compute an effective or average hydraulic conductivity for an aquifer.

2.4.2 Specific discharge. Darcy's law provides us with a method to calculate the total discharge or flow rate from a soil column, providing that we know the head gradient and hydraulic conductivity of the soil column. Specific discharge is defined as the total discharge rate divided by the cross-sectional area of the column. This means that the specific discharge is an average discharge value over the cross-sectional area. It does not represent the discharge from individual pores or areas smaller than the cross-sectional area. It is an average flux through a porous medium, at a scale at least as large as that of the REV.

2.4.3 Average fluid particle velocity. The average flow velocity of fluid particles is generally determined by the ratio of total discharge rate to the cross-sectional area of pore space through which flow occurs. This leads to the definition of average fluid particle velocity or average linear velocity in groundwater hydrology, which is:

$$v = \frac{q}{n_e} = \frac{Q}{An_e} \tag{2.4.9}$$

where q is the specific discharge and n_e is the effective porosity through which flow occurs. This is an average pore velocity over the total pore area in the cross section. Consequently, it does not represent the water velocity within individual

pores, because the areas of individual pores vary. As a result, if one uses the average fluid particle velocity to determine the arrival of a slug of tracer in the column test, the time of arrival would be the average arrival time of the tracer particles. Certainly, some of the tracer particles will move through larger pores and will arrive earlier than the predicted by the average time, and some of them will lag behind (Figure 2.6).

Generally, the average fluid particle velocity and the velocity deviations will vary with the size of the soil sample over which averaging takes place. If the sample is small enough to contain one soil, the velocity variation in a soil column tracer experiment, manifested in dispersion or spreading of tracer particle arrival times, will represent the velocity variation in the pore scale. If the sample is large enough to include several different soils, it will represent the combined effect of the variation in velocity among pores and among layers, and so on. Once again the velocity deviation is scale-dependent.

The average fluid particle velocity which is based on Darcy's law and effective hydraulic conductivity does not take into account the velocity variations at scales smaller than the scale at which the average fluid particle velocity is obtained. Then, how do hydrologists take account of the variation in velocity at the pore-scale or at any other scale? This question will be answered in the section that deals with dispersion.

2.4.4. Hydraulic Head. Now let us examine the physical meaning of hydraulic head in an equivalent homogeneous soil column. In the previous constant head permeameter examples (Section 2.4.1), a layered soil column was visualized as an equivalent homogeneous one (Figure 2.5). The effective hydraulic conductivity can be measured, and for flow perpendicular to the layering it is the harmonic mean of the two soil layers (equation 2.4.7). Certainly, one can use Darcy's equation and this effective hydraulic conductivity to determine a head distribution along the

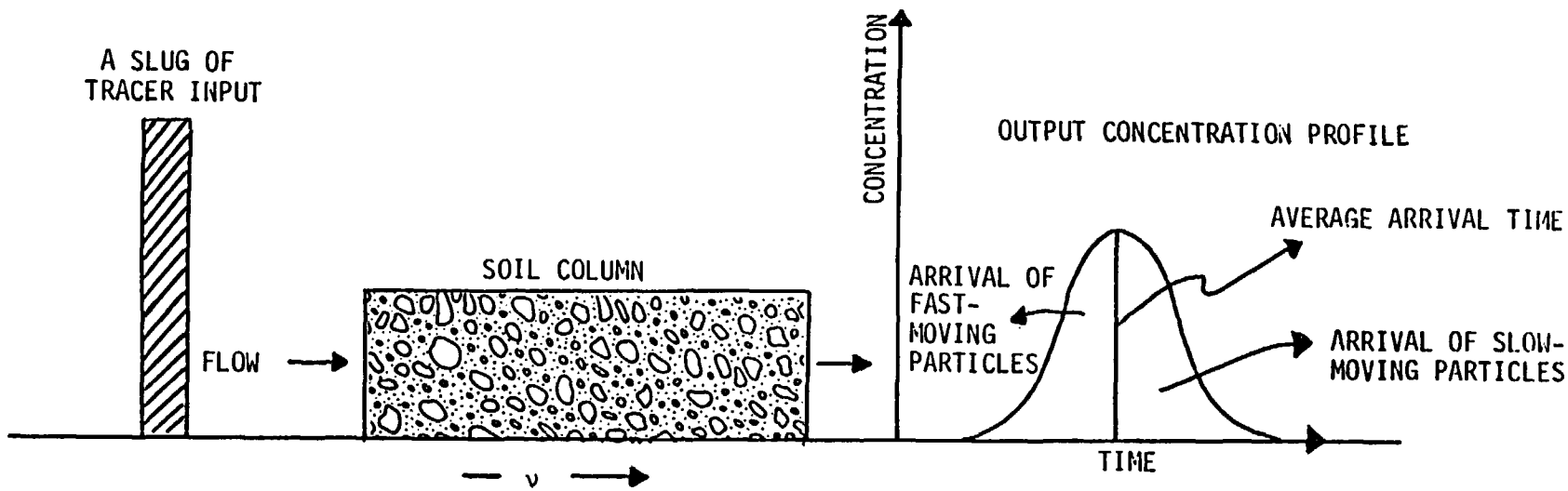


Figure 2.6. Effect of velocity variations in a soil column on outflow concentration.

equivalent, homogeneous soil column. Of course, the head distribution is a straight line, declining from the head at one boundary to the other (line C in Figure 2.7). However, owing to the layering, the head calculated by assuming that the two-layer column is homogenous is certainly different from actual head distribution along the soil column. Then, what does this calculated head distribution using the effective hydraulic conductivity represent? To answer this question, assume that the hydraulic conductivities of the two soils K_1 and K_2 are known. If $K_1 > K_2$, line A in the figure will represent the hydraulic head distribution along the layered soil column. If $K_1 < K_2$, line B is the head distribution. As illustrated in the figure, line C simply is the average of line A and Line B. This implies the head distribution determined from the effective hydraulic conductivity represents the average head distribution of all the possible head distributions; in this example there are only two possible head distributions. One can draw the same conclusion if the soil column consists of n layers of soils. In this case, the head distribution derived from the effective hydraulic conductivity will be the average of n possible hydraulic head distributions, resulting from all n! (n factorial) possible spatial arrangements of n K values along the soil column. This is equivalent to saying, in the jargon of stochastic hydrology, that the average is an "ensemble average" (see Section 4.0 or Appendix A).

From the simple example described above, one should see that a deterministic groundwater analysis is directly related to the stochastic concept that is used to deal with heterogeneity in field-scale problem, as will to be discussed in later sections. The discussion in this section is abstract and highly theoretical. However, it is crucial to understand the fundamentals of a theory before applying that theory to practical problems, such as the application of Theis' solution to aquifer tests (see Section 3.0).

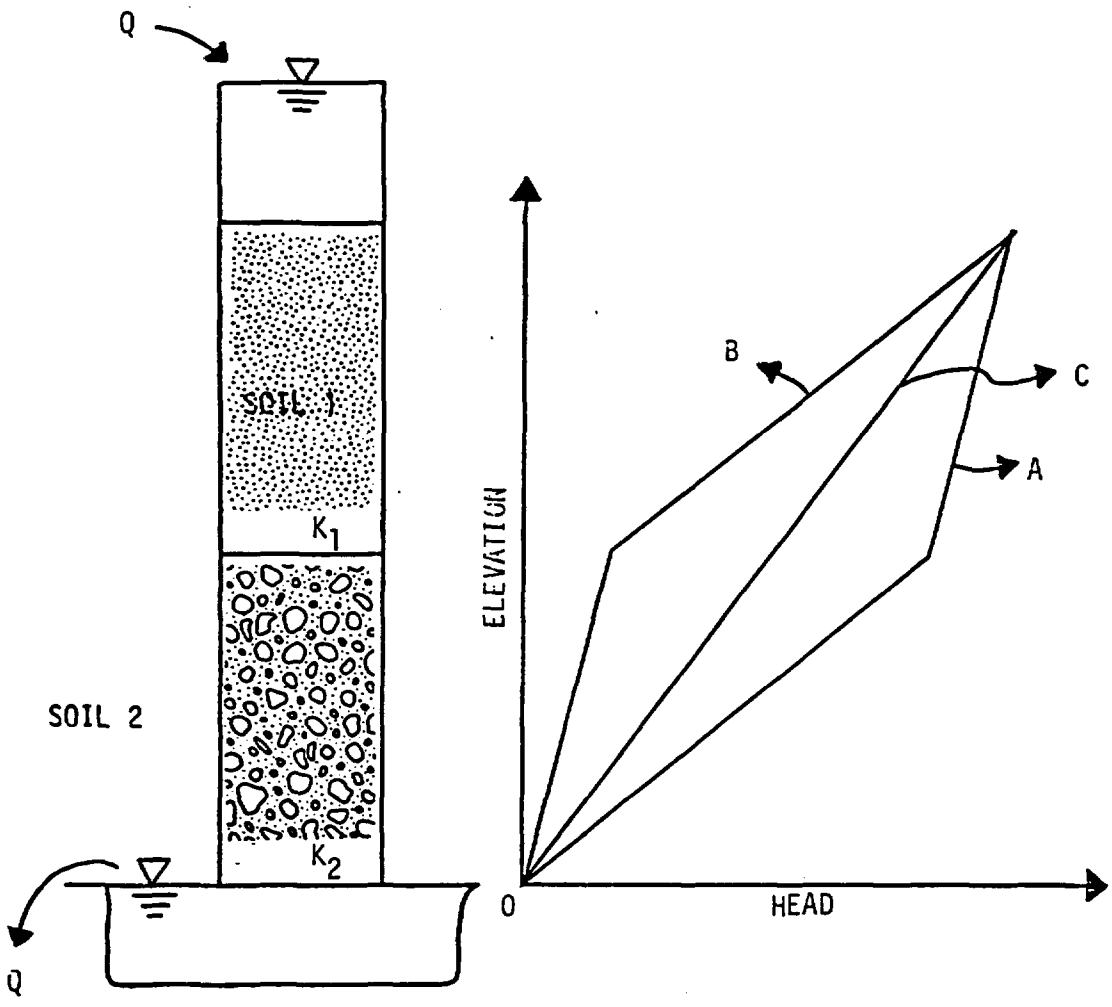


Figure 2.7. Concept of average hydraulic head distribution. Line A is for $K_1 > K_2$, line B is for $K_1 < K_2$, and line C is for K_{ave}.

2.5 Governing Groundwater Flow Equations

Estimating groundwater travel times in porous media requires the knowledge of the average fluid particle velocity which is determined by the gradient and the hydraulic conductivity values. Hydraulic gradients in groundwater problems are derived from hydraulic heads which may vary with time and space. Governing groundwater flow equations are used to predict the temporal and spatial variations of hydraulic heads. However, the equations are developed for the specific scales for Darcy's law and physical properties of groundwater discussed previously. Consequently, predictions from the equations, i.e., hydraulic heads, represent averages over some scale as well. Since groundwater travel times and paths are directly related to the hydraulic head distribution, understanding the meaning of the heads in equations of different scales is necessary. In the following sections, we will discuss the development of governing groundwater flow equations for various scales. Then, we will examine the physical meaning of head values. Meanwhile, some inconsistencies in the development of the equations which may contribute to uncertainties in predicting groundwater travel times will be elaborated on Appendix B.

2.5.1 Three-Dimensional Groundwater Flow Equation. To derive the governing groundwater flow equation, we start with the mass balance equation. Consider the mass balance of a stationary control volume at least as large as an REV (Figure 2.8) whose shape is fixed in space and time. The principle of mass conservation within this control volume requires that

$$\{ \text{rate of mass accumulation} \} = \{ \text{rate of mass in} \} - \{ \text{rate of mass out} \} \tag{2.5.1}$$

To apply the principle to the control volume, we begin by considering the pair of faces perpendicular to the x axis. The rate of mass in through the face at x is

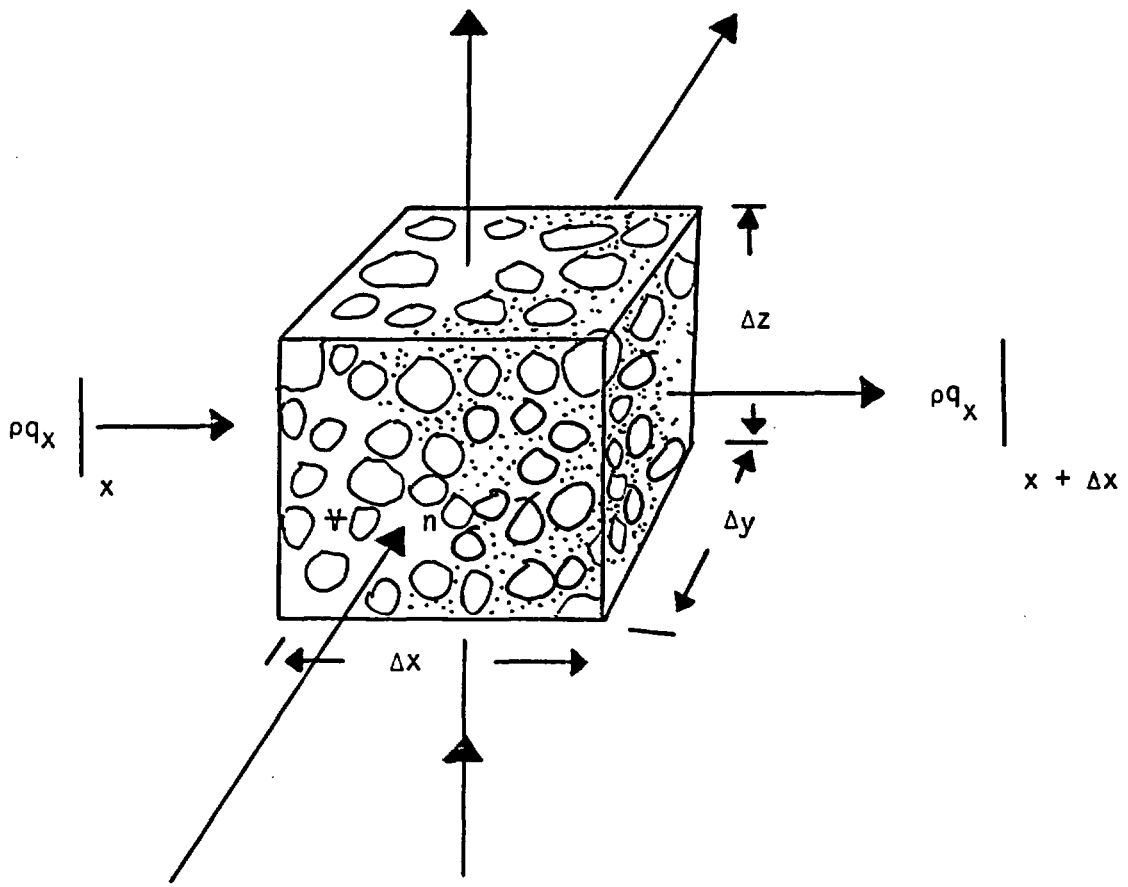


Figure 2.8. A control volume for mass balance.

$(\rho q_x)|_x \Delta y \Delta z$, and the rate of mass in through the face at $x+\Delta x$ is $(\rho q_x)|_{x+\Delta x} \Delta y \Delta z$. Similar expressions may be written for the other two pairs of faces. The rate of mass accumulation within the volume element is $(\Delta x \Delta y \Delta z)\left[\frac{\partial n\rho}{\partial t}\right]$, where n is the porosity of the control volume. The mass balance then becomes

$$\Delta x \Delta y \Delta z \left[\frac{\partial n\rho}{\partial t}\right] = \Delta y \Delta z[(\rho q_x)|_x - (\rho q_x)|_{x+\Delta x}] + \Delta x \Delta z[(\rho q_y)|_y - (\rho q_y)|_{y+\Delta y}] + \Delta x \Delta y[(\rho q_z)|_z - (\rho q_z)|_{z+\Delta z}] \tag{2.5.2}$$

By dividing this entire equation by $(\Delta x \Delta y \Delta z)$ and taking the limit as these dimensions approach zero, we get

$$\frac{\partial n\rho}{\partial t} = -\left[\frac{\partial \rho q_x}{\partial x} + \frac{\partial \rho q_y}{\partial y} + \frac{\partial \rho q_z}{\partial z}\right] \tag{2.5.3}$$

This is the equation of continuity for flow through porous media, which describes the rate of change of fluid density at a fixed point resulting from the changes in the mass flux $\rho \mathbf{q}$ (the bold type indicates a vector quantity, ie, a quantity having both magnitude and directions). Note that replacing the difference equation (2.5.2) by the partial differential equation (2.5.3) implies all the variables in (2.5.3) are continuous and differentiable in both space and time coordinates. regardless of whether the point of interest falls within a pore or solid. That is, the continuum assumption discussed previously has been used. Using the vector notation, equation (2.5.3) can be expressed as:

$$\frac{\partial n\rho}{\partial t} = -(\nabla \cdot \rho \mathbf{q}) \tag{2.5.4}$$

Here ($\nabla \cdot \rho q$) is called the "divergence" of ρq, sometimes written as div ρq. Note that the vector ρq is the mass flux, and its divergence has a simple significance: it is the net rate of mass efflux per unit volume. The equation (2.5.4) simply states that the rate of increase of the density within a small volume element fixed in the porous media is equal to the net rate of mass influx to the element. Note that the continuity equation applies to any arbitrary volume at this point.

Now if one assumes that the control volume is much larger than many pores, then the specific discharge, q, can be represented by Darcy's law. The substitution of a form of equation 2.4.1 (i.e., $q = -\nabla h$) for q in to equation 2.5.4 leads to the classical governing groundwater flow equation which is given as:

$$\nabla \cdot (K \cdot \nabla h) = \rho g(n\beta + \alpha) \frac{\partial h}{\partial t} = S_s \frac{\partial h}{\partial t} \qquad (2.5.5)$$

where K is the hydraulic conductivity tensor, h is the hydraulic head, and S_s is the specific storage coefficient. However, this equation is theoretically inconsistent since it mixes the expressions for both the fixed and moving coordinate systems as discussed in Appendix B.

Because of the use of Darcy's law, equation (2.5.5) is valid only for media whose volume is much larger than many pores. As a result, variables in the equation are continuous within the volume and represent average values. Certainly, these averages cannot account for the detailed variations of the variables at scales less than the volume, as we illustrated in section 2.4.4. Although the size of the averaging volume is restricted to be much larger than many pores, it could be enlarged to study any larger scale. Using equation (2.5.5), one can visualize an entire aquifer as a collection of many K values measured over a volume which is much larger than many pores but much smaller than the entire aquifer. On the

other hand, one can enlarge the REV so that the entire aquifer is considered homogeneous but the flow field remains three-dimensional. By reducing the size of the control volume, we obtain variables which are more representative of smaller scale variations within the volume.

2.5.2 Two-Dimensional Depth-Averaged Groundwater Flow Equation. Generally speaking, the three-dimensional groundwater flow equation is more representative of real flow fields than one- or two- dimensional equations. However, it may be impractical because a large number of data and a large amount of computer time are required for simulating three-dimensional flows in a field- or regional-scale aquifer system. Sometimes, it may be adequate to conceptualize such a three-dimensional flow field by a two-dimensional horizontal plane flow phenomenon. This conceptualization involves taking vertical averages of the three-dimensional groundwater flow equation, i.e.

$$\int_{z_0}^{z_0+b} \nabla\cdot(K\cdot\nabla h)\, dz = \int_{z_0}^{z_0+b} S_s \frac{\partial h}{\partial t}\, dz \qquad (2.5.6)$$

where z_0 is the elevation of the bottom of the aquifer, and b is the thickness of the aquifer Bear, (1979). Integration of (2.5.6) results in a two-dimensional depth-averaged equation,

$$\nabla'\cdot(T\cdot\nabla' H) = S\,\frac{\partial H}{\partial t}$$

where ∇' is the two-dimensional divergence

$$T = \int_{z_0}^{z_0+b} K(x,y,z)\ dz,$$

$$S = \int_{z_0}^{z_0+b} S_s(x,y,z)\ dz,$$

$$\text{and } H = \frac{1}{b} \int_{z_0}^{z_0+b} h(x,y,z)\ dz \qquad (2.5.7)$$

T, S, and H are transmissivity, storage coefficient, and the average hydraulic head, respectively. Note that T, S, and H are depth-averaged quantities which implies the vertical variations in these parameters are ignored. As an example, in a stratified aquifer the variation in hydraulic conductivities among layers is neglected. This implies that the vertical dimension of the REV of the aquifer properties, T and S, is at least equal to or much larger than the thickness of the layer in the aquifer. Certainly, one can conceptualize that T and S values are constant in both horizontal directions by enlarging the size of the REV. The aquifer is again considered homogeneous as in the three-dimensional case. However, even in homogeneous aquifers, the depth-average approach further restricts the flow to two horizontal dimensions only.

In fact, most field- and regional-scale aquifers have been characterized by aquifer tests which produce the depth-averaged T and S values. Since these data are abundant for most groundwater basins, Dagan (1986) argued that two-dimensional depth-averaged models are appropriate for field- or regional-scale problems.

2.5.3 One-Dimensional Flow Equation. A one-dimensional groundwater flow equation can be written as

$$\frac{\partial}{\partial x}\left[K\,\frac{\partial h}{\partial x}\right] = S_s\,\frac{\partial h}{\partial t} \qquad (2.5.8)$$

This equation is equivalent to conceptualizing an aquifer as a soil column (e.g. Figures 2.5 or 2.6) with flow in the aquifer being strictly unidirectional. If K is allowed to vary in the x direction, dimensions of the averaging volume (REV) in the other two directions, i.e. y, and z, are obviously as large as or larger than the width and thickness of heterogeneities (such as clay lenses) in the aquifer. If K is assumed constant in the x direction, the averaging volume must be much larger than the size of heterogeneities in the aquifer. Our scale of interest (such as the size of screen in a well) is much smaller than the entire aquifer. Such a large-scale averaging procedure may thus lose too much information pertinent to our interests. Therefore, this one-dimensional conceptualization may be considered of limited value.

2.5.4 Hydraulic Heads. Based on the discussion above, one can conclude that a three-dimensional equation (2.5.5) is most realistic. It allows us to describe aquifers as three-dimensional hydraulic conductivity fields using the small size average volume. The two-dimensional, depth-averaged equation (2.5.6), however, ignores the variations in hydraulic conductivity in the vertical direction. A one-dimensional equation (2.5.8) further averages the hydraulic conductivity variation in two directions (i.e., horizontal and vertical directions).

Groundwater flow equations for three-, two-, and one-dimensional problems (2.5.5, 2.5.6, and 2.5.8) allow us to conceptualize heterogeneous aquifers as homogeneous ones, using an appropriate REV. However, the flow fields (hydraulic heads) determined by each equation represent different averages. Because of the homogeneity assumption, the three-dimensional governing flow equation produces an ensemble-averaged three-dimensional head distribution. In other words, the head distribution is the average of all possible three-dimensional head distributions, as

discussed in Section 2.4.4. Note even though the aquifer is considered homogeneous, the head distribution may retain its three-dimensional characteristics, depending on type of flow field (i.e., uniform, converging, or diverging flow). Generally, the head determined by the three-dimensional flow equation for a homogeneous aquifer is analogous to the water level observed in a piezometer (Figure 2.9), if the aquifer is truly homogeneous (i.e, heterogeneity exists only at pore-level). However, if the heterogeneity is much larger than the opening of the piezometer, the head calculated by the three-dimensional equation with homogeneity assumption will differ from the one observed in the piezometer. The two-dimensional equation averages three-dimensional head distributions in the vertical to produce two-dimensional, depth-averaged heads. The depth-averaged head is equivalent to the water level observed in a well screened over the entire thickness of the aquifer (Figure 2.9). This depth-average procedure simply forces the head values along the vertical to be a constant value which is not identical to the ensemble average, unless the mean flow is parallel to stratifications. One-dimensional equations further reduce the two-dimensional head distribution to a one-dimensional one. The head resulting from the one-dimensional model is analogous to the water level in an excavation ditch which cuts completely through the aquifer, if there is no flow in the ditch.

As discussed above, each governing equation uses different averaged hydraulic properties of the aquifer. Each also gives hydraulic head values with different meanings. As a result, the fluid particle velocity determined from the averaged heads represents different averages. Moreover, these averages neglect variations in velocity at scales less than the scale where the averages apply. Therefore, one may ask: how can one include the effects of these variations smaller than the averaging scale to obtain a more realistic prediction of groundwater travel times and paths? We will try to address this equation in the next section that discusses the dispersion phenomena.

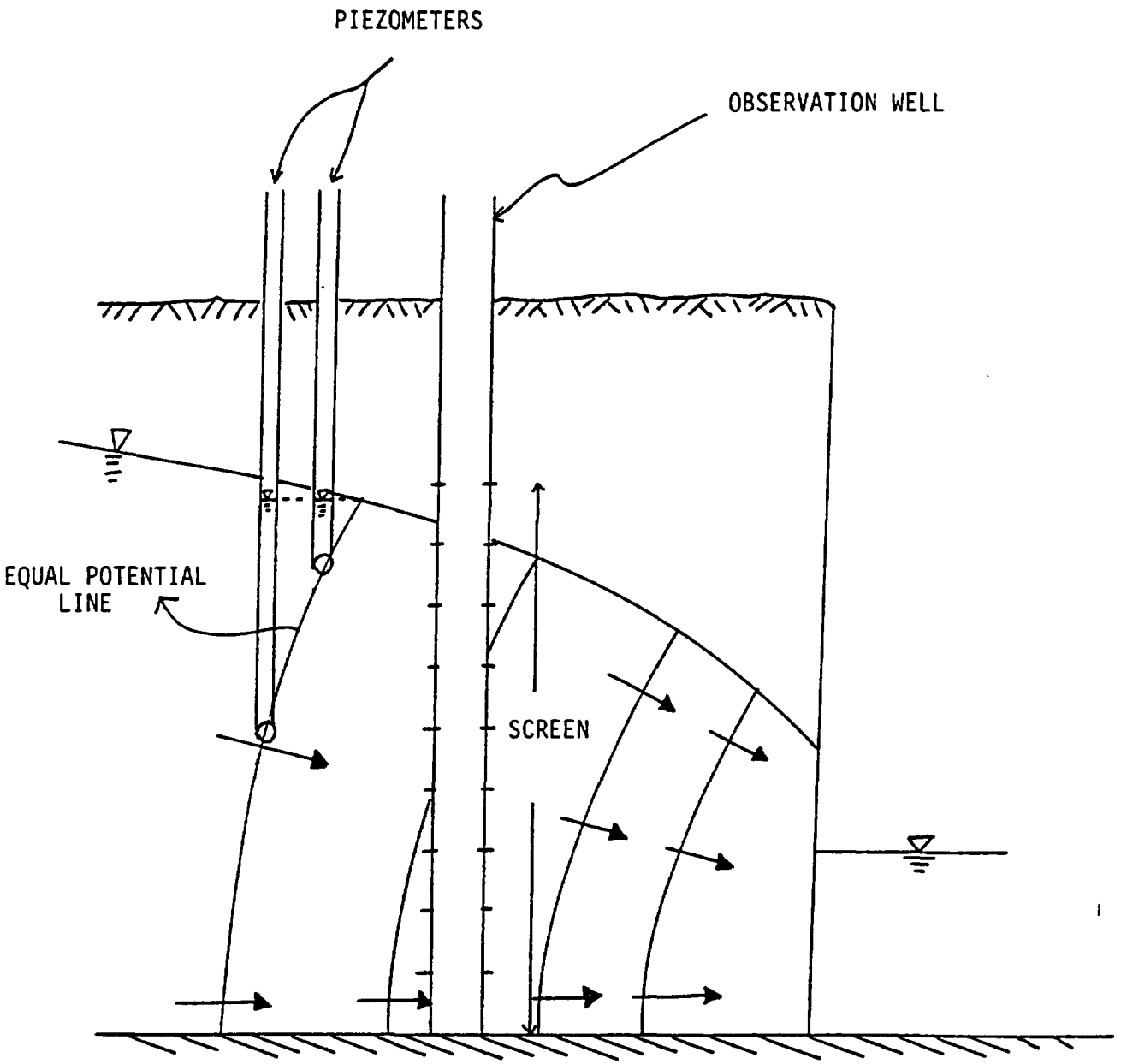


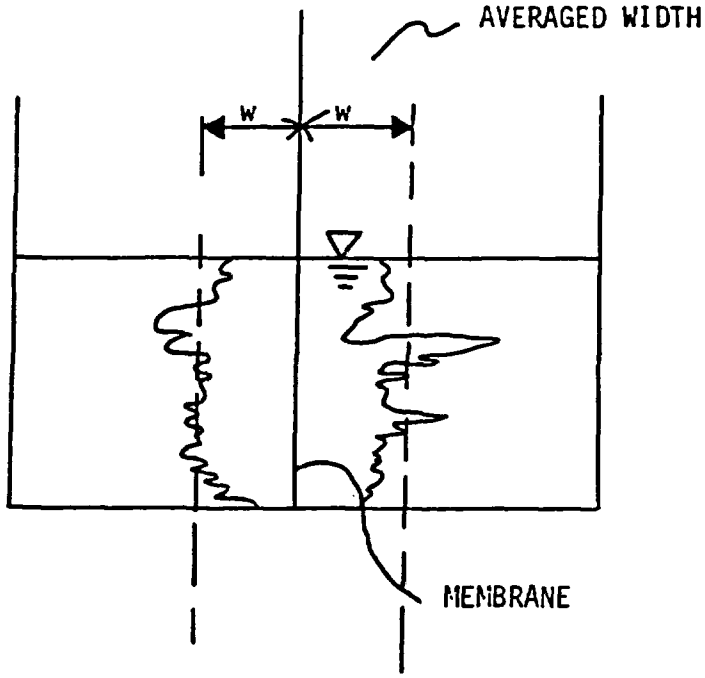
Figure 2.9. Water level in piezometers and a fully-screened observation well in a water table aquifer discharging to a ditch. Water level elevation in the observation well represents a depth-averaged head which is lower than the water table.

2.6 Hydrodynamic Dispersion

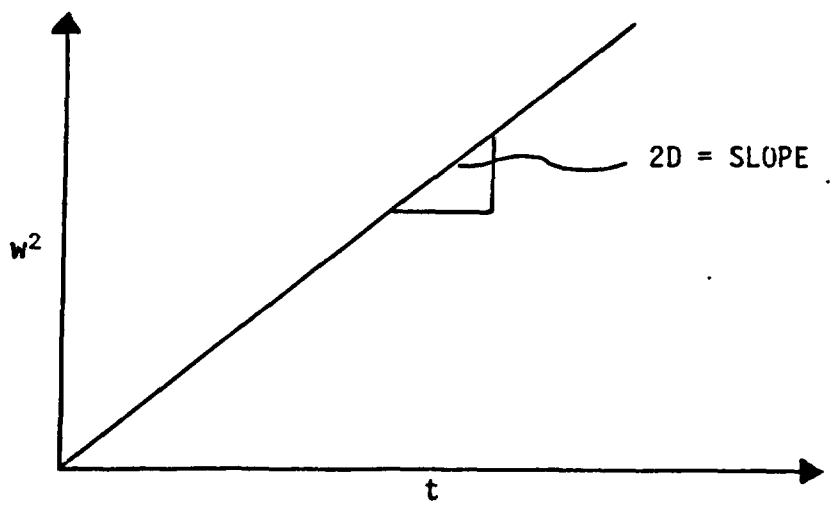
To include the variations in fluid particle motion at scales smaller than the scale at which the results of the flow equations apply, the concept of hydrodynamic dispersion must be introduced. However, before hydrodynamic dispersion is discussed, we will review the basic concept of molecular diffusion, which is analogous to hydrodynamic dispersion but at a much smaller scale.

2.6.1 Diffusion. Consider two fluids of the same chemical and physical properties but of different colors, separated in a tank by an impermeable membrane. The fluids in the tank are static, that is, there is no fluid flow. The membrane is then removed without disturbing the static condition. At early times, we would see an abrupt difference in color at the interface between the two fluids. As time passes, the abrupt interface diminishes and a smeared mixing zone develops (Figure 2.10a). The mixed color vanishes gradually away from the center, and fades into the initial color of the respective fluids. The width of this smeared zone grows continuously with time until the fluids are completely mixed. This process causing the smearing effect is called "molecular diffusion".

This diffusive process is generally attributed to the random motion of molecules of the two fluids. The term random motion is used because of the chaotic motion of molecules which seems to be unpredictable. In fact, if we apply kinetic theory to each molecule, the motion of a molecule in the fluid can then be described in a deterministic way. However, at the scale of our interest and instruments, it is of little practical use to describe the motion of each individual molecule. Nevertheless, such molecular-scale motions may have great impacts on phenomena at the scale larger than the size of molecules. Then, how can the diffusive process be quantified? This question was answered by Adolph Fick, a German physiologist, who in 1855 stated that the flux of solute mass, that is, the mass of a solute crossing a unit area per unit time in a given direction, is proportional to the gradient of



(a)



(b)

Figure 2.10. (a) Smearing effect in a tank, and (b) the linear relationship between w^2 and time.

solute concentration in that direction. This relationship is generally known as Fick's Law.

For a one-dimensional diffusion process, Fick's law can be stated mathematically as

$$q_m = -D_m \frac{\partial c}{\partial x} \tag{2.6.1}$$

where q_m is the solute mass flux; c, is the mass concentration of diffusing solute; D_m, is a coefficient of proportionality called the diffusion coefficient, and the minus sign indicates transport is from high to low concentrations. Fick's law is similar to Darcy's law in which the mass flux of water is related to the conductivity and hydraulic gradient. Similar to the hydraulic conductivity, the diffusion coefficient is a quantity averaged over a volume much larger than many molecules and the motion of individual molecules is ignored.

To illustrate the concept of averaging in a diffusion process, we will reexamine the case where two fluids are separated by a membrane. As mentioned earlier, the width of the mixing zone grows with time. Here, the width is defined as an average width of the mixing zone over the depth of the tank because the width may vary from depth to depth as shown in Figure 2.10a. This average is equivalent to the depth-average procedure discussed in section (2.5.2). If one repeatedly carries out the same experiment, the depth-average width may be different from one experiment to another because of the random motion of the molecules. However, if one averages the depth-averaged width of all the experiments, one obtains an average width which is an ensemble average, i.e., average over many possible outcomes. As a matter of fact, if the square of the ensemble-average width, w^2, is plotted as a function of time, a linear relationship is found (Figure 2.10b). The slope of the line

is generally related to the diffusion coefficient by

$$\frac{dw^2}{dt} = 2D_m \tag{2.6.2}$$

In other words, the diffusion coefficient, D_m, describes the rate of growth of the average width of the mixing zone over the depth of the tank, and over many experiments. It certainly does not intend to depict the rates at each depth and each experiment. Therefore, the coefficient of diffusion is merely a mean parameter. In view of the fact that our measuring devices, and human vision are limited, and the fact that repeated experiments are impractical, a diffusion coefficient obtained in one experiment is often considered adequate. This assumption implies the equivalence between the depth-average and the ensemble average (i.e. an ergodicity assumption; see Appendix A and Section 4.1). Since D_m is an average value, one should not expect that the concentration of the colored fluids can be predicted by using the diffusion coefficient at scales much smaller than the scale at which D_m is derived. Furthermore, one should not expect that the concentration predicted by the diffusion concept will be identical to the one observed in a single experiment.

The linear relationship shown in Figure 2.10b implies that the diffusion coefficient is a constant. This constant diffusion coefficient concept or the linear relation may be true, at least at the scale of our instruments but not at the microscopic scale. We now will illustrate this point by reviewing a statistical theory developed by G.I. Taylor (1922) for analyzing the random motion of molecules.

Inasmuch as the motion of each molecule is complex and "random", it is most appropriate to describe it by statistical means. That is, we will describe the position of molecules at any time in terms of probability, instead of the exact location of the particle. Again, we would like to reemphasize the fact that the motion of

molecules is deterministic but too complex for us to use any deterministic approach. Furthermore, we are not interested in how individual molecules move. Based on these reasons, we conceptualize the deterministic movement of molecules as a random process. To carry out this statistical analysis of random motion, we will assume that the velocity of a diffusing molecule is a stationary stochastic process in time (Csanady, 1973). This means that we do not know the velocity of the molecule at any time, but we could determine all the possible velocity values from the known statistical properties of the process, such as mean, variance, or probability distribution of the velocity (for definitions of statistical terms refer to Appendix A). Without loss of generality, we may say that the mean and variance of the velocity of a molecule are constant in time: i.e.,

$$E[v(t)] = \text{constant} = 0$$

$$\text{and} \quad E[v^2(t)] = \text{constant} = E[v^2],$$

respectively, where E[ ] stands for the expected value which represents the probablistic average of a random variable. Another important statistical parameter characterizing a stationary stochastic process is its autocorrelation function, $R_{vv}(\tau)$, where τ is the time lag between two times, t and $t+\tau$. The autocorrelation function of the velocity history of a molecule may be regarded as measuring the persistence of the velocity of a molecule throughout a period of time (Appendix A). In other words, it is a measure of the correlation of the velocities of a molecule between any time interval, τ. Thus, the velocity autocorrelation function is defined as:

$$R_{vv}(\tau) = \frac{E[\ v(t)\ v(t+\tau)\ ]}{E[\ v(0)^2]} \tag{2.6.3}$$

where $E[v(0)^2]$ is the variance of velocity. In a stationary stochastic process, the autocorrelation function is independent of time t but dependent on the time lag, τ. In the case of the velocity history of a diffusing molecule, such an autocorrelation function implies that once the molecule possesses a certain velocity, a short time τ later it is still likely to have a velocity of a similar magnitude and sign. For a given time lag τ, the velocity covariance, $E[v(t)v(t+\tau)]$ may be formed, which evidently tends to $E[v^2]$ as $\tau \to 0$. However, after a long enough time τ, the molecule tends to 'forget' the velocity at time t, in the sense that the value of v at $t+\tau$ will be quite independent of v(t). That is, at $\tau=0$, $R_{vv}(\tau)=1$, while as τ approaches ∞, $R_{vv}(\tau)$ becomes 0, as shown in Figure 2.11.

The displacement of an individual diffusing fluid or tracer molecule at any time, t, can be related to its velocity by

$$x(t) = \int_0^t v(s)ds \tag{2.6.4}$$

where x is the position. Now we imagine that there is more than one molecule moving "randomly" in fluid space. We further assume that the statistical characteristics (i.e., mean, variance, and covariance) of molecule's velocities are the same. After a period of time, the location of each molecule would, of course, be different. However, these molecules will spread around x=0,

$$E[x(t)] = \int_0^t E[v(s)]\, ds = 0 \tag{2.6.5}$$

because in a static system the mean velocity, E[v], is zero. As shown in Figure 2.10

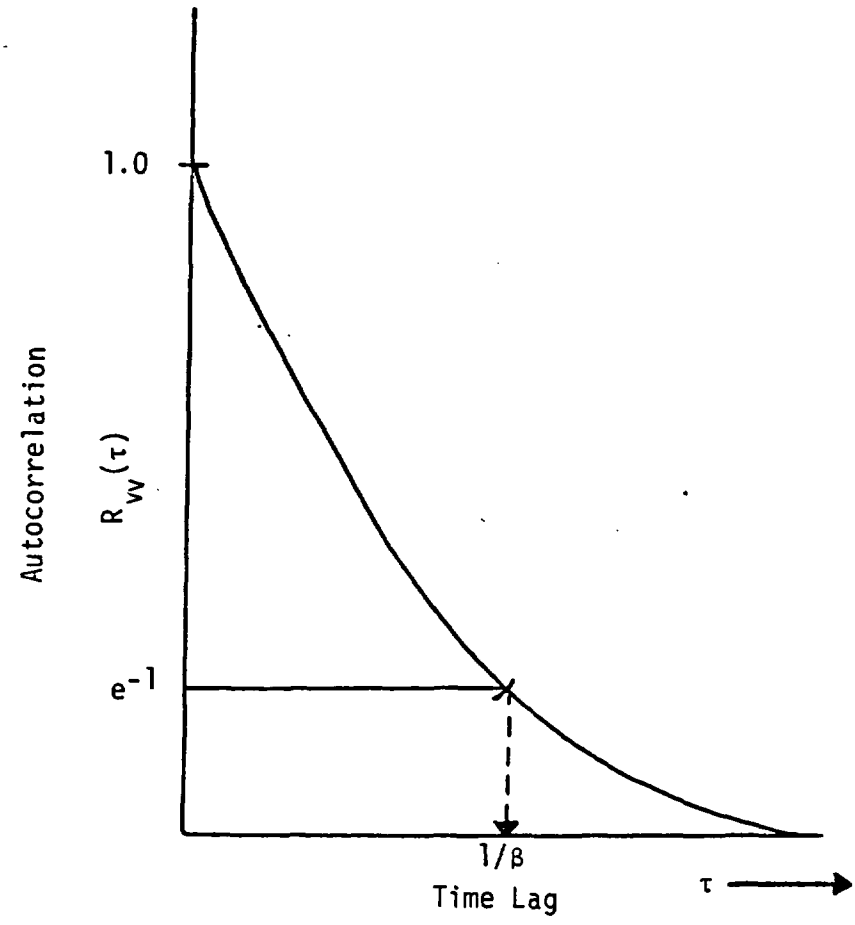


Figure 2.11. A hypothetical velocity autocorrelation function.

and equation 2.6.2, the spreading, the deviation of the position of a molecule from the mean position, at time t can be quantified by $x(t)^2$. The rate of change of $x(t)^2$ may then be written as:

$$\frac{dx^2(t)}{dt} = 2x\frac{dx}{dt} = 2\int_0^{t+\tau} v(t)\ v(t+s)\ ds \tag{2.6.6}$$

Since there are a large number of molecules, the average rate of change of $x^2(t)$ of all the molecules can be obtained by taking the expected value of (2.6.6) and the result is:

$$\frac{dE[x^2]}{dt} = 2\ E[v^2]\int_0^{t+\tau} R_{vv}(\tau)d\tau \tag{2.6.7}$$

where $E[x^2]$ is the variance of the molecule positions which is equivalent to the average width squared, w^2, in equation (2.6.2). The left-hand side of equation (2.6.7) represents the rate of change in variance of the molecule positions or $2D_m$ as shown in equation (2.6.2). In other words, the molecular diffusion coefficient, D_m, is directly related to the molecules' velocity autocorrelation function and it varies with time. However, due to numerous collisions with other molecules, the velocity of a molecule at time $t+\tau$ tends to forget its velocity at t, as τ becomes large. For simplicity, we assume that the velocity autocorrelation function takes the form:

$$R_{vv}(\tau) = e^{-\beta\tau} \tag{2.6.8}$$

where β^{-1} is considered as the persistence time for the velocities of the diffusing

molecules. This means that, on the average, molecules tend to forget their previous velocities after a period of time β^{-1}. This velocity autocorrelation function is shown in Figure 2.11 as a function of τ.

The integral of $R_{vv}(\tau)$ on the right hand-side of equation (2.6.7) represents the area under the curve bounded by 0 and $t+\tau$. It should be evident from Figure 2.11 that the value of the integral will increase initially but will approach a constant at large values of $t+\tau$, or $t+\tau$ approaches ∞. This result implies the rate of spreading of the diffusion molecules at large value of τ will be a constant according to equation (2.6.7). As a result, the diffusion coefficient, which is half of the rate of change in $E[x^2]$, will increase initially but at $t>>\beta^{-1}$ it tends to stabilize. For a particle of a radius, 10^{-4} cm, the persistence time, β^{-1}, is about 1.4×10^{-8} seconds (Csanady, 1973). Since the scale of our observation is likely much greater than 1.4×10^{-8} seconds, the time-dependent portion of the diffusion coefficient can be neglected and the diffusion coefficient can virtually be treated as a constant value. For much smaller scales of observations this may not be the case.

2.6.2 Advection-Diffusion Equation. Now suppose that an ideal fluid with a tracer is moving in a frictionless pipe. In this hypothetical frictionless pipe, there are no velocity variations caused by friction between the fluid and the wall of the pipe, so that the velocity recorded by small instruments is constant across the cross-section of the pipe, because friction does not exist. However, at the molecular level, molecules move at different velocities. The size of our instruments for measuring a flow velocity is generally much greater than the size of molecules. Obviously, the velocity we determined from the measurement is an average value over many molecules. This average velocity does not consider the variation in velocity of molecules. For example, consider a tracer experiment in a frictionless pipe (Figure 2.12a). If 10,000 tracer molecules are simultaneously released at one end of the pipe at time, t_0, then at various times the discharge at the other end of the pipe is

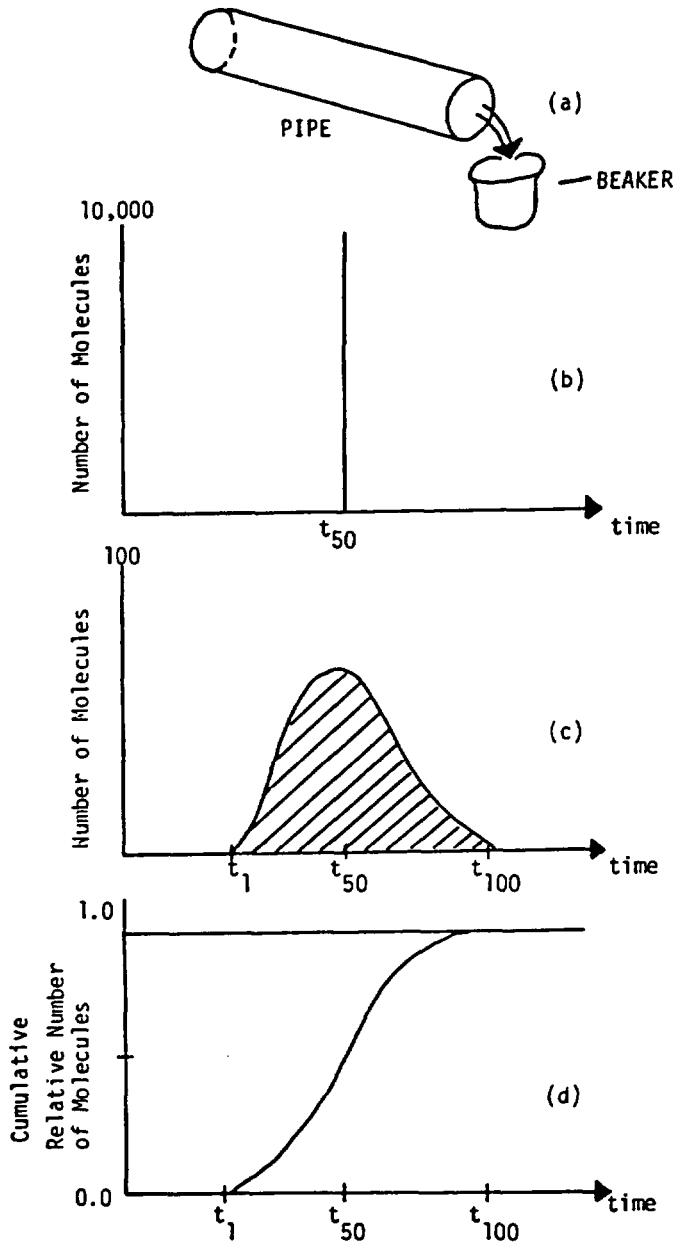


Figure 2.12. A tracer experiment in a frictionless pipe.

collected with a beaker, and the number of tracer molecules in the beaker is counted. We will observe the simultaneous arrival of all the molecules at time, t_{50} (Figure 2.12b), only if all the molecules move at the same velocity which is equal to the discharge rate divided by the cross-sectional area of the pipe. However, due to the random motion of molecules, some of the molecules will move faster than the others and some slower. If we plot the number of molecules in the beaker versus time, we shall have a molecule arrival time distribution shown in Figure 2.12c. This distribution represents the number of the tracer molecules arriving at the end of the pipe at any time, t. Figure 2.12d shows the cumulative, relative number of molecules (i.e., the ratio of the total number of molecules collected after t_0 to the total number of molecules released) as a function of time. Based on the figure, 50% of the tracer molecules exit the pipe at t_{50}, and all the molecules are removed at t_{100}. Time t_1 thus represents the arrival time of the fastest moving molecule, or the molecule travel time along the fastest path. However, we generally do not count the number of molecules due to the size of our instruments, and instead we use concentration, c, (i.e., the ratio of the mass of the tracer molecules to the volume or mass of the fluid in the beaker). Thus, Figure 2.12c is equivalent to the concentration-time distribution (breakthrough curve), and Figure 2.12d represents the cumulative concentration-time distribution. Obviously, the smearing or spread of the concentration distribution is due to variations in molecules' arrival time, which in turn are caused by variations in molecules' velocity. If the variation in velocity at the molecular level can be handled by the diffusion coefficient discussed previously in Section 2.6.1, the total rate of mass flux, q_m, across the instrument used to measure flow rate is thus the advective flux due to the average movement of the fluid plus the diffusive flux due to random motion of the fluid molecules. That is;

$$q_m = vc + \left[-D_m \frac{\partial c}{\partial x} \right] \tag{2.6.9}$$

where v is the average velocity of the fluid, and c is the concentration of tracer. The product term vc represents the advective tracer flux and $D_m \partial c/\partial x$ represents the diffusive flux. When (2.6.9) is substituted into the equation for conservation of mass (similar to equation 2.5.4) in one dimension, we obtain the advection-diffusion equation:

$$\frac{\partial c}{\partial t} + v\frac{\partial c}{\partial x} = D_m \frac{\partial^2 c}{\partial x^2} \tag{2.6.10}$$

where the second term on the left hand side of the equation represents the advection effect and the term on the right hand side of the equation represents the diffusion effect due to random motion of molecules. Thus, a concentration breakthrough curve which is the solution of Equation 2.6.10 in time domain reflects the arrival time of the tracer molecules. The molecular diffusion coefficient is simply a "fudge factor" accounting for velocity variations of molecules at a scale much smaller than the pipe.

Equation (2.6.10) is developed for tracer movement in a frictionless pipe. In the case where the wall of the pipe is not smooth but rough, velocities measured at a scale much larger than many molecules but smaller than the cross-section of the pipe (say, continuum scale in fluid mechanics) will vary across the cross-section of the pipe. The velocity is likely maximal in the center of the pipe and is minimal near the wall. This implies that the velocity determined by a discharge rate divided by the cross-sectional area of the pipe represents an average velocity value which neglects the velocity variation across the cross-sectional area due to friction. Furthermore, it also neglects the velocity variations among individual molecules.

Now, if we assume that the velocity variations at scales smaller than the cross-sectional area of the pipe and those at the molecular scale can be described by Fick's law as in the molecular diffusion process, then equation (2.6.10) is valid for this case as well. However, the diffusion coefficient, Dm, in equation (2.6.10) is replaced by a dispersion coefficient, D_d, which lumps together velocity variations at both the molecular scale and the continuum scale. Of course, the velocity, v, in equation (2.6.10) represents the average over the cross-sectional area. The concentration, c, then represents the total mass of a tracer in a volume of fluid discharging from the cross-sectional area of the pipe. Generally, this approach is valid for tracer movement in a long pipe as shown by G.I. Taylor (1953).

Following the above concept, surface-water hydrologists have frequently applied equation (2.6.10) to determine tracer movement in large-scale water bodies such as streams, rivers, estuaries, and oceans. Various successes have been reported in the literature for instance Fischer et al., (1979). Regardless of the validity of equation (2.6.10) for large-scale problems, the most important feature of the equation is that the parameters have different physical meanings, depending on the scale. Moreover, the dispersion coefficient always represents the effects of velocity variations at scales smaller than the scale at which the average velocity is defined.

2.6.3 Hydrodynamic Dispersion in Porous Media. Now consider flow in a porous medium (for example, a soil column). At the molecular level, each molecule has its own velocity. At the scale of a single pore, the velocity averaged over many molecules may not be constant over the pore space because of the roughness of the wall of the pore, just like flow in a frictional pipe. At the scale larger than a single pore variations in pore size, in addition to tortuosity of pore channels, will then cause an additional velocity variation. As discussed previously, the average fluid particle velocity defined in groundwater hydrology is the average value over many pores or heterogeneities of many different scales, depending on the size of the

control volume. The average fluid particle velocity does not take velocity variations at different scales into consideration. To account for the variation in velocity due to random motion of molecules, roughness of the pore walls, and the variation in size of pores and tortuosity in a flow path, groundwater hydrologists borrowed the advection-diffusion concept. In other words, in order to conserve mass, the mass flux which is not considered by the average fluid particle velocity is lumped into the dispersive flux term, similar to the way molecular diffusive flux was treated in the advection-diffusion process. The smearing effect due to the variation in velocity at a scale larger than the molecules, but smaller than the scale used to determine the average fluid particle velocity is then attributed to hydrodynamic dispersion. Therefore, the classic advection-diffusion equation (2.6.10) may then be directly applied to solute transport in porous media. However, the coefficient of hydrodynamic dispersion is used in lieu of the diffusion coefficient to represent the coefficient of proportionality between the mass flux and concentration gradient. The hydrodynamic dispersion coefficient thus includes the effect of variation in velocity at many different scales (from the molecular scale to the scale at which the average linear velocity is defined.) This approach is identical to convection-dispersion approaches used by surface-water hydrologists in dealing with solute transport in streams, rivers, and estuaries. However, causes of velocity variations or mechanisms of dispersion are different.

2.6.4 Mechanisms of Dispersion in Porous Media. Mixing of tracer particles due to dispersion is primarily an artifact related to the scale of averaging. In the REV, the hydraulic conductivity and porosity are assumed to be constants representing the average values over the volume. Consequently, the velocity determined from these parameters represents an average over the volume. This velocity describes the average solute movement as a piston type of displacement which exhibits a sharp interface with the fluid. Smearing effects observed in the

experiments are attributed to mixing due to subscale velocity variations within the REV which are treated as the dispersion process. Since the size of the REV varies with the scale of heterogeneity, mechanisms of dispersion are accordingly classified by the scale of heterogeneity.

At the microscopic scale, mixing is caused by random motion of fluid molecules. This process is called diffusion. At the laboratory scale, mixing is a result of the combined effects of diffusion and velocity variation within pores, among pores, and tortuous flow channels. This type of mixing is generally defined as local dispersion. If the concentration of tracer particles is measured in fully penetrating observation wells and one uses a two-dimensional depth-average flow and transport model to simulate the process, then the field-scale dispersion reflects mixing due to groundwater velocity variations between and within distinct hydrogeologic units, in addition to molecular diffusion and local dispersion. This type of dispersion is sometimes called two-dimensional macrodisperison (Gelhar et al., 1979). The term, macrodispersion, is also used in three-dimensional flow situations if one treats the entire aquifer as a homogeneous one. However, the two-dimensional macrodispersion is different from the three-dimensional one in the fact that it also includes the effects of averaging three-dimensional flow fields into two-dimensional fields (see section 2.5). Therefore, the mechanics causing dispersion vary with the scale of averaging.

2.6.5 Dispersivity. The dispersion concept in groundwater hydrology should become clear by now. Overall, the dispersion coefficient is merely a parameter in the classic convection-dispersion equation used to include variations in velocity at subscales. However, velocity variations are not controlled only by the heterogeneity at different scales of porous media, but also by the flow fields (directions of flow, and magnitudes of mean velocities). For example, consider an aquifer consisting of three homogeneous layers with equal thicknesses and with hydraulic conductivities,

K_1 = 10 cm/day, K_2 = 1cm/day, and K_3 = 100 cm/day. For simplicity, we will assume porosity values of the three layers are the same and equal to 0.5. If a constant hydraulic head gradient 0.01 is imposed on each layer, the average fluid particle velocity for layers 1, 2, and 3 is 0.2, 0.02, and 2 cm/day, respectively. The average velocity over the three layers is 0.74 cm/day and the variance is 1.2 cm^2/day^2. Now, if the gradient is increased to 0.1, the velocities are 2, 0.2, and 20 cm/day for layers 1, 2, and 3, respectively. The mean velocity is then 7.4 cm/day and variance is 119 cm^2/day^2. This simple example illustrates that velocity variations depend on the magnitude of gradient or mean velocity, as well as the hydraulic conductivity variation. Therefore, the hydrodynamic dispersion coefficient depends not only on the physical characteristic of porous media but also on the flow characteristics.

Inasmuch as flow is likely to vary with time and boundary conditions, how can this hydrodynamic dispersion coefficient be determined so that one can predict solute movement in porous media? One way to determine this parameter is to fit, by trial and error, the solution of the convection-dispersion equation to the results of tracer experiments. However, in a sense, the dispersion coefficient becomes a parameter which may vary from one experiment to another experiment even in the same porous medium, owing to differences in mean pore velocity. For predictive purposes, such an approach is not suitable.

To overcome this difficulty, many tracer experiments at the laboratory scale have been done in the past. The results of the experiments showed that the dispersion coefficient, D_d, is linearly proportional to the average velocity (Bear, 1979):

$$D_d = \alpha v \tag{2.6.11}$$

where v is the average velocity over the laboratory sample and α is the dispersivity.

For homogenous laboratory soil columns, the dispersivity can be further related to the particle size of porous media, and thus, can be considered constant. Because the dispersivity is a property of the medium, predicting movement of solutes in a porous medium under different flow fields now becomes possible.

2.6.6 Scale-Dependent Dispersivity. Taylor's (1922) analysis (Section 2.6.2) showed that the rate of spreading of molecules grows with time or distance because of the molecules' velocity persistence. However, the rate reaches a constant value in a relatively short period of time and distance compared to the measuring capacity of our instruments. As a result, molecular diffusion can virtually be represented by Fick's law (equation 2.6.1) with a constant diffusion coefficient.

By the same token, the spreading of a tracer plume in homogeneous soil columns will grow with time and distance because of the persistence of fluid particle velocity. This velocity refers to the velocity of a volume of water that is much larger than many molecules but smaller than the size of a pore. However, the persistence diminishes due to changes in pore geometries and mixing with water from other flow paths as the volume of water moves through many pores. Since the size of pores in soils is small compared to the size of the REV of a soil column, the classic convection-dispersion equation with a constant dispersion coefficient (or constant dispersivity) is generally considered adequate to describe solute transport in homogeneous soil columns.

In field scale problems, the effects of heterogeneity on velocity variations are controlled by large-scale heterogeneities such as clay lenses, facies changes, and layerings of sediments. If we assume that by averaging the hydraulic properties, the field-scale aquifer is, in effect, homogeneous, and we use the dispersion concept to represent the effect of the heterogeneity on solute transport, we would expect the dispersion coefficient to grow with distance and reach a constant value at some distance, as in the molecular diffusion process predicted by Taylor (1922) and

observed in homogeneous soil column tests. However, a problem arises from the fact that the size of heterogeneities (such as clay lenses) at the field-scale is many times larger than the size of irregular pore channels in soil columns. The travel distance which is sufficient to allow the solute particles to "forget" the influence of the previous velocity may thus be many times larger than the size of clay lenses or layerings. Furthermore, this distance is generally much larger than the length of our field tracer experiments. As a consequence, the dispersivity values estimated from the field tracer tests seem to grow with travel distance or time (Figure 2.13). This phenomenon is known as the scale-dependent dispersion. It should be evident by now that such a scale-dependent dispersion is a result of the scale of heterogeneity, the scale of averaging, and the scale of observation.

Many theories accounting for the scale-dependent dispersion have been developed in the past decade for example; Gelhar and Axness, (1983), Neuman et al., (1986), Dagan, (1987), Matheron and De Marsily, (1980), etc. Field experiments to validate the theory of scale-dependent dispersivity in aquifer systems are currently in progress at several locations in North America, for example, at the Borden land-fill in Canada (Sudicky, 1986 and Feryberg, 1986) and in Mississippi, (Betson, et al. 1985).

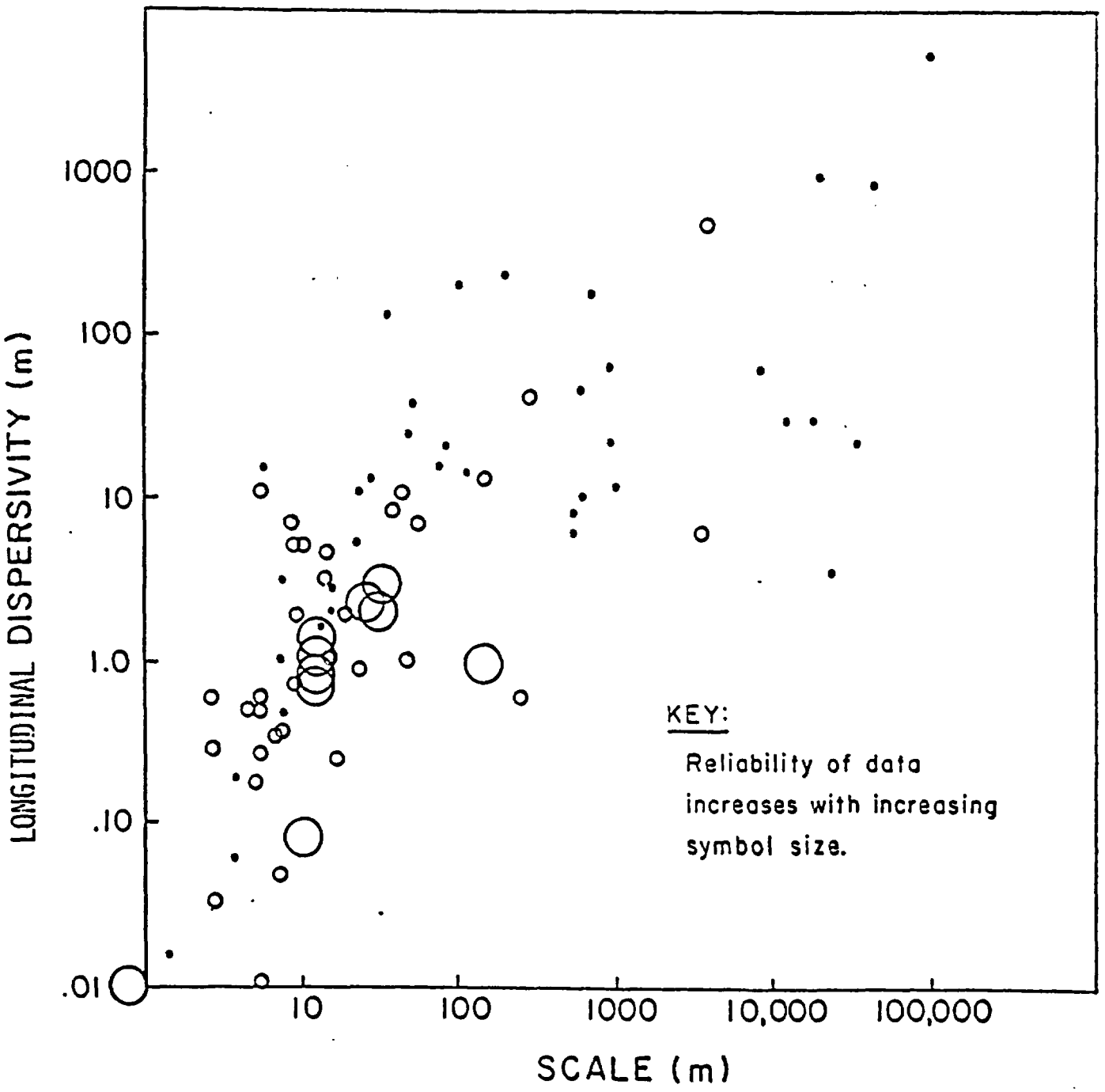


Figure 2.13. Data showing scale-dependent dispersivity (Gelhar, 1986).

2.7 Fracture Systems

In the previous sections of the review, we focused on laws and equations for flow and transport in porous media where large scale features such as fractures do not exist. Such media are representative of most aquifers which consist of unconsolidated sediments. However, most of the geologic materials at the proposed nuclear waste repository sites are generally consolidated sediments, volcanic or crystalline rocks. These geologic materials contain many fractures resulting from recent or past tectonic activities. Since groundwater flows through not only the rock matrix but also fractures, one certainly has to consider the effects of fractures in order to determine the groundwater travel times and paths in such geologic materials. Generally speaking, flow and transport phenomena in fractured rock are not as well understood and characterized as in porous media. This problem can be attributed partially to scale problems similar to those in porous media. That is, fractures are too small to be considered as discrete flow channels but too large to be considered as pore channels in porous media. In addition, the flow regime in fractures may vary from laminar to turbulent flow in which the classic groundwater flow equation based on Darcy's law is not valid. In the following sections, we will examine recent developments in conceptualization of flow and transport in such media under both saturated and unsaturated conditions.

2.7.1 Flow in Saturated Fractured Rocks. In fractured rocks, the size of a fracture is generally larger than the size of pores. The density of fractures at the macroscopic level, however, is much lower than the density of pore spaces. One has to enlarge the size of the REV defined for porous media in order to visualize fractured rock as a equivalent porous continuum at a large scale. In other words, the size of the REV for fractured rocks has to contain many fractures in the same way that the size of the REV for porous media must be much larger than many pores. Similarly, the detailed spatial distribution of individual fractures inside the

REV is ignored. However, if the knowledge of a detailed spatial distribution of fractures is available, and the behavior of flow in each fracture is what we are interested in, we may treat fractures as distinct flow channels embedded in a porous medium. The individual fracture is then visualized as a continuum with a smaller REV which ignores the much smaller scale flow channels within each fracture. Evidently, the size of the REV for individual fractures is not the same as that for the rock matrix.

Based on the discussion above, we can now classify the approaches of modeling flow and transport in fractured rocks into the continuum approach and the discrete approach. The continuum approach assumes that one can enlarge the REV so that the flow behavior in both the fracture and the porous matrix can be conceptualized as a flow system in an equivalent porous medium. This implies that the hydraulic properties of such an REV represents averages of the properties of the fractures and the rock matrix within the REV. Again, the detailed flow regimes in both fractures and rock matrix are ignored.

This continuum approach can be further divided into the single network approach and the double network approach. Such a division is necessary in fractured rock formations. In porous media, it is generally agreed that solids are impermeable and do not interact with the fluid in the void space. Thus, hydraulic conductivity is defined over many pores only. However, this may not be the case in a fractured rock system where both the fracture and the rock matrix are considered conductive. In a steady state flow situation, the conductivities of both the fractures and rock matrix may be represented by the notion of equivalent hydraulic conductivity. As a consequence, a single network approach is adequate. In this approach, a fractured medium is represented by a single network in which the hydraulic properties are averaged over both the fracture and the rock matrix. Thus, the general governing flow equation is written as:

$$\nabla\cdot(K\cdot\nabla h) = \frac{\partial S_s}{\partial t} \qquad (2.7.1)$$

where K, S_s, and h represent the average values of hydraulic conductivity, specific storage, and head over the fracture and the rock matrix within the volume of the REV, respectively. For steady state conditions, the right-hand side of equation 2.7.1 is zero. Although the hydraulic properties of such a REV are the averages over both the fracture and the rock matrix, they are dominated by the properties of fractures, and the influences of the porous matrix properties are negligible. (This is especially true for hydraulic conductivity, which is perhaps the most important property controlling groundwater travel time). Thus, this approach assumes that an equilibrium between the flows in both fractures and rock matrix exists, which may not be valid for most cases.

With the single network approach, one may conceptualize a large-scale fractured geologic formation as a heterogeneous continuum or a stochastic continuum if heterogeneities are represented by stochastic processes (Neuman, 1987). Because the volume over which the averaging takes place may contain several fractures and a vast number of pores in the rock matrix, the spatial distribution of the hydraulic properties thus becomes smooth and differentiable. The classic partial differential equations for flow in heterogeneous porous media can now appropriately applied.

In the transient state, owing to the relatively small storativity in fractures, the response of the fracture to pressure (or head changes) is much faster than in the matrix. The interaction between the fracture and the porous rock matrix becomes important. It therefore becomes necessary to define, inside the REV, two separate networks: one representing fractures and the other the rock matrix. Each network within the REV is considered a homogenous continuum. The spatial distribution of fractures or the rock matrix is not required to be specified within the REV. This

conceptualization is the so called double network or dual porosity model.

The double network approach has been used by many investigators such as Barenblatt et al. (1960), Warren and Root, (1963), Kazemi, (1969), Zhang, (1982), Huyakorn et al. (1983), and Moench (1984). The approach assumes that hydraulic responses of an REV result from two flow systems. One represents the flow in the rock matrix network, and the other the fracture network. Flow in each network is described by a governing flow equation. The influences of fractures on the flow regime in the rock matrix, or vice versa, are then entered as sink or source terms in the flow equations. More specifically, the governing differential equation for flow in the fracture network is assumed to be described by the classic groundwater flow equation with a source term to account for contributions from the matrix rock:

$$\nabla\cdot(K_f\cdot\nabla h_f) = \frac{\partial S_{sf}}{\partial t} + q \qquad (2.7.2)$$

where K_f is the hydraulic conductivity of the fractures, S_{sf} is the specific storage of the fractures, and h_f is the hydraulic head in the fracture network. These hydrologic properties represent averages over many fractures in the REV. The term q in equation 2.7.2 represents the contribution to or from the rock matrix. Similarly, for the rock matrix the governing flow equation is given as

$$\nabla\cdot(K_m\cdot\nabla h_m) = \frac{\partial S_{sm}}{\partial t} - q \qquad (2.7.3)$$

where K_m is the conductivity, S_{sm} is the specific storage, and h_m is the head in the rock matrix network, and q represents the contribution from or to the fractures and it is related to h_m and h_f. Generally speaking, this approach depicts the flow system better than the single network approach because the non-equilibrium interaction

between the rock matrix and the fracture is considered in the formulation of the governing equations.

Both single and double network approaches assume the medium is homogeneous within the REV. This assumption implies that the predicted flow behavior represents an average over the REV. For small-scale problems, this averaged approach may be of limited practical use and a discrete fracture approach may be necessary.

Many discrete fracture models for flow in saturated fractured media have been developed in the past few years (e.g., Huyakorn et al., 1983; Shapiro and Anderson, 1983; Elsworth, 1987; and Rasmussen et al., 1987). The discrete fracture approach is similar to the dual porosity approach. Both approaches treat the flow in fractures and the rock matrix as two separated systems with the exception that the discrete fracture approach assumes that an explicit knowledge of fracture distribution in the rock formation is available. Therefore, fractures are treated as a continuum in the same sense that a porous medium is a continuum representation of the interconnecting pore space. However, the REV for the fracture continuum is much smaller than the matrix. Generally, the parallel plate analogue is used to depict the flow in the fractures. The flow regime in the host rock is represented by the classic equations for flow in porous media. Since flow in the fracture and porous matrix may interact, these two flow regimes are not independent. Interaction is then entered through the coupling of the two equations, (2.7.2) and (2.7.3). However, the parameters in equation (2.7.2) represent hydrologic properties of individual fractures instead of averages over many fractures in the REV. An additional equation is then used to relate q to the heads in both the rock matrix and the fracture. In order to apply this discrete fracture approach to a field problem, the site has to be discretized into many rock matrix zones and fracture zones which are represented by either (2.7.2) or (2.7.3). As the number of zones increases, the number of equations (2.7.2)

and (2.7.3) increases accordingly. Solving such a large set of differential equations becomes a formidable task. This is one of the major drawbacks of the discrete fracture approach. However, if the flow in the rock matrix is steady, one may focus on the flow in the fracture system only. In this case, only the equation for the fracture network has to be solved. This may be an alternative to the double network discrete fracture approach.

2.7.2 Flow in Unsaturated Fractured Rocks. As mentioned previously, many flow and transport models based on the single or double network continuum approach and the discrete fracture approach have been developed for saturated fractured rocks in the past few years. However, models for flow and transport through unsaturated fractured rocks are rare. Existing models are based on the single continuum or discrete fracture conceptualization. No double network or dual porosity model has been developed. Available discrete fracture models for unsaturated fractured rocks generally use the single network approach without considering the interaction between the fracture and the rock matrix or assume some simplified flow system. This is mainly attributed to the inherent difficulty in the discrete fracture approach as discussed above, complexity of unsaturated flow, and difficulties in determining unsaturated hydraulic properties in fractured rocks. The complexity stems from the fact that unsaturated flow systems are generally nonlinear. The nonlinearity of the systems becomes even more severe due to the presence of the fractures, and high contrast in hydraulic conductivity between rock matrix and fractures.

An example of the application of this type of model is the work by Wang and Narasimhan (1985). They used the single heterogeneous continuum approach to simulate flow in a hypothetical, unsaturated fractured rock. A formula for calculating fracture conductivity under partially saturated conditions was developed. Saturated permeability of a fracture is assumed to be described by a generalized cubic law. Under partially saturated conditions, the effects of distortion of flow

paths by the air phase within a fracture plane were taken into account by a phase-separation constriction factor in the cubic law. The reduction of flow area in the plane was considered by summing the aperture distribution function to a saturation cutoff aperture, which is inversely proportional to the pressure head. Based on the theory and aperture distribution within fractures, they generated the fracture hydraulic conductivity-saturation, and saturation-suction curves for the densely welded tuff of the Topopah Spring Member at Yucca Mountain, southern Nevada. Moisture retention curves were measured from core samples. Using the relative permeability formula developed by van Genuchten (1980), and the retention curves, unsaturated hydraulic conductivity curves were estimated. These characteristic curves of fractures and porous matrix were then used to simulate the desaturation of a small fracture tuff column with discrete vertical and horizontal fractures with the aid of a computer model, TRUST.

The results of their study showed that the early transient changes from fully saturated conditions to partially saturated conditions were sensitive to fracture properties. However, the quasi-steady changes of the fluid flow of a partially saturated, fractured, porous system could be approximately simulated without taking the fractures into account. Peters et al. (1986), and Wang and Narasimhan (1985) derived the effective permeability of a partially saturated, fractured-porous medium and showed that the effective hydraulic conductivity was the sum of the fracture and matrix permeabilities weighted by the cross-sectional areas of the flow channels. They applied this effective continuum approximation to vertical infiltration problems.

Huang and Evans (1985) proposed a discrete fracture model to simulate flow and transport processes in three-dimensional fractured media. The model was developed to provide estimates of global hydraulic conductivity within a rock mass for specified distributions of fracture orientations, apertures, and densities. The model was also designed to calculate solute travel times and breakthrough curves.

However, the model assumed steady, saturated flow conditions, and used a piston flow approximation for simulating mass transport. The model later was extended with some simplified assumptions by Rasmussen (1987) for applications to variably-saturated fractured media. This was accomplished by defining a characteristic curve which related the total head within the fracture to a critical aperture using capillary theory. Also, an integrated air/water flow formulation was developed to explain hysteretic effects within the fracture rock network as the fluid potential changed. Finally, the ability to account for matrix diffusion of solutes into the walls of the fractures was added.

Neither the continuum nor the discrete fracture unsaturated flow models have been verified with either laboratory or field experiments. However, there is research in progress (e.g. at the University of Arizona) to characterize unsaturated flow in natural fractured rocks at laboratory scales. The results of this study may provide a means to verify the conceptual models discussed above. Other conceptual models with stochastic approaches (Yeh et al., 1985 a, b, and c) should be developed to improve our predictive capability related to flow through unsaturated fractured rocks.

3.0 GROUNDWATER TRAVEL TIMES AND PATHS

One of the NRC performance objectives for High Level Waste Repositories, commonly referred to as the "groundwater travel time (GWTT) objective," is stated in 10 CFR 60.113 (a)(2) as:

> "The geologic repository shall be located so that pre-waste-emplacement groundwater travel time along the fastest path of likely radionuclide travel from the disturbed zone to the accessible environment shall be at least 1,000 years or such other time as may be approved or specified by the Commission."

The definition of groundwater travel times and paths is not immune from the scale problems discussed previously. Generally speaking, groundwater travel path is known as the path along which groundwater travels. Consequently, groundwater travel time is defined as the time required for groundwater to travel along this path from one location to another. Mathematically, it is defined by

$$t = \int_0^x \frac{ds}{v} \tag{3.1}$$

where t is the groundwater travel time, x is the distance of the path which groundwater travels between the two locations, and v is the velocity of groundwater.

This definition seems to be quite clear, and, in fact, it is widely used by groundwater hydrologists. However, there are problems associated with this definition. First of all, what volume does the groundwater in the definition represent? Does it represent a cubic kilometer of groundwater, a cubic centimeter of groundwater, or maybe a molecule of the groundwater?

The need to define the volume of groundwater arises from the way the

groundwater velocity, v in equation (3.1), is determined in groundwater hydrology. As discussed in section 2.2, the continuum approach is the foundation of groundwater hydrology. That means we are not interested in, and in fact, are not able to determine how a volume of water smaller than a pore moves through intricately interconnected pore channels. Thus, the velocity of groundwater is defined over an REV which is much larger than many pores. If one can clearly define the size of an REV, the ambiguity in groundwater travel time and path may be partially resolved. However, the size of an REV may vary with the scale of heterogeneity which in turn depends on the scale of the problem that we deal with. The size of an REV may also depend on the scale of the hydrologic test we conduct to determine aquifer properties. Even if we could define an acceptable size of the REV, we may not be able to determine the exact manner in which a radionuclide travels, because the REV concept ignores the velocity variations smaller than the size of the REV. The velocity variation will cause some fluid or tracer particles to arrive earlier than the arrival time predicted from the average velocity for the REV. If we assume that the molecular diffusion is negligible, we may be able to define the REV to be several times larger than a molecule. If this is the case, then the groundwater travel time can be determined provided that the knowledge of the intricate pore channels is available. The question now is: how can one delineate the complex pore channels in a geologic formation over an area of 100 km^2? This approach is obviously impossible, and we are forced to characterize hydrogeologic properties at some scale which is much larger than the pore scale. However, the effects of the subscale velocity variations become more important as the size of the REV increases.

Based on the above discussion, pre-waste-emplacement groundwater travel times and paths are not clearly defined concepts. "The fastest path" described in 10 CFR 60.113 will vary with one's definition of scale. Therefore, the travel time criteria will be subject to interpretation and will be difficult to enforce. For

regulatory purposes, defining the occurrence of a threshold mass flux over a specified area of the accessible environment seems to be more appropriate. This is due to the fact that a concentration level reflects the total mass resulting from many different scale transport phenomena over a certain volume. Thus, the loophole in 10 CFR 60.113 can be eliminated. As a matter of fact, the fastest arrival of a certain concentration level at the accessible environment can be easily determined by application of the dispersion concept. The use of a cumulative concentration threshold is at the heart of the EPA criteria to evaluate the performance of a repository.

The NRC groundwater travel time criteria are specifically designed to pertain to pre-waste emplacement groundwater conditions. According to these criteria, the scale at which we want to delineate a flow path and characterize the hydraulic parameters appears to be arbitrary, but it is certainly less than 5 km. Whatever the scale chosen, it is essential to use consistent scales throughout the determination of the hydrogeologic parameters in the groundwater travel time equation. For example, it would not be appropriate to have a conceptual model in which the fastest path is along a sequence of voids in sandstone identified in thin sections and where the hydraulic conductivity is obtained from aquifer pumping tests which fully penetrate the sandstone. For practical purposes, the scale at which field measurements are made will limit the scale of the path that can be considered in the NRC travel time analysis. It does not seem reasonable to expect field investigations to result in characterization of single fractures or pore sequences as paths of likely radionuclide transport, at least over distance of 5 km. Although the volume of aquifer represented by a measurement is not known precisely, in most cases, the field measurement scale would seem to be on the order of meters or tens of meters. Therefore, paths of likely radionuclide transport will be one or more readily identifiable zones, such as layers within formations, major fault zones, or perhaps

entire formations. Stochastic methods would account for heterogeneity and travel time uncertainty within these paths.

3.1 Sources of Uncertainty in Predicting Groundwater Travel Times and Paths.

Regardless of the problems with the definition of groundwater travel time, we will assume that the groundwater travel time and path are defined for a specific size of an REV. We now will proceed to briefly discuss the sources of the uncertainty in predicting groundwater travel time and path. More in-depth discussion on this subject can be found in the paper by Bonano and Cranwell (1988).

To predict groundwater travel times and paths in geologic media, we first have to construct a conceptual model. The model generally simplifies the complex flow and transport processes in geologic media so that it can be represented with a tractable mathematical model. For example, flow through porous media is conceptualized as a continuum by the concept of the REV so that differential calculus applies. Continuum, discrete fracture, and dual porosity models are conceptual models which simplify the complex flow system in fractured rocks. Once the conceptual model has been formulated, it is then translated into mathematical expressions, usually partial differential equations with associated boundary and initial conditions. If the parameter values in the governing equations are well defined, analytical and numerical methods can then be employed to solve these equations for the flow system subject to any input stress. Once the flow behavior is determined, the travel time of groundwater can thus be calculated at a pre-determined scale of interest.

There is no uncertainty in groundwater travel times and paths themselves, but uncertainty in predicting them. If one uses the classic approach as outlined above to predict groundwater travel times and paths, it is evident that sources of uncertainties are attributed mainly to: (a) uncertainties in conceptualizing natural

processes, (b) uncertainties in mathematical models, and (c) uncertainties in data required by the mathematical model.

3.1.1. Uncertainty in Conceptualization. To describe groundwater flow in geologic media, we often rely on Darcy's law and the continuity equation. The law and the equation, as discussed earlier, are based on the concept of REV which is much larger than many pores. Thus, the law and equation are not strictly valid for groundwater flow through individual channels which are much smaller than the volume of an REV. Certainly, applying the REV concept for flow through individual pore channels will cause uncertainties in prediction. As an example, a heterogeneous aquifer can be conceptualized as effectively homogeneous by averaging the heterogeneities. As discussed in the previous section, the head determined from an equivalent homogeneous aquifer does not match the head from true heterogeneous one, unless a proper averaging procedure is used. Unquestionably, errors in conceptualization add uncertainties in prediction. Generally speaking, the major uncertainty in conceptualization lies in the area of flow through fractured rocks, especially flow through unsaturated fractured rocks. Although several conceptual models (such as discrete fracture, dual porosity, stochastic continuum approaches) have been proposed to conceptualize flow through fractured rocks, none of these have been verified with field experiments. Difficulties in monitoring flow behavior or in determining the fracture hydraulic properties of unsaturated, fractured rocks, even in the laboratory, further cast doubt on the validity of current conceptual models for flow through unsaturated, fractured rocks. Since there is no way to assess the validity of conceptual models at present, the uncertainty due to errors in conceptualization is entirely unknown.

3.1.2. Uncertainty in Mathematical Models. If one can somehow obtain a workable conceptual model or assume the uncertainty in the conceptualization of a natural flow process is negligible, the next source of uncertainty arises from the

formulation of mathematical equations based on the conceptual models and the solution of the mathematical model.

Uncertainties associated with the formulation of a mathematical model are generally attributed to mathematical simplifications during its formulation. For instance, neglecting the effects of fluid density gradients and changes in hydraulic conductivity due to deformation of porous media, and mixing expressions for moving and fixed coordinate systems (see Appendix B) causes uncertainties in the governing equation for three-dimensional groundwater flow. Similarly, the two-dimensional depth-averaged groundwater flow equation neglects the contribution from the product of hydraulic conductivity and head variations in the vertical direction (i.e., when horizontal flow is assumed). Stochastic models, such as those based on the first order analysis, (Gelhar and Axness, 1983, Dagan, 1987, Neuman, 1987, etc.) ignore higher order terms. All of these simplifications lead to uncertainties in mathematical models.

After a mathematical model is formulated, analytical methods often give exact solutions to a problem. However, the solutions are limited to simplified situations such as homogeneous aquifers of infinite lateral extent. More complex problems have to rely on numerical methods. No numerical method is completely error-free. Two basic types of errors which are inherent in a numerical computation are truncation and roundoff errors.

Finite difference, finite element, integrated finite difference, and boundary element methods generally are the numerical methods for solving groundwater flow and transport equations. They approximate the governing partial differential equations by a discrete formula; the solutions are thus subject to truncation errors. For instance, the finite difference groundwater flow model uses a Taylor series expansion to obtain the approximation of the head gradient:

$$\frac{dh}{dx} = \frac{h_{i+1} - h_i}{\Delta x} + O(\Delta x) \tag{3.2}$$

The term $O(\Delta x)$ represents the remaining higher order terms which are omitted in the formulation of the finite difference analog of the gradient. This type of error is called truncation error, since it is produced by truncating an infinite mathematical series. Numerical dispersion in the solution of a convection-dispersion equation is a typical result of the truncation error. In addition, a numerical analysis has to be conducted by a computational device such as a computer. The accuracy of the solution produced by the computational device depends on the number of significant figures available in the device. This type of error is called round-off error. These two sources of error add some uncertainties to the prediction of groundwater travel times and paths. Although these errors always exist, they can be minimized if a proper procedure such as small size grids, and small time steps is used.

The major problem associated with numerical models may lie in solving the governing equation of flow through unsaturated porous media or fractured rocks. The governing equation is generally nonlinear, i.e., the hydraulic properties in the governing equation, such as hydraulic conductivity, are functions of the dependent variable, so that the hydraulic property is unknown before the equation is solved. For nonlinear problems, an iterative scheme always must be used. There is no guarantee that the iterative scheme will give an exact solution or any solution at all. Furthermore, the nonlinearity of the equation becomes even more severe if the medium is heterogeneous, coarse textured, or fractured. Solutions often diverge, and in these cases no solution can be obtained (Freeze, 1971). If numerical solutions are obtained for complex problems, generally no exact analytical solution is available for assessing the accuracy of the solution. Thus, the uncertainty in mathematical modeling of flow in unsaturated porous and fractured materials is still a topic of

research.

3.1.3 Uncertainties in Data Required by Mathematical Models. Before mathematical models can be solved by either analytical or numerical methods, information about parameters in the equations, and boundary and initial conditions (for transient situations) must be specified. These parameters and conditions are generally tailored to physical or chemical properties of a specific site or geologic formation. The lack of a complete data base to characterize the properties of the site certainly introduces uncertainties in the solution of the mathematical models. This type of uncertainty is mainly a result of field heterogeneity.

In order to use any mathematical models to predict groundwater flow, values of the parameters and boundary conditions in the models have to be specified. These parameters include hydraulic conductivity, or transmissivity, storage coefficient, porosity, etc. If the aquifer is conceptualized as homogeneous, these parameter values should be easily obtained from a single hydraulic test. The aquifer can then be fully characterized. However, in reality, there is heterogeneity in aquifer hydrologic properties at all scales. For any field problem, virtually an unobtainable amount of data is required to completely specify the spatial distribution of these parameters everywhere in the aquifer. Only a limited amount of data will actually be available from a real site investigation. Furthermore, boundary and initial conditions are generally not clearly defined in most fields. For instance, recharge rate to groundwater reservoirs is generally difficult to measure, especially its temporal and spatial variability. Locations and types of boundaries are seldom known in field situations. Predictions based on few data values are thus characterized by uncertainty.

Incomplete information on the spatial distribution of the aquifer parameters also causes inconsistencies in the hydrologic data collected as inputs to mathematical models. The inconsistency in data is directly related to the scale problem discussed

previously. Hydraulic tests for determining hydraulic parameters of the aquifer material generally are aquifer tests, slug tests, or laboratory tests of core samples. Each of these tests determines the hydraulic properties of aquifer materials of different sizes. For example, the hydraulic properties determined from an aquifer test generally represents the effective properties of the aquifer material within the influence of the test. The zone of influence depends on the time scale of the aquifer test. Consequently, the hydraulic parameter values vary with the time and spatial scale of the test. On the other hand, the hydraulic parameter values obtained from a slug test may represent the properties of the aquifer material adjacent to the borehole. A laboratory test gives the value of the parameter for the size of the core sample. Thus, the inconsistent data set results in uncertainties in predictions.

Available field data for modeling groundwater flow are collected with various types of tests, and represent the parameter values of different sizes of aquifer material. It is inconsistent to use data collected from a test at one scale as input to a mathematical model at another scale to determine the groundwater flow. Furthermore, the size of grid used in the numerical model for a large basin generally exceeds by orders of magnitude the scale of hydraulic tests. Since aquifers are inherently heterogeneous, the parameter obtained from the hydraulic test may not be the representative one for the mathematical model. Such inconsistencies further augment the uncertainty in groundwater travel time and path predictions.

There is another problem regarding the use of data obtained from hydraulic tests as input to numerical models. Generally, the parameter values obtained from hydraulic tests represent effective properties of the area of influence. However, the effective properties may depend on the flow regime as well. For example, all hydraulic tests in boreholes involve radial flows. It is not known whether effective parameters estimated from radial flow tests in a heterogeneous aquifer are representative of parameter values for flow other than radial flow. It may not be

appropriate to input effective mean parameter values derived from radial flow into a numerical model to predict groundwater travel times and paths where uniform flow occurs.

Moreover, field heterogeneity introduces uncertainties in aquifer test data (Butler, 1986; Javandel and Witherspoon, 1969). The aquifer test is the standard method used by hydrogeologists to evaluate the transmissive and storage properties of subsurface material for groundwater resources evaluations. Driscoll (1986) and many others detailed the procedures for carrying out a successful test. Generally, the procedure is rather straightforward; a well is pumped, and water level responses are measured over space and time. The response data are then analyzed using methods based on analytical solutions to the problem of flow to a pumped well. The results from this analysis give us the transmissive and storage properties of the aquifer. The most common analytical solution used is the so-called Theis solution for confined-radial flow.

The Theis solution is derived for flow to a well in an extremely idealized aquifer. It is a mathematical model in which there are many simplifying assumptions, the major of which is the assumption that the aquifer is homogeneous. In fact, as pointed out earlier, aquifers are heterogeneous at all scales. Applying the Theis solution to a heterogeneous aquifer may, however, be justified if one replaces the heterogeneous aquifer by an equivalent homogeneous one. This substitution implies that parameters such as transmissivity and storage coefficient, obtained from the classical analysis of the aquifer test data should, therefore, represent the average values over the flow regime. As an example, based on numerical simulations of flow to a pumped well in a stratified aquifer, Javandel and Witherspoon (1969) concluded that the drawdown observed at any location in the aquifer virtually converges to the Theis solution at large times. This implies that the hydraulic conductivity estimated from the Theis solution corresponds to the arithmetic mean of the hydraulic

conductivity values of individual layers. In a perfectly stratified, confined aquifer, the drawdowns under steady state flow, at all the depths at a given radial distance must be the same because of constant head boundary conditions imposed at the well and at large distances. This analysis is identical to the soil column analysis where flow is parallel to the layering (section 2.4.1). Thus, it is clear that the effective hydraulic conductivity is the arithmetic mean. The results of their study are, however, not realistic because aquifers are generally not perfectly stratified.

Recent numerical experiments by Butler (1986) considered transmissivity as a stochastic field. In contrast to the finding of Javandel and Witherspoon (1969), Butler indicated that the geometric mean is a good approximation of the effective transmissivity obtained from aquifer tests in heterogeneous aquifers, if the drawdown in a fully penetrating well at large times is used. However, most observation wells do not fully penetrate the thickness of the aquifer. The head observed in a well tapped into a small portion of a thick heterogeneous aquifer does not represent the depth-averaged head (or the ensemble averaged head, if ergodicity is assumed). In section 4.3.1 (Figures 4.15 a, b and 4.16a) we will clearly illustrate this point. Figure 4.15a and b are the head distributions in two possible heterogeneous aquifers, and the head distribution in an equivalent homogeneous aquifer is shown in Figure 4.16a. Thus, the results of these studies are not conclusive. Regardless of exact type of average the effective hydraulic conductivity or transmissivity represents, the Theis solution based on these averaged aquifer properties predicts the drawdown in the equivalent homogeneous aquifer. Certainly, this drawdown does not correspond to the actual drawdown in the real aquifer which is heterogeneous, even if the head is a depth-averaged one. The drawdown determined from the Theis solution simply represents the average (ensemble average) of all possible drawdowns at a given radial distance in a plane. This concept is well illustrated in Figure 3.1 where dashed lines represent the actual irregular drawdown as may be expected in a heterogeneous

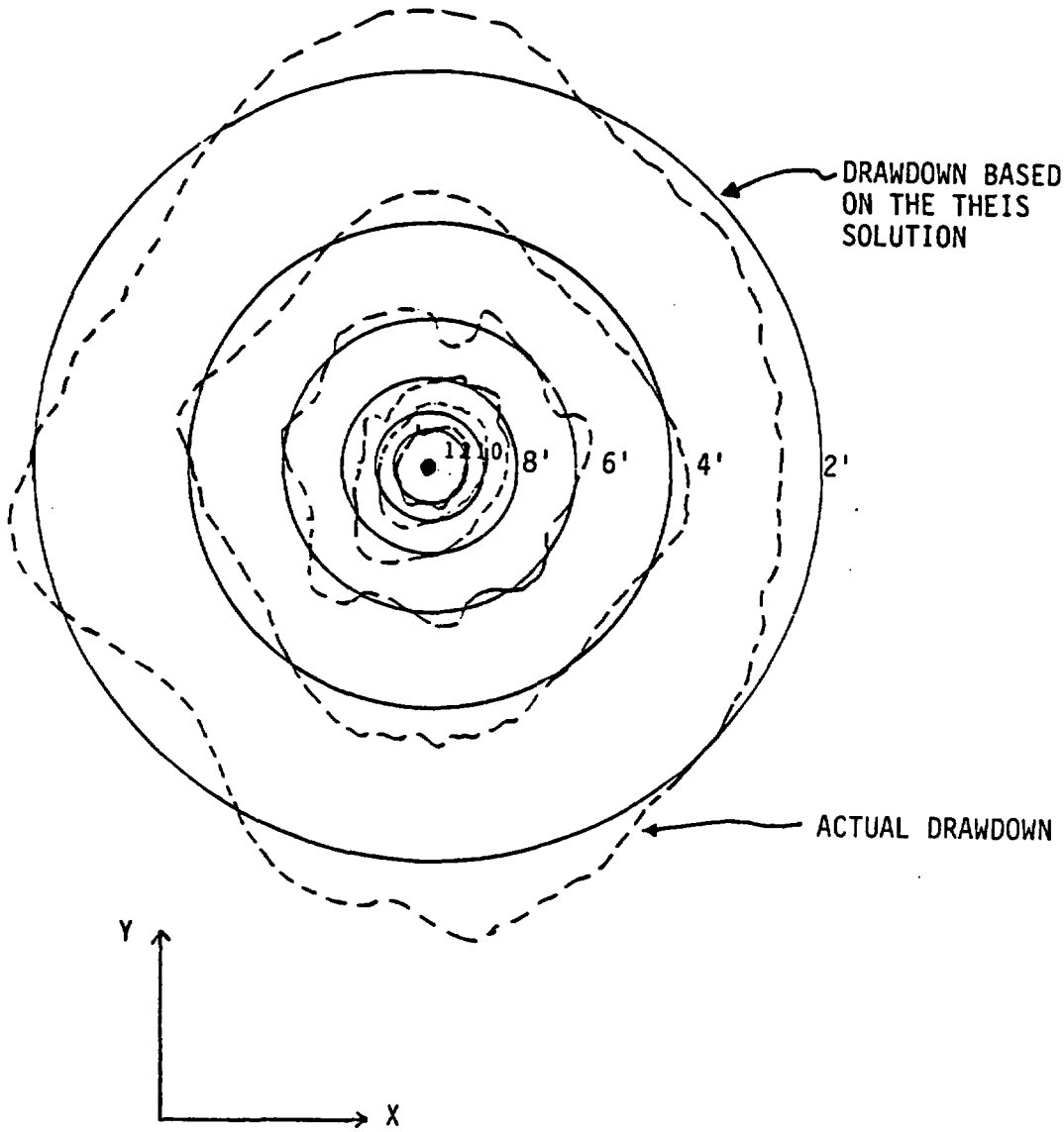


Figure 3.1. Plan view of the actual drawdown in a heterogeneous aquifer (dashed line) and the drawdown predicted from the Theis solution for an equivalent homogeneous aquifer (solid line). Dot shows the location of the pumping well.

aquifer, and solid lines represent the average drawdown. If one recognizes these limitations, then the application of the Theis solution to heterogeneous aquifers is appropriate in theory.

Limitations of the equivalent homogeneous aquifer concept are generally not well recognized. As a consequence, most procedures to analyze the aquifer test data are inconsistent with the theory. Again, if a heterogeneous aquifer is visualized as an equivalent homogeneous one, the drawdown predicted by the Theis solution should represent some kind of spatially averaged piezometric surface or drawdown at a radial distance. On the other hand, if one applies the Theis method to determine transmissivity and storage coefficient values of a heterogeneous aquifer, one has already replaced the heterogeneous aquifer by an equivalent homogeneous one. Thus, to be theoretically consistent, the spatially averaged drawdown from a very large number of observation wells at a given radial distance should be used to determine the aquifer properties. These properties should then represent the true effective properties of the equivalent homogeneous aquifer. However, there are only a limited amount of observation wells available in most field tests. As a matter of fact, many of the tests may have only one observation well. The drawdown observed in a single well does not necessarily represent the average drawdown at a certain radial distance, unless the aquifer has an uncorrelated random or statistically independent hydraulic conductivity field (for the definitions of the statistic terms, see section 4 or Appendix A). In these two cases, one may assume that the vertically averaged head value may be equivalent to the horizontally averaged one. Many recent field data have, however, shown that the hydraulic conductivity data in aquifers exhibit statistical anisotropy (layering). The transmissivity and storage coefficient values determined by the Theis solution with the drawdown data at a single well are thus not the effective ones. Therefore, a logical question one may ask is: What do the estimated transmissivity and storage coefficient values from the well hydrograph at a

single well represent? How much do the estimated values deviate from the true values? Are they reliable parameter values for determining the groundwater travel time and path?

Inconsistencies in interpreting aquifer test data have long been recognized. However, hydrogeologists have ignored these inconsistencies and still perform the analysis with the hydrograph from a single well. This is due to the fact that the estimated transmissivity and storage coefficient values, even though they may be erroneous, generally produce reasonably accurate piezometric surfaces or drawdowns. This surprising result may be attributed to the fact that the variation in head is relatively insensitive to the variation in T values. The groundwater system as far as head and T are concerned, is a filter. The error in T estimates is always damped out, and the calculated head using incorrect T values is often still in close agreement with the observed one. This filtering effect in groundwater systems has been clearly manifested in the results of stochastic analyses of groundwater flow through heterogeneous aquifers (Bakr et al. 1978; and Mizell et al. 1982). On the other hand, in an inverse problem (such as estimating T and S values using head data from aquifer tests), a tiny error in head or drawdown values may result in a significant departure of T values from the true one. Many hydrologists have experienced this type of problem. For instance, significantly different T estimates can be obtained by several groundwater hydrology experts using the same well hydrograph and the same procedures. Regardless of the significant differences in T values, the drawdown predicted with these T values is surprisingly close to the true drawdown value due to the damping effect. Therefore, one may draw the conclusion that the standard aquifer test analysis using one well may be adequate for the purpose of evaluating the well yield or drawdown of water levels. However, note that the primary interest in this case is the drawdown or head.

In the case of determining contaminant movement or groundwater travel time

and path in a groundwater system, the major controlling factor is not the hydraulic head but the hydraulic conductivity or transmissivity value, and the hydraulic gradient. Velocity of groundwater flow is determined by Darcy's law and is the product of conductivity, gradient and the reciprocal of the porosity. The variation in porosity and gradient are relatively small compared to the variation in conductivity. Therefore, the accuracy of predicted groundwater velocity may depend heavily on correct hydraulic conductivity or transmissivity values. An accurate prediction of groundwater velocity thus dictates correct estimates of transmissivity values from the standard aquifer test procedure.

Other sources of error are those due to instrument or human errors in estimating hydraulic parameters, even for a homogeneous aquifer. These types of errors could enter the modeling process and add uncertainty to the prediction of groundwater travel times and paths.

Of course, there are many other sources of errors in the prediction of groundwater travel times and paths which have not been discussed in this review. Generally speaking, sources of uncertainty in predicting groundwater travel time and path include: (a) uncertainties in conceptualization, (b) uncertainties in mathematical models, and (c) lack of a complete data base to characterize the variability of aquifer materials. For saturated porous media, uncertainties due to the errors in conceptualization and mathematical models are relatively small at the laboratory scale, or at least, it is believed their importance is relatively minor. This conclusion is supported by the fact that many small-scale laboratory experiments in the past have demonstrated the validity of mathematical models. Therefore, the major difficulty in the prediction of groundwater travel time in saturated porous media seems to lie in extrapolating these models to large-scale field problems where hydraulic properties of the aquifer materials vary spatially.

To predict groundwater travel times and paths in unsaturated, fractured

rocks, all of the sources of errors discussed above may play very important roles. This postulation stems from the fact that there is no satisfactory technology for measuring hydraulic properties for this type of material, because of the complexity of unsaturated flow and the scale of fractures. The lack of a demonstrated effective measurement technology hinders the development a workable conceptual model for flow in these complex types of media. Although there may have been some conceptual models (such as Wang and Narasimhan, 1985) developed in the past, none of them have been verified even with laboratory experiments, because of the difficulties in the development of a proper monitoring tool. If we can not verify the conceptual model in a small-scale laboratory experiment, we can not make predictions in field situations where the hydraulic properties of fractures and rock matrix are highly variable. In view of these difficulties, there are large uncertainties in predicting groundwater travel times and paths in unsaturated and fractured rocks.

Finally, "the groundwater travel time" and "the fastest path" as described in CFR 60.113 are not clearly defined concepts. Even if all the sources of uncertainties in predicting groundwater travel and path discussed above are identified and resolved, the GWTT criterion would vary with one's definition of scale; it will be subject to interpretation and will be difficult to enforce. As suggested in this report, defining the occurrence of a threshold mass flux over a specified area of the accessible environment is more appropiate for regulatory purposes. Unless this problem is clarified, uncertainty in groundwater travel time will always exist.

4.0 APPROACHES TO SPATIAL VARIABILITY

As discussed in section 3.0, spatial variabilities (heterogeneities) of geologic materials at various scales present difficulties for us to extrapolate our mathematical models to large-scale field problems. Therefore, spatial variability is the major source of the uncertainty in predicting groundwater travel times and paths. If the field heterogeneity problem can be resolved, the uncertainty in groundwater travel time and path prediction can be significantly reduced.

One approach to determine groundwater travel times and paths in a heterogeneous groundwater basin is to use the concept of REV. If one can define an REV that is large enough so that the entire aquifer within the accessible environment can be visualized as homogeneous, the mean groundwater travel time and path can then be determined through a deterministic simulation. However, this groundwater travel time represents only the average arrival time of groundwater particles and does not depict arrival times of groundwater particles along either the fastest or the slowest path, owing to variations in hydrologic properties at scales smaller than the size of REV.

To include the subscale variability, one must incorporate the dispersion process as discussed previously. However, this approach is not immune from scale problems. One of the problems is how to define an REV for effective (mean) hydrologic properties of the aquifer. More precisely, how can the effective hydraulic conductivity and dispersivity values be determined from hydrologic tests performed at a particular scale? Although a well controlled, large-scale hydraulic test (aquifer test) seems to be appropriate for this purpose (Williams, 1988), we do encounter problems. We must determine how to design such tests and how to analyze the data (see

Section 3.1.3, and Williams, 1985). Dispersivity values must also be determined. While a large-scale tracer test is desirable, the time, physical, and economic constraints of such a test make this approach impossible.

An alternative is to conduct many small-scale hydrologic tests to delineate spatial distributions of hydrologic properties at a specific scale of our interest (i.e., the size of our sample). Knowing the detailed spatial distributions of the properties, a deterministic model can adequately simulate a groundwater travel time and path distribution for fluid particles leaving the disturbed zone of a repository under pre-waste emplacement under given conditions. Such a simulated groundwater travel time distribution contains information about travel times pertaining to fast and slow paths of groundwater movement at the scale of our interest. However, the scale of the field problem, for example, the accessible environment (5 km), is generally much larger than the scale of our sampling device (i.e., an observation well is consider as a point compared with the accessible environment). To predict a groundwater travel time distribution from data collected at the scale of our instruments would require enormous manpower, time, and expense to collect information for such a degree of spatial resolution. Therefore, this deterministic approach is considered impractical in terms of the amount of data required to specify the actual complex three-dimensional heterogeneity. Thus, one has no choice but to use a limited amount of data to determine the groundwater travel time and path. Uncertainties always exist in the prediction, and an assessment of the uncertainties in predictions is necessary. However, the deterministic approach provides only one possible outcome from a given data set. It does not produce many possible groundwater travel times and paths resulting from many possible hydrologic properties at unsampled locations, and thus one can not evaluate the precision of the predictions.

Recent advances in stochastic groundwater hydrology and geostatistics have shed light on resolving the uncertainty problems due to spatial variability. In the

following sections, we will discuss the necessity of characterizing heterogeneity in terms of statistics, and will discuss methods to quantify the uncertainties in our predictions of hydrologic responses of groundwater systems due to field heterogeneity.

4.1 Stochastic Representation of Hydrologic Properties

Large-scale hydrologic tests to obtain the effective hydrologic properties at the scale of the accessible environment may be problematic and impractical. Accurate prediction of groundwater travel times and paths in a field-scale problem requires a large set of data obtained from small-scale tests. On the other hand, it is practically impossible to obtain such a large data set. So, a logical question to ask is: how can we obtain a meaningful or useful prediction using a limited amount of available data? Two approaches to address this question are to: (1) use effective hydrologic parameters derived from averaging the available data to predict the mean behavior of the aquifer and the deviation of the behavior from its mean, or (2) interpolate or extrapolate hydrologic parameter values measured at sample points to the locations where no measurements are available.

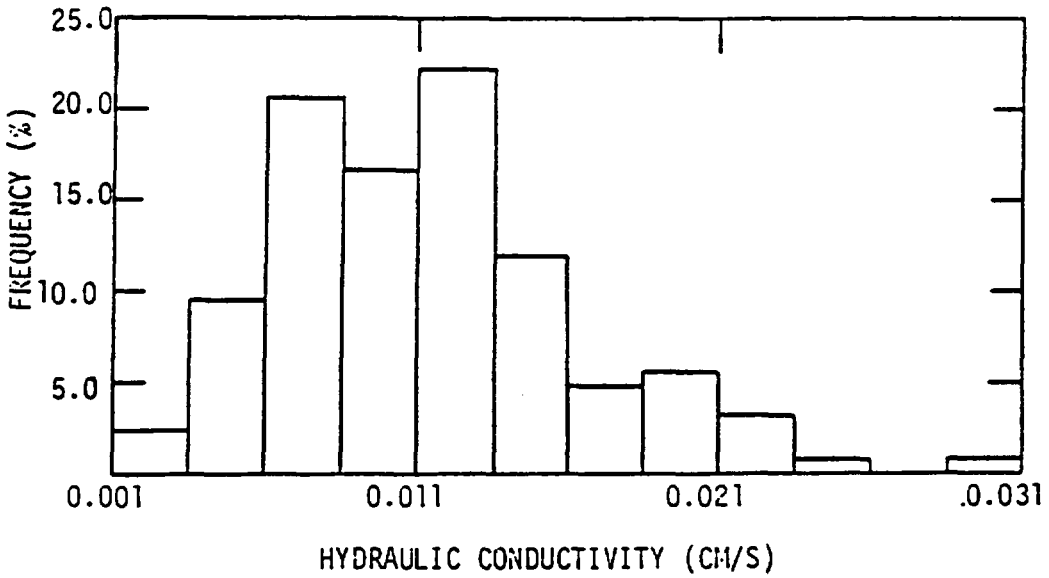
In the first approach, the effective properties are derived using theoretical formulas to combine data from small-scale tests. For example, the effective hydraulic conductivity of a layered aquifer can be determined from conductivity values of individual layers, using either harmonic or arithmetic means as discussed in Section 2.4.1. This approach is equivalent to the large-scale test approach but differs in the way that effective properties of an aquifer are derived. For instance, the large-scale test approach relies on observed responses of an aquifer and simplified equations, such as for instance, the Theis solution.

The second approach is similar to the small-scale test approach, but property values are estimated at unsampled locations by mathematical tools such as Kriging or

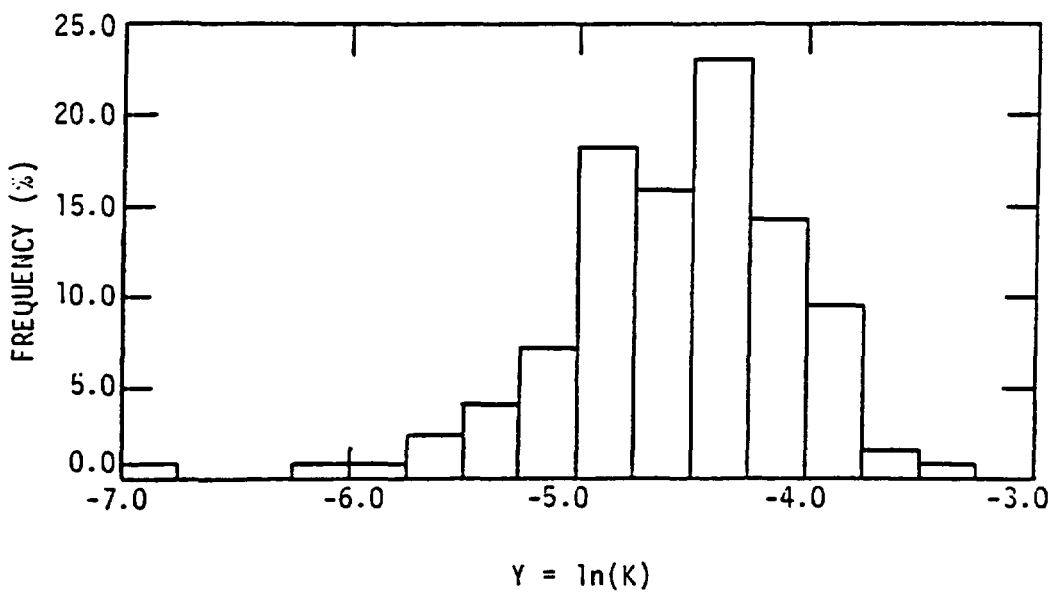
regression. However, the estimates are not exact and an evaluation of the deviation from the "true values" is required. Theories for both approaches require statistical information of the parameter values. This means that a statistical description of aquifer heterogeneity is necessary.

The statistical description of aquifer heterogeneity implies that hydraulic properties of the aquifer are viewed as random variables. Generally speaking, a random variable is a function whose values are real numbers and depend on "chance" or probability. To illustrate the application of the random variable concept to spatial variability of groundwater hydrology, let us consider the problem of estimating the hydraulic conductivity at a location where we have no experimental means to determine the hydraulic conductivity value. The value of hydraulic conductivity at this location may be guessed by examining the texture or other characteristics of drill cutting samples. Obviously, a variety of values may be assigned to the sample by different groundwater hydrologists. If we summarize all of the estimates by plotting the number of estimated values falling in different intervals, we observe a distribution (frequency distribution) of the guessed hydraulic conductivity values. As shown in Figure 4.1a, most values are clustered around some central value, and the frequency of occurrence declines away from this central point.

The random variable concept can also be interpreted in the following way. There are many different hydraulic conductivity values in a heterogeneous aquifer. If the hydraulic conductivity value at a location is unknown and we have to guess a value from all the possibilities, the chance of selecting a particular hydraulic conductivity value, K_i, may be expressed as the ratio n_i/n. n_i is the number of hydraulic conductivity values in the entire aquifer, which equal to K_i, and n is the total number of all possible hydraulic conductivity values in the aquifer. A plot of the probabilities of selecting different hydraulic conductivity values versus all the



(a)



(b)

Figure 4.1. Frequency distribution of (a) hydraulic conductivity, and (b) lnK data in the Borden aquifer (Sudicky, 1986).

possible hydraulic conductivity values is called a frequency or probability distribution of the hydraulic conductivity of the aquifer. Based on this conceptualization, the hydraulic conductivity value depends on probability or chance. Namely, it is not completely predictable: only proabilities can be associated with the possible values and hence the values are considered as realizations of a random variable. The frequency distribution determines the likelihood (or probability) that a specific hydraulic conductivity value will be found at a particular location.

Frequency distributions of most hydrologic properties of an aquifer generally are taken to be either normal or lognormal. A normal distribution is characterized by a symmetric bell shape. Lognormality implies that the distribution of the logarithms of a random variable has a normal distribution (Figure 4.1b). However, the distribution of a log-normal random variable itself is positively skewed (Figure 4.1a). Many field data have shown that the distribution of porosity data in a given aquifer is usually normal (Law, 1944 and Bennion and Griffiths, 1966), altough recent work by Hoeksema and Kitanidis (1985) suggests that the storage coefficient may be log normally distributed. Hydraulic conductivity data are usually reported to be approximately lognormal (Law, 1944; Bulness, 1946; Warren et al., 1961; Bennion and Griffiths, 1966; Ilyin, 1971; Bakr, 1976, and Freeze, 1975), as are transmissivity values (Delhomme, 1979; and Hoeksema and Kitanidis, 1985). There are exceptions however, as shown by Jensen et al., (1987). Figure 4.1 shows a skewed distribution of hydraulic conductivity values in a sandy aquifer and a more normal distribution of natural log of the hydraulic conductivity values, lnK.

Inasmuch as different aquifers are formed by different geologic processes, the distributions of hydrologic properties of different aquifers are likely to be different. To characterize the distribution one generally uses statistical moments of the random variable. The first moment refers to its mean, the second moment to the variance (the spread of the distribution) and the third moment to the skewness (a

measure of its symmetry). Figure 4.2 schematically illustrates distributions of the logarithms of hydraulic conductivity values in a sandstone and a shale unit. Although the hydraulic conductivity distribution of the two geologic materials is lognormal, the mean hydraulic conductivity value of the sandstone unit is larger than the shale unit and the variance is larger in the shale than in the sandstone.

The application of the random variable concept to hydraulic conductivity values seems to be valid only if no actual measurement of the parameter value is available. However, it is suitable for analysis of uncertainty in hydrologic property values. Even if one can determine hydrologic property values at every point in an aquifer, due to spatial variability of the property it is still appropriate to consider the hydraulic conductivity value as a random variable at the location. That is to say, the value represents only one of many possible geological materials that may have been deposited at a given point when the geological environment was created. This random variable concept can certainly be applied to other sample locations. Thus, hydraulic conductivity values of an aquifer may be considered as a collection of many random variables in space. This infinite sequence of random variables is generally referred to as a stochastic process (or a random process, random field or random function).

For example, the set of hydraulic conductivities along a transect can be considered as one possible outcome of a stochastic process. In a stochastic process the value of the quantity, say conductivity, $K(x)$, is a random variable for each location x. Namely, if conductivity is observed at locations x_1, x_2,....x_n, the $K(x_1)$ is a random variable, $K(x_2)$ another random variable, and so on out to $K(x_n)$. 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 transect depends not only on the probability distribution of the hydraulic conductivity at one location but also on those at other locations. This

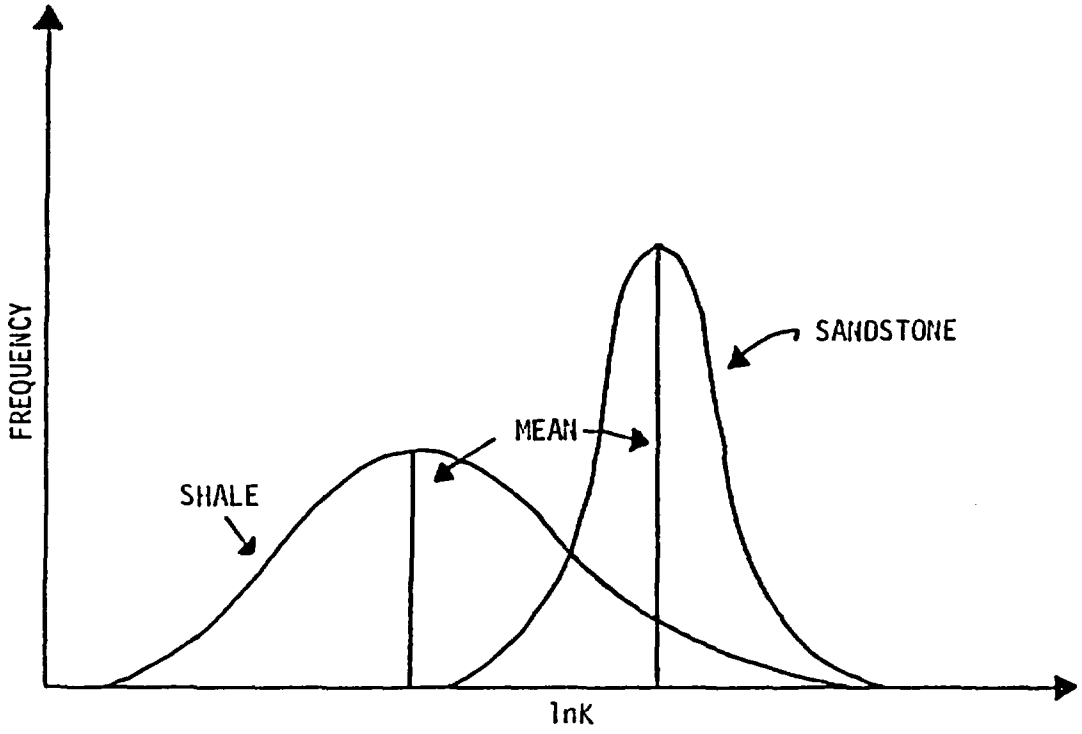


Figure 4.2. Frequency distributions of the hydraulic conductivity values of a sandstone and a shale unit.

implies that actual hydraulic conductivity values, along the transect are one possible sequence of K(x) out of all the possible sequences. In the vocabulary of stochastic processes, all these possible sequences are called an ensemble, and a realization refers to one of the possible sequences (Figure 4.3).

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. The joint distribution is completely defined only if the probabilities associated with all possible sequences of $K(x_i)$ values along the transect are known. Similar to the distribution of a single random variable, the joint distribution of random variables is also characterized by its moments. However, this joint distribution is seldom known in real-life situations because hydraulic conductivity values sampled along a transect, for instance, represent only one realization out of the ensemble of the hydraulic conductivity values along the transect. Therefore, one must usually resort to simplifying 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 (De Marsily, 1986). Since in reality one always deals with a specific geologic formation (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.

Because it is difficult to obtain all of the joint distributional information required and because in many cases important properties are assessed by moments like the mean, variance or other lower order moments, an assumption of weak or second order stationarity is often invoked. The first moment (mean) of K(x) is defined as:

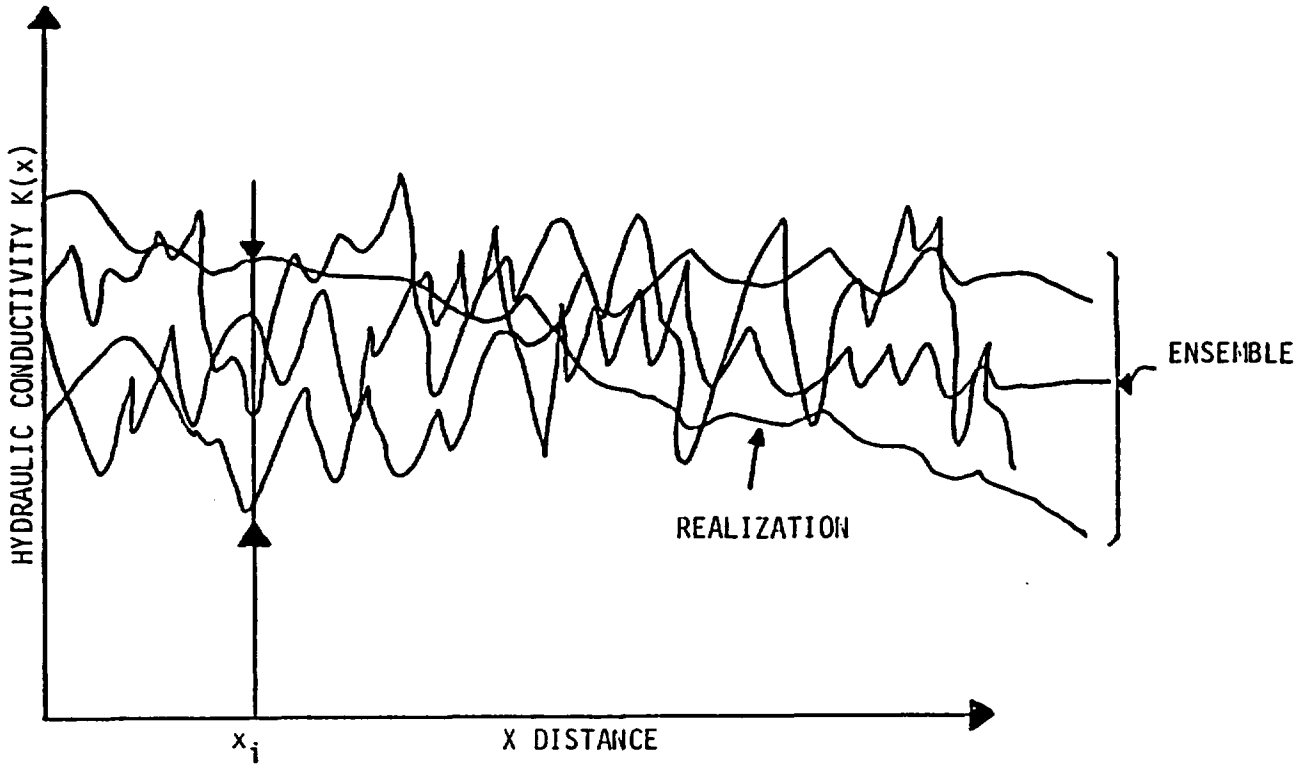


Figure 4.3. Schematic illustration of ensemble and realization concepts. Hydraulic conductivity at x_i is a random variable.

$$\mu = E[K] = \int_0^{\infty} K\ f(K)\ dK \tag{4.1.1}$$

where E[ ] stands for the expected value, and f(K) is the joint density distribution of K. This means that the expected value of a stochastic process is its probabilistic average (or ensemble average). The second moment (autocovariance or covariance function) is then defined as:

$$c(\xi)=\text{cov}\ [K(x+\xi),\ K(x)] = E[\ (K(x+\xi)-\mu)(K(x)-\mu)\ ] \tag{4.1.2}$$

The second-order stationarity assumptions are that (i) $\mu = E[K]$ is constant, and $\text{cov}[K(x+\xi),\ K(x)]$ only depends on ξ, (i.e., $c(\xi) = \text{cov}[K(x+\xi),K(x)]$) where ξ is called the separation distance. If the separation distance is set to zero, the covariance function becomes the variance, σ^2 . An autocorrelation function is simply defined as the ratio of covariance function to its variance, i.e.:

$$\rho(\xi) = \frac{c(\xi)}{\sigma^2} \tag{4.1.3}$$

Values of the autocorrelation function are always in the range between -1 and 1. The autocorrelation function represents the persistence of the value of a property in space.

To explain the idea of the autocorrelation function, we will consider two identical sine waves, w(x)=sinx, except they are separated by a distance ξ as shown in Figure 4.4a. Note that the sine waves are strictly deterministic functions. If a correlation coefficient, r, between these two waves is calculated, by regression

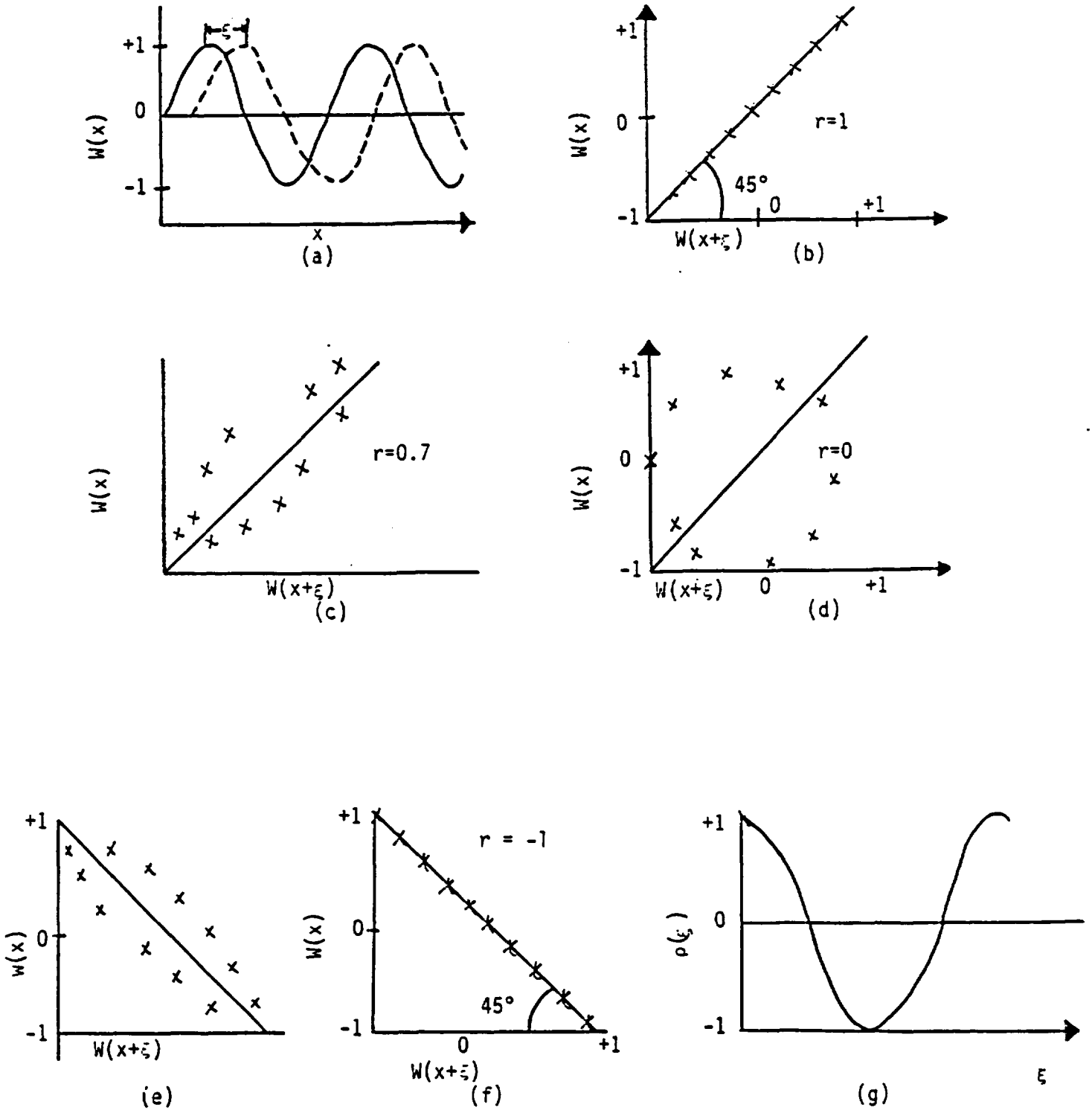


Figure 4.4. Diagrams to illustrate the concept of an autocorrelation function.

analysis, r has to be 1 if $\xi = 0$; if w(x) is plotted against $w(x+\xi)$ at $\xi = 0$, all the points will lie on a 45 degree line since they are identical (Figure 4.4b). As one of the waves is shifted by a distance $\xi \neq 0$, the plot of w(x) vs. $w(x+\xi)$ will start to scatter around the diagonal line as shown in Figure 4.4c. The correlation becomes less than unity because the values of the waves no longer correspond at every distance. As the wave moves out of phase exactly by one half of a wavelength, the scattering become even more significant and the correlation drops to zero (Figure 4.4d). This zero correlation indicates that the points of the two waves at this separation distance are completely different. Figure 4.4e shows that a further increase of the separation distance will reduce the scattering but the correlation becomes negative. As the separation distance approaches one half wavelength, i.e., the trough of one wave matches the peak of the other, and the correlation drops to -1 (Figure 4.4f). This r = -1 value implies that these two waves are identical but in an opposite manner. If one plots the r values at each separation distance vs. the separation distance, one obtains a plot of an autocorrelation function (Figure 4.4g). Therefore, the autocorrelation function is a measure of the similarity of the series at different separation distances.

Generally, the autocorrelation function of hydraulic conductivity data tends to drop rapidly as the separation distance increases. The decline of the correlation may be represented by many different autocorrelation models. The one commonly used is an exponential decay model (Bakr et al., 1978; Gutjahr et al., 1978, Gelhar et al., 1979, Yeh et al., 1985a, b, c):

$$\rho(\xi) = \exp\left[-\frac{\xi}{\lambda}\right] \tag{4.1.4}$$

where $\rho(\xi)$ is the correlation function, ξ is the separation distance, and λ is the

correlation scale. The correlation scale is a characteristic length beyond which the correlation between data is no longer considered significant. However, this definition is rather arbitrary and an integral scale is often used instead. The integral scale is defined as the area under a autocorrelation function if the area is a positive and nonzero value (Lumley and Panofsky, 1964). For the exponential model (equation 4.1.4), the integral scale is a separation distance at which the correlation drops to the exp(-1) level. At this level, the correlation between data is considered insignificant. That is, the data points separated by distances larger than the correlation scale are only weakly associated with each other.

On an intuitive basis, the correlation scale may be interpreted as the average length of clay lenses or sedimentary structures. Hydraulic property values of the 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 the spatial structure of hydrologic parameters. Table 1 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 pumping tests. We must point out that there has been very little published research to confirm the geologic significance of the correlation length (Byers and Stephens, 1983; MacMillan and Gutjahr, 1986).

For the sake of simplicity, the above discussion on autocorrelation function is restricted to one-dimensional data (i.e., data collected along a transect). The concept can be applied to a two- or three-dimensional data set as well. For example, a commonly used three-dimensional exponential autocorrelation function in groundwater hydrology is:

Table 1. Variances and correlation scales for log hydraulic conductivity or log transmissivity (Gelhar, 1986).

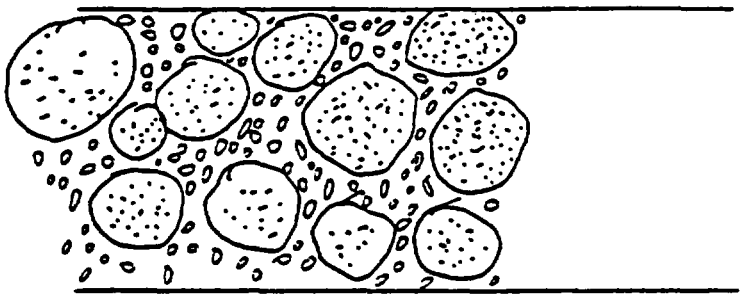
Source	Medium	σ_y^2	Correlation Scale, m	Overall Scale, m
Bakr [1976]	sandstone aquifer	1.5–2.2	0.3–1.0 V	100
Smith [1978]	outwash sand	0.8	0.4 V	20
Delhomme [1979]	limestone aquifer	2.3	6300 H	30,000
Binsariti [1980]	basin fill aquifer	1.0	800 H	20,000
Russo and Bressler [1981]	Hamra Red Mediterranean soil	0.4–1.1	14–39 H	100
Luxmoore et al. [1981]	weathered shale subsoil	0.8	< 2 H	14
Sisson and Wierenga [1981]	silty clay loam soil (alluvial)	0.6	0.1 H	5
Vieira et al. [1981]	Yolo soil (alluvial fan)	0.9	15 H	100
Delary and Doctor [1982]	alluvial aquifer (flood gravels)	0.8	820 H	5,000
Byers and Stephens [1983]	fluvial sand	0.9	0.1 V > 3 H	5 14
Hoeksema and Kitanidis [1985]	sandstone aquifer	0.6	45,000 H	5×10^3
Hutschmied [1985]	sand and gravel	1.9	0.5 V	20
Sudicky [1985]	outwash sand	0.6	0.1 V	20

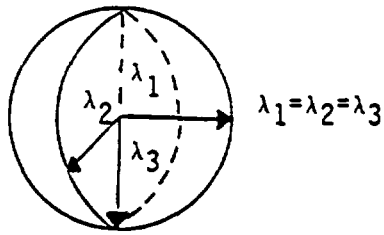
Correlation scales based on e^{-1} correlation distance: H, horizontal sampling, V, vertical sampling.

$$\rho(|\xi|) = \exp\left\{-\left[(\xi_1/\lambda_1)^2 + (\xi_2/\lambda_2)^2 + (\xi_3/\lambda_3)^2\right]^{1/2}\right\} \tag{4.1.5}$$

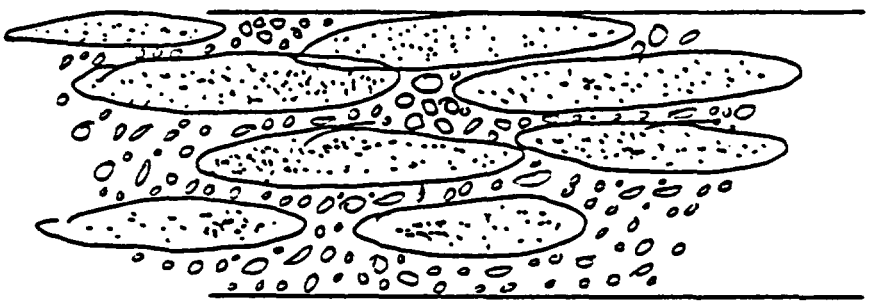
where ξ is the separation distance, and ξ_1, ξ_2, and ξ_3 are separation distances in x, y, z directions, respectively. Integral scales in the x, y, and z directions are λ_1, λ_2, and λ_3, respectively. If the integral scales are the same in all directions, then the stochastic process is called a statistically isotropic process. If these values are different, then it is called a statistically anisotropic process. Note that statistical isotropy and anisotropy are different from hydraulic conductivity anisotropy in classical hydrology. Statistical anisotropy simply implies that the hydrologic property (such as hydraulic conductivity) of an aquifer is correlated for a longer distance in one direction than in other two directions. For instance, in a perfectly stratified aquifer (e.g. laterally continuous "layer cake" sedimentary sequence), correlation scales in the horizontal directions are likely to be the same, but they will be much longer than the correlation scale in the vertical direction. This is due to the fact that within each layer, the material is considered to be effectively homogeneous. A short vertical correlation scale reflects a rapid lithologic change in the vertical direction. In Figures 4.5a and b, statistically isotropic and anisotropic aquifers are schematically illustrated. Figure 4.5c depicts an ellipsoid formed by anisotropic correlation scales. Hydrologic property values within the ellipsoid are considered correlated or similar, and those outside the ellipsoid are uncorrelated or dissimilar. A three-dimensional correlation function generally represents more closely the average physical dimensions of sediment bodies (such as clay lenses) than the one-dimensional correlation function.

If a stochastic process (e.g. hydraulic conductivity) has a constant mean we refer to the process as having no drift; that is, the first statistical moment is constant over distance. If a process exhibits no drift and its autocorrelation function depends

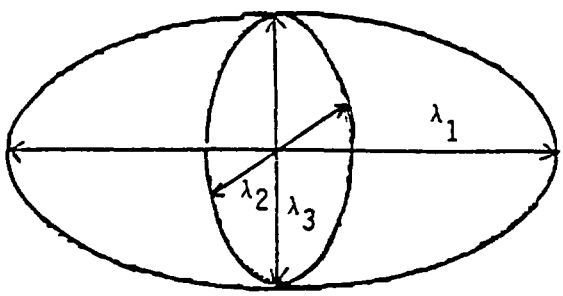




(a) Statistically isotropic aquifer and a sphere formed by an isotropic covariance function.



(b) Statistically anisotropic aquifer



(c) An ellipsoid formed by a three-dimensional anisotropic covariance function. $\lambda_1 \neq \lambda_2 \neq \lambda_3$.

Figure 4.5. Schematic diagrams illustrating stochastic concepts in ground-water hydrology.

on the separation distance only, the process is considered as a second-order stationary (or statistically homogeneous) process. If the spatial distribution of hydrologic data is second-order stationary, one is then able to use the first moment and its covariance function to characterize its spatial variability. On the other hand, data that do not fit the definition of the second-order stationarity process are considered as non-stationary processes. A non-stationary process describes data which has a definite trend in space (i.e., the mean varies with distance or the covariance depends not just on the separation distance). For example, in a sedimentary basin a formation may have facies changes which cause hydraulic conductivity to decrease gradually toward the center of the basin. However, for many cases the data with a trend may still be treated as a stationary process after the trend is removed.

Figure 4.6 schematically illustrates the meanings of stochastic terms discussed above. In Figure 4.6a, a regular sine wave and its autocorrelation function are shown. Figure 4.6b shows a signal created by a random number generator. The autocorrelation function drops rapidly from +1.0 at 0 separation distance, then fluctuates slightly about 0. This type of behavior indicates that the signal is uncorrelated or statistically independent from one point to the next. Both of these series are stationary: that is, no significant trend exists in the data, and the covariance presumably only depends on the separation distance. A non-stationary signal is shown in Figure 4.6c, where the data increase steadily in value along the sequence. The autocorrelation function shows steadily decreasing correlation. Figure 4.6d shows a combination of Figures 4.6a and b, a sine wave with superimposed noise (uncorrelated signal). Perfect autocorrelation does not occur except at 0 separation distance, but the periodic component of the series is revealed by the second peak in the autocorrelation function. Figure 4.6e is a combination of Figures 4.6a, b, and c, a sine wave combined with a linear trend with superimposed noise. Due to the existence of the trend, the series is non-stationary. Note that the trend

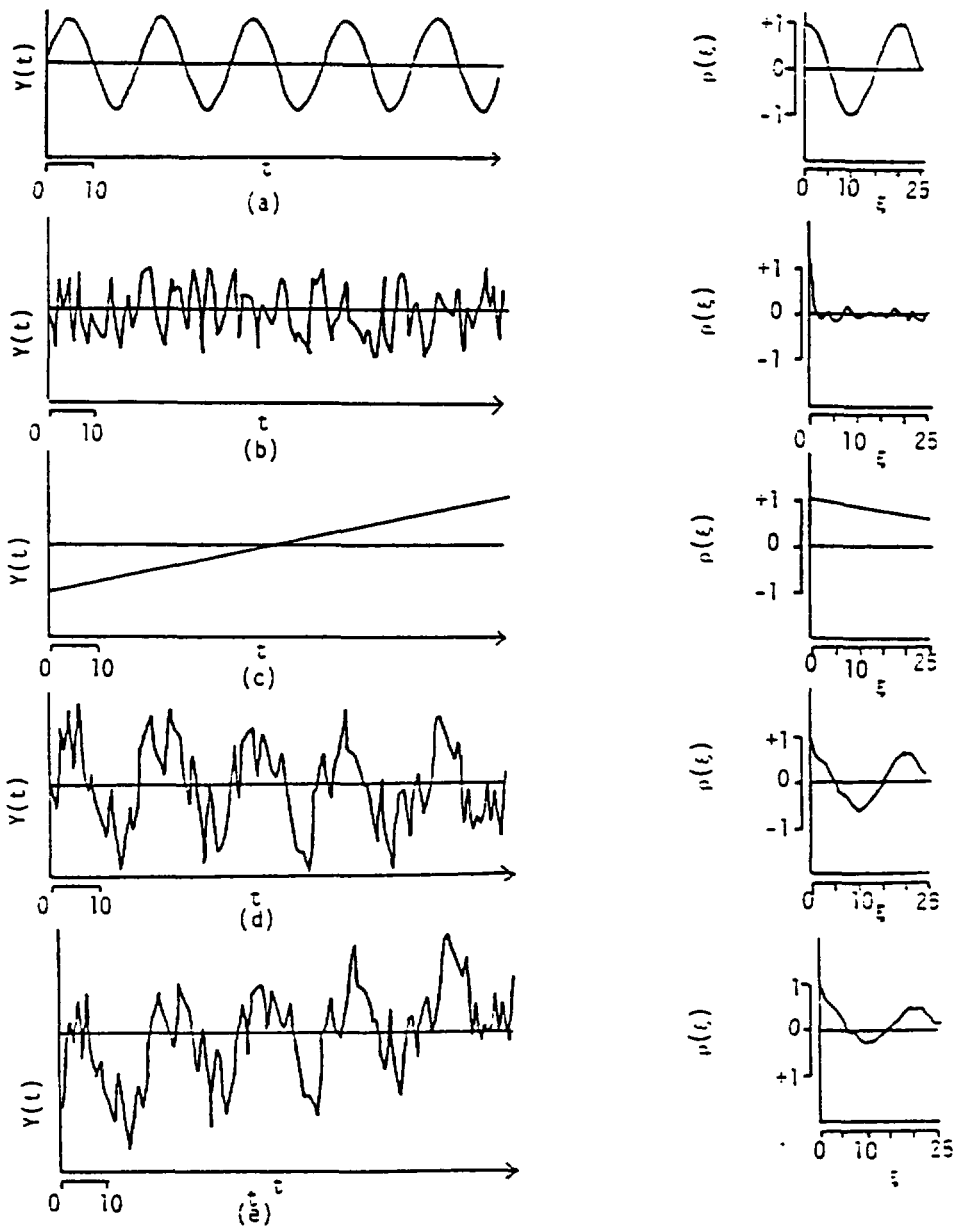


Figure 4.6. Some idealized time series, Y(t), and their autocorrelation functions, ρ(ξ). (a) Sine wave with wavelength of 20 units. (b) Sequence of random numbers or "noise". (c) Sequence of linearly increasing numbers of "trend". (d) Sine wave plus random noise (sequence a plus sequence b). (e) Sine wave plus random noise plus linear trend (sequence a plus sequence b plus sequence c). (Davis, 1973).

further reduces our ability to discern the periodic component in the series.

Using the stochastic concept, many field data have been collected and analyzed in the past decade. One typical example is the analysis of hydraulic conductivity data in the Borden sandy aquifer, collected by Sudicky (1986). Thirty-two core samples were taken from cross-sections of two perpendicular transects. Each core sample was cut into subsamples of 0.05m in length. A total of 1279 hydraulic conductivity measurements were made from these small samples. Figures 4.7 and 4.8 offer a view of the spatial variability of hydraulic conductivity in the aquifer. The results suggest that the Borden aquifer is heterogeneous over the distance that the measurements were performed with the local hydraulic conductivity field having a complex, lenticular structure. Several very distinct but thin lenses of low hydraulic conductivity are clearly visible in the profiles. A stochastic characterization of the spatial variability was carried out. The variance of lnK (the natural logarithms of K) was found to be 0.38, which included the variance due to uncorrelated variations below the scale of measurement (nugget effect; Section 4.2). Autocorrelation functions of the two cross-sections in the horizontal and vertical directions are illustrated in Figure 4.9 a,b,c and d. Using equation (4.1.5), Sudicky (1986) found that the autocorrelation function of lnK is anisotropic with $\lambda_1 = \lambda_2 = 2.8$ and $\lambda_3 = 0.12$ m, in horizontal and vertical directions, respectively.

4.2 Geostatistics

As mentioned in Section 4.1, there are two approaches to deal with aquifer heterogeneities: (1) the effective hydrologic property approach, and (2) estimation of property values at unsampled locations. The first approach will be explored in the later section dealing with spectral analysis. Here we will discuss some basic concepts and tools for the second approach. Detailed discussions can be found in textbooks by Journel and Huijbergts (1978) or De Marsily (1986).

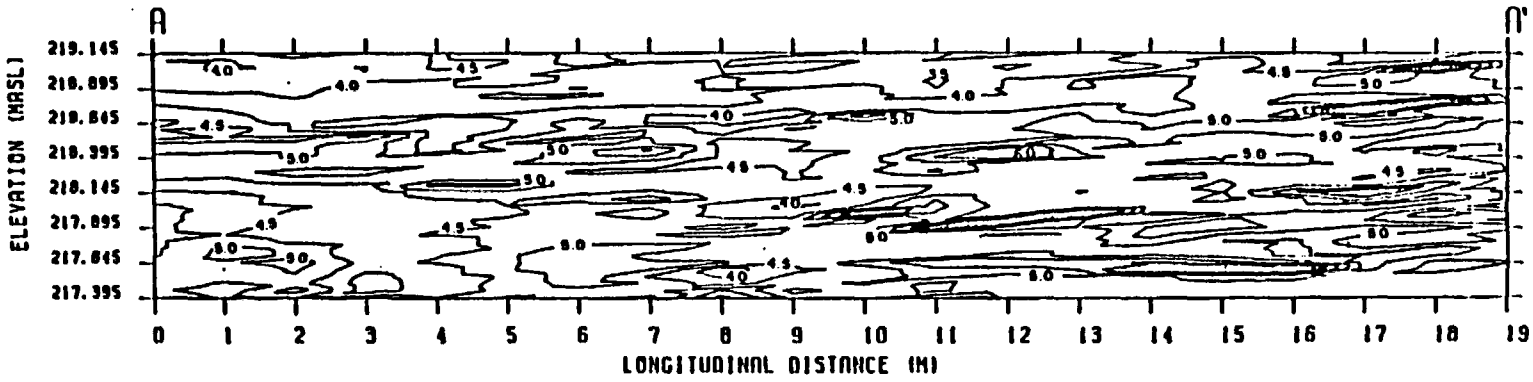


Figure 4.7. Cross-sectional view of the hydraulic conductivity distribution along a longitudinal direction in the Borden sandy aquifer (Sudicky, 1986).

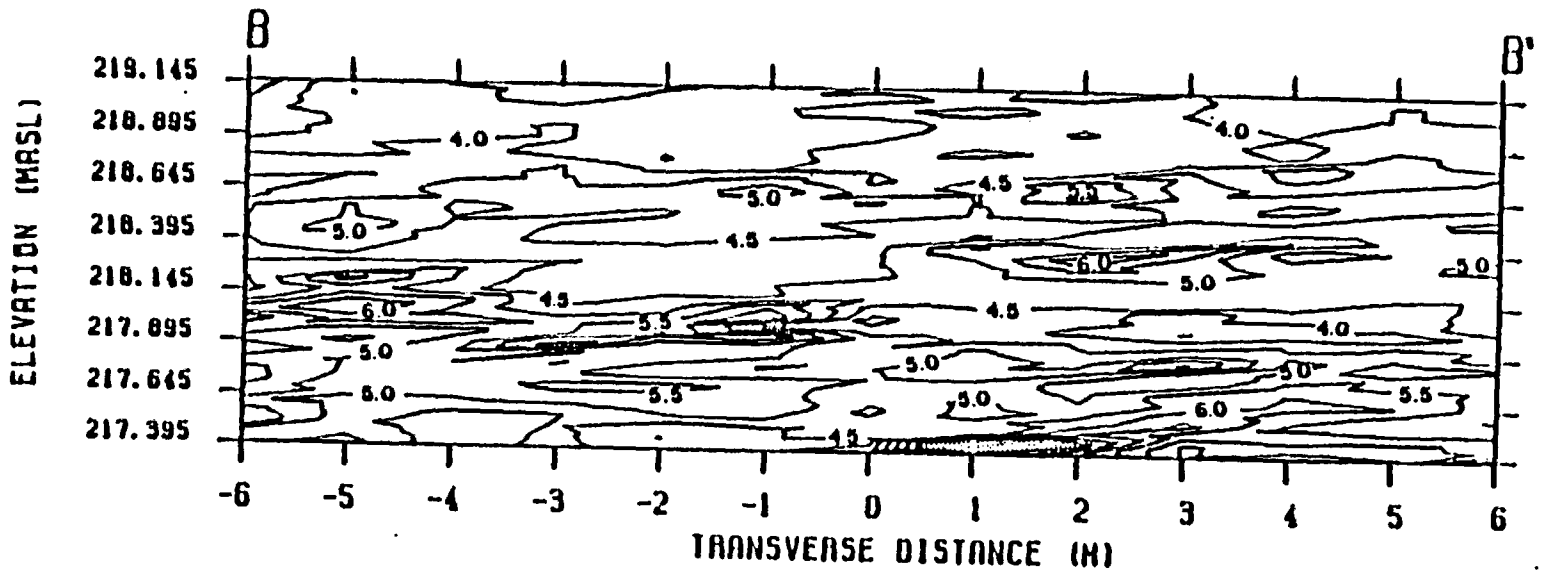


Figure 4.8 Cross-sectional view of the hydraulic conductivity distribution along a transverse direction in the Borden sandy aquifer (Sudicky, 1986).

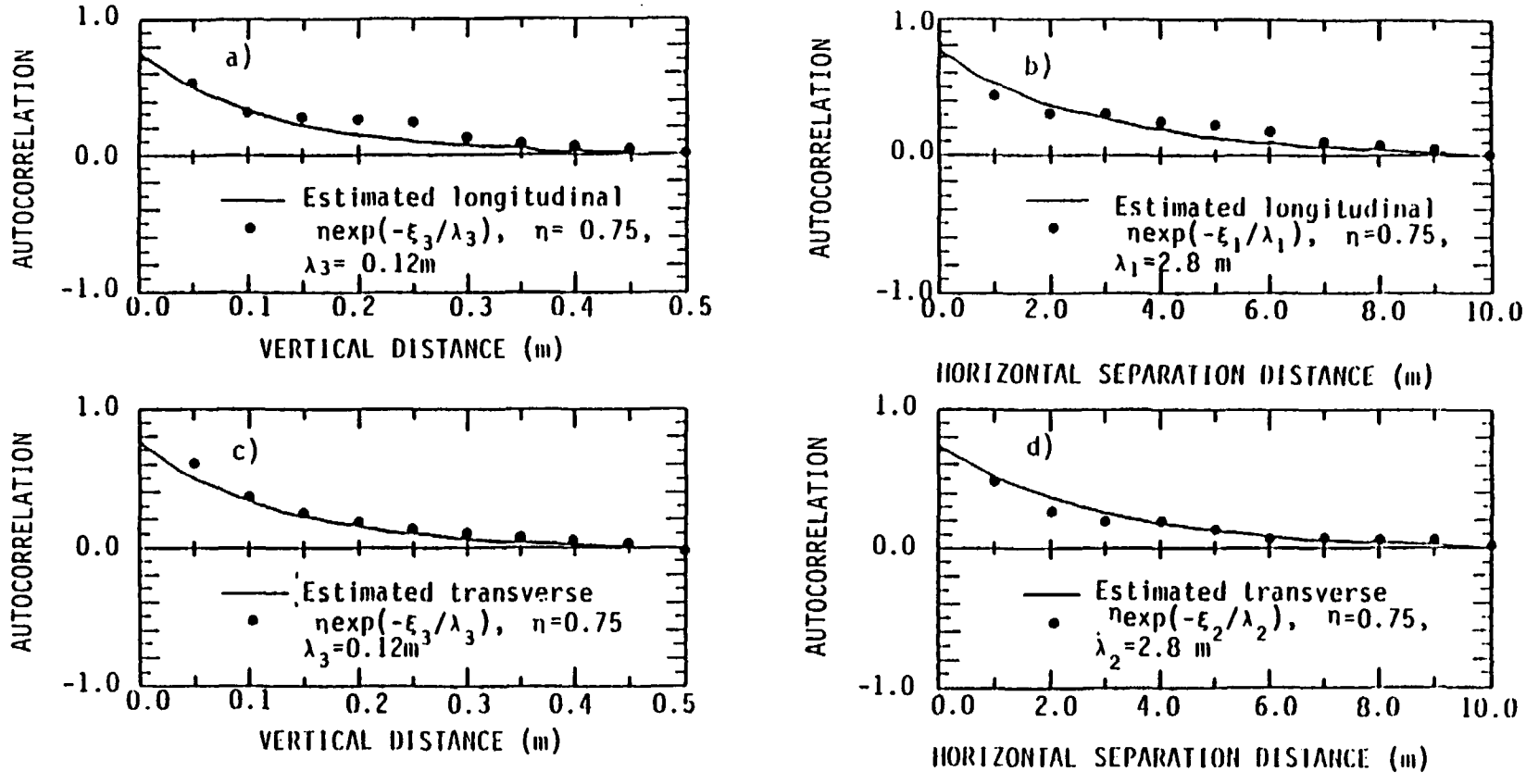


Figure 4.9. Vertical and horizontal autocorrelation functions for lnK along cross-sections in the longitudinal and transverse directions. n represents the ratio of the true variance (total variance minus the nugget effect) to the total variance.

Geostatistics is basically a statistical method 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 (Journel and Huijbergts, 1978). Recently, the technique has been applied to groundwater hydrology to deal with spatial variability problems. In principle, geostatistics concepts are similar to the stochastic concepts. They both are used to deal with variables distributed in space. However, some of the terminology is different. For example, the term "random function" is used in geostatistics to defined 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 $x_2+\xi$ are not independent but correlated. From 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). A regionalized variable is simply a particular realization of a certain random function or stochastic process. We will point out some other differences in the following text.

Two important parts of geostatistics are (1) identification of the spatial structure of the variable (variogram estimation, trend estimation, etc.) and (2) interpolation or estimating the value of a spatially distributed variable from neighboring values taking into account the spatial structure of the variable (kriging, co-kriging, etc., Davis, 1973).

Similar to 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 the covariance function depends on the separation

distance only. However, the intrinsic hypothesis requires only that the mean of the differences of the data values is constant, and the variance of the difference of data values depends on the separation distance, i.e. $[K(x+\xi) - K(x)]$ satisfies:

$$E[K(x+\xi) - K(x)] = m \tag{4.2.1}$$

$$\frac{1}{2}\,\mathrm{var}[K(x+\xi) - K(x)] = \gamma(\xi) \tag{4.2.2}$$

where K(x)'s are regionalized variables, and γ is a function of ξ, and not of x. $\gamma(\xi)$ is called the variogram, sometimes also called semivariogram. Figure 4.10 shows the general behavior 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 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 is a second-order stationary process.

The main types of variograms commonly used to fit sample variograms (variograms estimated from field data) are: linear, spherical, exponential, Gaussian, and cubic. Figure 4.11 shows the shapes and equations of these variograms. Generally, a linear variogram, as shown in Figure 4.11a, suggests that the process has an infinite variance and that there is no covariance function, i.e., it is not a second-order stationary process. In this case, one has to rely on the intrinsic hypothesis to analyze the data. Theoretically, all variogram plots pass through the origin; the variogram is zero at a separation distance of zero. However, variograms obtained

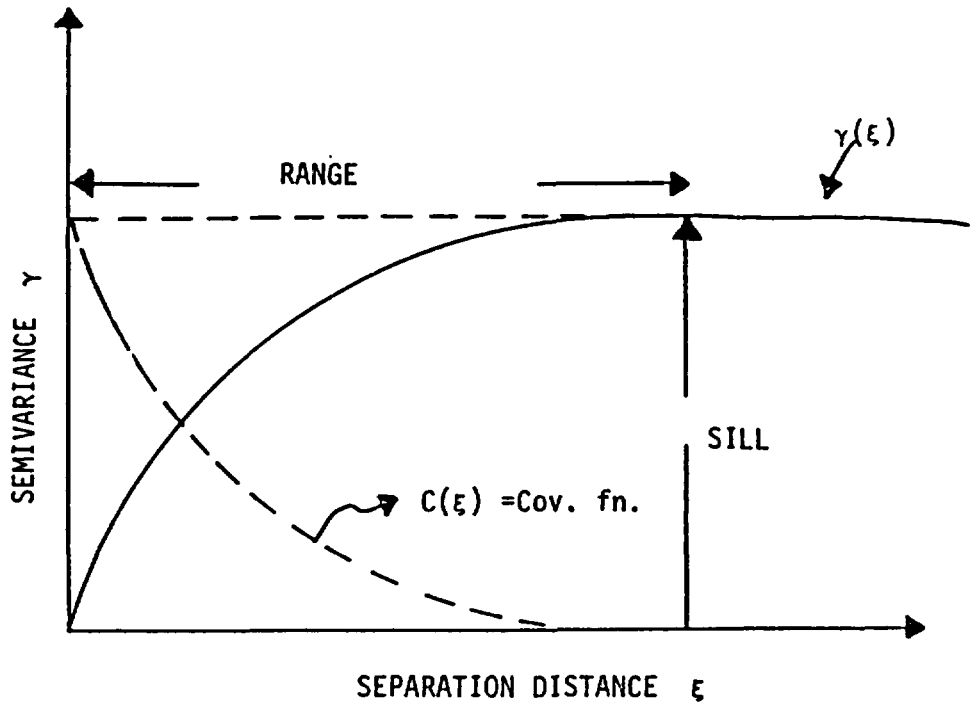
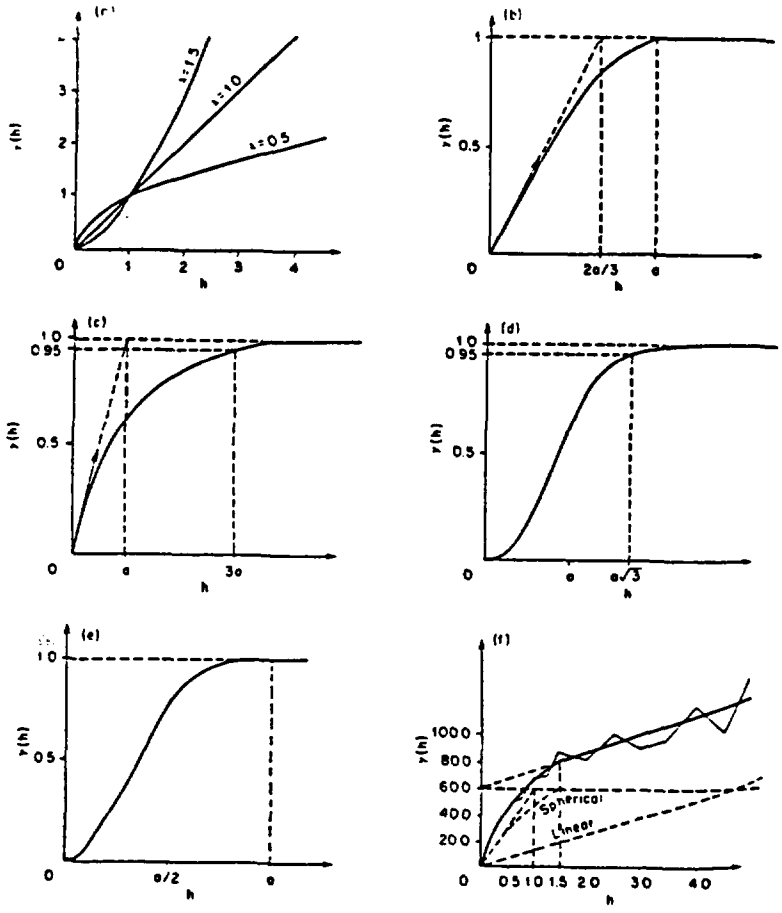


Figure 4.10. General behavior of a variogram.



(a) model in h^{λ}	ωh^{λ}	$\lambda < 2$
(b) spherical model	$\omega\left[\frac{3}{2}\left(\frac{h}{a}\right) - \frac{1}{2}\left(\frac{h}{a}\right)^3\right]$	$h < a$
	ω	$h > a$
(c) exponential model	$\omega[1 - \exp(-h/a)]$	
(d) Gaussian model	$\omega\{1 - \exp[-(h/a)^2]\}$	
(e) cubic model	$\omega\left[7\left(\frac{h}{a}\right) - 8.75\left(\frac{h}{a}\right)^3 + 3.5\left(\frac{h}{a}\right)^5 - 0.75\left(\frac{h}{a}\right)^7\right]$	$h < a$
	ω	$h < a$
(f) fitting on a "linear plus spherical" model (example)		
	$13.3h + 60\left[\frac{3}{2}\left(\frac{h}{1.5}\right) - \frac{1}{2}\left(\frac{h}{1.5}\right)^3\right]$	$h < 1.5$
	$13.3h + 60$	$h > 1.5$

Figure 4.11. A diagram showing the shapes and equations of various variograms (de Marsily, 1986).

from field data often exhibit a jump at the origin, as shown in Figure 4.12. This apparent jump is called the nugget effect and represents the uncorrelated subscale variability or measurement errors. The variogram can be either isotropic or anisotropic as in the covariance function. It is also likely that there are multiple correlation scales that appear when testing over different scales, ranging from laboratory to field to required scale, Figure 4.13, (Gelhar, 1986).

The other part of geostatistics is Kriging. The most general form of Kriging is termed "Universal Kriging," in which the values of points may be estimated from irregularly distributed samples in the presence of trends (or nonstationarity). If the data set is stationary, a less involved operation can be used to estimate the values of points. This technique is referred to simply as "Ordinary Kriging" or "Kriging" (see Bras and Rodriguez-Iturbe, 1985, and Journel and Huijbregts, 1978).

A common application of Kriging in groundwater hydrology is the estimation of hydraulic conductivity or transmissivity values at unsampled locations in between test wells (see Delhomme, 1979). For example, in an attempt to use a two-dimensional, finite difference, groundwater flow model to simulate flow fields in a groundwater basin, 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 objectively assign transmissivity values to the remaining nodes, one may have to resort to use of mathematical tools. Kriging is one of the possible tools.

To find the hydraulic conductivity estimate K^* of the unknown quantity K_0, Kriging uses a weighted sum of all the available sample values (measured hydraulic conductivity values):

$$K^* = \sum_{i=1}^{n} \lambda_i K_i \qquad (4.2.3)$$

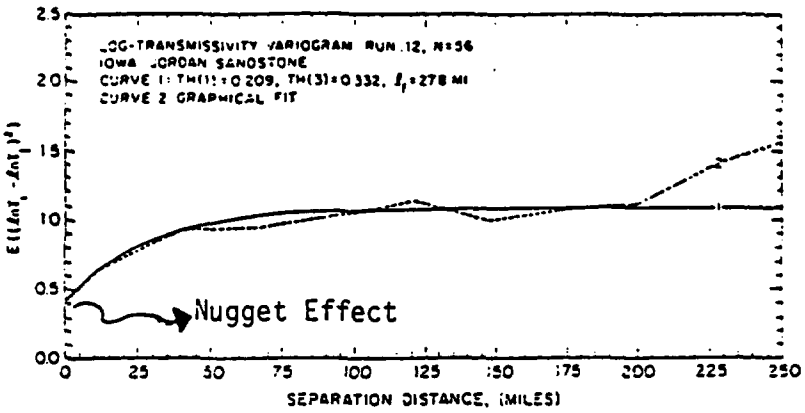


Figure 4.12. A variogram showing the nugget effect: a jump at the origin. (Hoeksema and Kitanidis, 1985).

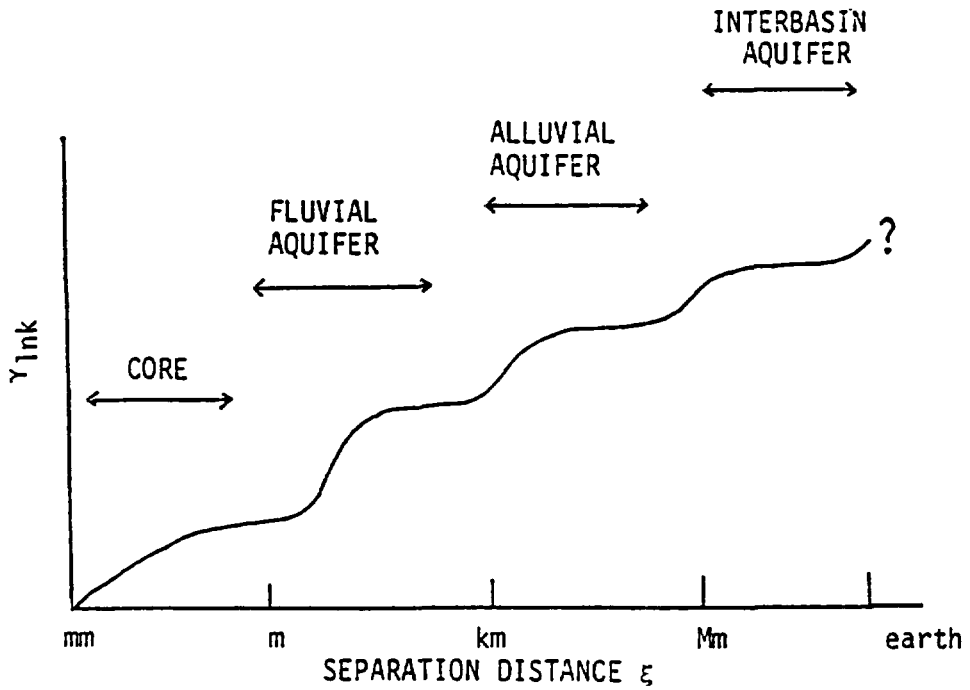


Figure 4.13. Hypothetical lnK variogram illustrating the notion of scale-dependent correlation scales (Gelhar, 1986).

where λ_i are the weighting factors, and K_i are sample values. In order to limit the choice of the weighting factors, we will impose two conditions. The first condition is that the expected value of the estimate of K should be the same as the expected value of K, i.e.,

$$E[\ K^*\ ] = E\ [\ K\ ] \tag{4.2.4}$$

It follows that in the constant mean case the sum of the weighting factors has to be unity.

$$\sum_{i=1}^{n} \lambda_i = 1 \tag{4.2.5}$$

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

$$E[\ (K^* - K)^2\ ] = \text{minimum} \tag{4.2.6}$$

This latter condition, along with 4.2.5 leads to a system of equations of the form:

$$\sum_{j=1}^{n} \lambda_j\ \gamma(x_i - x_j) + \mu = \gamma(\ x_i - x_0\ ) \tag{4.2.7}$$

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 between the point to be estimated and the point x_j. μ is a Lagrange multiplier. Combining the constraint that the weighting

coefficients must sum to one, the system of equations can be solved to obtain optimal λ_i values which can then be input to equation (4.2.3) to obtain the estimate of K*. The estimator, K* is a linear combination of the n data values (4.2.3). The n weights λ_i are calculated to ensure that the estimator is unbiased and that the estimation variance is minimal. Kriging is a best linear unbiased estimator (BLUE).

The Kriged estimate K* 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, K*, to be exact. The inexactitude of the estimate is the Kriging variance, σ_K^2, which is:

$$\sigma_K^2 (x_0) = \sum_{j=1}^{n} \lambda_j \, \gamma(x_i - x_0) + \mu \qquad (4.2.8)$$

The smaller the variance, the greater the reliability of the estimate K* . Conversely, an estimate with a large associated variance must be utilized with caution. One can also use the Kriging variance in determining the optional 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 could be a valuable tool in quantifying uncertainty in interpolated data and in assessing the value of additional data during 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 objections behind polynomial or surface fitting differ from those in kriging. For that reason a comparison between them 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.

Kriging can also be used in conjunction with numerical simulations that may be useful in calculating ground water travel time. 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, represent a much smaller scale than the grid blocks of the model. In contrast to ordinary Kriging described previously in this section, 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 an point or area basis. De Marsily et al. (1984) describes a method of identifying hydraulic characteristics of a reservoir from aquifer pumping tests which combines Kriging and numerical simulation. The approach allows one to utilize a variety of available hydrogeologic information at different scales. Kriging has also been 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 estimate pore velocity is described by Neuman (1984).

In most field problems, groundwater hydrologists are likely to have both transmissivity and hydraulic head, or the 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), Gutjahr (1981), and Kitanidis and Vomvoris (1983). Neuman (1984), Williams (1987), and Hoeksema and Kitanidis (1984) applied this approach to groundwater flow simulations.

4.3 Stochastic Analysis of Spatial Variability

The statistical description of spatial variability of hydraulic properties of subsurface materials has led many researchers to investigate the effect of randomly distributed parameters on the governing equations. The model used to investigate this type of problem is generally called a stochastic model. Although stochastic and deterministic models use the same governing flow and transport equations for porous media, the former differs from the latter in that its input functions are uncertain and, therefore, the model output must be described in probabilistic rather than deterministic terms (Neuman, 1982).

For example, a deterministic, three-dimensional, groundwater flow model requires values of hydraulic conductivity and storativity at every point in three-dimensional space, if we assume that the initial and boundary conditions and sink and source terms are prescribed. The output from the deterministic model is a realization of hydraulic head values corresponding to those parameters at each point in space. However, in a stochastic model, the hydraulic conductivity and storativity are considered as stochastic processes in space which are described in terms of means, covariances, and other statistical terms, instead of a value at each point. The output consists of many possible head distributions that relate to the input parameters. Therefore, the head is a stochastic process which can be described in terms of statistical parameters such as mean, variance, covariance, etc. In other words, the stochastic model produces a probabilistic result which can be utilized to assess the uncertainty in predictions due to heterogeneity of aquifer properties.

In the past few decades, many researchers in groundwater hydrology have applied stochastic models to study flow and transport through heterogeneous porous media. The following is a summary of these works which include Monte Carlo simulation, conditional simulation, spectral analysis, and fractal analysis.

4.3.1 Monte Carlo Simulation. The most intuitive approach to dealing with spatial variability in a stochastic sense is called Monte Carlo simulation. It is a very powerful method, since fewer assumptions are required than in all of the other stochastic methods. However, it may require extensive computer time and a careful analysis of the results. The principle of the method is rather simple. The method assumes that the probability distribution of the variable (for example, hydraulic conductivity) and its covariance function are known from measured field data. Then, many possible realizations of hydraulic conductivity values that conform to the assumed probability distribution can be generated by using a pseudorandom number generator with special techniques (Gutjahr, 1987; Smith and Freeze, 1979; Mantoglou and Wilson, 1982). Each realization of the parameter values is input to flow and transport equations which are then solved by either 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, there are N realizations of output from solving the governing equations. It is then possible to statistically analyze the output for each realization to obtain expected value, variance, covariance, and distribution. The idea is illustrated in Figure 4.14.

There are difficulties associated with the simulation method. First, a large number of realizations is necessary in order to obtain meaningful statistics. This implies that extensive computer CPU time is required, and this method is costly. Second, a groundwater basin has to 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 iterative methods. 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

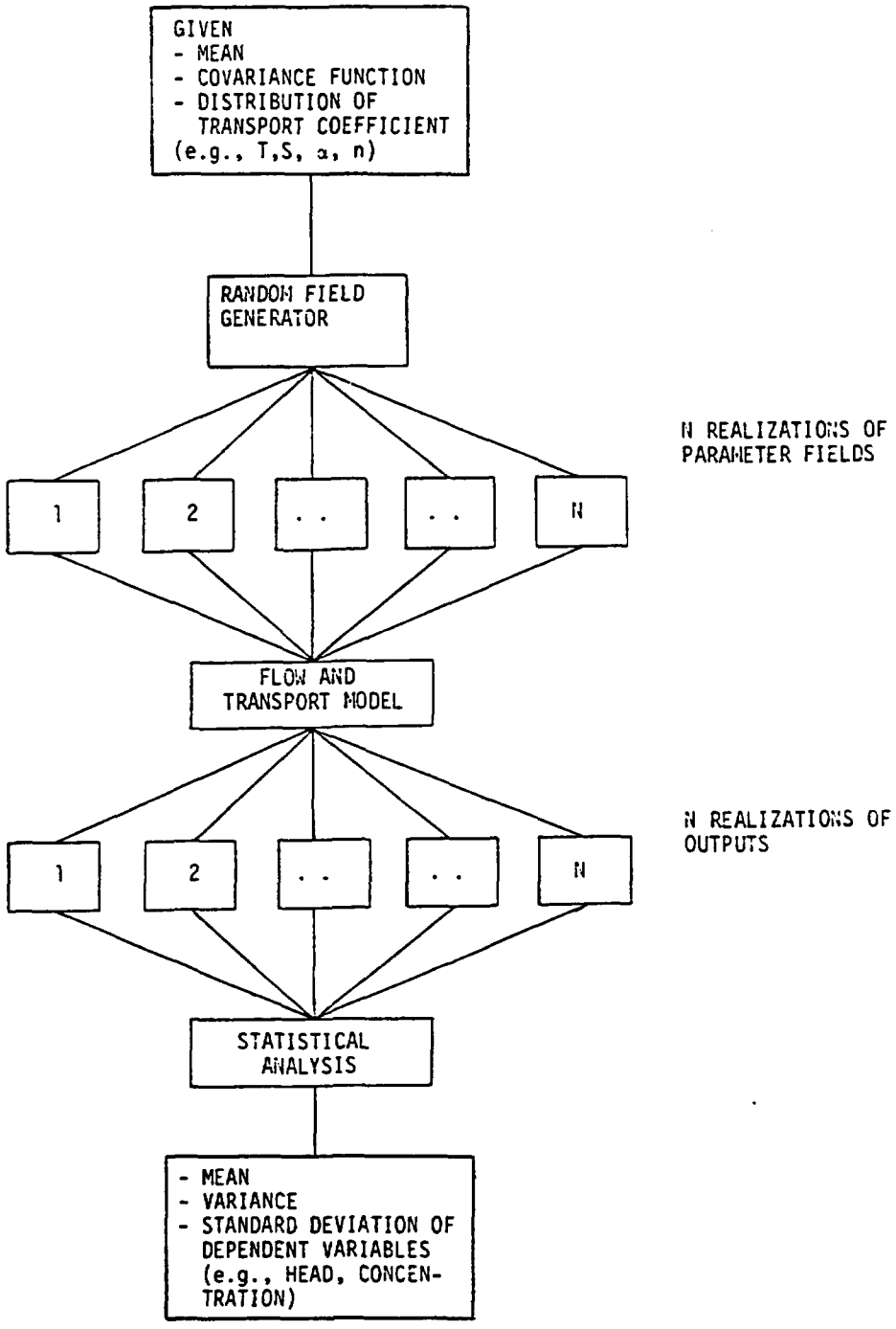


Figure 4.14. Schematic illustration of Monte Carlo simulation concept.

situations or other highly nonlinear 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 nonlinear systems with stochastic parameters are tremendous. Although these are 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.

Applications of Monte Carlo simulations to investigate the effect of heterogeneity on flow through porous media were first used by Warren and Price (1961). Following their work, studies were made by Warren and Skiba (1964), Bibby and Sunada (1971), and Heller (1972). All of these works are related to petroleum reservoirs. The first study directly related to groundwater hydrology was carried out by Freeze (1975). Freeze essentially extended the approach of Warren and Price (1961) to the multivariate case in which hydraulic conductivities, compressibilities, and porosities all vary randomly in space and are mutually correlated. The objective of his study was to investigate the uncertainty in hydraulic head prediction due to aquifer heterogeneity. Groundwater travel times and paths depend partially on the hydraulic gradient distribution, which in turn is related to hydraulic head distribution. Uncertainties in predictions of head distribution, of course, will result in uncertainties in prediction of groundwater travel times and paths. Thus, it is appropriate to discuss his work in detail in this section. Furthermore, discussion on the weakness of his work may lead to a better understanding and future utilization of Monte Carlo techniques to predict groundwater travel times and paths.

Freeze (1975) considered both steady-state flow under constant head boundary conditions and transient consolidation of a clay layer under similar boundary conditions and prescribed head at time zero. A one-dimensional flow domain was discretized into many blocks. Random hydrologic parameters (log

hydraulic conductivities, compressibilities, and porosities) were assigned to each block, and these parameter values were independent from those at adjacent blocks (i.e., no correlation structure was considered in generating the random hydraulic parameters). An analytical method and a numerical method were used to determine the hydraulic head distributions for steady and unsteady flow, respectively. Solutions were then analyzed for a given number of blocks and a given choice of statistical parameters such as mean parameter values, variances, and correlation coefficients between parameters.

Based on the Monte Carlo analysis, Freeze concluded that (1) there is no simple way to define an equivalent homogeneous porous medium for transient flow in a heterogeneous porous medium; and (2) the consideration of spatial variability of hydraulic properties in a stochastic sense may lead to very large fluctuations in the computed hydraulic head values. Therefore, he expressed the pessimistic view that the prediction of hydraulic head using any deterministic model may suffer from very large errors. He further questioned the usefulness of determining aquifer characteristics by means of aquifer test analyses, which rely on deterministic analytical solutions and the assumption that the aquifer is homogeneous.

Such pessimistic views on groundwater flow modeling by Freeze were challenged by Gelhar et al. (1976). They attributed the large variance in calculated hydraulic head in Freeze's work to the dimensionality of the model used. They indicated that the head variance will be reduced significantly in three-dimensional models. When a one-dimensional model is used, the flow must travel directly through impermeable layers. The hydraulic head gradient near an impermeable layer thus has to increase substantially to allow water to flow. In a three-dimensional problem, water takes the least resistant route and avoids the impermeable paths. Therefore, the head gradient is smaller than in the one-dimensional case. Head variance in a three-dimensional model is also much smaller than in the one-

dimensional case. Furthermore, Freeze's analysis assumed that hydrologic parameters in adjacent finite difference grids were independent, but within a grid the properties were constant. This assumption implies that the parameter values are correlated over a block; that is, the size of the block determines the correlation scale. Bakr et al. (1978) showed that the head variance is directly proportional to the square of the correlation scale. Consequently, the choice of the size of the block could significantly affect magnitude of the head variance. Therefore, Freeze's analysis was most likely overly pessimistic.

More realistic simulations than Freeze's study on uncertainties in hydraulic head were later conducted by Smith and Freeze (1979a and b) using a Monte Carlo technique. Steady flow through one- and two-dimensional random hydraulic conductivity fields was simulated using a finite element model. The hydraulic conductivity K was assumed to be lognormally distributed. Anisotropic spatial correlation structures (statistical anisotropic covariance function) of the random conductivity values were incorporated by using a first-order nearest-neighbor autoregressive model. One technical weakness of their work is that one has minimal control on the shape of covariance function generated by the nearest-neighbor model. In the two-dimensional analysis, a hypothetical rectangular aquifer was used in which constant hydraulic head boundaries were imposed on two opposite sides of the aquifer and no flow boundaries on the others.

The results of their simulations show that for the case of unidirectional (uniform) flow, the uncertainty in hydraulic head must be interpreted in light of the ratio of the correlation scale to length of size of the aquifer. The uncertainties in head (represented by the standard deviations of hydraulic head distribution) increase as the extent of the heterogeneity increases and/or as the correlation scale/length ratios increase. A comparison of the results of one- and two-dimensional flow regimes indicated that the standard deviation is smaller in the two-dimensional

problem. They also investigated the effects of nonuniform flows by rearranging the boundary conditions of the hypothetical aquifer. The results from nonuniform flow fields simulations led to the conclusion that the uncertainty in model predictions depends upon both the spatial heterogeneity in hydraulic conductivity and the flow regime. The uncertainty in the predicted head values is greatest where the mean hydraulic head gradient is large and the uncertainty in hydraulic head values tends to diminish near the constant head boundaries. Generally speaking, their results are in agreement with those obtained by a spectral method (Mizell et al., 1982). As pointed out by Neuman (1982), the results of Smith and Freeze (1979b) also illustrate that the concept of an equivalent uniform porous medium is not appropiate for the cases where the mean hydraulic gradient is not uniform (such as during a pumping test where the flow is convergent) or when the mean hydraulic conductivity varies in space.

In Smith and Freeze's work, they also addressed the problem of scale which is critical in determining groundwater travel times and paths. They pointed out that by using single conductivity values in the finite difference blocks or finite elements, spatial variations on a scale smaller than the block or element do not contribute to the variability in the finite element solution. They suggested that in order to obtain an accurate solution in modeling a given field situation, the finite difference or element model must reproduce all the significant scales of heterogeneity that contribute to the prediction uncertainties at the scale of the model. This statement concurs with the previously stated position in this review on the concept of groundwater travel times and paths. Dispersion representing subscale variability must be included in the analysis of groundwater travel times and paths.

Smith and Freeze (1979b) also emphasized that the scale at which heterogeneities are to be described in the analysis of uncertainties will be related to the scale of the flow analysis. They stated: "... in a regional flow the model would

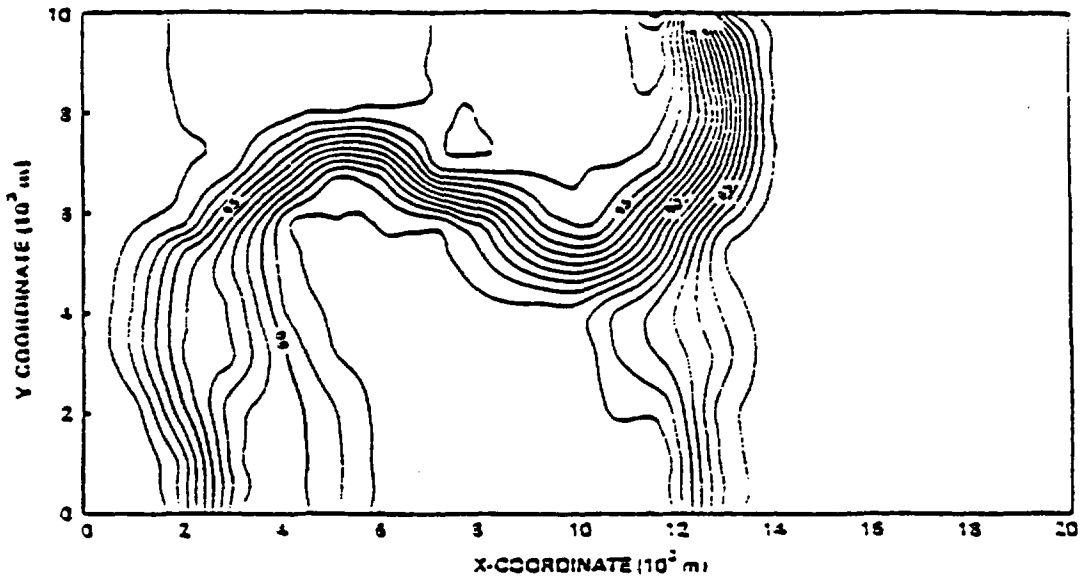
preserve the regional structures and patterns of conductivity variability. On the other hand, in considering flow to a tile drain, the description of the spatial heterogeneity would reflect the local dependence in the region about the drain." Such a statement seems to be a contradiction of their earlier statement that the effect of subscale variability should be considered in the simulation. In our opinion, the fastest path can best be predicted by characterizing local scale of heterogeneities. For example, if we are interested in the water level in a well, then the scale used to depict heterogeneities should be equal to the size of the screen in the well. Certainly, heterogeneities larger than the screen but much smaller than the size of heterogeneities forming the regional structures will affect the response of the well. As an example, the drawdown at a well tapped into a large sandstone lens embedded in a dolomite formation will be affected by the hydraulic conductivities of both the lens and the formation. Hydraulic conductivity variations smaller than the size of the screen (such as the conductivities of thin layers of gravel within the lens) can be ignored. This is because the water level is a quantity averaged over variabilities at scales much smaller than the screen. This is true for water level measurements in a well. However, in the case of groundwater travel times and paths, one may want to consider the variability at scales smaller than the screen, inasmuch as some fluid particles would move rapidly in those thin gravel layers.

One of the studies relevant to NRC's criterion of pre-waste emplacement groundwater travel times in a potential repository site was conducted by Clifton et al. (1985). He applied the Monte Carlo technique to examine the sensitivity of the travel time distribution predicted by a reference case model to: (1) scale of representation of the model parameters, (2) size of the model domain, (3) correlation range of log-transmissivity, and (4) cross-correlations between transmissivity and effective thickness.

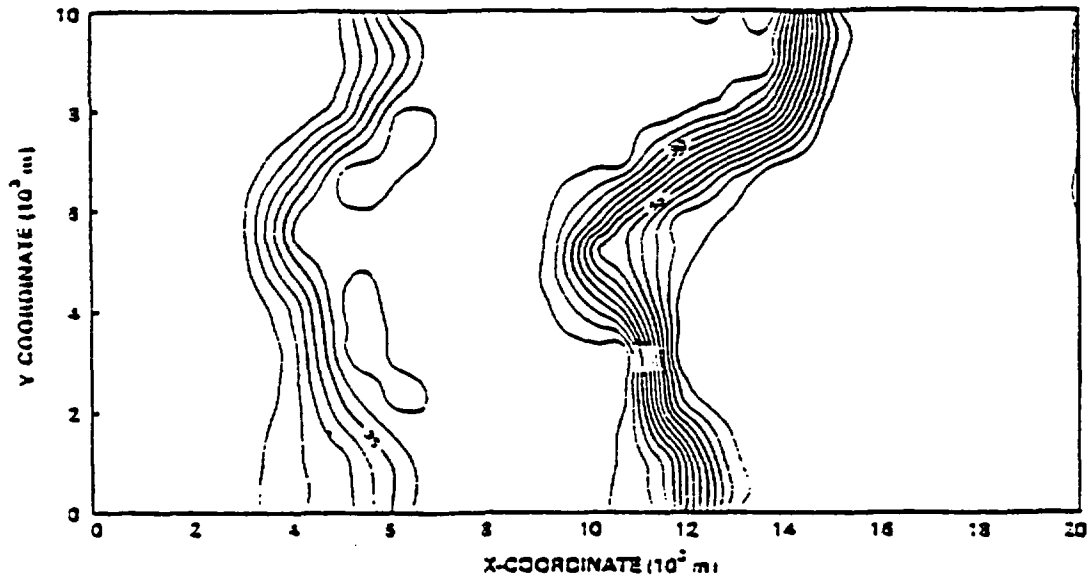
For this study, a rectangular area with dimensions 20 by 10 km was selected

as the reference case from the deep basalt beneath the Hanford site in southcentral Washington state. Impermeable boundaries were set along the two longer dimensions, and constant head boundaries were set along the shorter dimensions so that the regional hydraulic gradient was 10^{-3}. A steady-state, two-dimensional, horizontal groundwater flow regime was assumed. A finite difference flow model was used. The rectangular area was divided into square finite difference grids 1 km on a side. An effective thickness was defined as the product of the effective porosity and actual flow domain thickness. The effective thickness represents the area of effective, or hydraulically active, pore space in a vertical cross-section of the flow domain of unit width and thickness. Effective thickness of the area of the reference case was deterministically set at a uniform value of 4×10^{-2} m. Transmissivity was treated as a statistically isotropic stochastic process representing the uncertainties in inputs and was assumed to be log-normally distributed. Ten thousand random transmissivity fields were generated by using an unconditional estimator (Clifton and Neuman, 1982) with a spherical variogram model. The geometric mean of the transmissivity values was $0.153 m^2$/day, and the variance, and correlation scale of the log-transmissivity values were 3.35, and 5 km, respectively. These random hydrologic fields were input to the finite difference model to generate 10,000 hydraulic head fields.

Figures 4.15a and b show the hydraulic head distributions of realizations 3,899 and 5,120. In Figure 4.16a, the mean of the ensemble of 10,000 head field realizations is plotted. It is evident that the ensemble mean head field closely approximates the deterministic head field. This deterministic head field refers to the head field determined by assuming an equivalent homogeneous medium with the mean transmissivity. Interestingly, this result illustrates the fact that the head distribution in a constant head permeameter, calculated by using a single hydraulic conductivity value, represents an ensemble average. That is, it is an average head



(a) realization 3899



(b) realization 5120

Figure 4.15.. Simulated hydraulic head distribution in a two-dimensional aquifer with a random transmissivity field (Clifton et al., 1985).

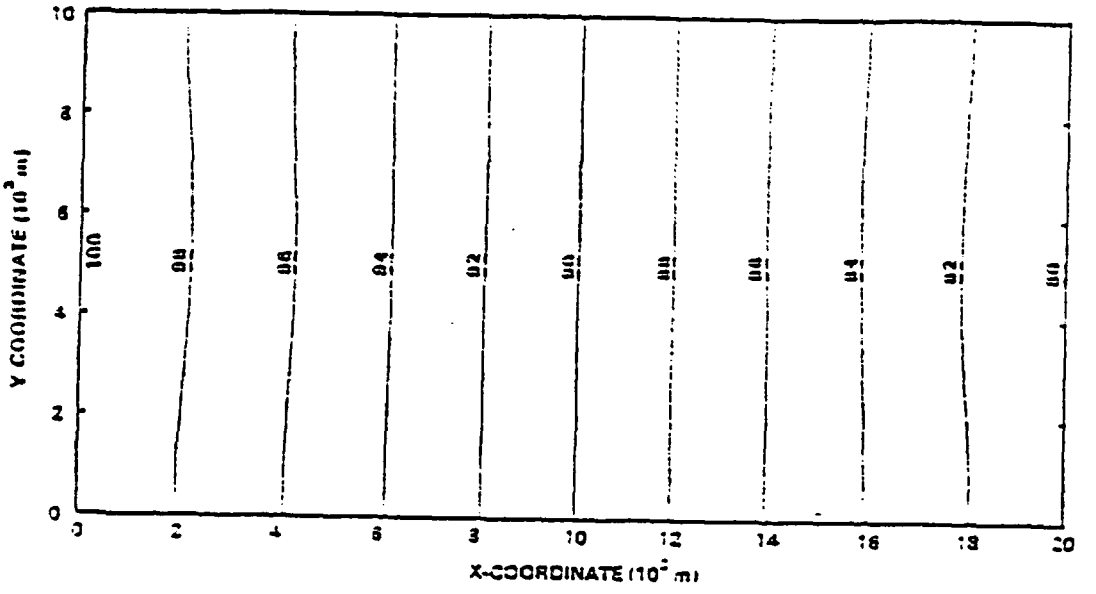


Figure 4.16a. Ensemble averaged head distribution. (Clifton et al., 1985).

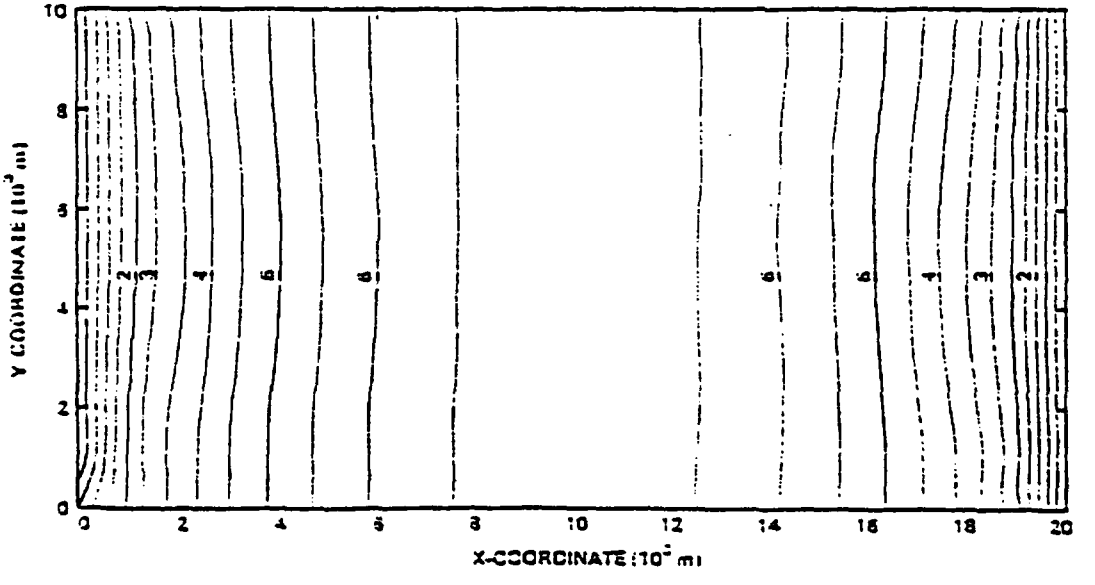


Figure 4.16b. The standard deviation distribution in a hypothetical aquifer. (Clifton et al., 1985).

distribution over many possible head realizations due to heterogeneities at scales smaller than the permeameter. Thus, it is clear that the deterministic approach (such as determining hydraulic conductivity from a soil column test) in groundwater hydrology is closely related to the stochastic approach. More importantly, the result here also supports the view that it is important to use head measurements averaged at many locations (observation wells) to determine mean hydraulic properties from aquifer test data (see section 3.1.3). Figure 4.16b shows the standard deviations of hydraulic head fields. The standard deviations decrease toward the specified constant head boundaries. This indicates the importance of boundary conditions on the uncertainty analysis.

In the analysis by Clifton et al., (1985) the average fluid particle velocity was determined from the transmissivity, hydraulic head gradient, and effective thickness values. The statistics of groundwater travel times were determined from a selected pathline in each of these 10,000 hydraulic head fields. Each pathline had the same starting location and same linear distance (10 km) between starting and termination points. The distribution of the groundwater travel times resulting from the 10,000 pathlines is shown in Figure 4.17. The median travel time (i.e., the travel time at 50% probability) is 21,500 yr. In other words, the probability that the predicted groundwater travel time between the two points is less than 21,500 yr is about 0.5, if the exact arrangement of transmissivity values within the flow domain is unknown. The standard deviation of the log-travel-time is 0.84 (one standard deviation above the mean). The results in Figure 4.17 indicate the probability of a predicted groundwater travel time less than 5000 yr (approximated from Figure 4.17) is 0.16 and less than 200,000 yr is 0.84. Such a groundwater travel time distribution thus provides us with a measure of the uncertainty in the predicted groundwater travel time.

One can also use this distribution to address the effect of heterogeneity on

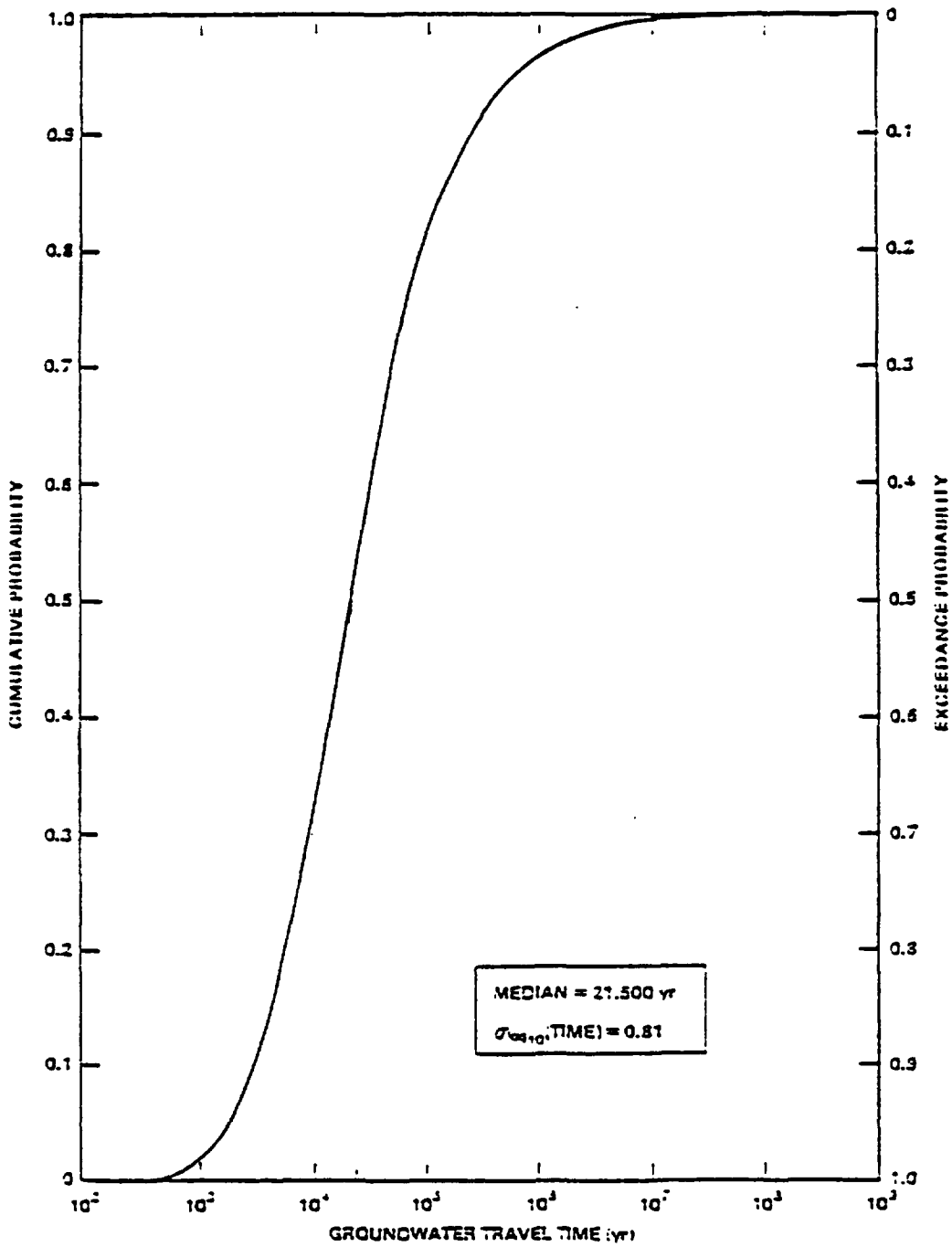


Figure 4.17. Cumulative probability of simulated groundwater travel times. (Clifton et al., 1985).

groundwater travel time, if the ergodicity assumption is used. That is, the probability distribution of ground-water travel time obtained from this analysis is equivalent to that of the time for a large number of groundwater particles released at the left boundary to travel across of the flow domain and exit the right boundary (e.g. Figure 4.15, and 4.16). This groundwater travel time distribution indicates that, on the average, 50% of the particles will arrive at the ending line within 21,500 yr. Due to the existence of some fast paths, 84% (one standard deviation less than the mean) of the groundwater particles will cross the flow domain in less than 200,000 yr. Therefore, the spread of groundwater travel times reflects spatial variations in fluid particle velocity, i.e., deviations of the velocities from the mean, within the flow field. In fact, this probability distribution is similar to the concentration distribution in a soil column tracer test discussed earlier with the exception that this distribution does not consider velocity variations at scales smaller than the finite difference block.

When a numerical groundwater flow model is used, the flow domain generally has to be discretized into many smaller grids. Because there are practical limits on the total number of grids used to represent a model domain, there will in turn be some limit on the minimum size of a block. Property values assigned to the block represent the averages over the block, and consequently variations at subscales are neglected. The larger the block is the more subscale variability is ignored. Therefore, the size of block used in the numerical simulation will influence results of the analysis, regardless of its impact on the accuracy of the numerical solution. Figure 4.18 illustrates the effect of the size of blocks (zones) on the probability distribution of groundwater travel time. As indicated in the figure, both the mean travel time and the standard deviation of log travel time (a measure of the arrival time variability) decrease as the size of the block increases. In the work by Clifton et al. (1985), the mean travel increased by 41%, from 16,000 to 23,500 years, when

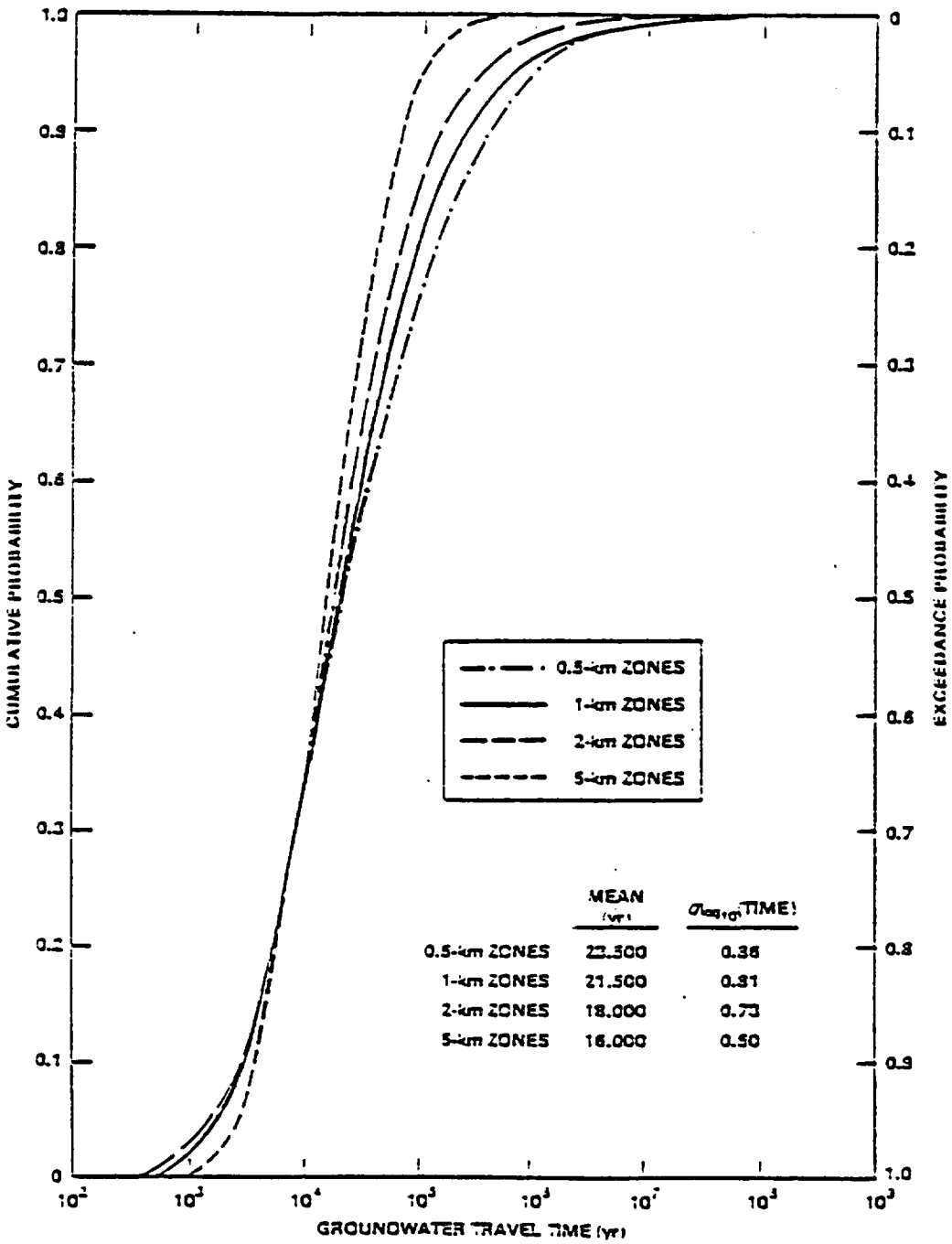


Figure 4.18. Effects of finite difference block (zone) size on the cumulative probability of groundwater travel time. (Clifton et al., 1985).

the grid blocks size in the model decreased from 5.0 to 0.5 km. This result is again illustrative of the importance of considering subscale variability in the prediction of the ground water travel time.

Impacts of the correlation scale of transmissivity values on the groundwater travel time distribution were also investigated in the study by Clifton et al. (1985). The travel time distributions from six random fields with different log-transmissivity correlation scales are illustrated in Figure 4.19. A constant variance in transmissivity was assumed in all six cases. As the correlation scale increases, the mean and standard deviation of log travel time also increase. At first inspection, this result may not seem intuitively correct, and an explanation is required. Generally speaking, the heterogeneity is characterized by the magnitudes of both variance and correlation. That is, a homogeneous medium has a zero variance and infinite correlation scale, and conversely, a highly heterogeneous medium has a large variance and small correlation scales. Thus, a variance assigned to a perfectly correlated medium (i.e., a medium with infinite correlation scale) may strictly represent uncertainty in measurements of the parameters. For other cases, one can explain the physical meaning of the results as follows. If the correlation scale is zero, spatial variations in transmissivity values between the starting and the ending points along the travel path are statistically independent. This implies that the heterogeneity encountered by a particle in each realization will be the same regardless of the sequential arrangement of the transmissivity values. Hence, the arrival times are identical among realizations. As the correlation scale increases, the sequential arrangement of the transmissivity values becomes important. This results in different arrival times among realizations.

Clifton et al. (1985) also found that an increase in the degree of cross-correlation between transmissivity and effective thickness causes a decrease in the variability of the predicted groundwater travel times. Independence between

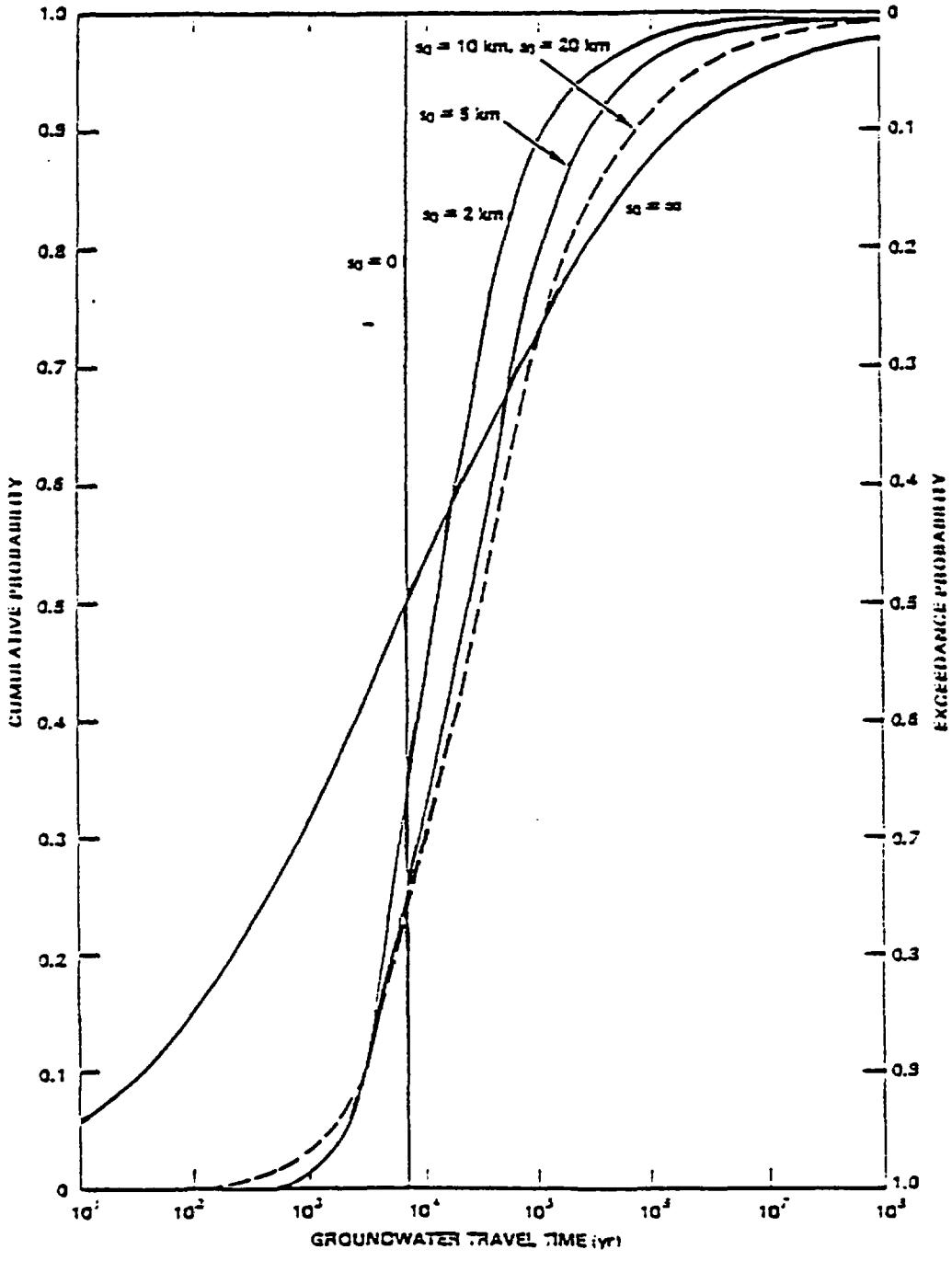


Figure 4.19. Effects of correlation scale of transmissivity on the cumulative probability of groundwater travel time. (From Clifton et al., 1985).

transmissivity and effective thickness results in a greater variability in the predicted travel times. The groundwater travel time distribution was found to be sensitive to the size of the model domain. The average travel time became longer as the width of the model domain decreased, and vice versa.

In summary, the results of the study by Clifton et al. (1985) shows that groundwater travel times are sensitive to parameters characterizing the spatial variability, the scale of representation of model parameters, and the size of model domain. A major technical drawback of the study is that the calculation of pathline was not clearly presented. This may have significant impacts on the accuracy of the predicted travel times, especially if the medium is heterogeneous. Comparisons of the relative importance of various factors on the groundwater travel time distribution was absent. This information would be helpful in the analysis of uncertainties in travel times. Overall, the results of the study are pertinent to the understanding of some sources of uncertainty in groundwater travel time calculations.

Another interesting analysis of uncertainties in groundwater travel times and paths due to sample size was carried out by Cole and Foote (1987). In their study, a hypothetical, two-dimensional, square aquifer with two realizations of hydraulic conductivity field was used. The first realization represented a real world analog of the hydraulic conductivity field. It was derived from a block of Nevada topographic data to ensure that it contained a variety of spatial correlation scales related in a natural way. The topographic data, which were nearly normally distributed, were scaled in order to allow them to represent a reasonable range for the logarithm of hydraulic conductivity. In the second realization, the hydraulic conductivity field was filtered using a simple moving average technique to remove the high spatial frequency perturbations in hydraulic conductivity data (i.e. small-scale variations in K). The filtered data could be viewed as the data collected from large-scale hydraulic tests in which small-scale phenomena are averaged out. The unfiltered log

K data set had a sample mean of 0.0814 and a standard deviation of 1.28, and the filtered data have a mean of 0.0821, and a standard deviation of 1.18. In Figure 4.20, a comparison of the unfiltered and filtered log K distribution along a cross-section is shown. The autocorrelation function for the data set was determined to be anisotropic. The longest axis of the correlation ellipse was nearly diagonal to the square aquifer, running from north to south. The anisotropy ratio of the correlation lengths was about 3. Two flow situations were examined: Case (1) east-west flow, where east and west sides of the square aquifer were assigned as prescribed head boundaries, and impermeable boundaries were assigned at the other two sides; Case (2) south-north flow, where south and north sides of the aquifer were assumed to be prescribed head boundaries and impermeable boundaries were set for the other two sides. The flow domain was discretized into 257x257 grids and hydraulic head and stream functions were calculated using a finite difference model for steady-state saturated flow. The convective velocity vector was calculated at each grid location from the stream function (or hydraulic gradient), hydraulic conductivity, and effective porosity. A particle tracking technique was used to determine groundwater travel times. Some of the results of the analysis are illustrated in Figure 4.21

Several conclusions were drawn from the results of the analysis by Cole and Foote (1987). The arrival times of 50% of the total number of particles in both Cases 1 and 2 were reduced if the filtered data set was used (Figure 4.21). The filtered hydraulic conductivity field produced a narrower arrival time distribution because filtering results in reducing the number of different pathways. According to Foote and Cole (1987), simulations using the filtered data tended to underestimate the first arrival of particles if flow was more nearly aligned with the longest correlation scale of the hydraulic conductivity field (Case 2), and to overestimate the time of arrival if flow was perpendicular to the direction of the longest correlation scale of the log K field (Case 1).

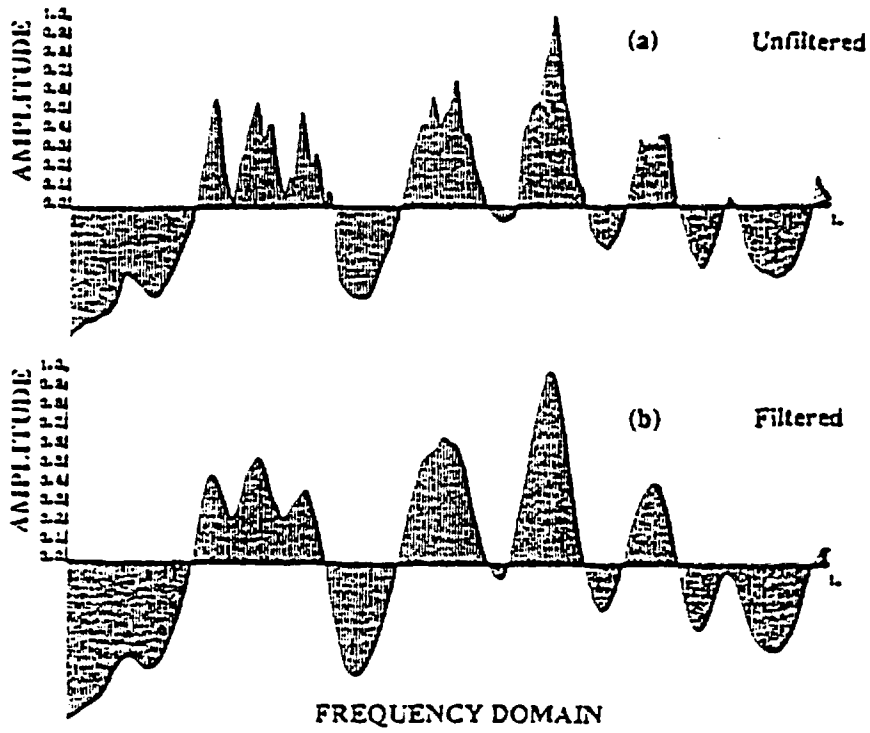


Figure 4.20. A comparison of the unfiltered (a) and filtered (b) log K data along a cross-section of a hypothetic aquifer. (Cole and Foote, 1987).

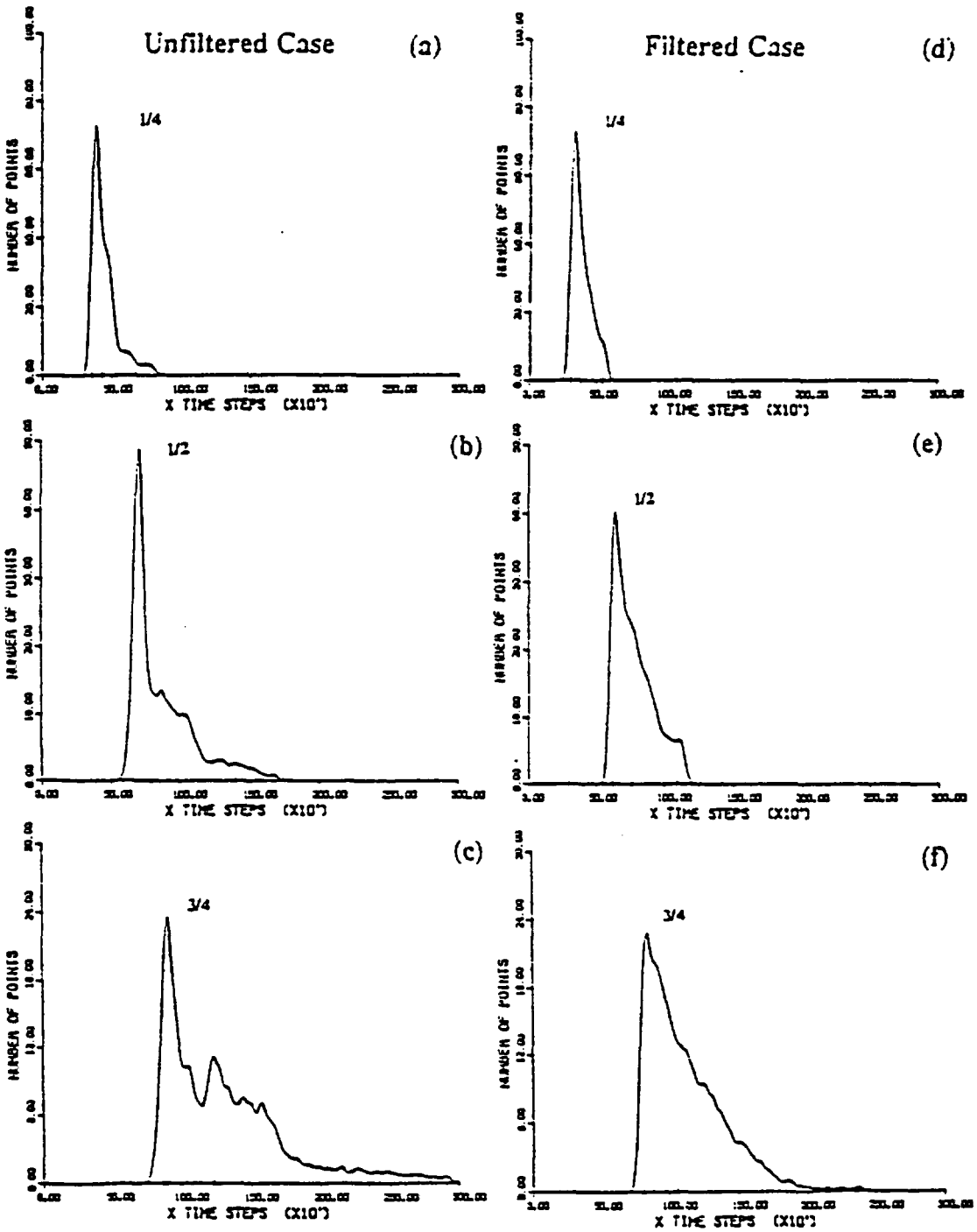


Figure 4.21. Particle arrival versus time curves (for the particles to travel 1/4, 1/2, and 3/4 of the distance across the domain) calculated for a pulse release of particles from a source in the east-west flow condition. Results are shown for the unfiltered data set (a-c) and for the filtered hydraulic conductivity data set (d-f). (Cole and Foote, 1987).

The results of the simulation are not conclusive because only two realizations of hydraulic conductivity fields (i.e., unfiltered and filtered) were employed. However, the effects of the REV assumption (i.e., the properties are uniformly distributed within the average volume), the scale of hydraulic testing, and size of spatial discretization in numerical simulations are well manifested in the analysis inasmuch as the filtering procedure is analogous to the averaging process in deriving hydraulic parameters from large-scale hydraulic tests. Similar spatial averaging procedures are often used in numerical models because hydraulic parameters assigned to each finite element or finite difference block represent the averaged values over the element or the block. These two conclusions agree with those by Clifton et al. (1985) (see Figure 4.18). The results of this study again demonstrate the problem with the groundwater travel times and paths concept.

As pointed out in section 2 dealing with basic concepts in groundwater hydrology, every property defined in groundwater hydrology involves a volume (REV). The property of the REV represents an average value over the volume, and the subscale variation in this property is ignored. The results of the analysis showed that ignoring the small-scale variability in hydraulic conductivity will result in underestimating the first arrival of tracer particles, overestimating the mean travel, and predicting a narrower arrival time distribution (Figure 4.18). Such effects may play a crucial role in regulating any nuclear waste repository facility, since the subscale velocity variation affects the fastest path by which groundwater travels. So, what is the proper volume for defining groundwater travel times and paths in order that the effects of subscale variations can be safely ignored? If one selects a volume that is large, then how do we account for subscale phenomena? On the other hand, if one selects a volume that is too small, then how do we characterize a large-scale aquifer with the properties defined over such a small volume? This is the dilemma we face if the concept of groundwater travel times and paths is to be used for

regulatory purposes.

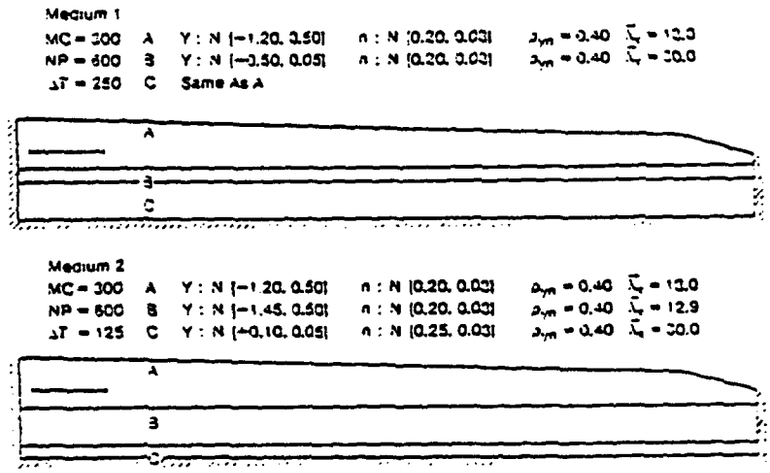
One of the key issues of the high-level nuclear waste repository site characterization program is determining if large-scale or small-scale hydraulic tests should be conducted to delineate the fastest path groundwater travel. This issue has been discussed earlier in various sections of this report, however, additional research addressing this issue has been presented by Smith and Schwartz (1981b). The objective of their study is to investigate the uncertainty in predicting mass transport due to three sources of uncertainties in data input to a model: (1) uncertainties due to the unknown spatial variation of the medium parameters, (2) uncertainties inherent in the particular model chosen to account for the heterogeneity, and (3) uncertainties related to the boundary conditions imposed on the flow domain.

A hypothetical water table aquifer was studied where the sides and bottom were assumed to be no-flow boundaries for both water and solute, and the water table represented the upper boundary for the region. A particle tracking model (Smith and Schwartz, 1980) was used to simulate the transport of a tracer in this aquifer. Monte Carlo simulation was used to form estimates of the probability distributions on model output. Hydraulic conductivity and porosity values of the aquifer were assumed to be statistically homogeneous, and their spatial structure was represented by a nearest-neighbor model (Smith and Freeze, 1979a). Furthermore, hydraulic conductivity and porosity were considered to be correlated and lognormally and normally distributed, respectively. Three hundred realizations of hydraulic conductivity and porosity fields were analyzed for transport of 600 particles. Statistics (mean and standard deviation) were computed for the first and last arrival times, as well as, for the arrival time of the maximum mass.

Most of the results are similar to those by Clifton et al. (1985), and Cole and Foote (1987). However, Smith and Schwartz (1980) also investigated cases where large, recognizable, geologic structures (such as stratifications) were present. The

aquifer consisted of layers of two distinct materials (sand and silt). Within each layer, hydrologic properties were assumed to be statistically homogeneous processes. Figure 4.22 shows the schematic diagram of the layered geologic formations with thin, relatively uniform higher-conductivity layers used in their simulation experiments. Table 2 summarizes the statistics of simulation results for the two scenarios shown in Figure 4.22. Results of the simulations showed that the fraction of mass which moves relatively quickly into the higher conductivity bed determined the initial arrival statistics. Because a small standard deviation in log hydraulic conductivity was assigned to the bed, the result is a smaller standard deviation in the initial arrival time than that in non-layered case. However, uncertainties in predicted arrival times can still be fairly large because of the sensitivity of transport to the within-layer heterogeneity. Again, this result is supportive of the position of this report on the importance of subscale variability. The result also sheds light on the high-level nuclear waste repository site characterization program. Large-scale permeable formations have to be identified by geologists or hydrogeologists as suggested by Williams (1988). However, small-scale tests are also necessary in order to define the variability within the formations. The subscale variability should then be treated stochastically.

Schwartz et al. (1983) employed a Monte Carlo technique to analyze macroscopic dispersion in fractured media. Mass transport in hypothetical two-dimensional, fractured aquifers was simulated using a particle tracking technique. Fractures in the aquifers are represented as linear features defined in terms of the location in space of their midpoints, their orientation with respect to the coordinate axes, their length, and their aperture. Some of these parameters were considered as random variables in the analysis. The fracture length distribution was assumed to have a negative exponential distribution. The distribution of fracture aperture was considered to be lognormal. Flow in the fractures was idealized as laminar flow



MC = number of realizations
NP = number of particles
ΔT = time step
Y:N[-1.20, 0.50] = log K; normally distributed with mean -1.20 and standard deviation 0.50
n = porosity
ρ_{yn} = cross-correlation between log K and n
$\bar{\lambda}_x$ = average correlation scale in the x direction

Figure 4.22. Schematic diagram of the layered geologic media with thin, relatively uniform higher conductivity layers used in the simulation experiments. (Smith and Schwartz, 1981).

Table 2. Comparison of transport behavior in systems with thin, relatively uniform higher conductivity layers extending across the basin. (Smith and Schwartz, 1981).

	Medium 1	Medium 2
Initial arrival		
$\bar{t}_i$	7.240	3.590
S_{t_i}	1.630	660
Time of maximum mass		
$\bar{t}_{max}$	11.440	4.240
$S_{t_{max}}$	5.760	1.050
Last arrival		
$\bar{t}_f$	32.200	7.740
S_{t_f}	7.310	2.590
Maximum mass at water table		
M_{max}	30.2	48.4
$S_{M_{max}}$	15.3	18.5
Mean location of arrival		
$\bar{z}$	299.0	299.4
$S_{\bar{z}}$	4.4	1.3
Standard deviation in location		
$\bar{S}_z$	1.0	0.4
Minimum location		
$\bar{z}_{min}$	294.9	298.0
$S_{z_{min}}$	20.4	3.8

through smooth parallel plates so that the cubic law which relates fracture hydraulic conductivity to fracture aperture could be applied. Sets of fractures were generated in a rectangular, two-dimensional aquifer with the assumption that the rock matrix had zero permeability. The aquifer was bounded by two constant head and two no-flow boundaries. A finite difference model was used to determine the hydraulic head distribution, and mass transport was then simulated using a particle tracking technique. The results of the study showed that the mass transport phenomena in fracture rocks are so complex that the classical macroscopic convection-dispersion equation does not seem to be appropriate. A single value of dispersivity or dispersivity function does not appear to characterize correctly the pattern of mass spreading in a fracture system.

4.3.2 Conditional Simulation. Conditional simulation is a special kind of Monte Carlo simulation technique. Unlike the Monte Carlo simulation discussed above, it imposes sample values at the sample points. That is, in each realization, parameter values are kept constant and equal to the measured values at a particular location. Thus, there will be no uncertainty at measurement points.

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 is shown in Figure 4.23. Briefly, the procedures of the conditional simulation are: (1) to generate nonconditional 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 of the simulations obtained in the first step by making the realizations consistent with the measured sample values. The first step is identical to the Monte Carlo simulation. For the second step, one has to employ kriging. From the actual sample values, kriging yields an estimate $K^*(x)$ (Figure 4.23a). If x is not a sample point, the true value K(x) is not available, and the kriging error $K(x) - K^*(x)$ remains unknown. However, the true value, K(x), equals the estimate plus the error in the estimate which we can write as:

$$K(x) = K^*(x) + [K(x) - K^*(x)] \tag{4.3.1}$$

Kriging can be performed using the measured values at the actual sample locations as data in a given nonconditional simulation (Figure 4.23b). The sample value of the given nonconditional simulation S(x) can be decomposed as the sum of the kriging estimate $S^*(x)$ and the kriging error, i.e., $S(x) = S^* + [S(x)-S^*(x)]$. Since this is derived from the nonconditional simulation, all terms are known. Note that $[S(x) - S^*(x) = 0]$ at the sample locations. By substituting $S(x)-S^*(x)$ for $K(x)- K^*(x)$, the

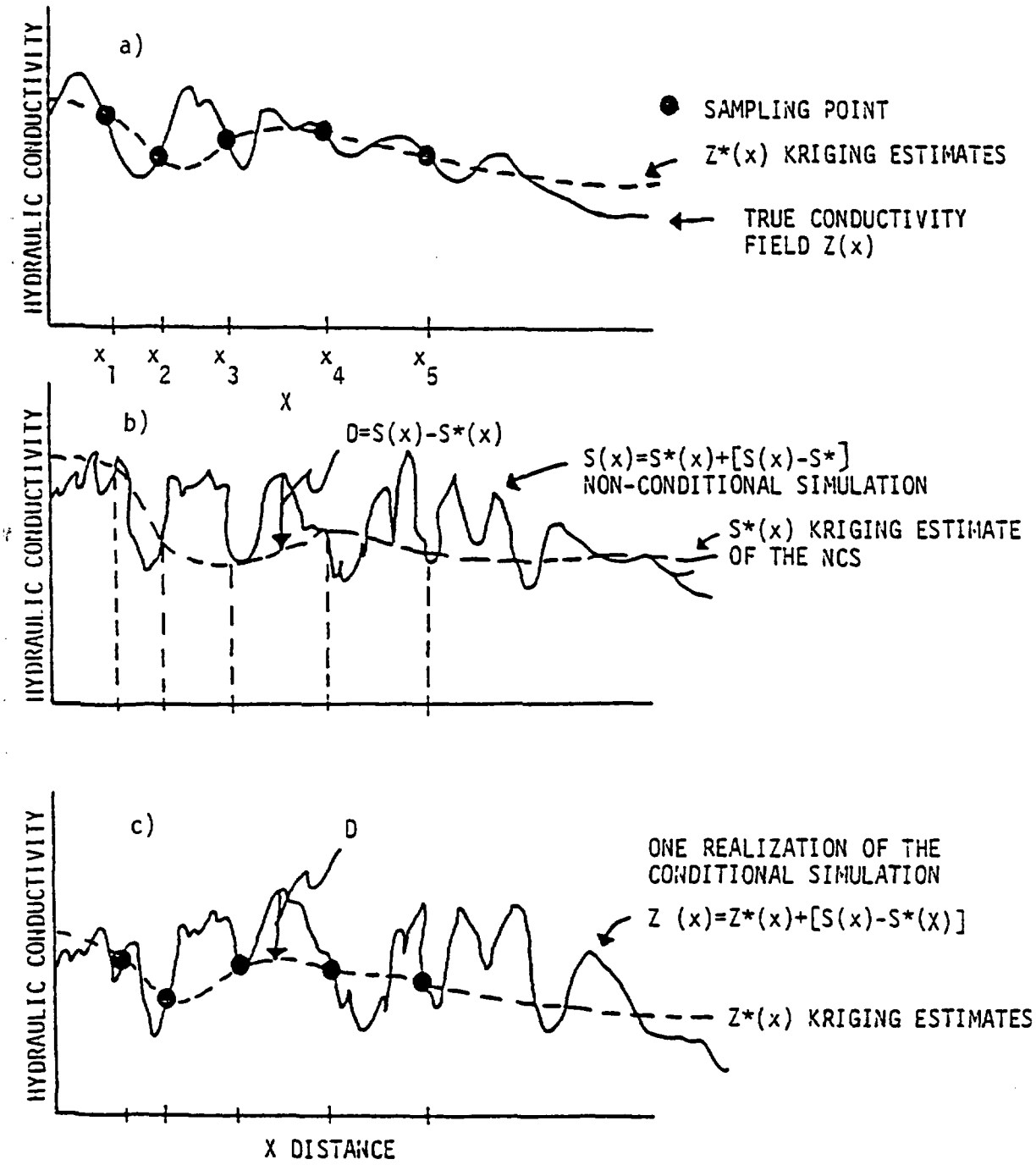


Figure 4.23. A schematic illustration of the conditional simulation.

K_s (x) for the conditional simulation is defined as:

$$K_s(x) = K^*(x) + [S(x) - S^*(x)] \qquad (4.3.2)$$

Therefore, K_s (x) is consistent with the measured values at the sample points, K_s (x) and K(x) have the same covariance functions. The average of many conditional simulations at a given point x is the kriging estimate, and their variance is the kriging variance.

Generally speaking, hydraulic property fields resulting from conditional simulation are; (1) smoother than unconditioned fields, but (2) more variable than kriged fields which essentially represent the conditional expected values.

The first application of conditional simulation to groundwater hydrology probably was the work by Delhomme (1979). He used 45 transmissivity data collected in the Bathonian aquifer in Normandy to investigate the effect of conditioning transmissivity values at sample locations on the uncertainty of the hydraulic head distribution. The first case he examined was steady- state flow through a rectangular hypothetical aquifer 10 km in length and 7.5 km in width. The aquifer was bounded by three impermeable boundaries and one constant head boundary. A uniform recharge over the aquifer area was assumed. Transmissivity values were considered to have a lognormal distribution with a spherical semivariogram as the spatial correlation structure. Thirty sample values were used with kriging to estimate the transmissivity at unsampled nodes of a 0.25 x 0.25 km regular grid. Fifty realizations of the logarithm of transmissivity (log T) fields incorporating the 30 samples were generated. Then, 50 head surfaces corresponding to the 50 transmissivity conditional simulations were produced by a numerical model. The results of the simulation indicated that conditioning by 30 log T samples did not lead to any significant decrease in uncertainty in head values at the center of the

aquifer. This was attributed to the fact that these 30 log T values were sampled far away from the outflow boundary which was a major controlling factor of the flow regime. Conclusions drawn from this study illustrate: (1) the importance of the locations of the log T samples with respect to the boundary conditions, and (2) that knowledge of head values at some locations and recharge rates. In addition, conditioning log T values may be helpful in reducing uncertainties in predicting hydraulic head values in heterogeneous aquifers.

Case 2 of the study by Delhomme (1979) is the Bathonian aquifer where it is bounded to the north by the sea. Steep hydraulic gradients occur in the southern part of the area which are due to local dewatering of mines. Discharge from wells, rainfall infiltration, interaction with streams, and leakage to or from overlying and underlying aquifers were considered in the simulation. Two possible sources of uncertainty on transmissivity were considered: (1) spatial variability and scattered sampling, and (2) measurement errors in T sample values. A similar approach to Case 1 was used. The conclusions drawn from the results of the analysis of Case 2 are: (1) the head surface cannot be reconstructed correctly from only the sample values of T, and (2) constraints on some head values tend to improve the agreement between simulated and observed head surfaces, without the transmissivity field necessarily being correct. Again, the flow rates to and from boundaries play important roles in reconstructing the head surface. Delhomme finally concluded that using conditioning on both head and log T values may be necessary in order to reduce the uncertainty in predicting the true head surface.

Conditional simulations pertinent to NRC's definition of groundwater travel time and path criterion were conducted by Smith and Schwartz (1981). They used this technique to study the role of hydraulic conductivity data in reduction of uncertainty in prediction of mass transport. Two cases were examined. In Case 1, they investigated the extent to which uncertainties in transport predictions are

reduced when hydraulic conductivity data act to constrain the possible arrangement of the heterogeneities. In Case 2, they investigated uncertainties in transport predictions using a hydraulic conductivity distribution estimated from a limited set of data.

In the first case, a hydraulic conductivity distribution along a two-dimensional, vertical cross-section of a hypothetical water table aquifer was generated using the nearest-neighbor model. They assumed statistical parameters (mean and variance) to characterize the variability of conductivity. This realization was assumed to be an analog of the site. Hydraulic conductivity values were sampled in this realization on a preselected grid, and this data set was used to estimate the parameters of the hydraulic conductivity distribution. The movement of contaminants from a hypothetical waste repository was simulated to determine various arrival times as solute mass exited from the aquifer.

As we described in the previous section (4.3.1), Monte Carlo simulations (300 realizations of hydraulic conductivity fields) were carried out based on the estimated statistical parameters without considering the conditioning at the sample grid using sample data. The movement of a swarm of 600 particles in each hydraulic conductivity realization was simulated using a transport model. The mean and coefficient of variation (i.e., standard deviation/mean) for each of the times of initial, maximum mass, and last arrival resulting from the 300 possible realizations were then analyzed. The results of this analysis represent the uncertainty in prediction. A small subset of the hydraulic conductivity values was sampled from the analog of a real-world site and was then used to constrain the hydraulic conductivity values at the sample locations. Three sample grids were used: Grid A had 12 sampling points, Grid B, 24 points, and Grid C, 36 points. Three hundred hydraulic conductivity fields were simulated in which the hydraulic conductivity values are identical to the sample values at the sample points.

Again, the mean and coefficient of variation for each of the arrival time distributions were analyzed. A comparison of the means and coefficients of variation of the unconditional and conditional simulations determined the effect of knowledge of hydraulic conductivity values at sample locations on uncertainty in prediction. That is, a decrease in the coefficient of variation can be taken as a measure of the reduction in the uncertainty in prediction. Effects of varying the number of samples were investigated. Surprisingly, for their data base, results of unconditional and conditional simulations indicated that knowledge of additional hydraulic conductivity data did not lead to large reductions in the uncertainty in the velocity field. This result is relevant to identifying uncertainties in groundwater travel time and in assessing data needs for site characterization.

The conditional simulations in Case 2 of Smith and Schwartz (1981) proceeded as follows. From a specified stochastic process with given parameters, a hydraulic conductivity field was constructed. Hydraulic conductivity values were sampled from this realization on a preselected grid, and this data set was used to estimate the parameters of the hydraulic conductivity distribution. A second realization was generated using these estimated parameters, while the hydraulic conductivity values were preserved at the measurement points. Mass transport was then simulated in this second realization. This two-step procedure was repeated over a set of trials in a Monte Carlo simulation to form the probability distributions of the arrival times.

Distinct differences exist between Cases 1 and 2. In Case 1, the parameters of the hydraulic conductivity distribution were estimated from the hydraulic conductivity values located on the sample grid. These estimated parameters and the data set were then fixed for all the realizations in that Monte Carlo experiment. For the simulation in Case 2, the estimated parameters of the stochastic process varied with each realization, as different sets of hydraulic conductivity values are located on

the sample grid. The statistical parameters estimated from the available hydraulic conductivity data are different from those prescribed as the properties of the ensemble. Thus, errors in estimating the parameters add additional sources of uncertainty in prediction. That is, a ratio formed between the coefficient of variation for the arrival times in the Case 2 simulations and a corresponding unconditional simulation will indicate the extent to which uncertainties are increased in estimating the mean and standard deviation in hydraulic conductivity. The larger the value of this ratio, the greater the importance of uncertainties in estimating the statistical parameters relative to the uncertainty introduced due to the unknown patterns of spatial variation in hydraulic conductivity. Table 3 summarizes the ratio for selected transport parameters for the Case 2 simulation. All the ratios are greater than 1, indicating additional uncertainties due to uncertainty in estimating the ensemble statistical parameters. However, such uncertainties are reduced as the number of samples increases.

A general conclusion drawn from the study by Smith and Schwartz (1981) is that unless a considerable number of field measurements are available to constrain the patterns of spatial variation in hydraulic conductivity, large uncertainties can be associated with seepage velocities. Individual hydraulic conductivity measurements do not reduce the uncertainty significantly because of the dependence of the local hydraulic gradient on the overall arrangement of heterogeneities within the flow domain. Smith and Schwartz (1981) suggested that more emphasis should be placed on in situ measurements of seepage velocity (fluid particle velocity). However, seepage velocity generally varies with time, and it is difficult to take any measurement in the field due to slow movement of groundwater. Therefore, their suggestion may not be practical. Finally, they emphasized that a careful selection of sample locations should focus on regions where the uncertainty in the seepage velocity is greatest. A carefully designed, integrated sampling program may play an

Table 3. Ratios of the coefficients of variation in various arrival times resulting from the conditional simulation to those from the unconditional simulation in Case 2 study (Smith and Schwartz, 1981).

	Sample Grid		
	A	B	C
Initial arrival	1.44	1.12	1.03
Time of maximum mass	1.59	1.22	1.13
Last arrival	1.61	1.32	1.30

Here $\mu_y = -1.45$, $\sigma_y = 0.50$, $\bar{\lambda}_x = 12.5$, $\bar{\lambda}_z = 6.3$.

important role in the reduction of uncertainties in solute transport predictions.

4.3.3 Spectral Analysis. Spectral analysis is generally an analytical approach which includes perturbation analysis. This approach has been used extensively by Gelhar and his co-workers (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, and c; Mantoglou and Gelhar, 1987a, b, and 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:

$$\frac{\partial}{\partial x_i}\left[K\frac{\partial h}{\partial x_i}\right] = 0, \qquad i=1,2,3 \tag{4.3.3}$$

where K is the 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 (4.3.3) can be rewritten as:

$$\frac{\partial^2 h}{\partial x_i \partial x_i} + \frac{\partial \ln K}{\partial x_i}\frac{\partial h}{\partial x_i} = 0 \tag{4.3.4}$$

If the natural log of hydraulic conductivity, lnK, and the hydraulic head, h, are assumed to be second-order stationary stochastic processes, the equation becomes a stochastic partial differential equation, and lnK and h can be represented by means and perturbations of these values about their means:

$$h = H + h' \qquad E[h] = H, \text{ and } E[h'] = 0 \tag{4.3.5a}$$

$$\ln K = F + f \qquad E[\ln K] = F, \text{ and } E[f] = 0 \tag{4.3.5b}$$

where H and F are the means of h and lnK, respectively. The perturbations are h' and f for h and lnK, respectively. By substituting the representations (equation 4.3.5) in equation (4.3.4), and taking the expected value of it, we obtain a mean equation:

$$\frac{\partial^2 H}{\partial x_i \partial x_i} + \frac{\partial F}{\partial x_i} + \frac{\partial F}{\partial x_i}\frac{\partial H}{\partial x_i} + E\left[\frac{\partial f}{\partial x_i}\frac{\partial h'}{\partial x_i}\right] = 0 \qquad (4.3.6)$$

Substracting the mean equation from equation (4.3.4) gives:

$$\frac{\partial^2 h'}{\partial x_i \partial x_i} + \frac{\partial f}{\partial x_i}\frac{\partial H}{\partial x_i} + \frac{\partial F}{\partial x_i}\frac{\partial h'}{\partial x_i} - E\left[\frac{\partial f}{\partial x_i}\frac{\partial h'}{\partial x_i}\right] + \frac{\partial f}{\partial x_i}\frac{\partial h'}{\partial x_i} = 0 \qquad (4.3.7)$$

If we assume that the log hydraulic conductivity perturbation f is small (aquifer is not highly heterogeneous, say, $\sigma_f^2 < 1.5$ (Ababou et al., 1988), it is logical to expect the head perturbation h will be small. Then, it is reasonable to neglect higher order terms so that the perturbation equation can be written as:

$$\frac{\partial f}{\partial x_i}\frac{\partial H}{\partial x_i} + \frac{\partial F}{\partial x_i}\frac{\partial h'}{\partial x_i} + \frac{\partial^2 h'}{\partial x_i \partial x_i} \cong 0 \qquad (4.3.8)$$

This approximate equation describes the relationship between the perturbations in lnK 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 (4.3.4) with stochastic parameters is tantamount to ignoring the details of the flow behavior in each element but examining the average behavior of the flow in all the interconnected elements. The perturbation equation thus depicts the deviation of the flow from the mean flow only.

Now, the problem is how to solve the perturbation equation (4.3.8) and here the spectral method comes into the play. The spectral representation theorem (Lumley and Panofsky, 1964) states that if a stochastic process y(x) is second-order stationary, there is an essentially unique complex-valued, random distribution Z(k) on the frequency axis such that:

$$y(x) = \int_{-\infty}^{\infty} e^{ikx} dZ(k) \tag{4.3.9}$$

where i is a complex number and dZ is a generalized derivative of Z(k). Equation (4.3.9) is an example of a Fourier-Stieltjes integral. Furthermore, this process Z(k) represents complex-value random variables in a wave number k domain. In addition, this Z(k) process is related to covariance behavior as discussed below. More specifically, equation (4.3.9) simply is the inverse Fourier transform of Z(k), or Z(k) is the Fourier transform of the variable y(x) in the spatial domain. By doing this transformation, we have tranformed the variable from the spatial domain to the wave number domain. A physical analogy can be drawn with the effect of a glass prism on sunlight, as shown in Figure 4.24. A beam of white light can be regarded as a complex wave form changing with time, and composed of many colors (or wavelengths) of light. A prism acts as a frequency analyzer and separates the beam into its components, which appear as a rainbow display. Each colored band is separated from its neighbor by an amount proportional to the difference in their

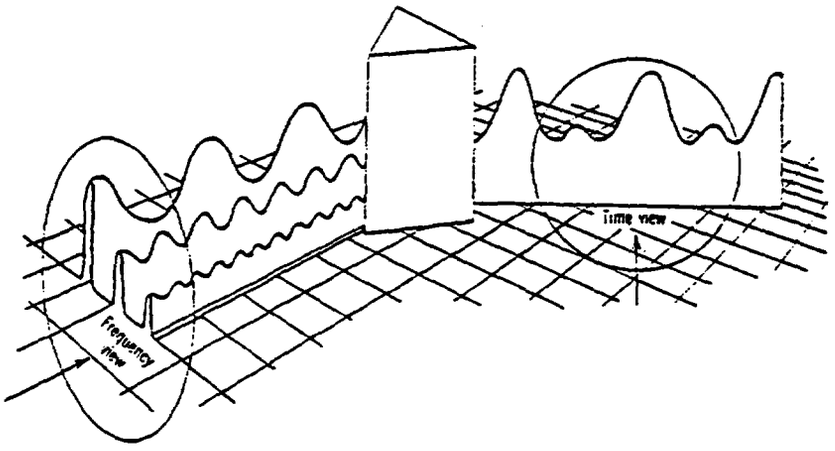


Figure 4.24.. A prism acts as a frequency analyzer, transforming white light (time domain) into its constituent spectrum of colors (frequency domain). Note the signals in the frequency domain are uncorrelated. (Davis, 1973).

wavelengths or frequencies, and the intensity of each band is proportional to the contribution of that particular wavelength to the total intensity of the original beam. Examining the spectrum of a light source may tell us many things: the composition of the source, its temperature, nature of the material through which the light passed, and so forth.

By the same token, examining the spectrum of spatial data may tell us a great deal about its nature and origin, information which may not be apparent in any other way. However, in this spectral analysis, the purpose of taking the Fourier tranform of the spatially correlated process y(x) is that after the transformation, Z(k) has been separated from its neighbor so that it is uncorrelated and the mathematics become easlier. Since Z(k) is uncorrelated, it has the following properties:

$$E[dZ(k_1)dZ^*(k_2)] = 0, \qquad \text{if } k_1 \neq k_2$$
$$E[dZ(k_1)dZ^*(k_2)] = S(k) \qquad k_1 = k_2 \tag{4.3.10}$$

where dZ^* is the complex conjugate, and S(k) is the spectrum of y which is merely the Fourier transform of its autocovariance function:

$$S(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-ik\xi}\, c(\xi)\, d\xi \tag{4.3.11}$$

Therefore, the inverse Fourier transform of the spectrum S(k) thus gives:

$$\text{cov}[\ y(x+\xi)', y(x)\ ] = c(\xi) = \int_{-\infty}^{\infty} e^{ik\xi}\, S(k)dk \tag{4.3.12}$$

Using the representation theorem for the perturbation terms f and h', and assuming uniform flow, equation (4.3.8) can be rewritten in terms of dZ processes:

$$dZ_h = \frac{iJ\ dZ_f}{k} \tag{4.3.13}$$

where J is the mean gradient in the x direction, $\partial H/\partial x$ and is assumed to be constant. Using the properties of the dZ processes, one can derive the relationship between the input and output spectrums, $S_{h'h'}$ and S_{ff}, respectively. That is:

$$S_{h'h'} = J^2 \frac{S_{ff}}{k^2} \tag{4.3.14}$$

By applying the inverse Fourier transform to the above equation, one thus obtains the head covariance functions, $c_{h'h'}(\xi)$, in terms of the hydraulic conductivity covariance function, $c_{ff}(\xi)$. If one uses a simple stationary three-dimensional covariance function for lnK, i.e.:

$$c_{ff}(\xi) = \sigma_f^2 \exp\left[-\left[\xi_1^2/\lambda_1^2 + \xi_2^2/\lambda_2^2 + \xi_3^2/\lambda_3^2 \right]^{1/2} \right] \tag{4.3.15}$$

where λ_1, λ_2, and λ_3 are the correlation scales in x_1, x_2, and x_3 respectively, the corresponding spectrum is

$$S_{ff}(k) = \frac{\sigma_f^2\ \lambda_1\lambda_2\lambda_3}{\pi^2 k^4 (1 + k^2\lambda^2)^2} \tag{4.3.16}$$

If we assume the hydraulic conductivity covariance function is isotropic (i.e., $\lambda_1 = \lambda_2 = \lambda_3$) and take the Fourier transform of (4.3.14), the head variance, $\sigma^2_{h'}$, is related to the variance of the hydraulic conductivity, σ^2_f , by:

$$\sigma^2_{h'} = c_{h'h'}(0) = \frac{1}{3} J^2 \sigma_f^2 \lambda^2 \tag{4.3.17}$$

The variance equation, (4.3.17), provides us with information on how the spatial variation in hydraulic conductivity affects the spatial variation in hydraulic head. In other words, it provides us with a measure of the deviation of hydraulic head from its mean value predicted using an effective hydraulic conductivity.

The spectral approach is also useful for deriving the effective hydraulic conductivity for such a stochastic random porous medium. To derive the effective hydraulic conductivity, we will again conceptualize the heterogenoeus aquifer as a collection of many finite elements with spatially correlated hydraulic conductivity values in which the flux is assumed to obey Darcy's law. Thus, the average flux over the entire heterogeneous aquifer then becomes the expected value of all the fluxes from each individual element within the aquifer. That is:

$$E[\, q_i \,] = -E\left[K \frac{\partial h}{\partial x_i} \right] = -E\left[K_g \, e^f \left[\frac{\partial H}{\partial x_i} + \frac{\partial h'}{\partial x_i} \right] \right] \tag{4.3.18a}$$

Using a series expansion for e^f, (4.3.18a) becomes:

$$= -K_g \, E\left[\left[1 + f + \frac{f^2}{2} + \cdots \right] \left[\frac{\partial H}{\partial x_i} + \frac{\partial h'}{\partial x_i} \right] \right]$$

$$= K_g \left[J_i \left(1+\frac{\sigma_f^2}{2}\right) - E\left[f\left(\frac{\partial h'}{\partial x_i}\right)\right]\right] \tag{4.3.18b}$$

where $K = K_g \exp(f)$ with $E(\ln K) = \ln K_g$. Equation (4.3.18b) represents the average of fluxes in all elements, or the ensemble average of the fluxes. The last term on the right-hand side of equation (4.3.18b), representing the cross-correlation between the log hydraulic conductivity and the hydraulic gradient perturbations, can be evaluated using the representation theorem as well. If we assume that Darcy's law (i.e., flux has to be linearly proportional to the hydraulic gradient) is valid for this ensemble flux, then:

$$E[\ q_i\ ] = K_{eff}\ J_i \tag{4.3.19}$$

where J_i is the mean gradient in direction i (i.e., $\partial H/\partial x_i$) and K_{eff} is the effective hydraulic conductivity. Based on equation (4.3.19), K_{eff} is merely a constant of proportionality between the ensemble flux and the mean gradient. In other words, K_{eff} is a parameter which produces the mean flux with the knowledge of the mean hydraulic gradient. By comparing equations (4.3.18) and (4.3.19), it is easy to see that:

$$K_{eff} = K_g \left[\left(1+\frac{\sigma_f^2}{2}\right) - \frac{E[f(\partial h'/\partial x_i)]}{J_i} \right] \tag{4.3.20}$$

As indicated in equation (4.3.20), the effective hydraulic conductivity clearly lumps together the variability of lnK, σ_f^2, and the covariance of f and $\partial h'/\partial x_i$, $E[f(\partial h'/\partial x_i)]$,

which varies with flow. Therefore, the effective hydraulic conductivity is not a simple arithmetic average of all hydraulic conductivity values of individual elements, but it depends on the flow regime as well.

Using the spectral technique discussed above, Bakr et al. (1978) analyzed the effects of spatial variability on steady-state groundwater flow. Closed forms of head variance expressions were derived for one- and three-dimensional flow fields in which hydraulic conductivity is a spatially-varying stochastic process. Several important conclusions were drawn from the results of the study. Hydraulic head distribution tends to be smooth due to the damping effect of the groundwater flow system. That is, the head values are correlated over a much longer distance than the hydraulic conductivity values. The head values are anisotropic (i.e., correlated over a longer distance in the direction perpendicular to the flow direction.), even if the hydraulic conductivity field is statistically isotropic. The head variance can be related to the variance of lnK by:

$$\sigma_{h'}^2 = \beta \sigma_f^2 \, J^2 \, \lambda^2 \tag{4.3.21}$$

where β is a constant: 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 logarithms of hydraulic conductivity, and λ is the correlation scale. The equation indicates that the variability in head predicted by a three-dimensional model is smaller than that predicted by a one-dimensional model. This means that a three-dimensional model would be much more appropriate for analyzing uncertainties in groundwater travel times and paths. Furthermore, it is manifest from equation (4.3.21) that studying the correlation scale is important in the calculation of head variance or uncertainty in head prediction as discussed in the section dealing with Monte Carlo simulation.

Gutjahr et al. (1978) extended Bakr's study to define effective hydraulic conductivity for heterogeneous lnK fields. They concluded that the effective hydraulic conductivity in one-dimensional flow, perpendicular to layerings, is the harmonic mean:

$$K_e = K_g \, e^{-\sigma_f^2/2} \tag{4.3.22}$$

where K_g is the geometric mean of K, and σ_f^2 is the variance of lnK, and the arithmetic mean for flow parallel to beddings, i.e.:

$$K_e = K_g \, e^{\sigma_f^2/2} \tag{4.3.23}$$

In the three-dimensional flow situation, the effective hydraulic conductivity is given by:

$$K_e = K_g \, e^{\sigma_f^2/6} \tag{4.3.24}$$

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.

Both analyses by Bakr et al. (1978) and Gutjahr et al. (1978) assumed statistical isotropy for the random hydraulic conductivity field. Gelhar and Axness (1983) extended the analyses by Bakr et al. (1978) and Gutjahr et al. (1978) to investigate 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 4.25 shows that the anisotropy ratio for the case with $\lambda_1 = \lambda_2 \neq \lambda_3$ is dependent on the degree of variability of hydraulic conductivity in terms of the variance of lnK as well as the geometry of the heterogeneity as characterized by the ratio of λ_1/λ_3.

The effective hydraulic conductivities and head variance derived from the spectral analysis may have important practical implications on the prediction of groundwater travel times and paths. Generally speaking, there is a limited number of hydraulic conductivity values available for determining accurately the groundwater travel times and paths. As a first step toward solving such a complex problem, one may use the limited amount of data to determine the variance of lnK, and thus the effective hydraulic conductivity, using one of the equations (4.3.22), (4.3.23), or (4.3.24), depending on the dimensionality of the model. The mean flow behavior thus can be determined. Correlation scales can be estimated from the available data by using autocorrelation analysis. With an estimated mean gradient, variance of lnK, and correlation scales, the head variance in a statistically isotropic medium can then be determined, using equation (4.3.21). If there is no hydraulic conductivity data available, one might be able to resort to the known variances and correlation scales of similar kinds of materials reported in the literature (see table 2). The calculated head variance can be used as a measure of the error in the model as the result of unmodeled aquifer heterogeneity (i.e., the result of using effective hydraulic conductivity). Therefore, the head variance is an appropriate model calibration target to study for defining the detailed hydraulic conductivity distribution, provided that other sources of error are also considered. The hydraulic conductivity field obtained from the calibration may then be used to determine groundwater travel times and paths. A similar application of the above spectral results to field problems was also illustrated in the paper by Gelhar (1986).

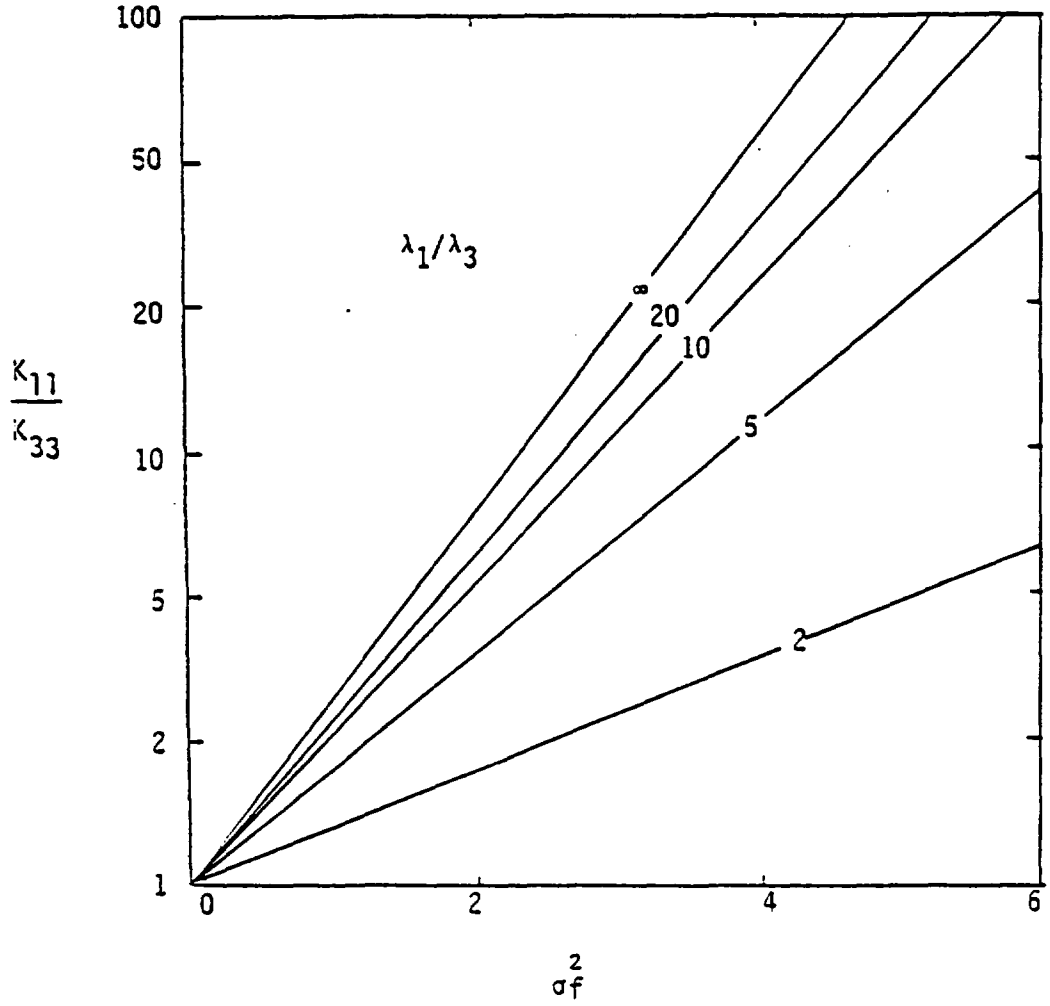


Figure 4.25. Anisotropy of effective hydraulic conductivity as a function of the variance of lnK, σ^2_f, and aspect ratio, λ_1/λ_3, for the case $\lambda_1=\lambda_2$. K_{11} and K_{33} are the principal effective hydraulic conductivies in x_1 and x_3 directions, respectively.

As emphasized many places in this report, the arrival time of a certain concentration of a tracer is similar to the groundwater travel time. The difference is that no tracer particles are involved, and the concentration is defined as the ratio of the weight of newly-arrived groundwater particles to the total weight of groundwater in the sample volume. If one has this concept in mind, it is clear that the nonreactive solute transport equation is the most appropriate model for determining the groundwater travel time. The use of the effective hydraulic conductivity predicts only the arrival of the center of the mass plume, and the arrival of fast moving groundwater particles due to subscale velocity variation is ignored. To analyze the effect of velocity variations on solute transport, the macrodispersion concept has to be introduced. This macrodispersion approach is analogous to the analysis of molecular diffusion at the microscopic scale discussed in section 2.6.

In order to use the macrodispersion approach, macrodispersivity must be defined. The dispersivity value at the laboratory scale can be related to the variation in grain size. Similarly, macrodispersivity can be related to the variation in hydraulic conductivity values at scales much smaller than the REV of the stochastic random field. The relationship between the macrodispersion and local-scale hydraulic conductivity variations was derived by Gelhar and Axness (1983) using a spectral analysis which will be discussed in the following section.

To examine the theory of macrodispersion, we will assume that the general equation describing transport of an ideal conservative solute by a fluid with constant density and viscosity in a saturated, homogeneous, three-dimensional porous media of constant porosity, n, is:

$$\frac{n\partial c}{\partial t} = E_{ij} \frac{\partial}{\partial x_i} \left[\frac{\partial c}{\partial x_j} - cq_i \right] \qquad i,j=1,2,3 \qquad (4.3.25)$$

where the standard Cartesian summation convention of Einstein is used and c is the concentration of the transported solute; q_i is specific discharge in the x_i direction; E_{ij} is a local bulk dispersion coefficient tensor equal to nD_{ij}; and D_{ij} is the local dispersion coefficient tensor. If D_{ij} is isotropic (i.e., the dispersion coefficient values are the same in all directions), then it is equivalent to D_d defined in Section (2.6). The local scale used here refers to the size of the volume (REV) over which the measured hydraulic conductivity is obtained. For example, if hydraulic conductivity is measured from a core sample, the local scale represents the size of the core. Thus, the local dispersion coefficient stands for the velocity variation at scales less than the size of the core sample (it includes molecular diffusion). Similarly, a local dispersion coefficient can be used to represent the velocity variation at scales much smaller than the scale at which the transmissivity is defined.

Conservation of total mass requires:

$$\frac{\partial q_i}{\partial x_i} = 0 \tag{4.3.26}$$

If a steady state condition is assumed (i.e., $n\partial c/\partial t = 0$), equation (4.3.25) becomes:

$$\frac{\partial c q_i}{\partial x_i} = E_{ij} \frac{\partial^2 c}{\partial x_i \partial x_j} \tag{4.3.27}$$

This equation is assumed to be adequate to describe the local-scale dispersion. In a large-scale heterogeneous aquifer, the log hydraulic conductivity, f; specific discharge, q; and concentration, c, are assumed to be stochastic processes. These parameters can be decomposed into a mean part and a perturbation part, i.e.:

$$c = \hat{c} + c,$$

$$f = \hat{f} + f'$$

$$q_i = \hat{q}_i + q'_i \qquad i=1,2,3 \tag{4.3.28}$$

where the head and the prime represent the mean and the perturbation, respectively. Substituting the above expressions into (4.3.27), one obtains:

$$\frac{\partial}{\partial x_i}\,[(\hat{c} + c')(\hat{q}_i + q'_i)] = E_{ij}\,\frac{\partial^2[\hat{c} + c']}{\partial x_i \partial x_j} \tag{4.3.29}$$

Because the parameters are stochastic processes, equation (4.3.29) describes concentration profiles in many realizations of possible heterogeneous aquifers (i.e., ensemble). Expanding terms and taking the expected value of the equation (i.e., taking the ensemble average) produces the mean equation:

$$\frac{\partial}{\partial x_i}\,\hat{q}_i\,\hat{c} + \frac{\partial}{\partial x_i} E[q'_i c'] = E_{ij}\,\frac{\partial^2 \hat{c}}{\partial x_i \partial x_j} \tag{4.3.30}$$

In other words, this is a transport equation which describes the mean profile of all the possible concentration profiles resulting from each realization of a heterogeneous hydraulic conductivity field. Comparing this equation to equation (4.3.25), which is the classic convection-dispersion equation, it should be evident that the first term in the left-hand side of the equation is the convective flux associated with the mean flow or specific discharge, and the second term is an additional flux, $E[q'_i c']$. This mass flux is defined as the macrodispersive flux resulting from the perturbation of velocity which is caused by the heterogeneity of the aquifer, neglected at the size where the effective hydraulic conductivity was defined.

If this macrodispersive flux is Fickian in nature, that is, this flux is linearly proportional to the mean concentration gradient (equation 2.6.1), and if the mean flow is aligned in the x_i direction so that $\hat{q}_1 = q \neq 0$ and $\hat{q}_2 = \hat{q}_3 = 0$, we may then write:

$$E[q'c'] = -q\, A_{ij} \frac{\partial \hat{c}}{\partial x_j} \tag{4.3.31}$$

where A_{ij} is the macrodispersivity tensor and q is the magnitude of the specific discharge vector. The work by Gelhar and Axness (1983) derived expressions for the A_{ij} term, relating A_{ij} to the variation in hydraulic conductivity, f'. This task was carried out by using the perturbation technique and the spectral representation theorem as used in the derivation of the effective hydraulic conductivity analysis. One of the results shows that:

$$A_{11} = \frac{\sigma_f^2 \lambda}{\gamma^2} \tag{4.3.32}$$

where A_{11} is the longitudinal macrodispersivity, σ_f^2 is the variance of f, λ is the correlation scale of statistically isotropic porous media, and γ is the flow correlation factor which depends on the direction of the mean flow and the orientation of the heterogeneity.

The practical implication of Gelhar and Axness's work is that the macrodispersivity values may be estimated from the knowledge of the variation of local-scale hydraulic conductivity values without conducting a large-scale field tracer experiment to determine the dispersivity values or the groundwater travel time. Generally speaking, a large-scale field tracer experiment is impractical in terms of

the time span required for such an experiment. However, local-scale hydraulic conductivity values are frequently measured in many aquifers. Data are available but limited. Hence, the macrodispersivity approach may provide a practical solution to many pollution problems (such as the high-level nuclear waste site characterization program).

However, the macrodispersivity approach produces the mean concentration profile only, as indicated by $\hat{c}$ in equation (4.3.30). The mean concentration profile represents the average values of concentration profiles occurring in many different aquifers (i.e., ensemble average, see section 2.6.1). As a result, the actual concentration profile observed in an aquifer may be quite different from the predicted one using the macrodispersivity. For example, Figure 4.26 shows the differences between an observed concentration distribution in the Borden sandy aquifer and an ensemble averaged (or mean) concentration distribution calculated from the classic convection-dispersion equation with macrodispersivity values. Determining the difference between the two profiles is necessary. To evaluate the difference, Vomvoris and Gelhar (1986) analyzed the mean concentration variance. They 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. The results imply that the concentration variance could be large depending on the magnitude of the parameters.

Before we illustrate the practical application of the macrodispersion theory to the groundwater travel time problem, recall that the concentration is simply the weight ratio of the newly arrived groundwater to the groundwater (including "new" and "old" water) in a sample volume. If the statistical parameters of the hydraulic conductivity distribution are known, either estimated from a limited amount of data or obtained from information from other similar aquifers, one can then calculate the breakthrough curve at the accessible environment using equation (4.3.30) and

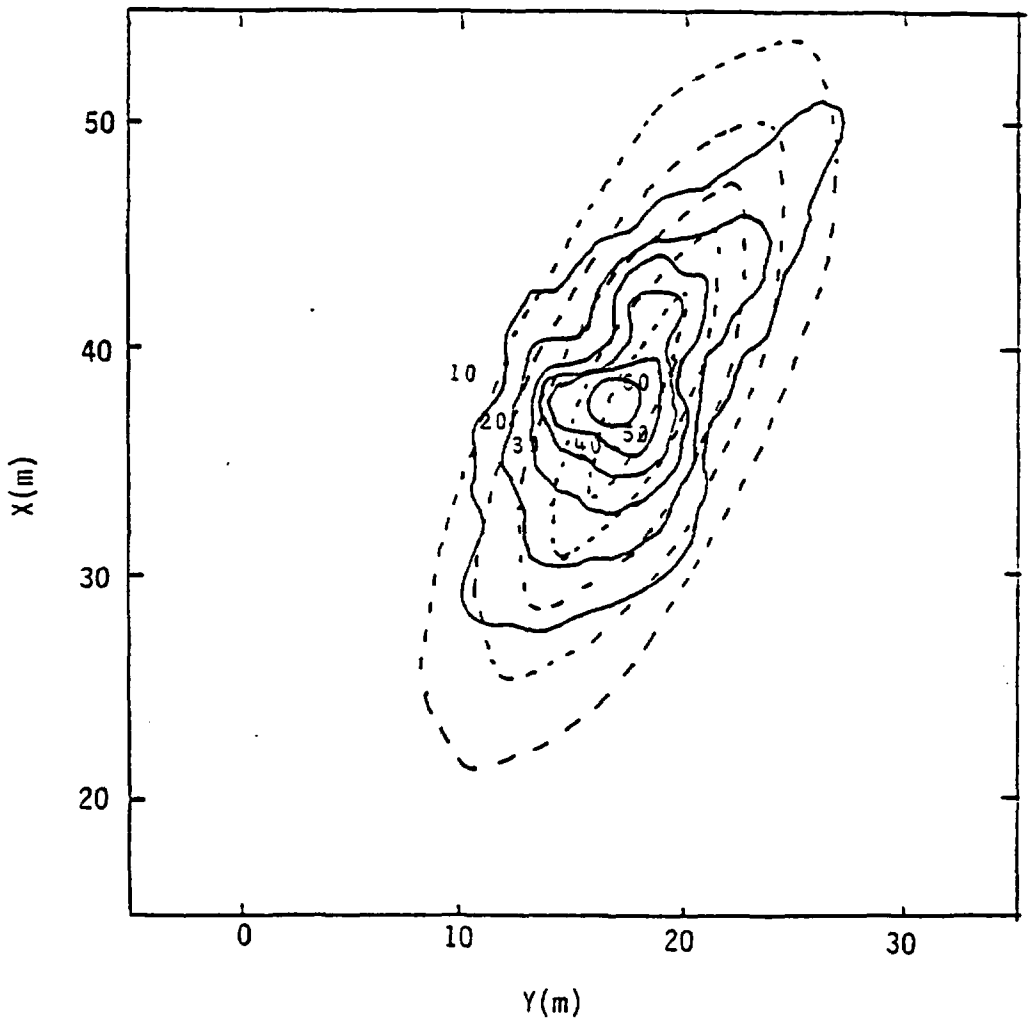


Figure 4.26. A schematic illustration of an observed depth-averaged concentration profile (solid) and a mean profile (dash), calculated from the macrodispersion equation (modified from Sudicky, 1986).

macrodispersivity values. This concentration breakthrough curve represents the arrival time distribution of different amounts of "new" water. Consequently, if a proper concentration of a tracer is defined as a criterion, then the arrival time can be defined. For the reason that the calculated concentration is the mean concentration, one should use the equations provided by Vomvoris and Gelhar (1986) to determine the variance of the mean concentration. An error band (plus or minus one concentration standard deviation about the mean concentration) can be calculated which indicates the range of the uncertainty in the mean concentration profile. Hence, the uncertainty in groundwater travel time is quantified.

Similar research on macrodispersion has been presented by many other researchers (e.g., Dagan, 1985, 1986, 1987; Neuman et al., 1986; Winter et al., 1984; Matheron and De Marsily, 1983). Dagan (1987) used the Eulerian velocity field to derive formulas for the time-dependent macrodispersivities in two-dimensional planes and three-dimensional aquifers. This approach is similar to Taylor's theorem on diffusion dicussed in section 2.6. However, in Dagan's analysis, the velocity field is related to the heterogeneity structure of the hydraulic conductivity field through the governing groundwater flow equation. The hydraulic conductivity field is considered to be statistically isotropic. For early time periods (i.e., $t << \lambda/v$), the spatial concentration variances (the square of the standard deviation of the plume concentration distribution: this is similar to the w^2 in section 2.6.1) are given by

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

$$\text{and } \sigma_{22}^2 (t) = \sigma_{33}^2 (t) = \frac{1}{15} \sigma_y^2 v^2 t^2 + 2 D_T t \qquad (4.3.33)$$

for three-dimensional flow, where σ_{11}^2, σ_{22}^2, and σ_{33}^2 are the concentration variances in

the direction of flow, and 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. σ_y^2 represents the variance of the natural log of 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 anaylsis are:

$$\sigma_{11}^2 = \frac{3}{8}\,\sigma_y^2\,v^2\,t^2$$

$$\sigma_{22}^2 = \frac{1}{8}\,\sigma_y^2\,v^2\,t^2 \qquad (4.3.34)$$

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

$$\sigma_{11}^2 \cong 2\sigma_y^2\,v\lambda t + 2D_L\,t$$

$$\sigma_{22}^2 = \sigma_{33}^2 \cong \frac{2}{3}\,\sigma_y^2\,\lambda^2\,t \qquad (4.3.35)$$

and the two-dimensional results,

$$\sigma_{11}^2 \cong 2\sigma_y^2\,\lambda vt\left[1 - \frac{3\ln(vt/\lambda)}{2vt/\lambda}\right]$$

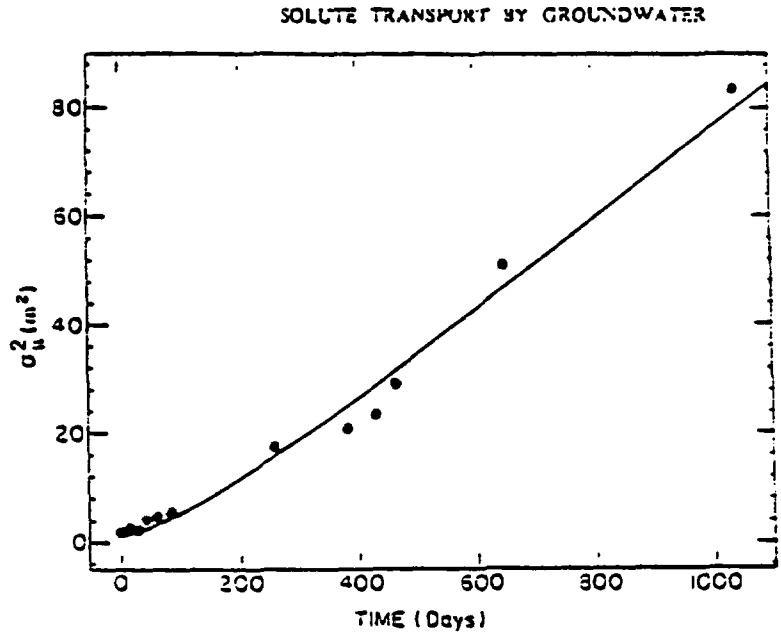
$$\sigma_{22}^2 \cong \sigma_y^2\,\lambda^2\,[\,\ln(vt/\lambda) + 0.933\,] \qquad (4.3.36)$$

Note that the concentration variances (equations (4.3.33) and (4.3.34)) for early time

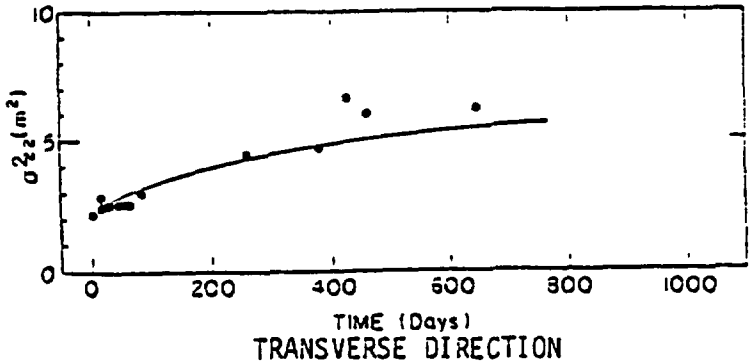
periods depend on t^2, implying the macrodispersion coefficient grows with time. For late time periods, the concentration variances (equations (4.3.35, and 4.3.36)) are a function of t only. This relationship implies that the macrodispersion coefficient is constant over time. Moreover, equations (4.3.33 - 4.3.36) do not predict the shape of the concentration plume but its relative size. Thus, no classic convection-dispersion which assumes the validity of Fick's law is used.

In generally, these results compare favorably with those obtained from a field tracer experiment (Sudicky, 1986) conducted in a sand aquifer in Canada (see Figure 4.27). A recent field tracer experiment by Garabedian (1987) in a glacial outwash aquifer also indicated that the stochastic results (i.e., Gelhar and Axness, 1983; and Dagan, 1987) are suprisingly robust, regardless of many assumptions used in the development. However, the robustness may be attributed to the fact that the variance of log hydraulic conductivity in those two aquifers is small so that the first-order approximation used in stochastic analysis is justifiable. The validity of the stochastic results, the reviewers of this report believe, still remains to be tested with tracer experiments in many different geologic environments.

Overall, the major advantage of the analytical approaches by Gelhar and Axness (1983), and Dagan (1987) is that they provide us with an explicit formula showing the relationship between the variance of inputs (such as hydraulic conductivity) and the head variance, or mean concentration profile and its variance, without conducting numerous computer experiments as required by the Monte Carlo simulations (such as Clifton et al., 1985; Smith and Schwartz, 1980, 1981a and b). Additionally, the results of the analytical approach (i.e., Gelhar and Axness, 1983) also give us an explicit way to 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)



LONGITUDINAL DIRECTION



TRANSVERSE DIRECTION

Figure 4.27. A comparison of observed (dots) and theoretical (line) spatial concentration variance in the longitudinal and transverse directions (Dagan, 1987).

may be valid only for small values of variations in hydraulic conductivity because of the omission of product terms in the analysis. Several studies have shown the results to be valid even for the variance of f = 1. Therefore, one may expect the results from the spectral analysis to be valid for most unconsolidated materials where the variance in f may be less than 1. For cases where a large variance in f is expected (such as in fractured rocks where the variance of lnK has been reported to be about 8.7, (Neuman, 1987), the validity of the method remains to be tested. The other drawback of the spectral approach is the stationarity assumption used in the analysis. In a basin-scale aquifer, the hydraulic conductivity field is likely to be nonstationary because of changes in deposition environments which may contain heterogeneities of a variety of scales, if the scale of our measurement is much smaller than the basin scale. Moreover, the validity of the classic convection-dispersion equation for large-scale problems is still under debate (see for example, Yeh, 1987). So, is it valid to apply such the results of the spectral analysis to these field problems?

It is generally agreed that the validity of the stochastic results still remains to be tested with tracer experiments in many different geologic environments. We previously noted a field experiment to validate the stochastic approach in an alluvial aquifer is currently in progress in Mississippi (Betson et al., 1985). We are unaware of similar experiments in unsaturated fractured rock. However, in the vadose zone there are two field-scale experiments in progress in New Mexico which are designed to evaluate multi-dimensional transport models in unsaturated media (Stephens et al., 1984; Wierenga et al., 1986).

4.3.4 Fractal Approach. In the past few years, geohydrologists and soil scientists have employed statistics to characterize the spatial variability of hydrological properties of geologic formations. Most of the hydrologic properties were found to be correlated over a large distance. Furthermore, many experimentally-determined variograms or autocorrelation functions of soils and geological data, exhibit some nugget effects. These nugget effects are generally viewed as a result of small-scale random noises which are spatially uncorrelated. This view implies that all variation within the closest sample spacing is infinitely erratic and possesses no spatial structure whatsoever. Although part of the nugget effect can be attributed to measurement errors which are likely to be spatially independent, experience shows that most of the noise at the macroscopic scale could be spatially correlated at the microscopic scale. This implies that the variability of hydrologic data exists in all scales and has a correlation structure at each scale (Dagan, 1986; and Gelhar, 1986). This scale phenomena was illustrated in Figure 4.13. In other words, the hydrologic data have a nested correlated structure. To analyze such a data set, a fractal approach has been proposed.

Fractals are based on the idea of 'self-similarity'; that is, the variations at one scale are manifested at another scale in similar ways. In other words, the irregularity of a process is independent of the scale of measurement. For example, the variation in effective hydraulic conductivity obtained from large-scale hydraulic tests should be similar to that from small-scale tests, at least according to the fractal concept. This self-similarity implies a long-range correlation structure in geostatistics terminology. That is, no matter how the size of the hydraulic test varies, the correlation between adjacent samples remains. For example, in Euclidean or classical geometry, the length, L, of a straight line can be easily determined by:

$$L = N \epsilon \tag{4.3.37}$$

where N is the number of measuring units of length ϵ. If we halve the size of ϵ, N will increase by a factor of two. Therefore, the length, L, is constant and independent of the scale of the measurement.

However, the Euclidean concept of a constant distance between two points independent from the scale of measurement may not be valid. Consider measuring the distance of a straight line between San Francisco and Washington, D.C. The distance as viewed by a person in outer space is essentially the length of a straight line between the two cities. The effects of topographic variation are completely neglected. However, the distance measured by a person on the ground will be much longer because this person has to consider the topographic variation of the land surface. Now, if we imagine the person is shrunk to the size of an ant, the distance between the two cities will then be even greater than that a normal-size person would experience, because an ant-size person has to consider not only the large-scale topographic variations such as hills, depressions, and mountains but also small-scale topographic variations such as heights of pebbles, rocks, and depths of cracks. The distance between the two cities, therefore, seems to grow infinitely as the scale of the measurement continuously decreases. This implies that the distance depends on the scale of the observation. This conclusion is based on the assumption that the small-scale topographic variation persists as the scale of the observation is reduced.

If the distance between two points varies with the scale of measurement, one may then ask the question: can we relate the distance between two points measured at our scale to those at scales different from ours? If the answer to the question is positive, we will then be able to predict phenomena at any scale, based on what we observed at our scale.

If we now assume that the topographic variations at all scales are self-similar, the distance between the two cities encountered by an ant-size person can then be scaled so that it is equivalent to that encountered by a normal-size person.

This concept is illustrated in Figure 4.28. Suppose the distance between two points A and B measured at a scale, ϵ, is defined as $L(\epsilon)$. A straight line distance, ℓ, represents the distance measured at a scale $\epsilon=\ell$ (Figure 4.28a). The number of measurements, N, is 1. If the measurement scale is reduced to $\ell/3$, the topographic variation at this scale will show up as indicated in Figure 4.28b. The distance between points A and B becomes $4\ell/3$ (i.e. N = 4). A further reduction of the measurement scale to 1/9 of ℓ reveals even more detailed topographic variation (Figure 4.28c). The number of measurements, N, required to measure the distance, then, is 16. If the measurement scale is further decreased to $\ell/27$, the topographic variation at this scale is shown in Figure 4.28d. In this case, N is 64. Note that the topographic variations in all the scales are similar in shape. Now, we plot the measurement scale, ϵ, versus N on log-log paper. A linear relationship between $\log\epsilon$ and log N is found (Figure 4.29). That is:

$$\log N = -D \log \epsilon \quad \text{or} \quad N = \epsilon^{-D} \tag{4.3.38}$$

where D is the slope of the line on the log-log plot. For the example, D is equal to 1.2618. This slope, D, is called the fractal dimension (Mandelbrot, 1983). In general, $1 < D < 2$. If $D = 1$, N is inversely proportional to the measurement scale ϵ, this indicates that the line is a topologically one-dimensional object. In other words, the topographic variation is independent of the scale of measurement. In the limiting case of $D = 2$, the line will be so irregular that it fills a plane (Mandelbrot, 1983). Again, here we are assuming that the topographic variation is self-similar at all scales. This is the most important property of the fractal geometry. Now, if we let:

$$F = N\epsilon^{D} \tag{4.3.39}$$

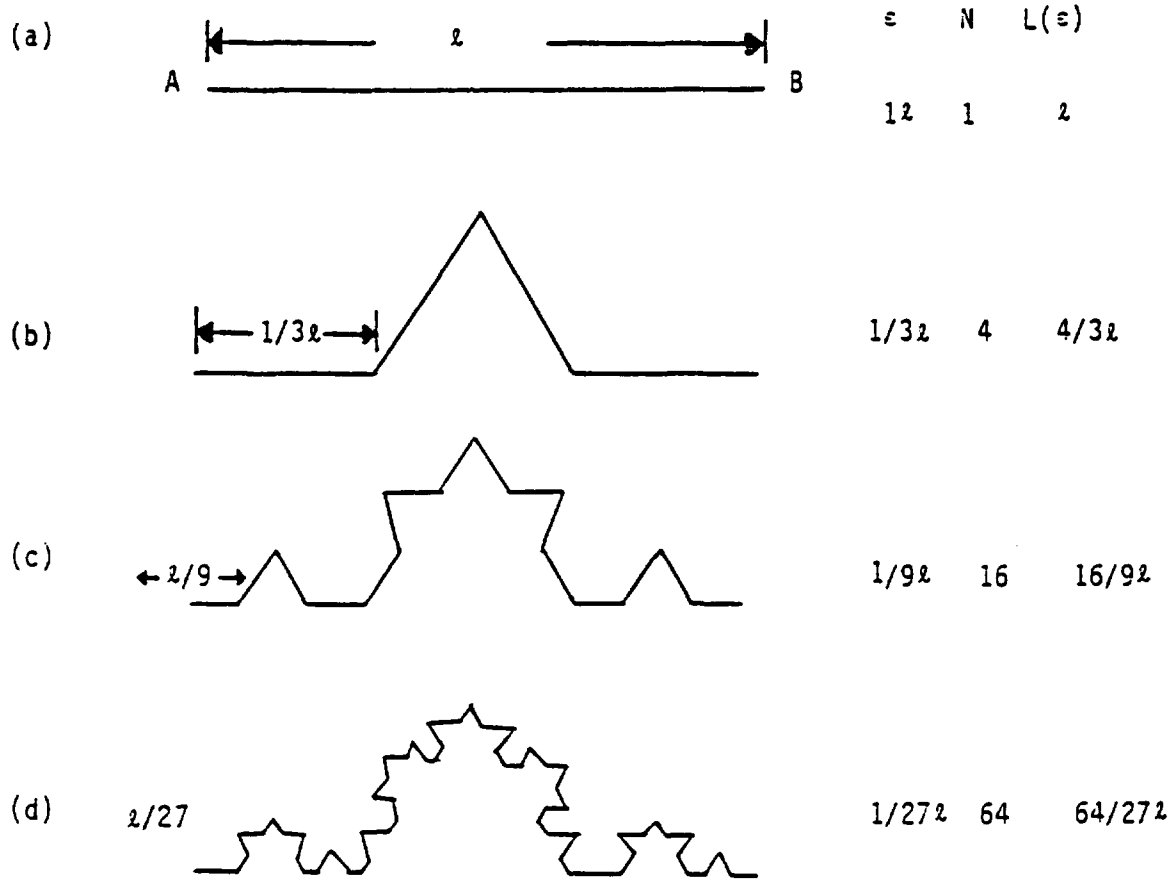


Figure 4.28. Schematic illustration of fractal concepts.
ξ is the measurement scale, N is the number of measuring units of length ξ, L is the total length, and ℓ is the straight line distance between A and B.

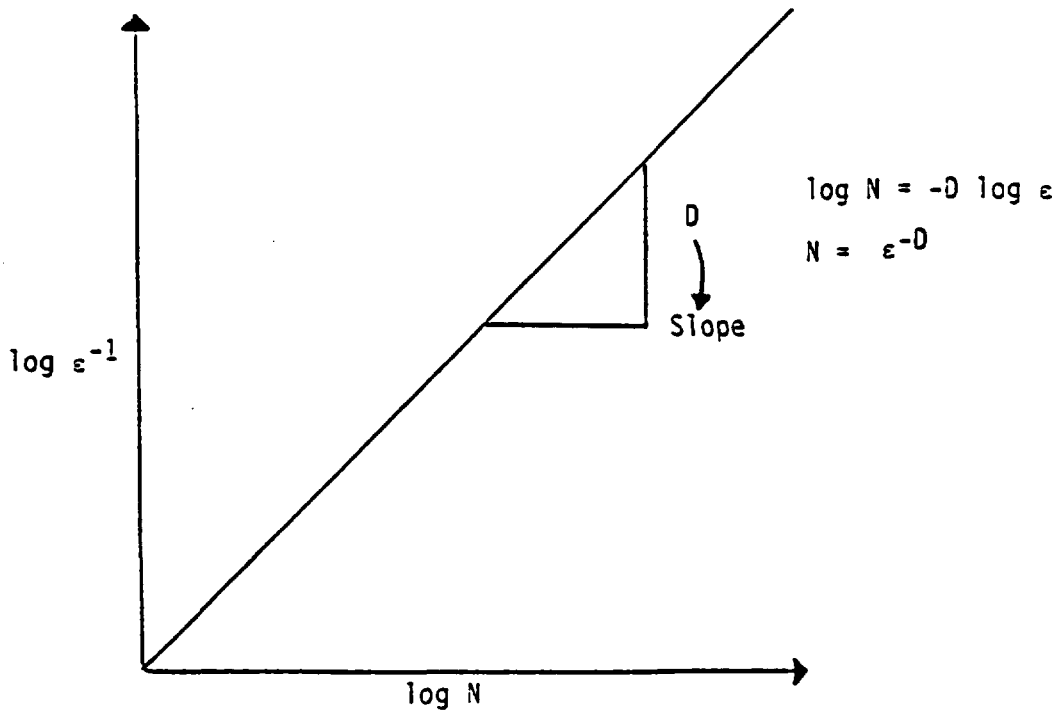


Figure 4.29. Schematic illustration of a linear relationship between log ε^{-1} and log N.

we can show that F is always a constant ($F = \ell^D$), no matter which scale of measurement is used. Thus, with the aid of the fractal dimension, we can properly scale the topographical variation at any scale to any measurement scale, if the variation is fractal, i.e. self-similar. The length of the distance between two points $L(\epsilon)$ at any measurement scale is then given as:

$$L(\epsilon) = F\ \epsilon^{1-D} \tag{4.3.40}$$

Equation (4.3.40) implies that as long as the distance between two points measured at a scale, ϵ, and the fractal dimension are known, one can determine the distance between two points as observed at any other scale. The practical implication of equation (4.3.40) is tremendous. We can predict large-or small-scale phenomena based on what we observe at our own measurement scale.

The fractal geometry concept has been recently applied to many scientific fields (Mandelbrot, 1967; Burrough, 1983a and b; Arya et al., 1985; Hewett, 1986) including groundwater hydrology (Wheatcraft and Tyler, 1988). Groundwater hydrologists, in general, rely on small-scale tests to obtain parameters for predicting flow or transport phenomena in large-scale geologic formations. Due to the spatial variability of the parameters, it is generally agreed that it is impractical to delineate the detailed spatial distribution of the hydrologic parameters in a deterministic sense. The alternative is to use effective, or mean parameters. This method is, however, not immune from difficulties. For example, there is field evidence showing that dispersivity, which is an effective parameter (see section 2.6.1), grows with the scale of experiment (Gelhar, 1986). So, how can dispersivity values obtained from small-scale laboratory experiments be scaled to large-scale problems?

To answer the above question, Wheatcraft and Tyler (1988) developed fractal scaling relationships to analyze dispersion in heterogeneous porous media. They

assumed that the path of a particle in a heterogeneous medium has fractal characteristics. The actual length a particle travels in a porous medium X_f can be related to the straight line distance of the medium, X_s, as:

$$X_f = \epsilon_c^{\,1-D} X_s^D \tag{4.3.41}$$

where ϵ_c is the fractal cutoff limit to ensure the actual length the particle travels is finite. The limit could be the smallest REV size. From equation (4.3.41), one can see that when the length between two points in a porous medium increases, the length of the actual travel path of a particle increases accordingly. Now, if we imagine a large-scale aquifer as a collection of many fractal stream tubes, the variance of the X_f is then given as:

$$\mathrm{var}(X_f) = \mathrm{var}\,(\epsilon_c^{\,1-D} X_s^D) \tag{4.3.42}$$

where X_s is constant. If we assume that the fractal dimension, D, is constant, then equation (4.3.42) can be rewritten as:

$$\mathrm{var}(X_f) = X_s^{2D}\,\mathrm{var}(\epsilon_c^{\,1-D}) \tag{4.3.43}$$

Equation (4.3.43) reveals that the variation in fractal length is due to the variation in the fractal cut-off limit and is related to the scale of the observation X_s. The variance of X_f can be considered as the spread of a plume in space. Then the macrodispersivity is:

$$A_x = \frac{1}{2}\,\mathrm{var}\,(\epsilon_c^{\,1-D})\,X_s\,\epsilon^{D-1} \tag{4.3.44}$$

This result, if D = 1, is consistent with that derived by Mercado (1967) in which the macrodispersivity of a perfectly-stratified aquifer is shown to grow linearly with travel distance. The expression (4.3.44) was also verified by using random walk models based on deterministic and stochastic fractal generators (Mandelbrot 1983). Gelhar et al. (1979) arrived at an expression for macrodispersivity that for early times is equivalent to Mercado's result, but for late times is equivalent to classical Taylor's dispersion, i.e., a constant dispersivity. The asymptotic approach to a constant dispersivity with distance predicted by Gelhar et al. (1979), Gelhar and Axness (1983), and Dagan (1987) is contrary to the fractal concept.

Finally, Wheatcraft and Tyler (1988) concluded that the dispersion model based on the fractal geometry concepts predicts that the field-measured dispersivity will be scale-dependent. The strength of the scale-dependence is directly related to the fractal dimension. They indicated that it is possible to obtain the fractal dimension from a tracer experiment in which the breakthrough curve is obtained for at least two travel distances. As long as the fractal dimension remains constant, it is then possible to predict solute migration at scales larger than the scale of the experiment in which the fractal dimension and the cutoff limit were obtained.

A direct application of fractal approach to the groundwater travel time position may be illustrated in the following example. If we agree that the actual travel path of a volume of groundwater is a fractal and can be adequately described by equation (4.3.41), i.e.:

$$X_f = \epsilon_c^{\,1-D} X_s^{D}$$

where, X_f is the total length of the tortuous groundwater path between two points with a straight line distance, X_s, and if one can assume that the velocity, v, of the groundwater is constant, the groundwater travel time is then given as:

$$\frac{X_f}{v} = t_f = \frac{1}{v} (\epsilon_c)^{1-D} (X_s)^D \tag{4.3.45}$$

where t_f is the actual groundwater travel time for the tortuous path between a straight line distance, X_s. If one further assume that a heterogenous aquifer can be represented by a bundle of such stream paths in a stochastic fashion, the variance in the arrival of tracer particles may be expressed as:

$$\mathrm{var}(t_f) = \frac{1}{v} X_s^{2D} \mathrm{var}[(\epsilon_c)^{1-D}] \tag{4.3.46}$$

The variance in t_f may thus represent the possible spreading in the arrival time of travel particles. This variance could be treated as a measure of uncertainties in groundwater travel time prediction. Based on the above equation, the variance in travel times will grow with X_s to the power of 2D and the variance of the fractal cutoff limit.

The fractal approach seems to be promising. Wheatcraft and Tyler, (1988) provided a new way of demonstrating the scale-dependent macrodispersion phenomena. Although, as they stated, considerable work still needs to be done to develop a more mature theory, there are some fundamental problems associated with the fractal approach.

One of the fundamental difficulties in the application of the fractal concept to groundwater hydrology arises from the self-similarity assumption in the fractal analysis. Self-similarity implies that the variations in hydrologic properties are similar at all scales. This assumption is a serious one and it still needs to be verified.

However, there is evidence supporting the self-similar nature of aquifer properties. An example is the porosity data reported by Hewett (1986). A sequence

of 2189 porosity values taken at intervals of 0.5 ft from a density porosity log in a well through a late Miocene-early Pleistocene sandstone formation (originally deposited in a deep submarine fan) was analyzed. The results showed that the porosity values may be correlated over 300 m. Hewett speculated an even larger range for horizontal correlations given the anisotropic nature of sedimentary formations. Such a long-range correlation suggests self-similarity in porosity data; the fractal approach is most suitable to represent the data.

On the other hand, Burrough (1983a, b) examined soil spatial data series in The Netherlands and the English Midlands that included percentage of clay, silt, pH, thickness, soil moisture capacity and topographic height. He concluded that soil does not vary exactly as an 'ideal' fractal but variation of physical properties is controlled by many independent processes that can cause abrupt transitions. Thus, soil does not possess the property of self-similarity at all scales. The spatial variation of soil properties is suggested to be a result of several closely spaced, nested scales of variation, occurring over short distances. He concluded that the geostatistical approach seems to be more appropriate than fractal analysis.

In groundwater transport cases, one may assume that the actual flow path of a particle in porous media is a fractal, as Wheatcraft and Tyler (1988) did. However, proving the validity of the assumption may be possible, but difficult. At present, we are somewhat skeptical of its validity. In fact, many stochastic analyses of dispersion in heterogeneous media (Gelhar et al., 1979; Gelhar and Axness, 1983; Dagan, 1987) showed that scale-dependent dispersion may exist only at early times of a transport process. An asymptotic dispersivity will develop after the plume is displaced at distances larger than the correlation scales of the hydraulic conductivity of media.

Results of the stochastic analyses by Gelhar and Axness (1983) and Dagan (1987) have been tested recently with carefully-designed large-scale field experiments

by Sudicky (1986), Freyberg (1986), and Garabedian (1987). Asymptotic macrodispersivities indeed occurred in these field experiments shortly after the injection of tracers. They all concluded that stochastic results by Gelhar and Axness (1983) and Dagan (1987) are robust and are in good agreement with field data. Although the robustness of the stochastic results may remain to be tested with many more large field experiments conducted at various geologic environments, it seems that continuously-growing dispersivity as predicted by the fractal approach may not exist, at least at a practical range of the size of aquifer. In fact, the boundless dispersivity predicted by the fractal analysis may arise from the fundamental assumption in the fractal approach which states that the variations in groundwater particle travel path are self-similar at all scales.

Regardless of whether the variation in flow channels in porous media (or the variation in intrinsic permeability which is determined by pore structure) is self-similar at all scales, the movement of the particles may not be self-similar. This is because the flow path of groundwater is also controlled by many other factors such as gradients, density variations, temperature variations, chemical variations, and degree of saturation under variable saturated flow conditions. Due to the influences of these factors, the travel path of a particle in the aquifer may likely be non-fractal, even if the pore channel is fractal. Theoretical analysis by Matheron and de Marsily (1980) seemed to demonstrate this conjecture. They showed that asymptotic macrodispersivity may develop at distances much less than the correlation scale of the hydraulic conductivity field if the flow is not parallel to the bedding. This results in an extra mixing effect and accelerates the development of an asymptotic macrodispersivity. This implies that the travel path no longer possesses the self-similar nature in properties of geologic formations. Deterministic numerical simulations of effects of heterogeneities on dispersion by Gannon and Yeh (1988) showed similar results. Hence, if the dispersivity depends on factors other than the

structure of porous media (which could be a fractal but needs to be proved), the fractal approach may face a formidable task as far as practical application is concerned.

Furthermore, it will be equally difficult to relate the parameters (such as fractal cutoff limit and fractal dimension) in Wheatcraft and Tyler's model to measurable physical parameters (such as hydraulic conductivity or porosity). This relationship needs to be explored.

5.0 SUMMARY AND CONCLUSION

There appears to be a fundamental problem with the NRC performance objectives for High Level Waste repositories, or "groundwater travel time (GWTT) objective" , which is stated in 10 CFR 60.113 (a)(2) as "...groundwater travel time along the fastest path of likely radionuclide travel from the disturbed zone to the accessible environment shall be at least 1000 years or such other time as may be approved or specified by the Commission." The "groundwater travel time along the fastest path" stated in the GWTT objective is an ambiguous phrase. The fastest path which groundwater travels can never be clearly defined because of the scale problem in groundwater hydrology. To circumvent this problem, the travel time of a certain concentration level of radionuclide should be used. The radionuclide or tracer would be a hypothetical release to the accessible environment which would travel under pre-waste emplacement hydrogeologic conditions. A concentration based standard is preferred because of the fact that the concentration represents the total mass flux (or total mass of newly-arrived groundwater) in a volume, resulting from flow phenomena of various scales. With this revised definition, a convection-dispersion equation can then be used to properly determine the arrival of the critical hyphotetical radionuclide or tracer concentration level. This approach overcomes the concern for data needed to compute the travel time for a particular molecule of radionuclide to arrive at the accesible environment. Unless this problem is resolved, the GWTT objectives will not be met.

In addition to the ambiguity of the GWTT objectives discussed above, there is another area of difficulty. Determining groundwater travel times and paths in a regional-scale problem is a difficult task based on the current monitoring and modeling techniques. There are large uncertainties in predictions. These uncertainties arise from many sources including those discussed previously. It is,

however, generally agreed that lack of complete knowledge of the spatial distribution of hydrologic parameters input to a mathematical models may be the major source of uncertainties in predicting the travel times and paths. Means of acquiring more detailed knowledge of the parameter distributions will certainly 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 fractal geometry techniques, macrodispersion methods, Monte Carlo approaches, and 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.

The fractal approach recognizes the existence of variability in all scales but assumes these variations are self-similar. With these assumptions, one can scale the results of experiments made at one scale to another. This approach is an easy way to estimate the uncertainty in groundwater travel times as indicated by equation (4.3.46). However, in this approach, the parameters lack physical meaning. What does the fractal dimension, D, mean? How can D and ϵ_c be related to the parameters (such as hydraulic conductivity, porosity, and their spatial variability) in the classic groundwater hydrology? More importantly, can we define clearly the volume of groundwater which we use to define the velocity? The tracer concentration of a volume of groundwater may be subject to changes due to mixing from subscale variations in groundwater velocity. Are we interested in the arrival of a volume of groundwater or a certain concentration of groundwater? Finally, the question which was posed in the section dealing with the fractal concept must be answered: is it true that the groundwater travel path is a fractal? Until these questions can be

resolved, the application of the fractal approach must be limited.

The approach using effective parameters with the macrodispersion concept may be attractive for relatively simple hydrogeologic systems. Recent field experiments (Sudicky, 1986; Freyberg, 1986; and Garabedian, 1987) 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 concentration variances are also in reasonable agreement with the stochastic results by Gelhar and Axness (1983) and Dagan (1987). However, the major concern with this effective parameter approach is its validity in analysis of flow and transport in highly heterogeneous aquifers where the variance of log saturated hydraulic conductivity is greater than 1. The variance of log saturated hydraulic conductivity in all the possible radioactive waste repository sites is likely much greater than 1, especially in fractured aquifers. The existing analytical solutions to stochastic differential equations are also only useful for simple flow fields, e.g., steady, uniform flow in a single aquifer. These stochastic results based on an analytical approach may serve as a tool for preliminary analyses but are not completely adequate for predictive purposes because of large variance associated with the results.

Furthermore, the spatial concentration variance formulas in the stochastic results (equations 4.3.33 to 4.3.36) provide us with the way to predict only the relative size of the plume. The shape of the concentration profile still remains unknown. The macrodispersivity defined in the stochastic analysis does not warrant the use of the classic convection-dispersion equation (Yeh, 1987) based on Fick's law. In addition, the variance of the predicted mean concentration profile may be large (Dagan, 1987). Most importantly, the number of samples required to obtain accurate estimates of the parameter values (correlation scales and covariance functions) for the

macrodispersivity models still must be investigated. Finally, the stochastic results need to be tested with many large-scale field tracer experiments in various geologic environments before they can be used for predictions.

Although the Monte Carlo simulation technique may be expensive because it requires a large number of simulations, it may be the most powerful tool among the available techniques for predicting groundwater travel times and paths or the arrival of the radionuclide concentration. Furthermore, conditional simulations which use available information at sample locations will enhance our ability to model the 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 hydraulic heads significantly, he suggested that using both hydraulic 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 (1981) showed that the locations of the 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 uncertainties in groundwater travel times and paths certainly deserves further investigation. Regardless of the amount of uncertainties that the conditional simulations (using both 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 seems to be the only tool that could bring us a step closer to reality.

As one approach to the problem of quantifying uncertainty in groundwater travel times and paths in porous media using stochastic methods, we suggest the following steps: (1) groundwater hydrologists should utilize the principles of structural

geology, stratigraphy, and sedimentology to delineate large-scale geologic units or structures which may contain the likely fast paths along which groundwater travels (Williams, 1988). (2) "Enough" data should be collected to characterize 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, porosity data from the geologic units identified in (1) using many small-scale tests (such as core samples from boreholes, or small-scale aquifer tests). (4) Groundwater hydrology modelers 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 behavior of the flow system or to calibrate flow models (see discussion in Section 4.3 or example in Gelhar, 1986). Note that the scale of samples should be consistent. That is, if one decides to use a certain scale, the entire characterization program should use that scale. Thus, the results of the calibration of models may provide a way to have 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 us with 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 assuming a release of a certain amount of radionuclides at a disturbed zone to determine the uncertainty in groundwater travel

times and paths. As more data become available, the same procedures should be repeated with the additional data. Such an iterative conditional simulation will bring our predictions close to reality step by step as more hydrologic parameter values are available. This suggested approach generally concurs with an earlier version of the NRC's draft generic position on groundwater travel time (Codell, 1986).

On the other hand, if the regulators would accept the mean groundwater travel time as a measure of the hydrologic integrity of a site, then the convection-dispersion equation would not be necessary. In this case, the ground water travel time criterion could be calculated from effective hydraulic properties and the groundwater flow equation.

Dr. Lynn W. Gelhar, who is one of the leaders in the field of stochastic hydrology, received the O. E. Meinzer Award from the Geological Society of America in 1987. In concluding this review, it seems appropiate to excerpt some of his remarks on the current status of stochastic theories and key issues which remain to be solved.

> "We now understand that this heterogeneity plays a central role regarding the large-scale mixing process in aquifers. The last decade witnessed a rapid development of mathematical, numerical, and statistical methodologies for evaluating the effects of heterogeneity on transport process. In spite of the confusion which seems to still persist in some recent literature, I believe that it is fair to say that we have arrived at a sound theoretical description of the dominant field-scale mixing process. Such stochastic theories provide a framework for predicting large-scale, long term behavior from observations of aquifer heterogeneity. Furthermore, such theories provide specific hypotheses which can be tested systematically by comparing independent theoretical predictions with the results of controlled field experiments.

This allows us to scape from the circular reasoning of the curve-fitting approach in ground-water hydrology. The stochastic approach not only provides a critical link between small-scale laboratory measurments, but also reveals features of the large-scale process which may not otherwise be apparent."

"....There is a need for controlled field experiments which explore more complex transport processes involving chemical heterogeneity, multi-phase flow, and fractured media. A fractured rock can be viewed as another type of heterogeneous medium which I suspect can be treated in some cases using stochastic continuum theory. Clearly, the problem of solute transport in fractured media is unresolved. Oversimplified matrix diffusion-type models have been extensively exercised using hyphotetical parameters to illustrate significant radionuclide retardation in the context of radioactive-waste disposal. As far as I can determine, there is no definitive field evidence which demonstrates such retardation effects. There is an obvious need for carefully designed field experiments to explore transport processes in fractured rock. Why aren't experiments of this type being developed in the United States?

A key unresolved issue is how we can characterize heterogeneity in practical sense. Research has shown that variances and correlation scales can be estimated using thousands of samples but our experience indicates that parameters can be estimated crudely from indirect geologic and geophysical observations and simple hydraulic tests. This more practical approach needs to be pursued in a number of different geologic environments. Heterogeneity remains a formidable difficulty in hydrogeology, but we now have a quantitative basis for evaluating

its effects." Gelhar (1988).

REFERENCES

Ababou, R. and L.W. Gelhar, Three-dimensional groundwater flow in random media: Direct simulation versus spectral theory, EOS, 68(44), Nov. 3, 1987.

Andersson, J. and A.M. Shapiro, Stochastic analysis of one-dimensional steady state unsaturated flow: a comparison of Monte Carlo and perturbation methods, Water Resour. Res., 19(1), 121 133, 1983.

Arya, A., T.A. Hewett, R. Larson, and L.W. Lake, Dispersion and reservoir heterogeneity, Society of Petroleum Engineers, SPE14364, Presented at the 60th Annual Technical Conference of the Society of Petroleum Engineers, Las Vegas, Nevada, Sept. 22-25, 1985.

Bakr, A.A., Stochastic analysis of the effect of spatial variations in hydraulic conductivity on groundwater flow, Ph.D. dissertation, New Mexico Institute of Mining and Technology, Socorro, July, 1976.

Bakr, A.A., L.W. Gelhar, A.L. Gutjahr, and J.R. MacMillan, Stochastic analysis of spatial variability in subsurface flows, 1:Comparison of one-dimensional flows, Water Resour. Res.,14, 263-271, 1978.

Barrenblat, G.E., I.P. Zheltov, and J.N. Kochina, Basic Concepts in the theory of homogeneous liquids in fissured rocks, J. Appl. Math. Mech. USSR, 24 (5):1286-1303, 1960.

Bear, J., Hydraulics of Groundwater, 569 pp., McGraw-Hill, New York, 1979.

Bennion, D.W., and J.C. Griffiths, A stochastic model for predicting variations in reservoir rock properties, Trans. AIME, No. 237, Part 2, 9-16, 1966,

Betson, R.P., J.M. Boggs, S.C. Young, L.W. Gelhar, Design of a field experiment to investigate groundwater saturated zone transport processes, Interim Rep., RP2485-05, 104pp., Elecr. Power, Res. Inst., Palo Alto, CA, 1985.

Bibby, R., and D.K. Sunada, Statistical error analysis of a numerical model of confined groundwater flow, in C.L. Chiu (ed.), Stochastic hydraulics, Proceedings, First International Symposium on Stochastic Hydraulics, 591-612, 1971.

Bonano, E.J., and R.M. Cranwell, Treatment of uncertainties in the performance assessment of geologic high-level radioactive waste repositories, Math. Geol., 20(5), 543-565, 1988.

Bras, R.L., and I. Rodriguez-Iturbe, Random functions and hydrology, Addison-Wesley publishing company, 559pp., 1985.

Bulnes, A.C., An application of statistical methods to core analysis data of dolomitic limestone, Trans. AIME, 165, 223-240, 1946.

Burrough, P.A., Multiscale sources of spatial variation in soil, I: The application of fractal concepts to nested levels of soil variation, J. Soil Science, 34, 577-597, 1983a.

Burrough, P.A., Multiscale sources of spatial variation in soil, II: A non-Brownian fractal model and its application in soil survey, J. Soil Science, 34, 599-620, 1983b.

Butler, Jr., J.J., Pumping tests in nonuniform aquifers: a deterministic/stochastic analysis, Ph.D. dissertation, Stanford University, Stanford, CA., 220 pp., December 1986.

Byers, E. and D.B. Stephens, Statistical and stochastic analysis of hydraulic conductivity and particle size in a fluivial sand, Soil Sci Soc. Am. J. 47, 1072-1081, 1983.

Clifton, P.M., and S.P. Neuman, Effects of kriging and inverse modeling on conditional simulation of the Avra Valley aquifer in southern Arizona, Water Resour. Res., 18, 1215-1234, 1982.

Clifton, P.M., B. Sagar, and R.G. Baca, Stochastic groundwater traveltime modeling using a Monte Carlo technique, In International Association of Hydrogeologists Memoires: Hydrogeology of Rocks of Low Permeability, Tucson, Arizona, 17(1), 319-329, 1985.

Codell, R., Draft generic position on groundwater travel time, Div. of Waste Manag., Office of Nuclear Material Safety and Safeguards, U.S. Nuclear Regulatory Commisssion, June 30, 1986.

Cole, C.R. and H.P. Foote, Use of a multigrid technique to study effects of limited sampling of heterogeneity on transport prediction, Presented at the National Water Well Association Conference, Solving Ground Water Problems with Models, Denver, Colorado, February 10-12, 1987.

Csanady, G.T., Turbulent diffusion in the environment, D. Reidel Publishing Co., 248 pp., 1973.

Dagan, G., Solute transport in heterogeneous porous formation, J. Fluid Mech., 145, 151-177, 1984.

Dagan, G., Statistical theory of groundwater flow and transport: pore-to laboratory-, laboratory-to formation-and formation-to regional-scale, Water Resour. Res., 22(9), 120S-134S, 1986.

Dagan, G., Theory of solute transport by groundwater, Ann. Rev. Fluid Mech., 19, 183-215, 1987.

Davis, J.C., Statistics and Data Analysis in Geology, 550 pp., John Wiley and Sons, Inc., New York, 1973.

Delhomme, J.P., Spatial variability and uncertainty in groundwater flow parameters: a geostatistical approach, Water Resour. Res., 15, 269-280, 1979.

De Marsily, G., G. Lavedan, M. Boucher, G. Fasamino, Interpretation of interference tests in a well field using geostatistical techniques to fit the permeability distribution in a reservoir model, "in" G. Verly etal (eds) Geostatistics for Natual Resources Characterization, Part 2, NATO Adv. Sci. Inst. Series C, vol 122, pp 831-849, Reidel Publ. Co., Dordrecht, 1984.

De Marsily, G., Quantitative Hydrogeology: Groundwater Hydrogeology for Engineers, 440 pp., Academic Press, Inc., Orlando, Florida, 1986.

Dooge, J.C.I., Scale problems in hydrology, Kisiel Memorial Lecture at Department of Hydrology and Water Resources, University of Arizona, Tucson, Arizona, February 19, 1986.

Driscoll, F.G., Groundwater and Wells, 1089 pp., Johnson Division, St. Paul, Minnesota., 1986.

Elsworth, D., A boundary element-finite element procedure for porous and fractured media flow, Water Resour. Res., 23(4), 551-560, 1987.

Fischer, H.B.,E.J. List, R.C.Y. Koh, J. Imberger, N.H. Brooks, Mixing in inland and coastal waters, Academic press, 483 pp., 1979.

Freeze, R.A., Three-dimensional, transient, saturated-unsaturated flow in a goundwater basin, Water Resour. Res., 7(2), 347-366, 1971.

Freeze, R.A., A stochastic-conceptual analysis of one-dimensional groundwater flow in non-uniform homogeneous media, Water Resour. Res., 725-741, 1975.

Freyberg, D.L., A natural gradient experiment of solute transport in a sand aquifer 2. Spatial moments and the advection and dispersion of nonreactive tracers, Water Resour. Res., 22, 2031-2046, 1986.

Gannon, J. M., and T.-C.J. Yeh, Numerical analysis of the effects of heterogeneities on dispersion, in prep., 1988.

Garabedian, S.P., Large-scale dispersive transport in aquifers: field experiments and reactive transport theory, PhD. dissertation, Massachusetts Institute of Technology, Cambridge, Massachusetts, July 1987.

Gelhar, L.W., Effects of hydraulic conductivity variations on groundwater flows, in Proceedings of the second interational IAHR symposium on stochastic hydraulic, Int. Ass. of Hydraul. Res., Lund, Sweden, 1976.

Gelhar, L.W., Stochastic subsurface hydrology from theory to applications, Water Resour. Res., 135S-145S, 1986.

Gelhar, L.W. and C.L. Axness, Three-dimensional stochastic analysis of macrodispersion in aquifers, Water Resour. Res., 19(1), 161-180, 1983.

Gelhar, L.W., A.A. Bakr, A.L. Gutjahr, and J.R. McMillan, Comments on stochastic conceptual analysis of one-dimensional groundwater flow in a non-unifrom homogeneous medium by Freeze, R.A., Water Resour. Res. 13(2), 477-480, 1977.

Gelhar, L.W., A.L. Gutjahr, and R.L. Naff, Stochastic analysis of macrodispersion in a stratified aquifer, Water Resour. Res., 15, 1387-1397, 1979.

Gelhar, L.W., Response to O.E. Meinzer Award, GSA Bulletin, July, P984, 1988.

Gutjahr, A.L., Kriging in stochastic hydrology: Assessing the worth of data, paper

presented at the Chapman Conference on Spatial Variability in Hydrologic Modeling, AGU, Fort Collins, Colorado., July 1981.

Gutjahr, A.L., L.W. Gelhar, A.A. Bakr, and J.R. MacMillan, Stochastic analysis of spatial variability in subsurface flows, 2: Evaluation and Applications, Water Resour. Res., 14, 953-960, 1978.

Gutjahr, A.L., D. McKay, and J.L. Wilson, Fast Fourier transform methods for random field generation, EOS, 68(44), Nov. 3, 1987.

Heller, J.P., Observations on diffusion and mixing in porous media, in Proceedings, Second International Symposium on Fundamentals of Transport Phenomena in Porous Media, IAHR and ISSS, Vol. 1, Guelph, University of Guelph, 1-26, 1972.

Hewett, T.A., Fractal distributions of reservoir heterogeneity and their influence on fluid transport, Society of Petroleum Engineers, SPE15386, Presented at the 61st Annual Technical Conference of the Society of Petroleum Engineers, New Orlans, Louisiana, October 5-8, 1986.

Hoeksema, R.J. and P.K. Kitanidis, An application of the geostatistical approach to the inverse problem in two-dimensional groundwater modeling, Water Resour. Res, 20(7), 1003-1020, 1984.

Hoeksema, R.J. and P.K. Kitanidis, Analysis of the spatial structure of properties of selected aquifers, Water Resour. Res, 21, 563-572, 1985.

Huang, C. and D.D. Evans, A 3-dimensional computer model to simulate fluid flow and contaminant transport through a rock fracture system, NUREG/CR-4042, U.S. Nuclear Regulatory Commission, 108 pp., 1985.

Hubbert, M.K., The theory of groundwater motion, J. of Geol., 48, 785-944, 1940.

Huyakorn, P.S., B.H. Lester, and C.R. Faust, Finite element techniques of modeling groundwater flow in fractured aquifers, Water Resour. Res., 19(4), 1019-1035, 1983a.

Huyakorn, P.S., B.H. Lester, and J.W. Mercer, An efficient finite element technique for modeling transport in fractured porous media, 1, Single Species Transport, Water Resour. Res., 19(3):841-854, 1983b.

Huyakorn, P.S., B.H. Lester and J.W. Mercer, An efficent finite element technique for modeling transport in fractured porous media, 2, Nuclide decay chain transport, Water Resour. Res., 19(3), 841-854, 1983c.

Ilyin, N.I., and others, Otsenka tochnosti opredeleniya vodopronitsayemosti gornykh porod, Moscow, Nedra, 1971.

Javandel, I., and P.A., Witherspoon, A method of analyzing transient fluid flow in multilayered aquifers, Water Resour. Res., 5(4), 1969.

Jenkins, G.M. and D.G. Watts, Spectral Analysis and its Applications, 525 pp., Holden-Day, Inc., San Francisco, 1968.

Jensen, J.L., D.V. Hinkley, L.W. Lake, A statistical study of reservoir permeability: distribution, correlation and averages, Soc. Petr. Eng. Formation Evaluation, 461-468, Dec. 1987.

Journel, A.G., and CH.J. Huijbregts, 600 pp., Mining Geostatistics, Academic Press, London, 1978.

Kazemi, H., M.S. Seth, and G.W. Thomas, The interpretation of interference tests in naturally fractured reservoirs with uniform fracture distribution, Soc. Pet. Eng. J., Dec., 463-472, 1969.

Kitanidis, P.K., and E.G. Vomvoris, A geostatistical approach to the inverse problem in groundwater modeliling (steady-state) and one-dimensional simulations, Water Resour. Res., 19(3), 677-690, 1983.

Law, J., A statistical approach to the interstitial heterogeneity of sand reservoirs, Trans AIME, v. 155, 202-222, 1944.

Lumley, J.L., and H.A. Panofsky, The Structure of Atmospheric Turbulence, John Wiley, New York, 1964.

MacMillan, J.R. and A.L., Gutjahr, Geological controls on spatial variability for one-dimensional arrays of porosity and permeability normal to layering, in Reservoir Characterization, edit by Haldorsen and Lake, 256-291, Academic Press, 1986.

Mandelbrot, B.B., The Fractal Geometry of Nature, 468 pp., W.H. Freeman, San Francisco, California, 1983.

Mandelbrot, B.B., How long is the coastline of Great Britain? Statistical self-similarity and fractional dimension, Science, 155, 636-638, 1967.

Mantoglou, A., and L.W. Gelhar, Stochastic modeling of large-scale transient unsaturated flow systems, Water Resour, Res., 23(1), 37-46, 1987a.

Mantoglou, A., and L.W. Gelhar, Capillary tension head variance, mean soil moistsure content, and effctive specific soil moisture capacity of transient unsaturated flow in stratified soils, Water Resour. Res., 23(1), 47-56, 1987b.

Mantoglou, A. and L.W. Gelhar, Effective hydraulic conductivities of transient unsaturated flow in stratified soils, Water Resour. Res., 23(1), 57-68, 1987c.

Mantoglou, A., and J.L. Wilson, The turning bands method for simulation of random fields using line generation by a spectral method, Water Resour. Res., 18(5), 1379-1394, 1982.

Marle, C., Ecoulements polyphasiques en milieu poreux, Rev. Inst. Fr. Pet, 22(10), 1471-1509, 1967.

Matheron, G., The intrinsic random functions and their applications, Advan. Appl. Probab., 5, 438-468, 1973.

Matheron, G., and G. de Marsily, Is transport in porous media always diffusive? A conunter example, Water Resour. Res., 16(5), 901-917, 1980.

Mercado, A., The spreading pattern of injected water in a permeability-stratified aquifer, p. 23, Proc. Int. Assoc. Sci. Hydrol. Symp., Haifa Pub. 72, 1967.

Mizell, S.A., A.L. Gutjahr, and L.W. Gelhar, Stochastic analysis of spatial variability in two-dimensional steady groundwater flow assuming stationary and non-stationary heads, Water Resour. Res., 19, 1853-1867, 1982.

Moench, A.F., Double-porosity models for a fissured groundwater reservoir with fracture skin, Water Resour. Res., 20(7), 831-846, 1984.

Morrison, P., and P. Morrison, Powers of Ten, Scientific American Books, New York, 1982.

Neuman, S.P., Stochastic continuum representation of fractured rock permeability as an alternative to the REV and fracture network concepts, 533-561, 28th U.S. symposium on rock mechanics, Tucson, Arizona, 29 June -1 July, 1987.

Neuman, S.P., Role of geostatistics in subsurface hydrology, in G. Verly, M. David, A.G. Journel, and A. Marechal, eds., Geostatistics for Natural Resources Characterization, Part 2, p787-816, D. Roede; Publ. Co., Boston, MA, 1072 pp., 1984.

Neuman, S.P., C.L. Winter, and C.M. Newman, Stochastic theory of field-scale Fickian dispersion in anisotropic porous media, Water Resour. Res., 23, 453-466, 1987.

Neuman, S.P., Statistical Characterization of aquifer heterogeneities, in Recent Trends in Hydrogeology, Geol. Soc. Amer. Spec. Paper 189, 81-102, 1982.

Parsons, A.M., E.D. Mattson, D.B. Stephens, K. Flanigan, K. Black, Field simulation of waste impoundment seepage in the vadoze zone, Proc. Flows on Southwestern Groundwater Issues Conf., Nat. Water Well Assoc., Albuquerque, March 23-25, 1988.

Peters, R.R., J.H. Gauthier, and A.L. Dudley, The effect of percolation rate on water-travel time in deep, partially saturated zones, Sandia Report, SAND85-0854, 1986.

Rasmussen, T.C., Computer simulation of steady fluid flow and solute transport through three-dimensional networks of variably saturated, discrete fractures, in Evans, D.D. and T.J. Nicholson (Eds.), Flow and Transport Through Unsaturated Fractured Rock, AGU Geophysical Monograph 42, 107-114, 1987.

Schwartz, F.W., L. Smith, and A.S. Crowe, 1983. A stochastic analysis of macroscopic dispersion in fractured media, Water Resour. Res., 19,1253-1265, 1983.

Shapiro, A. M., and J. Andersson, Steady-state fluid reposnes in fractured rock: A boundary element solution for a coupled, discrete fracture continuum model, Water Resour. Res. 19(4), 959-969, 1983.

Smith, L., and R.A. Freeze, Stochastic analysis of steady state groundwater flow in

a bounded domain, 1: One-dimensional simulations, Water Resour. Res., 15, 521-528, 1979a.

Smith, L., and R.A. Freeze, Stochastic analysis of steady state groundwater flow in a bounded domain, 2: Two-dimensional simulations, Water Resour. Res., 15, 1543-1559, 1979b.

Smith, L. and F.W. Schwartz, Mass transport, 1. A stochastic analysis of macroscopic dispersion, Water Resour. Res., 16, 303-313, 1980.

Smith, L. and F.W. Schwartz, Mass transport, 2. Analysis of uncertainty in prediction, Water Resour. Res., 17(2), 351-368, 1981a.

Smith, L. and F.W. Schwartz, Mass transport, 3. Role of hydraulic conductivity in prediction, Water Resour. Res., 17(5), 1463-1479, 1981b.

Stephens, D.B., L.W. Gelhar, S. Young, Field experiment to evaluate disperison in unsaturated media, EOS, 65(16), 106, 1984.

Sudicky, E.A., A natural gradient experiment on solute transport in a sand aquifer: spatial variability of hydraulic conductivity and its role in the dispersion process, Water Resour. Res., 22, 2069-2082, 1986.

Taylor, G.I., Diffusion by continuous movements, Proc. London. Math. Soc. Ser. A20, 196-211, 1922.

Taylor, G.I., Dispersion of soluble matter in solvent flowing slowly through a tube, Proc. London. Math. Soc. Ser. A219, 186-203, 1953.

van Genuchten, M.T., A closed-form equation for predicting the hydraulic conductivity of unsaturated soils, Soil Sci. Soc. Am. J., 44, 892-898, 1980.

Vomvoris, E.G., and L.W. Gelhar, Stochastic prediction of dispersive contaminant transport, U.S. Department of Commerce National Technical Information Service, Cooperative Agreement, CR-811135-01-2, Dec., 1986.

Wang, J.S.Y., and T.N. Narasimhan, Hydrologic mechanisms governing fluid flow in a partially saturated, fractured, porous medium, Water Resour. Res., 21(12), 1861-1874, 1985.

Warren, J.E., and H.S. Price, Flow in heterogeneous porous media, Society of Petroleum Engineers Journal, 1, 153-169, 1961.

Warren, J.E., and P.J. Root, Behavior of naturally fractured reservoirs, Society of Petroleum Engineers Journal, 9, 245-255, 1963.

Warren, J.E., and F.F. Skiba, Macroscopic dispersion, Trans AIME, 231, 215-230, 1964.

Warren, J.E., F.F. Skiba, and H.S. Price, An evaluation of the significance of permeability measurements, Journal Petroleum Technology, 13, 739-744, 1961.

Wheatcraft, S.W. and S.W. Tyler, An explanation of scale-dependent dispersivity in

heterogeneous aquifers using concepts of fractal geometry, Water Resour. Res., 24(4), 525-532, 1988.

Wierenga, P.J., L.W. Gelhar, C.S. Simmons, G.W. Gee, T.J. Nicholson, Validation of stochastic flow and transport models for unsaturated soil: a comprehensive field study, U.S. Nuc. Reg. Comm. Reprt, NUREG/CR-4622, 1986.

Williams, D., Geostatistical analysis and inverse modeling of the Upper Santa Cruz Basin, Arizona, Master Thesis, Univ. of Arizona, pp149, 1987.

Williams, R.E., Comment on "Statistical theory of groundwater flow and transport: Pore to Laboratory, Laboratory to Formation, and Formation to Regional Scale" by Gedeon Dagan, Water Resour. Res., 24(7), 1197-1200, 1988.

Williams, R.E., Comment on "Double-porosity models for a fissured groundwater reservoir with fracture skin" by Allen F. Moench, Water Resour. Res., 21(6), 889-891, 1985.

Winter, C.L., C.M. Newman, and S.P. Neuman, A perturbation expansion for diffusion in a random velocity field, SIAM J. Appl. Math, 44(2), 411-424, 1984.

Yeh, T.-C.J., L.W. Gelhar and A.L. Gutjahr, Stochastic analysis of unsaturated flow in heterogeneous soils, 1, Statistically isotropic media, Water Resour. Res., 21(4), 447-456, 1985a.

Yeh, T.-C.J., L.W. Gelhar and A.L. Gutjahr, Stochastic analysis of unsaturated flow in heterogeneous soils, 2, Statistically anisotropic media with variable alpha, Water Resour. Res., 21(4), 457-464, 1985b.

Yeh, T.-C.J., L.W. Gelhar and A.L. Gutjahr, Stochastic analysis of unsaturated flow in heterogeneous soils, 3, Observations and applications, Water Resour. Res., 21(4), 465-472, 1985c.

Yeh, T.-C.J., Comment on "Modeling of scale-dependent dispersion in hydrogelogic systems" by J.F. Pickens and G.E. Grisak, Water Resour. Res., 23(3), 522, 1987.

Zhang, Y., Double porocity model and its finite element solution for the flow in fractured-Karst Rocks, Hydrogeology and Engineering Geology, 4, 1982.

APPENDIX A

Glossary

Note that the glossary provided here is intended to clarify the concepts or physical meanings of terms, instead of rigorous definitions. Although most of the definitions refer to space series, they can be applied to time series as well.

Autocorrelation function: A function which depicts the linear correlation between a space series at all ranges of offset distance. For example, an autocorrelation function of hydraulic conductivity values along a transect is a measure of the intensity of association or interdependence among the values at all ranges of separation distances. Syn: autocorrelation, correlation function.

Autocovariance function: A function which describes the behavior of the covariances of two identical spatial series offset at various separation distances.

Correlation (correlation coefficient): the ratio of the covariance of two random variables to the product of their standard deviations. The correlation coefficient ranges from +1 to -1. A correlation of +1 indicates a perfect direct relationship between two random variables; a correlation of -1 indicates that one variable changes inversely with relation to the other. Between the two extremes is a spectrum of less than-perfect relationships, including a correlation coefficient of zero which indicates the lack of any linear relationship.

Correlation scale: A separation distance beyond which the random variables are no

longer considered correlated. Physically, it can be related to the average size of all sedimentary structures (for example, clay lenses) in an aquifer.

Cross-correlation function: A function which describes the correlation between two different data series at all separation distances. For example, a cross-correlation function of hydraulic conductivity and head values along a transect shows the relationship between the conductivity and head values along the transect at various separation distance. Syn: cross-correlation.

Cross-covariance function: A function which characterizes the covariances of spatial series of two different properties (e.g., hydraulic conductivity and porosity) at different separation distances. Syn: cross-covariance.

Co-Kriging: A method for estimating the value of a spatially distributed variable (e.g. transmissivity) from adjacent values of two variables (such as transmissivity and well capacity) while considering the spatial interdependence (cross-covariance) of the two variables.

Conditional probability: The probability of occurrence of a property value at an unsampled location if the property values at other location are known.

Conditional simulation: A data-generating technique, used with Monte Carlo simulation. However, sample values at sample locations are preserved in the generated data by this technique.

Covariance: A measure of the distribution of values of two properties around a common mean and thus of their mutual variability.

Ensemble: A collection of an infinite number of space series measuring the same variable.

Ensemble average: An average of the property at a point in space over many possible space series. Syn. expected value.

Ergodicity: A property of a stochastic process which says the ensemble moments equal the corresponding averages calculated from a single realization. These averages in turn can be approximated from a finite part of the realization.

Expected value: see ensemble average.

First moment: see mean

Frequency distribution: A table or a plot which divides a set of data into a number of classes, and shows the number of data belonging in each class.

Geostatistics: Statistics as applied to geology generally including correlated processes. In groundwater hydrology, it is the application of random function concepts to study the hydrologic properties in space.

Integral scale: A convenient measure of autocorrelation of a stochastic process. It carries the same physical meaning as the correlation scale but is defined more rigorously. Mathematically, it is defined as the area under the autocorrelation function.

Intrinsic hypothesis: A less stringent hypothesis than that of second-order stationarity. It states that a random field is intrinsic only if the variance of the increments of the random field is finite and these increments are second-order stationary. Variogram analysis is then applicable.

Joint probability function: A function which describes the behavior of the joint probability distribution of many random variables (i.e., the probabilities of occurrence of many random variables).

Kriging: A method for estimating the value of a spatially distributed variable from adjacent values while considering the spatial interdependence of the variables.

Log hydraulic conductivity: The natural logarithm of a hydraulic conductivity value, (lnK) or the logarithm of a hydraulic conductivity value to the base 10, (logK).

Log transmissivity: The natural logarithm of a transmissivity value, (lnT), or the logarithm of a transmissivity value to the base 10, (logT).

Lognormal distribution: A frequency distribution whose logarithms follow a normal distribution.

Mean: The sum of all observations divided by the number of observations.

Median: The value of the middle term in a set of data arranged in rank order.

Mode: The value or group of values that occurs with greatest frequency in a set of data; the most typical observation.

Monte Carlo simulation: A data-generating technique. It generates large samples of data from known probability distributions.

Nonstationary process: A stochastic process which does not possess stationary properties. Generally, it refers to a process which contains a significant trend or where the covariance depends on location as well as separation distance.

Normal distribution: A frequency distribution whose plot is a continuous, infinite, bell-shape curve that is symmetrical about its arithmetic mean, mode, and median. Syn: Gaussian distribution; bell-shaped distribution.

Nugget effect: A jump exhibited at the origin of a variogram. It generally represents uncorrelated measurement errors or subscale variability.

Perfectly correlated process: A process which has infinitely large correlation scales. Generally, this process has a constant value over space.

Probability: A term to describe the frequency of occurrence of an event.

Probability distribution: A distribution of frequencies of occurrence of many events. It is approximated by a frequency distribution.

Random variable: A function whose values are real numbers and depend on

"chance" or probability.

Random field: see stochastic process.

Random function: see stochastic process.

Range: The distance beyond which the value of the variogram equals the variance of the random field. Similar to the correlation scale, it is the distance beyond which the interdependence of values in a space series is considered insignificant.

Realization: A single space series in an ensemble. For example, a set of porosity values measured in an aquifer is considered as a realization of all the possible porosity values of the aquifer.

Regionalized variable: A variable which is distributed in space. It is equivalent to a realization of a stochastic process. Examples are porosity, hydraulic conductivity, and other hydrologic properties of an aquifer.

Representation theorem: A theorem which allows a second-order stationary stochastic process to be decomposed into sums of uncorrelated (or orthogonal) increments in the frequency domain.

Second moment: see variance.

Second-order stationary (weakly stationary) process: A stochastic process in which the ensemble mean (expected value) of the process is constant over space, and

the autocovariance function depends only on the separation distance.

Separation distance: The amount of offset in distance between the two space series being compared.

Sill: The asymptotic value of a variogram at a separation distance equal to or greater than the range. It is the variance of the random field.

Spectral Method: A mathematical tool used to solve partial differential equations which contain stochastic parameters.

Spectrum: The inverse Fourier transform of a covariance function. In other words, the covariance function has been transformed from a space domain to a wave number domain.

Standard deviation: Square root of the variance; it describes dispersion or spread of data around the mean.

Statistical moment: A convenient measure of the location and the shape of a probability distribution. First, second, and third moments of a probability distribution correspond to mean, variance, and skewness of the distribution.

Statistically anisotropic process: A stochastic process in which the covariance function depends not only on the magnitude of the separation distance but also on the direction of the separation distance. That is, the correlation scales of the process varies with change in direction.

Statistically homogeneous process: see second-order stationary process.

Statistically heterogeneous process: Any process that does not possess the properties of a second-order stationary process.

Statistically isotropic process: A stochastic process in which the covariance function depends only on the magnitude of the separation distance, regardless of the direction. That is, the correlation scales of the process are invariant in all directions.

Statistically independent: Two random variables are statistically independent if and only if the joint distribution of the two random variables equals the product of the individual probability distributions of the two random variables. That is, one random variable conveys no information about the other random variable.

Stationary process: If the statistical properties of a spatial stochastic process do not change over the spatial coordinates, then the stochastic process is a stationary process. Syn. Strictly stationary process.

Stochastic process: A collection of an infinite number of random variables in space.

Variance: The average squared deviations of all possible observations from the population mean.

Variogram: A plot of the semivariance of a random field versus separation distances. Like a covariance function, a variogram is used to define the spatial

interdependence of two random variables. However, variogram is not restricted to only stationary or second-order stationary process.

APPENDIX B

B.1 Inconsistency in the Development of Governing Groundwater Flow Equations

The purpose of this appendix is to clarify some confusions in the development of governing groundwater flow equation in saturated porous media. Therefore, some of the inconsistencies in the derivation will be discussed.

To derive the governing groundwater flow equation, we start with the mass balance equation. Consider the mass balance of a stationary control volume, V_T (Figure 2.4) whose shape is fixed in space and time. The principle of mass conservation states that

$$\{ \text{ rate of mass accumulation } \} = \{ \text{ rate of mass in } \} - \{ \text{ rate of mass out } \} \quad \text{(B.1)}$$

To apply the principle to the control volume, we begin by considering the pair of faces perpendicular to the x axis. The rate of mass in through the face at x is $(\rho q_x)|_x \ \Delta y \Delta z$, and the rate of mass out through the face at $x+\Delta x$ is $(\rho q_x)|_{x+\Delta x} \ \Delta y \Delta z$. Similar expressions may be written for the other two pairs of faces. The rate of mass accumulation within the volume element is $(\Delta x \Delta y \Delta z)(\partial n\rho/\partial t)$, where n is the porosity of the control volume. The mass balance then becomes

$$\Delta x \Delta y \Delta z \left[\frac{\partial n\rho}{\partial t}\right] = \Delta y \Delta z[(\rho q_x)|_x - (\rho q_x)|_{x+\Delta x}] + \Delta x \Delta z[(\rho q_y)|_y - (\rho q_y)|_{y+\Delta y}] + \Delta x \Delta y[(\rho q_z)|_z - (\rho q_z)|_{z+\Delta z}] \quad \text{(B.2)}$$

By dividing this entire equation by $(\Delta x \Delta y \Delta z)$ and taking the limit as these dimensions approach zero, we get

$$\frac{\partial n\rho}{\partial t} = -\left[\frac{\partial \rho q_x}{\partial x} + \frac{\partial \rho q_y}{\partial y} + \frac{\partial \rho q_z}{\partial z}\right] \tag{B.3}$$

This is the equation of continuity for flow through porous media, which describes the rate of change of fluid density at a fixed point resulting from the changes in the mass flux ρq. Using the vector notation, equation (B.3) can be expressed as:

$$\frac{\partial n\rho}{\partial t} = -(\nabla \cdot \rho q) \tag{B.4}$$

Here $(\nabla \cdot \rho q)$ is called the "divergence" of ρq, sometimes written as div ρq. Note that the vector ρq is the mass flux, and its divergence has a simple significance: it is the net rate of mass efflux per unit volume. The equation (B.4) simply states that the rate of increase of the density within a small volume element fixed in the porous media is equal to the net rate of mass influx to the element divided by its volume.

Since the ρ and q are functions of spatial coordinates, equation (B.3) can be written as:

$$\frac{\partial n\rho}{\partial t} + q_x \frac{\partial \rho}{\partial x} + q_y \frac{\partial \rho}{\partial y} + q_z \frac{\partial \rho}{\partial z} = -\rho \left[\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z}\right] \tag{B.5}$$

The first term on the left-hand side of equation (B.5) represents the rate of change in fluid mass in the control volume at a fix position in space. The second term reflects the rate of change in fluid mass as the fluid moves from one control volume to the other at another location (change in mass due to convection). The combination of these two changes is equivalent ot the substantial derivative (or total derivative) of mass density in the control volume, that is, the time derivative for a path following the fluid motion. Hence, equation (B.5) can be abbreviated thus:

$$\frac{Dn\rho}{Dt} = -\rho(\nabla \cdot \mathbf{q}) \tag{B.6}$$

This is the continuity equation describing the rate of change of density in the fixed control volume as seen by an observer "floating along" with the fluid (or Lagrangian point of view as oppose to Eulerian point of view, i.e., equation (B.4)). Both equations (B.4) and (B.6) describe conservation of mass in the control volume.

For an incompressible fluid, and a rigid porous medium (i.e., ρ and n are constant over time), equation (B.4) can be expressed as

$$(\nabla \cdot \mathbf{q}) = 0 \tag{B.7}$$

B.1.1 The Eulerian Point of View. The governing partial differential equation describing flow through porous media can be derived from the Eulerian or the Lagrangian point of view. If the Eulerian approach is used (i.e., we consider mass balance and fluid motion in a control volume with a fixed shape and at a fixed location in porous media), the continuity equation is

$$\frac{\partial n\rho}{\partial t} = -(\nabla \cdot \rho \mathbf{q}_a) \tag{B.8}$$

where $\mathbf{q}_a$ is the specific discharge at the Eulerian point of view. Considering the media deformable, and the fluid compressible, one can express equation (B.8) as:

$$-\nabla \cdot \rho \mathbf{q}_a = n \frac{\partial \rho}{\partial t} + \rho \frac{\partial n}{\partial t} \tag{B.9}$$

The first and second terms at the right-hand side of equation (B.9) represent the rate

of change of fluid density and the rate of change of porosity, respectively, in the fixed control volume as seen by an observer at a fixed location. Recall that the compressibility of fluid is

$$\beta = \frac{1}{\rho}\frac{d\rho}{dp} \tag{B.10}$$

and if ρ is a function of p only, i.e., $\rho(p)$, then

$$n\frac{\partial\rho}{\partial t} = n\frac{\partial\rho}{\partial p}\frac{\partial p}{\partial t} = n\rho\beta\frac{\partial p}{\partial t} \tag{B.11}$$

The second term at the right-hand side of equation (B.9) can be related to the rate of change in pressure. Since the control volume does not deform, i.e., V_T, remains constant, the volume of solids in the control volume, V_s, may change if the porous medium deforms. The coefficient of compressibility of porous matrix is then

$$\alpha = \frac{1}{V_s}\frac{\partial V_s}{\partial\sigma_e} = -\frac{1}{1-n}\frac{\partial n}{\partial\sigma_e} = \frac{1}{1-n}\frac{\partial n}{\partial p} \tag{B.12}$$

This definition results in the same α as defined previously, assuming the control volume deforms under stress. Therefore,

$$\rho\frac{\partial n}{\partial t} = \rho\frac{\partial n}{\partial p}\frac{\partial p}{\partial t} = \rho\,\alpha\,(1-n)\frac{\partial p}{\partial t} \tag{B.13}$$

By making use of (B.11) and (B.13), equation (B.9) becomes

$$-\nabla\cdot\rho q_a = n\rho\beta \frac{\partial p}{\partial t} + \rho\alpha(1-n) \frac{\partial p}{\partial t}$$

or

$$-\nabla\cdot\rho q_a = \rho^2 g[n\beta + \alpha(1-n)] \frac{\partial h}{\partial t} \tag{B.14}$$

since

$$h = z + \frac{p}{\rho g} \quad \text{and} \quad \frac{\partial h}{\partial t} = \frac{\partial z}{\partial t} + \frac{1}{\rho g} \frac{\partial p}{\partial t} \tag{B.15}$$

where the $\partial z/\partial t$ is zero because the location of the control volume is fixed in time. Let $S_s = \rho g(n\beta + \alpha (1-n))$, specific storage, equation (B.15) expressed as:

$$-\rho\nabla\cdot q_a - q_a\cdot\nabla\rho = \rho S_s \frac{\partial h}{\partial t} \tag{B.16}$$

Generally, the second term at left-hand side of equation (B.16) is much smaller than the first term. It can be neglected although we still assume the fluid is compressible. Thus, the governing partial differential equation for groundwater flow is

$$-\nabla\cdot q_a = S_s \frac{\partial h}{\partial t} \tag{B.17}$$

where $q_a = -K\cdot\nabla h$, Darcy's law. This equation simply describes the flow through porous media as seen by an observer at a fixed location in space.

B.1.2 The Lagrangian Point of View. Generally speaking, the Lagrangian

approach in fluid mechanics implies that observations are made by following the fluid flow. Flow in deformable porous media, however, involves the movement of both fluid and solids. Since most of our monitoring devices such as observation wells are installed in the geologic formations, our observations are likely following the movement of solid grains as the formations undergo deformation. In this section, we will derive the governing groundwater flow equation from the Lagrangian point of view (i.e., by following the mean displacement of the solid grains instead of the fluid.)

The classical form of Darcy's law applies in effect to the velocity of the fluid in relation to that of the solid and not in relation to stationary space. From the Eulerian point of view, the specific discharge, q_a, is then

$$q_a = q_w + nv_s \tag{B.18}$$

where q_w represents the specific discharge of the fluid in the classical Darcy's law, n is the porosity, and v_s is the solid velocity in the vertical direction since we will assume the porous medium undergoes vertical deformation only.

Using (B.18), the continuity equation defined in relation to a fixed point in space, (B.8), becomes

$$-\nabla\cdot\rho(q_w + nv_s) = -\nabla\cdot\rho q_w - \frac{\partial \rho n v_s}{\partial z} = \frac{\partial \rho n}{\partial t} \tag{B.19}$$

where the second term represents the net solid mass flux over the control volume. Equation (B.19) can be further expanded to

$$-\nabla\cdot\rho q_w - nv_s \frac{\partial \rho}{\partial z} - \rho v_s \frac{\partial n}{\partial z} - \rho n \frac{\partial v_s}{\partial z} = n \frac{\partial \rho}{\partial t} + \rho \frac{\partial n}{\partial t}$$

$$-\nabla\cdot\rho q_w = n\,\frac{d\rho}{dt} + \rho\,\frac{dn}{dt} + \rho n\,\frac{\partial v_s}{\partial z} \tag{B.20}$$

where $d\rho/dt$ and dn/dt are the substantial derivatives of ρ and n, respectively, with respect to the v_s. That is, the rate of changes in fluid density and porosity as seen by an observer moving at the mean velocity of solid grains.

The substantial derivative of ρ can be expressed as

$$\frac{d\rho}{dt} = \frac{\partial\rho}{\partial t} + v_s\cdot\nabla\rho$$

Since the second term on the right-hand side of the equation is small, it can be neglected. The rate of change in fluid density can be related to compressibility of the fluid as we did previously.

$$n\,\frac{d\rho}{dt} = n\,\frac{d\rho}{dp}\,\frac{dp}{dt} = n\rho\beta\,\frac{dp}{dt} \tag{B.21}$$

However, the rate of change of porosity deserves some elaboration. Consider solid volume conservation in a control volume. The continuity equation is

$$\frac{\partial V_s}{\partial t} = -(\nabla\cdot V_s\ v_s) \tag{B.22}$$

Recognizing that $V_s = (1-n)V_T$ and V_T is constant, equation (B.22) can be rewritten in the form of

$$(1-n)\ \frac{\partial v_s}{\partial z} = \frac{\partial n}{\partial t} + v_s\ \frac{\partial n}{\partial z} = \frac{dn}{dt} \tag{B.23}$$

Assuming each individual solid grain does not deform, the density of solids should remain constant. A solid mass balance leads to

$$-\nabla \cdot m_s\ v_s = \frac{\partial m_s}{\partial t} \quad \text{and}$$

$$\frac{\partial m_s}{\partial t} + v_s\ \frac{\partial m_s}{\partial z} = \frac{dm_s}{dt} = -m_s\ \frac{\partial v_s}{\partial z} \tag{B.24}$$

and

$$-\frac{1}{m_s\ /\rho_s}\ \frac{d(m_s\ /\rho_s)}{dt} = -\frac{1}{V_s}\ \frac{dV_s}{dt} = -\frac{1}{V_s}\ \frac{dV_s}{d\sigma_e}\ \frac{d\sigma_e}{dt} = -\frac{\alpha d\sigma_e}{dt} = \alpha\ \frac{dp}{dt} \tag{B.25}$$

Substituting (B.21),(B.23), and (B.25) into (B.20), one obtains

$$-\nabla \cdot \rho q_w = \rho(n\beta + \alpha)\ \frac{dp}{dt} \tag{B.26}$$

Note that

$$h = z + \frac{p}{\rho g} \quad \text{and} \quad \frac{dh}{dt} = \frac{dz}{dt} + \frac{1}{\rho g}\ \frac{dp}{dt} \tag{B.27}$$

and the dz/dt is zero because the location of the reference point is stationary as seen by an observer following the displacement of the solid. Equation (B.27) thus becomes:

$$-\rho\nabla\cdot q_w - q_w \cdot\nabla\rho = \rho^2 g(n\beta + \alpha) \frac{dh}{dt} \tag{B.28}$$

Assuming that $\rho\nabla\cdot q_w >> q_w \cdot\nabla\rho$ and applying Darcy's law to (B.28), one obtain the governing groundwater flow equation from the Lagrangian point of view:

$$\nabla\cdot(K\cdot\nabla h) = S_s \frac{dh}{dt} \tag{B.29}$$

where $S_s = \rho g(n\beta + \alpha)$ and is called specific storage. Note the expression of specific storage is different from the one in equation (B.17) which is derived from the Eulerian point of view. Theoretically, equation (B.29) is the correct one for field applications because our observations generally follow the displacement of the grains as the aquifer deforms.

However, the velocity of the solid is small. Many convenient but misleading assumptions have been employed for practical purposes. For example, the coefficients of compressibility of water, β, and porous matrix, α, in the fixed coordinate system are assumed the same as those in the moving coordinate system. They are, in effect, different. Moreover, based on the same argument, the dh/dt is replaced by $\partial h/\partial t$ and hydraulic conductivity is assumed constant in time even if the porous medium is deformable. These misleading assumptions lead to the classical governing groundwater flow equation which is given as:

$$\nabla\cdot(K\cdot\nabla h) = \rho g(n\beta + \alpha) \frac{\partial h}{\partial t} = S_s \frac{\partial h}{\partial t} \tag{B.30}$$

This equation is theoretically inconsistent since it mixes the expressions for both the fixed and moving coordinate systems.

The inconsistency of the classic groundwater equation may not, however, have significant impacts on the analysis of groundwater flow. This results from the fact that the hydraulic head in the field is indeed observed following the displacement of the solid grains. The specific storage is often estimated from aquifer tests and the analysis of the test data does not require the use of the expressions for S_s. Furthermore, the error in the estimation of Ss and K from field data may be so large that misleading assumptions may not play any critical role in the analysis of groundwater flow.

Bibliography on Geostatistical and Stochastic Methods Related to Groundwater-Hydrology

Ababou, R. and L.W. Gelhar, Three-dimensional groundwater flow in random media: Direct simulation versus spectral theory, EOS, 68(44), Nov. 3, 1987.

Ahlstrom, S.W., 1975, Modeling the transport of selected rationuclides in subsurface water systems using the discrete-parcel-random-walk approach, Trans. Am. Geophys. Union, V56(12), 979

Ahlstrom, S.W. and H.P. Foote, 1976, Transport modeling in the environment using the discrete-parcel-walk approach, NTIS Accession No. BNWLSA-5528

Alpay, O.A., 1972, A practical approach to defining reservoir hereogeneity, J. Petrol. Technol., V20(7), 841-848

Anderson, M.P., 1979, Using models to simulate the movement of contaminants through groundwater flow systems, Crit. Rev. in Env. Controls 9(2):97-156

Andersson, J. and A.M. Shapiro, 1983, Stochastic analysis of one-dimensional steady state unsaturated flow: a comparison of Monte Carlo and perturbation methods, Water Resour. Res., 19(1), 121 133

Arya, A., T.A. Hewett, R. Larson, and L.W. Lake, 1985, Dispersion and reservoir heterogeneity, Society of Petroleum Engineers, SPE14364, Presented at the 60th Annual Technical Conference of the Society of Petroleum Engineers, Las Vegas, Nevada, Sept. 22-25

Bachmat, Y., 1969, Hydrodynamic dispersion in a saturated homogeneous porous medium at low Peclet numbers and nonhomogeneous solution, Water Resour. Res., V5(1), 139-143

Bachmat, Y., 1972, Spatial macroscopization of processes in heterogeneous systems, Israel J. of Technology, V10(5), 391

Bachmat, Y., 1976, Annual operation of a coastal groundwater basin at a prescribed reliability level, J. Hydrol., V31 (1-2), 97-118

Bachmat, Y. and J. Bear, 1964, The general equations of hydrodynamic dispersion in homogeneous isotropic porous mediums, J. Geophy. Res. V69(12), 2561-2567

Bakr, A.A., Stochastic analysis of the effect of spatial variations in hydraulic conductivity on groundwater flow, Ph.D. dissertation, New Mexico Institute of Mining and Technology, Socorro, July 1976

Bakr, A.A., L.W. Gelhar, A.L. Gutjahr, and J.R. MacMillan, 1978, Stochastic analysis of spatial variability in subsurface flows, 1, Comparison of one- and three-dimensional flows, Water Resour. Res., V14(2), 263-271

Barrenblat, G.E., I.P. Zheltov, and J.N. Kochina, 1960, Basic Concepts in the theory of homogeneous liquids in fissured rocks, J. Appl. Math. Mech. USSR, 24 (5):1286-1303

Bastin, G., Stochastic parameter estimation of a steady-state groundwater flow model,

Paper presented at the Congress on Simulation of Systems, Sorrento, Italy, September 24-28, 1979

Batchelor, G.K., 1974, Transport properties of two-phase materials with random structure, Annu. Rev. Fluid Mech., V6, 227-257

Bathala, C.T., A.R. Rao, and J.A. Spooner, 1977, Application of linear systems analysis to ground water evaluation studies, Tech. Rep. No. 91, Water Resour. Res. Center, Purdue Univ., West Lafayette, Indiana, 128

Bathala, C.T., A.R. Rao, and J.A. Spooner, 1977, Stochastic- models for groundwater levels using causal relationships, Abstract in Hydraulics in the Coastal Zone, ASCE, New York, p. 211

Bathala, C.T., J.A. Spooner, and A.R. Rao, 1976, Regional aquifer evaluation studies with stochastic inputs, Tech. Rep. No. 72, Purdue Univ., Water Resour. Res. Center, West Lafayette, Indiana

Bear, J., 1961, On the tensor form of dispersion in porous media, J. Geophys. Res., V66(4), 1185-1197

Bear, J., 1961, Some experiments in dispersion, J. Geophys. Res., V66(8), 2455-2468

Bear, J., 1972, Dynamics of fluids in porous media, 764 p., American Elsevier, New York

Bear, J., 1979, Hydraulics of Groundwater, 569 pp., McGraw-Hill, New York

Bear, J. and Y. Bachmat, 1967, A generalized thoery on hydrodynamic dispersion in porous media, Int. Assn Sci. Hydrol Symp., Haifa, Publ. 72, 7-16, March 1967

Bellomo, N. and R. Monaco, 1979, Mathematical models for the time-evolution of stochastic systems in two-phase flow, Appl. Math Modeling, V3(1), 41-44
Bennion, D.W., and J.C. Griffiths, 1966, A stochastic model for predicting variations in reservoir rock properties, Trans. AIME, No. 237, Part 2, 9-16

Bennion, D.W., and J.C. Griffiths, A stochastic model for predicting variations in reservoir rock properties, Trans. AIME, No. 237, Part 2, 9-16, 1966.

Beran, M.J., 1957, Dispersion of soluble matter in flow through granular media, J. Chem. Phys., V27, 270-274

Beran, M.J., 1968, Statistical continuum theories, Interscience, New York

Betson, R.P., J.M. Boggs, S.C. Young, L.W. Gelhar, 1985, Design of a field experiment to investigate groundwater saturated zone transport processes, Interim rpt, RP2485-05, 104pp., Elecr. Power, Res. Inst., Palo Alto, CA

Bhattacharya, R.N., V.K. Gupta, and G. Sposito, 1976, Markovian stochastic basis for tranport of water through unsaturated soil, Soil Sci. Soc. Am. J., V40(3), 465-467

Bhattacharya, R.N., V.K. Gupta, and G. Sposito, 1976, On the stochastic foundations

of the theory of water flow through unsaturated soil, Water Resour. Res., V12(3), 503-512

Bhattacharya, R.N., V.K. Gupta, and G. Sposito, 1976, Physical interpretation of soil-water diffusivity in terms of theory of Markov-processes, Soil Sci., V121(5) 313-314

Bhattacharya, R.N., V.K. Gupta, 1979, Statistical-theory of solute transport in porous media, SIAM J. on Applied Math., V37(3), 485-498

Bibby, R. and D.K. Sunada, 1971, Statistcal error analysis of a numerical model of confined groundwater flow, in Stochastic Hydraulics: Proc. First Int. Symp. on Stochastic Hydraul., C.L. Chiu, ed., 591-612, 1971, School of Engineering, University of Pittsburgh, Pittsburgh, Pennsylvania

Black, T.C. and D.L. Freyberg, 1987, Stochastic modeling of vertically averaged concentration uncertainity in a perfectly stratified aquifer, Water Resour. Res. 23(6): 997-1004

Bogardi, I. and L. Duckstein, Design of a foundation subject of random groundwater levels, in Hydraulic Engineering for Improved Water Mangement, Proc. 17th Congress of Int. Assn for Hydraul. Res., 15-19 August 1977, Vol 6, 383-389

Bogardi, I., L. Duckstein, A. Schmieder, and F. Szidarovszky, 1980, Stochastic forecasting of minewater inrushes, Adv. in Water Resour., V3(1), 3-8

Bonano, E.J. and R.M. Cranwell, 1988, Treatment of uncertainties in the performance assessment of geologic high-level radioactive waste repositories, Math. Geol., 20(5), 543-565

Bonano, E.J., L.R. Shipers, A.L. Gutjahr, 1987, Stochastic analysis of contaminant transport in porous media: analysis of a two-member ratio nuclide chain, Water Resour. Res. 23(6):1063-1078

Boreli, M., M. Radojkovic, and S. Jovic, Some fundamental problems of underground water pollution, in Hydraulic Engineering for Improved Water Management, Proc. 17th Congress of Int. Assn for Hydraul. Res., 15-19 August 1977, Vol 6, 714-717

Bouwer, H., 1969, Planning and interpreting soil permeability measurements, J. Irr Drain Div., ASCE, V95(3), 391-402

Bras, R.L. and I. Rodriguez-Iturbe, 1985, Random functions and hydrology, Addison-Wesley publishing company, 559pp.

Bresler, E., H. Bielorai, and A. Laufer, 1979, Field test of solution flow models in a herogeneous irrigated cropped soil, Water Resour. Res., V15(3), 645-652

Bresler, E. and G. Dagan, 1979, Solute dispersion in unsaturated heterogeneous soil at field scale, 2. Applications, Soil Sci. Soc. Am. J. 43:467-472

Broadbent, S.R. and J.M. Hammersley, 1957, Percolation processes, crystals and mazes, Proc. Cambridge Phil. Soc., V53, 629-641

Brown, M.C., 1973, Mass balance and spectral analysis applied to karst hydraulic networks, Water Resources Res., V9(3), 749-752

Bulnes, A.C., 1946, An application of statistical methods to core analysis data of dolomitic limestone, Trans. AIME, 165, 223-240

Burrough, P.A., 1983a, Multiscale sources of spatial variation in soil, I: The application of fractal concepts to nested levels of soil variation, J. Soil Science, 34, 577-597

Burrough, P.A., 1983b, Multiscale sources of spatial variation in soil, II: A non-Brownian fractal model and its application in soil survey, J. Soil Science, 34, 599-620

Butler, Jr., J.J., Pumping tests in nonuniform aquifers: a deterministic/stochastic analysis, Ph.D. dissertation, Stanford University, Stanford, CA., 220 pp., December 1986

Butler, S.S. and D.L. Gundlach, 1972, Discharge and travel time for nonuniform groundwater conduits, Trans. Am. Geophys. Union, V53(11), 980 Buyevich, Y.A., A.I. Lenov, and V.M. Safrai, 1969, Variations in filtration velocity due to random large scale fluctuations in porosity, J. Fluid Mech., V37(2), 371-381

Byers, E. and D.B. Stephens, 1983, Statistical and stochastic analysis of hydraulic conductivity and particle size in a fluivial sand, Soil Sci Soc Am J., 47:1072-1081

Carnahan, C.L., 1976, Nonequilibrium thermodynamics of groundwater flow systems--symmetry properties of phenomenological coefficients and conservations of hydrodynamic dispersion, J. Hydrol, V31(1-2), 125-150

Carrera, J. and S.P. Neuman, 1986, Estimation of aquifer parameters under transient and steady state conditions, 1. Maximum likelihood method incorporating prior information, Water Resour. Res. 22(2):199-210

Carrera, J. and S.P. Neuman, 1986, Estimation of aquifer parameters under transient and steady state conditions, 2. Uniqueness, stability, and solution algorithms, Water Resour. Res. 22(2):211-227

Carrera, J. and S.P. Neuman, 1986, Estimation of aquifer parameters under transient and steady state conditions, 3. Application to synthetic and field data, Water Resour. Res. 22(2):228-242

Cavazza, S., 1964, Relationship between rainfall intensity and groundwater movement in subfluvial aquifers, in General Assembly of Berkeley, August 1963, Int. Assn Sci. Hydrol. Publ. No. 64, 390-401

Chander, S., P.N. Kapoor, and S.K. Goyal, 1981, Aquifer parameter estimation using Kalman filters, J. Irrigation and Drainage Div., ASCE, V107(IR1), 25-33

Charbeneau, R.J., and H-D. Yeh, 1979, Conditional simulation of groundwater flow fields with emphasis on regional dispersion, Trans. Am. Geophys. Union, V60(46), 821

Chaudhari, N.M. and A.E. Scheidegger, 1965, Statistical mechanics of certain hyrodynamic dispersion phenomena, Can. J. Phys., V43(10), 1776-1794

Chirlin, G.R. and G. Dagan, 1980, Theoretical head variograms for steady flow in statiscally homogeneous aquifers, Water Resour. Res., V16(6), 1001-1015

Chirlin, G.R. and E.F. Wood, 1979, Some theoretical and practical problems in variogram estimation and application, Trans Am. Geophys. Union, V60(46), 820 Chow, V.T. and S.J. Kareliotis, 1970, Analysis of stochastic hydrological systems, Water Resour. Res., V6(6), 1569-1582

Chu, S.T., 1977, Water table response to a sequence of recharges, Water Resour. Res., V13(4), 739-742

Clapp, R.B., G.M. Hornberger, and B.J. Cosby, 1981, Estimating spatial variability in soil moisture with a dynamic cmodel and Monte-Carlo simulation, Trans. Am. Geophys. Union, V62(17), 287

Clifton, P.M., and S.P. Neuman, 1982, Effects of kriging and inverse modeling on conditional simulation of the Avra Valley aquifer in southern Arizona, Water Resour. Res., 18, 1215-1234

Clifton, P.M., B. Sagar, and R.G. Baca, 1985, Stochastic groundwater traveltime modeling using a Monte Carlo technique, In International Association of Hydrogeologists Memoires: Hydrogeology of Rocks of Low Permeability, Tucson, Arizona, 17(1), 319-329

Codell, R., Draft generic position on groundwater travel time, Div. of Waste Manag., Office of Nuclear Material Safety and Safeguards, U.S. Nuclear Regulatory Commisssion, June 30, 1986

Cole, C.R. and H.P. Foote, Use of a multigrid technique to study effects of limited sampling of heterogeneity on transport prediction, Presented at the National Water Well Association Conference, Solving Ground Water Problems with Models, Denver, Colorado, February 10-12, 1987

Cooley, R.L., 1979, A method of estimating parameters and assessing reliability for models of steady-state groundwater flow, 2. Application of statistical analysis, Water Resour. Res., V15(3), 603-617

Cooley, R.L., J.W. Fordham, and J.A. Westphal, 1973, Some applications of statistical methods to groundwater flow system analysis, Tech. Rept. Series H-W, Hydrology and Water Resources Pub. No. 14, 53 p., Desert Research Institute, University of Nevada, Reno, Nevada

Csanady, G.T., 1973, Turbulent diffusion in the environment, D. Reidel Publishing Co., 248 pp.

Cushman, J.H., 1983, Volume averaging, probabilistic averaging, and ergodicity, Adv. Water Resour. 6:182-184

Cushman, J.H., 1984, On unifying the concepts of scale, instrumentation, and stochastics in the development of multiphase transport theory, Water Resour. Res. 20( ): 1668-1676

Cushman, J.H., 1986, On measurement, scale, and scaling, Water Resour. Res. 22:129-134

Cushman, J.H., 1987, More on stochastic models, Water Resour. Res. 23(4):750-752

Dagan, G., 1967, Hydrodynamic dispersion in a nonhomogeneous porous column, J. Geophys. Res., V72(4), 4075-4080

Dagan, G., 1976, Comment on "A stochastic-cnceptual analysis of one-dimensional groundwater flow in nonuniform homogeneous media" by R.A. Freeze, Water Resour. Res., V12(3), p 567

Dagan, G., 1979, Generalization of Darcy law for nonuniform flows, Water Resour. Res., V15(1), 1-7

Dagan, G., 1979, Models of groundwater flow in statistically homogeneous porous formations, Water Resour. Res., V15(1), 47-63

Dagan, G., 1980, Correction, Water Resour. Res., V16(1), 255, to: Models of groundwater flow in statistically homogenous porous formations, Water Resour. Res., 15(1), 1979

Dagan, G., 1981, Analysis of flow through heterogeneous random aquifers by the method of embedding matrix, 1, Steady flow, Water Resour Res., V17(1), 107-121

Dagan, G., Solute transport in heterogeneous porous formation, J. Fluid Mech., 145, 151-177, 1984.

Dagan, G., 1986, Statistical theory of groundwater flow: pore - to laboratory -, laboratory - to formation, and formation - to regional scale, Water Resour. Res. 22(9):1205-1345

Dagan, G., 1987, Theory of solute transport by groundwater, Ann. Rev. Fluid Mech., 19, 183-215

Dagan, G. and E. Bresler, 1979, Solute-dispersion in unsaturated heterogeheous soil at field scale, 1. theory, Soil Sci. Soc. Am. J., V43(3), 461-467

Davidson, M.R. and B.L. Dickson, 1986, A porous flow model for steady state transport of radium in groundwater, Water Resour. Res. 22(1):34-44

Davis, J.C., 1973, Statistics and Data Analysis in Geology, 550 pp., John Wiley and Sons, Inc., New York

Debouche, Ch., S. Gaspar, and L. Sine, 1974, Diffusivite de l'eau dans un milieu non sature heterogene, J. Hydrol. V22(1-2), 35-51

DeJosselin de Jong, G., 1958, Longitudinal and transverse diffusion in granular deposits, Trans. Am. Geophys. Union, V39(1), 67-74

DeJosselin de Jong, G., 1972, The tensor characteristics of the dispersion coefficient in anisotropic porous media, in Fundamentals of Transport Phenomena in Porous Media, Elsevier, Amsterdam, 1972, 259-267

DeJosselin de Jong, G. and M.J. Bossen, 1961, Discussion of paper by Jacob Bear "On the tensor form of dispersion in porous media", J. Geophys. Res., V66(10), 3623-3624

Delhomme, J.P., 1978, Kriging in the hydrosciences, Adv. in Water Resour., V1(5), 251-266

Delhomme, J.P., 1979, Kriging under boundary conditions, Trans. Am. Geophy., Union, V60(46), 820

Delhomme, J.P., 1979, Spatial variability and uncertainty in groundwater flow parameters: A geostatistical approach, Water Resour. Res., V15(2), 269-280

De Marsily, G., 1984, Spatial variability of properties in porous media: a stochastic approach, in Fundamentals of Transport in Porous Media, J. Bear, Y. Corapcioglu (eds.), Nijhoff, Dordrecht, pp. 721-769

De Marsily, G., G. Lauedan, M. Boucher, G. Fasanino, 1984, Interpretation of intereference tests in a well field using geostatistical techniques to fit the permeability distribution in a reservoir model, in Geostatistics for Natural Resources Characterization, Proc. NATO-ASI, Berly et al. (eds.) Part 2, Reidel Pub. Co. Dordrecht, The Netherlands

De Marsily, G., 1985, Flow and transport in fractured rocks: connectivity and scale effect, Mem. Int. Assoc. Hydrogeol. 17:267-277

De Marsily, G., 1986, Quantitative Hydrogeology: Groundwater Hydrogeology for Engineers, 440 pp., Academic Press, Inc., Orlando, Florida

Dendrou, B.A., E.N. Houstis, and S.A. Dendrou, 1979, Site selection using a kriging-FEM scheme, Trans. Am. Geophys. Union, V60(46), 821

Desbarats, A.J., 1987, Numerical estimation of effective permeability in sand-shale formations, Water Resour. Res. 23(2):273-286 Dettinger, M.D. and J.L. Wilson, 1981, First-order analysis of uncertainty in numerical models of groundwater flow, 1. Mathematical description, Water Resour. Res. 17:149-161

Devary, J.L. and P.G. Doctor, 1982, Pore velocity estimation uncertainties, Water Resour. Res. 18(4):1157-1164

Dievlin, A., G. Matheson, G. de Marsily, 1981, Growth of the dispersion coefficient with the mean travelled distance in porous media, Sci. Total Env. 21:319-328

Domenico, P.A. and G.A. Robbins, 1984, A dispersion scale effect in model calibrations and field tracer experiments, J. Hydrol. 70:132-

Dooge, J.C.I., Scale problems in hydrology, Kisiel Memorial Lecture at Department of Hydrology and Water Resources, University of Arizona, Tucson, Arizona, February 19, 1986

Dracup, J.A., O.E. Drummond, and P.R. Westlake, 1978, Kalman filtering of water well fluctuations, in Applications of Kalman Filter to Hydrology, Hydraulics, and Water Resouces, C.L. Chiu, ed., Stochastic Hydraulics Program,

University of Pittsburg, Pennsylvania, 693-275

Driscoll, F.G., 1986, Groundwater and Wells, 1089 pp., Johnson Division, St. Paul, Minnesota

Duerbaum, H.J. and K. Trippler, 1972, Comparison of statistical and deterministic approaches in the determinationof hydrological parameters of aquifers, in Proc. Int. Symp. on Uncertainties in Hydrologic and Water Resource Systems, Vol. 3, 3.3-1-3.3-20, Department of Hydrol. and Water Resour., University of Arizona, Tucson

Duffy, C.J. and L.W. Gelhar, 1986, A frequency domain analysis of groundwater quality fluctuations: interpretations of field data, Water Resour. Res. 22(7):1115-1128

Duffy, C.J. and J. Harrison, 1987, The statistical structure and filter characteristics of tritium fluctuations in fractured basalt, Water Resour. Res. 23(5):894-902

Dullien, F.A.L., 1979, orous media-fluid transport and pore structure, 396 p., Academic Press, New York, NY

Elgizawi, M.G., 1974, Use of cross-correlation techniques for determining the relationship between groundwater levels and sources in the Nile delta area, in Mathematical Models in Hydrology, Proc. of the Warsaw Symp., July 1971, Int. Assn Hydrol. Sci. Publ. No. 100, 319-325

Elsworth, D., A boundary element-finite element procedure for porous and fractured media flow, Water Resour. Res., 23(4), 551-560, 1987

Eriksson, G., 1970, Cross-spectrum analysis of groundwater levels in an esker, Nord. Hydrol., V1(4), 245-259

Eriksson, G., 1970, Groundwater time-series: An exercise in stochastic hydrology, Nord. Hydrol. V1(3), 181-205

Fara, H.D., and A.E. Scheidegger, 1961, Statistical geometry of porous media, J. Geophys. Res., V66(10), 3279-3284

Ferrandon, J., 1948, Lew lois de l'ecoulement de filtration, Le Genie Civil, V 125, 24-28

Ferraund, L.A. P.C.D. Milly, G.F. Pinder, 1986, Dual-gamma attenuation for the determination of porous medium saturation with respect to three fluids, Water Resour. Res. 22(12):1657-1663

Fischer, H.B.,E.J. List, R.C.Y. Koh, J. Imberger, N.H. Brooks, 1979, Mixing in inland and coastal waters, Academic press, 483 pp.

Flores, W., E.Z., A.L. Gutjarh, and L.W. Gelhar, 1978, A stochastic model of the operation of a stream-aquifer system, Water Resour. Res., V14(1), 30-38

Fogg, G.E., 1986, Groundwater flow and sand body interconnectedness in a thick multiple-aquifer system, Water Resour. Res. 22(5):679-694

Freeze, R.A., 1971, Three-dimensional, transient, saturated-unsaturated flow in a goundwater basin, Water Resour. Res., 7(2), 347-366

Freeze, R.A., 1975, A stochastic-conceptual analysis of one- dimentional groundwater flow innonuniform homogeneous media, Water Resourc. Res., V11(5), 725-741

Freeze,, R.A., L.W. Gelhar,and T. Maddock, 1978, Geostatistical concepts and stochastic methods in hydrogeology, Geology, V6(5), 297-298

Freyberg, D.L., 1986, A natural gradient experiment of solute transport in a sand aquifer 2. Spatial moments and the advection and dispersion of nonreactive tracers, Water Resour. Res., 22, 2031-2046

Fried, J.J. and M.A. Combarnous, 1971, Dispersionin porous media, in Advances in Hydroscience, V 7, 169-282

Frisch, H.L., and J.M. Hammersley, 1963, Percolation processes and related topics, J. Soc. Ind. Appl. Math., V11(4), 894-918

Gambolati, G., 1979, Kriging in the environmental applications: results and shortcomings, Trans. Am. Geophys. Union, V60(45), 821

Gambolati, G. and G. Volpi, 1979, A conceptual deterministic analysis of the Kriging technique inhydrology, Water Resour, Res., V15(3), 625-629

Gambolati, G. and G. Volpi, 1979, Groundwater countour mapping in Venice by stochastic interpolators, 1, Theory, Water Resour, Res., V15(2), 281-290

Ganoulis, J. and C. Thirriot, 1973, Sur un modele probabiliste de l'equilibre capillaire en milieu poreux C. R. Acad. Sc. Paris, T. 276, Ser. A, 1573-76

Ganoulis, J. and C. Thirriot, 1977, Stochastic study of the entrance of a non-wetting fluid in a pourous medium, under the influence of capillarity in "Hydraulic probems solved by stochastic methods", Proc. 2e Int. IAHR Symp. on Stochastic Hydraulics, Lund, Sweden, Aug. 2-4, 1976,Water Res. Publ., pp 22.1-22.18, Fort Collins, Colorado 80522

Gannon, John M., and T.-C.J. Yeh, Numerical analysis of the effects of heterogeneities on dispersion, in prep 1988.

Garabedian, S.P., Large-scale dispersive transport in aquifers: field experiments and reactive transport theory, PhD. dissertation, Massachusetts Institute of Technology, Cambridge, Massachusetts, July 1987

Gavalas, G.T., P.C. Shah, and J.H. Seinfeld, 1976, Reservoir history matching by Bayesian estimation, Soc. Petrol. Eng. J., V16(6), 337-350

Gelhar, L.W., 1974, Stochastic analysis of phreatic aquifers, Water Resour. Res., V10(3), 539-545

Gelhar, L.W., 1976, Effects of hydraulic conductivity variations on groundwater flows, in Hydraulic Problems Solved by Stochastic Methods, Proc. Second Int. IAHR Symp on Stochas- tic Hydraulics, Lund, Sweden, 409, 429,Water Resourc. Publications, Fort Collins, CO

Gelhar, L.W., A.A. Bakr, A.L. Gutjahr, and J.R. McMillan, Comments on stochastic conceptual analysis of one-dimensional groundwater flow in a non-unifrom homogeneous medium by Freeze, R.A., Water Resour. Res. 13(2), 477-480, 1977.

Gelhar, L.W., A.L. Gutjahr, and R.L. Naff, Stochastic analysis of macrodispersion in a stratified aquifer, Water Resour. Res., 15, 1387-1397, 1979.

Gelhar, L.W., 1984, Stochastic analysis of flow in heterogeneous porous media in Fundamentals of Transport Pheonmena in Porous Media, J. Bear and M.Y. Corapcioglau (eds.), Martinus Nijhoff Publishers, Dordrecht, The Netherlands

Gelhar, L.W., 1986, Stochastic subsurface hydrology: from theory to applications, Water Resour. Res. 22(9):1355-1455

Gelhar, L.W., 1988, Response to O.E. Meinzer Award, GSA Bulletin, July, p. 948.

Gelhar, L.W. and C.L. Axness, 1983, Three-dimensional stochastic analysis of macrodispersion in aquifers, Water Resour. Res., 19(1), 161-180

Gelhar, L.W., A.A. Bakr, A.L. Gutjahr, and J.R. MacMillan, 1977, Comments on "A stochastic-conceptual analysis of one- dimensional groundwater flow in nonuniform homogeneous media" by R.A. Freeze, Water Resourc. Res., V13(2), 477-479

Gelhar, L.W. and M.S. Collins, 1971, General analysis of longitudinal dispersion in nonuniform flow, Water Resour. Res., V7(6), 1511-1521

Gelhar, L.W., G.W. Gross, and C.J. Duffy, 1979, Stochastic methods of analyzing groundwater recharge, in the Hydrology of Areas of Low Precipitation, Proc. of Canberra Symp., Int. Assn Hydrol Sci Publ No. 128, 313-321

Gelhar, L.W., A.L. Gutjahr, and R.L. Naff, 1979, Stochastic analysis of macrodispersion in a stratified aquifer, Water Resour. Res., V15(6), 1387-1397

Gelhar, L.W., P.Y. Ko, H.H. Kwai, and J.L. Wilson, 1974, Stochastic modelling of groundwater systems, 313 p., Rep. 189, R.M. Parsons Lab for Water Resour. and Hydrodynamics, Massachusetts Institute of Technology, Cambridge, Massachusetts

Gelhar, L.W., J.L. Wilson, and A.L. Gutjahr, 1979, Comments on "Simulation of groundwater flow and mass transport under uncertainty" by D.H. Tang and G.F. Pinder, Adv. in Water Resourc., 2(2), 101

Gillham, R.W., E.A. Sudicky, J.A. Cherry, E.O. Frind, 1984, An advection-diffusion concept for solute transport in heterogeneous unconsolidated geological deposits, Water Resour. Res. 20(3):369-378

Golden, J.M., 1980, Percolation theory and models of unsaturated porous media, Water Resour. Res., V16(1), 201-109

Greenkorn, R.A. and D.P. Kessler, 1969, Dispersion in heterogeneous nonuniform anisotropic porous media, Ind. Eng. Chem., V61(9), 14-32

Gupta, V.K. and R.N. Bhattacharya, 1986, Solute dispersion in multidimensional periodic saturated media, Water Resour. Res. 22(2):156-164

Gutjahr, A.L., Kriging in stochastic hydrology: Assessing the worth of data, paper presented at the Chapman Conference on Spatial Variability in Hydrologic Modeling, AGU, Fort Collins, Colorado, July 1981

Gutjahr, A.L. and L.W. Gelhar, 1981, Stochastic models of subsurface flow: Infinite versus finite domains and stationarity, Water Resour. Res., V17(2), 337-350

Gutjahr, A.L., E.J. Bonano, R.M. Cranwell, 1985, Treatment of parameter uncertainties in modeling contaminant transport in geologic media: stochastic models versus determination models with statistical parameter sampling, in Proc. Int's Assoc. Hydraulic Research Symp. in the Stochastic Approach to Subsurface Flow, G. de Marsily (ed.), Montvillargenne, France, June 3-6, 1985, pp. 332-350

Gutjahr, A.L., L.W. Gelhar, A.A. Bakr, and J.R. MacMillan, 1978, Stochastic analysis of spatial variability in subsurface flows, 2, Evaluation and application, Water Resourc. Res., V14(5), 953-960

Gutjahr, A.L., D. McKay, and J.L. Wilson, Fast Fourier transform methods for random field generation, EOS, 68(44), Nov. 3, 1987.

Guven, O., F.J. Molz, J.G. Melville, 1984, An analysis of dispersion in a stratifed aquifer, Water Resour. Res. 20: 1337-1354

Guven, O., F.J. Molz, J.G. Melville, 1986, Comment on "an advection-diffusion concept for solute transport in heterogeneous unconsolidated geological deposit" by Gillham et al., Water Resour. Res. 22(1):89-91

Guven, O. and F.J. Molz, 1986, Deterministic and stochastic analysis of dispersion in an unbounded stratified porous medium, Water Resour. Res. 22(11):1565-1574

Haldorsen, H.H. and L.W. Lake, 1982, A new approach to shale management in field scale simulation models, Paper presented at the 57th Annual Technical Conference, Soc. Pet. Eng., New Orleans, Sept. 26-29

Haring, R.E. and R.A. Greenkorn, 1970, A statistical model of a porous medium with nonuniform pores, AIChE J., V16(3), 447-483

Harleman, D.R.F. and R.R. Rumer, 1963, Longitudinal and lateral dispersion in an isotropic porous medium, F. Fluid Mech., V16(3), 385-394

Heller, J.P., 1972, Observations of mixing and diffusion in porous media, Proc. Second Int Symp on Fund of Trans Phen in Porpous Media, Int. Assn' Hydraulic Res., 1-26, University of Guelph, Guelph, Ontario, Canada

Hewett, T.A., Fractal distributions of reservoir heterogeneity and their influence on fluid transport, Society of Petroleum Engineers, SPE15386, Presented at the 61st Annual Technical Conference of the Society of Petroleum Engineers, New Orlans, Louisiana, October 5-8, 1986

Hoeksema, R.J. and P.K. Kitanidis, 1984, An application of the geostatistical approach

to the inverse problem in two- dimensional groundwater modeling, Water Resour. Res. 19(3):677-690

Hoeksema, R.J. and P.K. Kitanidis, 1985, Analysis of the spatial structure of properties of selected aquifers, Water Resour. Res, 21, 563-572

Horton, R., M.C. Thompson, J.F. McBride, 1987, Method of estimating the travel time of noninteracting solutes through compacted soil material, Soil Sci. Soc. Am. J. 51(1):48-53

Huang, C. and D.D. Evans, 1985, A 3-dimensional computer model to simulate fluid flow and contaminant transport through a rock fracture system, NUREG/CR-4042, U.S. Nuclear Regulatory Commission, 108 pp.

Hubbert, M.K., 1940, The theory of groundwater motion, J. of Geol., 48, 785-944

Huyakorn, P.S., B.H. Lester, and C.R. Faust, 1983a, Finite element techniques of modeling groundwater flow in fractured aquifers, Water Resour. Res., 19(4), 1019-1035

Huyakorn, P.S., B.H. Lester, and J.W. Mercer, 1983b, An efficient finite element technique for modeling transport in fractured porous media, 1, Single Species Transport, Water Resour. Res., 19(3):841-854

Huyakorn, P.S., B.H. Lester and J.W. Mercer, 1983c, An efficent finite element technique for modeling transport in fractured porous media, 2, Nuclide decay chain transport, Water Resour. Res., 19(3), 841-854

Ilyin, N.I., and others, 1971, tsenka tochnosti opredeleniya vodopronitsayemosti gornykh porod, Moscow, Nedra

Iwasa, Y. and H. Takeuchi, 1971, Dispersive characteristics of flows through porous media, in Stochastic Hydraulics, C.L. Chiu, ed., School of Engineering, University of Pittsburg, 613-631

Jackson, R.E., 1973, Evapotranspiration of groundwater, Scientific Series No. 17, Department of the Environment, Inland Waters Directorate, Ottawa, Canada, 40p.

Jackson, R.E., 1974, Time-series analysis of groundwater hydrographs from surficial deposits on Canadian shield, Can. J. Earth Sci., V11(1), 177-188.

Jackson, R.E., J.A. Gilliland and K. Adamowski, 1973, Time series analysis of the hydrologic regimen of a groundwater recharge area, Water Resour. Res., V9(5), 1411-1419

Javandel, I., and P.A., 1969, Witherspoon, A method of analyzing transient fluid flow in multilayered aquifers, Water Resour. Res., 5(4), 1969

Jenkins, G.M. and D.G. Watts, 1968, Spectral Analysis and its Applications, 525 pp., Holden-Day, Inc., San Francisco

Jensen, J.L., D.V. Hinkley, L.W. Lake, 1987, A statistical study of reservoir permeability: distributions, correlations and averages, Soc. Petr. Eng.,

Formation Evaluation, December, pp. 461-468. Journel, A.G., and CH.J. Huijbregts, 1978, Mining Geostatistics, 600 pp., Academic Press, London

Journel, A.G., and CH.J. Huijbregts, 600 pp., Mining Geostatistics, Academic Press, London, 1978.

Julian, P.R., 1967, Variance spectrum analysis, Water Resourc. Res., V3(3), 831-845

Kasansky, A.B., 1974, A statistical filtration model for the inseepage of melt water into frozen ground, in Mathematical Models in Hydrology, Proc. of the Warsaw Symp., July 1971, Int. Assn Hydrol. Sci. Publ. No. 100, 241-245. Discussion by S. Dyck, Publ No. 102, 1175-1176

Kazemi, H., M.S. Seth, and G.W. Thomas, 1969, The interpretation of interference tests in naturally fractured reservoirs with uniform fracture distribution, Soc. Pet. Eng. J., Dec., 463-472

Kilbury, R.K., T.C. Rasmussen, D.V. Evans, A.W. Warrick, 1986, Water and air intake of surface exposed rock fractures in situ, Water Resour. Res. 22(10):1431-1443

Kipp, K.C., K.G. Stollenwerk, D.B. Grove, 1986, Groundwater transport of strontium 90 in a glacial outwash environment, Water Resour. Res. 22(4):519-530

Kiremidjian, A.S. and P. Kruger, 1979, A stochastic model of radionuclide migration from natural and engineered repositories, in Scientific Basis for Nuclear Waste Management, V 2, 779-785

Kitanidis, P.K., 1986, Comment on "Stochastic modeling of groundwater flow by unconditional and conditional probabilities: the inverse problem" by G. Dagan, Water Resour. Res. 22(6):984-986

Kitanidis, P.K., 1986, Parameter uncertainty in estimation of spatial functions: Boysian analysis, Water Resour. Res. 22(4):499-507

Kitanidis, P.K., and E.G. Vomvoris, 1983, A geostatistical approach to the inverse problem in groundwater modeliling (steady-state) and one-dimensional simulations, Water Resour. Res., 19(3), 677-690

Koval, E.J., 1963, A method for predicting the performance of unstable miscible displacement in heterogeneous media, Soc. Petrol Eng. J. V392), 145-154

Kriz, H., 1972, Statistical processing of long-term observations of groundwaters, J. Hydrol., V16(1), 17-37

Labadie, J.W. and D.R. Hampton, 1979, Estimation of hydrogeologic parameters for optimal groundwater basin development, in Mathematical Programming with Data Perturbations, A.V. Fiacco, ed., Lecture Notest in Pure and Applied mathematics, Marcel Dekker, Inc., New York sched. pub. date, 1981

Larson, R.G., L.E. Scriven, and H.T. Davis, 1981, Percolation theory of two phase flow inporous media, Chem. Eng. Sci., V36, 57-73

Lau, L.K., W.J. Kaufman, and D.K. Todd, 1959, Dispersion of a water tracer in

radial laminar flow through porous media, Inst. Eng. Research Rept 93-5, University of California, Berkeley, 78 p.

Law, A.G., 1974, Stochastic analysis of groundwater level time series in the western United States, Hydrology Paper No. 68, Colorado State University, Fort Collins, CO

Law, J., 1944, A statistical approach to the interstitial heterogeneity of sand reservoirs, Trans AIME, v. 155, 202-222

Liao, K.H. and A.E. Scheidegger, 1968, A computer model for some branching-type phenomena in hydrology, Bull. Int. Assn. Sci. Hydrol., V13(1), 5-13

Liao, K.H. and A.E. Scheidegger, 1969, Branching-type models of flow through porous media, Bull Int Assn Sci Hydrol, V14(4), 137-145

Liao, K.H. and A.E. Scheidegger, 1970, Statistical models of flow through porous media, Pure and Appl. Geophys., V83(6), 74-81

Lippmann, M.J., 1974, Two-dimensional stochastic model of a heterogeneous geologic system, Ph.D. thesis, 135 p., University of California, Berkelye, University Microfilms order no 75-5810

Lippmann, M.J., and P.A. Witherspoon, 1974, Stochastic model to simulate cross sections of layered heterogeneous groundwater systems, Trans. Am. Geophys. Union, V55(12), 1118.

Lumley, J.L., and H.A. Panofsky, 1964, The Structure of Atmospheric Turbulence, John Wiley, New York

Maddock, T., III, 1974, The operation of a stream-aquifer sytem under stochastic demand,s Water Resour. Res., V10(1), 1-10

Maddock, T., III, 1976, A drawdown prediction model based on regression analysis, Water Resour. Res., V12(4), 818-822

Mandel, S. and Z. Weinberger, 1972, Analysis of a network-model for dispersive flow, J. Hydrol., V16(2), 147-157

Mandelbrot, B.B., 1967, How long is the coastline of Great Britain? Statistical self-similarity and fractional dimension, Science, 155, 636-638

Mandelbrot, B.B., 1983, The Fractal Geometry of Nature, 468 pp., W.H. Freeman, San Francisco, California

Mantoglou, A., and J.L. Wilson, 1982, The turning bands method for simulation of random fields using line generation by a spectral method, Water Resour. Res., 18(5), 1379-1394

Mantoglou, A., and L.W. Gelhar, 1987a, Stochastic modeling of large-scale transient unsaturated flow systems, Water Resour, Res., 23(1), 37-46

Mantoglou, A., and L.W. Gelhar, 1987b, Capillary tension head variance, mean soil moistsure content, and effctive specific soil moisture capacity of transient

unsaturated flow in stratified soils, Water Resour. Res., 23(1), 47-56

Mantoglou, A. and L.W. Gelhar, 1987c, Effective hydraulic conductivities of transient unsaturated flow in stratified soils, Water Resour. Res., 23(1), 57-68

Marle, C., 1967, Ecoulements polyphasiques en milieu poreux, Rev. Inst. Fr. Pet, 22(10), 1471-1509

Marle, C., P. Simandoux, J. Pacsirsky, and C. Gaulier, 1967, Etude du deplacement de fluides miscibles en milieu poreux startifie, Rev. Inst. Francais Petrole, V2292), 272-294

Massman, J. and R.A. Freeze, 1987, Groundwater contamination from waste management site: the interaction between risk-based engineering design and regulatory policy, 1. Methodology, Water Resour. Res. 23(2):351-367

Massman, J. and R.A. Freeze, 1987, Groundwater contamination from waste management sites: the interaction between risk-based engineering design and regulatory policy, 2. Results, Water Resour. Res. 23(2):368-380

Matheron, G., 1967, Composition des permeabilities en milieu poreux heterogene methode de Schwydler et regles de ponderation, Rev. Inst. Francais Petrole, V 22, 443-466

Matheron, G., 1967, Elements pour une theorie des milieux poreux, Masson et Cie, Paris.

Matheron, G., 1973, The intrinsic random functions and their applications, Advan. Appl. Probab., 5, 438-468

Matheron, G., and G. de Marsily, 1980, Is transport in porous media always diffusive? A counter example, Water Resour. Res., 16(5), 901-917

McLaughlin, D., 1978, Potential applications of Kalman filtering concepts to gorundwater basin management, in Applications of Kalman Filter to Hydrology, Hydraulics, and Water Resources, C.L. Chiu, ed., Stochastic Hydraulics Program, University of Pittsburg, Pennsylvania, 639-655

McLaughlin, D. 1979, Application of kriging to a groundwater plume mapping problem, Trans, Am. Geophys. Union, V60(46), 820

McMillan, W.D., 1966, Theoretical analysis of groundwater basin operations, Contrib. 114, 167 p., University of California, Water Resour. Center, Berkeley, California

Mercado, A., 1967, The spreading pattern of injected waters in a permeable stratified aquifer, Symp. of Haifa, Artificial Recharge and mangement of Aquifers, IASH Publ. 72, 23-36, Int Assn Hydrol Sci., Gentbrugge, Belgium

Mizell, S.A., A.L. Gutjahr, and L.W. Gelhar, 1982, Stochastic analysis of spatial variability in two-dimensional steady groundwater flow assuming stationary and non-stationary heads, Water Resour. Res., 19, 1853-1867

Moench, A.F., 1984, Double-porosity models for a fissured groundwater reservoir

with fracture skin, Water Resour. Res., 20(7), 831-846

Moltyaner, G.L., 1985, Stochastic versus determinate: a case study, in Proc. Int'l Assoc. Hydraulic Research Symp. on The Stochastic Approach to Subsurface Flow, G. de Marsily (ed.), Montuillargenne, France, June 3-6, pp. 362-364

Molz, F.J., O. Guven, J.G. Melville, R.D. Crocker, K.T. Matteson, 1986, Performance, analysis and simulation of a two-well tracer test at the Mobile site, Water Resour. Res. 22(7):1031-1037

Morel-Seytoux, H.J., 1976, Water resources planning (an illustration on management of surface and groundwaters), in Stochastic Approaches to Water Resources, Vol 1., H.W. Shen, ed., pp 10-1-10-61

Moreno, L. and A. Rasmuson, 1986, Contaminant transport through a fractured porous rock: impact of the inlet boundary condition on the concentration profile in a rock matrix, Water Resour. Res. 22(12):1728-1730

Morrison, P., and P. Morrison, 1982, Powers of Ten, Scientific American Books, New York

Musy, A. and L. Duckstein, 1976, Bayesian approach to tile drain design, J. Irr. Drain Div., ASCE, V102(3), 317-334

Naff, R.L. and A.V. Vecchia, 1986, Stochastic analysis of three- dimensional flow in a bounded domain, Water Resour. Res. 22(5):695-704

Naff, R.L. and A.V. Vecchia, 1987, Depth-averaging effects on hydraulic head for media with stochastic hydraulic conductivity, Water Resour. Res. 23(4):5612-570

Nelson, R.W., 1964, Stream functions for three-dimentional flow in heterogeneous porous media, in General Assembly of Berkeley, August 1963, Int. Assn. Sci. Hydrol. Publ. No. 64, 290-297

Nelson, R.W., 1966, Flow in heterogeneous porous mediums, 1, Darcian-type description of two-phase systems, Water Resour. Res. V2(3), 487-495

Neretnieks, I., 1985, Transport in fractured rocks, Mem. Int. Assoc. Hydrogeol., 17:301-318

Neuman, S.P., 1979, Statistical characterization of aquifer heterogeneities: An overview, Recent Trends in Hydrogeology, Geol. Soc. Am. Spec. Pap., in press

Neuman, S.P., 1980, Statistical analysis and stochastic modeling of the Cortaro aquifer in southern Arizona, Trans. Am. Geophys. Union, V61(46), 952

Neuman, S.P., 1980, A statistical approach to the inverse problem of aquifer hydrology, 3, Improved solution method and added perspetive, Water Resour. Res., V16(2), 331-346

Neuman, S.P., 1982, Statistical characterization of aquifer heterogeneitics: an overview, in Recent Trends in Hydrogeology (T.N. Narasimham, ed.), Spec.

Pap. Geol. Soc. Amer. v. 189, pp. 81-102, Boulder, CO

Neuman, S.P., 1984, Role of geostatistics in subsurface hydrology in Geostatistics for Natural Resources Characterization, Proc. NATO-ASI, Verly, G., David, M., Journel, A.G., and Marechal, A. (eds.), Part 1, pp. 781-817, Reidel, Dordrecth, The Netherlands

Neuman, S.P., Stochastic continuum representation of fractured rock permeability as an alternative to the REV and fracture network concepts, 533-561, 28th U.S. symposium on rock mechanics, Tucson, Arizona, 29 June -1 July, 1987.

Neuman, S.P., and S. Yakowitz, 1979, A statistical approach to the inverse problem of aquifer hydrology, 1, Theory, Water Resour. Res., V15(4), 845-860

Neuman, S.P., G.E. Fogg, and E.A. Jacobson, 1980, A statistical approach to the inverse probelm of aquifer hydrology: 2. Case study, Water Resour. Res., V16(1), 33-58

Neuman, S.P., C.L. Winter, C.M. Newman, 1987, Stochastic theory of field-scale fickian dispersion in anisotropic porous media, Water Resour. Res. 23(3):453-466

Neuzil, C.E., 1986, Groundwater flow in low-permeability environments, Water Resour. Res. 22(8):1163-1195

Nielsen, D.R., 1979, Analyzing the spatial variability of soil parameters infield soils, Trans. Am. Geophys. Union, V60(32), 583-584

Nielsen, D.R., J.W. Biggar, and K.T. Erh, 1973, Spatial variability of field measured soil-water properties, Hilgardia, V. 42:215-260

Nielsen, D.R., J. W. Biggar, and C.S. Simmons, 1979, Analysis of water and solute movement in field soils, Trans. Am. Geophys. Union, V60(7), 113

Nikolaevskii, V.N., 1959, Convective diffusion in porous media, Prikl, Matem. Mekhan, V23(6), 1042-1050

Olbrisch, H-D., 1977, Modeling of groundwater recharge according to infiltration measurements by lysimeters, in Hydraulic Engineering for Improved Water Management, Proc. 17th Congress of Int. Assn for Hydraul Res., 15-19 August 1977, Vol 6, 718-722

Osborn, J.F., 1966, The prediction fo piezometric groundwater levels in observation wells based on prior occurrences, Water Resour. Res., V2(1), 139-144 Oster, C.A., A.G. Gibbs, and D.H. Tang, 1981, Analysis of a numerical solution to the one-dimentional stochastic convection equation, Adv. in Water Resour., V4(1), 2-8

Parker, J.C., and K.A. Albrecht, 1987, Sample volume effects on solute transport predictions, Water Resour. Res. 23(12): 2293-2301

Parsons, A.M., E.D. Mattson, D.B. Stephens, K. Flamigan, K. Black, 1988, Field simulation of waste impoundment seepage in the vadose zone, Proc. Focus on Groundwater Issues, Conf. Nat. Water Well Assoc., March 23-35,

Albuquerque. Peck, A.J., R.J. Luxmoore, and J.L. Stolzy, 1977, Effects of spatial variability of soil hydraulic properties in water budget modeling, Water Resour. Res., V13(2), 348-354

Perkins, T.K. and O.E. Johnston, 1963, A review of diffusion and dispersion in porous media, Soc. Petrol. Eng. J., V3(1), 70-84f

Philip, J.R., 1967, Sorption and infiltration in heterogeneous media, Aust. J. Soil Res., V5, 1-10Peters, R.R., J.H. Gauthier, and A.L. Dudley, The effect of percolation rate on water-travel time in deep, partially saturated zones, Sandia Report, SAND85-0854, 1986

Philip, J.R., 1980, Field heterogeneity: Some basic issues, Water Resour. Res., V16(2), 443-448

Philip, J.R., 1984, Travel times from buried and surface infiltration point sources, Water Resour. Res. 20( ): 990-994

Pickens, J.F. and G.E. Grisak, 1981, Modeling of scale-dependent dispersion in hydrogeologic systems, Water Resour. Res. 17(6):1701-1711

Pickens, J.F. and G.E. Grisak, 1981, Scale-dependent dispersion in a stratified granular aquifer, Water Resour. Res. 17: 1191-1211

Pimentel, K.D., 1978, Asymptotic estimation error growth applied to monitoring, in Applications of Kalman Filter to Hydrology, Hydraulics, and Water Resources, C.L. Chiu, ed., Stochastic Hydraulics Program, University of Pittsburg, Pennsylvania, 681-691

Pimentel, K.D., J.V. Candy, S.G. Azevedo, and T.A. Doerr, 1980, Simplified groundwater flow modeling: An application of Kalman filter based identification, NTIS Accession No. UCRL- 82649.

Pollock, D.W., 1986, Simulation of fluid flow and energy transport processes associated with high-level radioactive waste disposal in unsaturated alluvium, Water Resour. Res. 22(5):765-777

Poreh, M., 1965, The dispersivitytensor inisotropic and axisymmetric mediums, J. Geophys. Res., V70(16), 3909-3914

Prager, S., 1961, Viscous flow through porous media, Phys Fluids, V4(12), 1477-1482

Raats, P.A.C., 1975, Continuum interpretation of discrete, structured and probabilistic models for transport of solutes in prous media, Trans. Am. Geophys. Union, V56(12), 978

Rao, A.R., R.G.S. Rao, and R.L. Kashyap, 1975, Stochastic models for groundwater levels, Tech. Rep. No. 67, Water Resour. Res. Center, Purdue Univ.,West Lafayette, Indiana

Rao, P.S.C, P.V. Rao, J.M. Davidson, 1977, Estimation of the spatial variability of soil-water flux, Soil Sci. Soc. Am. J. 41:1208-1209

Rao, P.V., K.M. Portier, and P.S.C. Rao, 1981, A stochastic approach for describing

convective-dispersive solute transport in saturated porous media. Water Resour. Res., V17, in press

Rasmuson, A. and I. Neretnieks, 1986, Radionuclide migration in strongly fissured zones: the sensitivity to some assumptions and parameters, Water Resour. Res. 22(4):559-569

Rasmuson, A. and I. Neretnieks, 1986, Radionuclide transport in fast channels in crystaline rock, Water Resour. Res. 22(8):1247-1256

Rasmussen, T.C., 1987, Computer simulation of steady fluid flow and solute transport through three-dimensional networks of variably saturated, discrete fractures, in Evans, D.D. and T.J. Nicholson (Eds.), Flow and Transport Through Unsaturated Fractured Rock, AGU Geophysical Monograph 42, 107-114

Remson, I. and J.R. Randolph, 1958, Application of statistical methods to the analysis of groundwater levels, Trans. Am. Geophys. union, V39(1), 75-83

Rifai, E.M.N., W.J. Kaufman, and D.K. Todd, 1956, Dispersion phenomena in laminar flow through porous media, Progr. Report 3, Sanitary Eng. Research Lab., University of California, Berkeley, 156 p.

Robbins, G.A. and P.A. Domenico, 1985, Determining dispersion coefficients and sources of model-dependent scaling, J. Hydrol. 75:195-211

Rockaway, J.D., Jr., 1970, Trend-surface analysis of ground- water fluctuations, Ground Water, May-June 1970, 29-36

Ross, B. and C.M. Kopllik, 1978, A statistical approach to modeling transport of pollutants in ground water, J. Int. Assn. Math Geology, V10(6), 657-672

Ross, B. and C.M. Koplik, 1979, A new numerical method for solving the solute transport equation, Water Resour. Res., V15(4), 949-955

Ross, B., 1986, Dispersion in fractal fracture networks, Water Resour. Res. 22(5):823-827

Russo, D. and E. Bresler, 1980, Field determinations of soil hydraulic properties for statistical analyses, Soil Sci. Soc. Am. J., V44(4), 697-702

Russo, D. and E. Bresler, 1980, Scaling soil hydraulic properties of heterogeneous field, Soil Sci Soc Am J., V44(4), 681-684

Saffman, P.G., 1959, A theory of dispersion in a porous medium, J. Fluid Mech., V6(3), 321-349

Saffman, P.G., 1960, Dispersion due to molecular diffusion and macroscopic mixing inflow through a network of capillaries, J. Fluid Mech., V7(2), 194-208

Sager, B., 1978, Analysis of dynamic aquifers with stochastic forcing function, Water Resour. Res., V14(2), 207-216

Sager, B., 1978, Galerkin finite element procedure for analyzing flow through random media, Water Resour. Res., V14(6), 1035- 1044

Sager, B., 1979, Solution of lineraized Boussineq equation with stochastic boundaries and recharge, Water Resour. Res. V15(3), 618-624

Sagar, B. and C.C. Kiesiel, 1972, Limits of deterministic predictability of saturated flow equations, in Proc. Second Int. Symp. on Fund of Trans. Phen. in Porous Media, V 1, 194-205, Int. Assn Hydraul. Res., University of Guelph, Guelph, Ontario, Canada

Sager, B. and C. Preller, 1980, Stochastic model of water table under drainage, J. Irr. Drain. Div., ASCE, V106(3), 189-202

Sager, B. and S.R. Singh, 1979, Aquifer diffusivity from noisy boundary data, J. Hydraul. Div., ASCE, V105(8), 943-954

Scheidegger, A.E., 1954, Statistical hydrodynamics in porous media, J. Appl Phy., V25(8), 994-1001

Scheidegger, A.E., 1958, The random-walk model with autocorrelation of flow through porous media, Can. J. Phys., V36, 649-658

Scheidegger, A.E., 1959, Statistical approach to miscible displacement in porous media, Can. Mining Met. Bull., V 52(561), 26-30

Scheidegger, A.E., 1960, The physics of flow through porous media, revised edition, University of Toronto Press, Toronto, Ontario, Canada

Scheidegger, A.E., 1961, General theory of dispersion in porous media, J. Geophys. Res., V66(10), 3273-3278

Scheidegger, A.E., 1961, On the statistical properties of some transport equations, Can. J. Phys., V39(11), 1573-1582

Scheidegger, A.E., 1964, Statistical hydrodynamics in porous media, Advan. Hydrosci., V1, 161-181, V.T. Chow, ed., Academic Press, New York, NY

Scheidegger, A.E., 1967, Solitary dispersion, Can. J. Phys., V45(5), 1783-1789

Scheidegger, A.E., 1974, The physics of flow through porous media, 3rd ed., University of Toronto Press, Toronto, Ontario, Canada

Scheidegger, A.E., and N.M. Chandhari, 1964, Some statistical properties of certain geophysical transport equations, Pure and Appl. Geophys., V59(3), 45

Schmidtke, K., E.A. McBean, and J.F. Sykes, 1980, Stochastic estimation of states in unconfined aquifers subject to artificial recharge, Trans. Am. Geophys. Union, V61(46), 954

Schwartz, F.W., 1977, Macroscopic dispersion in porous media: The controlling factors, Water Resour. Res., V13(4), 743-752

Schwartz, F.W., L. Smith, and A.S. Crowe, 1983, A stochastic analysis of macroscopic dispersion in fractured media, Water Resour. Res., 19,1253-1265

Schwydler, M.I., 1962, Flow inheterogeheous media (in Russian), Izv. Akad. Nauk

SSSR Mekh Zhidk. Gaza., V 3, 185

Shapiro, A. M., and J. Andersson, 1983, Steady-state fluid response in fractured rock: A boundary element solution for a coupled, discrete fracture continuum model, Water Resour. Res. 19(4), 959-969

Shih, S.F., 1973, Modified Monte Carlo application to groundwater movement--the simultaneity procedures, Water Resour. Res., V9(4), 1029-1038

Shvidler, M.I., 1975, Dispersion of a filtration stream in a medium with random in homogeneities, Sov. Phys. Doklady, V20(3), 171-173

Siddiqui, S.H. and R.R. Parizek, 1974, An application of parametric statistical tests to well-yield data from carbonates of central Pennsylvania, J. Hydrol., V21(1),1-14

Simmons, C.S., 1982, A stochastic-convective ensemble method for representing dispersive transport in groundwater, EPRI, Palo Alto CA, Tech. Rept. CS-2558, RP 1406-1

Simmons, C.S., 1982, A stochastic-convective transport representation of dispersion in one-dimensional porous media systems, Water Resour. Res. 18(4):1193-1214

Simmons, C.S., D.R. Nielsen and J.W. Biggar, 1979, Scaling of field-measured soil-water properties, Hilgardia, V47(4), 77-173

Simpson, E.S., 1962, Transverse dispersion in liquid flow through porous media, USGS Prof. Paper 411-C, Washington, D.C.

Simpson, E.S., 1970, On the dispersivity of real aquifers, Trans. Am. Geophys. Union, V51(4), 284

Sitar, N., J.D. Cawlfield, A. Der Kiureghian, 1987, First-order reliability approach to stochastic analysis of flow and contaminant transport, Water Resour. Res. 23(5):794-804

Skagius, K. and I. Neretnieks, 1986, Porosities and diffusivities of some nonsorbing species in crystalline rocks, Water Resour. Res. 22(3):389-398

Smith, D.V., 1972, Comments on "A chance-constrained approach to the conjunctive use of surface waters and groundwaters" by G.H. Nieswand and M.L. Granstrom, Water Resour. Res., V8(6), 1621-1622. Nieswand, G.H. and M.L. Granstrom, 1972, Reply, Water Resourc. Res., V8(6), 1623-1625

Smith, L. and R.A. Freeze, 1979a, Stochastic analysis of steady state groundwater flow in a bounded domain, 1, One- dimensional simulations, Water Resour. Res., V15(3), 521-528

Smith, L. and R.A. Freeze, 1979b, Stochastic analysis of steady state groundwater flow in a bounded domain, 2, Two- dimensional simulations, Water Resour. Res., V15(6), 1543-1559

Smith, L. and F.W. Schwartz, 1980, Role of laboratory-scale measurements in mass-transport modeling, Trans. Am. Geophys. Union, V61(17), 232

Smith, L. and F.W. Schwartz, 1980, Mass transport, 1. A stochastic analysis of macroscopic dispersion, Water Resour. Res. 16:303-313

Smith, L., F.W. Schwartz, 1981a, Mass transport, 2. Analysis of uncertanity in prediction, Water Resour. Res. 17(2): 351-369

Smith, L. and F.W. Schwartz, 1981b, Mass transport, 3. Role of hydraulic conductivity in prediction, Water Resour. Res., 17(5), 1463-1479

Smith, L., 1981, Spatial variability of flow parameters in a stratified sand, Int. J. Math. Geol., V13(1), 1-21

Smith, R.E., 1976, Effects of random variation in soil parameters relating to infiltration patterns, Trans. Am. Geophys. Union, V57(12), 914

Snyder, W.M. and L.E. Asmussen, 1972, Subsurface hydrograph analysis by convolution, J. Irr. Drain. Div., ASCE, V98(3), 405-418,Smith,R.E., 1973, Discussion, V99(3), 404-406

Sposito, G., 1981, The statistical mechanical theory of groundwater flow, Water Resour. Res., V 17, in press

Sposito, G., W.A. Jury, V.K. Gupta, 1986, Fundamental problems in the stochastic convection-dispersion model of solute transport in aquifers and field soils, Water Resour. Res. 22(1):77-88

Sposito, G., P.J. Sullivan, and V.K. Gupta, 1977, Experimental test of Langevin equation as a model for waterflow through unsaturated soil, SoilSci. Soc. Am. J., V41(4), 820-822

Stephens, D.B., L.W. Gelhar, S. Young, 1984, Field experiment to evaluate dispersion in unsaturated media (Abs.) EOS, 65(16):106.

Strecker, E.W., W.-S. Chaurd, D.P. Lettenmaier, 1986, Parameter identification of ground-water contamination transport model, Groundwater 24(1):56-62

Sudicky, E.A., 1986, A natural gradient experiment on solute transport in a sand aquifer: spatial variability of hydraulic conductivity and its role in the dispersion process, Water Resour. Res., 22, 2069-2082

Sunada, D.K., 1976, Statistical applications in groundwater systems, in Stochastic Approaches to Water Resources, Vol. 2, H.W. Shen, ed., pp 20-1-20-17Taylor, G.I., Diffusion by continuous movements, Proc. London. Math. Soc. Ser. A20, 196-211, 1922

Tang, D.H. and G.F. Pinder, 1977, Simulation of groundwater flow and mass transport under uncertainty, Adv. in Water Resources 1(1):25-30

Tang, D.H., and G.F. Pinder, 1979, Analysis of mass transport with uncertain physical parameters, Water Resourc. Res., V15(5), 1147-1155

Tang, D.H., F.W. Schwartz, L. Smith, 1982, Stochastic modeling of mass transport in a random velocity field, Water Resour. Res. 18( ):231-244

Taylor, G. I., Diffusion by continuous movements, Proc. London. Math. Soc. Ser. A20, 196-211, 1922.

Taylor, G.I., Dispersion of soluble matter in solvent flowing slowly through a tube, Proc. London. Math. Soc. Ser. A219, 186-203, 1953.

Thirriot, C., R. Gaudu, and j. Valiantzas, 1979, Microscopic and macroscopic aspects of heterogeneity in porous media, Trans., Am. Geophys. Union,V60(7), 116-117

Todorovic, P., 1970, A stochastic model of longitudinal diffusion in porous media, Water Resour. Res.,V6(1), 211-222

Todorovic, P.N., 1971, A stochastic model of lateral diffusion in a porous medium, in Stochastic Hydraulics, C.L. Chiu, ed., School of Engineering, University of Pittsburg, 632-653

Todorovic, P., 1975, A stochastic model of dispersion in a porous medium, Water Resourc. Res., V11(2), 348-354

Tomkoria, B.N. and A.E. Scheidegger, 1967, A complete thermo- dynamic analogy for transport processes, Can., J. Phys., V45(11), 3569-3587

Torelli, L. and A.E. Scheidegger,1971, A review of the stochastic approach to flow through porous media, in Stochastic Hydraulics, C.L. Chiu, ed., School of Engineering, University of Pittsburg, 644-666.

Torelli, L. and A.E. Scheidegger, 1972, Three-dimensional branching-type models of flow through porous media, J. Hydrol. V15(1), 23-35

Torelli, L., 1972, Computer simultaion of the dispersion phenomena occurring during flow through porous media, using a random maze model, Pure and Appl. Geophys. V96(4), 75-88

Torelli, L. and P. Tomasi, 1977, Interpolation and trend analysis, two geohydrological applications, J. Int. Ass'n for Math. Geol., V995), 529-542

van Genuchten, M.T., A closed-form equation for predicting the hydraulic conductivity of unsaturated soils, Soil Sci. Soc. Am. J., 44, 892-898, 1980.

Vomvoris, E.G., and L.W. Gelhar, Stochastic prediction of dispersive contaminant transport, U.S. Department of Commerce National Technical Information Service, Cooperative Agreement, CR-811135-01-2, Dec., 1986.

Vanmarke, E. 1983, Random fields: analysis and synthesis, MIT Press, Cambridge, MA

Vauclin, M., Imbernon, J., Vachaud, G. and C. Danceete, 1983, Description experimentale et modelisation stochastique des transferts par la mise en echelle des proprietes hydrodynamiques. In: Isotope and radiation techniques in Soil Physics and irrigation studies 1983, IAEA, Vienne 1983

Vauclin, M., 1983, Methods d'etude de la variabilite spatiale des proprietes d' un sol, Variabilite spatiale des processus de transfert dans les sols, Avignon, 24-25

Juin 1982 Ed. INRA Publ. 1983 (Les Colloques de l' INRA, no 15). Vetier, A., 1978, Covariance function of a stochastic process, Periodica Polytech., Electr. Eng., V22(2-3), 85-89

Volpi, G. and G. Gambolati, 1978, On the use of main trend for the kriging technique in hydrology, Adv. in Water Resour., V1(6), 345-349

Wagner, B.J. and S.M. Gorelick, 1986, A statistical methodology for estimating transport parameters: theory and applications to one-dimensional advective-dispersive systems, Water Resour. Res. 22(8):1303-1315

Wang, J.S.Y., and T.N. Narasimhan, Hydrologic mechanisms governing fluid flow in a partially saturated, fractured, porous medium, Water Resour. Res., 21(12), 1861-1874, 1985.

Warren, J.E., and H.S. Price, Flow in heterogeneous porous media, Society of Petroleum Engineers Journal, 1, 153-169, 1961.

Warren, J.E., and P.J. Root, Behavior of naturally fractured reservoirs, Society of Petroleum Engineers Journal, 9, 245-255, 1963.

Warren, J.E., and F.F. Skiba, Macroscopic dispersion, Trans AIME, 231, 215-230, 1964.

Warren, J.E., F.F. Skiba, and H.S. Price, An evaluation of the significance of permeability measurements, Journal Petroleum Technology, 13, 739-744, 1961.

Warrick, A.W., G.J. Mullen, and D.R. Nielsen, 1977, Scaling field-measured soil hydraulic properties using a similar media concept, Water Resour. Res., V13(2), 355-362

Wen-Sen, C., E.W. Strecker, D.P. Lettenmaier, 1987, An evaluation of data requirements for groundwater contaminant transport modeling, Water Resour. Res. 23(3): 408-424

Wheatcraft, S.W. and S.W. Tyler, An explanation of scale- dependent dispersivity in heterogeneous aquifers using concepts of fractal geometry, Water Resour. Res., 24(4), 525-532, 1988.

Wierenga, P.J., L.W. Gelhar, C.S. Simmons, G.W.Gee, T.J. Nicholson, 1986, Validation of stochastical flow and transport models for unsaturated soil: a comprehensive field study, U.S. Nuc. Reg. Comm. Report NUREG/CR-4622.

Williams, D., Geostatistical analysis and inverse modeling of the Upper Santa Cruz Basin, Arizona, Master Thesis, Univ. of Arizona, pp149, 1987.

Williams, R.E., Comment on "Statistical theory of groundwater flow and transport: Pore to Laboratory, Laboratory to Formation, and Formation to Regional Scale" by Gedeon Dagan, Water Resour. Res., 24(7), 1197-1200, 1988.

Williams, R.E., Comment on "Double-porosity models for a fissured groundwater reservoir with fracture skin" by Allen F. Moench, Water Resour. Res., 21(6), 889-891, 1985.

Wilson, J.L., and L.W. Gelhar, 1974, Dispersive mixing in a partially saturated porous medium, 353 p., Rep. 191, R.M. Parsons Lab. for Water Resour. and Hydrodynamics, Massachusetts Institute of Technology, Cambridge

Wilson, J.L., P.K. Kitanidis, and M.D. Dettinger, 1978, State and parameter estimation in groundwater models, in Applications of Kalman Filter to Hydrology, Hydraulics, and Water Resources, C.L. Chin, ed., Stochastic Hydraulics Program, University of Pittsburg, 657-679

Wilson, J.L., 1979, Piezometric head prediction: Conditional simulation vs. first-order analysis, Trans. Am. Geophys. union, V60(46), 820.

Wilson, J.L., 1981, The unified approach to groundwater modeling, Trans. Am. Geophys. Union, V62(17), 281

Winter, C.L., C.M. Newman, and S.P. Neuman, A perturbation expansion for diffusion in a random velocity field, SIAM J. Appl. Math, 44(2), 411-424, 1984.

Wood, E.F., 1981, The unified approach to groundwater modeling, Trans. Am. Geophys. Union, V62(17), 281

Wu, T.H., S.K. Vyas, and N.Y. Change, 1973, Probabilistic analysis of seepage, J. Soil Mech. Found. Div.,ASCE, V99(4), 323-240

Yakowitz, S., 1976, Model-free statistical methods for water table prediction, Water Resour. Res., V12(5), 836-844

Yakowitz, S. and L. Duckstein, 1980, Instability in aquifer identification: Theory and case studies, Water Resour. Res., V1696), 1045-1064

Yeh, T.-C.J., L.W. Gelhar, A.L. Gutjahr, 1985a, Stochastic analysis of unsaturated flow in heterogeneous soils, 1, Statistically isotropic media, Water Resour. Res., 21(4), 447-456

Yeh, T.-C.J., L. W. Gelhar and A.L. Gutjahr, 1985b, Stochastic analysis of unsaturated flow in heterogeneous soils, 2, Statistically anisotropic media with variable alpha, Water Resour. Res., 21(4), 457-464

Yeh, T.-C.J., L.W. Gelhar and A.L. Gutjahr, 1985c, Stochastic analysis of unsaturated flow in heterogeneous soils, 3, Observations and applications, Water Resour. Res., 21(4), 465-472

Yeh, T.-C.J., L.W. Gelhar, A.L. Gutjahr, 1986, Correction to "Stochastic analysis of unsaturated flow in heterogeneous soils, 1 and 2", Water Resour. Res. 22(5):843

Yeh, T.-C.J., 1987, Comment on "modeling of scale dependent dispersion in hydrogeologic systems" by J.F. Pickens and G.E. Grisak, Water Resour. Res. 23(3):522

Yeh, W.W.-G., 1986, Review of parameter identification procedures in groundwater hydrology: the inverse problem, Water Resour. Res. 22(2):95-108

Yoon, Y.S. and W. W-G. Yeh, 1979, Identification of aquifer parameters with the kriging technique, Trans. Am. Geophys. Union, V60(46), 821.

Zal'tsberg, E.A., 1975, Application of the theory of stationary random functions to hydrogeologic forecasting, Soviet Hydrology-Selected papers, 1975, No. 4, 216-219

Zaporozec, A., 1980, Statistical analysis as a tool in evaluating the effect of drought on shallow ground-water levels, Trans. Am. Geophys. Union, V61(17), 229-230 Zhang, Y., 1982, Double Porosity Model and its Finite Element Solution for the flow in Fractured-Karst Rocks, Hydrogeology and Engineering Geology, 4.

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A REVIEW OF THE SCALE PROBLEM AND APPLICATIONS OF STOCHASTIC METHODS TO DETERMINE GROUNDWATER TRAVEL TIME AND PATH

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ABSTRACT

The groundwater travel time along the fastest path of likely radionuclide transport is a regulatory criterion used to assess the hydrogeologic quality of a high-level radioactive waste repository. Hydrologists and engineers are limited in their ability to define with confidence the fastest path, owing to the heterogeneous nature of geologic materials. Field measurements of hydraulic properties such as in test or observation wells, are inherently averages of properties at scales smaller than the scale of the field measurement. As a result of averaging, subscale information is lost and there is uncertainty in defining the fastest trajectory of groundwater. This scale problem is explained through a review of the continuum and REV concepts in groundwater hydrology. The application of hydrodynamic dispersion concepts is recommended as a means of incorporating the effect of subscale heterogeneity on the fastest groundwater travel time.

Sources of uncertainties in predicting groundwater travel time are discussed in the report. The uncertainties are mainly attributed to the heterogeneous nature of geologic formations. The heterogeneity of geologic materials can, however, be characterized quantitatively using geostatistical methods. Important statistical parameters include mean and variance, as well as the spatial correlation structures of the hydrologic properties within the hydrogeologic system. These parameters may be obtained from limited data base. Stochastic methods, reviewed and explained in this report, can take advantage of the geostatistical characterization to predict large-scale groundwater flow and solute transport. Several examples from recent scientific literature are provided to illustrate the application of stochastic methods to the groundwater travel time analysis.

Stochastic methods in subsurface hydrology have only recently been evaluated under field conditions for a few locations, and validation of the theories is

incomplete, especially in unsaturated fractured rocks. Nevertheless, research efforts should continue to improve the state-of-the art. Geostatistics and stochastic methods will be valuable tools in addressing the groundwater travel time objective.

1.0 INTRODUCTION

1.1 Purpose and Scope

Daniel B. Stephens & Associates, Inc. was requested by the U.S. Nuclear Regulatory Commission (NRC), through Nuclear Waste Consultants, to conduct a review of the literature pertaining to stochastic approaches for characterizing the uncertainty in predicting groundwater travel path and travel time in saturated media. Enclosed is the draft final report of this study. As directed by the NRC, the report addresses the following:

- -review of uncertainties in groundwater travel time and path which are attributed to hydrogeologic parameters
- -critical reviews of relevant scientific articles relevant to the analysis of uncertainties in prediction of groundwater travel time and path
- -a discussion of the significance of the findings to the NRC's waste management program
- -explanations and illustrations of the stochastic concept and methods of stochastic analysis
- -a glossary of terms relevant to stochastic analyses

In addition, the report discusses the concept of the representative elementary volume (REV). The report also attempts to clarify the relationships between the REV scale, the measurement scale of hydraulic properties and scale of modeling.

The proposed work is motivated in large part by federal regulations pertaining to the performance of high level waste repositories, in particular, the groundwater travel time (GWTT) objective. As stated in 10 CFR 60.113(a)(2), the GWTT performance objective is:

"The geologic repository shall be located so that pre-waste-emplacement groundwater travel time along the fastest path of likely

radionuclide travel from the disturbed zone to the accessible environment shall be at least 1,000 years or such other time as may be approved or specified by the Commission."

The NRC has drafted generic technical positions on groundwater travel time to help explain this phase, as well as the rest of the regulation (NRC, 1986, 1988). One of the key points requiring clarification is the definition of "the fastest path of likely radionuclide transport". Hydrogeologists are well aware that there are many possible pathways, but which one is the fastest and how fast does groundwater travel along it? Herein, enters the element of uncertainty. There is uncertainty not only in identifying the fastest path from limited subsurface data but also in travel time owing to the uncertainty in path length as well as in data or approaches used to compute travel time.

As our report will illustrate, stochastic methods are well-suited to deal with uncertainty in groundwater travel time and travel path analysis. However, they have only been developed for groundwater problems within the last decade. The mathematical complexities presented in theoretical articles in the scientific literature are not easily assimilated by most practitioners. Moreover, because field tests to validate stochastic models have not been completed, most hydrogeologists are still reluctant to apply these models. One of the underlying purposes of our review is to explain the principles of stochastic models without resorting to the mathematical details and give examples of how the stochastic methods may be applied in the analysis of groundwater travel time and travel path.

1.2 Background

Uncertainties in predicting groundwater travel times and paths arise primarily from heterogeneity of aquifer materials. Heterogeneity is a continuous phenomenon; it exists at all scales (from microscale to megascale). However, heterogeneous materials may be treated as homogeneous at one observation scale, and

heterogeneous at a different scale. That is, the definition of heterogeneity is a relative one, depending on the scale of observation. Thus, the heterogeneity observed is directly related to the scale of the problem.

The problem of scale does not exist only in hydrology (Dooge, 1986), but poses many difficulties for every branch of science and every one of us living in the universe. It controls our perception of everything that we see and feel. The scale problem is best illustrated in the book entitled "Powers of Ten" by Morrison and Morrison (1982). The book contains visual images ranging from a scale of 10^{25} meters to 10^{-14} meters. At a scale of 10^{25} meters galaxies are seen as tiny clusters in empty space. At a scale of 10^{23} meters, the Milky Way appears as one of a number of bright spots in empty space. The spiral structure of the Milky Way becomes apparent at a scale of 10^{21} meters. A scale of 10^{13} meters encompasses the orbits and all the planets of the solar system. At the scale between 10^{-7} and 10^{-9} meters, we see the various structures of DNA molecules, and so on. Similarly, in groundwater hydrology, at a scale of 10^{6} meters one may observe variations among groundwater basins. Various geologic formations become noticeable at a scale of 10^{3} meters. A scale of 10 meters may encompass various layers of clay, sand, and gravel. We can no longer recognize the irregularity of layers, but we do recognize pore structures at a scale of 10^{-6} meters. Water molecules within pores are visible at a scale of 10^{-8} meters, and so on as the scale of observation decreases.

Heterogeneity exists in groundwater hydrology at all scales. However, once we select a scale of observation, we often neglect phenomena at subscales. This is exactly the way our formulas, equations, and laws are developed in all sciences, including groundwater hydrology. Subscale phenomena we ignored, however, may play vital roles in solving or studying the problems of interest. Furthermore, different laws and equations may be developed or discovered at different scales and may not be appropriate for studying problems at another scale. For instance, a

representative elementary volume as used in the study of flow through porous media would be different from that for flow through fractures or karsts. When predicting groundwater travel times and paths, we may face the difficulty of extrapolating equations and laws developed for a small scale to solve problems at a larger scale, for example over distances of 10 km or more.

In the following chapters, we will first discuss of the continuum hypothesis in fluid mechanics and groundwater hydrology, and then we will show the development of equations for groundwater flow at different scales. We will then discuss the uncertainties in predicting groundwater travel times and paths and finally review some recent advances in groundwater hydrology to tackle the scale related problems.

2.0 BASIC CONCEPTS IN GROUNDWATER HYDROLOGY

2.1 Continuum Assumption in Fluid Mechanics

The most fundamental assumption in fluid mechanics is the continuum assumption in which the fluid is assumed to behave as if it were continuous in space at the macroscopic scale, say 10^{-2} meters.

For example, at the macroscopic scale, one can see water in a garden hose, and the water is continuous throughout the hose. However, if we examine a fluid at the microscopic scale, say 10^{-8} meters, the mass of the material in a fluid is concentrated in the nuclei of the atoms composing a molecule and is not uniformly distributed over the column occupied by the liquid. Using the garden hose example, we can view the velocity of water moving through the hose in perhaps two ways, depending upon the scale of interest. In the first case, at the macroscopic scale, the velocity is simply the volumetric discharge rate per unit cross-sectional area. For steady-state conditions, the velocity is constant in space along the hose. In the second case, at the microscopic scale, the velocity of individual fluid molecules is highly variable along their path through the hose. This molecular velocity is virtually impossible to measure. However, we are normally concerned with the behavior of matter on a macroscopic scale which is much larger than the distance between molecules. Accordingly, the properties of a fluid defined in fluid mechanics have to represent the property values over such a macroscopic volume. The properties contained in this volume are thus regarded as the average values being spread uniformly over that volume instead of, as at the microscopic scale, being concentrated in a small fraction of it. This macroscopic representation of the fluid makes it possible to treat the fluid as a continuum in space. This approach in fluid mechanics is known as the continuum approach and the associated hypothesis that the

fluid can be so represented is called the continuum approach.

Indeed, the properties of the fluid at the macroscopic scale are continuous and smoothly varying, if observed with any of the conventional measuring devices. When a measuring device is inserted in a fluid, it responds in some way to a property of the fluid within some small neighboring volume, and provides a measure which is effectively an average of that property over the volume. The device, such as a pitometer for measuring velocity, is normally chosen so that the volume is small enough for the measurement to be a local one; that is, further reduction of the volume does not change the reading of the device. However, the volume is large enough to contain an enormous number of molecules so that the fluctuations arising from the different properties of molecules have no effect on the observed average. Therefore, we can define a reproducible property of the fluid. Of course, if the averaging volume is so small as to contain only a few molecules, the number and kind of molecules in the volume at the instant of observation will fluctuate from one observation to another, and the measurement will vary in an irregular way, with the size of the averaging volume corresponding to the measuring device. Figure 2.1 illustrates the way in which a measurement of velocity of the fluid would depend on the averaging volume of the device. We are able to regard the fluid as a continuum when, as shown in the figure, the measured fluid property is constant for volumes which are small on the macroscopic scale but large on the microscopic scale.

The continuum assumption allows us to attach a precise meaning to the various physical properties at any point in space. The various fluid properties such as density, velocity, and temperature can thus be treated as continuous functions of time and position in the fluid which satisfy the requirements of differential calculus. On this basis, we shall be able to establish differential equations governing the motion of the fluid. The equations are macroscopic equations that are independent of the nature of the particle structure which is generally discontinuous in space and

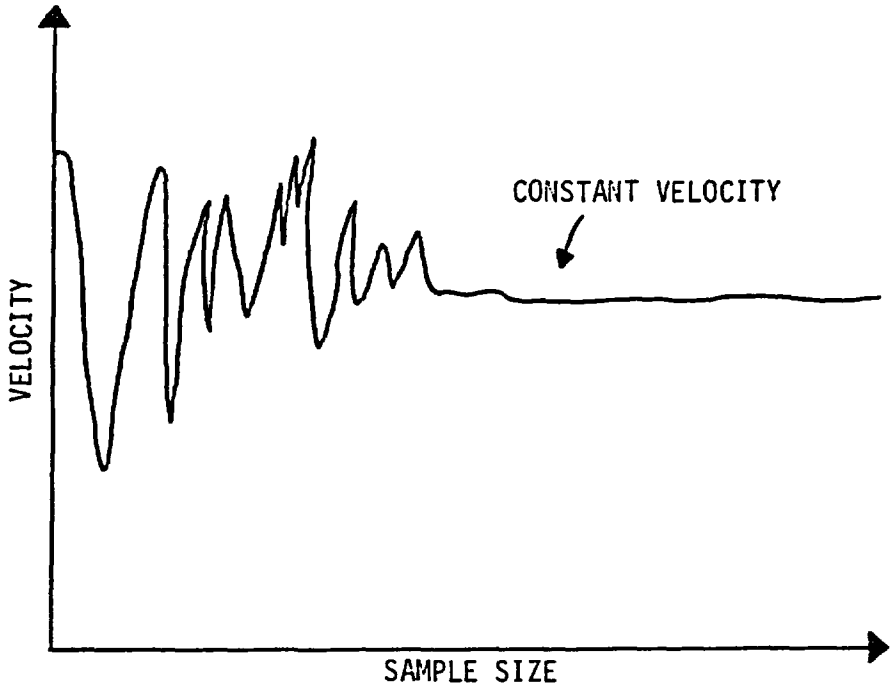


Figure 2.1. Dependence of velocity measurements upon sample size within a fluid.

time.

2.2 Continuum Assumption in Groundwater Hydrology

In saturated porous media (granular materials), flow takes place through a complex network of interconnected pores or openings. Although the fluid itself may be considered as a continuum by the continuum hypothesis used in fluid mechanics, the flow path may be discontinuous because of the complex nature of the pore geometry. 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. By doing so, they are employing the concept of a continuum, which is analogous to the concept used in fluid mechanics and other branches of sciences. The minimum volume over which the continuum assumption applies in flow through porous media, however, is much larger than the one defined in fluid mechanics (Figure 2.2). In groundwater hydrology, this volume is called the representative elementary volume (REV) (Bear, 1979). Using the REV concept, we essentially bypass both the microscopic level, at which we consider what happens to each molecule in the fluid, 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 which only averaged phenomena over the REV are considered. Thus, a REV is simply a volume over which we carry out the averaging process, as shown in Figure 2.2.

A more practical definition of the REV may be given as follows: an REV is a volume that is sufficiently large to contain a great number of pores so that a mean property exists, and it is sufficiently small so that the parameter variations at a scale

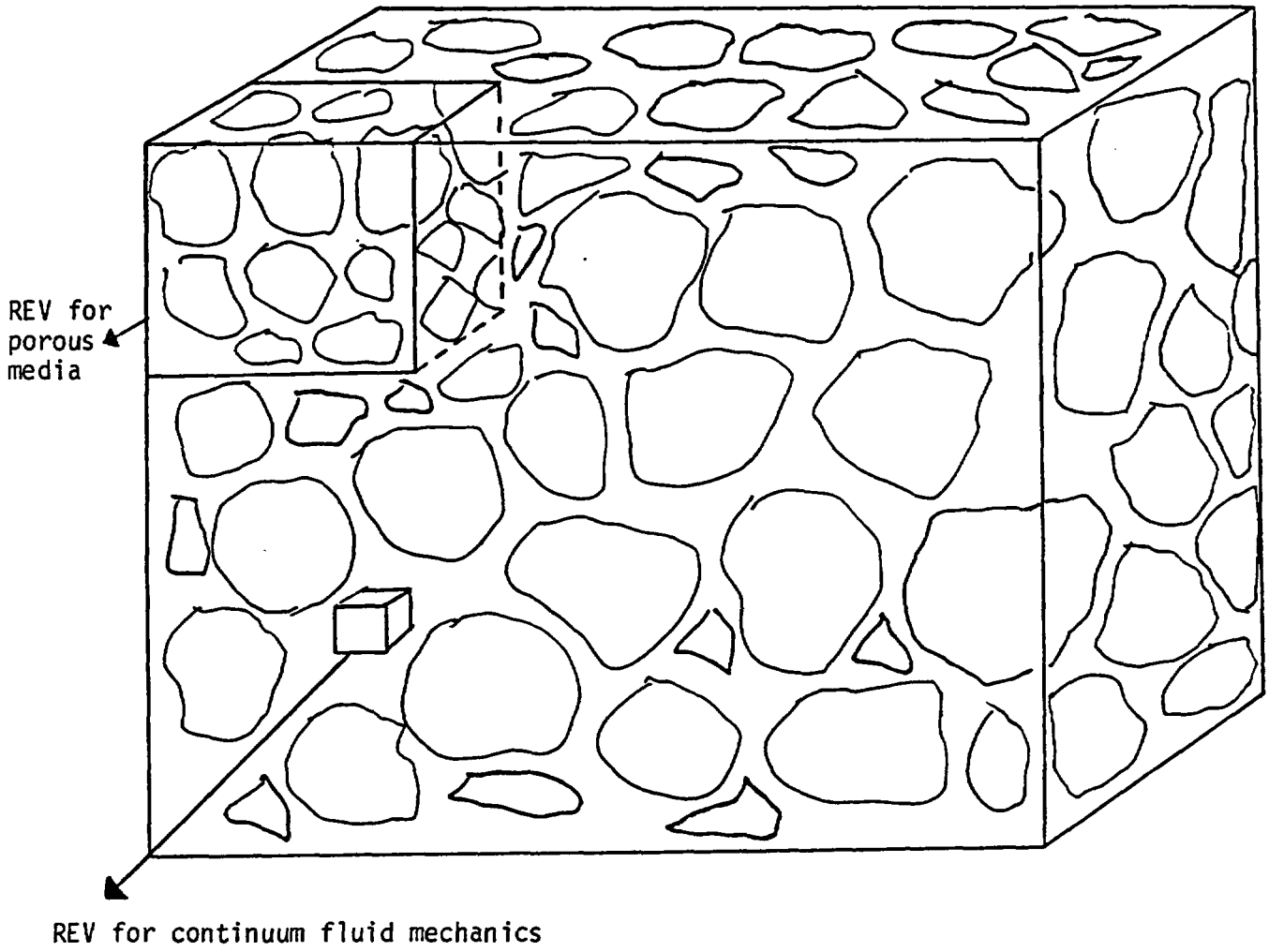


Figure 2.2. Different averaging volumes in fluid mechanics and porous media.

larger than the size of REV can be represented by continuous functions which satisfy the requirements of the classic differential calculus (De Marsily, 1986).

The REV concept is also defined through a rigorous mathematical expression suggested by Marle (1967). At pore-scale, the spatial distribution of pore openings could be highly erratic, analogous to electronic signals superimposed with random noises. Then, an REV is merely a noise filter similar to the one in electrical engineering that filters out the random noises and produces a smooth signal (Figure 2.3). Mathematically, this process can be formulated as:

$$H(x) = \int h(x + \eta)\, f(\eta)\, d\eta \qquad (2.2.1)$$

where H(x) is the smoothed, continuous, output signal, h(x) is the original, noisy, and erratic signal, and $f(\eta)$ is the filter or a weighting factor. Figure 2.3a shows a filter function which eliminates high frequency noises but retains the smooth sinusoidal signal. Some filter functions can smooth noises and signal as shown in Figure 2.3b. In groundwater hydrology, H(x) is the macroscopic property of porous media and $f(\eta)$ is the weighting function used within the volume or window over which the pore-scale properties are averaged, i.e., the REV. For example,

$$f(\eta) = \begin{cases} \frac{1}{V}, & \text{within the volume } V \\ 0, & \text{otherwise} \end{cases} \qquad (2.2.2)$$

2.3 Homogeneity, Heterogeneity, and Scale

The definitions of homogeneity and heterogeneity follow from the concept of the REV. From the previous discussion, it should be clear that as the size of the

window or the volume over which the averaging takes place increases, the noise level in the output will decrease (Figures 2.3). Therefore, if one properly chooses the size of the averaging volume, a material with a spatially-varying property may thus be treated as a material with a spatially-constant property. This material is then defined as homogeneous. This situation is analogous to that in Figure 2.3b. Now, consider a porosity distribution of a hypothetical porous medium. If one chooses a pin point as the sample size to define porosity, let us assume that Figure 2.4a would represent the porosity distribution along a transect of the porous medium. At a point, the void has a porosity value one, and the solid zero. If one averages the values of porosity over a window that is larger than a point, say, as large as one solid or void space, the "new" porosity distribution of the aquifer will look like that shown in Figure 2.4b where the sharp boundary between voids and solid is smeared out due to the averaging over the window. It should be evident that if a window slightly larger than one solid space is used, the porosity values of the aquifer will still vary in space but the variation will be relatively smooth and continuous. Therefore, the aquifer is heterogeneous and it can be described by our continuum mathematics. If one chooses a window which is equal to two void spaces to define the porosity values at every point within the medium, the medium should obviously have a constant porosity over the entire medium. In fact, the porosity will be 0.5 everywhere if the averaging window is equal to two void or solid spaces. Hence, the medium as far as porosity is concerned is a homogeneous medium (Figure 2.4c). This window can be considered as the minimum size of the REV for conceptualizing the medium as a homogeneous one. Suppose one applies this window to another porous medium which has a checkerboard porosity distribution but with larger void and solid sizes. The porosity distribution defined by the average porosity over the same window becomes nonuniform. In other words, the medium now is considered heterogeneous. But, if one again chooses a window that is equal to the size of the

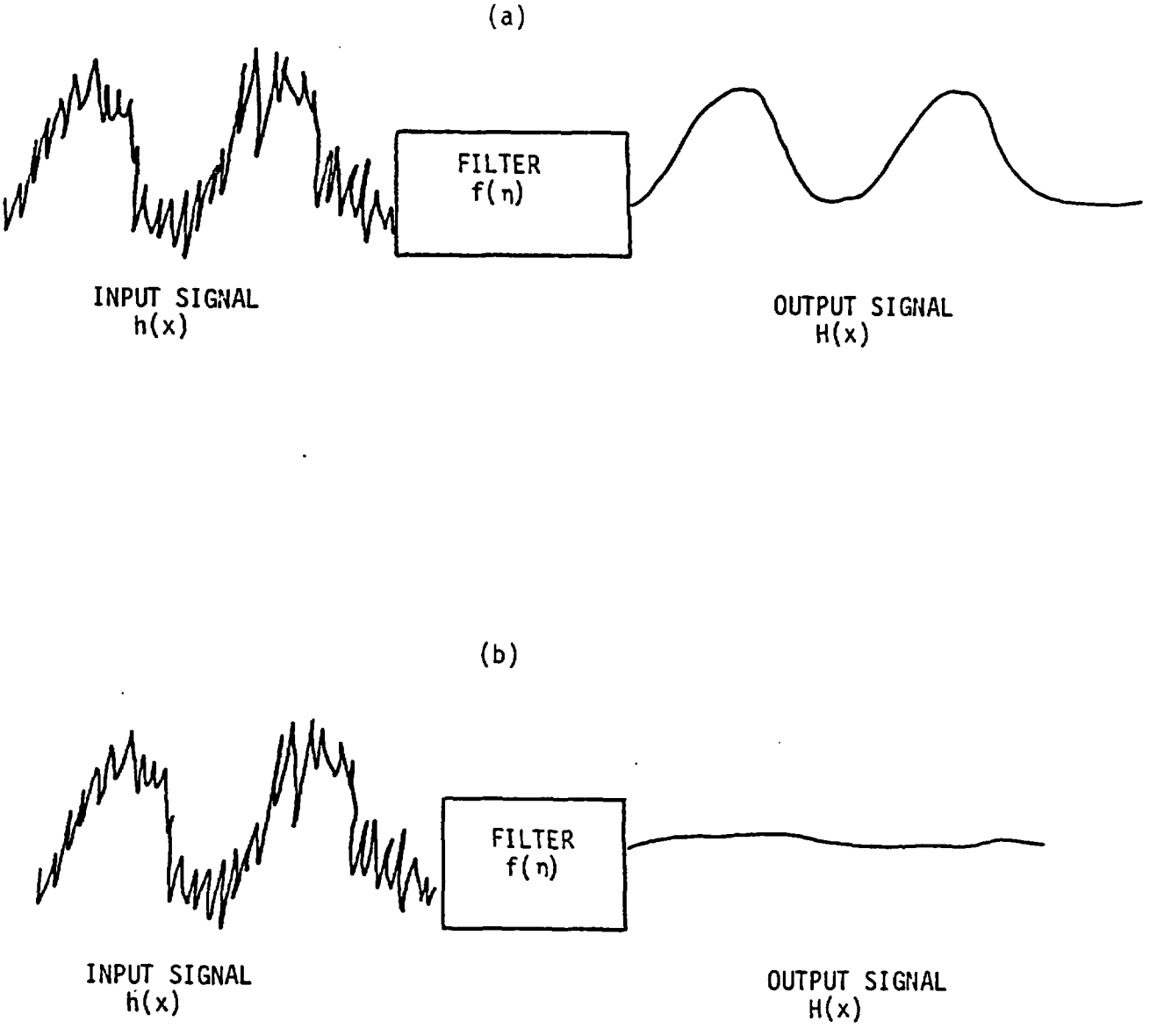


Figure 2.3. Effects of filters on noisy signals.
a) Filter affects noise only, and b) filter affects noise and most of signal.

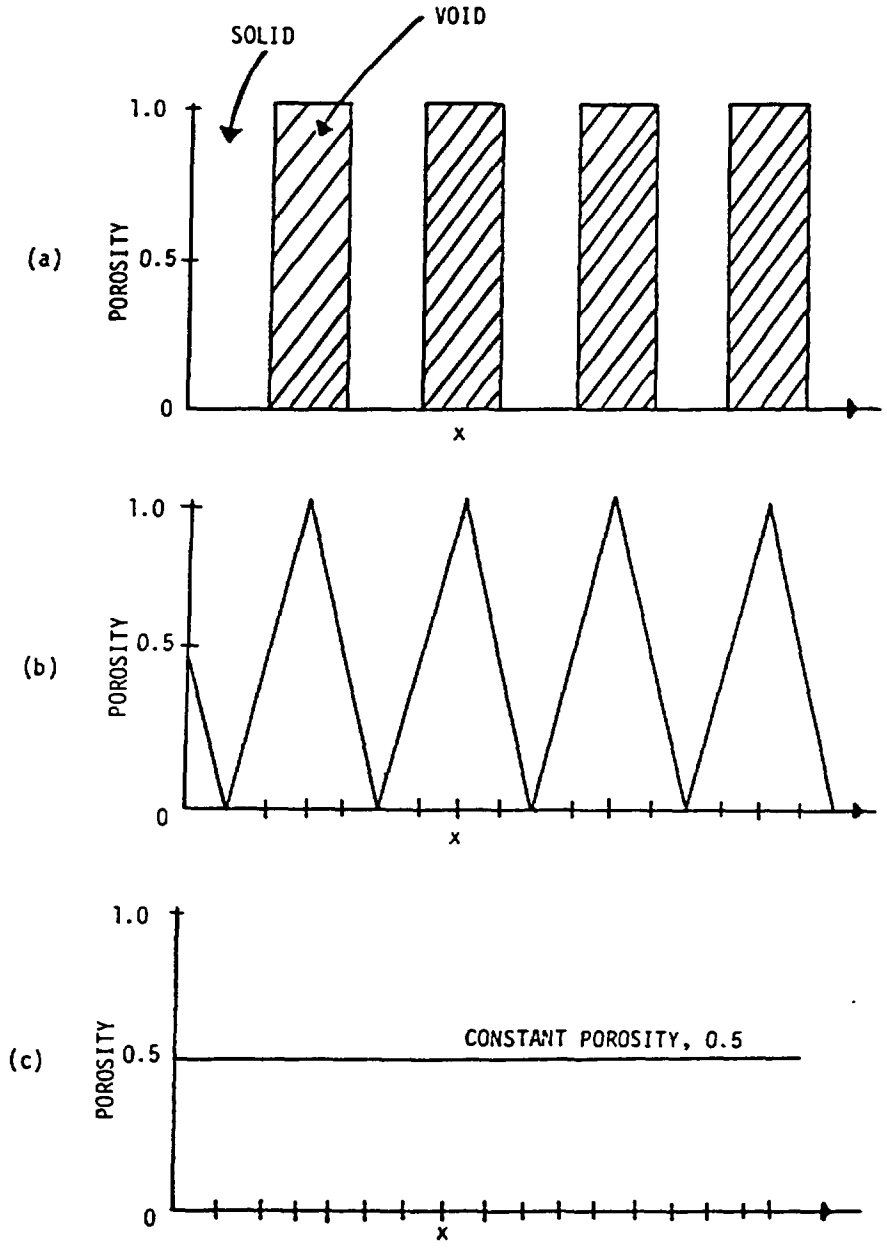


Figure 2.4. Effects of averaging volume on porosity distribution. (a) A hypothetical solid and void distribution. (b) Size of averaging volume equals one void volume. (c) Size of averaging volume equals two void volumes.

two void or solid spaces of this checkerboard, one can define this medium as a homogeneous porous medium. From this simple example, it can be seen that in order to obtain the homogeneity, the size or the REV has to be much larger than the size of heterogeneity.

The size of the REV varies with the size of the blocks in the examples or the size of heterogeneity in reality. The size of heterogeneity depends on the scale of the problem that we encounter. For instance, the heterogeneity within core samples is likely due to the variation in grain size. We may call this variability the laboratory-scale heterogeneity. Heterogeneity due to geologic stratification or layering in a formation may be classified as the field-scale heterogeneity. The regional-scale heterogeneity then represents the variation of geologic formations or facies. Furthermore, variations among sedimentary basins may be classified as the global-scale heterogeneity, and so on. Similar definitions of the scale of heterogeneity were given by Dagan (1986) and Gelhar (1986). Regardless of the definition of the scale of heterogeneity, one has to recognize that the heterogeneity is a continuous phenomenon which exists at all scales.

2.4 Darcy's Law

With the concept of the REV in mind, one should recognize that every property defined in groundwater hydrology (such as volumetric flow rate, hydraulic head, porosity, hydraulic conductivity, and storativity, etc.) involves measurement over a certain volume. The same is true for the principles and laws used in groundwater hydrology. The most important example would be Darcy's law, which states that groundwater specific discharge is linearly proportional to the hydraulic gradient with a constant of proportionality:

$$q = \frac{Q}{A} = KI \qquad (2.4.1)$$

where q is the specific discharge with dimensions of (LT^{-1}), Q is the volumetric flow rate (L^3T^{-1}), I is the gradient (LL^{-1}), A is the cross-sectional area perpendicular to the direction of flow (L^2), and K is a constant of proportionality which is usually called hydraulic conductivity (LT^{-1}). Darcy's law is an empirical equation, although one can prove the validity of the equation using rigorous mathematics and physics (Hubbert, 1940). Nevertheless, it is simply a linear regression equation showing the relationship between gradient and specific discharge through a column of soil of a certain volume. Therefore, Darcy's law is a macroscopic law because the volume where the law applies is obviously much larger than many pores.

2.4.1 Hydraulic conductivity. In the laboratory, hydraulic conductivity is generally determined from a column test which uses either a constant head permeameter or a falling head permeameter. Regardless of whether one uses a constant or falling head permeameter, the measured hydraulic conductivity is an average value over the length of the column. To illustrate this point, we will examine the case where the column consists of a single homogeneous soil. If a constant head permeameter is used, then steady-state flow will be established. The flow rate through the column is, according to Darcy's law:

$$Q = KAI = KA \frac{h_1 - h_2}{L} \tag{2.4.2}$$

where h_1 and h_2 are the hydraulic heads measured at points 1 and 2, and L is the distance between the two points (Figure 2.5). If we measure Q, A, and I, we certainly can determine the K value, the hydraulic conductivity. Obviously, in a core sample, the calculated hydraulic conductivity, K, represents some average small-scale hydraulic conductivity variations within the core. To illustrate the concept of an average K, we consider a second case where the porous medium contains layered

heterogeneity (Figure 2.5). Again, if a constant head permeameter is used, steady flow exists. This implies that the flow rates across any cross-section of the column must be equal. That is:

$$Q_1 = Q_2$$

$$K_1 \; A \; \frac{h_1 - h}{L_1} = K_2 \; A \; \frac{h - h_2}{L_2} \qquad (2.4.3)$$

where K_1 and K_2 are the hydraulic conductivity values of soils 1 and 2, respectively; h_1 is the water level at reservoir 1, and h_2 is the water level at reservoir 2; h is the head value at the interface between the two soils; and L_1 and L_2 are the thicknesses of layer 1 and layer 2, respectively. If the head at the interface is not measure, one can solve Equation (2.4.3) for h at the interface by knowing the hydraulic conductivities and thickness of the individual layers:

$$h = \frac{L_1 L_2}{K_1 L_2 + K_2 L_1} \; \frac{(K_1/L_1)\, h_1 + (K_2/L_2)\, h_2}{L} \qquad (2.4.4)$$

where L is $L_1 + L_2$. If this expression for h is substituted into the left-hand side of equation (2.4.3), one obtains:

$$Q = A \; \frac{K_1 K_2 L}{K_1 L_2 + K_2 L_1} \; \frac{h_1 - h_2}{L} \qquad (2.4.5)$$

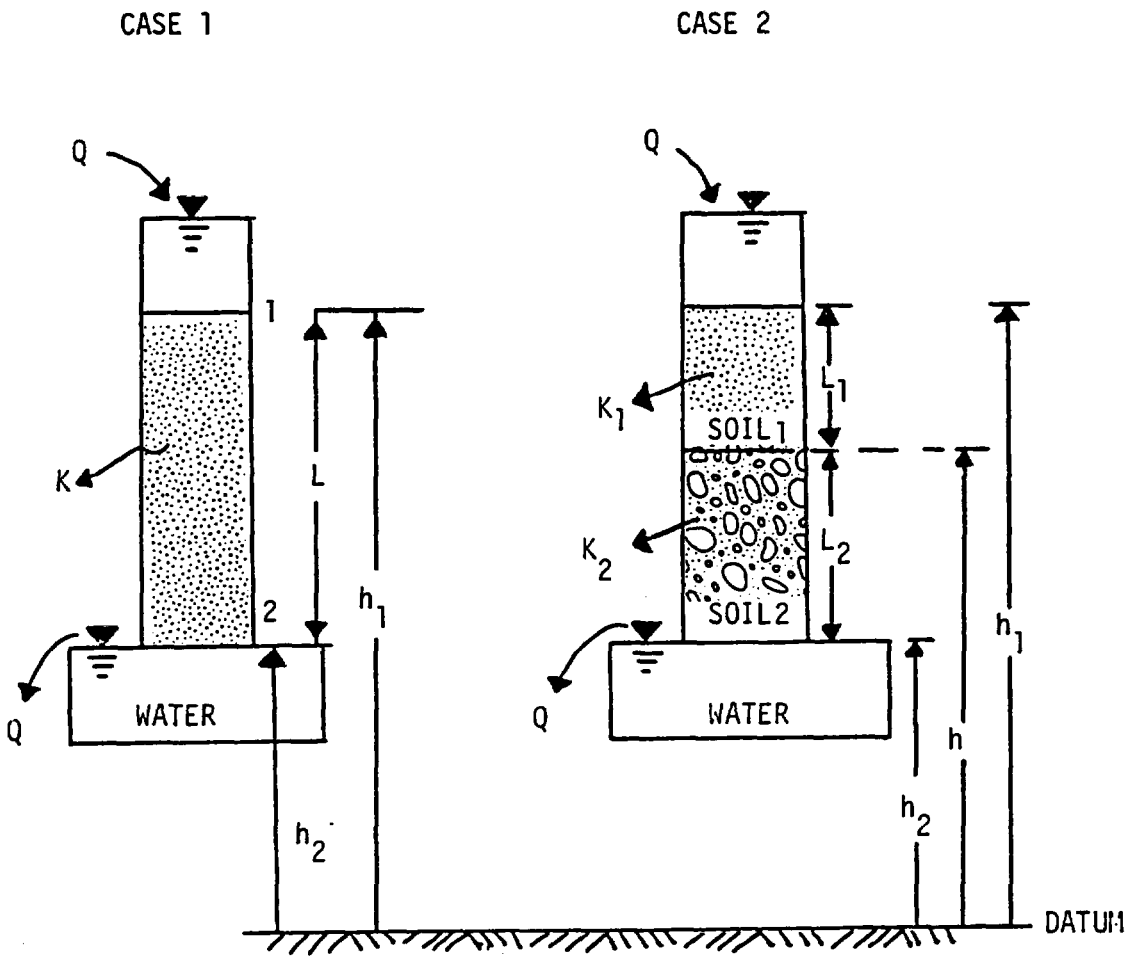


Figure 2.5. Hydraulic conductivity measurements using soil columns. Case 1 is a homogeneous(or equivalent homogeneous) soil column, and Case 2 is a two layer soil column.

This is the formula to determine the flow rate through the core sample from the permeameter. Let us attempt to determine the average hydraulic conductivity of this two-layer soil column. If a constant head permeameter is used, we can measure heads at the two ends of the column and the discharge from the column. Using the measured heads and discharge rate, from Darcy's law (2.4.2), the hydraulic conductivity can be easily determined by:

$$K_{ave} = \frac{QL}{A(h_1 - h_2)} \tag{2.4.6}$$

When equation (2.4.6) is used, we evidently assume that there is an equivalent homogeneous soil which should transmit the same amount of discharge as the layered soil column under the same head drop. Therefore, the K_{ave} value obtained from this calculation represents the K value of the equivalent homogeneous soil column and ignores the K values of each layer.

So, how is the K_{ave} value related to the K values of each individual soil? From a comparison of equation (2.4.2) and (2.4.5), one can see that:

$$K_{ave} = \frac{L}{L_1/K_1 + L_2/K_2} \tag{2.4.7}$$

As indicated in equation (2.4.7), the K value of the equivalent homogeneous soil column is the harmonic mean of the K's of individual soil layers. A similar analysis can be done where flow is parallel to the layers in the soil column. In this case, the average K obtained from the soil column will correspond to the arithmetic mean of the K's of the individual layers. That is:

$$K_{ave} = \frac{K_1 L_1 + K_2 L_2}{L} \qquad (2.4.8)$$

Based on the above discussion, one can see that the K values measured from a soil column test may vary with the size of the soil column. For instance, if the soil column is small enough to contain one soil layer, the value of K estimated is certainly the hydraulic conductivity of the layer. If the column contains more than one layer of soil, the estimated value of K is an average of the K for the individual layers. Furthermore, the average hydraulic conductivity depends on the direction of layering and the direction of flow. The average hydraulic conductivity should be the harmonic mean if the flow is perpendicular to the bedding, and the arithmetic mean if the flow is parallel to the bedding (Bear, 1979). Thus, we can draw a few conclusions about the hydraulic conductivity of a material, namely; it is an average over many small-scale values, it depends on the size of averaging volume (i.e., the total length of the soil column), the heterogeneity (i.e., the K values of individual layers), the size of the heterogeneity (i.e., the thickness of each layer), and the flow direction.

The average hydraulic conductivity can be easily determined from a soil column test. However, one should recognize two important facts in the column test. First, the heads at the ends of the soil column are kept constant over the cross section of the soil column, so the heads represent averages over the cross sections. Second, the discharge is measured with respect to the entire cross-sectional area of the soil column, including voids and solids. In essence, to calculate hydraulic conductivity, one needs to know the average hydraulic head over the cross-sectional area of porous media through which flow rate is measured. Without measurements of head and flow rate at the same scale, one may not be able to define an average or effective hydraulic conductivity. This is especially problematic for a large-scale

field site. Inasmuch as in the field problem analogous to the column in figure 2.5, the hydraulic head measured by a piezometer is generally regarded as a "point" measurement, and we usually do not have an instrument to measure the total discharge from a large aquifer. Hence the limitations of the measuring capacity of our instruments may restrain us from using the averaging rules discussed above, or at least from using Darcy's equation directly to compute an effective or average hydraulic conductivity for an aquifer.

2.4.2 Specific discharge. Darcy's law provides us with a method to calculate the total discharge or flow rate from a soil column, providing that we know the head gradient and hydraulic conductivity of the soil column. Specific discharge is defined as the total discharge rate divided by the cross-sectional area of the column. This means that the specific discharge is an average discharge value over the cross-sectional area. It does not represent the discharge from individual pores or areas smaller than the cross-sectional area. It is an average flux through a porous medium, at a scale at least as large as that of the REV.

2.4.3 Average fluid particle velocity. The average flow velocity of fluid particles is generally determined by the ratio of total discharge rate to the cross-sectional area of pore space through which flow occurs. This leads to the definition of average fluid particle velocity or average linear velocity in groundwater hydrology, which is:

$$v = \frac{q}{n_e} = \frac{Q}{An_e} \tag{2.4.9}$$

where q is the specific discharge and n_e is the effective porosity through which flow occurs. This is an average pore velocity over the total pore area in the cross section. Consequently, it does not represent the water velocity within individual

pores, because the areas of individual pores vary. As a result, if one uses the average fluid particle velocity to determine the arrival of a slug of tracer in the column test, the time of arrival would be the average arrival time of the tracer particles. Certainly, some of the tracer particles will move through larger pores and will arrive earlier than the predicted by the average time, and some of them will lag behind (Figure 2.6).

Generally, the average fluid particle velocity and the velocity deviations will vary with the size of the soil sample over which averaging takes place. If the sample is small enough to contain one soil, the velocity variation in a soil column tracer experiment, manifested in dispersion or spreading of tracer particle arrival times, will represent the velocity variation in the pore scale. If the sample is large enough to include several different soils, it will represent the combined effect of the variation in velocity among pores and among layers, and so on. Once again the velocity deviation is scale-dependent.

The average fluid particle velocity which is based on Darcy's law and effective hydraulic conductivity does not take into account the velocity variations at scales smaller than the scale at which the average fluid particle velocity is obtained. Then, how do hydrologists take account of the variation in velocity at the pore-scale or at any other scale? This question will be answered in the section that deals with dispersion.

2.4.4. Hydraulic Head. Now let us examine the physical meaning of hydraulic head in an equivalent homogeneous soil column. In the previous constant head permeameter examples (Section 2.4.1), a layered soil column was visualized as an equivalent homogeneous one (Figure 2.5). The effective hydraulic conductivity can be measured, and for flow perpendicular to the layering it is the harmonic mean of the two soil layers (equation 2.4.7). Certainly, one can use Darcy's equation and this effective hydraulic conductivity to determine a head distribution along the

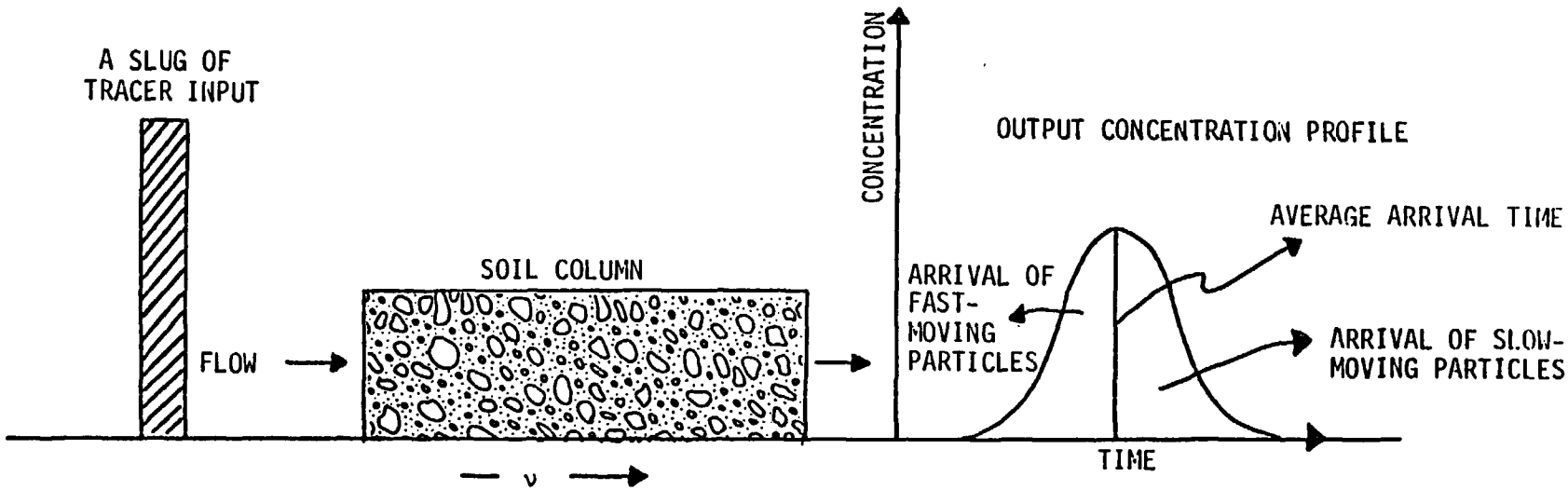


Figure 2.6. Effect of velocity variations in a soil column on outflow concentration.

equivalent, homogeneous soil column. Of course, the head distribution is a straight line, declining from the head at one boundary to the other (line C in Figure 2.7). However, owing to the layering, the head calculated by assuming that the two-layer column is homogenous is certainly different from actual head distribution along the soil column. Then, what does this calculated head distribution using the effective hydraulic conductivity represent? To answer this question, assume that the hydraulic conductivities of the two soils K_1 and K_2 are known. If $K_1 > K_2$, line A in the figure will represent the hydraulic head distribution along the layered soil column. If $K_1 < K_2$, line B is the head distribution. As illustrated in the figure, line C simply is the average of line A and Line B. This implies the head distribution determined from the effective hydraulic conductivity represents the average head distribution of all the possible head distributions; in this example there are only two possible head distributions. One can draw the same conclusion if the soil column consists of n layers of soils. In this case, the head distribution derived from the effective hydraulic conductivity will be the average of n possible hydraulic head distributions, resulting from all n! (n factorial) possible spatial arrangements of n K values along the soil column. This is equivalent to saying, in the jargon of stochastic hydrology, that the average is an "ensemble average" (see Section 4.0 or Appendix A).

From the simple example described above, one should see that a deterministic groundwater analysis is directly related to the stochastic concept that is used to deal with heterogeneity in field-scale problem, as will to be discussed in later sections. The discussion in this section is abstract and highly theoretical. However, it is crucial to understand the fundamentals of a theory before applying that theory to practical problems, such as the application of Theis' solution to aquifer tests (see Section 3.0).

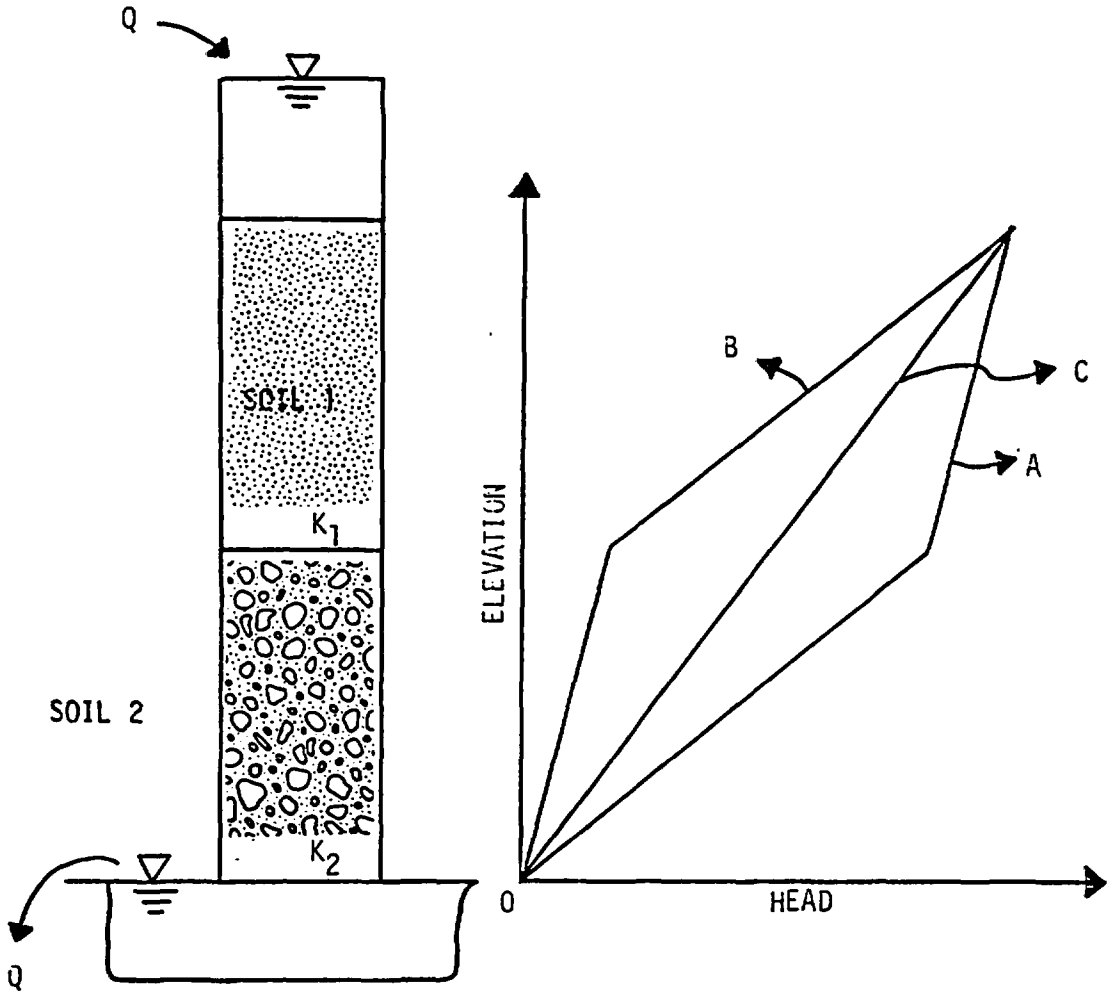


Figure 2.7. Concept of average hydraulic head distribution. Line A is for $K_1 > K_2$, line B is for $K_1 < K_2$, and line C is for K_{ave}.

2.5 Governing Groundwater Flow Equations

Estimating groundwater travel times in porous media requires the knowledge of the average fluid particle velocity which is determined by the gradient and the hydraulic conductivity values. Hydraulic gradients in groundwater problems are derived from hydraulic heads which may vary with time and space. Governing groundwater flow equations are used to predict the temporal and spatial variations of hydraulic heads. However, the equations are developed for the specific scales for Darcy's law and physical properties of groundwater discussed previously. Consequently, predictions from the equations, i.e., hydraulic heads, represent averages over some scale as well. Since groundwater travel times and paths are directly related to the hydraulic head distribution, understanding the meaning of the heads in equations of different scales is necessary. In the following sections, we will discuss the development of governing groundwater flow equations for various scales. Then, we will examine the physical meaning of head values. Meanwhile, some inconsistencies in the development of the equations which may contribute to uncertainties in predicting groundwater travel times will be elaborated on Appendix B.

2.5.1 Three-Dimensional Groundwater Flow Equation. To derive the governing groundwater flow equation, we start with the mass balance equation. Consider the mass balance of a stationary control volume at least as large as an REV (Figure 2.8) whose shape is fixed in space and time. The principle of mass conservation within this control volume requires that

$$\{ \text{rate of mass accumulation} \} = \{ \text{rate of mass in} \} - \{ \text{rate of mass out} \} \tag{2.5.1}$$

To apply the principle to the control volume, we begin by considering the pair of faces perpendicular to the x axis. The rate of mass in through the face at x is

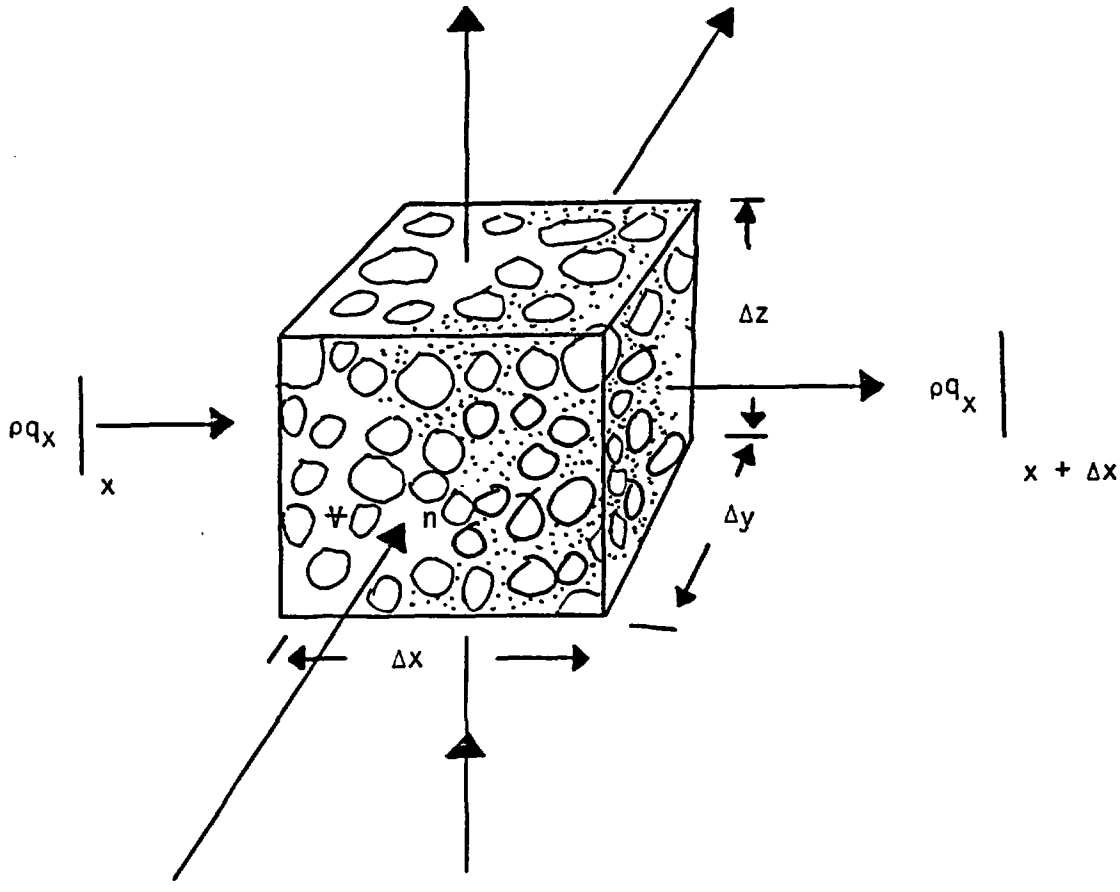


Figure 2.8. A control volume for mass balance.

$(\rho q_x)|_x \ \Delta y \Delta z$, and the rate of mass in through the face at $x+\Delta x$ is $(\rho q_x)|_{x+\Delta x} \ \Delta y \Delta z$. Similar expressions may be written for the other two pairs of faces. The rate of mass accumulation within the volume element is $(\Delta x \Delta y \Delta z)\left[\frac{\partial n\rho}{\partial t}\right]$, where n is the porosity of the control volume. The mass balance then becomes

$$\Delta x \Delta y \Delta z \left[\frac{\partial n\rho}{\partial t}\right] = \Delta y \Delta z[(\rho q_x)|_x - (\rho q_x)|_{x+\Delta x}] + \Delta x \Delta z[(\rho q_y)|_y - (\rho q_y)|_{y+\Delta y}] + \Delta x \Delta y[(\rho q_z)|_z - (\rho q_z)|_{z+\Delta z}] \tag{2.5.2}$$

By dividing this entire equation by $(\Delta x \Delta y \Delta z)$ and taking the limit as these dimensions approach zero, we get

$$\frac{\partial n\rho}{\partial t} = -\left[\frac{\partial \rho q_x}{\partial x} + \frac{\partial \rho q_y}{\partial y} + \frac{\partial \rho q_z}{\partial z}\right] \tag{2.5.3}$$

This is the equation of continuity for flow through porous media, which describes the rate of change of fluid density at a fixed point resulting from the changes in the mass flux $\rho \mathbf{q}$ (the bold type indicates a vector quantity, ie, a quantity having both magnitude and directions). Note that replacing the difference equation (2.5.2) by the partial differential equation (2.5.3) implies all the variables in (2.5.3) are continuous and differentiable in both space and time coordinates. regardless of whether the point of interest falls within a pore or solid. That is, the continuum assumption discussed previously has been used. Using the vector notation, equation (2.5.3) can be expressed as:

$$\frac{\partial n\rho}{\partial t} = -(\nabla \cdot \rho \mathbf{q}) \tag{2.5.4}$$

Here ($\nabla \cdot \rho q$) is called the "divergence" of ρq, sometimes written as div ρq. Note that the vector ρq is the mass flux, and its divergence has a simple significance: it is the net rate of mass efflux per unit volume. The equation (2.5.4) simply states that the rate of increase of the density within a small volume element fixed in the porous media is equal to the net rate of mass influx to the element. Note that the continuity equation applies to any arbitrary volume at this point.

Now if one assumes that the control volume is much larger than many pores, then the specific discharge, q, can be represented by Darcy's law. The substitution of a form of equation 2.4.1 (i.e., $q = -\nabla h$) for q in to equation 2.5.4 leads to the classical governing groundwater flow equation which is given as:

$$\nabla \cdot (K \cdot \nabla h) = \rho g(n\beta + \alpha) \frac{\partial h}{\partial t} = S_s \frac{\partial h}{\partial t} \qquad (2.5.5)$$

where K is the hydraulic conductivity tensor, h is the hydraulic head, and S_s is the specific storage coefficient. However, this equation is theoretically inconsistent since it mixes the expressions for both the fixed and moving coordinate systems as discussed in Appendix B.

Because of the use of Darcy's law, equation (2.5.5) is valid only for media whose volume is much larger than many pores. As a result, variables in the equation are continuous within the volume and represent average values. Certainly, these averages cannot account for the detailed variations of the variables at scales less than the volume, as we illustrated in section 2.4.4. Although the size of the averaging volume is restricted to be much larger than many pores, it could be enlarged to study any larger scale. Using equation (2.5.5), one can visualize an entire aquifer as a collection of many K values measured over a volume which is much larger than many pores but much smaller than the entire aquifer. On the

other hand, one can enlarge the REV so that the entire aquifer is considered homogeneous but the flow field remains three-dimensional. By reducing the size of the control volume, we obtain variables which are more representative of smaller scale variations within the volume.

2.5.2 Two-Dimensional Depth-Averaged Groundwater Flow Equation. Generally speaking, the three-dimensional groundwater flow equation is more representative of real flow fields than one- or two- dimensional equations. However, it may be impractical because a large number of data and a large amount of computer time are required for simulating three-dimensional flows in a field- or regional-scale aquifer system. Sometimes, it may be adequate to conceptualize such a three-dimensional flow field by a two-dimensional horizontal plane flow phenomenon. This conceptualization involves taking vertical averages of the three-dimensional groundwater flow equation, i.e.

$$\int_{z_0}^{z_0+b} \nabla\cdot(K\cdot\nabla h)\, dz = \int_{z_0}^{z_0+b} S_s \frac{\partial h}{\partial t}\, dz \qquad (2.5.6)$$

where z_0 is the elevation of the bottom of the aquifer, and b is the thickness of the aquifer Bear, (1979). Integration of (2.5.6) results in a two-dimensional depth-averaged equation,

$$\nabla'\cdot(T\cdot\nabla' H) = S\,\frac{\partial H}{\partial t}$$

where ∇' is the two-dimensional divergence

$$T = \int_{z_0}^{z_0+b} K(x,y,z)\, dz,$$

$$S = \int_{z_0}^{z_0+b} S_s(x,y,z)\, dz,$$

$$\text{and } H = \frac{1}{b} \int_{z_0}^{z_0+b} h(x,y,z)\, dz \qquad (2.5.7)$$

T, S, and H are transmissivity, storage coefficient, and the average hydraulic head, respectively. Note that T, S, and H are depth-averaged quantities which implies the vertical variations in these parameters are ignored. As an example, in a stratified aquifer the variation in hydraulic conductivities among layers is neglected. This implies that the vertical dimension of the REV of the aquifer properties, T and S, is at least equal to or much larger than the thickness of the layer in the aquifer. Certainly, one can conceptualize that T and S values are constant in both horizontal directions by enlarging the size of the REV. The aquifer is again considered homogeneous as in the three-dimensional case. However, even in homogeneous aquifers, the depth-average approach further restricts the flow to two horizontal dimensions only.

In fact, most field- and regional-scale aquifers have been characterized by aquifer tests which produce the depth-averaged T and S values. Since these data are abundant for most groundwater basins, Dagan (1986) argued that two-dimensional depth-averaged models are appropriate for field- or regional-scale problems.

2.5.3 One-Dimensional Flow Equation. A one-dimensional groundwater flow equation can be written as

$$\frac{\partial}{\partial x}\left[K\,\frac{\partial h}{\partial x}\right] = S_s\,\frac{\partial h}{\partial t} \qquad (2.5.8)$$

This equation is equivalent to conceptualizing an aquifer as a soil column (e.g. Figures 2.5 or 2.6) with flow in the aquifer being strictly unidirectional. If K is allowed to vary in the x direction, dimensions of the averaging volume (REV) in the other two directions, i.e. y, and z, are obviously as large as or larger than the width and thickness of heterogeneities (such as clay lenses) in the aquifer. If K is assumed constant in the x direction, the averaging volume must be much larger than the size of heterogeneities in the aquifer. Our scale of interest (such as the size of screen in a well) is much smaller than the entire aquifer. Such a large-scale averaging procedure may thus lose too much information pertinent to our interests. Therefore, this one-dimensional conceptualization may be considered of limited value.

2.5.4 Hydraulic Heads. Based on the discussion above, one can conclude that a three-dimensional equation (2.5.5) is most realistic. It allows us to describe aquifers as three-dimensional hydraulic conductivity fields using the small size average volume. The two-dimensional, depth-averaged equation (2.5.6), however, ignores the variations in hydraulic conductivity in the vertical direction. A one-dimensional equation (2.5.8) further averages the hydraulic conductivity variation in two directions (i.e., horizontal and vertical directions).

Groundwater flow equations for three-, two-, and one-dimensional problems (2.5.5, 2.5.6, and 2.5.8) allow us to conceptualize heterogeneous aquifers as homogeneous ones, using an appropriate REV. However, the flow fields (hydraulic heads) determined by each equation represent different averages. Because of the homogeneity assumption, the three-dimensional governing flow equation produces an ensemble-averaged three-dimensional head distribution. In other words, the head distribution is the average of all possible three-dimensional head distributions, as

discussed in Section 2.4.4. Note even though the aquifer is considered homogeneous, the head distribution may retain its three-dimensional characteristics, depending on type of flow field (i.e., uniform, converging, or diverging flow). Generally, the head determined by the three-dimensional flow equation for a homogeneous aquifer is analogous to the water level observed in a piezometer (Figure 2.9), if the aquifer is truly homogeneous (i.e, heterogeneity exists only at pore-level). However, if the heterogeneity is much larger than the opening of the piezometer, the head calculated by the three-dimensional equation with homogeneity assumption will differ from the one observed in the piezometer. The two-dimensional equation averages three-dimensional head distributions in the vertical to produce two-dimensional, depth-averaged heads. The depth-averaged head is equivalent to the water level observed in a well screened over the entire thickness of the aquifer (Figure 2.9). This depth-average procedure simply forces the head values along the vertical to be a constant value which is not identical to the ensemble average, unless the mean flow is parallel to stratifications. One-dimensional equations further reduce the two-dimensional head distribution to a one-dimensional one. The head resulting from the one-dimensional model is analogous to the water level in an excavation ditch which cuts completely through the aquifer, if there is no flow in the ditch.

As discussed above, each governing equation uses different averaged hydraulic properties of the aquifer. Each also gives hydraulic head values with different meanings. As a result, the fluid particle velocity determined from the averaged heads represents different averages. Moreover, these averages neglect variations in velocity at scales less than the scale where the averages apply. Therefore, one may ask: how can one include the effects of these variations smaller than the averaging scale to obtain a more realistic prediction of groundwater travel times and paths? We will try to address this equation in the next section that discusses the dispersion phenomena.

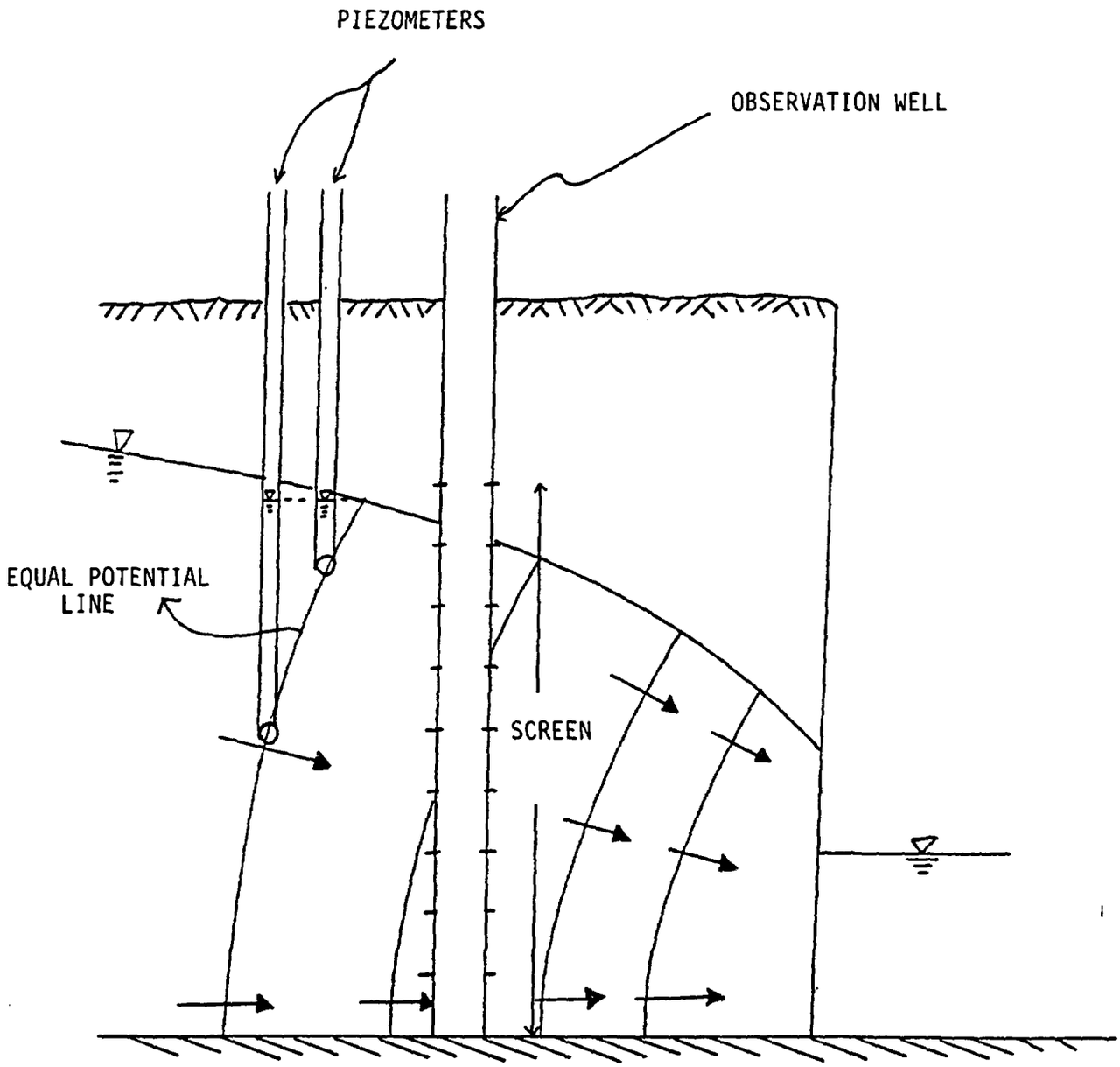


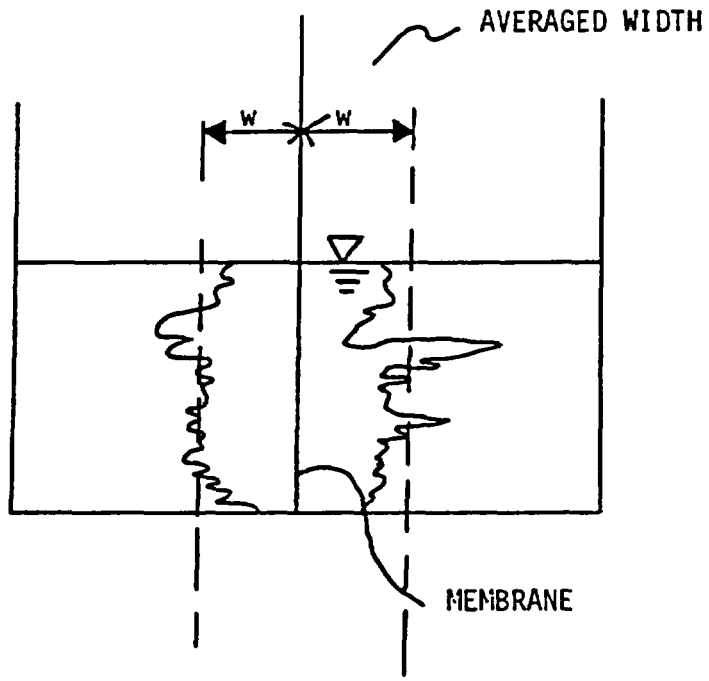
Figure 2.9. Water level in piezometers and a fully-screened observation well in a water table aquifer discharging to a ditch. Water level elevation in the observation well represents a depth-averaged head which is lower than the water table.

2.6 Hydrodynamic Dispersion

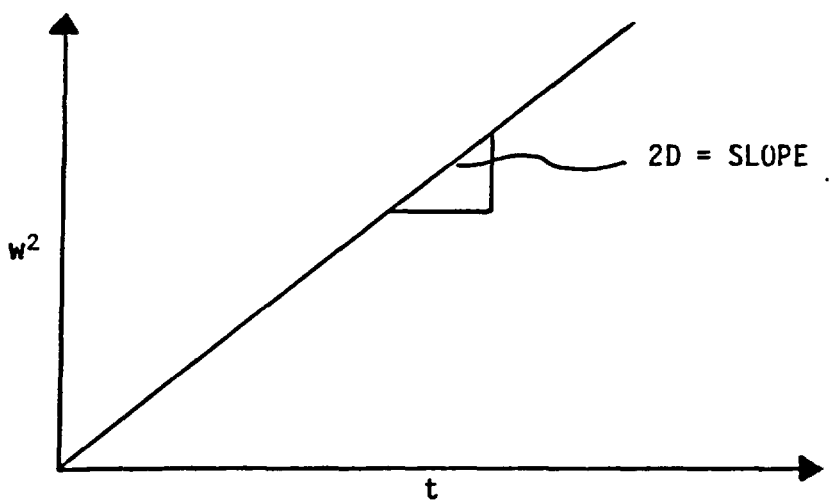
To include the variations in fluid particle motion at scales smaller than the scale at which the results of the flow equations apply, the concept of hydrodynamic dispersion must be introduced. However, before hydrodynamic dispersion is discussed, we will review the basic concept of molecular diffusion, which is analogous to hydrodynamic dispersion but at a much smaller scale.

2.6.1 Diffusion. Consider two fluids of the same chemical and physical properties but of different colors, separated in a tank by an impermeable membrane. The fluids in the tank are static, that is, there is no fluid flow. The membrane is then removed without disturbing the static condition. At early times, we would see an abrupt difference in color at the interface between the two fluids. As time passes, the abrupt interface diminishes and a smeared mixing zone develops (Figure 2.10a). The mixed color vanishes gradually away from the center, and fades into the initial color of the respective fluids. The width of this smeared zone grows continuously with time until the fluids are completely mixed. This process causing the smearing effect is called "molecular diffusion".

This diffusive process is generally attributed to the random motion of molecules of the two fluids. The term random motion is used because of the chaotic motion of molecules which seems to be unpredictable. In fact, if we apply kinetic theory to each molecule, the motion of a molecule in the fluid can then be described in a deterministic way. However, at the scale of our interest and instruments, it is of little practical use to describe the motion of each individual molecule. Nevertheless, such molecular-scale motions may have great impacts on phenomena at the scale larger than the size of molecules. Then, how can the diffusive process be quantified? This question was answered by Adolph Fick, a German physiologist, who in 1855 stated that the flux of solute mass, that is, the mass of a solute crossing a unit area per unit time in a given direction, is proportional to the gradient of



(a)



(b)

Figure 2.10. (a) Smearing effect in a tank, and (b) the linear relationship between w^2 and time.

solute concentration in that direction. This relationship is generally known as Fick's Law.

For a one-dimensional diffusion process, Fick's law can be stated mathematically as

$$q_m = -D_m \frac{\partial c}{\partial x} \tag{2.6.1}$$

where q_m is the solute mass flux; c, is the mass concentration of diffusing solute; D_m, is a coefficient of proportionality called the diffusion coefficient, and the minus sign indicates transport is from high to low concentrations. Fick's law is similar to Darcy's law in which the mass flux of water is related to the conductivity and hydraulic gradient. Similar to the hydraulic conductivity, the diffusion coefficient is a quantity averaged over a volume much larger than many molecules and the motion of individual molecules is ignored.

To illustrate the concept of averaging in a diffusion process, we will reexamine the case where two fluids are separated by a membrane. As mentioned earlier, the width of the mixing zone grows with time. Here, the width is defined as an average width of the mixing zone over the depth of the tank because the width may vary from depth to depth as shown in Figure 2.10a. This average is equivalent to the depth-average procedure discussed in section (2.5.2). If one repeatedly carries out the same experiment, the depth-average width may be different from one experiment to another because of the random motion of the molecules. However, if one averages the depth-averaged width of all the experiments, one obtains an average width which is an ensemble average, i.e., average over many possible outcomes. As a matter of fact, if the square of the ensemble-average width, w^2, is plotted as a function of time, a linear relationship is found (Figure 2.10b). The slope of the line

is generally related to the diffusion coefficient by

$$\frac{dw^2}{dt} = 2D_m \tag{2.6.2}$$

In other words, the diffusion coefficient, D_m, describes the rate of growth of the average width of the mixing zone over the depth of the tank, and over many experiments. It certainly does not intend to depict the rates at each depth and each experiment. Therefore, the coefficient of diffusion is merely a mean parameter. In view of the fact that our measuring devices, and human vision are limited, and the fact that repeated experiments are impractical, a diffusion coefficient obtained in one experiment is often considered adequate. This assumption implies the equivalence between the depth-average and the ensemble average (i.e. an ergodicity assumption; see Appendix A and Section 4.1). Since D_m is an average value, one should not expect that the concentration of the colored fluids can be predicted by using the diffusion coefficient at scales much smaller than the scale at which D_m is derived. Furthermore, one should not expect that the concentration predicted by the diffusion concept will be identical to the one observed in a single experiment.

The linear relationship shown in Figure 2.10b implies that the diffusion coefficient is a constant. This constant diffusion coefficient concept or the linear relation may be true, at least at the scale of our instruments but not at the microscopic scale. We now will illustrate this point by reviewing a statistical theory developed by G.I. Taylor (1922) for analyzing the random motion of molecules.

Inasmuch as the motion of each molecule is complex and "random", it is most appropriate to describe it by statistical means. That is, we will describe the position of molecules at any time in terms of probability, instead of the exact location of the particle. Again, we would like to reemphasize the fact that the motion of

molecules is deterministic but too complex for us to use any deterministic approach. Furthermore, we are not interested in how individual molecules move. Based on these reasons, we conceptualize the deterministic movement of molecules as a random process. To carry out this statistical analysis of random motion, we will assume that the velocity of a diffusing molecule is a stationary stochastic process in time (Csanady, 1973). This means that we do not know the velocity of the molecule at any time, but we could determine all the possible velocity values from the known statistical properties of the process, such as mean, variance, or probability distribution of the velocity (for definitions of statistical terms refer to Appendix A). Without loss of generality, we may say that the mean and variance of the velocity of a molecule are constant in time: i.e.,

$$E[v(t)] = \text{constant} = 0$$

$$\text{and} \quad E[v^2(t)] = \text{constant} = E[v^2],$$

respectively, where E[ ] stands for the expected value which represents the probablistic average of a random variable. Another important statistical parameter characterizing a stationary stochastic process is its autocorrelation function, $R_{vv}(\tau)$, where τ is the time lag between two times, t and $t+\tau$. The autocorrelation function of the velocity history of a molecule may be regarded as measuring the persistence of the velocity of a molecule throughout a period of time (Appendix A). In other words, it is a measure of the correlation of the velocities of a molecule between any time interval, τ. Thus, the velocity autocorrelation function is defined as:

$$R_{vv}(\tau) = \frac{E[\ v(t)\ v(t+\tau)\ ]}{E[\ v(0)^2]} \tag{2.6.3}$$

where $E[v(0)^2]$ is the variance of velocity. In a stationary stochastic process, the autocorrelation function is independent of time t but dependent on the time lag, τ. In the case of the velocity history of a diffusing molecule, such an autocorrelation function implies that once the molecule possesses a certain velocity, a short time τ later it is still likely to have a velocity of a similar magnitude and sign. For a given time lag τ, the velocity covariance, $E[v(t)v(t+\tau)]$ may be formed, which evidently tends to $E[v^2]$ as $\tau \to 0$. However, after a long enough time τ, the molecule tends to 'forget' the velocity at time t, in the sense that the value of v at $t+\tau$ will be quite independent of v(t). That is, at $\tau=0$, $R_{vv}(\tau)=1$, while as τ approaches ∞, $R_{vv}(\tau)$ becomes 0, as shown in Figure 2.11.

The displacement of an individual diffusing fluid or tracer molecule at any time, t, can be related to its velocity by

$$x(t) = \int_0^t v(s)ds \tag{2.6.4}$$

where x is the position. Now we imagine that there is more than one molecule moving "randomly" in fluid space. We further assume that the statistical characteristics (i.e., mean, variance, and covariance) of molecule's velocities are the same. After a period of time, the location of each molecule would, of course, be different. However, these molecules will spread around x=0,

$$E[x(t)] = \int_0^t E[v(s)]\, ds = 0 \tag{2.6.5}$$

because in a static system the mean velocity, E[v], is zero. As shown in Figure 2.10

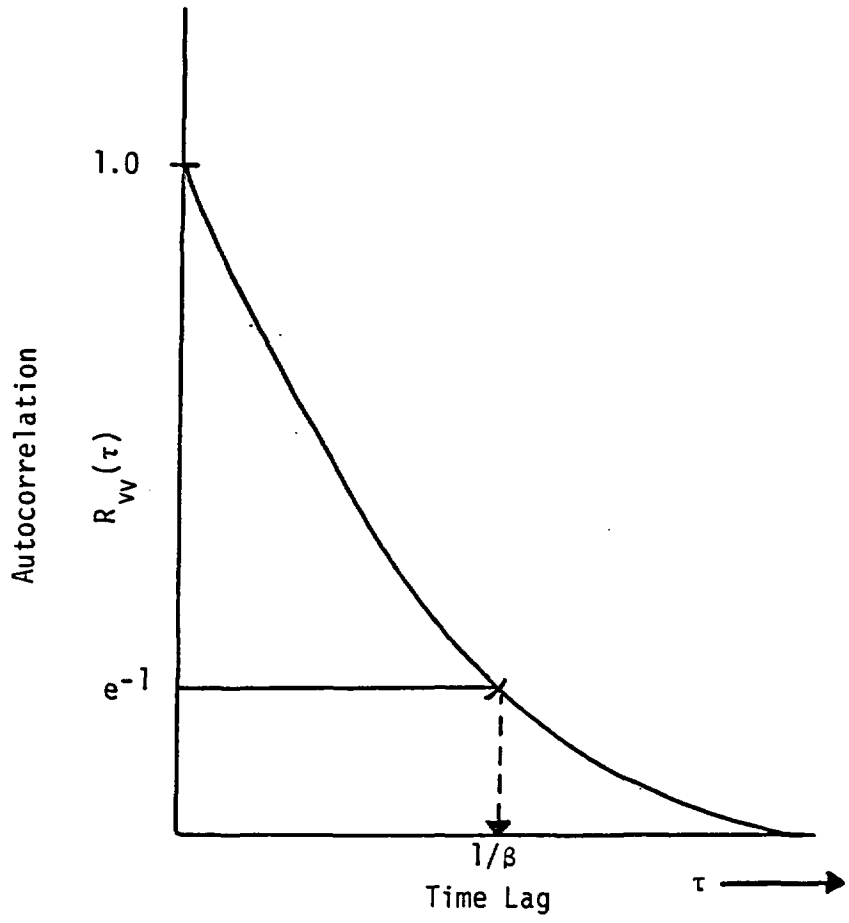


Figure 2.11. A hypothetical velocity autocorrelation function.

and equation 2.6.2, the spreading, the deviation of the position of a molecule from the mean position, at time t can be quantified by $x(t)^2$. The rate of change of $x(t)^2$ may then be written as:

$$\frac{dx^2(t)}{dt} = 2x\frac{dx}{dt} = 2\int_0^{t+\tau} v(t)\ v(t+s)\ ds \tag{2.6.6}$$

Since there are a large number of molecules, the average rate of change of $x^2(t)$ of all the molecules can be obtained by taking the expected value of (2.6.6) and the result is:

$$\frac{dE[x^2]}{dt} = 2\ E[v^2]\int_0^{t+\tau} R_{vv}(\tau)d\tau \tag{2.6.7}$$

where $E[x^2]$ is the variance of the molecule positions which is equivalent to the average width squared, w^2, in equation (2.6.2). The left-hand side of equation (2.6.7) represents the rate of change in variance of the molecule positions or $2D_m$ as shown in equation (2.6.2). In other words, the molecular diffusion coefficient, D_m, is directly related to the molecules' velocity autocorrelation function and it varies with time. However, due to numerous collisions with other molecules, the velocity of a molecule at time $t+\tau$ tends to forget its velocity at t, as τ becomes large. For simplicity, we assume that the velocity autocorrelation function takes the form:

$$R_{vv}(\tau) = e^{-\beta\tau} \tag{2.6.8}$$

where β^{-1} is considered as the persistence time for the velocities of the diffusing

molecules. This means that, on the average, molecules tend to forget their previous velocities after a period of time β^{-1}. This velocity autocorrelation function is shown in Figure 2.11 as a function of τ.

The integral of $R_{vv}(\tau)$ on the right hand-side of equation (2.6.7) represents the area under the curve bounded by 0 and $t+\tau$. It should be evident from Figure 2.11 that the value of the integral will increase initially but will approach a constant at large values of $t+\tau$, or $t+\tau$ approaches ∞. This result implies the rate of spreading of the diffusion molecules at large value of τ will be a constant according to equation (2.6.7). As a result, the diffusion coefficient, which is half of the rate of change in $E[x^2]$, will increase initially but at $t \gg \beta^{-1}$ it tends to stabilize. For a particle of a radius, 10^{-4} cm, the persistence time, β^{-1}, is about 1.4×10^{-8} seconds (Csanady, 1973). Since the scale of our observation is likely much greater than 1.4×10^{-8} seconds, the time-dependent portion of the diffusion coefficient can be neglected and the diffusion coefficient can virtually be treated as a constant value. For much smaller scales of observations this may not be the case.

2.6.2 Advection-Diffusion Equation. Now suppose that an ideal fluid with a tracer is moving in a frictionless pipe. In this hypothetical frictionless pipe, there are no velocity variations caused by friction between the fluid and the wall of the pipe, so that the velocity recorded by small instruments is constant across the cross-section of the pipe, because friction does not exist. However, at the molecular level, molecules move at different velocities. The size of our instruments for measuring a flow velocity is generally much greater than the size of molecules. Obviously, the velocity we determined from the measurement is an average value over many molecules. This average velocity does not consider the variation in velocity of molecules. For example, consider a tracer experiment in a frictionless pipe (Figure 2.12a). If 10,000 tracer molecules are simultaneously released at one end of the pipe at time, t_0, then at various times the discharge at the other end of the pipe is

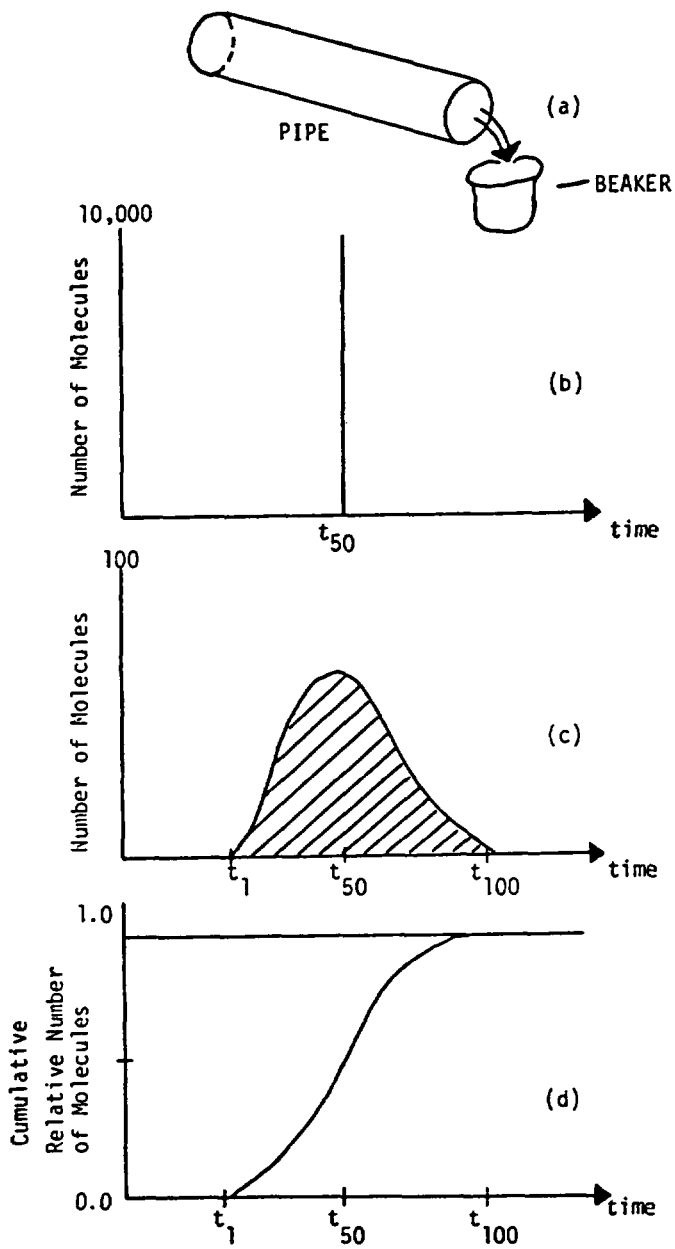


Figure 2.12. A tracer experiment in a frictionless pipe.

collected with a beaker, and the number of tracer molecules in the beaker is counted. We will observe the simultaneous arrival of all the molecules at time, t_{50} (Figure 2.12b), only if all the molecules move at the same velocity which is equal to the discharge rate divided by the cross-sectional area of the pipe. However, due to the random motion of molecules, some of the molecules will move faster than the others and some slower. If we plot the number of molecules in the beaker versus time, we shall have a molecule arrival time distribution shown in Figure 2.12c. This distribution represents the number of the tracer molecules arriving at the end of the pipe at any time, t. Figure 2.12d shows the cumulative, relative number of molecules (i.e., the ratio of the total number of molecules collected after t_0 to the total number of molecules released) as a function of time. Based on the figure, 50% of the tracer molecules exit the pipe at t_{50}, and all the molecules are removed at t_{100}. Time t_1 thus represents the arrival time of the fastest moving molecule, or the molecule travel time along the fastest path. However, we generally do not count the number of molecules due to the size of our instruments, and instead we use concentration, c, (i.e., the ratio of the mass of the tracer molecules to the volume or mass of the fluid in the beaker). Thus, Figure 2.12c is equivalent to the concentration-time distribution (breakthrough curve), and Figure 2.12d represents the cumulative concentration-time distribution. Obviously, the smearing or spread of the concentration distribution is due to variations in molecules' arrival time, which in turn are caused by variations in molecules' velocity. If the variation in velocity at the molecular level can be handled by the diffusion coefficient discussed previously in Section 2.6.1, the total rate of mass flux, q_m, across the instrument used to measure flow rate is thus the advective flux due to the average movement of the fluid plus the diffusive flux due to random motion of the fluid molecules. That is;

$$q_m = vc + \left[-D_m \frac{\partial c}{\partial x} \right] \tag{2.6.9}$$

where v is the average velocity of the fluid, and c is the concentration of tracer. The product term vc represents the advective tracer flux and $D_m \partial c/\partial x$ represents the diffusive flux. When (2.6.9) is substituted into the equation for conservation of mass (similar to equation 2.5.4) in one dimension, we obtain the advection-diffusion equation:

$$\frac{\partial c}{\partial t} + v\frac{\partial c}{\partial x} = D_m \frac{\partial^2 c}{\partial x^2} \tag{2.6.10}$$

where the second term on the left hand side of the equation represents the advection effect and the term on the right hand side of the equation represents the diffusion effect due to random motion of molecules. Thus, a concentration breakthrough curve which is the solution of Equation 2.6.10 in time domain reflects the arrival time of the tracer molecules. The molecular diffusion coefficient is simply a "fudge factor" accounting for velocity variations of molecules at a scale much smaller than the pipe.

Equation (2.6.10) is developed for tracer movement in a frictionless pipe. In the case where the wall of the pipe is not smooth but rough, velocities measured at a scale much larger than many molecules but smaller than the cross-section of the pipe (say, continuum scale in fluid mechanics) will vary across the cross-section of the pipe. The velocity is likely maximal in the center of the pipe and is minimal near the wall. This implies that the velocity determined by a discharge rate divided by the cross-sectional area of the pipe represents an average velocity value which neglects the velocity variation across the cross-sectional area due to friction. Furthermore, it also neglects the velocity variations among individual molecules.

Now, if we assume that the velocity variations at scales smaller than the cross-sectional area of the pipe and those at the molecular scale can be described by Fick's law as in the molecular diffusion process, then equation (2.6.10) is valid for this case as well. However, the diffusion coefficient, Dm, in equation (2.6.10) is replaced by a dispersion coefficient, D_d, which lumps together velocity variations at both the molecular scale and the continuum scale. Of course, the velocity, v, in equation (2.6.10) represents the average over the cross-sectional area. The concentration, c, then represents the total mass of a tracer in a volume of fluid discharging from the cross-sectional area of the pipe. Generally, this approach is valid for tracer movement in a long pipe as shown by G.I. Taylor (1953).

Following the above concept, surface-water hydrologists have frequently applied equation (2.6.10) to determine tracer movement in large-scale water bodies such as streams, rivers, estuaries, and oceans. Various successes have been reported in the literature for instance Fischer et al., (1979). Regardless of the validity of equation (2.6.10) for large-scale problems, the most important feature of the equation is that the parameters have different physical meanings, depending on the scale. Moreover, the dispersion coefficient always represents the effects of velocity variations at scales smaller than the scale at which the average velocity is defined.

2.6.3 Hydrodynamic Dispersion in Porous Media. Now consider flow in a porous medium (for example, a soil column). At the molecular level, each molecule has its own velocity. At the scale of a single pore, the velocity averaged over many molecules may not be constant over the pore space because of the roughness of the wall of the pore, just like flow in a frictional pipe. At the scale larger than a single pore variations in pore size, in addition to tortuosity of pore channels, will then cause an additional velocity variation. As discussed previously, the average fluid particle velocity defined in groundwater hydrology is the average value over many pores or heterogeneities of many different scales, depending on the size of the

control volume. The average fluid particle velocity does not take velocity variations at different scales into consideration. To account for the variation in velocity due to random motion of molecules, roughness of the pore walls, and the variation in size of pores and tortuosity in a flow path, groundwater hydrologists borrowed the advection-diffusion concept. In other words, in order to conserve mass, the mass flux which is not considered by the average fluid particle velocity is lumped into the dispersive flux term, similar to the way molecular diffusive flux was treated in the advection-diffusion process. The smearing effect due to the variation in velocity at a scale larger than the molecules, but smaller than the scale used to determine the average fluid particle velocity is then attributed to hydrodynamic dispersion. Therefore, the classic advection-diffusion equation (2.6.10) may then be directly applied to solute transport in porous media. However, the coefficient of hydrodynamic dispersion is used in lieu of the diffusion coefficient to represent the coefficient of proportionality between the mass flux and concentration gradient. The hydrodynamic dispersion coefficient thus includes the effect of variation in velocity at many different scales (from the molecular scale to the scale at which the average linear velocity is defined.) This approach is identical to convection-dispersion approaches used by surface-water hydrologists in dealing with solute transport in streams, rivers, and estuaries. However, causes of velocity variations or mechanisms of dispersion are different.

2.6.4 Mechanisms of Dispersion in Porous Media. Mixing of tracer particles due to dispersion is primarily an artifact related to the scale of averaging. In the REV, the hydraulic conductivity and porosity are assumed to be constants representing the average values over the volume. Consequently, the velocity determined from these parameters represents an average over the volume. This velocity describes the average solute movement as a piston type of displacement which exhibits a sharp interface with the fluid. Smearing effects observed in the

experiments are attributed to mixing due to subscale velocity variations within the REV which are treated as the dispersion process. Since the size of the REV varies with the scale of heterogeneity, mechanisms of dispersion are accordingly classified by the scale of heterogeneity.

At the microscopic scale, mixing is caused by random motion of fluid molecules. This process is called diffusion. At the laboratory scale, mixing is a result of the combined effects of diffusion and velocity variation within pores, among pores, and tortuous flow channels. This type of mixing is generally defined as local dispersion. If the concentration of tracer particles is measured in fully penetrating observation wells and one uses a two-dimensional depth-average flow and transport model to simulate the process, then the field-scale dispersion reflects mixing due to groundwater velocity variations between and within distinct hydrogeologic units, in addition to molecular diffusion and local dispersion. This type of dispersion is sometimes called two-dimensional macrodisperison (Gelhar et al., 1979). The term, macrodispersion, is also used in three-dimensional flow situations if one treats the entire aquifer as a homogeneous one. However, the two-dimensional macrodispersion is different from the three-dimensional one in the fact that it also includes the effects of averaging three-dimensional flow fields into two-dimensional fields (see section 2.5). Therefore, the mechanics causing dispersion vary with the scale of averaging.

2.6.5 Dispersivity. The dispersion concept in groundwater hydrology should become clear by now. Overall, the dispersion coefficient is merely a parameter in the classic convection-dispersion equation used to include variations in velocity at subscales. However, velocity variations are not controlled only by the heterogeneity at different scales of porous media, but also by the flow fields (directions of flow, and magnitudes of mean velocities). For example, consider an aquifer consisting of three homogeneous layers with equal thicknesses and with hydraulic conductivities,

K_1 = 10 cm/day, K_2 = 1cm/day, and K_3 = 100 cm/day. For simplicity, we will assume porosity values of the three layers are the same and equal to 0.5. If a constant hydraulic head gradient 0.01 is imposed on each layer, the average fluid particle velocity for layers 1, 2, and 3 is 0.2, 0.02, and 2 cm/day, respectively. The average velocity over the three layers is 0.74 cm/day and the variance is 1.2 cm^2/day^2. Now, if the gradient is increased to 0.1, the velocities are 2, 0.2, and 20 cm/day for layers 1, 2, and 3, respectively. The mean velocity is then 7.4 cm/day and variance is 119 cm^2/day^2. This simple example illustrates that velocity variations depend on the magnitude of gradient or mean velocity, as well as the hydraulic conductivity variation. Therefore, the hydrodynamic dispersion coefficient depends not only on the physical characteristic of porous media but also on the flow characteristics.

Inasmuch as flow is likely to vary with time and boundary conditions, how can this hydrodynamic dispersion coefficient be determined so that one can predict solute movement in porous media? One way to determine this parameter is to fit, by trial and error, the solution of the convection-dispersion equation to the results of tracer experiments. However, in a sense, the dispersion coefficient becomes a parameter which may vary from one experiment to another experiment even in the same porous medium, owing to differences in mean pore velocity. For predictive purposes, such an approach is not suitable.

To overcome this difficulty, many tracer experiments at the laboratory scale have been done in the past. The results of the experiments showed that the dispersion coefficient, D_d, is linearly proportional to the average velocity (Bear, 1979):

$$D_d = \alpha v \tag{2.6.11}$$

where v is the average velocity over the laboratory sample and α is the dispersivity.

For homogenous laboratory soil columns, the dispersivity can be further related to the particle size of porous media, and thus, can be considered constant. Because the dispersivity is a property of the medium, predicting movement of solutes in a porous medium under different flow fields now becomes possible.

2.6.6 Scale-Dependent Dispersivity. Taylor's (1922) analysis (Section 2.6.2) showed that the rate of spreading of molecules grows with time or distance because of the molecules' velocity persistence. However, the rate reaches a constant value in a relatively short period of time and distance compared to the measuring capacity of our instruments. As a result, molecular diffusion can virtually be represented by Fick's law (equation 2.6.1) with a constant diffusion coefficient.

By the same token, the spreading of a tracer plume in homogeneous soil columns will grow with time and distance because of the persistence of fluid particle velocity. This velocity refers to the velocity of a volume of water that is much larger than many molecules but smaller than the size of a pore. However, the persistence diminishes due to changes in pore geometries and mixing with water from other flow paths as the volume of water moves through many pores. Since the size of pores in soils is small compared to the size of the REV of a soil column, the classic convection-dispersion equation with a constant dispersion coefficient (or constant dispersivity) is generally considered adequate to describe solute transport in homogeneous soil columns.

In field scale problems, the effects of heterogeneity on velocity variations are controlled by large-scale heterogeneities such as clay lenses, facies changes, and layerings of sediments. If we assume that by averaging the hydraulic properties, the field-scale aquifer is, in effect, homogeneous, and we use the dispersion concept to represent the effect of the heterogeneity on solute transport, we would expect the dispersion coefficient to grow with distance and reach a constant value at some distance, as in the molecular diffusion process predicted by Taylor (1922) and

observed in homogeneous soil column tests. However, a problem arises from the fact that the size of heterogeneities (such as clay lenses) at the field-scale is many times larger than the size of irregular pore channels in soil columns. The travel distance which is sufficient to allow the solute particles to "forget" the influence of the previous velocity may thus be many times larger than the size of clay lenses or layerings. Furthermore, this distance is generally much larger than the length of our field tracer experiments. As a consequence, the dispersivity values estimated from the field tracer tests seem to grow with travel distance or time (Figure 2.13). This phenomenon is known as the scale-dependent dispersion. It should be evident by now that such a scale-dependent dispersion is a result of the scale of heterogeneity, the scale of averaging, and the scale of observation.

Many theories accounting for the scale-dependent dispersion have been developed in the past decade for example; Gelhar and Axness, (1983), Neuman et al., (1986), Dagan, (1987), Matheron and De Marsily, (1980), etc. Field experiments to validate the theory of scale-dependent dispersivity in aquifer systems are currently in progress at several locations in North America, for example, at the Borden land-fill in Canada (Sudicky, 1986 and Feryberg, 1986) and in Mississippi, (Betson, et al. 1985).

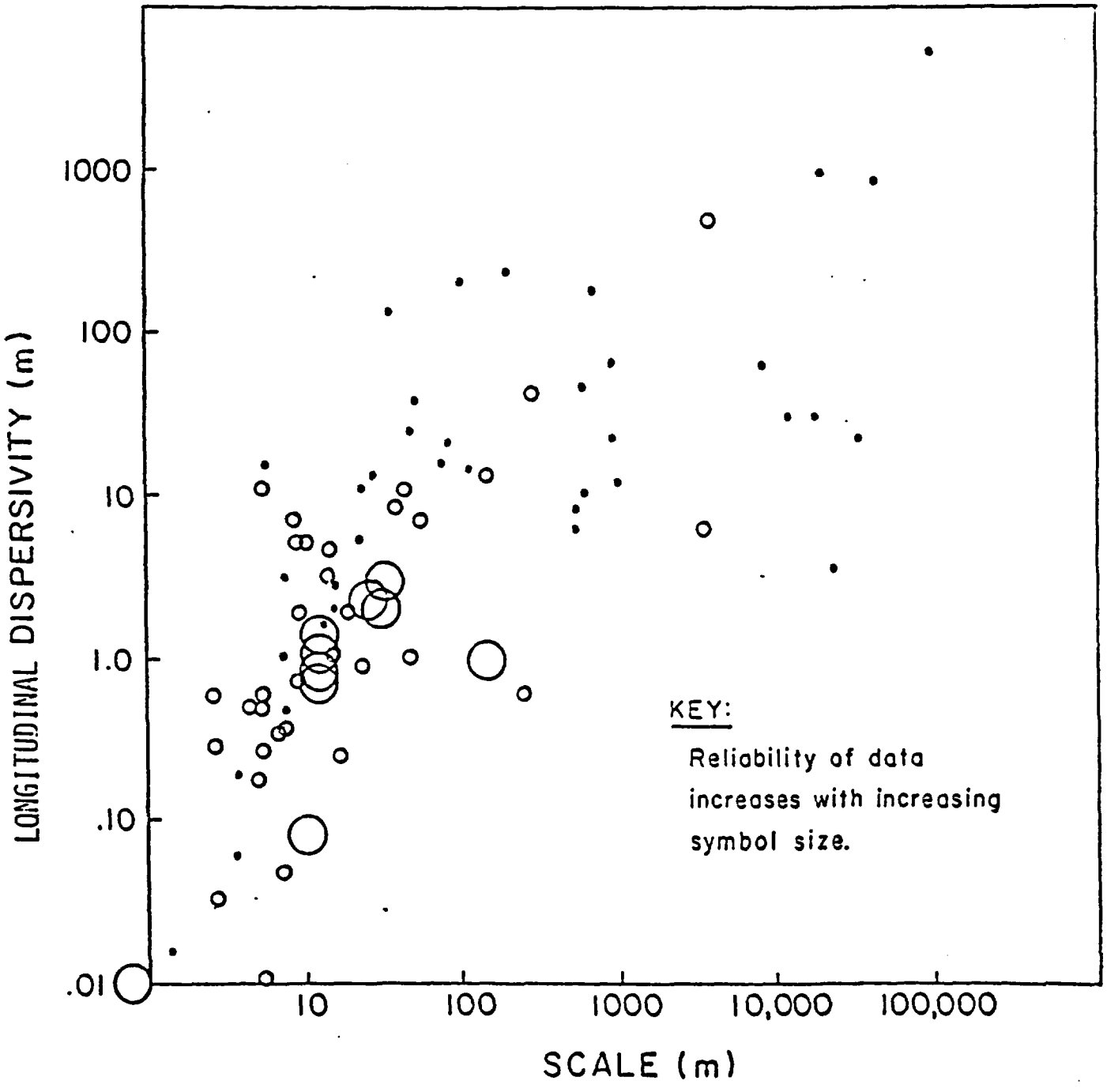


Figure 2.13. Data showing scale-dependent dispersivity (Gelhar, 1986).

2.7 Fracture Systems

In the previous sections of the review, we focused on laws and equations for flow and transport in porous media where large scale features such as fractures do not exist. Such media are representative of most aquifers which consist of unconsolidated sediments. However, most of the geologic materials at the proposed nuclear waste repository sites are generally consolidated sediments, volcanic or crystalline rocks. These geologic materials contain many fractures resulting from recent or past tectonic activities. Since groundwater flows through not only the rock matrix but also fractures, one certainly has to consider the effects of fractures in order to determine the groundwater travel times and paths in such geologic materials. Generally speaking, flow and transport phenomena in fractured rock are not as well understood and characterized as in porous media. This problem can be attributed partially to scale problems similar to those in porous media. That is, fractures are too small to be considered as discrete flow channels but too large to be considered as pore channels in porous media. In addition, the flow regime in fractures may vary from laminar to turbulent flow in which the classic groundwater flow equation based on Darcy's law is not valid. In the following sections, we will examine recent developments in conceptualization of flow and transport in such media under both saturated and unsaturated conditions.

2.7.1 Flow in Saturated Fractured Rocks. In fractured rocks, the size of a fracture is generally larger than the size of pores. The density of fractures at the macroscopic level, however, is much lower than the density of pore spaces. One has to enlarge the size of the REV defined for porous media in order to visualize fractured rock as a equivalent porous continuum at a large scale. In other words, the size of the REV for fractured rocks has to contain many fractures in the same way that the size of the REV for porous media must be much larger than many pores. Similarly, the detailed spatial distribution of individual fractures inside the

REV is ignored. However, if the knowledge of a detailed spatial distribution of fractures is available, and the behavior of flow in each fracture is what we are interested in, we may treat fractures as distinct flow channels embedded in a porous medium. The individual fracture is then visualized as a continuum with a smaller REV which ignores the much smaller scale flow channels within each fracture. Evidently, the size of the REV for individual fractures is not the same as that for the rock matrix.

Based on the discussion above, we can now classify the approaches of modeling flow and transport in fractured rocks into the continuum approach and the discrete approach. The continuum approach assumes that one can enlarge the REV so that the flow behavior in both the fracture and the porous matrix can be conceptualized as a flow system in an equivalent porous medium. This implies that the hydraulic properties of such an REV represents averages of the properties of the fractures and the rock matrix within the REV. Again, the detailed flow regimes in both fractures and rock matrix are ignored.

This continuum approach can be further divided into the single network approach and the double network approach. Such a division is necessary in fractured rock formations. In porous media, it is generally agreed that solids are impermeable and do not interact with the fluid in the void space. Thus, hydraulic conductivity is defined over many pores only. However, this may not be the case in a fractured rock system where both the fracture and the rock matrix are considered conductive. In a steady state flow situation, the conductivities of both the fractures and rock matrix may be represented by the notion of equivalent hydraulic conductivity. As a consequence, a single network approach is adequate. In this approach, a fractured medium is represented by a single network in which the hydraulic properties are averaged over both the fracture and the rock matrix. Thus, the general governing flow equation is written as:

$$\nabla\cdot(K\cdot\nabla h) = \frac{\partial S_s}{\partial t} \qquad (2.7.1)$$

where K, S_s, and h represent the average values of hydraulic conductivity, specific storage, and head over the fracture and the rock matrix within the volume of the REV, respectively. For steady state conditions, the right-hand side of equation 2.7.1 is zero. Although the hydraulic properties of such a REV are the averages over both the fracture and the rock matrix, they are dominated by the properties of fractures, and the influences of the porous matrix properties are negligible. (This is especially true for hydraulic conductivity, which is perhaps the most important property controlling groundwater travel time). Thus, this approach assumes that an equilibrium between the flows in both fractures and rock matrix exists, which may not be valid for most cases.

With the single network approach, one may conceptualize a large-scale fractured geologic formation as a heterogeneous continuum or a stochastic continuum if heterogeneities are represented by stochastic processes (Neuman, 1987). Because the volume over which the averaging takes place may contain several fractures and a vast number of pores in the rock matrix, the spatial distribution of the hydraulic properties thus becomes smooth and differentiable. The classic partial differential equations for flow in heterogeneous porous media can now appropriately applied.

In the transient state, owing to the relatively small storativity in fractures, the response of the fracture to pressure (or head changes) is much faster than in the matrix. The interaction between the fracture and the porous rock matrix becomes important. It therefore becomes necessary to define, inside the REV, two separate networks: one representing fractures and the other the rock matrix. Each network within the REV is considered a homogenous continuum. The spatial distribution of fractures or the rock matrix is not required to be specified within the REV. This

conceptualization is the so called double network or dual porosity model.

The double network approach has been used by many investigators such as Barenblatt et al. (1960), Warren and Root, (1963), Kazemi, (1969), Zhang, (1982), Huyakorn et al. (1983), and Moench (1984). The approach assumes that hydraulic responses of an REV result from two flow systems. One represents the flow in the rock matrix network, and the other the fracture network. Flow in each network is described by a governing flow equation. The influences of fractures on the flow regime in the rock matrix, or vice versa, are then entered as sink or source terms in the flow equations. More specifically, the governing differential equation for flow in the fracture network is assumed to be described by the classic groundwater flow equation with a source term to account for contributions from the matrix rock:

$$\nabla\cdot(K_f\cdot\nabla h_f) = \frac{\partial S_{sf}}{\partial t} + q \qquad (2.7.2)$$

where K_f is the hydraulic conductivity of the fractures, S_{sf} is the specific storage of the fractures, and h_f is the hydraulic head in the fracture network. These hydrologic properties represent averages over many fractures in the REV. The term q in equation 2.7.2 represents the contribution to or from the rock matrix. Similarly, for the rock matrix the governing flow equation is given as

$$\nabla\cdot(K_m\cdot\nabla h_m) = \frac{\partial S_{sm}}{\partial t} - q \qquad (2.7.3)$$

where K_m is the conductivity, S_{sm} is the specific storage, and h_m is the head in the rock matrix network, and q represents the contribution from or to the fractures and it is related to h_m and h_f. Generally speaking, this approach depicts the flow system better than the single network approach because the non-equilibrium interaction

between the rock matrix and the fracture is considered in the formulation of the governing equations.

Both single and double network approaches assume the medium is homogeneous within the REV. This assumption implies that the predicted flow behavior represents an average over the REV. For small-scale problems, this averaged approach may be of limited practical use and a discrete fracture approach may be necessary.

Many discrete fracture models for flow in saturated fractured media have been developed in the past few years (e.g., Huyakorn et al., 1983; Shapiro and Anderson, 1983; Elsworth, 1987; and Rasmussen et al., 1987). The discrete fracture approach is similar to the dual porosity approach. Both approaches treat the flow in fractures and the rock matrix as two separated systems with the exception that the discrete fracture approach assumes that an explicit knowledge of fracture distribution in the rock formation is available. Therefore, fractures are treated as a continuum in the same sense that a porous medium is a continuum representation of the interconnecting pore space. However, the REV for the fracture continuum is much smaller than the matrix. Generally, the parallel plate analogue is used to depict the flow in the fractures. The flow regime in the host rock is represented by the classic equations for flow in porous media. Since flow in the fracture and porous matrix may interact, these two flow regimes are not independent. Interaction is then entered through the coupling of the two equations, (2.7.2) and (2.7.3). However, the parameters in equation (2.7.2) represent hydrologic properties of individual fractures instead of averages over many fractures in the REV. An additional equation is then used to relate q to the heads in both the rock matrix and the fracture. In order to apply this discrete fracture approach to a field problem, the site has to be discretized into many rock matrix zones and fracture zones which are represented by either (2.7.2) or (2.7.3). As the number of zones increases, the number of equations (2.7.2)

and (2.7.3) increases accordingly. Solving such a large set of differential equations becomes a formidable task. This is one of the major drawbacks of the discrete fracture approach. However, if the flow in the rock matrix is steady, one may focus on the flow in the fracture system only. In this case, only the equation for the fracture network has to be solved. This may be an alternative to the double network discrete fracture approach.

2.7.2 Flow in Unsaturated Fractured Rocks. As mentioned previously, many flow and transport models based on the single or double network continuum approach and the discrete fracture approach have been developed for saturated fractured rocks in the past few years. However, models for flow and transport through unsaturated fractured rocks are rare. Existing models are based on the single continuum or discrete fracture conceptualization. No double network or dual porosity model has been developed. Available discrete fracture models for unsaturated fractured rocks generally use the single network approach without considering the interaction between the fracture and the rock matrix or assume some simplified flow system. This is mainly attributed to the inherent difficulty in the discrete fracture approach as discussed above, complexity of unsaturated flow, and difficulties in determining unsaturated hydraulic properties in fractured rocks. The complexity stems from the fact that unsaturated flow systems are generally nonlinear. The nonlinearity of the systems becomes even more severe due to the presence of the fractures, and high contrast in hydraulic conductivity between rock matrix and fractures.

An example of the application of this type of model is the work by Wang and Narasimhan (1985). They used the single heterogeneous continuum approach to simulate flow in a hypothetical, unsaturated fractured rock. A formula for calculating fracture conductivity under partially saturated conditions was developed. Saturated permeability of a fracture is assumed to be described by a generalized cubic law. Under partially saturated conditions, the effects of distortion of flow

paths by the air phase within a fracture plane were taken into account by a phase-separation constriction factor in the cubic law. The reduction of flow area in the plane was considered by summing the aperture distribution function to a saturation cutoff aperture, which is inversely proportional to the pressure head. Based on the theory and aperture distribution within fractures, they generated the fracture hydraulic conductivity-saturation, and saturation-suction curves for the densely welded tuff of the Topopah Spring Member at Yucca Mountain, southern Nevada. Moisture retention curves were measured from core samples. Using the relative permeability formula developed by van Genuchten (1980), and the retention curves, unsaturated hydraulic conductivity curves were estimated. These characteristic curves of fractures and porous matrix were then used to simulate the desaturation of a small fracture tuff column with discrete vertical and horizontal fractures with the aid of a computer model, TRUST.

The results of their study showed that the early transient changes from fully saturated conditions to partially saturated conditions were sensitive to fracture properties. However, the quasi-steady changes of the fluid flow of a partially saturated, fractured, porous system could be approximately simulated without taking the fractures into account. Peters et al. (1986), and Wang and Narasimhan (1985) derived the effective permeability of a partially saturated, fractured-porous medium and showed that the effective hydraulic conductivity was the sum of the fracture and matrix permeabilities weighted by the cross-sectional areas of the flow channels. They applied this effective continuum approximation to vertical infiltration problems.

Huang and Evans (1985) proposed a discrete fracture model to simulate flow and transport processes in three-dimensional fractured media. The model was developed to provide estimates of global hydraulic conductivity within a rock mass for specified distributions of fracture orientations, apertures, and densities. The model was also designed to calculate solute travel times and breakthrough curves.

However, the model assumed steady, saturated flow conditions, and used a piston flow approximation for simulating mass transport. The model later was extended with some simplified assumptions by Rasmussen (1987) for applications to variably-saturated fractured media. This was accomplished by defining a characteristic curve which related the total head within the fracture to a critical aperture using capillary theory. Also, an integrated air/water flow formulation was developed to explain hysteretic effects within the fracture rock network as the fluid potential changed. Finally, the ability to account for matrix diffusion of solutes into the walls of the fractures was added.

Neither the continuum nor the discrete fracture unsaturated flow models have been verified with either laboratory or field experiments. However, there is research in progress (e.g. at the University of Arizona) to characterize unsaturated flow in natural fractured rocks at laboratory scales. The results of this study may provide a means to verify the conceptual models discussed above. Other conceptual models with stochastic approaches (Yeh et al., 1985 a, b, and c) should be developed to improve our predictive capability related to flow through unsaturated fractured rocks.

3.0 GROUNDWATER TRAVEL TIMES AND PATHS

One of the NRC performance objectives for High Level Waste Repositories, commonly referred to as the "groundwater travel time (GWTT) objective," is stated in 10 CFR 60.113 (a)(2) as:

> "The geologic repository shall be located so that pre-waste-emplacement groundwater travel time along the fastest path of likely radionuclide travel from the disturbed zone to the accessible environment shall be at least 1,000 years or such other time as may be approved or specified by the Commission."

The definition of groundwater travel times and paths is not immune from the scale problems discussed previously. Generally speaking, groundwater travel path is known as the path along which groundwater travels. Consequently, groundwater travel time is defined as the time required for groundwater to travel along this path from one location to another. Mathematically, it is defined by

$$t = \int_0^x \frac{ds}{v} \tag{3.1}$$

where t is the groundwater travel time, x is the distance of the path which groundwater travels between the two locations, and v is the velocity of groundwater.

This definition seems to be quite clear, and, in fact, it is widely used by groundwater hydrologists. However, there are problems associated with this definition. First of all, what volume does the groundwater in the definition represent? Does it represent a cubic kilometer of groundwater, a cubic centimeter of groundwater, or maybe a molecule of the groundwater?

The need to define the volume of groundwater arises from the way the

groundwater velocity, v in equation (3.1), is determined in groundwater hydrology. As discussed in section 2.2, the continuum approach is the foundation of groundwater hydrology. That means we are not interested in, and in fact, are not able to determine how a volume of water smaller than a pore moves through intricately interconnected pore channels. Thus, the velocity of groundwater is defined over an REV which is much larger than many pores. If one can clearly define the size of an REV, the ambiguity in groundwater travel time and path may be partially resolved. However, the size of an REV may vary with the scale of heterogeneity which in turn depends on the scale of the problem that we deal with. The size of an REV may also depend on the scale of the hydrologic test we conduct to determine aquifer properties. Even if we could define an acceptable size of the REV, we may not be able to determine the exact manner in which a radionuclide travels, because the REV concept ignores the velocity variations smaller than the size of the REV. The velocity variation will cause some fluid or tracer particles to arrive earlier than the arrival time predicted from the average velocity for the REV. If we assume that the molecular diffusion is negligible, we may be able to define the REV to be several times larger than a molecule. If this is the case, then the groundwater travel time can be determined provided that the knowledge of the intricate pore channels is available. The question now is: how can one delineate the complex pore channels in a geologic formation over an area of 100 km^2? This approach is obviously impossible, and we are forced to characterize hydrogeologic properties at some scale which is much larger than the pore scale. However, the effects of the subscale velocity variations become more important as the size of the REV increases.

Based on the above discussion, pre-waste-emplacement groundwater travel times and paths are not clearly defined concepts. "The fastest path" described in 10 CFR 60.113 will vary with one's definition of scale. Therefore, the travel time criteria will be subject to interpretation and will be difficult to enforce. For

regulatory purposes, defining the occurrence of a threshold mass flux over a specified area of the accessible environment seems to be more appropriate. This is due to the fact that a concentration level reflects the total mass resulting from many different scale transport phenomena over a certain volume. Thus, the loophole in 10 CFR 60.113 can be eliminated. As a matter of fact, the fastest arrival of a certain concentration level at the accessible environment can be easily determined by application of the dispersion concept. The use of a cumulative concentration threshold is at the heart of the EPA criteria to evaluate the performance of a repository.

The NRC groundwater travel time criteria are specifically designed to pertain to pre-waste emplacement groundwater conditions. According to these criteria, the scale at which we want to delineate a flow path and characterize the hydraulic parameters appears to be arbitrary, but it is certainly less than 5 km. Whatever the scale chosen, it is essential to use consistent scales throughout the determination of the hydrogeologic parameters in the groundwater travel time equation. For example, it would not be appropriate to have a conceptual model in which the fastest path is along a sequence of voids in sandstone identified in thin sections and where the hydraulic conductivity is obtained from aquifer pumping tests which fully penetrate the sandstone. For practical purposes, the scale at which field measurements are made will limit the scale of the path that can be considered in the NRC travel time analysis. It does not seem reasonable to expect field investigations to result in characterization of single fractures or pore sequences as paths of likely radionuclide transport, at least over distance of 5 km. Although the volume of aquifer represented by a measurement is not known precisely, in most cases, the field measurement scale would seem to be on the order of meters or tens of meters. Therefore, paths of likely radionuclide transport will be one or more readily identifiable zones, such as layers within formations, major fault zones, or perhaps

entire formations. Stochastic methods would account for heterogeneity and travel time uncertainty within these paths.

3.1 Sources of Uncertainty in Predicting Groundwater Travel Times and Paths.

Regardless of the problems with the definition of groundwater travel time, we will assume that the groundwater travel time and path are defined for a specific size of an REV. We now will proceed to briefly discuss the sources of the uncertainty in predicting groundwater travel time and path. More in-depth discussion on this subject can be found in the paper by Bonano and Cranwell (1988).

To predict groundwater travel times and paths in geologic media, we first have to construct a conceptual model. The model generally simplifies the complex flow and transport processes in geologic media so that it can be represented with a tractable mathematical model. For example, flow through porous media is conceptualized as a continuum by the concept of the REV so that differential calculus applies. Continuum, discrete fracture, and dual porosity models are conceptual models which simplify the complex flow system in fractured rocks. Once the conceptual model has been formulated, it is then translated into mathematical expressions, usually partial differential equations with associated boundary and initial conditions. If the parameter values in the governing equations are well defined, analytical and numerical methods can then be employed to solve these equations for the flow system subject to any input stress. Once the flow behavior is determined, the travel time of groundwater can thus be calculated at a pre-determined scale of interest.

There is no uncertainty in groundwater travel times and paths themselves, but uncertainty in predicting them. If one uses the classic approach as outlined above to predict groundwater travel times and paths, it is evident that sources of uncertainties are attributed mainly to: (a) uncertainties in conceptualizing natural

processes, (b) uncertainties in mathematical models, and (c) uncertainties in data required by the mathematical model.

3.1.1. Uncertainty in Conceptualization. To describe groundwater flow in geologic media, we often rely on Darcy's law and the continuity equation. The law and the equation, as discussed earlier, are based on the concept of REV which is much larger than many pores. Thus, the law and equation are not strictly valid for groundwater flow through individual channels which are much smaller than the volume of an REV. Certainly, applying the REV concept for flow through individual pore channels will cause uncertainties in prediction. As an example, a heterogeneous aquifer can be conceptualized as effectively homogeneous by averaging the heterogeneities. As discussed in the previous section, the head determined from an equivalent homogeneous aquifer does not match the head from true heterogeneous one, unless a proper averaging procedure is used. Unquestionably, errors in conceptualization add uncertainties in prediction. Generally speaking, the major uncertainty in conceptualization lies in the area of flow through fractured rocks, especially flow through unsaturated fractured rocks. Although several conceptual models (such as discrete fracture, dual porosity, stochastic continuum approaches) have been proposed to conceptualize flow through fractured rocks, none of these have been verified with field experiments. Difficulties in monitoring flow behavior or in determining the fracture hydraulic properties of unsaturated, fractured rocks, even in the laboratory, further cast doubt on the validity of current conceptual models for flow through unsaturated, fractured rocks. Since there is no way to assess the validity of conceptual models at present, the uncertainty due to errors in conceptualization is entirely unknown.

3.1.2. Uncertainty in Mathematical Models. If one can somehow obtain a workable conceptual model or assume the uncertainty in the conceptualization of a natural flow process is negligible, the next source of uncertainty arises from the

formulation of mathematical equations based on the conceptual models and the solution of the mathematical model.

Uncertainties associated with the formulation of a mathematical model are generally attributed to mathematical simplifications during its formulation. For instance, neglecting the effects of fluid density gradients and changes in hydraulic conductivity due to deformation of porous media, and mixing expressions for moving and fixed coordinate systems (see Appendix B) causes uncertainties in the governing equation for three-dimensional groundwater flow. Similarly, the two-dimensional depth-averaged groundwater flow equation neglects the contribution from the product of hydraulic conductivity and head variations in the vertical direction (i.e., when horizontal flow is assumed). Stochastic models, such as those based on the first order analysis, (Gelhar and Axness, 1983, Dagan, 1987, Neuman, 1987, etc.) ignore higher order terms. All of these simplifications lead to uncertainties in mathematical models.

After a mathematical model is formulated, analytical methods often give exact solutions to a problem. However, the solutions are limited to simplified situations such as homogeneous aquifers of infinite lateral extent. More complex problems have to rely on numerical methods. No numerical method is completely error-free. Two basic types of errors which are inherent in a numerical computation are truncation and roundoff errors.

Finite difference, finite element, integrated finite difference, and boundary element methods generally are the numerical methods for solving groundwater flow and transport equations. They approximate the governing partial differential equations by a discrete formula; the solutions are thus subject to truncation errors. For instance, the finite difference groundwater flow model uses a Taylor series expansion to obtain the approximation of the head gradient:

$$\frac{dh}{dx} = \frac{h_{i+1} - h_i}{\Delta x} + O(\Delta x) \tag{3.2}$$

The term $O(\Delta x)$ represents the remaining higher order terms which are omitted in the formulation of the finite difference analog of the gradient. This type of error is called truncation error, since it is produced by truncating an infinite mathematical series. Numerical dispersion in the solution of a convection-dispersion equation is a typical result of the truncation error. In addition, a numerical analysis has to be conducted by a computational device such as a computer. The accuracy of the solution produced by the computational device depends on the number of significant figures available in the device. This type of error is called round-off error. These two sources of error add some uncertainties to the prediction of groundwater travel times and paths. Although these errors always exist, they can be minimized if a proper procedure such as small size grids, and small time steps is used.

The major problem associated with numerical models may lie in solving the governing equation of flow through unsaturated porous media or fractured rocks. The governing equation is generally nonlinear, i.e., the hydraulic properties in the governing equation, such as hydraulic conductivity, are functions of the dependent variable, so that the hydraulic property is unknown before the equation is solved. For nonlinear problems, an iterative scheme always must be used. There is no guarantee that the iterative scheme will give an exact solution or any solution at all. Furthermore, the nonlinearity of the equation becomes even more severe if the medium is heterogeneous, coarse textured, or fractured. Solutions often diverge, and in these cases no solution can be obtained (Freeze, 1971). If numerical solutions are obtained for complex problems, generally no exact analytical solution is available for assessing the accuracy of the solution. Thus, the uncertainty in mathematical modeling of flow in unsaturated porous and fractured materials is still a topic of

research.

3.1.3 Uncertainties in Data Required by Mathematical Models. Before mathematical models can be solved by either analytical or numerical methods, information about parameters in the equations, and boundary and initial conditions (for transient situations) must be specified. These parameters and conditions are generally tailored to physical or chemical properties of a specific site or geologic formation. The lack of a complete data base to characterize the properties of the site certainly introduces uncertainties in the solution of the mathematical models. This type of uncertainty is mainly a result of field heterogeneity.

In order to use any mathematical models to predict groundwater flow, values of the parameters and boundary conditions in the models have to be specified. These parameters include hydraulic conductivity, or transmissivity, storage coefficient, porosity, etc. If the aquifer is conceptualized as homogeneous, these parameter values should be easily obtained from a single hydraulic test. The aquifer can then be fully characterized. However, in reality, there is heterogeneity in aquifer hydrologic properties at all scales. For any field problem, virtually an unobtainable amount of data is required to completely specify the spatial distribution of these parameters everywhere in the aquifer. Only a limited amount of data will actually be available from a real site investigation. Furthermore, boundary and initial conditions are generally not clearly defined in most fields. For instance, recharge rate to groundwater reservoirs is generally difficult to measure, especially its temporal and spatial variability. Locations and types of boundaries are seldom known in field situations. Predictions based on few data values are thus characterized by uncertainty.

Incomplete information on the spatial distribution of the aquifer parameters also causes inconsistencies in the hydrologic data collected as inputs to mathematical models. The inconsistency in data is directly related to the scale problem discussed

previously. Hydraulic tests for determining hydraulic parameters of the aquifer material generally are aquifer tests, slug tests, or laboratory tests of core samples. Each of these tests determines the hydraulic properties of aquifer materials of different sizes. For example, the hydraulic properties determined from an aquifer test generally represents the effective properties of the aquifer material within the influence of the test. The zone of influence depends on the time scale of the aquifer test. Consequently, the hydraulic parameter values vary with the time and spatial scale of the test. On the other hand, the hydraulic parameter values obtained from a slug test may represent the properties of the aquifer material adjacent to the borehole. A laboratory test gives the value of the parameter for the size of the core sample. Thus, the inconsistent data set results in uncertainties in predictions.

Available field data for modeling groundwater flow are collected with various types of tests, and represent the parameter values of different sizes of aquifer material. It is inconsistent to use data collected from a test at one scale as input to a mathematical model at another scale to determine the groundwater flow. Furthermore, the size of grid used in the numerical model for a large basin generally exceeds by orders of magnitude the scale of hydraulic tests. Since aquifers are inherently heterogeneous, the parameter obtained from the hydraulic test may not be the representative one for the mathematical model. Such inconsistencies further augment the uncertainty in groundwater travel time and path predictions.

There is another problem regarding the use of data obtained from hydraulic tests as input to numerical models. Generally, the parameter values obtained from hydraulic tests represent effective properties of the area of influence. However, the effective properties may depend on the flow regime as well. For example, all hydraulic tests in boreholes involve radial flows. It is not known whether effective parameters estimated from radial flow tests in a heterogeneous aquifer are representative of parameter values for flow other than radial flow. It may not be

appropriate to input effective mean parameter values derived from radial flow into a numerical model to predict groundwater travel times and paths where uniform flow occurs.

Moreover, field heterogeneity introduces uncertainties in aquifer test data (Butler, 1986; Javandel and Witherspoon, 1969). The aquifer test is the standard method used by hydrogeologists to evaluate the transmissive and storage properties of subsurface material for groundwater resources evaluations. Driscoll (1986) and many others detailed the procedures for carrying out a successful test. Generally, the procedure is rather straightforward; a well is pumped, and water level responses are measured over space and time. The response data are then analyzed using methods based on analytical solutions to the problem of flow to a pumped well. The results from this analysis give us the transmissive and storage properties of the aquifer. The most common analytical solution used is the so-called Theis solution for confined-radial flow.

The Theis solution is derived for flow to a well in an extremely idealized aquifer. It is a mathematical model in which there are many simplifying assumptions, the major of which is the assumption that the aquifer is homogeneous. In fact, as pointed out earlier, aquifers are heterogeneous at all scales. Applying the Theis solution to a heterogeneous aquifer may, however, be justified if one replaces the heterogeneous aquifer by an equivalent homogeneous one. This substitution implies that parameters such as transmissivity and storage coefficient, obtained from the classical analysis of the aquifer test data should, therefore, represent the average values over the flow regime. As an example, based on numerical simulations of flow to a pumped well in a stratified aquifer, Javandel and Witherspoon (1969) concluded that the drawdown observed at any location in the aquifer virtually converges to the Theis solution at large times. This implies that the hydraulic conductivity estimated from the Theis solution corresponds to the arithmetic mean of the hydraulic

conductivity values of individual layers. In a perfectly stratified, confined aquifer, the drawdowns under steady state flow, at all the depths at a given radial distance must be the same because of constant head boundary conditions imposed at the well and at large distances. This analysis is identical to the soil column analysis where flow is parallel to the layering (section 2.4.1). Thus, it is clear that the effective hydraulic conductivity is the arithmetic mean. The results of their study are, however, not realistic because aquifers are generally not perfectly stratified.

Recent numerical experiments by Butler (1986) considered transmissivity as a stochastic field. In contrast to the finding of Javandel and Witherspoon (1969), Butler indicated that the geometric mean is a good approximation of the effective transmissivity obtained from aquifer tests in heterogeneous aquifers, if the drawdown in a fully penetrating well at large times is used. However, most observation wells do not fully penetrate the thickness of the aquifer. The head observed in a well tapped into a small portion of a thick heterogeneous aquifer does not represent the depth-averaged head (or the ensemble averaged head, if ergodicity is assumed). In section 4.3.1 (Figures 4.15 a, b and 4.16a) we will clearly illustrate this point. Figure 4.15a and b are the head distributions in two possible heterogeneous aquifers, and the head distribution in an equivalent homogeneous aquifer is shown in Figure 4.16a. Thus, the results of these studies are not conclusive. Regardless of exact type of average the effective hydraulic conductivity or transmissivity represents, the Theis solution based on these averaged aquifer properties predicts the drawdown in the equivalent homogeneous aquifer. Certainly, this drawdown does not correspond to the actual drawdown in the real aquifer which is heterogeneous, even if the head is a depth-averaged one. The drawdown determined from the Theis solution simply represents the average (ensemble average) of all possible drawdowns at a given radial distance in a plane. This concept is well illustrated in Figure 3.1 where dashed lines represent the actual irregular drawdown as may be expected in a heterogeneous

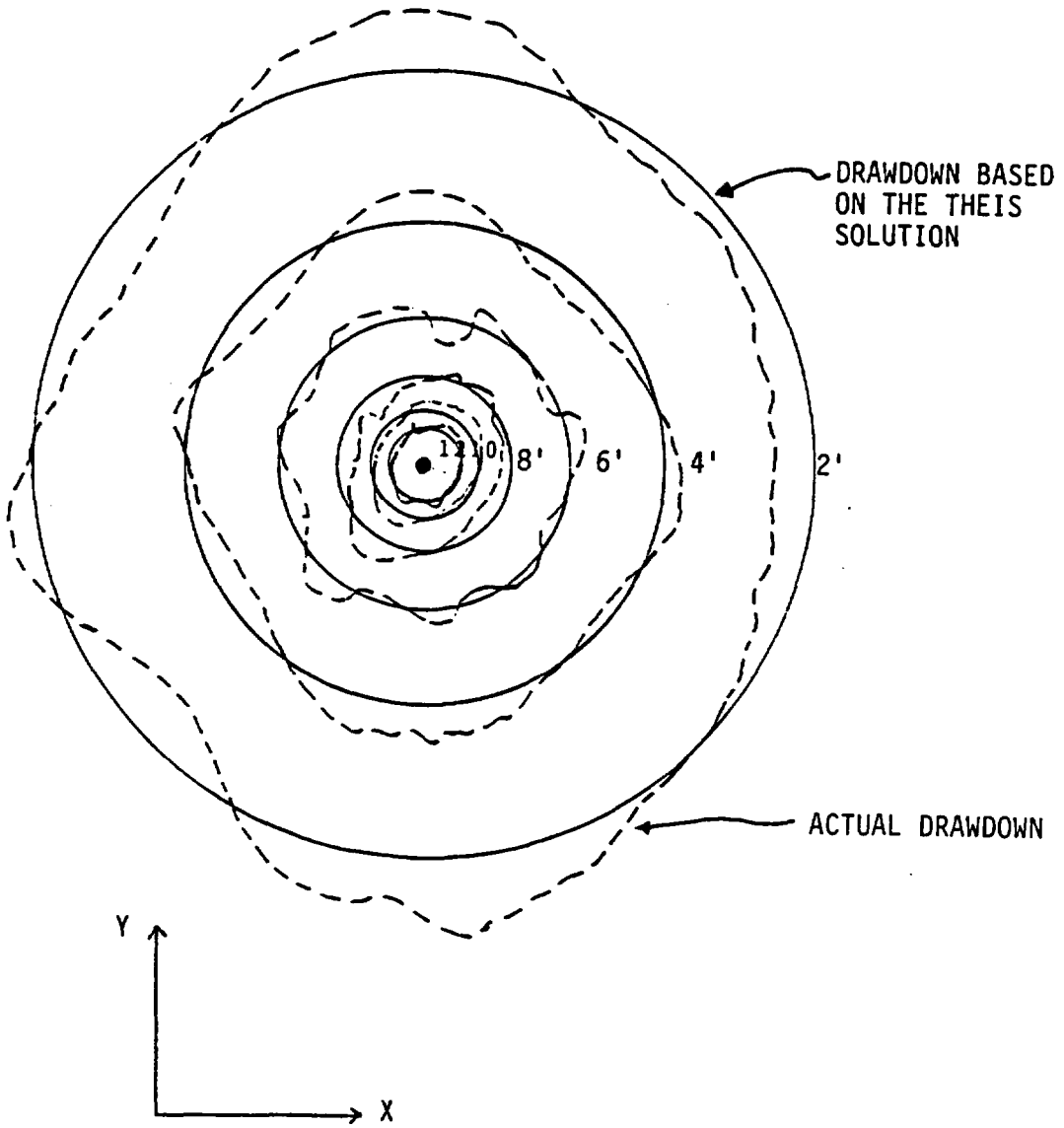


Figure 3.1. Plan view of the actual drawdown in a heterogeneous aquifer (dashed line) and the drawdown predicted from the Theis solution for an equivalent homogeneous aquifer (solid line). Dot shows the location of the pumping well.

aquifer, and solid lines represent the average drawdown. If one recognizes these limitations, then the application of the Theis solution to heterogeneous aquifers is appropriate in theory.

Limitations of the equivalent homogeneous aquifer concept are generally not well recognized. As a consequence, most procedures to analyze the aquifer test data are inconsistent with the theory. Again, if a heterogeneous aquifer is visualized as an equivalent homogeneous one, the drawdown predicted by the Theis solution should represent some kind of spatially averaged piezometric surface or drawdown at a radial distance. On the other hand, if one applies the Theis method to determine transmissivity and storage coefficient values of a heterogeneous aquifer, one has already replaced the heterogeneous aquifer by an equivalent homogeneous one. Thus, to be theoretically consistent, the spatially averaged drawdown from a very large number of observation wells at a given radial distance should be used to determine the aquifer properties. These properties should then represent the true effective properties of the equivalent homogeneous aquifer. However, there are only a limited amount of observation wells available in most field tests. As a matter of fact, many of the tests may have only one observation well. The drawdown observed in a single well does not necessarily represent the average drawdown at a certain radial distance, unless the aquifer has an uncorrelated random or statistically independent hydraulic conductivity field (for the definitions of the statistic terms, see section 4 or Appendix A). In these two cases, one may assume that the vertically averaged head value may be equivalent to the horizontally averaged one. Many recent field data have, however, shown that the hydraulic conductivity data in aquifers exhibit statistical anisotropy (layering). The transmissivity and storage coefficient values determined by the Theis solution with the drawdown data at a single well are thus not the effective ones. Therefore, a logical question one may ask is: What do the estimated transmissivity and storage coefficient values from the well hydrograph at a

single well represent? How much do the estimated values deviate from the true values? Are they reliable parameter values for determining the groundwater travel time and path?

Inconsistencies in interpreting aquifer test data have long been recognized. However, hydrogeologists have ignored these inconsistencies and still perform the analysis with the hydrograph from a single well. This is due to the fact that the estimated transmissivity and storage coefficient values, even though they may be erroneous, generally produce reasonably accurate piezometric surfaces or drawdowns. This surprising result may be attributed to the fact that the variation in head is relatively insensitive to the variation in T values. The groundwater system as far as head and T are concerned, is a filter. The error in T estimates is always damped out, and the calculated head using incorrect T values is often still in close agreement with the observed one. This filtering effect in groundwater systems has been clearly manifested in the results of stochastic analyses of groundwater flow through heterogeneous aquifers (Bakr et al. 1978; and Mizell et al. 1982). On the other hand, in an inverse problem (such as estimating T and S values using head data from aquifer tests), a tiny error in head or drawdown values may result in a significant departure of T values from the true one. Many hydrologists have experienced this type of problem. For instance, significantly different T estimates can be obtained by several groundwater hydrology experts using the same well hydrograph and the same procedures. Regardless of the significant differences in T values, the drawdown predicted with these T values is surprisingly close to the true drawdown value due to the damping effect. Therefore, one may draw the conclusion that the standard aquifer test analysis using one well may be adequate for the purpose of evaluating the well yield or drawdown of water levels. However, note that the primary interest in this case is the drawdown or head.

In the case of determining contaminant movement or groundwater travel time

and path in a groundwater system, the major controlling factor is not the hydraulic head but the hydraulic conductivity or transmissivity value, and the hydraulic gradient. Velocity of groundwater flow is determined by Darcy's law and is the product of conductivity, gradient and the reciprocal of the porosity. The variation in porosity and gradient are relatively small compared to the variation in conductivity. Therefore, the accuracy of predicted groundwater velocity may depend heavily on correct hydraulic conductivity or transmissivity values. An accurate prediction of groundwater velocity thus dictates correct estimates of transmissivity values from the standard aquifer test procedure.

Other sources of error are those due to instrument or human errors in estimating hydraulic parameters, even for a homogeneous aquifer. These types of errors could enter the modeling process and add uncertainty to the prediction of groundwater travel times and paths.

Of course, there are many other sources of errors in the prediction of groundwater travel times and paths which have not been discussed in this review. Generally speaking, sources of uncertainty in predicting groundwater travel time and path include: (a) uncertainties in conceptualization, (b) uncertainties in mathematical models, and (c) lack of a complete data base to characterize the variability of aquifer materials. For saturated porous media, uncertainties due to the errors in conceptualization and mathematical models are relatively small at the laboratory scale, or at least, it is believed their importance is relatively minor. This conclusion is supported by the fact that many small-scale laboratory experiments in the past have demonstrated the validity of mathematical models. Therefore, the major difficulty in the prediction of groundwater travel time in saturated porous media seems to lie in extrapolating these models to large-scale field problems where hydraulic properties of the aquifer materials vary spatially.

To predict groundwater travel times and paths in unsaturated, fractured

rocks, all of the sources of errors discussed above may play very important roles. This postulation stems from the fact that there is no satisfactory technology for measuring hydraulic properties for this type of material, because of the complexity of unsaturated flow and the scale of fractures. The lack of a demonstrated effective measurement technology hinders the development a workable conceptual model for flow in these complex types of media. Although there may have been some conceptual models (such as Wang and Narasimhan, 1985) developed in the past, none of them have been verified even with laboratory experiments, because of the difficulties in the development of a proper monitoring tool. If we can not verify the conceptual model in a small-scale laboratory experiment, we can not make predictions in field situations where the hydraulic properties of fractures and rock matrix are highly variable. In view of these difficulties, there are large uncertainties in predicting groundwater travel times and paths in unsaturated and fractured rocks.

Finally, "the groundwater travel time" and "the fastest path" as described in CFR 60.113 are not clearly defined concepts. Even if all the sources of uncertainties in predicting groundwater travel and path discussed above are identified and resolved, the GWTT criterion would vary with one's definition of scale; it will be subject to interpretation and will be difficult to enforce. As suggested in this report, defining the occurrence of a threshold mass flux over a specified area of the accessible environment is more appropiate for regulatory purposes. Unless this problem is clarified, uncertainty in groundwater travel time will always exist.

4.0 APPROACHES TO SPATIAL VARIABILITY

As discussed in section 3.0, spatial variabilities (heterogeneities) of geologic materials at various scales present difficulties for us to extrapolate our mathematical models to large-scale field problems. Therefore, spatial variability is the major source of the uncertainty in predicting groundwater travel times and paths. If the field heterogeneity problem can be resolved, the uncertainty in groundwater travel time and path prediction can be significantly reduced.

One approach to determine groundwater travel times and paths in a heterogeneous groundwater basin is to use the concept of REV. If one can define an REV that is large enough so that the entire aquifer within the accessible environment can be visualized as homogeneous, the mean groundwater travel time and path can then be determined through a deterministic simulation. However, this groundwater travel time represents only the average arrival time of groundwater particles and does not depict arrival times of groundwater particles along either the fastest or the slowest path, owing to variations in hydrologic properties at scales smaller than the size of REV.

To include the subscale variability, one must incorporate the dispersion process as discussed previously. However, this approach is not immune from scale problems. One of the problems is how to define an REV for effective (mean) hydrologic properties of the aquifer. More precisely, how can the effective hydraulic conductivity and dispersivity values be determined from hydrologic tests performed at a particular scale? Although a well controlled, large-scale hydraulic test (aquifer test) seems to be appropriate for this purpose (Williams, 1988), we do encounter problems. We must determine how to design such tests and how to analyze the data (see

Section 3.1.3, and Williams, 1985). Dispersivity values must also be determined. While a large-scale tracer test is desirable, the time, physical, and economic constraints of such a test make this approach impossible.

An alternative is to conduct many small-scale hydrologic tests to delineate spatial distributions of hydrologic properties at a specific scale of our interest (i.e., the size of our sample). Knowing the detailed spatial distributions of the properties, a deterministic model can adequately simulate a groundwater travel time and path distribution for fluid particles leaving the disturbed zone of a repository under pre-waste emplacement under given conditions. Such a simulated groundwater travel time distribution contains information about travel times pertaining to fast and slow paths of groundwater movement at the scale of our interest. However, the scale of the field problem, for example, the accessible environment (5 km), is generally much larger than the scale of our sampling device (i.e., an observation well is consider as a point compared with the accessible environment). To predict a groundwater travel time distribution from data collected at the scale of our instruments would require enormous manpower, time, and expense to collect information for such a degree of spatial resolution. Therefore, this deterministic approach is considered impractical in terms of the amount of data required to specify the actual complex three-dimensional heterogeneity. Thus, one has no choice but to use a limited amount of data to determine the groundwater travel time and path. Uncertainties always exist in the prediction, and an assessment of the uncertainties in predictions is necessary. However, the deterministic approach provides only one possible outcome from a given data set. It does not produce many possible groundwater travel times and paths resulting from many possible hydrologic properties at unsampled locations, and thus one can not evaluate the precision of the predictions.

Recent advances in stochastic groundwater hydrology and geostatistics have shed light on resolving the uncertainty problems due to spatial variability. In the

following sections, we will discuss the necessity of characterizing heterogeneity in terms of statistics, and will discuss methods to quantify the uncertainties in our predictions of hydrologic responses of groundwater systems due to field heterogeneity.

4.1 Stochastic Representation of Hydrologic Properties

Large-scale hydrologic tests to obtain the effective hydrologic properties at the scale of the accessible environment may be problematic and impractical. Accurate prediction of groundwater travel times and paths in a field-scale problem requires a large set of data obtained from small-scale tests. On the other hand, it is practically impossible to obtain such a large data set. So, a logical question to ask is: how can we obtain a meaningful or useful prediction using a limited amount of available data? Two approaches to address this question are to: (1) use effective hydrologic parameters derived from averaging the available data to predict the mean behavior of the aquifer and the deviation of the behavior from its mean, or (2) interpolate or extrapolate hydrologic parameter values measured at sample points to the locations where no measurements are available.

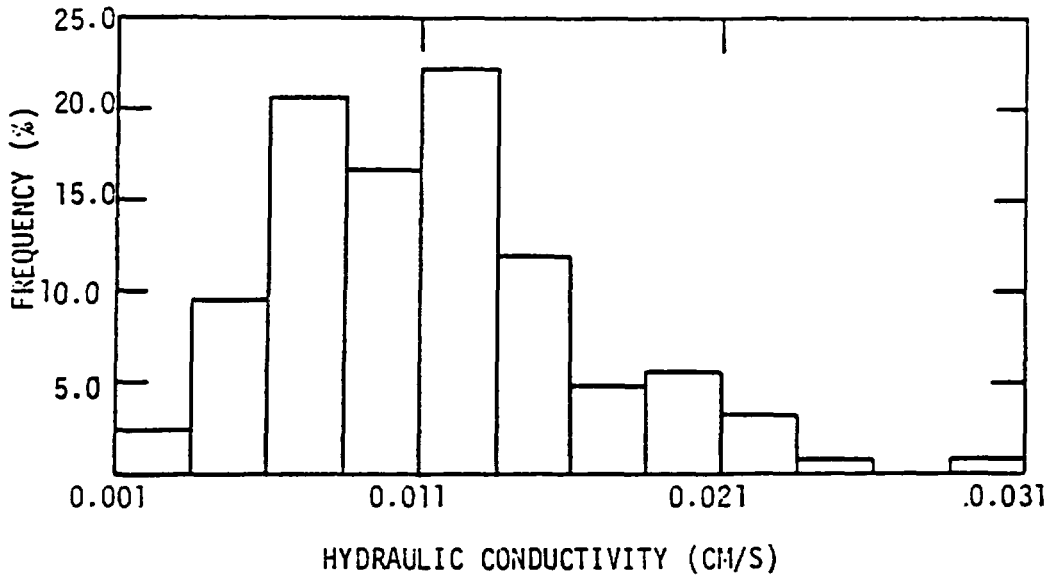
In the first approach, the effective properties are derived using theoretical formulas to combine data from small-scale tests. For example, the effective hydraulic conductivity of a layered aquifer can be determined from conductivity values of individual layers, using either harmonic or arithmetic means as discussed in Section 2.4.1. This approach is equivalent to the large-scale test approach but differs in the way that effective properties of an aquifer are derived. For instance, the large-scale test approach relies on observed responses of an aquifer and simplified equations, such as for instance, the Theis solution.

The second approach is similar to the small-scale test approach, but property values are estimated at unsampled locations by mathematical tools such as Kriging or

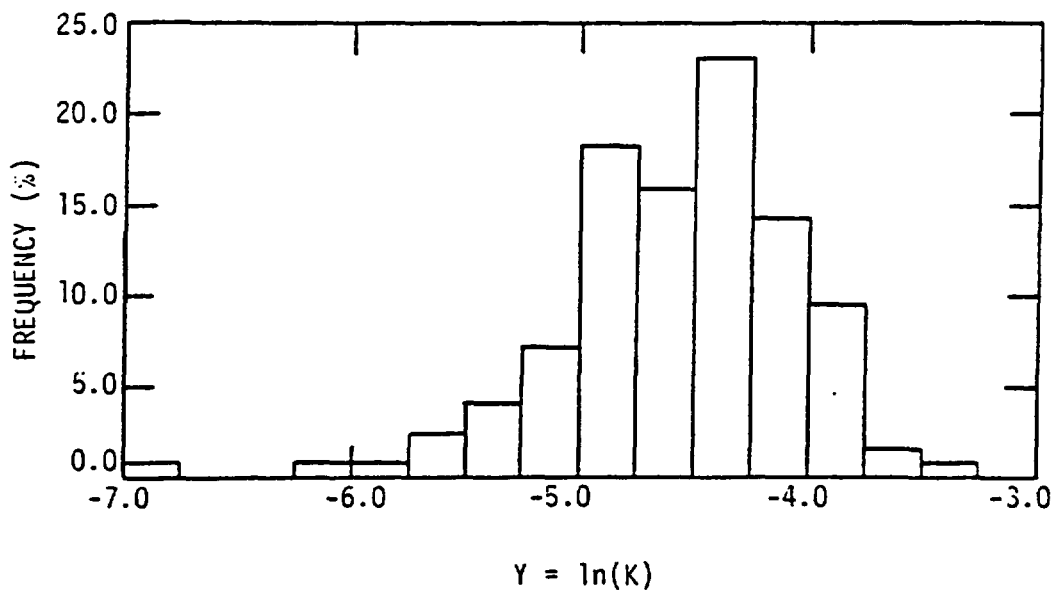
regression. However, the estimates are not exact and an evaluation of the deviation from the "true values" is required. Theories for both approaches require statistical information of the parameter values. This means that a statistical description of aquifer heterogeneity is necessary.

The statistical description of aquifer heterogeneity implies that hydraulic properties of the aquifer are viewed as random variables. Generally speaking, a random variable is a function whose values are real numbers and depend on "chance" or probability. To illustrate the application of the random variable concept to spatial variability of groundwater hydrology, let us consider the problem of estimating the hydraulic conductivity at a location where we have no experimental means to determine the hydraulic conductivity value. The value of hydraulic conductivity at this location may be guessed by examining the texture or other characteristics of drill cutting samples. Obviously, a variety of values may be assigned to the sample by different groundwater hydrologists. If we summarize all of the estimates by plotting the number of estimated values falling in different intervals, we observe a distribution (frequency distribution) of the guessed hydraulic conductivity values. As shown in Figure 4.1a, most values are clustered around some central value, and the frequency of occurrence declines away from this central point.

The random variable concept can also be interpreted in the following way. There are many different hydraulic conductivity values in a heterogeneous aquifer. If the hydraulic conductivity value at a location is unknown and we have to guess a value from all the possibilities, the chance of selecting a particular hydraulic conductivity value, K_l, may be expressed as the ratio n_l/n. n_l is the number of hydraulic conductivity values in the entire aquifer, which equal to K_l, and n is the total number of all possible hydraulic conductivity values in the aquifer. A plot of the probabilities of selecting different hydraulic conductivity values versus all the



(a)



(b)

Figure 4.1. Frequency distribution of (a) hydraulic conductivity, and (b) lnK data in the Borden aquifer (Sudicky, 1986).

possible hydraulic conductivity values is called a frequency or probability distribution of the hydraulic conductivity of the aquifer. Based on this conceptualization, the hydraulic conductivity value depends on probability or chance. Namely, it is not completely predictable: only proabilities can be associated with the possible values and hence the values are considered as realizations of a random variable. The frequency distribution determines the likelihood (or probability) that a specific hydraulic conductivity value will be found at a particular location.

Frequency distributions of most hydrologic properties of an aquifer generally are taken to be either normal or lognormal. A normal distribution is characterized by a symmetric bell shape. Lognormality implies that the distribution of the logarithms of a random variable has a normal distribution (Figure 4.1b). However, the distribution of a log-normal random variable itself is positively skewed (Figure 4.1a). Many field data have shown that the distribution of porosity data in a given aquifer is usually normal (Law, 1944 and Bennion and Griffiths, 1966), altough recent work by Hoeksema and Kitanidis (1985) suggests that the storage coefficient may be log normally distributed. Hydraulic conductivity data are usually reported to be approximately lognormal (Law, 1944; Bulness, 1946; Warren et al., 1961; Bennion and Griffiths, 1966; Ilyin, 1971; Bakr, 1976, and Freeze, 1975), as are transmissivity values (Delhomme, 1979; and Hoeksema and Kitanidis, 1985). There are exceptions however, as shown by Jensen et al., (1987). Figure 4.1 shows a skewed distribution of hydraulic conductivity values in a sandy aquifer and a more normal distribution of natural log of the hydraulic conductivity values, lnK.

Inasmuch as different aquifers are formed by different geologic processes, the distributions of hydrologic properties of different aquifers are likely to be different. To characterize the distribution one generally uses statistical moments of the random variable. The first moment refers to its mean, the second moment to the variance (the spread of the distribution) and the third moment to the skewness (a

measure of its symmetry). Figure 4.2 schematically illustrates distributions of the logarithms of hydraulic conductivity values in a sandstone and a shale unit. Although the hydraulic conductivity distribution of the two geologic materials is lognormal, the mean hydraulic conductivity value of the sandstone unit is larger than the shale unit and the variance is larger in the shale than in the sandstone.

The application of the random variable concept to hydraulic conductivity values seems to be valid only if no actual measurement of the parameter value is available. However, it is suitable for analysis of uncertainty in hydrologic property values. Even if one can determine hydrologic property values at every point in an aquifer, due to spatial variability of the property it is still appropriate to consider the hydraulic conductivity value as a random variable at the location. That is to say, the value represents only one of many possible geological materials that may have been deposited at a given point when the geological environment was created. This random variable concept can certainly be applied to other sample locations. Thus, hydraulic conductivity values of an aquifer may be considered as a collection of many random variables in space. This infinite sequence of random variables is generally referred to as a stochastic process (or a random process, random field or random function).

For example, the set of hydraulic conductivities along a transect can be considered as one possible outcome of a stochastic process. In a stochastic process the value of the quantity, say conductivity, $K(x)$, is a random variable for each location x. Namely, if conductivity is observed at locations x_1, x_2,....x_n, the $K(x_1)$ is a random variable, $K(x_2)$ another random variable, and so on out to $K(x_n)$. 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 transect depends not only on the probability distribution of the hydraulic conductivity at one location but also on those at other locations. This

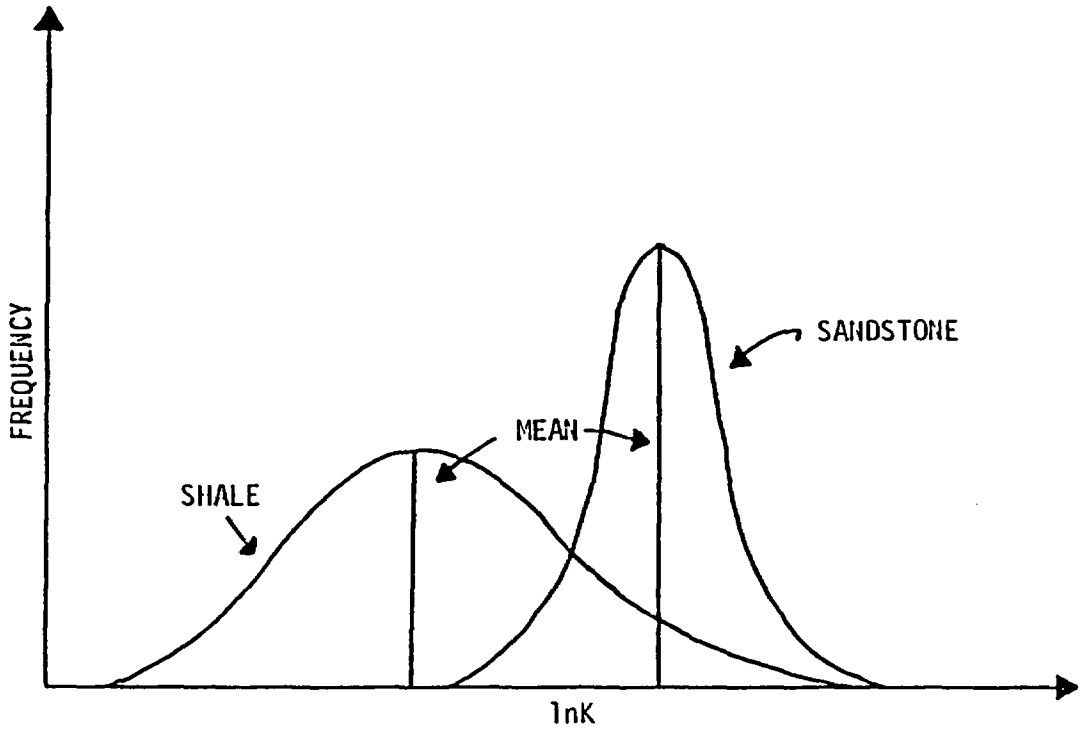


Figure 4.2. Frequency distributions of the hydraulic conductivity values of a sandstone and a shale unit.

implies that actual hydraulic conductivity values, along the transect are one possible sequence of K(x) out of all the possible sequences. In the vocabulary of stochastic processes, all these possible sequences are called an ensemble, and a realization refers to one of the possible sequences (Figure 4.3).

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. The joint distribution is completely defined only if the probabilities associated with all possible sequences of $K(x_i)$ values along the transect are known. Similar to the distribution of a single random variable, the joint distribution of random variables is also characterized by its moments. However, this joint distribution is seldom known in real-life situations because hydraulic conductivity values sampled along a transect, for instance, represent only one realization out of the ensemble of the hydraulic conductivity values along the transect. Therefore, one must usually resort to simplifying 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 (De Marsily, 1986). Since in reality one always deals with a specific geologic formation (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.

Because it is difficult to obtain all of the joint distributional information required and because in many cases important properties are assessed by moments like the mean, variance or other lower order moments, an assumption of weak or second order stationarity is often invoked. The first moment (mean) of K(x) is defined as:

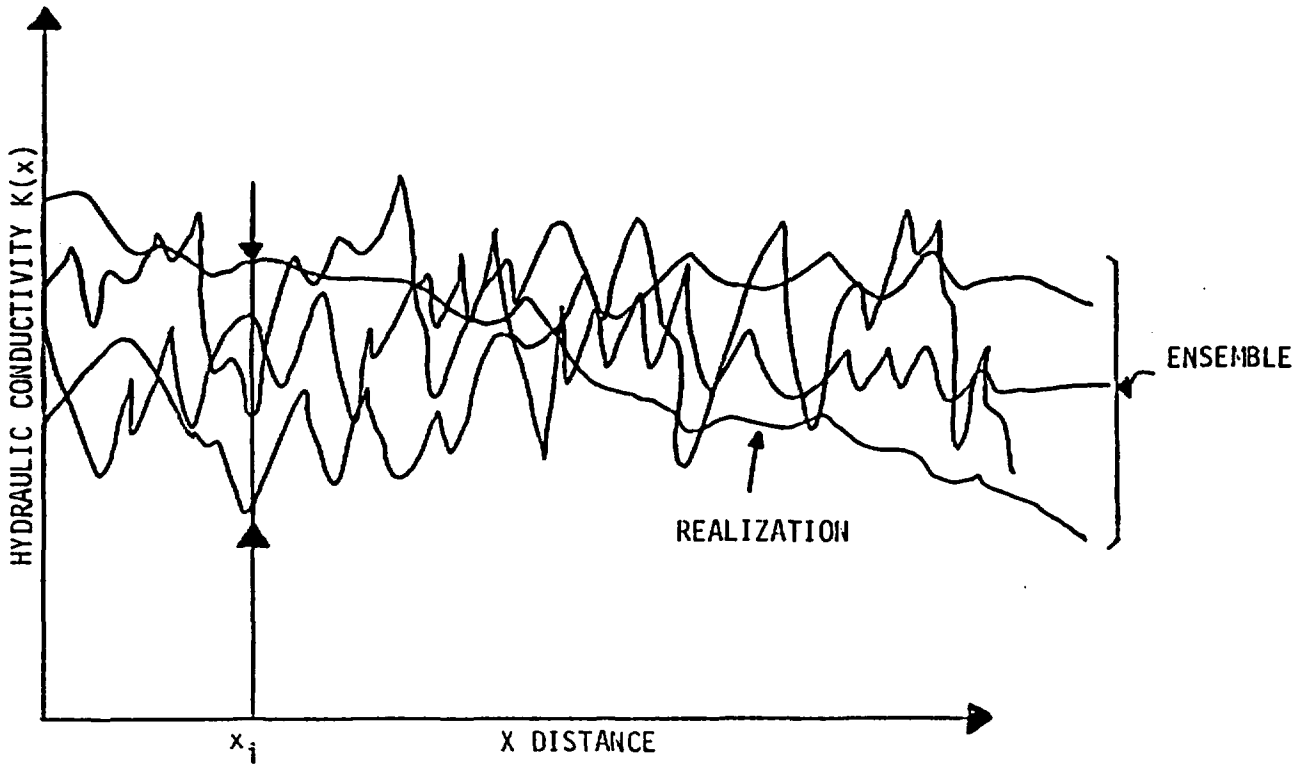


Figure 4.3. Schematic illustration of ensemble and realization concepts. Hydraulic conductivity at x_i is a random variable.

$$\mu = E[K] = \int_0^{\infty} K\ f(K)\ dK \tag{4.1.1}$$

where E[ ] stands for the expected value, and f(K) is the joint density distribution of K. This means that the expected value of a stochastic process is its probabilistic average (or ensemble average). The second moment (autocovariance or covariance function) is then defined as:

$$c(\xi)=\text{cov}\ [K(x+\xi),\ K(x)] = E[\ (K(x+\xi)-\mu)(K(x)-\mu)\ ] \tag{4.1.2}$$

The second-order stationarity assumptions are that (i) $\mu = E[K]$ is constant, and $\text{cov}[K(x+\xi),\ K(x)]$ only depends on ξ, (i.e., $c(\xi) = \text{cov}[K(x+\xi),K(x)]$) where ξ is called the separation distance. If the separation distance is set to zero, the covariance function becomes the variance, σ^2 . An autocorrelation function is simply defined as the ratio of covariance function to its variance, i.e.:

$$\rho(\xi) = \frac{c(\xi)}{\sigma^2} \tag{4.1.3}$$

Values of the autocorrelation function are always in the range between -1 and 1. The autocorrelation function represents the persistence of the value of a property in space.

To explain the idea of the autocorrelation function, we will consider two identical sine waves, w(x)=sinx, except they are separated by a distance ξ as shown in Figure 4.4a. Note that the sine waves are strictly deterministic functions. If a correlation coefficient, r, between these two waves is calculated, by regression

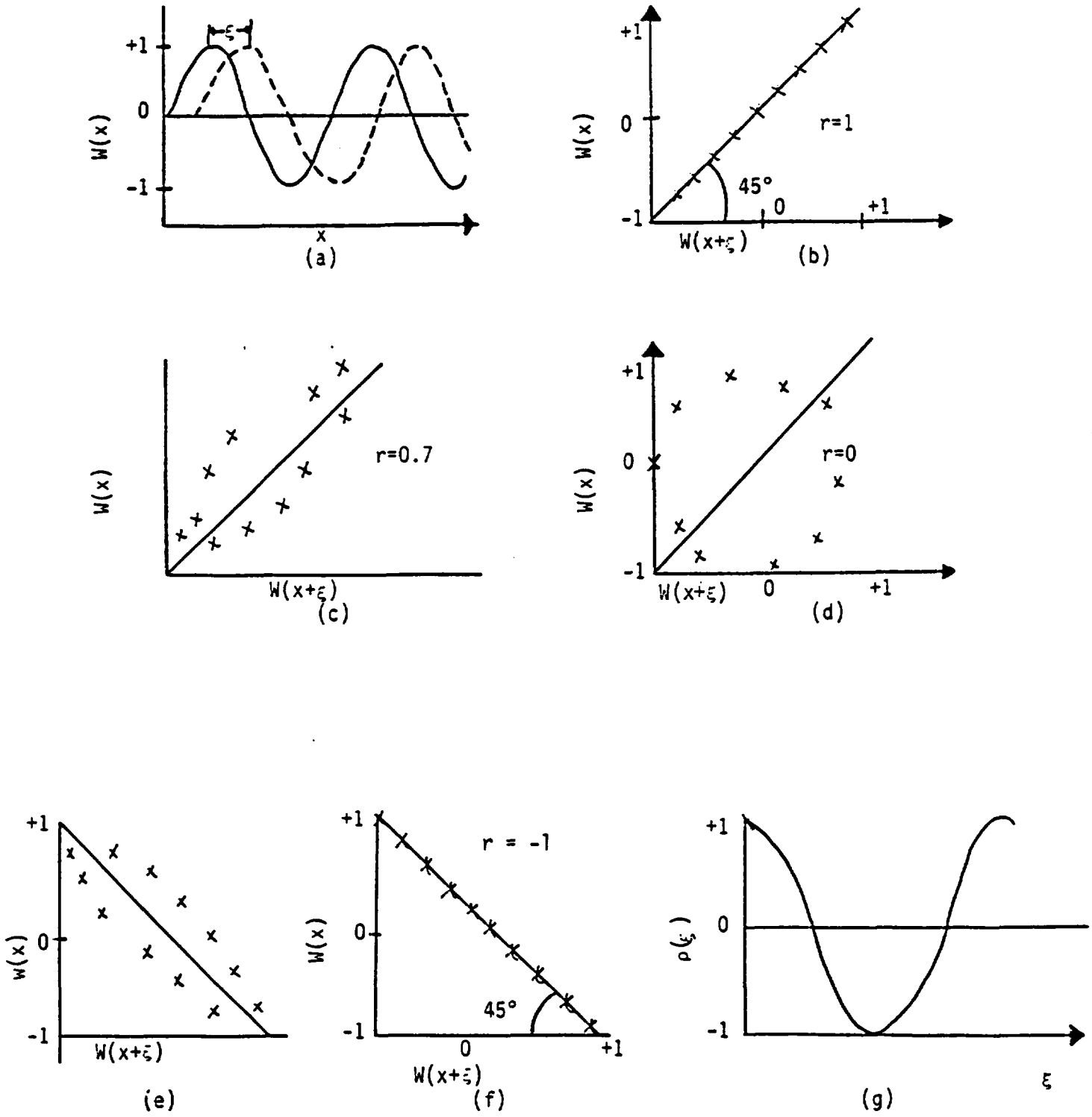


Figure 4.4. Diagrams to illustrate the concept of an autocorrelation function.

analysis, r has to be 1 if $\xi = 0$; if w(x) is plotted against $w(x+\xi)$ at $\xi = 0$, all the points will lie on a 45 degree line since they are identical (Figure 4.4b). As one of the waves is shifted by a distance $\xi \neq 0$, the plot of w(x) vs. $w(x+\xi)$ will start to scatter around the diagonal line as shown in Figure 4.4c. The correlation becomes less than unity because the values of the waves no longer correspond at every distance. As the wave moves out of phase exactly by one half of a wavelength, the scattering become even more significant and the correlation drops to zero (Figure 4.4d). This zero correlation indicates that the points of the two waves at this separation distance are completely different. Figure 4.4e shows that a further increase of the separation distance will reduce the scattering but the correlation becomes negative. As the separation distance approaches one half wavelength, i.e., the trough of one wave matches the peak of the other, and the correlation drops to -1 (Figure 4.4f). This r = -1 value implies that these two waves are identical but in an opposite manner. If one plots the r values at each separation distance vs. the separation distance, one obtains a plot of an autocorrelation function (Figure 4.4g). Therefore, the autocorrelation function is a measure of the similarity of the series at different separation distances.

Generally, the autocorrelation function of hydraulic conductivity data tends to drop rapidly as the separation distance increases. The decline of the correlation may be represented by many different autocorrelation models. The one commonly used is an exponential decay model (Bakr et al., 1978; Gutjahr et al., 1978, Gelhar et al., 1979, Yeh et al., 1985a, b, c):

$$\rho(\xi) = \exp\left[-\frac{\xi}{\lambda}\right] \tag{4.1.4}$$

where $\rho(\xi)$ is the correlation function, ξ is the separation distance, and λ is the

correlation scale. The correlation scale is a characteristic length beyond which the correlation between data is no longer considered significant. However, this definition is rather arbitrary and an integral scale is often used instead. The integral scale is defined as the area under a autocorrelation function if the area is a positive and nonzero value (Lumley and Panofsky, 1964). For the exponential model (equation 4.1.4), the integral scale is a separation distance at which the correlation drops to the exp(-1) level. At this level, the correlation between data is considered insignificant. That is, the data points separated by distances larger than the correlation scale are only weakly associated with each other.

On an intuitive basis, the correlation scale may be interpreted as the average length of clay lenses or sedimentary structures. Hydraulic property values of the 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 the spatial structure of hydrologic parameters. Table 1 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 pumping tests. We must point out that there has been very little published research to confirm the geologic significance of the correlation length (Byers and Stephens, 1983; MacMillan and Gutjahr, 1986).

For the sake of simplicity, the above discussion on autocorrelation function is restricted to one-dimensional data (i.e., data collected along a transect). The concept can be applied to a two- or three-dimensional data set as well. For example, a commonly used three-dimensional exponential autocorrelation function in groundwater hydrology is:

Table 1. Variances and correlation scales for log hydraulic conductivity or log transmissivity (Gelhar, 1986).

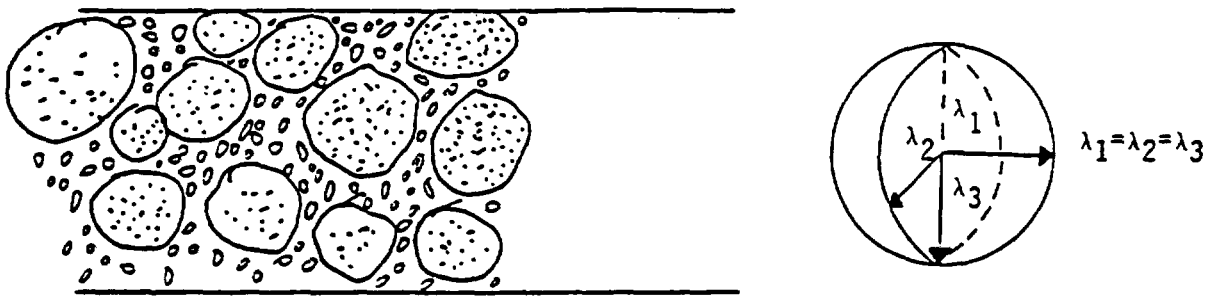
Source	Medium	σ_f^2	Correlation Scale, m	Overall Scale, m
Bakr [1976]	sandstone aquifer	1.5–2.2	0.3–1.0 V	100
Smith [1978]	outwash sand	0.8	0.4 V	30
Delhomme [1979]	limestone aquifer	2.3	6300 H	30,000
Binsariti [1980]	basin fill aquifer	1.0	800 H	20,000
Russo and Bressler [1981]	Hamra Red Mediterranean soil	0.4–1.1	14–39 H	100
Luxmoore et al. [1981]	weathered shale subsoil	0.8	< 2 H	14
Sisson and Wierenga [1981]	silty clay loam soil (alluvial)	0.6	0.1 H	5
Viera et al. [1981]	Yolo soil (alluvial fan)	0.9	15 H	100
Devary and Doctor [1982]	alluvial aquifer (flood gravels)	0.8	820 H	5,000
Byers and Stephens [1983]	fluvial sand	0.9	0.1 V > 3 H	5 14
Hoeksema and Kitanidis [1985]	sandstone aquifer	0.6	45,000 H	5×10^3
Hufschmied [1985]	sand and gravel	1.9	0.5 V	20
Sudicky [1985]	outwash sand	0.6	0.1 V	20

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

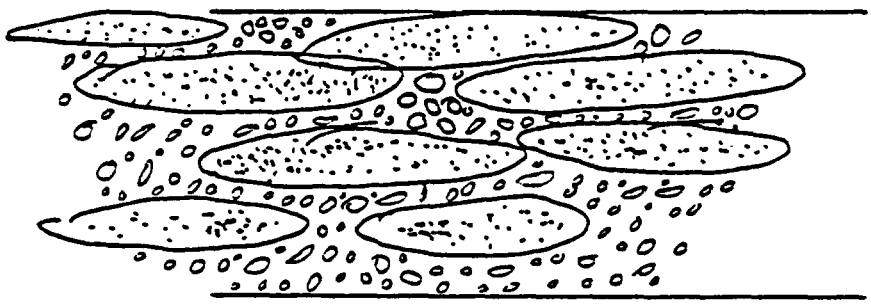
$$\rho(|\xi|) = \exp\left\{-\left[(\xi_1/\lambda_1)^2 + (\xi_2/\lambda_2)^2 + (\xi_3/\lambda_3)^2\right]^{1/2}\right\} \tag{4.1.5}$$

where ξ is the separation distance, and ξ_1, ξ_2, and ξ_3 are separation distances in x, y, z directions, respectively. Integral scales in the x, y, and z directions are λ_1, λ_2, and λ_3, respectively. If the integral scales are the same in all directions, then the stochastic process is called a statistically isotropic process. If these values are different, then it is called a statistically anisotropic process. Note that statistical isotropy and anisotropy are different from hydraulic conductivity anisotropy in classical hydrology. Statistical anisotropy simply implies that the hydrologic property (such as hydraulic conductivity) of an aquifer is correlated for a longer distance in one direction than in other two directions. For instance, in a perfectly stratified aquifer (e.g. laterally continuous "layer cake" sedimentary sequence), correlation scales in the horizontal directions are likely to be the same, but they will be much longer than the correlation scale in the vertical direction. This is due to the fact that within each layer, the material is considered to be effectively homogeneous. A short vertical correlation scale reflects a rapid lithologic change in the vertical direction. In Figures 4.5a and b, statistically isotropic and anisotropic aquifers are schematically illustrated. Figure 4.5c depicts an ellipsoid formed by anisotropic correlation scales. Hydrologic property values within the ellipsoid are considered correlated or similar, and those outside the ellipsoid are uncorrelated or dissimilar. A three-dimensional correlation function generally represents more closely the average physical dimensions of sediment bodies (such as clay lenses) than the one-dimensional correlation function.

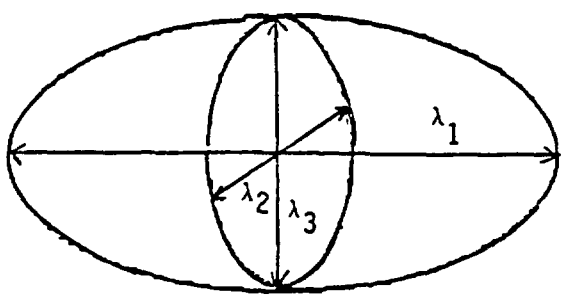
If a stochastic process (e.g. hydraulic conductivity) has a constant mean we refer to the process as having no drift; that is, the first statistical moment is constant over distance. If a process exhibits no drift and its autocorrelation function depends



(a) Statistically isotropic aquifer and a sphere formed by an isotropic covariance function.



(b) Statistically anisotropic aquifer



(c) An ellipsoid formed by a three-dimensional anisotropic covariance function. $\lambda_1 \neq \lambda_2 \neq \lambda_3$.

Figure 4.5. Schematic diagrams illustrating stochastic concepts in ground-water hydrology.

on the separation distance only, the process is considered as a second-order stationary (or statistically homogeneous) process. If the spatial distribution of hydrologic data is second-order stationary, one is then able to use the first moment and its covariance function to characterize its spatial variability. On the other hand, data that do not fit the definition of the second-order stationarity process are considered as non-stationary processes. A non-stationary process describes data which has a definite trend in space (i.e., the mean varies with distance or the covariance depends not just on the separation distance). For example, in a sedimentary basin a formation may have facies changes which cause hydraulic conductivity to decrease gradually toward the center of the basin. However, for many cases the data with a trend may still be treated as a stationary process after the trend is removed.

Figure 4.6 schematically illustrates the meanings of stochastic terms discussed above. In Figure 4.6a, a regular sine wave and its autocorrelation function are shown. Figure 4.6b shows a signal created by a random number generator. The autocorrelation function drops rapidly from +1.0 at 0 separation distance, then fluctuates slightly about 0. This type of behavior indicates that the signal is uncorrelated or statistically independent from one point to the next. Both of these series are stationary: that is, no significant trend exists in the data, and the covariance presumably only depends on the separation distance. A non-stationary signal is shown in Figure 4.6c, where the data increase steadily in value along the sequence. The autocorrelation function shows steadily decreasing correlation. Figure 4.6d shows a combination of Figures 4.6a and b, a sine wave with superimposed noise (uncorrelated signal). Perfect autocorrelation does not occur except at 0 separation distance, but the periodic component of the series is revealed by the second peak in the autocorrelation function. Figure 4.6e is a combination of Figures 4.6a, b, and c, a sine wave combined with a linear trend with superimposed noise. Due to the existence of the trend, the series is non-stationary. Note that the trend

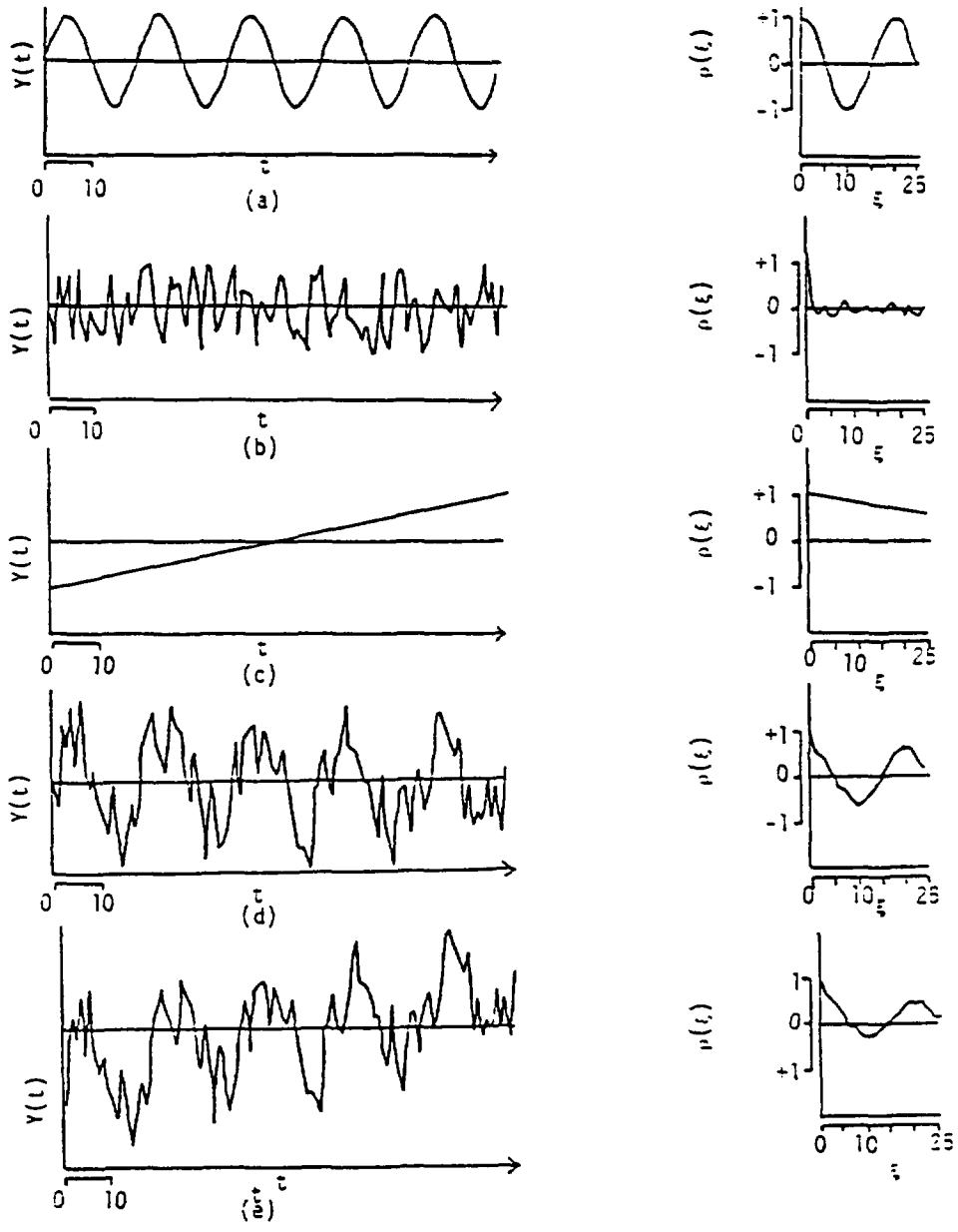


Figure 4.6. Some idealized time series, Y(t), and their autocorrelation functions, $\rho(\xi)$. (a) Sine wave with wavelength of 20 units. (b) Sequence of random numbers or "noise". (c) Sequence of linearly increasing numbers of "trend". (d) Sine wave plus random noise (sequence a plus sequence b). (e) Sine wave plus random noise plus linear trend (sequence a plus sequence b plus sequence c). (Davis, 1973).

further reduces our ability to discern the periodic component in the series.

Using the stochastic concept, many field data have been collected and analyzed in the past decade. One typical example is the analysis of hydraulic conductivity data in the Borden sandy aquifer, collected by Sudicky (1986). Thirty-two core samples were taken from cross-sections of two perpendicular transects. Each core sample was cut into subsamples of 0.05m in length. A total of 1279 hydraulic conductivity measurements were made from these small samples. Figures 4.7 and 4.8 offer a view of the spatial variability of hydraulic conductivity in the aquifer. The results suggest that the Borden aquifer is heterogeneous over the distance that the measurements were performed with the local hydraulic conductivity field having a complex, lenticular structure. Several very distinct but thin lenses of low hydraulic conductivity are clearly visible in the profiles. A stochastic characterization of the spatial variability was carried out. The variance of lnK (the natural logarithms of K) was found to be 0.38, which included the variance due to uncorrelated variations below the scale of measurement (nugget effect; Section 4.2). Autocorrelation functions of the two cross-sections in the horizontal and vertical directions are illustrated in Figure 4.9 a,b,c and d. Using equation (4.1.5), Sudicky (1986) found that the autocorrelation function of lnK is anisotropic with $\lambda_1 = \lambda_2 = 2.8$ and $\lambda_3 = 0.12$ m, in horizontal and vertical directions, respectively.

4.2 Geostatistics

As mentioned in Section 4.1, there are two approaches to deal with aquifer heterogeneities: (1) the effective hydrologic property approach, and (2) estimation of property values at unsampled locations. The first approach will be explored in the later section dealing with spectral analysis. Here we will discuss some basic concepts and tools for the second approach. Detailed discussions can be found in textbooks by Journel and Huijbergts (1978) or De Marsily (1986).

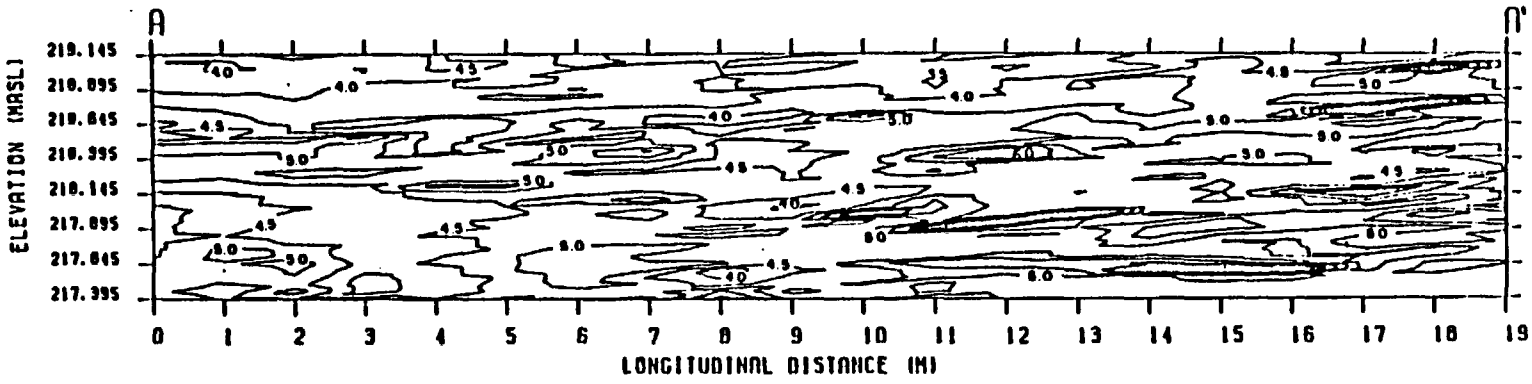


Figure 4.7. Cross-sectional view of the hydraulic conductivity distribution along a longitudinal direction in the Borden sandy aquifer (Sudicky, 1986).

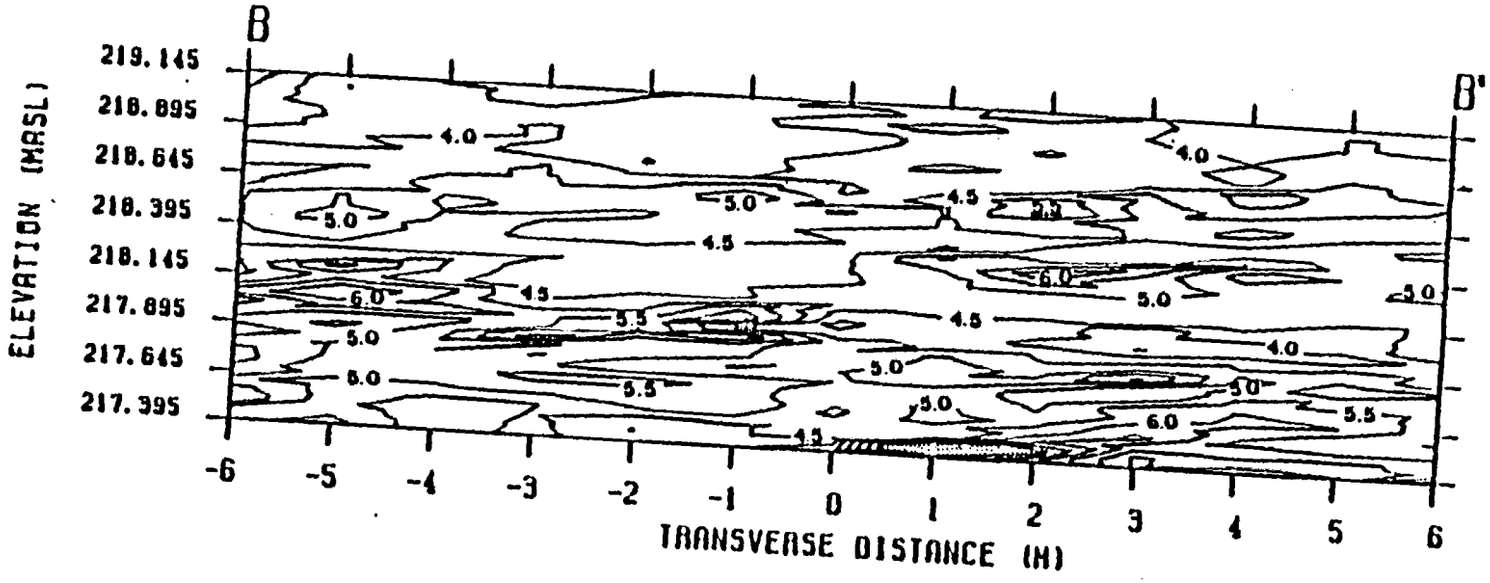


Figure 4.8 Cross-sectional view of the hydraulic conductivity distribution along a transverse direction in the Borden sandy aquifer (Sudicky, 1986).

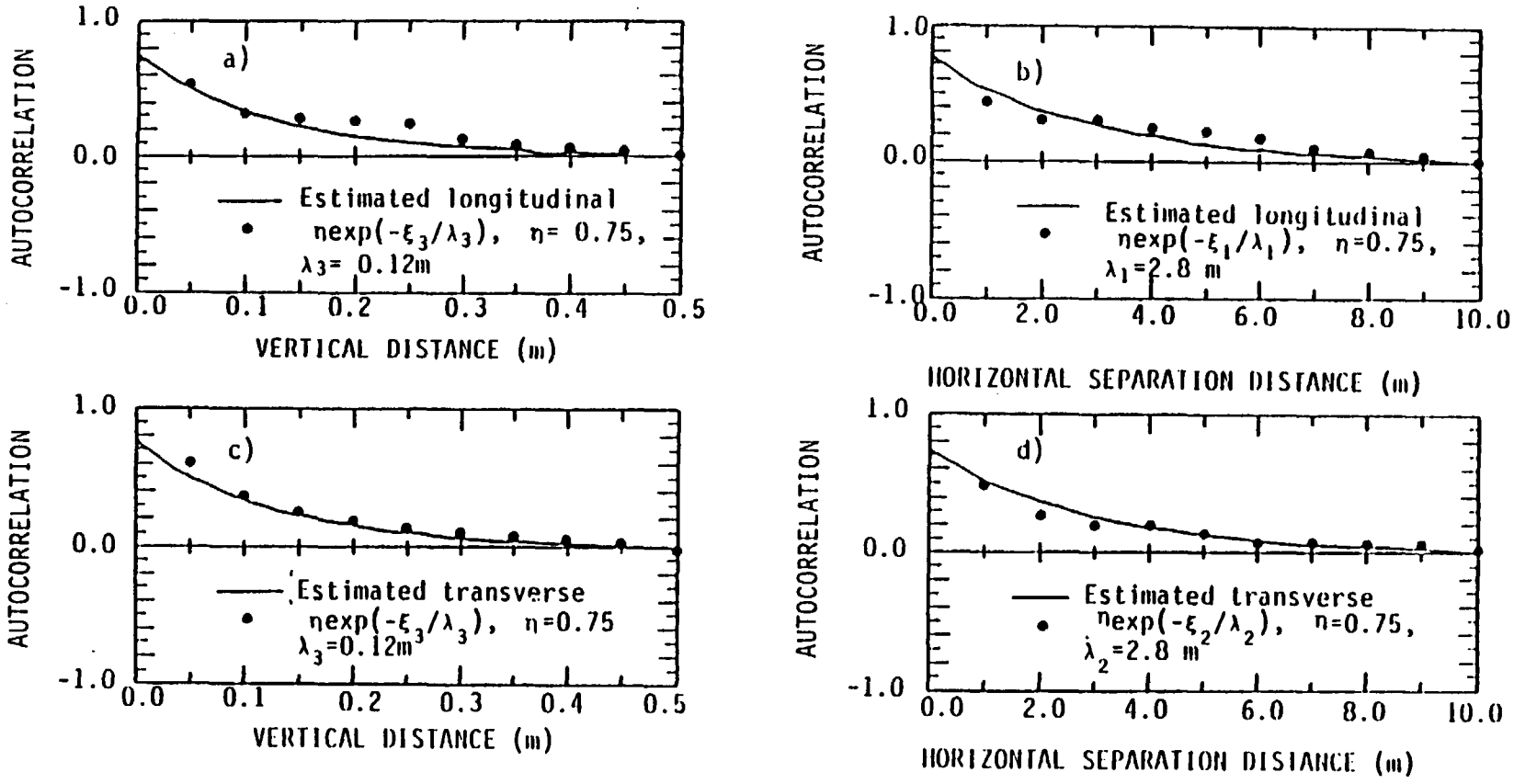


Figure 4.9. Vertical and horizontal autocorrelation functions for lnK along cross-sections in the longitudinal and transverse directions. η represents the ratio of the true variance (total variance minus the nugget effect) to the total variance.

Geostatistics is basically a statistical method 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 (Journel and Huijbergts, 1978). Recently, the technique has been applied to groundwater hydrology to deal with spatial variability problems. In principle, geostatistics concepts are similar to the stochastic concepts. They both are used to deal with variables distributed in space. However, some of the terminology is different. For example, the term "random function" is used in geostatistics to defined 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 $x_2+\xi$ are not independent but correlated. From 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). A regionalized variable is simply a particular realization of a certain random function or stochastic process. We will point out some other differences in the following text.

Two important parts of geostatistics are (1) identification of the spatial structure of the variable (variogram estimation, trend estimation, etc.) and (2) interpolation or estimating the value of a spatially distributed variable from neighboring values taking into account the spatial structure of the variable (kriging, co-kriging, etc., Davis, 1973).

Similar to 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 the covariance function depends on the separation

distance only. However, the intrinsic hypothesis requires only that the mean of the differences of the data values is constant, and the variance of the difference of data values depends on the separation distance, i.e. $[K(x+\xi) - K(x)]$ satisfies:

$$E[K(x+\xi) - K(x)] = m \tag{4.2.1}$$

$$\frac{1}{2}\,\mathrm{var}[K(x+\xi) - K(x)] = \gamma(\xi) \tag{4.2.2}$$

where K(x)'s are regionalized variables, and γ is a function of ξ, and not of x. $\gamma(\xi)$ is called the variogram, sometimes also called semivariogram. Figure 4.10 shows the general behavior 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 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 is a second-order stationary process.

The main types of variograms commonly used to fit sample variograms (variograms estimated from field data) are: linear, spherical, exponential, Gaussian, and cubic. Figure 4.11 shows the shapes and equations of these variograms. Generally, a linear variogram, as shown in Figure 4.11a, suggests that the process has an infinite variance and that there is no covariance function, i.e., it is not a second-order stationary process. In this case, one has to rely on the intrinsic hypothesis to analyze the data. Theoretically, all variogram plots pass through the origin; the variogram is zero at a separation distance of zero. However, variograms obtained

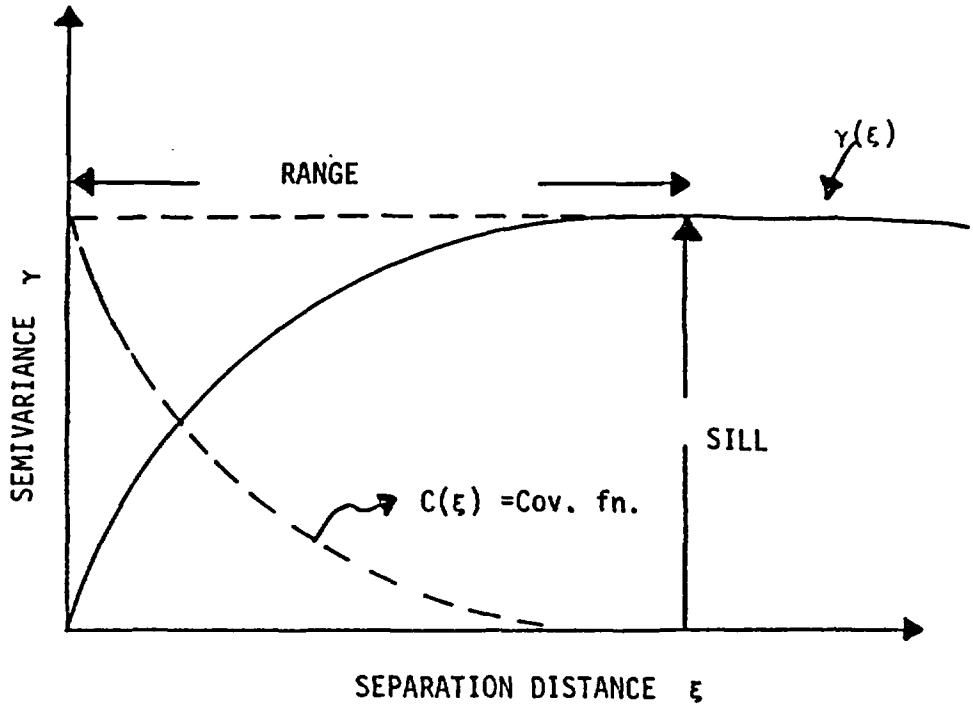
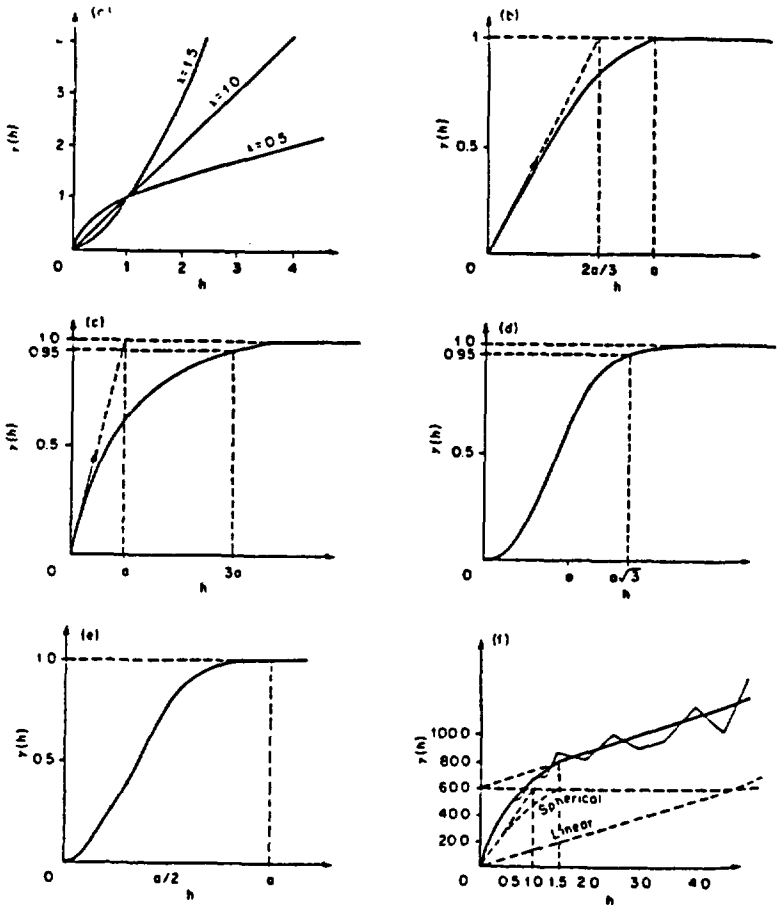


Figure 4.10. General behavior of a variogram.



(a) model in h^{λ}	ωh^{λ}	$\lambda < 2$
(b) spherical model	$\omega\left[\frac{3}{2}\left(\frac{h}{a}\right) - \frac{1}{2}\left(\frac{h}{a}\right)^3\right]$	$h < a$
	ω	$h > a$
(c) exponential model	$\omega[1 - \exp(-h/a)]$	
(d) Gaussian model	$\omega\{1 - \exp[-(h/a)^2]\}$	
(e) cubic model	$\omega\left[7\left(\frac{h}{a}\right) - 8.75\left(\frac{h}{a}\right)^3 + 3.5\left(\frac{h}{a}\right)^5 - 0.75\left(\frac{h}{a}\right)^7\right]$	$h < a$
	ω	$h < a$
(f) fitting on a "linear plus spherical" model (example)		
	$13.3\,h + 60\left[\frac{3}{2}\left(\frac{h}{1.5}\right) - \frac{1}{2}\left(\frac{h}{1.5}\right)^3\right]$	$h < 1.5$
	$13.3\,h + 60$	$h > 1.5$

Figure 4.11. A diagram showing the shapes and equations of various variograms (de Marsily, 1986).

from field data often exhibit a jump at the origin, as shown in Figure 4.12. This apparent jump is called the nugget effect and represents the uncorrelated subscale variability or measurement errors. The variogram can be either isotropic or anisotropic as in the covariance function. It is also likely that there are multiple correlation scales that appear when testing over different scales, ranging from laboratory to field to required scale, Figure 4.13, (Gelhar, 1986).

The other part of geostatistics is Kriging. The most general form of Kriging is termed "Universal Kriging," in which the values of points may be estimated from irregularly distributed samples in the presence of trends (or nonstationarity). If the data set is stationary, a less involved operation can be used to estimate the values of points. This technique is referred to simply as "Ordinary Kriging" or "Kriging" (see Bras and Rodriguez-Iturbe, 1985, and Journel and Huijbregts, 1978).

A common application of Kriging in groundwater hydrology is the estimation of hydraulic conductivity or transmissivity values at unsampled locations in between test wells (see Delhomme, 1979). For example, in an attempt to use a two-dimensional, finite difference, groundwater flow model to simulate flow fields in a groundwater basin, 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 objectively assign transmissivity values to the remaining nodes, one may have to resort to use of mathematical tools. Kriging is one of the possible tools.

To find the hydraulic conductivity estimate K^* of the unknown quantity K_0, Kriging uses a weighted sum of all the available sample values (measured hydraulic conductivity values):

$$K^* = \sum_{i=1}^{n} \lambda_i K_i \qquad (4.2.3)$$

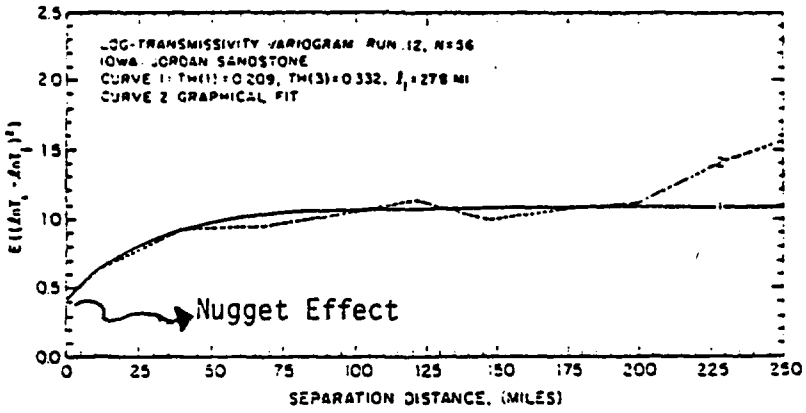


Figure 4.12. A variogram showing the nugget effect: a jump at the origin. (Hoeksema and Kitanidis, 1985).

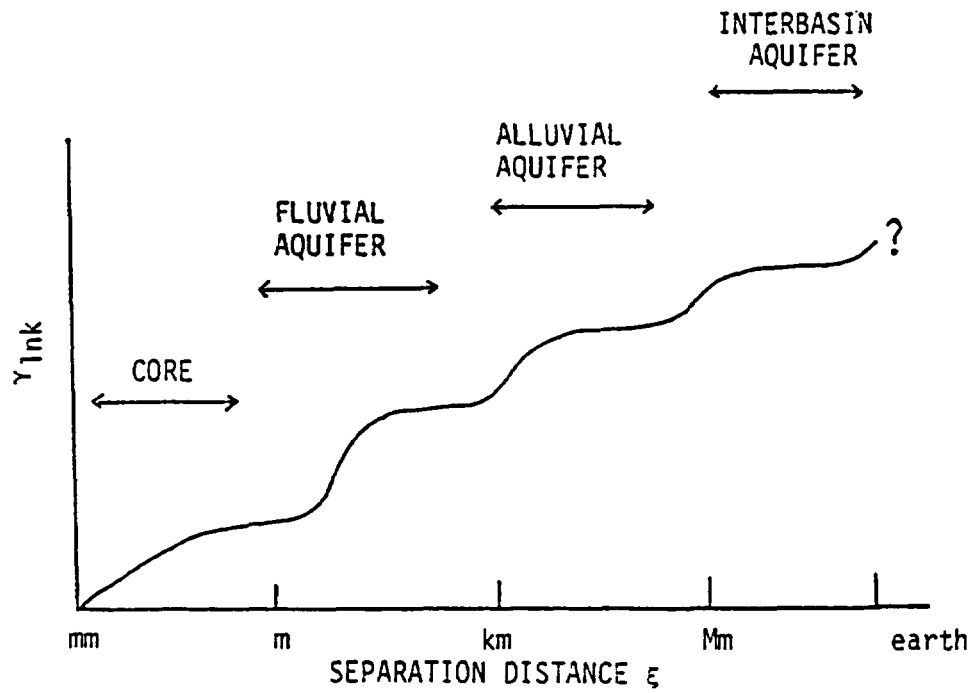


Figure 4.13. Hypothetical lnK variogram illustrating the notion of scale-dependent correlation scales (Gelhar, 1986).

where λ_i are the weighting factors, and K_i are sample values. In order to limit the choice of the weighting factors, we will impose two conditions. The first condition is that the expected value of the estimate of K should be the same as the expected value of K, i.e.,

$$E[\ K^*\ ] = E\ [\ K\ ] \tag{4.2.4}$$

It follows that in the constant mean case the sum of the weighting factors has to be unity.

$$\sum_{i=1}^{n} \lambda_i = 1 \tag{4.2.5}$$

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

$$E[\ (K^* - K)^2\ ] = \text{minimum} \tag{4.2.6}$$

This latter condition, along with 4.2.5 leads to a system of equations of the form:

$$\sum_{j=1}^{n} \lambda_j\ \gamma(x_i - x_j) + \mu = \gamma(\ x_i - x_0\ ) \tag{4.2.7}$$

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 between the point to be estimated and the point x_j. μ is a Lagrange multiplier. Combining the constraint that the weighting

coefficients must sum to one, the system of equations can be solved to obtain optimal λ_i values which can then be input to equation (4.2.3) to obtain the estimate of K'. The estimator, K' is a linear combination of the n data values (4.2.3). The n weights λ_i are calculated to ensure that the estimator is unbiased and that the estimation variance is minimal. Kriging is a best linear unbiased estimator (BLUE).

The Kriged estimate K^* 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, K^*, to be exact. The inexactitude of the estimate is the Kriging variance, σ_K^2, which is:

$$\sigma_K^2 (x_0) = \sum_{j=1}^{n} \lambda_j \gamma(x_i - x_0) + \mu \qquad (4.2.8)$$

The smaller the variance, the greater the reliability of the estimate K^*. Conversely, an estimate with a large associated variance must be utilized with caution. One can also use the Kriging variance in determining the optional 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 could be a valuable tool in quantifying uncertainty in interpolated data and in assessing the value of additional data during 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 objections behind polynomial or surface fitting differ from those in kriging. For that reason a comparison between them 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.

Kriging can also be used in conjunction with numerical simulations that may be useful in calculating ground water travel time. 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, represent a much smaller scale than the grid blocks of the model. In contrast to ordinary Kriging described previously in this section, 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 an point or area basis. De Marsily et al. (1984) describes a method of identifying hydraulic characteristics of a reservoir from aquifer pumping tests which combines Kriging and numerical simulation. The approach allows one to utilize a variety of available hydrogeologic information at different scales. Kriging has also been 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 estimate pore velocity is described by Neuman (1984).

In most field problems, groundwater hydrologists are likely to have both transmissivity and hydraulic head, or the 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), Gutjahr (1981), and Kitanidis and Vomvoris (1983). Neuman (1984), Williams (1987), and Hoeksema and Kitanidis (1984) applied this approach to groundwater flow simulations.

4.3 Stochastic Analysis of Spatial Variability

The statistical description of spatial variability of hydraulic properties of subsurface materials has led many researchers to investigate the effect of randomly distributed parameters on the governing equations. The model used to investigate this type of problem is generally called a stochastic model. Although stochastic and deterministic models use the same governing flow and transport equations for porous media, the former differs from the latter in that its input functions are uncertain and, therefore, the model output must be described in probabilistic rather than deterministic terms (Neuman, 1982).

For example, a deterministic, three-dimensional, groundwater flow model requires values of hydraulic conductivity and storativity at every point in three-dimensional space, if we assume that the initial and boundary conditions and sink and source terms are prescribed. The output from the deterministic model is a realization of hydraulic head values corresponding to those parameters at each point in space. However, in a stochastic model, the hydraulic conductivity and storativity are considered as stochastic processes in space which are described in terms of means, covariances, and other statistical terms, instead of a value at each point. The output consists of many possible head distributions that relate to the input parameters. Therefore, the head is a stochastic process which can be described in terms of statistical parameters such as mean, variance, covariance, etc. In other words, the stochastic model produces a probabilistic result which can be utilized to assess the uncertainty in predictions due to heterogeneity of aquifer properties.

In the past few decades, many researchers in groundwater hydrology have applied stochastic models to study flow and transport through heterogeneous porous media. The following is a summary of these works which include Monte Carlo simulation, conditional simulation, spectral analysis, and fractal analysis.

4.3.1 Monte Carlo Simulation. The most intuitive approach to dealing with spatial variability in a stochastic sense is called Monte Carlo simulation. It is a very powerful method, since fewer assumptions are required than in all of the other stochastic methods. However, it may require extensive computer time and a careful analysis of the results. The principle of the method is rather simple. The method assumes that the probability distribution of the variable (for example, hydraulic conductivity) and its covariance function are known from measured field data. Then, many possible realizations of hydraulic conductivity values that conform to the assumed probability distribution can be generated by using a pseudorandom number generator with special techniques (Gutjahr, 1987; Smith and Freeze, 1979; Mantoglou and Wilson, 1982). Each realization of the parameter values is input to flow and transport equations which are then solved by either 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, there are N realizations of output from solving the governing equations. It is then possible to statistically analyze the output for each realization to obtain expected value, variance, covariance, and distribution. The idea is illustrated in Figure 4.14.

There are difficulties associated with the simulation method. First, a large number of realizations is necessary in order to obtain meaningful statistics. This implies that extensive computer CPU time is required, and this method is costly. Second, a groundwater basin has to 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 iterative methods. 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

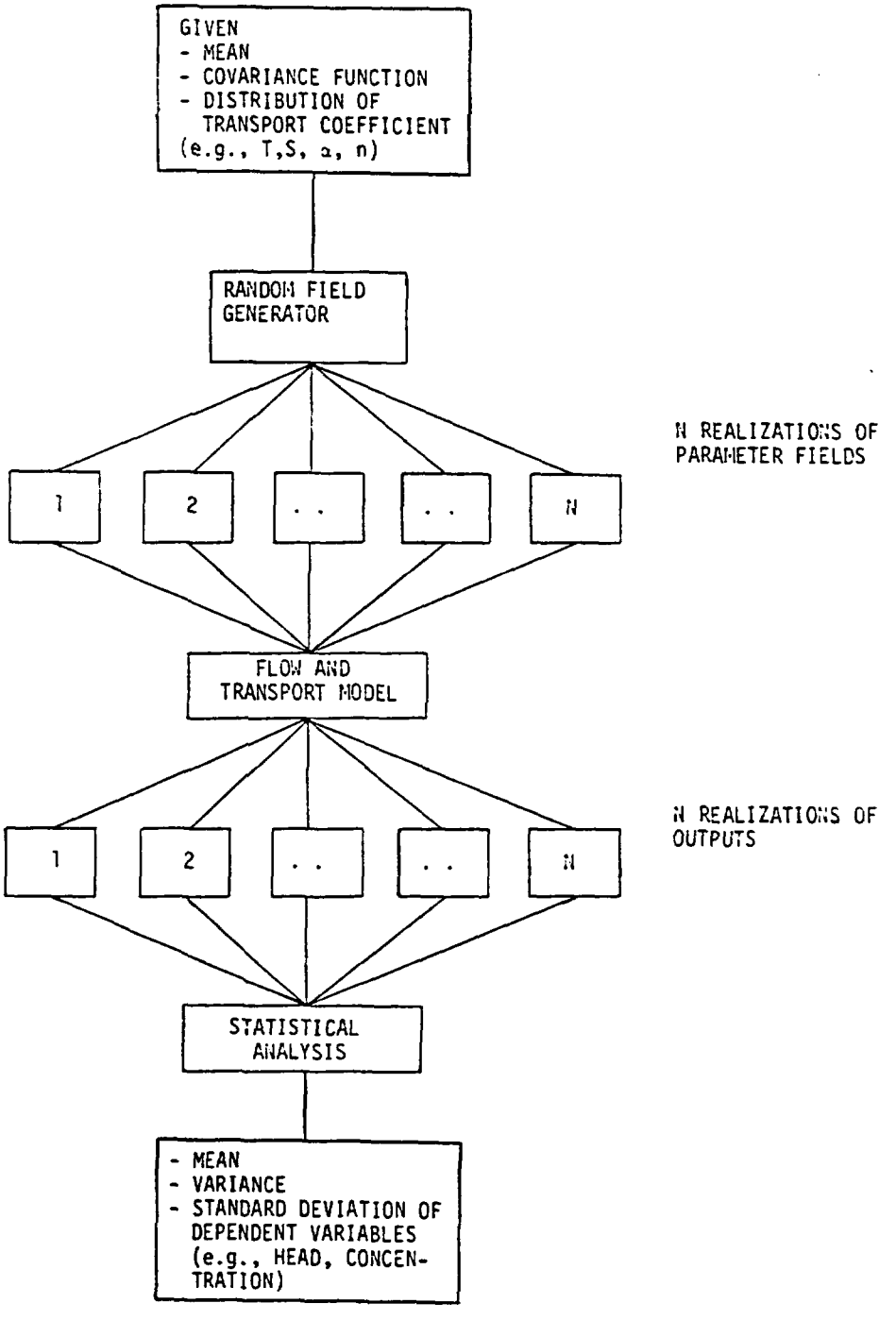


Figure 4.14. Schematic illustration of Monte Carlo simulation concept.

situations or other highly nonlinear 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 nonlinear systems with stochastic parameters are tremendous. Although these are 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.

Applications of Monte Carlo simulations to investigate the effect of heterogeneity on flow through porous media were first used by Warren and Price (1961). Following their work, studies were made by Warren and Skiba (1964), Bibby and Sunada (1971), and Heller (1972). All of these works are related to petroleum reservoirs. The first study directly related to groundwater hydrology was carried out by Freeze (1975). Freeze essentially extended the approach of Warren and Price (1961) to the multivariate case in which hydraulic conductivities, compressibilities, and porosities all vary randomly in space and are mutually correlated. The objective of his study was to investigate the uncertainty in hydraulic head prediction due to aquifer heterogeneity. Groundwater travel times and paths depend partially on the hydraulic gradient distribution, which in turn is related to hydraulic head distribution. Uncertainties in predictions of head distribution, of course, will result in uncertainties in prediction of groundwater travel times and paths. Thus, it is appropriate to discuss his work in detail in this section. Furthermore, discussion on the weakness of his work may lead to a better understanding and future utilization of Monte Carlo techniques to predict groundwater travel times and paths.

Freeze (1975) considered both steady-state flow under constant head boundary conditions and transient consolidation of a clay layer under similar boundary conditions and prescribed head at time zero. A one-dimensional flow domain was discretized into many blocks. Random hydrologic parameters (log

hydraulic conductivities, compressibilities, and porosities) were assigned to each block, and these parameter values were independent from those at adjacent blocks (i.e., no correlation structure was considered in generating the random hydraulic parameters). An analytical method and a numerical method were used to determine the hydraulic head distributions for steady and unsteady flow, respectively. Solutions were then analyzed for a given number of blocks and a given choice of statistical parameters such as mean parameter values, variances, and correlation coefficients between parameters.

Based on the Monte Carlo analysis, Freeze concluded that (1) there is no simple way to define an equivalent homogeneous porous medium for transient flow in a heterogeneous porous medium; and (2) the consideration of spatial variability of hydraulic properties in a stochastic sense may lead to very large fluctuations in the computed hydraulic head values. Therefore, he expressed the pessimistic view that the prediction of hydraulic head using any deterministic model may suffer from very large errors. He further questioned the usefulness of determining aquifer characteristics by means of aquifer test analyses, which rely on deterministic analytical solutions and the assumption that the aquifer is homogeneous.

Such pessimistic views on groundwater flow modeling by Freeze were challenged by Gelhar et al. (1976). They attributed the large variance in calculated hydraulic head in Freeze's work to the dimensionality of the model used. They indicated that the head variance will be reduced significantly in three-dimensional models. When a one-dimensional model is used, the flow must travel directly through impermeable layers. The hydraulic head gradient near an impermeable layer thus has to increase substantially to allow water to flow. In a three-dimensional problem, water takes the least resistant route and avoids the impermeable paths. Therefore, the head gradient is smaller than in the one-dimensional case. Head variance in a three-dimensional model is also much smaller than in the one-

dimensional case. Furthermore, Freeze's analysis assumed that hydrologic parameters in adjacent finite difference grids were independent, but within a grid the properties were constant. This assumption implies that the parameter values are correlated over a block; that is, the size of the block determines the correlation scale. Bakr et al. (1978) showed that the head variance is directly proportional to the square of the correlation scale. Consequently, the choice of the size of the block could significantly affect magnitude of the head variance. Therefore, Freeze's analysis was most likely overly pessimistic.

More realistic simulations than Freeze's study on uncertainties in hydraulic head were later conducted by Smith and Freeze (1979a and b) using a Monte Carlo technique. Steady flow through one- and two-dimensional random hydraulic conductivity fields was simulated using a finite element model. The hydraulic conductivity K was assumed to be lognormally distributed. Anisotropic spatial correlation structures (statistical anisotropic covariance function) of the random conductivity values were incorporated by using a first-order nearest-neighbor autoregressive model. One technical weakness of their work is that one has minimal control on the shape of covariance function generated by the nearest-neighbor model. In the two-dimensional analysis, a hypothetical rectangular aquifer was used in which constant hydraulic head boundaries were imposed on two opposite sides of the aquifer and no flow boundaries on the others.

The results of their simulations show that for the case of unidirectional (uniform) flow, the uncertainty in hydraulic head must be interpreted in light of the ratio of the correlation scale to length of size of the aquifer. The uncertainties in head (represented by the standard deviations of hydraulic head distribution) increase as the extent of the heterogeneity increases and/or as the correlation scale/length ratios increase. A comparison of the results of one- and two-dimensional flow regimes indicated that the standard deviation is smaller in the two-dimensional

problem. They also investigated the effects of nonuniform flows by rearranging the boundary conditions of the hypothetical aquifer. The results from nonuniform flow fields simulations led to the conclusion that the uncertainty in model predictions depends upon both the spatial heterogeneity in hydraulic conductivity and the flow regime. The uncertainty in the predicted head values is greatest where the mean hydraulic head gradient is large and the uncertainty in hydraulic head values tends to diminish near the constant head boundaries. Generally speaking, their results are in agreement with those obtained by a spectral method (Mizell et al., 1982). As pointed out by Neuman (1982), the results of Smith and Freeze (1979b) also illustrate that the concept of an equivalent uniform porous medium is not appropiate for the cases where the mean hydraulic gradient is not uniform (such as during a pumping test where the flow is convergent) or when the mean hydraulic conductivity varies in space.

In Smith and Freeze's work, they also addressed the problem of scale which is critical in determining groundwater travel times and paths. They pointed out that by using single conductivity values in the finite difference blocks or finite elements, spatial variations on a scale smaller than the block or element do not contribute to the variability in the finite element solution. They suggested that in order to obtain an accurate solution in modeling a given field situation, the finite difference or element model must reproduce all the significant scales of heterogeneity that contribute to the prediction uncertainties at the scale of the model. This statement concurs with the previously stated position in this review on the concept of groundwater travel times and paths. Dispersion representing subscale variability must be included in the analysis of groundwater travel times and paths.

Smith and Freeze (1979b) also emphasized that the scale at which heterogeneities are to be described in the analysis of uncertainties will be related to the scale of the flow analysis. They stated: "... in a regional flow the model would

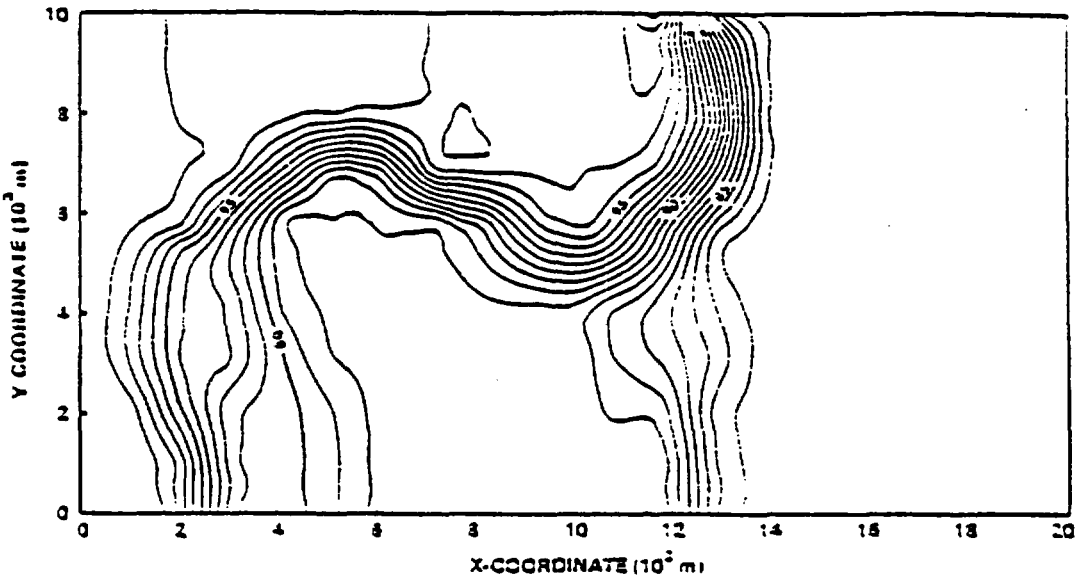
preserve the regional structures and patterns of conductivity variability. On the other hand, in considering flow to a tile drain, the description of the spatial heterogeneity would reflect the local dependence in the region about the drain." Such a statement seems to be a contradiction of their earlier statement that the effect of subscale variability should be considered in the simulation. In our opinion, the fastest path can best be predicted by characterizing local scale of heterogeneities. For example, if we are interested in the water level in a well, then the scale used to depict heterogeneities should be equal to the size of the screen in the well. Certainly, heterogeneities larger than the screen but much smaller than the size of heterogeneities forming the regional structures will affect the response of the well. As an example, the drawdown at a well tapped into a large sandstone lens embedded in a dolomite formation will be affected by the hydraulic conductivities of both the lens and the formation. Hydraulic conductivity variations smaller than the size of the screen (such as the conductivities of thin layers of gravel within the lens) can be ignored. This is because the water level is a quantity averaged over variabilities at scales much smaller than the screen. This is true for water level measurements in a well. However, in the case of groundwater travel times and paths, one may want to consider the variability at scales smaller than the screen, inasmuch as some fluid particles would move rapidly in those thin gravel layers.

One of the studies relevant to NRC's criterion of pre-waste emplacement groundwater travel times in a potential repository site was conducted by Clifton et al. (1985). He applied the Monte Carlo technique to examine the sensitivity of the travel time distribution predicted by a reference case model to: (1) scale of representation of the model parameters, (2) size of the model domain, (3) correlation range of log-transmissivity, and (4) cross-correlations between transmissivity and effective thickness.

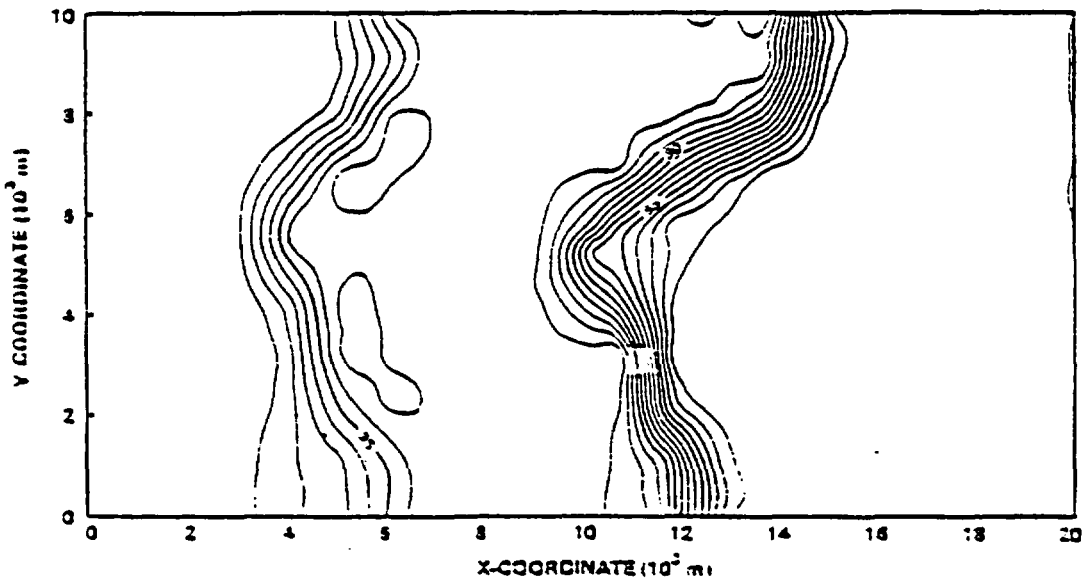
For this study, a rectangular area with dimensions 20 by 10 km was selected

as the reference case from the deep basalt beneath the Hanford site in southcentral Washington state. Impermeable boundaries were set along the two longer dimensions, and constant head boundaries were set along the shorter dimensions so that the regional hydraulic gradient was 10^{-3}. A steady-state, two-dimensional, horizontal groundwater flow regime was assumed. A finite difference flow model was used. The rectangular area was divided into square finite difference grids 1 km on a side. An effective thickness was defined as the product of the effective porosity and actual flow domain thickness. The effective thickness represents the area of effective, or hydraulically active, pore space in a vertical cross-section of the flow domain of unit width and thickness. Effective thickness of the area of the reference case was deterministically set at a uniform value of 4×10^{-2} m. Transmissivity was treated as a statistically isotropic stochastic process representing the uncertainties in inputs and was assumed to be log-normally distributed. Ten thousand random transmissivity fields were generated by using an unconditional estimator (Clifton and Neuman, 1982) with a spherical variogram model. The geometric mean of the transmissivity values was $0.153 m^2$/day, and the variance, and correlation scale of the log-transmissivity values were 3.35, and 5 km, respectively. These random hydrologic fields were input to the finite difference model to generate 10,000 hydraulic head fields.

Figures 4.15a and b show the hydraulic head distributions of realizations 3,899 and 5,120. In Figure 4.16a, the mean of the ensemble of 10,000 head field realizations is plotted. It is evident that the ensemble mean head field closely approximates the deterministic head field. This deterministic head field refers to the head field determined by assuming an equivalent homogeneous medium with the mean transmissivity. Interestingly, this result illustrates the fact that the head distribution in a constant head permeameter, calculated by using a single hydraulic conductivity value, represents an ensemble average. That is, it is an average head



(a) realization 3899



(b) realization 5120

Figure 4.15. Simulated hydraulic head distribution in a two-dimensional aquifer with a random transmissivity field (Clifton et al., 1985).

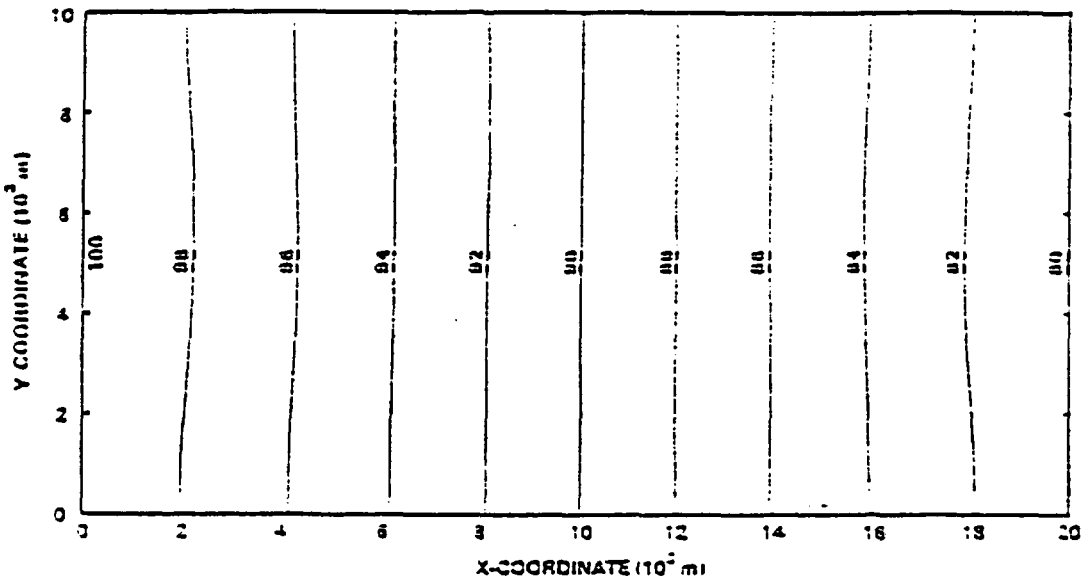


Figure 4.16a. Ensemble averaged head distribution. (Clifton et al., 1985).

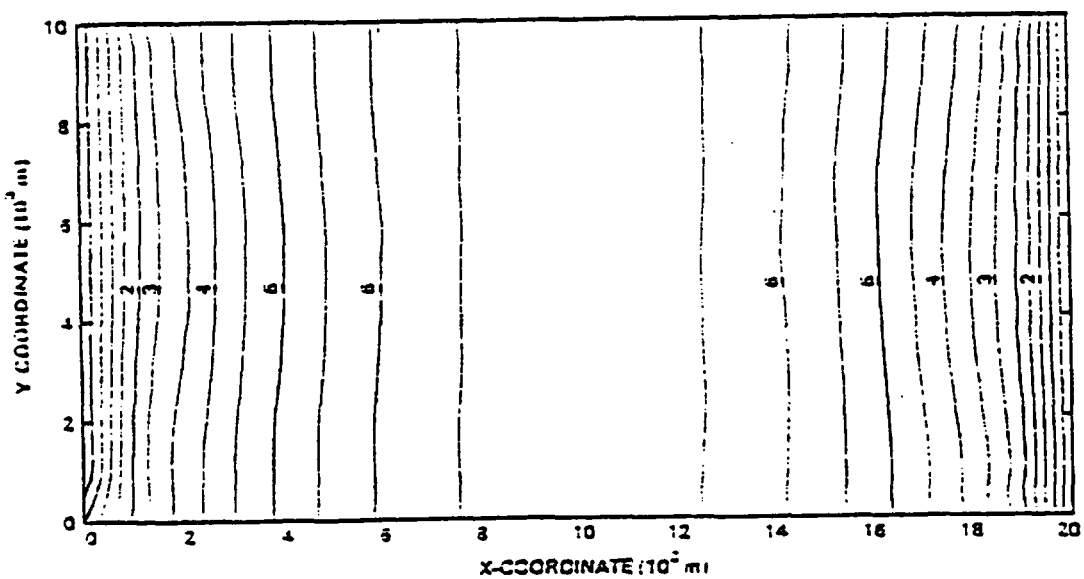


Figure 4.16b. The standard deviation distribution in a hypothetical aquifer. (Clifton et al., 1985).

distribution over many possible head realizations due to heterogeneities at scales smaller than the permeameter. Thus, it is clear that the deterministic approach (such as determining hydraulic conductivity from a soil column test) in groundwater hydrology is closely related to the stochastic approach. More importantly, the result here also supports the view that it is important to use head measurements averaged at many locations (observation wells) to determine mean hydraulic properties from aquifer test data (see section 3.1.3). Figure 4.16b shows the standard deviations of hydraulic head fields. The standard deviations decrease toward the specified constant head boundaries. This indicates the importance of boundary conditions on the uncertainty analysis.

In the analysis by Clifton et al., (1985) the average fluid particle velocity was determined from the transmissivity, hydraulic head gradient, and effective thickness values. The statistics of groundwater travel times were determined from a selected pathline in each of these 10,000 hydraulic head fields. Each pathline had the same starting location and same linear distance (10 km) between starting and termination points. The distribution of the groundwater travel times resulting from the 10,000 pathlines is shown in Figure 4.17. The median travel time (i.e., the travel time at 50% probability) is 21,500 yr. In other words, the probability that the predicted groundwater travel time between the two points is less than 21,500 yr is about 0.5, if the exact arrangement of transmissivity values within the flow domain is unknown. The standard deviation of the log-travel-time is 0.84 (one standard deviation above the mean). The results in Figure 4.17 indicate the probability of a predicted groundwater travel time less than 5000 yr (approximated from Figure 4.17) is 0.16 and less than 200,000 yr is 0.84. Such a groundwater travel time distribution thus provides us with a measure of the uncertainty in the predicted groundwater travel time.

One can also use this distribution to address the effect of heterogeneity on

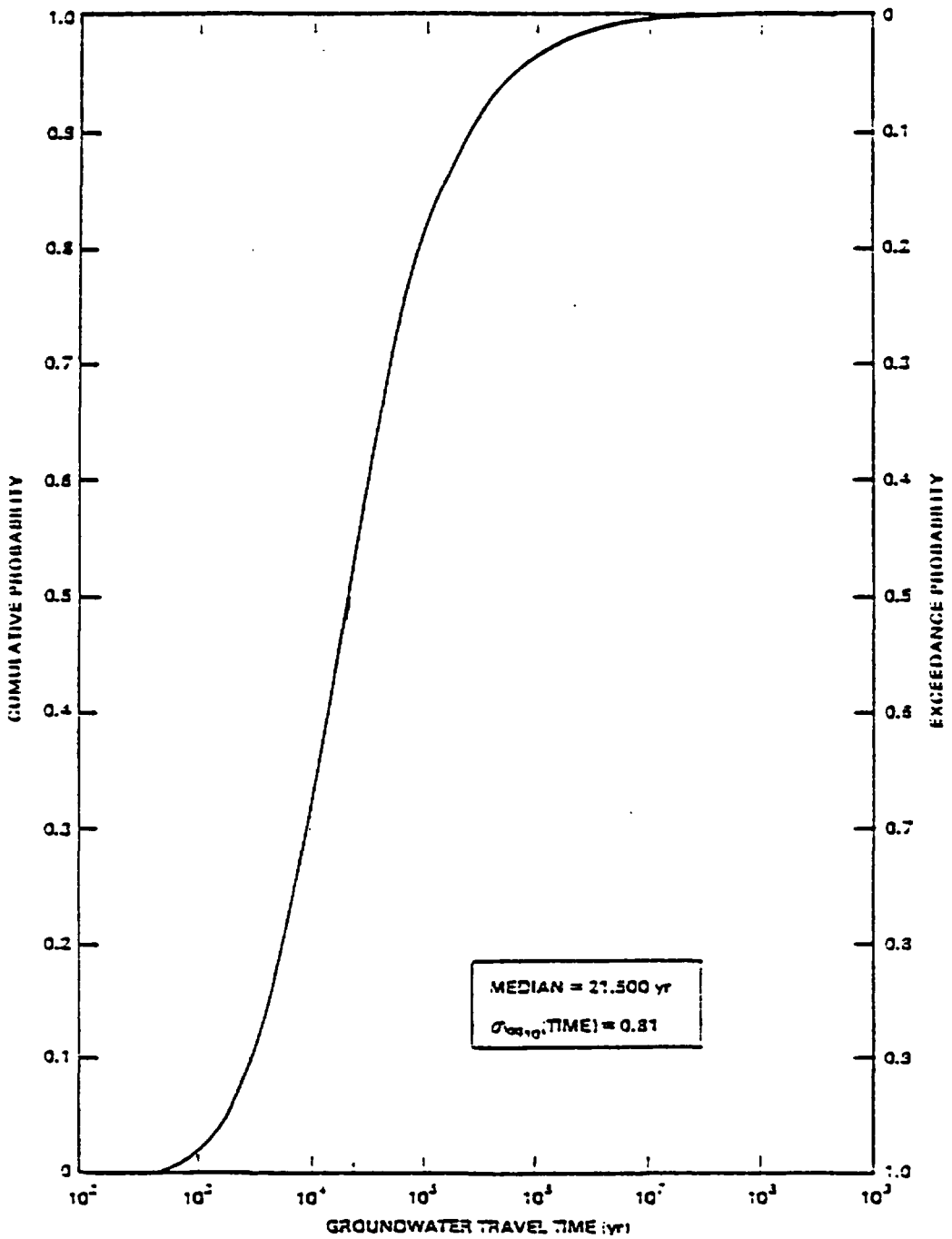


Figure 4.17. Cumulative probability of simulated groundwater travel times. (Clifton et al., 1985).

groundwater travel time, if the ergodicity assumption is used. That is, the probability distribution of ground-water travel time obtained from this analysis is equivalent to that of the time for a large number of groundwater particles released at the left boundary to travel across of the flow domain and exit the right boundary (e.g. Figure 4.15, and 4.16). This groundwater travel time distribution indicates that, on the average, 50% of the particles will arrive at the ending line within 21,500 yr. Due to the existence of some fast paths, 84% (one standard deviation less than the mean) of the groundwater particles will cross the flow domain in less than 200,000 yr. Therefore, the spread of groundwater travel times reflects spatial variations in fluid particle velocity, i.e., deviations of the velocities from the mean, within the flow field. In fact, this probability distribution is similar to the concentration distribution in a soil column tracer test discussed earlier with the exception that this distribution does not consider velocity variations at scales smaller than the finite difference block.

When a numerical groundwater flow model is used, the flow domain generally has to be discretized into many smaller grids. Because there are practical limits on the total number of grids used to represent a model domain, there will in turn be some limit on the minimum size of a block. Property values assigned to the block represent the averages over the block, and consequently variations at subscales are neglected. The larger the block is the more subscale variability is ignored. Therefore, the size of block used in the numerical simulation will influence results of the analysis, regardless of its impact on the accuracy of the numerical solution. Figure 4.18 illustrates the effect of the size of blocks (zones) on the probability distribution of groundwater travel time. As indicated in the figure, both the mean travel time and the standard deviation of log travel time (a measure of the arrival time variability) decrease as the size of the block increases. In the work by Clifton et al. (1985), the mean travel increased by 41%, from 16,000 to 23,500 years, when

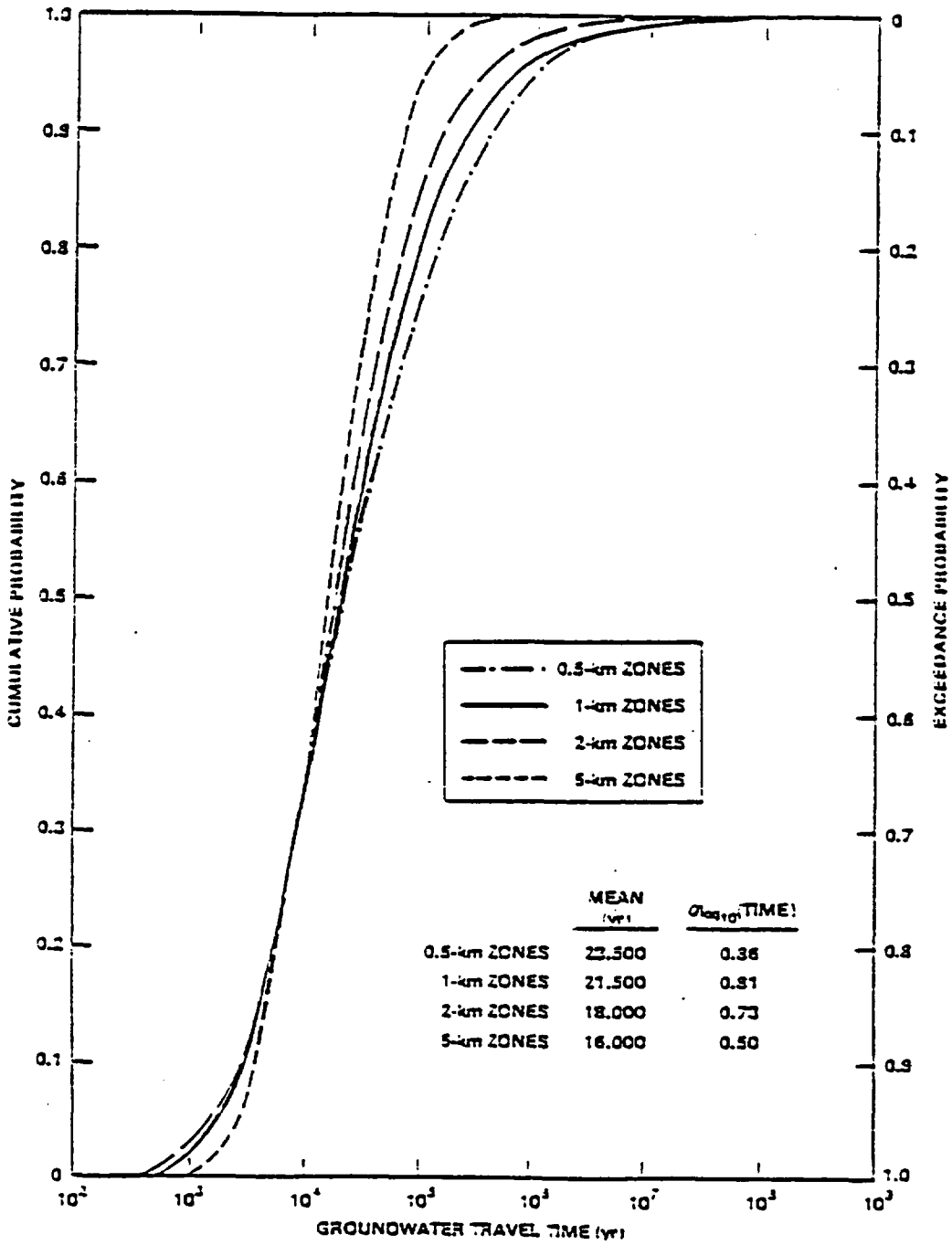


Figure 4.18. Effects of finite difference block (zone) size on the cumulative probability of groundwater travel time. (Clifton et al., 1985).

the grid blocks size in the model decreased from 5.0 to 0.5 km. This result is again illustrative of the importance of considering subscale variability in the prediction of the ground water travel time.

Impacts of the correlation scale of transmissivity values on the groundwater travel time distribution were also investigated in the study by Clifton et al. (1985). The travel time distributions from six random fields with different log-transmissivity correlation scales are illustrated in Figure 4.19. A constant variance in transmissivity was assumed in all six cases. As the correlation scale increases, the mean and standard deviation of log travel time also increase. At first inspection, this result may not seem intuitively correct, and an explanation is required. Generally speaking, the heterogeneity is characterized by the magnitudes of both variance and correlation. That is, a homogeneous medium has a zero variance and infinite correlation scale, and conversely, a highly heterogeneous medium has a large variance and small correlation scales. Thus, a variance assigned to a perfectly correlated medium (i.e., a medium with infinite correlation scale) may strictly represent uncertainty in measurements of the parameters. For other cases, one can explain the physical meaning of the results as follows. If the correlation scale is zero, spatial variations in transmissivity values between the starting and the ending points along the travel path are statistically independent. This implies that the heterogeneity encountered by a particle in each realization will be the same regardless of the sequential arrangement of the transmissivity values. Hence, the arrival times are identical among realizations. As the correlation scale increases, the sequential arrangement of the transmissivity values becomes important. This results in different arrival times among realizations.

Clifton et al. (1985) also found that an increase in the degree of cross-correlation between transmissivity and effective thickness causes a decrease in the variability of the predicted groundwater travel times. Independence between

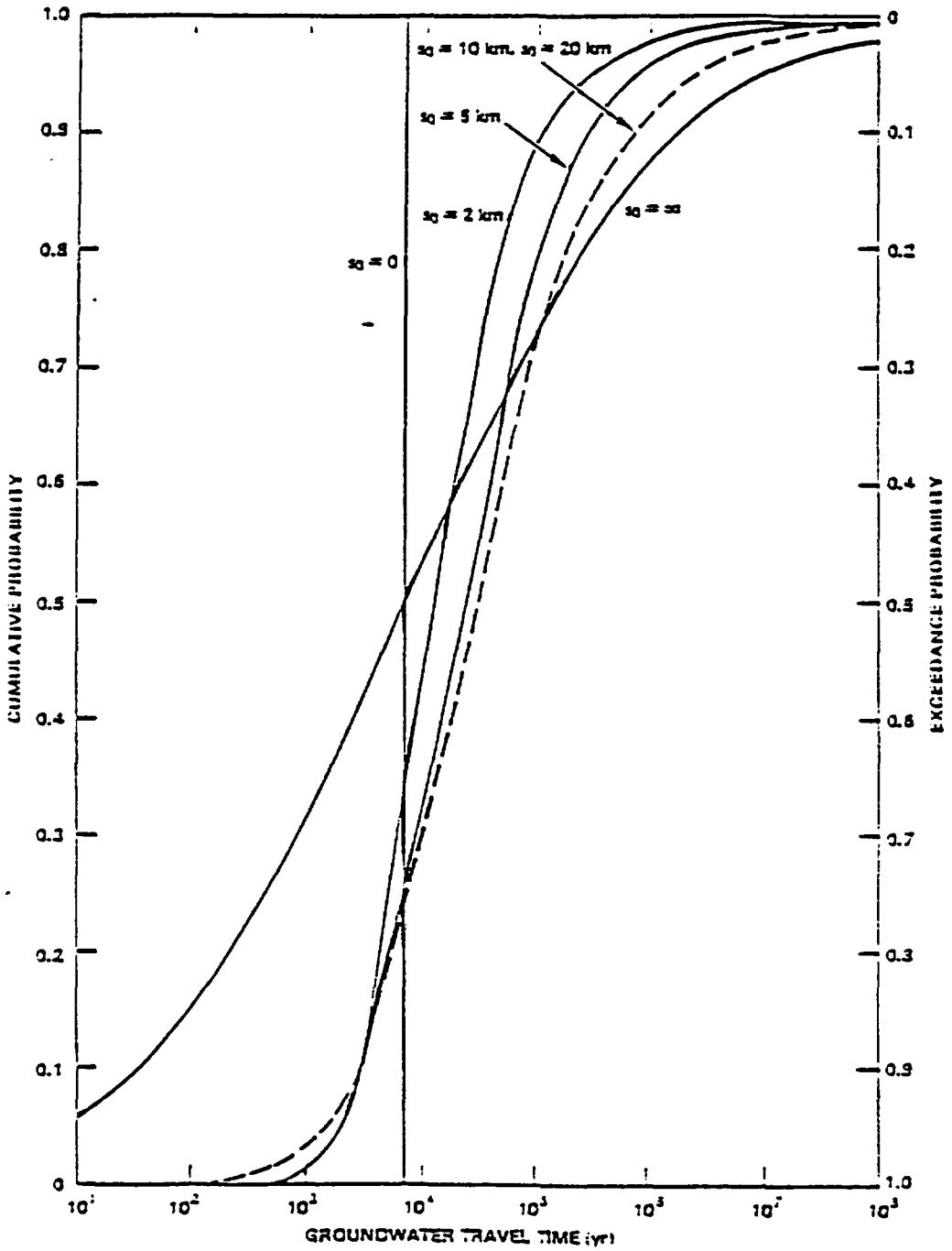


Figure 4.19. Effects of correlation scale of transmissivity on the cumulative probability of groundwater travel time. (From Clifton et al., 1985).

transmissivity and effective thickness results in a greater variability in the predicted travel times. The groundwater travel time distribution was found to be sensitive to the size of the model domain. The average travel time became longer as the width of the model domain decreased, and vice versa.

In summary, the results of the study by Clifton et al. (1985) shows that groundwater travel times are sensitive to parameters characterizing the spatial variability, the scale of representation of model parameters, and the size of model domain. A major technical drawback of the study is that the calculation of pathline was not clearly presented. This may have significant impacts on the accuracy of the predicted travel times, especially if the medium is heterogeneous. Comparisons of the relative importance of various factors on the groundwater travel time distribution was absent. This information would be helpful in the analysis of uncertainties in travel times. Overall, the results of the study are pertinent to the understanding of some sources of uncertainty in groundwater travel time calculations.

Another interesting analysis of uncertainties in groundwater travel times and paths due to sample size was carried out by Cole and Foote (1987). In their study, a hypothetical, two-dimensional, square aquifer with two realizations of hydraulic conductivity field was used. The first realization represented a real world analog of the hydraulic conductivity field. It was derived from a block of Nevada topographic data to ensure that it contained a variety of spatial correlation scales related in a natural way. The topographic data, which were nearly normally distributed, were scaled in order to allow them to represent a reasonable range for the logarithm of hydraulic conductivity. In the second realization, the hydraulic conductivity field was filtered using a simple moving average technique to remove the high spatial frequency perturbations in hydraulic conductivity data (i.e. small-scale variations in K). The filtered data could be viewed as the data collected from large-scale hydraulic tests in which small-scale phenomena are averaged out. The unfiltered log

K data set had a sample mean of 0.0814 and a standard deviation of 1.28, and the filtered data have a mean of 0.0821, and a standard deviation of 1.18. In Figure 4.20, a comparison of the unfiltered and filtered log K distribution along a cross-section is shown. The autocorrelation function for the data set was determined to be anisotropic. The longest axis of the correlation ellipse was nearly diagonal to the square aquifer, running from north to south. The anisotropy ratio of the correlation lengths was about 3. Two flow situations were examined: Case (1) east-west flow, where east and west sides of the square aquifer were assigned as prescribed head boundaries, and impermeable boundaries were assigned at the other two sides; Case (2) south-north flow, where south and north sides of the aquifer were assumed to be prescribed head boundaries and impermeable boundaries were set for the other two sides. The flow domain was discretized into 257x257 grids and hydraulic head and stream functions were calculated using a finite difference model for steady-state saturated flow. The convective velocity vector was calculated at each grid location from the stream function (or hydraulic gradient), hydraulic conductivity, and effective porosity. A particle tracking technique was used to determine groundwater travel times. Some of the results of the analysis are illustrated in Figure 4.21

Several conclusions were drawn from the results of the analysis by Cole and Foote (1987). The arrival times of 50% of the total number of particles in both Cases 1 and 2 were reduced if the filtered data set was used (Figure 4.21). The filtered hydraulic conductivity field produced a narrower arrival time distribution because filtering results in reducing the number of different pathways. According to Foote and Cole (1987), simulations using the filtered data tended to underestimate the first arrival of particles if flow was more nearly aligned with the longest correlation scale of the hydraulic conductivity field (Case 2), and to overestimate the time of arrival if flow was perpendicular to the direction of the longest correlation scale of the log K field (Case 1).

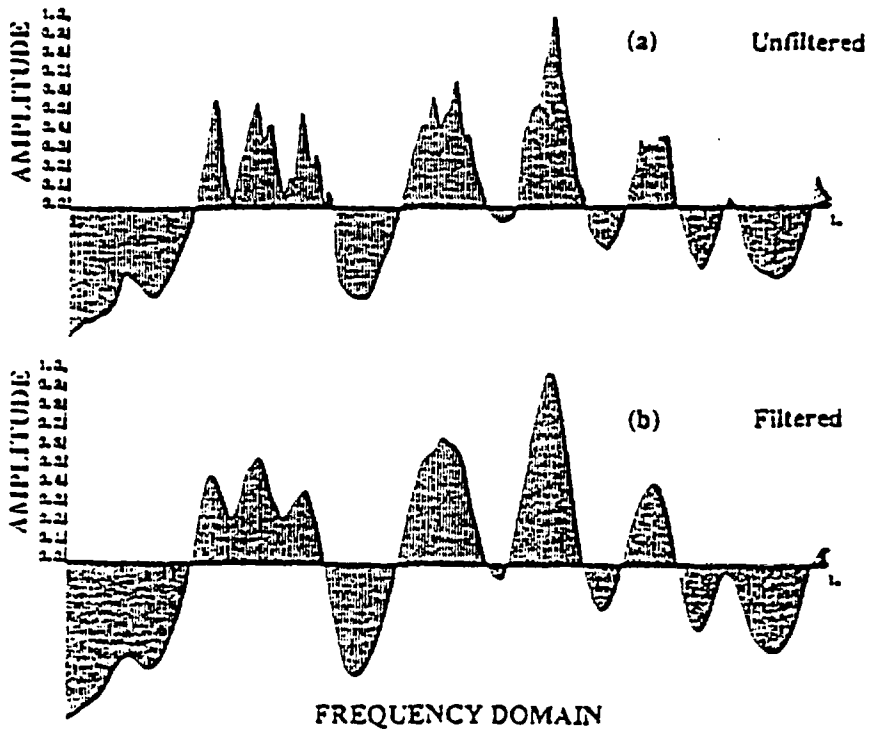


Figure 4.20. A comparison of the unfiltered (a) and filtered (b) log K data along a cross-section of a hypothetic aquifer. (Cole and Foote, 1987).

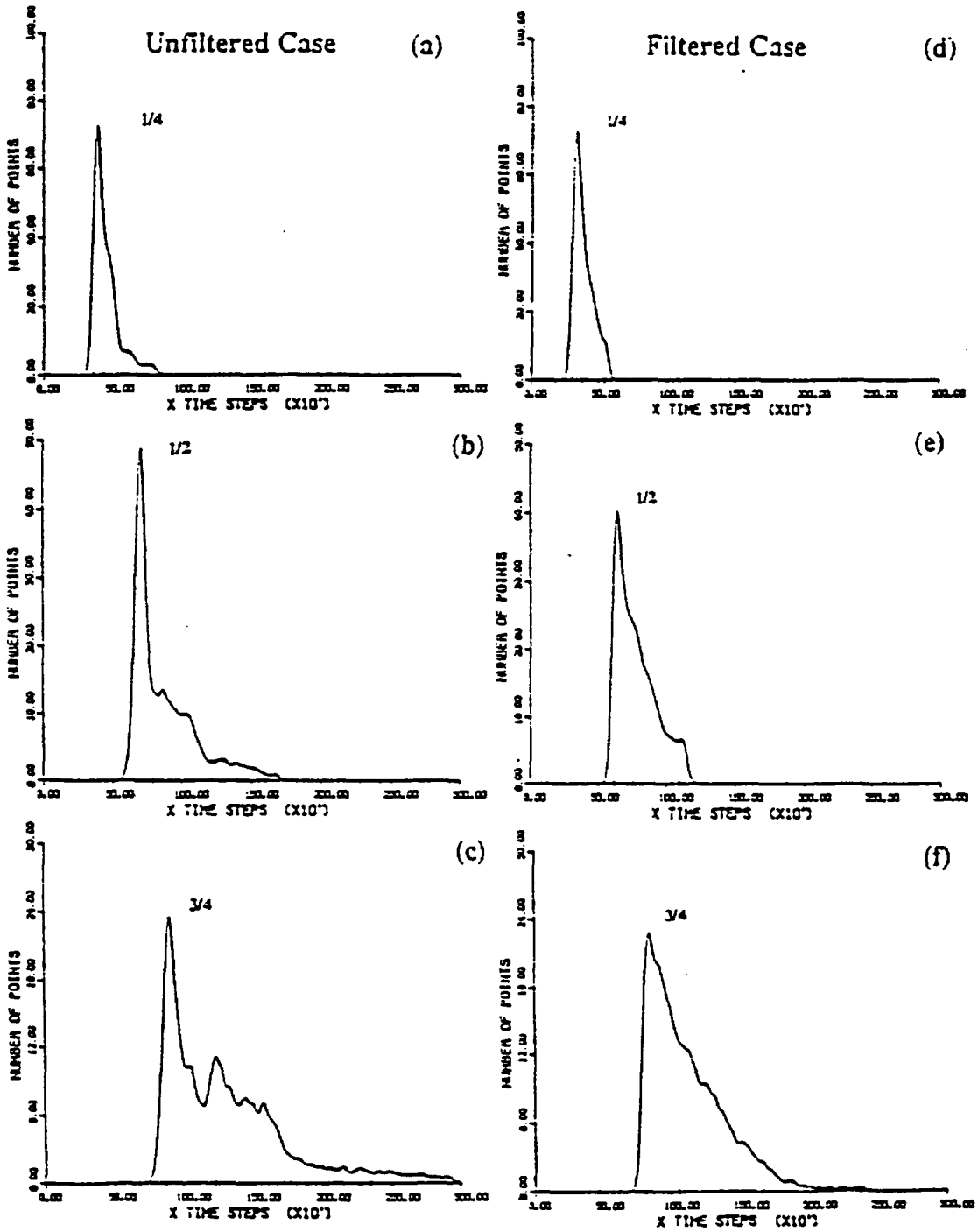


Figure 4.21. Particle arrival versus time curves (for the particles to travel 1/4, 1/2, and 3/4 of the distance across the domain) calculated for a pulse release of particles from a source in the east-west flow condition. Results are shown for the unfiltered data set (a-c) and for the filtered hydraulic conductivity data set (d-f). (Cole and Foote, 1987).

The results of the simulation are not conclusive because only two realizations of hydraulic conductivity fields (i.e., unfiltered and filtered) were employed. However, the effects of the REV assumption (i.e., the properties are uniformly distributed within the average volume), the scale of hydraulic testing, and size of spatial discretization in numerical simulations are well manifested in the analysis inasmuch as the filtering procedure is analogous to the averaging process in deriving hydraulic parameters from large-scale hydraulic tests. Similar spatial averaging procedures are often used in numerical models because hydraulic parameters assigned to each finite element or finite difference block represent the averaged values over the element or the block. These two conclusions agree with those by Clifton et al. (1985) (see Figure 4.18). The results of this study again demonstrate the problem with the groundwater travel times and paths concept.

As pointed out in section 2 dealing with basic concepts in groundwater hydrology, every property defined in groundwater hydrology involves a volume (REV). The property of the REV represents an average value over the volume, and the subscale variation in this property is ignored. The results of the analysis showed that ignoring the small-scale variability in hydraulic conductivity will result in underestimating the first arrival of tracer particles, overestimating the mean travel, and predicting a narrower arrival time distribution (Figure 4.18). Such effects may play a crucial role in regulating any nuclear waste repository facility, since the subscale velocity variation affects the fastest path by which groundwater travels. So, what is the proper volume for defining groundwater travel times and paths in order that the effects of subscale variations can be safely ignored? If one selects a volume that is large, then how do we account for subscale phenomena? On the other hand, if one selects a volume that is too small, then how do we characterize a large-scale aquifer with the properties defined over such a small volume? This is the dilemma we face if the concept of groundwater travel times and paths is to be used for

regulatory purposes.

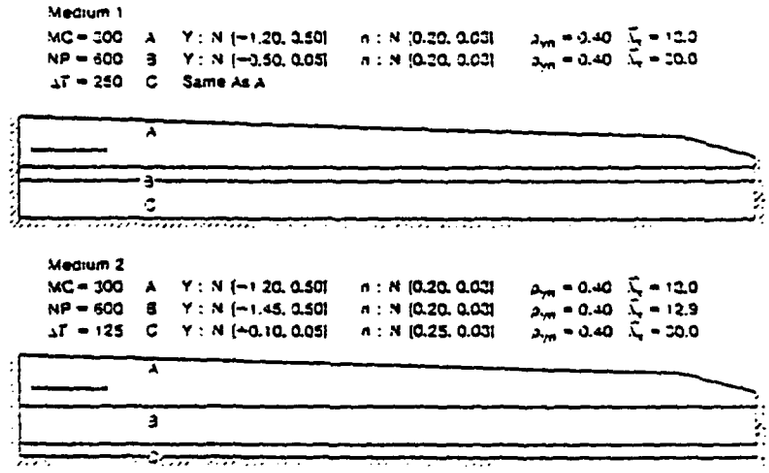
One of the key issues of the high-level nuclear waste repository site characterization program is determining if large-scale or small-scale hydraulic tests should be conducted to delineate the fastest path groundwater travel. This issue has been discussed earlier in various sections of this report, however, additional research addressing this issue has been presented by Smith and Schwartz (1981b). The objective of their study is to investigate the uncertainty in predicting mass transport due to three sources of uncertainties in data input to a model: (1) uncertainties due to the unknown spatial variation of the medium parameters, (2) uncertainties inherent in the particular model chosen to account for the heterogeneity, and (3) uncertainties related to the boundary conditions imposed on the flow domain.

A hypothetical water table aquifer was studied where the sides and bottom were assumed to be no-flow boundaries for both water and solute, and the water table represented the upper boundary for the region. A particle tracking model (Smith and Schwartz, 1980) was used to simulate the transport of a tracer in this aquifer. Monte Carlo simulation was used to form estimates of the probability distributions on model output. Hydraulic conductivity and porosity values of the aquifer were assumed to be statistically homogeneous, and their spatial structure was represented by a nearest-neighbor model (Smith and Freeze, 1979a). Furthermore, hydraulic conductivity and porosity were considered to be correlated and lognormally and normally distributed, respectively. Three hundred realizations of hydraulic conductivity and porosity fields were analyzed for transport of 600 particles. Statistics (mean and standard deviation) were computed for the first and last arrival times, as well as, for the arrival time of the maximum mass.

Most of the results are similar to those by Clifton et al. (1985), and Cole and Foote (1987). However, Smith and Schwartz (1980) also investigated cases where large, recognizable, geologic structures (such as stratifications) were present. The

aquifer consisted of layers of two distinct materials (sand and silt). Within each layer, hydrologic properties were assumed to be statistically homogeneous processes. Figure 4.22 shows the schematic diagram of the layered geologic formations with thin, relatively uniform higher-conductivity layers used in their simulation experiments. Table 2 summarizes the statistics of simulation results for the two scenarios shown in Figure 4.22. Results of the simulations showed that the fraction of mass which moves relatively quickly into the higher conductivity bed determined the initial arrival statistics. Because a small standard deviation in log hydraulic conductivity was assigned to the bed, the result is a smaller standard deviation in the initial arrival time than that in non-layered case. However, uncertainties in predicted arrival times can still be fairly large because of the sensitivity of transport to the within-layer heterogeneity. Again, this result is supportive of the position of this report on the importance of subscale variability. The result also sheds light on the high-level nuclear waste repository site characterization program. Large-scale permeable formations have to be identified by geologists or hydrogeologists as suggested by Williams (1988). However, small-scale tests are also necessary in order to define the variability within the formations. The subscale variability should then be treated stochastically.

Schwartz et al. (1983) employed a Monte Carlo technique to analyze macroscopic dispersion in fractured media. Mass transport in hypothetical two-dimensional, fractured aquifers was simulated using a particle tracking technique. Fractures in the aquifers are represented as linear features defined in terms of the location in space of their midpoints, their orientation with respect to the coordinate axes, their length, and their aperture. Some of these parameters were considered as random variables in the analysis. The fracture length distribution was assumed to have a negative exponential distribution. The distribution of fracture aperture was considered to be lognormal. Flow in the fractures was idealized as laminar flow



MC = number of realizations
NP = number of particles
ΔT = time step
Y:N[-1.20, 0.50] = log K; normally distributed with mean -1.20 and standard deviation 0.50
n = porosity
ρ_{yn} = cross-correlation between log K and n
$\bar{\lambda}_x$ = average correlation scale in the x direction

Figure 4.22. Schematic diagram of the layered geologic media with thin, relatively uniform higher conductivity layers used in the simulation experiments. (Smith and Schwartz, 1981).

Table 2. Comparison of transport behavior in systems with thin, relatively uniform higher conductivity layers extending across the basin. (Smith and Schwartz, 1981).

	Medium 1	Medium 2
Initial arrival		
$\bar{t}_i$	7.240	3.590
S_{t_i}	1.630	660
Time of maximum mass		
$\bar{t}_{max}$	11.440	4.240
$S_{t_{max}}$	5.760	1.050
Last arrival		
$\bar{t}_f$	32.200	7.740
S_{t_f}	7.310	2.590
Maximum mass at water table		
M_{max}	30.2	48.4
$S_{M_{max}}$	15.3	18.5
Mean location of arrival		
$\bar{z}$	299.0	299.4
$S_{\bar{z}}$	4.4	1.5
Standard deviation in location		
$\bar{S}_z$	1.0	0.4
Minimum location		
$\bar{z}_{min}$	294.9	298.0
$S_{z_{min}}$	20.4	3.3

through smooth parallel plates so that the cubic law which relates fracture hydraulic conductivity to fracture aperture could be applied. Sets of fractures were generated in a rectangular, two-dimensional aquifer with the assumption that the rock matrix had zero permeability. The aquifer was bounded by two constant head and two no-flow boundaries. A finite difference model was used to determine the hydraulic head distribution, and mass transport was then simulated using a particle tracking technique. The results of the study showed that the mass transport phenomena in fracture rocks are so complex that the classical macroscopic convection-dispersion equation does not seem to be appropriate. A single value of dispersivity or dispersivity function does not appear to characterize correctly the pattern of mass spreading in a fracture system.

4.3.2 Conditional Simulation. Conditional simulation is a special kind of Monte Carlo simulation technique. Unlike the Monte Carlo simulation discussed above, it imposes sample values at the sample points. That is, in each realization, parameter values are kept constant and equal to the measured values at a particular location. Thus, there will be no uncertainty at measurement points.

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 is shown in Figure 4.23. Briefly, the procedures of the conditional simulation are: (1) to generate nonconditional 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 of the simulations obtained in the first step by making the realizations consistent with the measured sample values. The first step is identical to the Monte Carlo simulation. For the second step, one has to employ kriging. From the actual sample values, kriging yields an estimate $K^*(x)$ (Figure 4.23a). If x is not a sample point, the true value K(x) is not available, and the kriging error $K(x) - K^*(x)$ remains unknown. However, the true value, K(x), equals the estimate plus the error in the estimate which we can write as:

$$K(x) = K^*(x) + [K(x) - K^*(x)] \tag{4.3.1}$$

Kriging can be performed using the measured values at the actual sample locations as data in a given nonconditional simulation (Figure 4.23b). The sample value of the given nonconditional simulation S(x) can be decomposed as the sum of the kriging estimate $S^*(x)$ and the kriging error, i.e., $S(x) = S^* + [S(x)-S^*(x)]$. Since this is derived from the nonconditional simulation, all terms are known. Note that $[S(x) - S^*(x) = 0]$ at the sample locations. By substituting $S(x)-S^*(x)$ for $K(x)- K^*(x)$, the

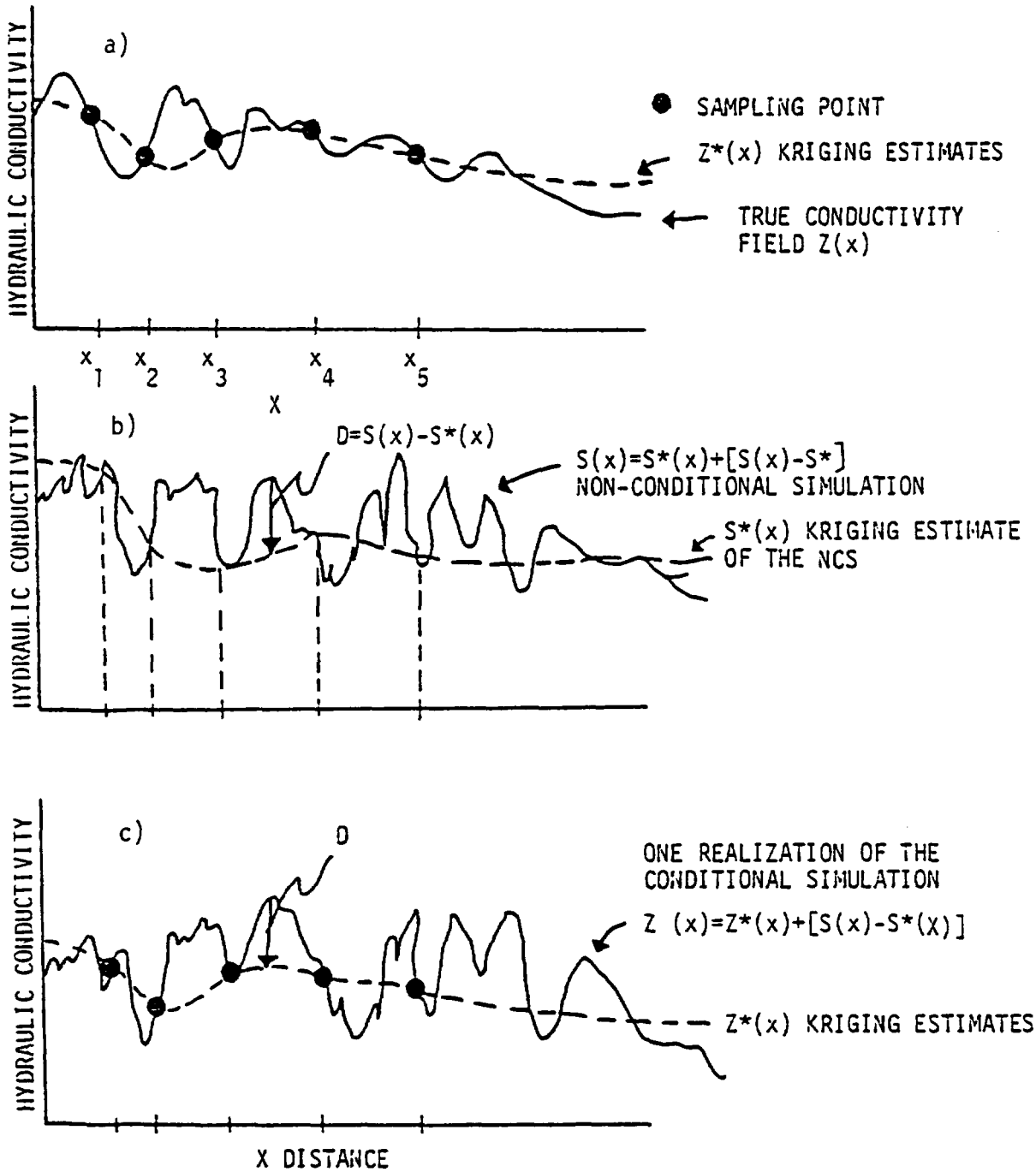


Figure 4.23. A schematic illustration of the conditional simulation.

K_s (x) for the conditional simulation is defined as:

$$K_s(x) = K^*(x) + [S(x) - S^*(x)] \qquad (4.3.2)$$

Therefore, K_s (x) is consistent with the measured values at the sample points, K_s (x) and K(x) have the same covariance functions. The average of many conditional simulations at a given point x is the kriging estimate, and their variance is the kriging variance.

Generally speaking, hydraulic property fields resulting from conditional simulation are; (1) smoother than unconditioned fields, but (2) more variable than kriged fields which essentially represent the conditional expected values.

The first application of conditional simulation to groundwater hydrology probably was the work by Delhomme (1979). He used 45 transmissivity data collected in the Bathonian aquifer in Normandy to investigate the effect of conditioning transmissivity values at sample locations on the uncertainty of the hydraulic head distribution. The first case he examined was steady- state flow through a rectangular hypothetical aquifer 10 km in length and 7.5 km in width. The aquifer was bounded by three impermeable boundaries and one constant head boundary. A uniform recharge over the aquifer area was assumed. Transmissivity values were considered to have a lognormal distribution with a spherical semivariogram as the spatial correlation structure. Thirty sample values were used with kriging to estimate the transmissivity at unsampled nodes of a 0.25 x 0.25 km regular grid. Fifty realizations of the logarithm of transmissivity (log T) fields incorporating the 30 samples were generated. Then, 50 head surfaces corresponding to the 50 transmissivity conditional simulations were produced by a numerical model. The results of the simulation indicated that conditioning by 30 log T samples did not lead to any significant decrease in uncertainty in head values at the center of the

aquifer. This was attributed to the fact that these 30 log T values were sampled far away from the outflow boundary which was a major controlling factor of the flow regime. Conclusions drawn from this study illustrate: (1) the importance of the locations of the log T samples with respect to the boundary conditions, and (2) that knowledge of head values at some locations and recharge rates. In addition, conditioning log T values may be helpful in reducing uncertainties in predicting hydraulic head values in heterogeneous aquifers.

Case 2 of the study by Delhomme (1979) is the Bathonian aquifer where it is bounded to the north by the sea. Steep hydraulic gradients occur in the southern part of the area which are due to local dewatering of mines. Discharge from wells, rainfall infiltration, interaction with streams, and leakage to or from overlying and underlying aquifers were considered in the simulation. Two possible sources of uncertainty on transmissivity were considered: (1) spatial variability and scattered sampling, and (2) measurement errors in T sample values. A similar approach to Case 1 was used. The conclusions drawn from the results of the analysis of Case 2 are: (1) the head surface cannot be reconstructed correctly from only the sample values of T, and (2) constraints on some head values tend to improve the agreement between simulated and observed head surfaces, without the transmissivity field necessarily being correct. Again, the flow rates to and from boundaries play important roles in reconstructing the head surface. Delhomme finally concluded that using conditioning on both head and log T values may be necessary in order to reduce the uncertainty in predicting the true head surface.

Conditional simulations pertinent to NRC's definition of groundwater travel time and path criterion were conducted by Smith and Schwartz (1981). They used this technique to study the role of hydraulic conductivity data in reduction of uncertainty in prediction of mass transport. Two cases were examined. In Case 1, they investigated the extent to which uncertainties in transport predictions are

reduced when hydraulic conductivity data act to constrain the possible arrangement of the heterogeneities. In Case 2, they investigated uncertainties in transport predictions using a hydraulic conductivity distribution estimated from a limited set of data.

In the first case, a hydraulic conductivity distribution along a two-dimensional, vertical cross-section of a hypothetical water table aquifer was generated using the nearest-neighbor model. They assumed statistical parameters (mean and variance) to characterize the variability of conductivity. This realization was assumed to be an analog of the site. Hydraulic conductivity values were sampled in this realization on a preselected grid, and this data set was used to estimate the parameters of the hydraulic conductivity distribution. The movement of contaminants from a hypothetical waste repository was simulated to determine various arrival times as solute mass exited from the aquifer.

As we described in the previous section (4.3.1), Monte Carlo simulations (300 realizations of hydraulic conductivity fields) were carried out based on the estimated statistical parameters without considering the conditioning at the sample grid using sample data. The movement of a swarm of 600 particles in each hydraulic conductivity realization was simulated using a transport model. The mean and coefficient of variation (i.e., standard deviation/mean) for each of the times of initial, maximum mass, and last arrival resulting from the 300 possible realizations were then analyzed. The results of this analysis represent the uncertainty in prediction. A small subset of the hydraulic conductivity values was sampled from the analog of a real-world site and was then used to constrain the hydraulic conductivity values at the sample locations. Three sample grids were used: Grid A had 12 sampling points, Grid B, 24 points, and Grid C, 36 points. Three hundred hydraulic conductivity fields were simulated in which the hydraulic conductivity values are identical to the sample values at the sample points.

Again, the mean and coefficient of variation for each of the arrival time distributions were analyzed. A comparison of the means and coefficients of variation of the unconditional and conditional simulations determined the effect of knowledge of hydraulic conductivity values at sample locations on uncertainty in prediction. That is, a decrease in the coefficient of variation can be taken as a measure of the reduction in the uncertainty in prediction. Effects of varying the number of samples were investigated. Surprisingly, for their data base, results of unconditional and conditional simulations indicated that knowledge of additional hydraulic conductivity data did not lead to large reductions in the uncertainty in the velocity field. This result is relevant to identifying uncertainties in groundwater travel time and in assessing data needs for site characterization.

The conditional simulations in Case 2 of Smith and Schwartz (1981) proceeded as follows. From a specified stochastic process with given parameters, a hydraulic conductivity field was constructed. Hydraulic conductivity values were sampled from this realization on a preselected grid, and this data set was used to estimate the parameters of the hydraulic conductivity distribution. A second realization was generated using these estimated parameters, while the hydraulic conductivity values were preserved at the measurement points. Mass transport was then simulated in this second realization. This two-step procedure was repeated over a set of trials in a Monte Carlo simulation to form the probability distributions of the arrival times.

Distinct differences exist between Cases 1 and 2. In Case 1, the parameters of the hydraulic conductivity distribution were estimated from the hydraulic conductivity values located on the sample grid. These estimated parameters and the data set were then fixed for all the realizations in that Monte Carlo experiment. For the simulation in Case 2, the estimated parameters of the stochastic process varied with each realization, as different sets of hydraulic conductivity values are located on

the sample grid. The statistical parameters estimated from the available hydraulic conductivity data are different from those prescribed as the properties of the ensemble. Thus, errors in estimating the parameters add additional sources of uncertainty in prediction. That is, a ratio formed between the coefficient of variation for the arrival times in the Case 2 simulations and a corresponding unconditional simulation will indicate the extent to which uncertainties are increased in estimating the mean and standard deviation in hydraulic conductivity. The larger the value of this ratio, the greater the importance of uncertainties in estimating the statistical parameters relative to the uncertainty introduced due to the unknown patterns of spatial variation in hydraulic conductivity. Table 3 summarizes the ratio for selected transport parameters for the Case 2 simulation. All the ratios are greater than 1, indicating additional uncertainties due to uncertainty in estimating the ensemble statistical parameters. However, such uncertainties are reduced as the number of samples increases.

A general conclusion drawn from the study by Smith and Schwartz (1981) is that unless a considerable number of field measurements are available to constrain the patterns of spatial variation in hydraulic conductivity, large uncertainties can be associated with seepage velocities. Individual hydraulic conductivity measurements do not reduce the uncertainty significantly because of the dependence of the local hydraulic gradient on the overall arrangement of heterogeneities within the flow domain. Smith and Schwartz (1981) suggested that more emphasis should be placed on in situ measurements of seepage velocity (fluid particle velocity). However, seepage velocity generally varies with time, and it is difficult to take any measurement in the field due to slow movement of groundwater. Therefore, their suggestion may not be practical. Finally, they emphasized that a careful selection of sample locations should focus on regions where the uncertainty in the seepage velocity is greatest. A carefully designed, integrated sampling program may play an

Table 3. Ratios of the coefficients of variation in various arrival times resulting from the conditional simulation to those from the unconditional simulation in Case 2 study (Smith and Schwartz, 1981).

	Sample Grid		
	A	B	C
Initial arrival	1.44	1.12	1.03
Time of maximum mass	1.59	1.22	1.13
Last arrival	1.61	1.32	1.30

Here $\mu_y = -1.45$, $\sigma_y = 0.50$, $\bar{\lambda}_x = 12.5$, $\bar{\lambda}_z = 6.3$.

important role in the reduction of uncertainties in solute transport predictions.

4.3.3 Spectral Analysis. Spectral analysis is generally an analytical approach which includes perturbation analysis. This approach has been used extensively by Gelhar and his co-workers (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, and c; Mantoglou and Gelhar, 1987a, b, and 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:

$$\frac{\partial}{\partial x_i}\left[K\frac{\partial h}{\partial x_i}\right] = 0, \qquad i=1,2,3 \tag{4.3.3}$$

where K is the 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 (4.3.3) can be rewritten as:

$$\frac{\partial^2 h}{\partial x_i \partial x_i} + \frac{\partial \ln K}{\partial x_i}\frac{\partial h}{\partial x_i} = 0 \tag{4.3.4}$$

If the natural log of hydraulic conductivity, lnK, and the hydraulic head, h, are assumed to be second-order stationary stochastic processes, the equation becomes a stochastic partial differential equation, and lnK and h can be represented by means and perturbations of these values about their means:

$$h = H + h' \qquad E[h] = H, \text{ and } E[h'] = 0 \tag{4.3.5a}$$

$$\ln K = F + f \qquad E[\ln K] = F, \text{ and } E[f] = 0 \tag{4.3.5b}$$

where H and F are the means of h and lnK, respectively. The perturbations are h' and f for h and lnK, respectively. By substituting the representations (equation 4.3.5) in equation (4.3.4), and taking the expected value of it, we obtain a mean equation:

$$\frac{\partial^2 H}{\partial x_i \partial x_i} + \frac{\partial F}{\partial x_i} + \frac{\partial F}{\partial x_i}\frac{\partial H}{\partial x_i} + E\left[\frac{\partial f}{\partial x_i}\frac{\partial h'}{\partial x_i}\right] = 0 \qquad (4.3.6)$$

Substracting the mean equation from equation (4.3.4) gives:

$$\frac{\partial^2 h'}{\partial x_i \partial x_i} + \frac{\partial f}{\partial x_i}\frac{\partial H}{\partial x_i} + \frac{\partial F}{\partial x_i}\frac{\partial h'}{\partial x_i} - E\left[\frac{\partial f}{\partial x_i}\frac{\partial h'}{\partial x_i}\right] + \frac{\partial f}{\partial x_i}\frac{\partial h'}{\partial x_i} = 0 \qquad (4.3.7)$$

If we assume that the log hydraulic conductivity perturbation f is small (aquifer is not highly heterogeneous, say, $\sigma_f^2 < 1.5$ (Ababou et al., 1988), it is logical to expect the head perturbation h will be small. Then, it is reasonable to neglect higher order terms so that the perturbation equation can be written as:

$$\frac{\partial f}{\partial x_i}\frac{\partial H}{\partial x_i} + \frac{\partial F}{\partial x_i}\frac{\partial h'}{\partial x_i} + \frac{\partial^2 h'}{\partial x_i \partial x_i} \cong 0 \qquad (4.3.8)$$

This approximate equation describes the relationship between the perturbations in lnK 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 (4.3.4) with stochastic parameters is tantamount to ignoring the details of the flow behavior in each element but examining the average behavior of the flow in all the interconnected elements. The perturbation equation thus depicts the deviation of the flow from the mean flow only.

Now, the problem is how to solve the perturbation equation (4.3.8) and here the spectral method comes into the play. The spectral representation theorem (Lumley and Panofsky, 1964) states that if a stochastic process y(x) is second-order stationary, there is an essentially unique complex-valued, random distribution Z(k) on the frequency axis such that:

$$y(x) = \int_{-\infty}^{\infty} e^{ikx} dZ(k) \tag{4.3.9}$$

where i is a complex number and dZ is a generalized derivative of Z(k). Equation (4.3.9) is an example of a Fourier-Stieltjes integral. Furthermore, this process Z(k) represents complex-value random variables in a wave number k domain. In addition, this Z(k) process is related to covariance behavior as discussed below. More specifically, equation (4.3.9) simply is the inverse Fourier transform of Z(k), or Z(k) is the Fourier transform of the variable y(x) in the spatial domain. By doing this transformation, we have tranformed the variable from the spatial domain to the wave number domain. A physical analogy can be drawn with the effect of a glass prism on sunlight, as shown in Figure 4.24. A beam of white light can be regarded as a complex wave form changing with time, and composed of many colors (or wavelengths) of light. A prism acts as a frequency analyzer and separates the beam into its components, which appear as a rainbow display. Each colored band is separated from its neighbor by an amount proportional to the difference in their

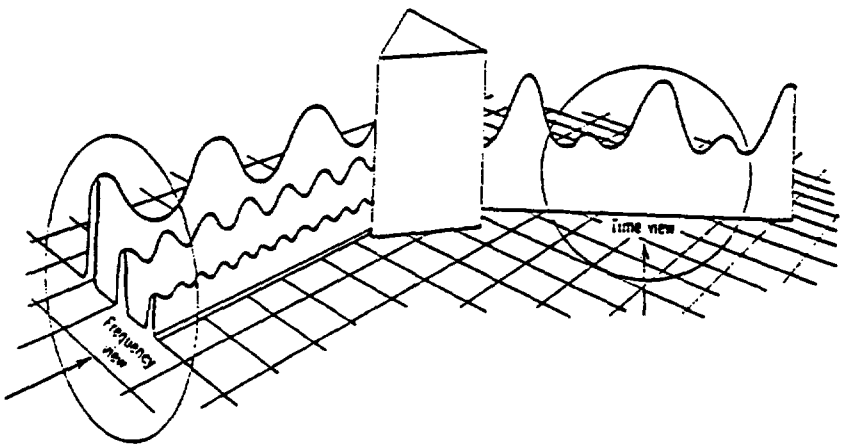


Figure 4.24.. A prism acts as a frequency analyzer, transforming white light (time domain) into its constituent spectrum of colors (frequency domain). Note the signals in the frequency domain are uncorrelated. (Davis, 1973).

wavelengths or frequencies, and the intensity of each band is proportional to the contribution of that particular wavelength to the total intensity of the original beam. Examining the spectrum of a light source may tell us many things: the composition of the source, its temperature, nature of the material through which the light passed, and so forth.

By the same token, examining the spectrum of spatial data may tell us a great deal about its nature and origin, information which may not be apparent in any other way. However, in this spectral analysis, the purpose of taking the Fourier tranform of the spatially correlated process y(x) is that after the transformation, Z(k) has been separated from its neighbor so that it is uncorrelated and the mathematics become easlier. Since Z(k) is uncorrelated, it has the following properties:

$$E[dZ(k_1)dZ^*(k_2)] = 0, \qquad \text{if } k_1 \neq k_2$$
$$E[dZ(k_1)dZ^*(k_2)] = S(k) \qquad k_1 = k_2 \tag{4.3.10}$$

where dZ^* is the complex conjugate, and S(k) is the spectrum of y which is merely the Fourier transform of its autocovariance function:

$$S(k) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-ik\xi}\, c(\xi)\, d\xi \tag{4.3.11}$$

Therefore, the inverse Fourier transform of the spectrum S(k) thus gives:

$$\text{cov}[\ y(x+\xi)', y(x)\ ] = c(\xi) = \int_{-\infty}^{\infty} e^{ik\xi}\, S(k)dk \tag{4.3.12}$$

Using the representation theorem for the perturbation terms f and h', and assuming uniform flow, equation (4.3.8) can be rewritten in terms of dZ processes:

$$dZ_h = \frac{iJ\ dZ_f}{k} \tag{4.3.13}$$

where J is the mean gradient in the x direction, $\partial H/\partial x$ and is assumed to be constant. Using the properties of the dZ processes, one can derive the relationship between the input and output spectrums, $S_{h'h'}$ and S_{ff}, respectively. That is:

$$S_{h'h'} = J^2 \frac{S_{ff}}{k^2} \tag{4.3.14}$$

By applying the inverse Fourier transform to the above equation, one thus obtains the head covariance functions, $c_{h'h'}(\xi)$, in terms of the hydraulic conductivity covariance function, $c_{ff}(\xi)$. If one uses a simple stationary three-dimensional covariance function for lnK, i.e.:

$$c_{ff}(\xi) = \sigma_f^2 \exp\left[-\left[\xi_1^2/\lambda_1^2 + \xi_2^2/\lambda_2^2 + \xi_3^2/\lambda_3^2 \right]^{1/2} \right] \tag{4.3.15}$$

where λ_1, λ_2, and λ_3 are the correlation scales in x_1, x_2, and x_3 respectively, the corresponding spectrum is

$$S_{ff}(k) = \frac{\sigma_f^2\ \lambda_1\lambda_2\lambda_3}{\pi^2 k^4 (1 + k^2\lambda^2)^2} \tag{4.3.16}$$

If we assume the hydraulic conductivity covariance function is isotropic (i.e., $\lambda_1 = \lambda_2 = \lambda_3$) and take the Fourier transform of (4.3.14), the head variance, $\sigma^2_{h'}$, is related to the variance of the hydraulic conductivity, σ^2_f , by:

$$\sigma^2_{h'} = c_{h'h'}(0) = \frac{1}{3} J^2 \sigma_f^2 \lambda^2 \tag{4.3.17}$$

The variance equation, (4.3.17), provides us with information on how the spatial variation in hydraulic conductivity affects the spatial variation in hydraulic head. In other words, it provides us with a measure of the deviation of hydraulic head from its mean value predicted using an effective hydraulic conductivity.

The spectral approach is also useful for deriving the effective hydraulic conductivity for such a stochastic random porous medium. To derive the effective hydraulic conductivity, we will again conceptualize the heterogenoeus aquifer as a collection of many finite elements with spatially correlated hydraulic conductivity values in which the flux is assumed to obey Darcy's law. Thus, the average flux over the entire heterogeneous aquifer then becomes the expected value of all the fluxes from each individual element within the aquifer. That is:

$$E[\, q_i \,] = -E\left[K \frac{\partial h}{\partial x_i} \right] = -E\left[K_g \, e^f \left(\frac{\partial H}{\partial x_i} + \frac{\partial h'}{\partial x_i} \right) \right] \tag{4.3.18a}$$

Using a series expansion for e^f, (4.3.18a) becomes:

$$= -K_g \, E\left[\left(1 + f + \frac{f^2}{2} + \cdots \right) \left(\frac{\partial H}{\partial x_i} + \frac{\partial h'}{\partial x_i} \right) \right]$$

$$= K_g \left[J_i \left(1+\frac{\sigma_f^2}{2}\right) - E\left[f\left(\frac{\partial h'}{\partial x_i}\right)\right]\right] \tag{4.3.18b}$$

where $K = K_g \exp(f)$ with $E(\ln K) = \ln K_g$. Equation (4.3.18b) represents the average of fluxes in all elements, or the ensemble average of the fluxes. The last term on the right-hand side of equation (4.3.18b), representing the cross-correlation between the log hydraulic conductivity and the hydraulic gradient perturbations, can be evaluated using the representation theorem as well. If we assume that Darcy's law (i.e., flux has to be linearly proportional to the hydraulic gradient) is valid for this ensemble flux, then:

$$E[\ q_i\ ] = K_{eff}\ J_i \tag{4.3.19}$$

where J_i is the mean gradient in direction i (i.e., $\partial H/\partial x_i$) and K_{eff} is the effective hydraulic conductivity. Based on equation (4.3.19), K_{eff} is merely a constant of proportionality between the ensemble flux and the mean gradient. In other words, K_{eff} is a parameter which produces the mean flux with the knowledge of the mean hydraulic gradient. By comparing equations (4.3.18) and (4.3.19), it is easy to see that:

$$K_{eff} = K_g \left[\left(1+\frac{\sigma_f^2}{2}\right) - \frac{E[f(\partial h'/\partial x_i)]}{J_i} \right] \tag{4.3.20}$$

As indicated in equation (4.3.20), the effective hydraulic conductivity clearly lumps together the variability of lnK, σ_f^2, and the covariance of f and $\partial h'/\partial x_i$, $E[f(\partial h'/\partial x_i)]$,

which varies with flow. Therefore, the effective hydraulic conductivity is not a simple arithmetic average of all hydraulic conductivity values of individual elements, but it depends on the flow regime as well.

Using the spectral technique discussed above, Bakr et al. (1978) analyzed the effects of spatial variability on steady-state groundwater flow. Closed forms of head variance expressions were derived for one- and three-dimensional flow fields in which hydraulic conductivity is a spatially-varying stochastic process. Several important conclusions were drawn from the results of the study. Hydraulic head distribution tends to be smooth due to the damping effect of the groundwater flow system. That is, the head values are correlated over a much longer distance than the hydraulic conductivity values. The head values are anisotropic (i.e., correlated over a longer distance in the direction perpendicular to the flow direction.), even if the hydraulic conductivity field is statistically isotropic. The head variance can be related to the variance of lnK by:

$$\sigma_{h'}^2 = \beta\sigma_f^2 \, J^2 \, \lambda^2 \tag{4.3.21}$$

where β is a constant: 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 logarithms of hydraulic conductivity, and λ is the correlation scale. The equation indicates that the variability in head predicted by a three-dimensional model is smaller than that predicted by a one-dimensional model. This means that a three-dimensional model would be much more appropriate for analyzing uncertainties in groundwater travel times and paths. Furthermore, it is manifest from equation (4.3.21) that studying the correlation scale is important in the calculation of head variance or uncertainty in head prediction as discussed in the section dealing with Monte Carlo simulation.

Gutjahr et al. (1978) extended Bakr's study to define effective hydraulic conductivity for heterogeneous lnK fields. They concluded that the effective hydraulic conductivity in one-dimensional flow, perpendicular to layerings, is the harmonic mean:

$$K_e = K_g \, e^{-\sigma_f^2/2} \tag{4.3.22}$$

where K_g is the geometric mean of K, and σ_f^2 is the variance of lnK, and the arithmetic mean for flow parallel to beddings, i.e.:

$$K_e = K_g \, e^{\sigma_f^2/2} \tag{4.3.23}$$

In the three-dimensional flow situation, the effective hydraulic conductivity is given by:

$$K_e = K_g \, e^{\sigma_f^2/6} \tag{4.3.24}$$

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.

Both analyses by Bakr et al. (1978) and Gutjahr et al. (1978) assumed statistical isotropy for the random hydraulic conductivity field. Gelhar and Axness (1983) extended the analyses by Bakr et al. (1978) and Gutjahr et al. (1978) to investigate 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 4.25 shows that the anisotropy ratio for the case with $\lambda_1 = \lambda_2 \neq \lambda_3$ is dependent on the degree of variability of hydraulic conductivity in terms of the variance of lnK as well as the geometry of the heterogeneity as characterized by the ratio of λ_1/λ_3.

The effective hydraulic conductivities and head variance derived from the spectral analysis may have important practical implications on the prediction of groundwater travel times and paths. Generally speaking, there is a limited number of hydraulic conductivity values available for determining accurately the groundwater travel times and paths. As a first step toward solving such a complex problem, one may use the limited amount of data to determine the variance of lnK, and thus the effective hydraulic conductivity, using one of the equations (4.3.22), (4.3.23), or (4.3.24), depending on the dimensionality of the model. The mean flow behavior thus can be determined. Correlation scales can be estimated from the available data by using autocorrelation analysis. With an estimated mean gradient, variance of lnK, and correlation scales, the head variance in a statistically isotropic medium can then be determined, using equation (4.3.21). If there is no hydraulic conductivity data available, one might be able to resort to the known variances and correlation scales of similar kinds of materials reported in the literature (see table 2). The calculated head variance can be used as a measure of the error in the model as the result of unmodeled aquifer heterogeneity (i.e., the result of using effective hydraulic conductivity). Therefore, the head variance is an appropriate model calibration target to study for defining the detailed hydraulic conductivity distribution, provided that other sources of error are also considered. The hydraulic conductivity field obtained from the calibration may then be used to determine groundwater travel times and paths. A similar application of the above spectral results to field problems was also illustrated in the paper by Gelhar (1986).

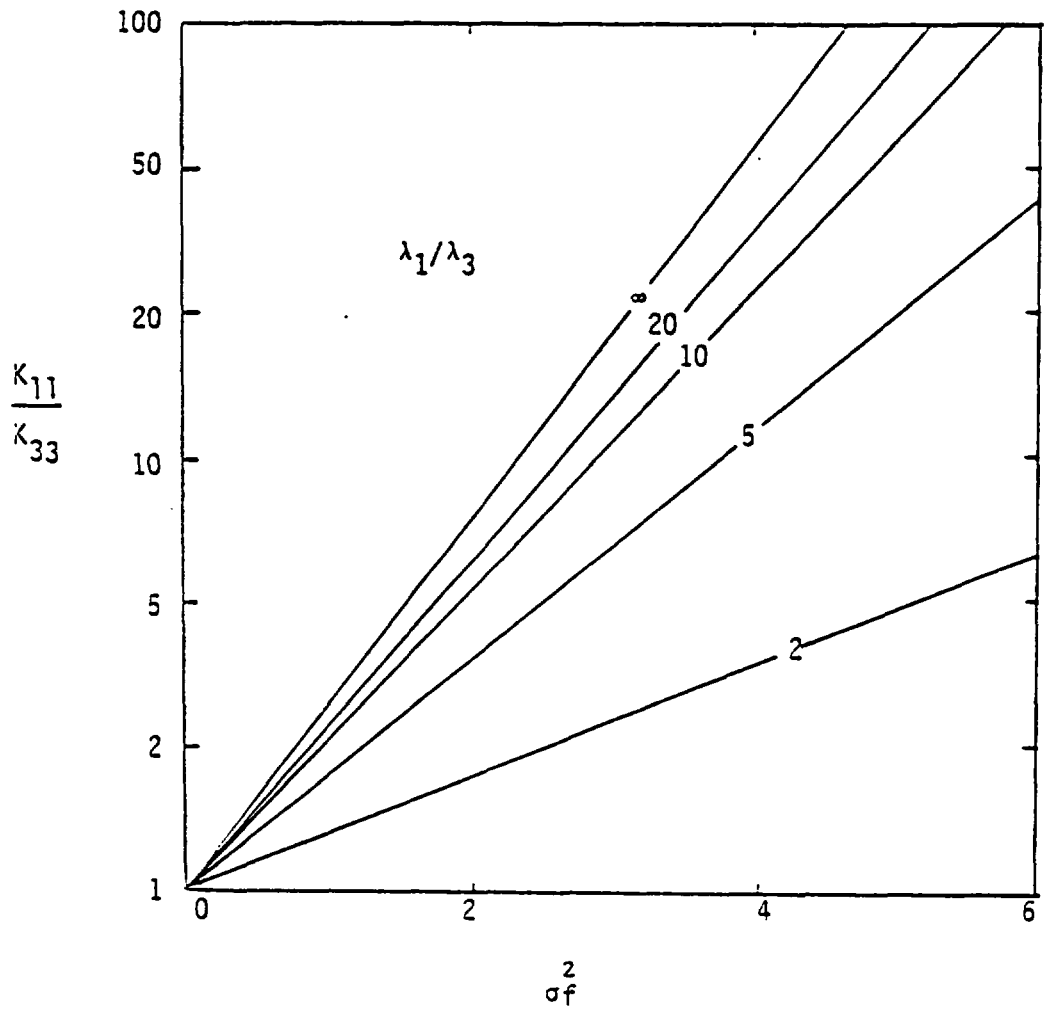


Figure 4.25. Anisotropy of effective hydraulic conductivity as a function of the variance of lnK, σ^2_f, and aspect ratio, λ_1/λ_3, for the case $\lambda_1=\lambda_2$. K_{11} and K_{33} are the principal effective hydraulic conductivies in x_1 and x_3 directions, respectively.

As emphasized many places in this report, the arrival time of a certain concentration of a tracer is similar to the groundwater travel time. The difference is that no tracer particles are involved, and the concentration is defined as the ratio of the weight of newly-arrived groundwater particles to the total weight of groundwater in the sample volume. If one has this concept in mind, it is clear that the nonreactive solute transport equation is the most appropriate model for determining the groundwater travel time. The use of the effective hydraulic conductivity predicts only the arrival of the center of the mass plume, and the arrival of fast moving groundwater particles due to subscale velocity variation is ignored. To analyze the effect of velocity variations on solute transport, the macrodispersion concept has to be introduced. This macrodispersion approach is analogous to the analysis of molecular diffusion at the microscopic scale discussed in section 2.6.

In order to use the macrodispersion approach, macrodispersivity must be defined. The dispersivity value at the laboratory scale can be related to the variation in grain size. Similarly, macrodispersivity can be related to the variation in hydraulic conductivity values at scales much smaller than the REV of the stochastic random field. The relationship between the macrodispersion and local-scale hydraulic conductivity variations was derived by Gelhar and Axness (1983) using a spectral analysis which will be discussed in the following section.

To examine the theory of macrodispersion, we will assume that the general equation describing transport of an ideal conservative solute by a fluid with constant density and viscosity in a saturated, homogeneous, three-dimensional porous media of constant porosity, n, is:

$$\frac{n\partial c}{\partial t} = E_{ij} \frac{\partial}{\partial x_i} \left[\frac{\partial c}{\partial x_j} - cq_i \right] \qquad i,j=1,2,3 \qquad (4.3.25)$$

where the standard Cartesian summation convention of Einstein is used and c is the concentration of the transported solute; q_i is specific discharge in the x_i direction; E_{ij} is a local bulk dispersion coefficient tensor equal to nD_{ij}; and D_{ij} is the local dispersion coefficient tensor. If D_{ij} is isotropic (i.e., the dispersion coefficient values are the same in all directions), then it is equivalent to D_d defined in Section (2.6). The local scale used here refers to the size of the volume (REV) over which the measured hydraulic conductivity is obtained. For example, if hydraulic conductivity is measured from a core sample, the local scale represents the size of the core. Thus, the local dispersion coefficient stands for the velocity variation at scales less than the size of the core sample (it includes molecular diffusion). Similarly, a local dispersion coefficient can be used to represent the velocity variation at scales much smaller than the scale at which the transmissivity is defined.

Conservation of total mass requires:

$$\frac{\partial q_i}{\partial x_i} = 0 \tag{4.3.26}$$

If a steady state condition is assumed (i.e., $n\partial c/\partial t = 0$), equation (4.3.25) becomes:

$$\frac{\partial c q_i}{\partial x_i} = E_{ij} \frac{\partial^2 c}{\partial x_i \partial x_j} \tag{4.3.27}$$

This equation is assumed to be adequate to describe the local-scale dispersion. In a large-scale heterogeneous aquifer, the log hydraulic conductivity, f; specific discharge, q; and concentration, c, are assumed to be stochastic processes. These parameters can be decomposed into a mean part and a perturbation part, i.e.:

$$c = \hat{c} + c,$$

$$f = \hat{f} + f'$$

$$q_i = \hat{q}_i + q'_i \qquad i=1,2,3 \tag{4.3.28}$$

where the head and the prime represent the mean and the perturbation, respectively. Substituting the above expressions into (4.3.27), one obtains:

$$\frac{\partial}{\partial x_i}[(\hat{c} + c')(\hat{q}_i + q'_i)] = E_{ij}\frac{\partial^2[\hat{c} + c']}{\partial x_i \partial x_j} \tag{4.3.29}$$

Because the parameters are stochastic processes, equation (4.3.29) describes concentration profiles in many realizations of possible heterogeneous aquifers (i.e., ensemble). Expanding terms and taking the expected value of the equation (i.e., taking the ensemble average) produces the mean equation:

$$\frac{\partial}{\partial x_i}\hat{q}_i\,\hat{c} + \frac{\partial}{\partial x_i}E[q'_i c'] = E_{ij}\frac{\partial^2 \hat{c}}{\partial x_i \partial x_j} \tag{4.3.30}$$

In other words, this is a transport equation which describes the mean profile of all the possible concentration profiles resulting from each realization of a heterogeneous hydraulic conductivity field. Comparing this equation to equation (4.3.25), which is the classic convection-dispersion equation, it should be evident that the first term in the left-hand side of the equation is the convective flux associated with the mean flow or specific discharge, and the second term is an additional flux, $E[q'_i c']$. This mass flux is defined as the macrodispersive flux resulting from the perturbation of velocity which is caused by the heterogeneity of the aquifer, neglected at the size where the effective hydraulic conductivity was defined.

If this macrodispersive flux is Fickian in nature, that is, this flux is linearly proportional to the mean concentration gradient (equation 2.6.1), and if the mean flow is aligned in the x_i direction so that $\hat{q}_1 = q \neq 0$ and $\hat{q}_2 = \hat{q}_3 = 0$, we may then write:

$$E[q'c'] = -q\, A_{ij} \frac{\partial \hat{c}}{\partial x_j} \tag{4.3.31}$$

where A_{ij} is the macrodispersivity tensor and q is the magnitude of the specific discharge vector. The work by Gelhar and Axness (1983) derived expressions for the A_{ij} term, relating A_{ij} to the variation in hydraulic conductivity, f'. This task was carried out by using the perturbation technique and the spectral representation theorem as used in the derivation of the effective hydraulic conductivity analysis. One of the results shows that:

$$A_{11} = \frac{\sigma_f^2 \lambda}{\gamma^2} \tag{4.3.32}$$

where A_{11} is the longitudinal macrodispersivity, σ_f^2 is the variance of f, λ is the correlation scale of statistically isotropic porous media, and γ is the flow correlation factor which depends on the direction of the mean flow and the orientation of the heterogeneity.

The practical implication of Gelhar and Axness's work is that the macrodispersivity values may be estimated from the knowledge of the variation of local-scale hydraulic conductivity values without conducting a large-scale field tracer experiment to determine the dispersivity values or the groundwater travel time. Generally speaking, a large-scale field tracer experiment is impractical in terms of

the time span required for such an experiment. However, local-scale hydraulic conductivity values are frequently measured in many aquifers. Data are available but limited. Hence, the macrodispersivity approach may provide a practical solution to many pollution problems (such as the high-level nuclear waste site characterization program).

However, the macrodispersivity approach produces the mean concentration profile only, as indicated by $\hat{c}$ in equation (4.3.30). The mean concentration profile represents the average values of concentration profiles occurring in many different aquifers (i.e., ensemble average, see section 2.6.1). As a result, the actual concentration profile observed in an aquifer may be quite different from the predicted one using the macrodispersivity. For example, Figure 4.26 shows the differences between an observed concentration distribution in the Borden sandy aquifer and an ensemble averaged (or mean) concentration distribution calculated from the classic convection-dispersion equation with macrodispersivity values. Determining the difference between the two profiles is necessary. To evaluate the difference, Vomvoris and Gelhar (1986) analyzed the mean concentration variance. They 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. The results imply that the concentration variance could be large depending on the magnitude of the parameters.

Before we illustrate the practical application of the macrodispersion theory to the groundwater travel time problem, recall that the concentration is simply the weight ratio of the newly arrived groundwater to the groundwater (including "new" and "old" water) in a sample volume. If the statistical parameters of the hydraulic conductivity distribution are known, either estimated from a limited amount of data or obtained from information from other similar aquifers, one can then calculate the breakthrough curve at the accessible environment using equation (4.3.30) and

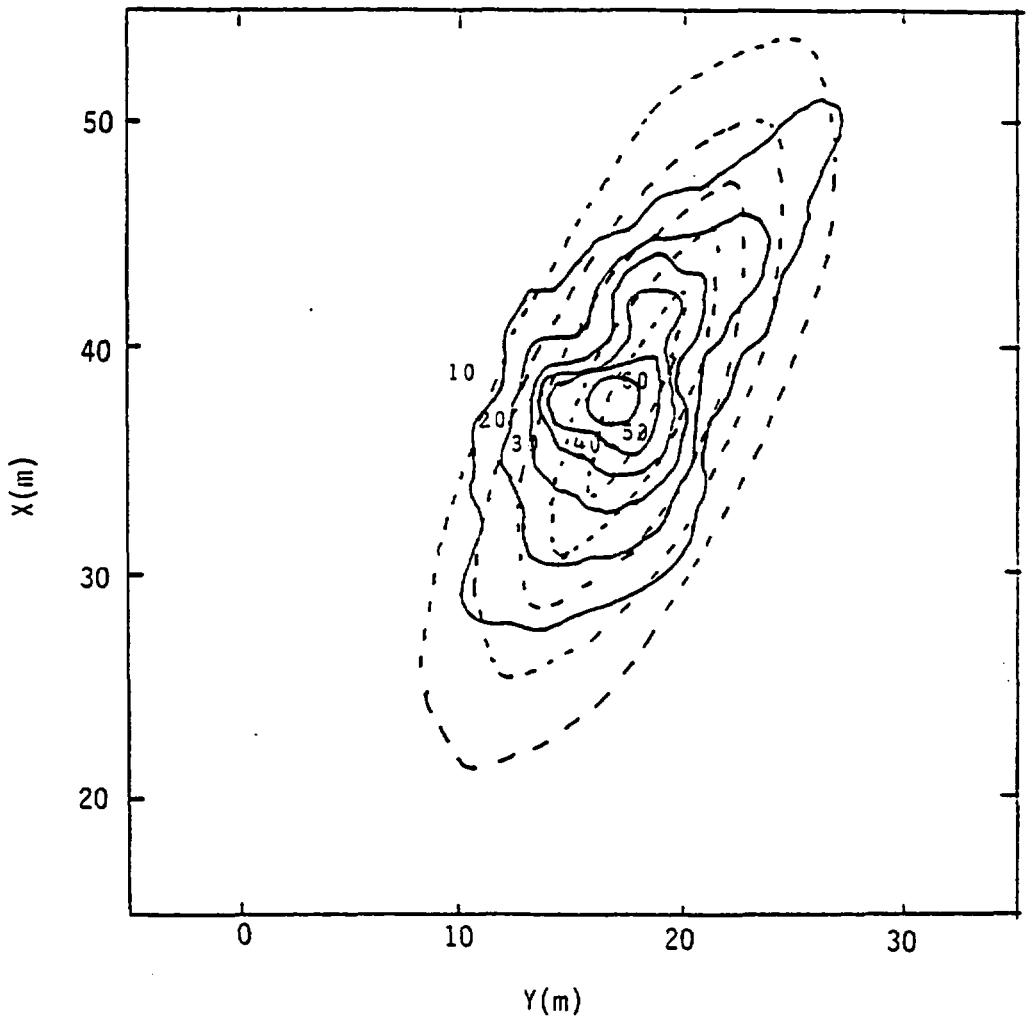


Figure 4.26. A schematic illustration of an observed depth-averaged concentration profile (solid) and a mean profile (dash), calculated from the macrodispersion equation (modified from Sudicky, 1986).

macrodispersivity values. This concentration breakthrough curve represents the arrival time distribution of different amounts of "new" water. Consequently, if a proper concentration of a tracer is defined as a criterion, then the arrival time can be defined. For the reason that the calculated concentration is the mean concentration, one should use the equations provided by Vomvoris and Gelhar (1986) to determine the variance of the mean concentration. An error band (plus or minus one concentration standard deviation about the mean concentration) can be calculated which indicates the range of the uncertainty in the mean concentration profile. Hence, the uncertainty in groundwater travel time is quantified.

Similar research on macrodispersion has been presented by many other researchers (e.g., Dagan, 1985, 1986, 1987; Neuman et al., 1986; Winter et al., 1984; Matheron and De Marsily, 1983). Dagan (1987) used the Eulerian velocity field to derive formulas for the time-dependent macrodispersivities in two-dimensional planes and three-dimensional aquifers. This approach is similar to Taylor's theorem on diffusion dicussed in section 2.6. However, in Dagan's analysis, the velocity field is related to the heterogeneity structure of the hydraulic conductivity field through the governing groundwater flow equation. The hydraulic conductivity field is considered to be statistically isotropic. For early time periods (i.e., $t \ll \lambda/v$), the spatial concentration variances (the square of the standard deviation of the plume concentration distribution: this is similar to the w^2 in section 2.6.1) are given by

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

$$\text{and } \sigma_{22}^2 (t) = \sigma_{33}^2 (t) = \frac{1}{15} \sigma_y^2 v^2 t^2 + 2 D_T t \qquad (4.3.33)$$

for three-dimensional flow, where σ_{11}^2, σ_{22}^2, and σ_{33}^2 are the concentration variances in

the direction of flow, and 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. σ_y^2 represents the variance of the natural log of 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 anaylsis are:

$$\sigma_{11}^2 = \frac{3}{8}\,\sigma_y^2\,v^2\,t^2$$

$$\sigma_{22}^2 = \frac{1}{8}\,\sigma_y^2\,v^2\,t^2 \qquad (4.3.34)$$

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

$$\sigma_{11}^2 \cong 2\sigma_y^2\,v\lambda t + 2D_L\,t$$

$$\sigma_{22}^2 = \sigma_{33}^2 \cong \frac{2}{3}\,\sigma_y^2\,\lambda^2\,t \qquad (4.3.35)$$

and the two-dimensional results,

$$\sigma_{11}^2 \cong 2\sigma_y^2\,\lambda vt\left[1 - \frac{3\ln(vt/\lambda)}{2vt/\lambda}\right]$$

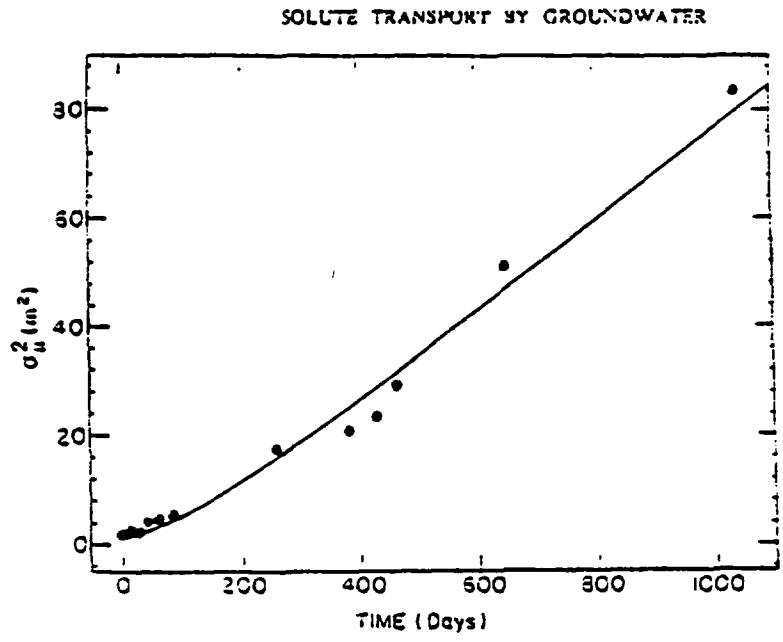
$$\sigma_{22}^2 \cong \sigma_y^2\,\lambda^2\,[\,\ln(vt/\lambda) + 0.933\,] \qquad (4.3.36)$$

Note that the concentration variances (equations (4.3.33) and (4.3.34)) for early time

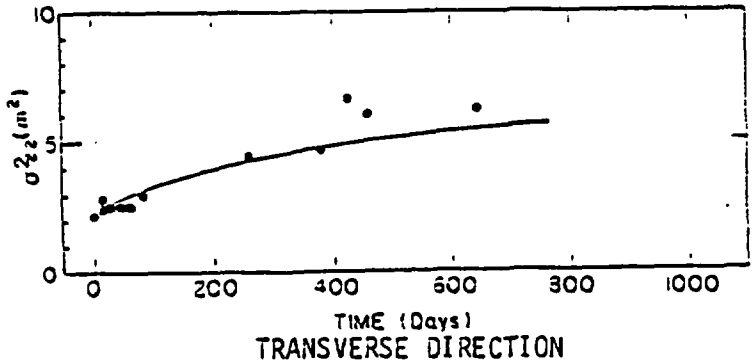
periods depend on t^2, implying the macrodispersion coefficient grows with time. For late time periods, the concentration variances (equations (4.3.35, and 4.3.36)) are a function of t only. This relationship implies that the macrodispersion coefficient is constant over time. Moreover, equations (4.3.33 - 4.3.36) do not predict the shape of the concentration plume but its relative size. Thus, no classic convection-dispersion which assumes the validity of Fick's law is used.

In generally, these results compare favorably with those obtained from a field tracer experiment (Sudicky, 1986) conducted in a sand aquifer in Canada (see Figure 4.27). A recent field tracer experiment by Garabedian (1987) in a glacial outwash aquifer also indicated that the stochastic results (i.e., Gelhar and Axness, 1983; and Dagan, 1987) are suprisingly robust, regardless of many assumptions used in the development. However, the robustness may be attributed to the fact that the variance of log hydraulic conductivity in those two aquifers is small so that the first-order approximation used in stochastic analysis is justifiable. The validity of the stochastic results, the reviewers of this report believe, still remains to be tested with tracer experiments in many different geologic environments.

Overall, the major advantage of the analytical approaches by Gelhar and Axness (1983), and Dagan (1987) is that they provide us with an explicit formula showing the relationship between the variance of inputs (such as hydraulic conductivity) and the head variance, or mean concentration profile and its variance, without conducting numerous computer experiments as required by the Monte Carlo simulations (such as Clifton et al., 1985; Smith and Schwartz, 1980, 1981a and b). Additionally, the results of the analytical approach (i.e., Gelhar and Axness, 1983) also give us an explicit way to 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)



LONGITUDINAL DIRECTION



TRANSVERSE DIRECTION

Figure 4.27. A comparison of observed (dots) and theoretical (line) spatial concentration variance in the longitudinal and transverse directions (Dagan, 1987).

may be valid only for small values of variations in hydraulic conductivity because of the omission of product terms in the analysis. Several studies have shown the results to be valid even for the variance of f = 1. Therefore, one may expect the results from the spectral analysis to be valid for most unconsolidated materials where the variance in f may be less than 1. For cases where a large variance in f is expected (such as in fractured rocks where the variance of lnK has been reported to be about 8.7, (Neuman, 1987), the validity of the method remains to be tested. The other drawback of the spectral approach is the stationarity assumption used in the analysis. In a basin-scale aquifer, the hydraulic conductivity field is likely to be nonstationary because of changes in deposition environments which may contain heterogeneities of a variety of scales, if the scale of our measurement is much smaller than the basin scale. Moreover, the validity of the classic convection-dispersion equation for large-scale problems is still under debate (see for example, Yeh, 1987). So, is it valid to apply such the results of the spectral analysis to these field problems?

It is generally agreed that the validity of the stochastic results still remains to be tested with tracer experiments in many different geologic environments. We previously noted a field experiment to validate the stochastic approach in an alluvial aquifer is currently in progress in Mississippi (Betson et al., 1985). We are unaware of similar experiments in unsaturated fractured rock. However, in the vadose zone there are two field-scale experiments in progress in New Mexico which are designed to evaluate multi-dimensional transport models in unsaturated media (Stephens et al., 1984; Wierenga et al., 1986).

4.3.4 Fractal Approach. In the past few years, geohydrologists and soil scientists have employed statistics to characterize the spatial variability of hydrological properties of geologic formations. Most of the hydrologic properties were found to be correlated over a large distance. Furthermore, many experimentally-determined variograms or autocorrelation functions of soils and geological data, exhibit some nugget effects. These nugget effects are generally viewed as a result of small-scale random noises which are spatially uncorrelated. This view implies that all variation within the closest sample spacing is infinitely erratic and possesses no spatial structure whatsoever. Although part of the nugget effect can be attributed to measurement errors which are likely to be spatially independent, experience shows that most of the noise at the macroscopic scale could be spatially correlated at the microscopic scale. This implies that the variability of hydrologic data exists in all scales and has a correlation structure at each scale (Dagan, 1986; and Gelhar, 1986). This scale phenomena was illustrated in Figure 4.13. In other words, the hydrologic data have a nested correlated structure. To analyze such a data set, a fractal approach has been proposed.

Fractals are based on the idea of 'self-similarity'; that is, the variations at one scale are manifested at another scale in similar ways. In other words, the irregularity of a process is independent of the scale of measurement. For example, the variation in effective hydraulic conductivity obtained from large-scale hydraulic tests should be similar to that from small-scale tests, at least according to the fractal concept. This self-similarity implies a long-range correlation structure in geostatistics terminology. That is, no matter how the size of the hydraulic test varies, the correlation between adjacent samples remains. For example, in Euclidean or classical geometry, the length, L, of a straight line can be easily determined by:

$$L = N \epsilon \tag{4.3.37}$$

where N is the number of measuring units of length ϵ. If we halve the size of ϵ, N will increase by a factor of two. Therefore, the length, L, is constant and independent of the scale of the measurement.

However, the Euclidean concept of a constant distance between two points independent from the scale of measurement may not be valid. Consider measuring the distance of a straight line between San Francisco and Washington, D.C. The distance as viewed by a person in outer space is essentially the length of a straight line between the two cities. The effects of topographic variation are completely neglected. However, the distance measured by a person on the ground will be much longer because this person has to consider the topographic variation of the land surface. Now, if we imagine the person is shrunk to the size of an ant, the distance between the two cities will then be even greater than that a normal-size person would experience, because an ant-size person has to consider not only the large-scale topographic variations such as hills, depressions, and mountains but also small-scale topographic variations such as heights of pebbles, rocks, and depths of cracks. The distance between the two cities, therefore, seems to grow infinitely as the scale of the measurement continuously decreases. This implies that the distance depends on the scale of the observation. This conclusion is based on the assumption that the small-scale topographic variation persists as the scale of the observation is reduced.

If the distance between two points varies with the scale of measurement, one may then ask the question: can we relate the distance between two points measured at our scale to those at scales different from ours? If the answer to the question is positive, we will then be able to predict phenomena at any scale, based on what we observed at our scale.

If we now assume that the topographic variations at all scales are self-similar, the distance between the two cities encountered by an ant-size person can then be scaled so that it is equivalent to that encountered by a normal-size person.

This concept is illustrated in Figure 4.28. Suppose the distance between two points A and B measured at a scale, ϵ, is defined as $L(\epsilon)$. A straight line distance, ℓ, represents the distance measured at a scale $\epsilon=\ell$ (Figure 4.28a). The number of measurements, N, is 1. If the measurement scale is reduced to $\ell/3$, the topographic variation at this scale will show up as indicated in Figure 4.28b. The distance between points A and B becomes $4\ell/3$ (i.e. N = 4). A further reduction of the measurement scale to 1/9 of ℓ reveals even more detailed topographic variation (Figure 4.28c). The number of measurements, N, required to measure the distance, then, is 16. If the measurement scale is further decreased to $\ell/27$, the topographic variation at this scale is shown in Figure 4.28d. In this case, N is 64. Note that the topographic variations in all the scales are similar in shape. Now, we plot the measurement scale, ϵ, versus N on log-log paper. A linear relationship between $\log\epsilon$ and log N is found (Figure 4.29). That is:

$$\log N = -D \log \epsilon \quad \text{or} \quad N = \epsilon^{-D} \tag{4.3.38}$$

where D is the slope of the line on the log-log plot. For the example, D is equal to 1.2618. This slope, D, is called the fractal dimension (Mandelbrot, 1983). In general, $1 < D < 2$. If $D = 1$, N is inversely proportional to the measurement scale ϵ, this indicates that the line is a topologically one-dimensional object. In other words, the topographic variation is independent of the scale of measurement. In the limiting case of $D = 2$, the line will be so irregular that it fills a plane (Mandelbrot, 1983). Again, here we are assuming that the topographic variation is self-similar at all scales. This is the most important property of the fractal geometry. Now, if we let:

$$F = N\epsilon^{D} \tag{4.3.39}$$

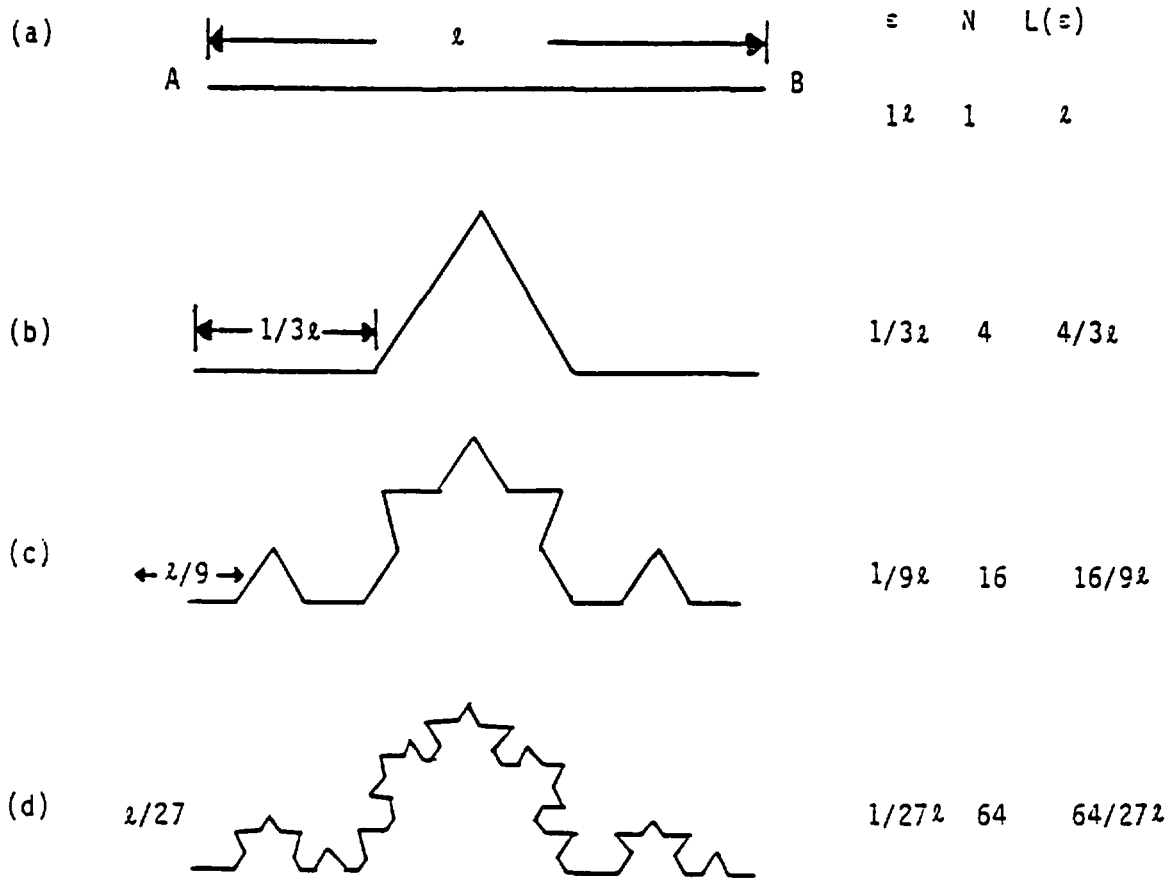


Figure 4.28. Schematic illustration of fractal concepts.
ξ is the measurement scale, N is the number of measuring units of length ξ, L is the total length, and ℓ is the straight line distance between A and B.

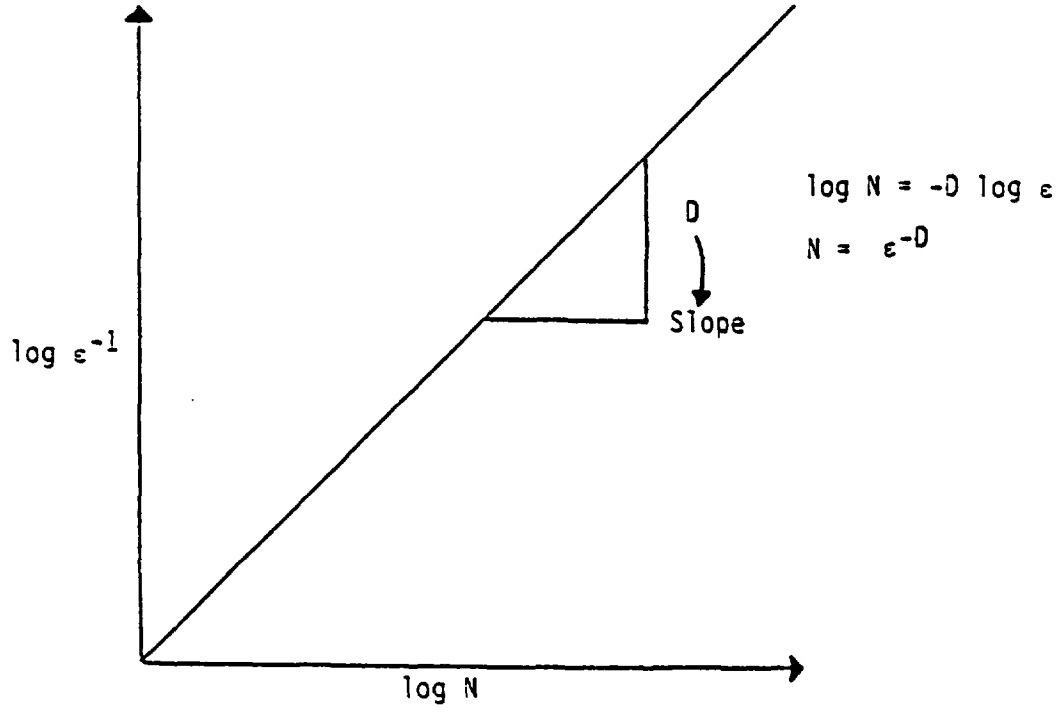


Figure 4.29. Schematic illustration of a linear relationship between log ε^{-1} and log N.

we can show that F is always a constant ($F = \ell^D$), no matter which scale of measurement is used. Thus, with the aid of the fractal dimension, we can properly scale the topographical variation at any scale to any measurement scale, if the variation is fractal, i.e. self-similar. The length of the distance between two points $L(\epsilon)$ at any measurement scale is then given as:

$$L(\epsilon) = F\ \epsilon^{1-D} \tag{4.3.40}$$

Equation (4.3.40) implies that as long as the distance between two points measured at a scale, ϵ, and the fractal dimension are known, one can determine the distance between two points as observed at any other scale. The practical implication of equation (4.3.40) is tremendous. We can predict large-or small-scale phenomena based on what we observe at our own measurement scale.

The fractal geometry concept has been recently applied to many scientific fields (Mandelbrot, 1967; Burrough, 1983a and b; Arya et al., 1985; Hewett, 1986) including groundwater hydrology (Wheatcraft and Tyler, 1988). Groundwater hydrologists, in general, rely on small-scale tests to obtain parameters for predicting flow or transport phenomena in large-scale geologic formations. Due to the spatial variability of the parameters, it is generally agreed that it is impractical to delineate the detailed spatial distribution of the hydrologic parameters in a deterministic sense. The alternative is to use effective, or mean parameters. This method is, however, not immune from difficulties. For example, there is field evidence showing that dispersivity, which is an effective parameter (see section 2.6.1), grows with the scale of experiment (Gelhar, 1986). So, how can dispersivity values obtained from small-scale laboratory experiments be scaled to large-scale problems?

To answer the above question, Wheatcraft and Tyler (1988) developed fractal scaling relationships to analyze dispersion in heterogeneous porous media. They

assumed that the path of a particle in a heterogeneous medium has fractal characteristics. The actual length a particle travels in a porous medium X_f can be related to the straight line distance of the medium, X_s, as:

$$X_f = \epsilon_c^{\,1-D} X_s^D \tag{4.3.41}$$

where ϵ_c is the fractal cutoff limit to ensure the actual length the particle travels is finite. The limit could be the smallest REV size. From equation (4.3.41), one can see that when the length between two points in a porous medium increases, the length of the actual travel path of a particle increases accordingly. Now, if we imagine a large-scale aquifer as a collection of many fractal stream tubes, the variance of the X_f is then given as:

$$\mathrm{var}(X_f) = \mathrm{var}\,(\epsilon_c^{1-D} X_s^D) \tag{4.3.42}$$

where X_s is constant. If we assume that the fractal dimension, D, is constant, then equation (4.3.42) can be rewritten as:

$$\mathrm{var}(X_f) = X_s^{2D}\,\mathrm{var}(\epsilon_c^{1-D}) \tag{4.3.43}$$

Equation (4.3.43) reveals that the variation in fractal length is due to the variation in the fractal cut-off limit and is related to the scale of the observation X_s. The variance of X_f can be considered as the spread of a plume in space. Then the macrodispersivity is:

$$A_x = \frac{1}{2}\,\mathrm{var}\,(\epsilon_c^{1-D})\,X_s\,\epsilon^{D-1} \tag{4.3.44}$$

This result, if D = 1, is consistent with that derived by Mercado (1967) in which the macrodispersivity of a perfectly-stratified aquifer is shown to grow linearly with travel distance. The expression (4.3.44) was also verified by using random walk models based on deterministic and stochastic fractal generators (Mandelbrot 1983). Gelhar et al. (1979) arrived at an expression for macrodispersivity that for early times is equivalent to Mercado's result, but for late times is equivalent to classical Taylor's dispersion, i.e., a constant dispersivity. The asymptotic approach to a constant dispersivity with distance predicted by Gelhar et al. (1979), Gelhar and Axness (1983), and Dagan (1987) is contrary to the fractal concept.

Finally, Wheatcraft and Tyler (1988) concluded that the dispersion model based on the fractal geometry concepts predicts that the field-measured dispersivity will be scale-dependent. The strength of the scale-dependence is directly related to the fractal dimension. They indicated that it is possible to obtain the fractal dimension from a tracer experiment in which the breakthrough curve is obtained for at least two travel distances. As long as the fractal dimension remains constant, it is then possible to predict solute migration at scales larger than the scale of the experiment in which the fractal dimension and the cutoff limit were obtained.

A direct application of fractal approach to the groundwater travel time position may be illustrated in the following example. If we agree that the actual travel path of a volume of groundwater is a fractal and can be adequately described by equation (4.3.41), i.e.:

$$X_f = \epsilon_c^{\,1-D} X_s^{D}$$

where, X_f is the total length of the tortuous groundwater path between two points with a straight line distance, X_s, and if one can assume that the velocity, v, of the groundwater is constant, the groundwater travel time is then given as:

$$\frac{X_f}{v} = t_f = \frac{1}{v} (\epsilon_c)^{1-D} (X_s)^D \tag{4.3.45}$$

where t_f is the actual groundwater travel time for the tortuous path between a straight line distance, X_s. If one further assume that a heterogenous aquifer can be represented by a bundle of such stream paths in a stochastic fashion, the variance in the arrival of tracer particles may be expressed as:

$$\mathrm{var}(t_f) = \frac{1}{v} X_s^{2D} \mathrm{var}[(\epsilon_c)^{1-D}] \tag{4.3.46}$$

The variance in t_f may thus represent the possible spreading in the arrival time of travel particles. This variance could be treated as a measure of uncertainties in groundwater travel time prediction. Based on the above equation, the variance in travel times will grow with X_s to the power of 2D and the variance of the fractal cutoff limit.

The fractal approach seems to be promising. Wheatcraft and Tyler, (1988) provided a new way of demonstrating the scale-dependent macrodispersion phenomena. Although, as they stated, considerable work still needs to be done to develop a more mature theory, there are some fundamental problems associated with the fractal approach.

One of the fundamental difficulties in the application of the fractal concept to groundwater hydrology arises from the self-similarity assumption in the fractal analysis. Self-similarity implies that the variations in hydrologic properties are similar at all scales. This assumption is a serious one and it still needs to be verified.

However, there is evidence supporting the self-similar nature of aquifer properties. An example is the porosity data reported by Hewett (1986). A sequence

of 2189 porosity values taken at intervals of 0.5 ft from a density porosity log in a well through a late Miocene-early Pleistocene sandstone formation (originally deposited in a deep submarine fan) was analyzed. The results showed that the porosity values may be correlated over 300 m. Hewett speculated an even larger range for horizontal correlations given the anisotropic nature of sedimentary formations. Such a long-range correlation suggests self-similarity in porosity data; the fractal approach is most suitable to represent the data.

On the other hand, Burrough (1983a, b) examined soil spatial data series in The Netherlands and the English Midlands that included percentage of clay, silt, pH, thickness, soil moisture capacity and topographic height. He concluded that soil does not vary exactly as an 'ideal' fractal but variation of physical properties is controlled by many independent processes that can cause abrupt transitions. Thus, soil does not possess the property of self-similarity at all scales. The spatial variation of soil properties is suggested to be a result of several closely spaced, nested scales of variation, occurring over short distances. He concluded that the geostatistical approach seems to be more appropriate than fractal analysis.

In groundwater transport cases, one may assume that the actual flow path of a particle in porous media is a fractal, as Wheatcraft and Tyler (1988) did. However, proving the validity of the assumption may be possible, but difficult. At present, we are somewhat skeptical of its validity. In fact, many stochastic analyses of dispersion in heterogeneous media (Gelhar et al., 1979; Gelhar and Axness, 1983; Dagan, 1987) showed that scale-dependent dispersion may exist only at early times of a transport process. An asymptotic dispersivity will develop after the plume is displaced at distances larger than the correlation scales of the hydraulic conductivity of media.

Results of the stochastic analyses by Gelhar and Axness (1983) and Dagan (1987) have been tested recently with carefully-designed large-scale field experiments

by Sudicky (1986), Freyberg (1986), and Garabedian (1987). Asymptotic macrodispersivities indeed occurred in these field experiments shortly after the injection of tracers. They all concluded that stochastic results by Gelhar and Axness (1983) and Dagan (1987) are robust and are in good agreement with field data. Although the robustness of the stochastic results may remain to be tested with many more large field experiments conducted at various geologic environments, it seems that continuously-growing dispersivity as predicted by the fractal approach may not exist, at least at a practical range of the size of aquifer. In fact, the boundless dispersivity predicted by the fractal analysis may arise from the fundamental assumption in the fractal approach which states that the variations in groundwater particle travel path are self-similar at all scales.

Regardless of whether the variation in flow channels in porous media (or the variation in intrinsic permeability which is determined by pore structure) is self-similar at all scales, the movement of the particles may not be self-similar. This is because the flow path of groundwater is also controlled by many other factors such as gradients, density variations, temperature variations, chemical variations, and degree of saturation under variable saturated flow conditions. Due to the influences of these factors, the travel path of a particle in the aquifer may likely be non-fractal, even if the pore channel is fractal. Theoretical analysis by Matheron and de Marsily (1980) seemed to demonstrate this conjecture. They showed that asymptotic macrodispersivity may develop at distances much less than the correlation scale of the hydraulic conductivity field if the flow is not parallel to the bedding. This results in an extra mixing effect and accelerates the development of an asymptotic macrodispersivity. This implies that the travel path no longer possesses the self-similar nature in properties of geologic formations. Deterministic numerical simulations of effects of heterogeneities on dispersion by Gannon and Yeh (1988) showed similar results. Hence, if the dispersivity depends on factors other than the

structure of porous media (which could be a fractal but needs to be proved), the fractal approach may face a formidable task as far as practical application is concerned.

Furthermore, it will be equally difficult to relate the parameters (such as fractal cutoff limit and fractal dimension) in Wheatcraft and Tyler's model to measurable physical parameters (such as hydraulic conductivity or porosity). This relationship needs to be explored.

5.0 SUMMARY AND CONCLUSION

There appears to be a fundamental problem with the NRC performance objectives for High Level Waste repositories, or "groundwater travel time (GWTT) objective" , which is stated in 10 CFR 60.113 (a)(2) as "...groundwater travel time along the fastest path of likely radionuclide travel from the disturbed zone to the accessible environment shall be at least 1000 years or such other time as may be approved or specified by the Commission." The "groundwater travel time along the fastest path" stated in the GWTT objective is an ambiguous phrase. The fastest path which groundwater travels can never be clearly defined because of the scale problem in groundwater hydrology. To circumvent this problem, the travel time of a certain concentration level of radionuclide should be used. The radionuclide or tracer would be a hypothetical release to the accessible environment which would travel under pre-waste emplacement hydrogeologic conditions. A concentration based standard is preferred because of the fact that the concentration represents the total mass flux (or total mass of newly-arrived groundwater) in a volume, resulting from flow phenomena of various scales. With this revised definition, a convection-dispersion equation can then be used to properly determine the arrival of the critical hyphotetical radionuclide or tracer concentration level. This approach overcomes the concern for data needed to compute the travel time for a particular molecule of radionuclide to arrive at the accesible environment. Unless this problem is resolved, the GWTT objectives will not be met.

In addition to the ambiguity of the GWTT objectives discussed above, there is another area of difficulty. Determining groundwater travel times and paths in a regional-scale problem is a difficult task based on the current monitoring and modeling techniques. There are large uncertainties in predictions. These uncertainties arise from many sources including those discussed previously. It is,

however, generally agreed that lack of complete knowledge of the spatial distribution of hydrologic parameters input to a mathematical models may be the major source of uncertainties in predicting the travel times and paths. Means of acquiring more detailed knowledge of the parameter distributions will certainly 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 fractal geometry techniques, macrodispersion methods, Monte Carlo approaches, and 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.

The fractal approach recognizes the existence of variability in all scales but assumes these variations are self-similar. With these assumptions, one can scale the results of experiments made at one scale to another. This approach is an easy way to estimate the uncertainty in groundwater travel times as indicated by equation (4.3.46). However, in this approach, the parameters lack physical meaning. What does the fractal dimension, D, mean? How can D and ϵ_c be related to the parameters (such as hydraulic conductivity, porosity, and their spatial variability) in the classic groundwater hydrology? More importantly, can we define clearly the volume of groundwater which we use to define the velocity? The tracer concentration of a volume of groundwater may be subject to changes due to mixing from subscale variations in groundwater velocity. Are we interested in the arrival of a volume of groundwater or a certain concentration of groundwater? Finally, the question which was posed in the section dealing with the fractal concept must be answered: is it true that the groundwater travel path is a fractal? Until these questions can be

resolved, the application of the fractal approach must be limited.

The approach using effective parameters with the macrodispersion concept may be attractive for relatively simple hydrogeologic systems. Recent field experiments (Sudicky, 1986; Freyberg, 1986; and Garabedian, 1987) 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 concentration variances are also in reasonable agreement with the stochastic results by Gelhar and Axness (1983) and Dagan (1987). However, the major concern with this effective parameter approach is its validity in analysis of flow and transport in highly heterogeneous aquifers where the variance of log saturated hydraulic conductivity is greater than 1. The variance of log saturated hydraulic conductivity in all the possible radioactive waste repository sites is likely much greater than 1, especially in fractured aquifers. The existing analytical solutions to stochastic differential equations are also only useful for simple flow fields, e.g., steady, uniform flow in a single aquifer. These stochastic results based on an analytical approach may serve as a tool for preliminary analyses but are not completely adequate for predictive purposes because of large variance associated with the results.

Furthermore, the spatial concentration variance formulas in the stochastic results (equations 4.3.33 to 4.3.36) provide us with the way to predict only the relative size of the plume. The shape of the concentration profile still remains unknown. The macrodispersivity defined in the stochastic analysis does not warrant the use of the classic convection-dispersion equation (Yeh, 1987) based on Fick's law. In addition, the variance of the predicted mean concentration profile may be large (Dagan, 1987). Most importantly, the number of samples required to obtain accurate estimates of the parameter values (correlation scales and covariance functions) for the

macrodispersivity models still must be investigated. Finally, the stochastic results need to be tested with many large-scale field tracer experiments in various geologic environments before they can be used for predictions.

Although the Monte Carlo simulation technique may be expensive because it requires a large number of simulations, it may be the most powerful tool among the available techniques for predicting groundwater travel times and paths or the arrival of the radionuclide concentration. Furthermore, conditional simulations which use available information at sample locations will enhance our ability to model the 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 hydraulic heads significantly, he suggested that using both hydraulic 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 (1981) showed that the locations of the 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 uncertainties in groundwater travel times and paths certainly deserves further investigation. Regardless of the amount of uncertainties that the conditional simulations (using both 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 seems to be the only tool that could bring us a step closer to reality.

As one approach to the problem of quantifying uncertainty in groundwater travel times and paths in porous media using stochastic methods, we suggest the following steps: (1) groundwater hydrologists should utilize the principles of structural

geology, stratigraphy, and sedimentology to delineate large-scale geologic units or structures which may contain the likely fast paths along which groundwater travels (Williams, 1988). (2) "Enough" data should be collected to characterize 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, porosity data from the geologic units identified in (1) using many small-scale tests (such as core samples from boreholes, or small-scale aquifer tests). (4) Groundwater hydrology modelers 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 behavior of the flow system or to calibrate flow models (see discussion in Section 4.3 or example in Gelhar, 1986). Note that the scale of samples should be consistent. That is, if one decides to use a certain scale, the entire characterization program should use that scale. Thus, the results of the calibration of models may provide a way to have 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 us with 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 assuming a release of a certain amount of radionuclides at a disturbed zone to determine the uncertainty in groundwater travel

times and paths. As more data become available, the same procedures should be repeated with the additional data. Such an iterative conditional simulation will bring our predictions close to reality step by step as more hydrologic parameter values are available. This suggested approach generally concurs with an earlier version of the NRC's draft generic position on groundwater travel time (Codell, 1986).

On the other hand, if the regulators would accept the mean groundwater travel time as a measure of the hydrologic integrity of a site, then the convection-dispersion equation would not be necessary. In this case, the ground water travel time criterion could be calculated from effective hydraulic properties and the groundwater flow equation.

Dr. Lynn W. Gelhar, who is one of the leaders in the field of stochastic hydrology, received the O. E. Meinzer Award from the Geological Society of America in 1987. In concluding this review, it seems appropiate to excerpt some of his remarks on the current status of stochastic theories and key issues which remain to be solved.

> "We now understand that this heterogeneity plays a central role regarding the large-scale mixing process in aquifers. The last decade witnessed a rapid development of mathematical, numerical, and statistical methodologies for evaluating the effects of heterogeneity on transport process. In spite of the confusion which seems to still persist in some recent literature, I believe that it is fair to say that we have arrived at a sound theoretical description of the dominant field-scale mixing process. Such stochastic theories provide a framework for predicting large-scale, long term behavior from observations of aquifer heterogeneity. Furthermore, such theories provide specific hypotheses which can be tested systematically by comparing independent theoretical predictions with the results of controlled field experiments.

This allows us to scape from the circular reasoning of the curve-fitting approach in ground-water hydrology. The stochastic approach not only provides a critical link between small-scale laboratory measurments, but also reveals features of the large-scale process which may not otherwise be apparent."

"....There is a need for controlled field experiments which explore more complex transport processes involving chemical heterogeneity, multi-phase flow, and fractured media. A fractured rock can be viewed as another type of heterogeneous medium which I suspect can be treated in some cases using stochastic continuum theory. Clearly, the problem of solute transport in fractured media is unresolved. Oversimplified matrix diffusion-type models have been extensively exercised using hyphotetical parameters to illustrate significant radionuclide retardation in the context of radioactive-waste disposal. As far as I can determine, there is no definitive field evidence which demonstrates such retardation effects. There is an obvious need for carefully designed field experiments to explore transport processes in fractured rock. Why aren't experiments of this type being developed in the United States?

A key unresolved issue is how we can characterize heterogeneity in practical sense. Research has shown that variances and correlation scales can be estimated using thousands of samples but our experience indicates that parameters can be estimated crudely from indirect geologic and geophysical observations and simple hydraulic tests. This more practical approach needs to be pursued in a number of different geologic environments. Heterogeneity remains a formidable difficulty in hydrogeology, but we now have a quantitative basis for evaluating

its effects." Gelhar (1988).

REFERENCES

Ababou, R. and L.W. Gelhar, Three-dimensional groundwater flow in random media: Direct simulation versus spectral theory, EOS, 68(44), Nov. 3, 1987.

Andersson, J. and A.M. Shapiro, Stochastic analysis of one-dimensional steady state unsaturated flow: a comparison of Monte Carlo and perturbation methods, Water Resour. Res., 19(1), 121 133, 1983.

Arya, A., T.A. Hewett, R. Larson, and L.W. Lake, Dispersion and reservoir heterogeneity, Society of Petroleum Engineers, SPE14364, Presented at the 60th Annual Technical Conference of the Society of Petroleum Engineers, Las Vegas, Nevada, Sept. 22-25, 1985.

Bakr, A.A., Stochastic analysis of the effect of spatial variations in hydraulic conductivity on groundwater flow, Ph.D. dissertation, New Mexico Institute of Mining and Technology, Socorro, July, 1976.

Bakr, A.A., L.W. Gelhar, A.L. Gutjahr, and J.R. MacMillan, Stochastic analysis of spatial variability in subsurface flows, 1:Comparison of one-dimensional flows, Water Resour. Res.,14, 263-271, 1978.

Barrenblat, G.E., I.P. Zheltov, and J.N. Kochina, Basic Concepts in the theory of homogeneous liquids in fissured rocks, J. Appl. Math. Mech. USSR, 24 (5):1286-1303, 1960.

Bear, J., Hydraulics of Groundwater, 569 pp., McGraw-Hill, New York, 1979.

Bennion, D.W., and J.C. Griffiths, A stochastic model for predicting variations in reservoir rock properties, Trans. AIME, No. 237, Part 2, 9-16, 1966,

Betson, R.P., J.M. Boggs, S.C. Young, L.W. Gelhar, Design of a field experiment to investigate groundwater saturated zone transport processes, Interim Rep., RP2485-05, 104pp., Elecr. Power, Res. Inst., Palo Alto, CA, 1985.

Bibby, R., and D.K. Sunada, Statistical error analysis of a numerical model of confined groundwater flow, in C.L. Chiu (ed.), Stochastic hydraulics, Proceedings, First International Symposium on Stochastic Hydraulics, 591-612, 1971.

Bonano, E.J., and R.M. Cranwell, Treatment of uncertainties in the performance assessment of geologic high-level radioactive waste repositories, Math. Geol., 20(5), 543-565, 1988.

Bras, R.L., and I. Rodriguez-Iturbe, Random functions and hydrology, Addison-Wesley publishing company, 559pp., 1985.

Bulnes, A.C., An application of statistical methods to core analysis data of dolomitic limestone, Trans. AIME, 165, 223-240, 1946.

Burrough, P.A., Multiscale sources of spatial variation in soil, I: The application of fractal concepts to nested levels of soil variation, J. Soil Science, 34, 577-597, 1983a.

Burrough, P.A., Multiscale sources of spatial variation in soil, II: A non-Brownian fractal model and its application in soil survey, J. Soil Science, 34, 599-620, 1983b.

Butler, Jr., J.J., Pumping tests in nonuniform aquifers: a deterministic/stochastic analysis, Ph.D. dissertation, Stanford University, Stanford, CA., 220 pp., December 1986.

Byers, E. and D.B. Stephens, Statistical and stochastic analysis of hydraulic conductivity and particle size in a fluivial sand, Soil Sci Soc. Am. J. 47, 1072-1081, 1983.

Clifton, P.M., and S.P. Neuman, Effects of kriging and inverse modeling on conditional simulation of the Avra Valley aquifer in southern Arizona, Water Resour. Res., 18, 1215-1234, 1982.

Clifton, P.M., B. Sagar, and R.G. Baca, Stochastic groundwater traveltime modeling using a Monte Carlo technique, In International Association of Hydrogeologists Memoires: Hydrogeology of Rocks of Low Permeability, Tucson, Arizona, 17(1), 319-329, 1985.

Codell, R., Draft generic position on groundwater travel time, Div. of Waste Manag., Office of Nuclear Material Safety and Safeguards, U.S. Nuclear Regulatory Commisssion, June 30, 1986.

Cole, C.R. and H.P. Foote, Use of a multigrid technique to study effects of limited sampling of heterogeneity on transport prediction, Presented at the National Water Well Association Conference, Solving Ground Water Problems with Models, Denver, Colorado, February 10-12, 1987.

Csanady, G.T., Turbulent diffusion in the environment, D. Reidel Publishing Co., 248 pp., 1973.

Dagan, G., Solute transport in heterogeneous porous formation, J. Fluid Mech., 145, 151-177, 1984.

Dagan, G., Statistical theory of groundwater flow and transport: pore-to laboratory-, laboratory-to formation-and formation-to regional-scale, Water Resour. Res., 22(9), 120S-134S, 1986.

Dagan, G., Theory of solute transport by groundwater, Ann. Rev. Fluid Mech., 19, 183-215, 1987.

Davis, J.C., Statistics and Data Analysis in Geology, 550 pp., John Wiley and Sons, Inc., New York, 1973.

Delhomme, J.P., Spatial variability and uncertainty in groundwater flow parameters: a geostatistical approach, Water Resour. Res., 15, 269-280, 1979.

De Marsily, G., G. Lavedan, M. Boucher, G. Fasamino, Interpretation of interference tests in a well field using geostatistical techniques to fit the permeability distribution in a reservoir model, "in" G. Verly etal (eds) Geostatistics for Natual Resources Characterization, Part 2, NATO Adv. Sci. Inst. Series C, vol 122, pp 831-849, Reidel Publ. Co., Dordrecht, 1984.

De Marsily, G., Quantitative Hydrogeology: Groundwater Hydrogeology for Engineers, 440 pp., Academic Press, Inc., Orlando, Florida, 1986.

Dooge, J.C.I., Scale problems in hydrology, Kisiel Memorial Lecture at Department of Hydrology and Water Resources, University of Arizona, Tucson, Arizona, February 19, 1986.

Driscoll, F.G., Groundwater and Wells, 1089 pp., Johnson Division, St. Paul, Minnesota., 1986.

Elsworth, D., A boundary element-finite element procedure for porous and fractured media flow, Water Resour. Res., 23(4), 551-560, 1987.

Fischer, H.B.,E.J. List, R.C.Y. Koh, J. Imberger, N.H. Brooks, Mixing in inland and coastal waters, Academic press, 483 pp., 1979.

Freeze, R.A., Three-dimensional, transient, saturated-unsaturated flow in a goundwater basin, Water Resour. Res., 7(2), 347-366, 1971.

Freeze, R.A., A stochastic-conceptual analysis of one-dimensional groundwater flow in non-uniform homogeneous media, Water Resour. Res., 725-741, 1975.

Freyberg, D.L., A natural gradient experiment of solute transport in a sand aquifer 2. Spatial moments and the advection and dispersion of nonreactive tracers, Water Resour. Res., 22, 2031-2046, 1986.

Gannon, J. M., and T.-C.J. Yeh, Numerical analysis of the effects of heterogeneities on dispersion, in prep., 1988.

Garabedian, S.P., Large-scale dispersive transport in aquifers: field experiments and reactive transport theory, PhD. dissertation, Massachusetts Institute of Technology, Cambridge, Massachusetts, July 1987.

Gelhar, L.W., Effects of hydraulic conductivity variations on groundwater flows, in Proceedings of the second interational IAHR symposium on stochastic hydraulic, Int. Ass. of Hydraul. Res., Lund, Sweden, 1976.

Gelhar, L.W., Stochastic subsurface hydrology from theory to applications, Water Resour. Res., 135S-145S, 1986.

Gelhar, L.W. and C.L. Axness, Three-dimensional stochastic analysis of macrodispersion in aquifers, Water Resour. Res., 19(1), 161-180, 1983.

Gelhar, L.W., A.A. Bakr, A.L. Gutjahr, and J.R. McMillan, Comments on stochastic conceptual analysis of one-dimensional groundwater flow in a non-unifrom homogeneous medium by Freeze, R.A., Water Resour. Res. 13(2), 477-480, 1977.

Gelhar, L.W., A.L. Gutjahr, and R.L. Naff, Stochastic analysis of macrodispersion in a stratified aquifer, Water Resour. Res., 15, 1387-1397, 1979.

Gelhar, L.W., Response to O.E. Meinzer Award, GSA Bulletin, July, P984, 1988.

Gutjahr, A.L., Kriging in stochastic hydrology: Assessing the worth of data, paper

presented at the Chapman Conference on Spatial Variability in Hydrologic Modeling, AGU, Fort Collins, Colorado., July 1981.

Gutjahr, A.L., L.W. Gelhar, A.A. Bakr, and J.R. MacMillan, Stochastic analysis of spatial variability in subsurface flows, 2: Evaluation and Applications, Water Resour. Res., 14, 953-960, 1978.

Gutjahr, A.L., D. McKay, and J.L. Wilson, Fast Fourier transform methods for random field generation, EOS, 68(44), Nov. 3, 1987.

Heller, J.P., Observations on diffusion and mixing in porous media, in Proceedings, Second International Symposium on Fundamentals of Transport Phenomena in Porous Media, IAHR and ISSS, Vol. 1, Guelph, University of Guelph, 1-26, 1972.

Hewett, T.A., Fractal distributions of reservoir heterogeneity and their influence on fluid transport, Society of Petroleum Engineers, SPE15386, Presented at the 61st Annual Technical Conference of the Society of Petroleum Engineers, New Orlans, Louisiana, October 5-8, 1986.

Hoeksema, R.J. and P.K. Kitanidis, An application of the geostatistical approach to the inverse problem in two-dimensional groundwater modeling, Water Resour. Res, 20(7), 1003-1020, 1984.

Hoeksema, R.J. and P.K. Kitanidis, Analysis of the spatial structure of properties of selected aquifers, Water Resour. Res, 21, 563-572, 1985.

Huang, C. and D.D. Evans, A 3-dimensional computer model to simulate fluid flow and contaminant transport through a rock fracture system, NUREG/CR-4042, U.S. Nuclear Regulatory Commission, 108 pp., 1985.

Hubbert, M.K., The theory of groundwater motion, J. of Geol., 48, 785-944, 1940.

Huyakorn, P.S., B.H. Lester, and C.R. Faust, Finite element techniques of modeling groundwater flow in fractured aquifers, Water Resour. Res., 19(4), 1019-1035, 1983a.

Huyakorn, P.S., B.H. Lester, and J.W. Mercer, An efficient finite element technique for modeling transport in fractured porous media, 1, Single Species Transport, Water Resour. Res., 19(3):841-854, 1983b.

Huyakorn, P.S., B.H. Lester and J.W. Mercer, An efficent finite element technique for modeling transport in fractured porous media, 2, Nuclide decay chain transport, Water Resour. Res., 19(3), 841-854, 1983c.

Ilyin, N.I., and others, Otsenka tochnosti opredeleniya vodopronitsayemosti gornykh porod, Moscow, Nedra, 1971.

Javandel, I., and P.A., Witherspoon, A method of analyzing transient fluid flow in multilayered aquifers, Water Resour. Res., 5(4), 1969.

Jenkins, G.M. and D.G. Watts, Spectral Analysis and its Applications, 525 pp., Holden-Day, Inc., San Francisco, 1968.

Jensen, J.L., D.V. Hinkley, L.W. Lake, A statistical study of reservoir permeability: distribution, correlation and averages, Soc. Petr. Eng. Formation Evaluation, 461-468, Dec. 1987.

Journel, A.G., and CH.J. Huijbregts, 600 pp., Mining Geostatistics, Academic Press, London, 1978.

Kazemi, H., M.S. Seth, and G.W. Thomas, The interpretation of interference tests in naturally fractured reservoirs with uniform fracture distribution, Soc. Pet. Eng. J., Dec., 463-472, 1969,

Kitanidis, P.K., and E.G. Vomvoris, A geostatistical approach to the inverse problem in groundwater modeliling (steady-state) and one-dimensional simulations, Water Resour. Res., 19(3), 677-690, 1983.

Law, J., A statistical approach to the interstitial heterogeneity of sand reservoirs, Trans AIME, v. 155, 202-222, 1944.

Lumley, J.L., and H.A. Panofsky, The Structure of Atmospheric Turbulence, John Wiley, New York, 1964.

MacMillan, J.R. and A.L., Gutjahr, Geological controls on spatial variability for one-dimensional arrays of porosity and permeability normal to layering, in Reservoir Characterization, edit by Haldorsen and Lake, 256-291, Academic Press, 1986.

Mandelbrot, B.B., The Fractal Geometry of Nature, 468 pp., W.H. Freeman, San Francisco, California, 1983.

Mandelbrot, B.B., How long is the coastline of Great Britain? Statistical self-similarity and fractional dimension, Science, 155, 636-638, 1967.

Mantoglou, A., and L.W. Gelhar, Stochastic modeling of large-scale transient unsaturated flow systems, Water Resour. Res., 23(1), 37-46, 1987a.

Mantoglou, A., and L.W. Gelhar, Capillary tension head variance, mean soil moistsure content, and effctive specific soil moisture capacity of transient unsaturated flow in stratified soils, Water Resour. Res., 23(1), 47-56, 1987b.

Mantoglou, A. and L.W. Gelhar, Effective hydraulic conductivities of transient unsaturated flow in stratified soils, Water Resour. Res., 23(1), 57-68, 1987c.

Mantoglou, A., and J.L. Wilson, The turning bands method for simulation of random fields using line generation by a spectral method, Water Resour. Res., 18(5), 1379-1394, 1982.

Marle, C., Ecoulements polyphasiques en milieu poreux, Rev. Inst. Fr. Pet, 22(10), 1471-1509, 1967.

Matheron, G., The intrinsic random functions and their applications, Advan. Appl. Probab., 5, 438-468, 1973.

Matheron, G., and G. de Marsily, Is transport in porous media always diffusive? A conunter example, Water Resour. Res., 16(5), 901-917, 1980.

Mercado, A., The spreading pattern of injected water in a permeability-stratified aquifer, p. 23, Proc. Int. Assoc. Sci. Hydrol. Symp., Haifa Pub. 72, 1967.

Mizell, S.A., A.L. Gutjahr, and L.W. Gelhar, Stochastic analysis of spatial variability in two-dimensional steady groundwater flow assuming stationary and non-stationary heads, Water Resour. Res., 19, 1853-1867, 1982.

Moench, A.F., Double-porosity models for a fissured groundwater reservoir with fracture skin, Water Resour. Res., 20(7), 831-846, 1984.

Morrison, P., and P. Morrison, Powers of Ten, Scientific American Books, New York, 1982.

Neuman, S.P., Stochastic continuum representation of fractured rock permeability as an alternative to the REV and fracture network concepts, 533-561, 28th U.S. symposium on rock mechanics, Tucson, Arizona, 29 June -1 July, 1987.

Neuman, S.P., Role of geostatistics in subsurface hydrology, in G. Verly, M. David, A.G. Journel, and A. Marechal, eds., Geostatistics for Natural Resources Characterization, Part 2, p787-816, D. Roede; Publ. Co., Boston, MA, 1072 pp., 1984.

Neuman, S.P., C.L. Winter, and C.M. Newman, Stochastic theory of field-scale Fickian dispersion in anisotropic porous media, Water Resour. Res., 23, 453-466, 1987.

Neuman, S.P., Statistical Characterization of aquifer heterogeneities, in Recent Trends in Hydrogeology, Geol. Soc. Amer. Spec. Paper 189, 81-102, 1982.

Parsons, A.M., E.D. Mattson, D.B. Stephens, K. Flanigan, K. Black, Field simulation of waste impoundment seepage in the vadoze zone, Proc. Flows on Southwestern Groundwater Issues Conf., Nat. Water Well Assoc., Albuquerque, March 23-25, 1988.

Peters, R.R., J.H. Gauthier, and A.L. Dudley, The effect of percolation rate on water-travel time in deep, partially saturated zones, Sandia Report, SAND85-0854, 1986.

Rasmussen, T.C., Computer simulation of steady fluid flow and solute transport through three-dimensional networks of variably saturated, discrete fractures, in Evans, D.D. and T.J. Nicholson (Eds.), Flow and Transport Through Unsaturated Fractured Rock, AGU Geophysical Monograph 42, 107-114, 1987.

Schwartz, F.W., L. Smith, and A.S. Crowe, 1983. A stochastic analysis of macroscopic dispersion in fractured media, Water Resour. Res., 19,1253-1265, 1983.

Shapiro, A. M., and J. Andersson, Steady-state fluid reposnes in fractured rock: A boundary element solution for a coupled, discrete fracture continuum model, Water Resour. Res. 19(4), 959-969, 1983.

Smith, L., and R.A. Freeze, Stochastic analysis of steady state groundwater flow in

a bounded domain, 1: One-dimensional simulations, Water Resour. Res., 15, 521-528, 1979a.

Smith, L., and R.A. Freeze, Stochastic analysis of steady state groundwater flow in a bounded domain, 2: Two-dimensional simulations, Water Resour. Res., 15, 1543-1559, 1979b.

Smith, L. and F.W. Schwartz, Mass transport, 1. A stochastic analysis of macroscopic dispersion, Water Resour. Res., 16, 303-313, 1980.

Smith, L. and F.W. Schwartz, Mass transport, 2. Analysis of uncertainty in prediction, Water Resour. Res., 17(2), 351-368, 1981a.

Smith, L. and F.W. Schwartz, Mass transport, 3. Role of hydraulic conductivity in prediction, Water Resour. Res., 17(5), 1463-1479, 1981b.

Stephens, D.B., L.W. Gelhar, S. Young, Field experiment to evaluate disperison in unsaturated media, EOS, 65(16), 106, 1984.

Sudicky, E.A., A natural gradient experiment on solute transport in a sand aquifer: spatial variability of hydraulic conductivity and its role in the dispersion process, Water Resour. Res., 22, 2069-2082, 1986.

Taylor, G.I., Diffusion by continuous movements, Proc. London. Math. Soc. Ser. A20, 196-211, 1922.

Taylor, G.I., Dispersion of soluble matter in solvent flowing slowly through a tube, Proc. London. Math. Soc. Ser. A219, 186-203, 1953.

van Genuchten, M.T., A closed-form equation for predicting the hydraulic conductivity of unsaturated soils, Soil Sci. Soc. Am. J., 44, 892-898, 1980.

Vomvoris, E.G., and L.W. Gelhar, Stochastic prediction of dispersive contaminant transport, U.S. Department of Commerce National Technical Information Service, Cooperative Agreement, CR-811135-01-2, Dec., 1986.

Wang, J.S.Y., and T.N. Narasimhan, Hydrologic mechanisms governing fluid flow in a partially saturated, fractured, porous medium, Water Resour. Res., 21(12), 1861-1874, 1985.

Warren, J.E., and H.S. Price, Flow in heterogeneous porous media, Society of Petroleum Engineers Journal, 1, 153-169, 1961.

Warren, J.E., and P.J. Root, Behavior of naturally fractured reservoirs, Society of Petroleum Engineers Journal, 9, 245-255, 1963.

Warren, J.E., and F.F. Skiba, Macroscopic dispersion, Trans AIME, 231, 215-230, 1964.

Warren, J.E., F.F. Skiba, and H.S. Price, An evaluation of the significance of permeability measurements, Journal Petroleum Technology, 13, 739-744, 1961.

Wheatcraft, S.W. and S.W. Tyler, An explanation of scale-dependent dispersivity in

heterogeneous aquifers using concepts of fractal geometry, Water Resour. Res., 24(4), 525-532, 1988.

Wierenga, P.J., L.W. Gelhar, C.S. Simmons, G.W. Gee, T.J. Nicholson, Validation of stochastic flow and transport models for unsaturated soil: a comprehensive field study, U.S. Nuc. Reg. Comm. Reprt, NUREG/CR-4622, 1986.

Williams, D., Geostatistical analysis and inverse modeling of the Upper Santa Cruz Basin, Arizona, Master Thesis, Univ. of Arizona, pp149, 1987.

Williams, R.E., Comment on "Statistical theory of groundwater flow and transport: Pore to Laboratory, Laboratory to Formation, and Formation to Regional Scale" by Gedeon Dagan, Water Resour. Res., 24(7), 1197-1200, 1988.

Williams, R.E., Comment on "Double-porosity models for a fissured groundwater reservoir with fracture skin" by Allen F. Moench, Water Resour. Res., 21(6), 889-891, 1985.

Winter, C.L., C.M. Newman, and S.P. Neuman, A perturbation expansion for diffusion in a random velocity field, SIAM J. Appl. Math, 44(2), 411-424, 1984.

Yeh, T.-C.J., L.W. Gelhar and A.L. Gutjahr, Stochastic analysis of unsaturated flow in heterogeneous soils, 1, Statistically isotropic media, Water Resour. Res., 21(4), 447-456, 1985a.

Yeh, T.-C.J., L.W. Gelhar and A.L. Gutjahr, Stochastic analysis of unsaturated flow in heterogeneous soils, 2, Statistically anisotropic media with variable alpha, Water Resour. Res., 21(4), 457-464, 1985b.

Yeh, T.-C.J., L.W. Gelhar and A.L. Gutjahr, Stochastic analysis of unsaturated flow in heterogeneous soils, 3, Observations and applications, Water Resour. Res., 21(4), 465-472, 1985c.

Yeh, T.-C.J., Comment on "Modeling of scale-dependent dispersion in hydrogelogic systems" by J.F. Pickens and G.E. Grisak, Water Resour. Res., 23(3), 522, 1987.

Zhang, Y., Double porocity model and its finite element solution for the flow in fractured-Karst Rocks, Hydrogeology and Engineering Geology, 4, 1982.

APPENDIX A

Glossary

Note that the glossary provided here is intended to clarify the concepts or physical meanings of terms, instead of rigorous definitions. Although most of the definitions refer to space series, they can be applied to time series as well.

Autocorrelation function: A function which depicts the linear correlation between a space series at all ranges of offset distance. For example, an autocorrelation function of hydraulic conductivity values along a transect is a measure of the intensity of association or interdependence among the values at all ranges of separation distances. Syn: autocorrelation, correlation function.

Autocovariance function: A function which describes the behavior of the covariances of two identical spatial series offset at various separation distances.

Correlation (correlation coefficient): the ratio of the covariance of two random variables to the product of their standard deviations. The correlation coefficient ranges from +1 to -1. A correlation of +1 indicates a perfect direct relationship between two random variables; a correlation of -1 indicates that one variable changes inversely with relation to the other. Between the two extremes is a spectrum of less than-perfect relationships, including a correlation coefficient of zero which indicates the lack of any linear relationship.

Correlation scale: A separation distance beyond which the random variables are no

longer considered correlated. Physically, it can be related to the average size of all sedimentary structures (for example, clay lenses) in an aquifer.

Cross-correlation function: A function which describes the correlation between two different data series at all separation distances. For example, a cross-correlation function of hydraulic conductivity and head values along a transect shows the relationship between the conductivity and head values along the transect at various separation distance. Syn: cross-correlation.

Cross-covariance function: A function which characterizes the covariances of spatial series of two different properties (e.g., hydraulic conductivity and porosity) at different separation distances. Syn: cross-covariance.

Co-Kriging: A method for estimating the value of a spatially distributed variable (e.g. transmissivity) from adjacent values of two variables (such as transmissivity and well capacity) while considering the spatial interdependence (cross-covariance) of the two variables.

Conditional probability: The probability of occurrence of a property value at an unsampled location if the property values at other location are known.

Conditional simulation: A data-generating technique, used with Monte Carlo simulation. However, sample values at sample locations are preserved in the generated data by this technique.

Covariance: A measure of the distribution of values of two properties around a common mean and thus of their mutual variability.

Ensemble: A collection of an infinite number of space series measuring the same variable.

Ensemble average: An average of the property at a point in space over many possible space series. Syn. expected value.

Ergodicity: A property of a stochastic process which says the ensemble moments equal the corresponding averages calculated from a single realization. These averages in turn can be approximated from a finite part of the realization.

Expected value: see ensemble average.

First moment: see mean

Frequency distribution: A table or a plot which divides a set of data into a number of classes, and shows the number of data belonging in each class.

Geostatistics: Statistics as applied to geology generally including correlated processes. In groundwater hydrology, it is the application of random function concepts to study the hydrologic properties in space.

Integral scale: A convenient measure of autocorrelation of a stochastic process. It carries the same physical meaning as the correlation scale but is defined more rigorously. Mathematically, it is defined as the area under the autocorrelation function.

Intrinsic hypothesis: A less stringent hypothesis than that of second-order stationarity. It states that a random field is intrinsic only if the variance of the increments of the random field is finite and these increments are second-order stationary. Variogram analysis is then applicable.

Joint probability function: A function which describes the behavior of the joint probability distribution of many random variables (i.e., the probabilities of occurrence of many random variables).

Kriging: A method for estimating the value of a spatially distributed variable from adjacent values while considering the spatial interdependence of the variables.

Log hydraulic conductivity: The natural logarithm of a hydraulic conductivity value, (lnK) or the logarithm of a hydraulic conductivity value to the base 10, (logK).

Log transmissivity: The natural logarithm of a transmissivity value, (lnT), or the logarithm of a transmissivity value to the base 10, (logT).

Lognormal distribution: A frequency distribution whose logarithms follow a normal distribution.

Mean: The sum of all observations divided by the number of observations.

Median: The value of the middle term in a set of data arranged in rank order.

Mode: The value or group of values that occurs with greatest frequency in a set of data; the most typical observation.

Monte Carlo simulation: A data-generating technique. It generates large samples of data from known probability distributions.

Nonstationary process: A stochastic process which does not possess stationary properties. Generally, it refers to a process which contains a significant trend or where the covariance depends on location as well as separation distance.

Normal distribution: A frequency distribution whose plot is a continuous, infinite, bell-shape curve that is symmetrical about its arithmetic mean, mode, and median. Syn: Gaussian distribution; bell-shaped distribution.

Nugget effect: A jump exhibited at the origin of a variogram. It generally represents uncorrelated measurement errors or subscale variability.

Perfectly correlated process: A process which has infinitely large correlation scales. Generally, this process has a constant value over space.

Probability: A term to describe the frequency of occurrence of an event.

Probability distribution: A distribution of frequencies of occurrence of many events. It is approximated by a frequency distribution.

Random variable: A function whose values are real numbers and depend on

"chance" or probability.

Random field: see stochastic process.

Random function: see stochastic process.

Range: The distance beyond which the value of the variogram equals the variance of the random field. Similar to the correlation scale, it is the distance beyond which the interdependence of values in a space series is considered insignificant.

Realization: A single space series in an ensemble. For example, a set of porosity values measured in an aquifer is considered as a realization of all the possible porosity values of the aquifer.

Regionalized variable: A variable which is distributed in space. It is equivalent to a realization of a stochastic process. Examples are porosity, hydraulic conductivity, and other hydrologic properties of an aquifer.

Representation theorem: A theorem which allows a second-order stationary stochastic process to be decomposed into sums of uncorrelated (or orthogonal) increments in the frequency domain.

Second moment: see variance.

Second-order stationary (weakly stationary) process: A stochastic process in which the ensemble mean (expected value) of the process is constant over space, and

the autocovariance function depends only on the separation distance.

Separation distance: The amount of offset in distance between the two space series being compared.

Sill: The asymptotic value of a variogram at a separation distance equal to or greater than the range. It is the variance of the random field.

Spectral Method: A mathematical tool used to solve partial differential equations which contain stochastic parameters.

Spectrum: The inverse Fourier transform of a covariance function. In other words, the covariance function has been transformed from a space domain to a wave number domain.

Standard deviation: Square root of the variance; it describes dispersion or spread of data around the mean.

Statistical moment: A convenient measure of the location and the shape of a probability distribution. First, second, and third moments of a probability distribution correspond to mean, variance, and skewness of the distribution.

Statistically anisotropic process: A stochastic process in which the covariance function depends not only on the magnitude of the separation distance but also on the direction of the separation distance. That is, the correlation scales of the process varies with change in direction.

Statistically homogeneous process: see second-order stationary process.

Statistically heterogeneous process: Any process that does not possess the properties of a second-order stationary process.

Statistically isotropic process: A stochastic process in which the covariance function depends only on the magnitude of the separation distance, regardless of the direction. That is, the correlation scales of the process are invariant in all directions.

Statistically independent: Two random variables are statistically independent if and only if the joint distribution of the two random variables equals the product of the individual probability distributions of the two random variables. That is, one random variable conveys no information about the other random variable.

Stationary process: If the statistical properties of a spatial stochastic process do not change over the spatial coordinates, then the stochastic process is a stationary process. Syn. Strictly stationary process.

Stochastic process: A collection of an infinite number of random variables in space.

Variance: The average squared deviations of all possible observations from the population mean.

Variogram: A plot of the semivariance of a random field versus separation distances. Like a covariance function, a variogram is used to define the spatial

interdependence of two random variables. However, variogram is not restricted to only stationary or second-order stationary process.

APPENDIX B

B.1 Inconsistency in the Development of Governing Groundwater Flow Equations

The purpose of this appendix is to clarify some confusions in the development of governing groundwater flow equation in saturated porous media. Therefore, some of the inconsistencies in the derivation will be discussed.

To derive the governing groundwater flow equation, we start with the mass balance equation. Consider the mass balance of a stationary control volume, V_T (Figure 2.4) whose shape is fixed in space and time. The principle of mass conservation states that

$$\{ \text{ rate of mass accumulation } \} = \{ \text{ rate of mass in } \} - \{ \text{ rate of mass out } \} \quad \text{(B.1)}$$

To apply the principle to the control volume, we begin by considering the pair of faces perpendicular to the x axis. The rate of mass in through the face at x is $(\rho q_x)|_x \ \Delta y \Delta z$, and the rate of mass out through the face at $x+\Delta x$ is $(\rho q_x)|_{x+\Delta x} \ \Delta y \Delta z$. Similar expressions may be written for the other two pairs of faces. The rate of mass accumulation within the volume element is $(\Delta x \Delta y \Delta z)(\partial n\rho/\partial t)$, where n is the porosity of the control volume. The mass balance then becomes

$$\Delta x \Delta y \Delta z \left[\frac{\partial n\rho}{\partial t}\right] = \Delta y \Delta z[(\rho q_x)|_x - (\rho q_x)|_{x+\Delta x}] + \Delta x \Delta z[(\rho q_y)|_y - (\rho q_y)|_{y+\Delta y}] + \Delta x \Delta y[(\rho q_z)|_z - (\rho q_z)|_{z+\Delta z}] \quad \text{(B.2)}$$

By dividing this entire equation by $(\Delta x \Delta y \Delta z)$ and taking the limit as these dimensions approach zero, we get

$$\frac{\partial n\rho}{\partial t} = -\left[\frac{\partial \rho q_x}{\partial x} + \frac{\partial \rho q_y}{\partial y} + \frac{\partial \rho q_z}{\partial z}\right] \tag{B.3}$$

This is the equation of continuity for flow through porous media, which describes the rate of change of fluid density at a fixed point resulting from the changes in the mass flux ρq. Using the vector notation, equation (B.3) can be expressed as:

$$\frac{\partial n\rho}{\partial t} = -(\nabla \cdot \rho q) \tag{B.4}$$

Here $(\nabla \cdot \rho q)$ is called the "divergence" of ρq, sometimes written as div ρq. Note that the vector ρq is the mass flux, and its divergence has a simple significance: it is the net rate of mass efflux per unit volume. The equation (B.4) simply states that the rate of increase of the density within a small volume element fixed in the porous media is equal to the net rate of mass influx to the element divided by its volume.

Since the ρ and q are functions of spatial coordinates, equation (B.3) can be written as:

$$\frac{\partial n\rho}{\partial t} + q_x \frac{\partial \rho}{\partial x} + q_y \frac{\partial \rho}{\partial y} + q_z \frac{\partial \rho}{\partial z} = -\rho \left[\frac{\partial q_x}{\partial x} + \frac{\partial q_y}{\partial y} + \frac{\partial q_z}{\partial z}\right] \tag{B.5}$$

The first term on the left-hand side of equation (B.5) represents the rate of change in fluid mass in the control volume at a fix position in space. The second term reflects the rate of change in fluid mass as the fluid moves from one control volume to the other at another location (change in mass due to convection). The combination of these two changes is equivalent ot the substantial derivative (or total derivative) of mass density in the control volume, that is, the time derivative for a path following the fluid motion. Hence, equation (B.5) can be abbreviated thus:

$$\frac{Dn\rho}{Dt} = -\rho(\nabla \cdot q) \tag{B.6}$$

This is the continuity equation describing the rate of change of density in the fixed control volume as seen by an observer "floating along" with the fluid (or Lagrangian point of view as oppose to Eulerian point of view, i.e., equation (B.4)). Both equations (B.4) and (B.6) describe conservation of mass in the control volume.

For an incompressible fluid, and a rigid porous medium (i.e., ρ and n are constant over time), equation (B.4) can be expressed as

$$(\nabla \cdot q) = 0 \tag{B.7}$$

B.1.1 The Eulerian Point of View. The governing partial differential equation describing flow through porous media can be derived from the Eulerian or the Lagrangian point of view. If the Eulerian approach is used (i.e., we consider mass balance and fluid motion in a control volume with a fixed shape and at a fixed location in porous media), the continuity equation is

$$\frac{\partial n\rho}{\partial t} = -(\nabla \cdot \rho q_a) \tag{B.8}$$

where q_a is the specific discharge at the Eulerian point of view. Considering the media deformable, and the fluid compressible, one can express equation (B.8) as:

$$-\nabla \cdot \rho q_a = n \frac{\partial \rho}{\partial t} + \rho \frac{\partial n}{\partial t} \tag{B.9}$$

The first and second terms at the right-hand side of equation (B.9) represent the rate

of change of fluid density and the rate of change of porosity, respectively, in the fixed control volume as seen by an observer at a fixed location. Recall that the compressibility of fluid is

$$\beta = \frac{1}{\rho}\frac{d\rho}{dp} \tag{B.10}$$

and if ρ is a function of p only, i.e., $\rho(p)$, then

$$n\frac{\partial\rho}{\partial t} = n\frac{\partial\rho}{\partial p}\frac{\partial p}{\partial t} = n\rho\beta\frac{\partial p}{\partial t} \tag{B.11}$$

The second term at the right-hand side of equation (B.9) can be related to the rate of change in pressure. Since the control volume does not deform, i.e., V_T, remains constant, the volume of solids in the control volume, V_s, may change if the porous medium deforms. The coefficient of compressibility of porous matrix is then

$$\alpha = \frac{1}{V_s}\frac{\partial V_s}{\partial\sigma_e} = -\frac{1}{1-n}\frac{\partial n}{\partial\sigma_e} = \frac{1}{1-n}\frac{\partial n}{\partial p} \tag{B.12}$$

This definition results in the same α as defined previously, assuming the control volume deforms under stress. Therefore,

$$\rho\frac{\partial n}{\partial t} = \rho\frac{\partial n}{\partial p}\frac{\partial p}{\partial t} = \rho\,\alpha\,(1-n)\frac{\partial p}{\partial t} \tag{B.13}$$

By making use of (B.11) and (B.13), equation (B.9) becomes

$$-\nabla\cdot\rho q_a = n\rho\beta \frac{\partial p}{\partial t} + \rho\alpha(1-n) \frac{\partial p}{\partial t}$$

or

$$-\nabla\cdot\rho q_a = \rho^2 g[n\beta + \alpha(1-n)] \frac{\partial h}{\partial t} \tag{B.14}$$

since

$$h = z + \frac{p}{\rho g} \quad \text{and} \quad \frac{\partial h}{\partial t} = \frac{\partial z}{\partial t} + \frac{1}{\rho g} \frac{\partial p}{\partial t} \tag{B.15}$$

where the $\partial z/\partial t$ is zero because the location of the control volume is fixed in time. Let $S_s = \rho g(n\beta + \alpha (1-n))$, specific storage, equation (B.15) expressed as:

$$-\rho\nabla\cdot q_a - q_a\cdot\nabla\rho = \rho S_s \frac{\partial h}{\partial t} \tag{B.16}$$

Generally, the second term at left-hand side of equation (B.16) is much smaller than the first term. It can be neglected although we still assume the fluid is compressible. Thus, the governing partial differential equation for groundwater flow is

$$-\nabla\cdot q_a = S_s \frac{\partial h}{\partial t} \tag{B.17}$$

where $q_a = -K\cdot\nabla h$, Darcy's law. This equation simply describes the flow through porous media as seen by an observer at a fixed location in space.

B.1.2 The Lagrangian Point of View. Generally speaking, the Lagrangian

approach in fluid mechanics implies that observations are made by following the fluid flow. Flow in deformable porous media, however, involves the movement of both fluid and solids. Since most of our monitoring devices such as observation wells are installed in the geologic formations, our observations are likely following the movement of solid grains as the formations undergo deformation. In this section, we will derive the governing groundwater flow equation from the Lagrangian point of view (i.e., by following the mean displacement of the solid grains instead of the fluid.)

The classical form of Darcy's law applies in effect to the velocity of the fluid in relation to that of the solid and not in relation to stationary space. From the Eulerian point of view, the specific discharge, q_a, is then

$$q_a = q_w + nv_s \tag{B.18}$$

where q_w represents the specific discharge of the fluid in the classical Darcy's law, n is the porosity, and v_s is the solid velocity in the vertical direction since we will assume the porous medium undergoes vertical deformation only.

Using (B.18), the continuity equation defined in relation to a fixed point in space, (B.8), becomes

$$-\nabla\cdot\rho(q_w + nv_s) = -\nabla\cdot\rho q_w - \frac{\partial \rho n v_s}{\partial z} = \frac{\partial \rho n}{\partial t} \tag{B.19}$$

where the second term represents the net solid mass flux over the control volume. Equation (B.19) can be further expanded to

$$-\nabla\cdot\rho q_w - nv_s \frac{\partial \rho}{\partial z} - \rho v_s \frac{\partial n}{\partial z} - \rho n \frac{\partial v_s}{\partial z} = n \frac{\partial \rho}{\partial t} + \rho \frac{\partial n}{\partial t}$$

$$-\nabla\cdot\rho q_w = n\,\frac{d\rho}{dt} + \rho\,\frac{dn}{dt} + \rho n\,\frac{\partial v_s}{\partial z} \tag{B.20}$$

where $d\rho/dt$ and dn/dt are the substantial derivatives of ρ and n, respectively, with respect to the v_s. That is, the rate of changes in fluid density and porosity as seen by an observer moving at the mean velocity of solid grains.

The substantial derivative of ρ can be expressed as

$$\frac{d\rho}{dt} = \frac{\partial\rho}{\partial t} + v_s\cdot\nabla\rho$$

Since the second term on the right-hand side of the equation is small, it can be neglected. The rate of change in fluid density can be related to compressibility of the fluid as we did previously.

$$n\,\frac{d\rho}{dt} = n\,\frac{d\rho}{dp}\,\frac{dp}{dt} = n\rho\beta\,\frac{dp}{dt} \tag{B.21}$$

However, the rate of change of porosity deserves some elaboration. Consider solid volume conservation in a control volume. The continuity equation is

$$\frac{\partial V_s}{\partial t} = -(\nabla\cdot V_s\ v_s) \tag{B.22}$$

Recognizing that $V_s = (1-n)V_T$ and V_T is constant, equation (B.22) can be rewritten in the form of

$$(1-n)\ \frac{\partial v_s}{\partial z} = \frac{\partial n}{\partial t} + v_s\ \frac{\partial n}{\partial z} = \frac{dn}{dt} \tag{B.23}$$

Assuming each individual solid grain does not deform, the density of solids should remain constant. A solid mass balance leads to

$$-\nabla \cdot m_s\ v_s = \frac{\partial m_s}{\partial t} \quad \text{and}$$

$$\frac{\partial m_s}{\partial t} + v_s\ \frac{\partial m_s}{\partial z} = \frac{dm_s}{dt} = -m_s\ \frac{\partial v_s}{\partial z} \tag{B.24}$$

and

$$-\frac{1}{m_s\ /\rho_s}\ \frac{d(m_s\ /\rho_s)}{dt} = -\frac{1}{V_s}\ \frac{dV_s}{dt} = -\frac{1}{V_s}\ \frac{dV_s}{d\sigma_e}\ \frac{d\sigma_e}{dt} = -\frac{\alpha d\sigma_e}{dt} = \alpha\ \frac{dp}{dt} \tag{B.25}$$

Substituting (B.21),(B.23), and (B.25) into (B.20), one obtains

$$-\nabla \cdot \rho q_w = \rho(n\beta + \alpha)\ \frac{dp}{dt} \tag{B.26}$$

Note that

$$h = z + \frac{p}{\rho g} \quad \text{and} \quad \frac{dh}{dt} = \frac{dz}{dt} + \frac{1}{\rho g}\ \frac{dp}{dt} \tag{B.27}$$

and the dz/dt is zero because the location of the reference point is stationary as seen by an observer following the displacement of the solid. Equation (B.27) thus becomes:

$$-\rho\nabla\cdot q_w - q_w \cdot\nabla\rho = \rho^2 g(n\beta + \alpha) \frac{dh}{dt} \tag{B.28}$$

Assuming that $\rho\nabla\cdot q_w >> q_w \cdot\nabla\rho$ and applying Darcy's law to (B.28), one obtain the governing groundwater flow equation from the Lagrangian point of view:

$$\nabla\cdot(K\cdot\nabla h) = S_s \frac{dh}{dt} \tag{B.29}$$

where $S_s = \rho g(n\beta + \alpha)$ and is called specific storage. Note the expression of specific storage is different from the one in equation (B.17) which is derived from the Eulerian point of view. Theoretically, equation (B.29) is the correct one for field applications because our observations generally follow the displacement of the grains as the aquifer deforms.

However, the velocity of the solid is small. Many convenient but misleading assumptions have been employed for practical purposes. For example, the coefficients of compressibility of water, β, and porous matrix, α, in the fixed coordinate system are assumed the same as those in the moving coordinate system. They are, in effect, different. Moreover, based on the same argument, the dh/dt is replaced by $\partial h/\partial t$ and hydraulic conductivity is assumed constant in time even if the porous medium is deformable. These misleading assumptions lead to the classical governing groundwater flow equation which is given as:

$$\nabla\cdot(K\cdot\nabla h) = \rho g(n\beta + \alpha) \frac{\partial h}{\partial t} = S_s \frac{\partial h}{\partial t} \tag{B.30}$$

This equation is theoretically inconsistent since it mixes the expressions for both the fixed and moving coordinate systems.

The inconsistency of the classic groundwater equation may not, however, have significant impacts on the analysis of groundwater flow. This results from the fact that the hydraulic head in the field is indeed observed following the displacement of the solid grains. The specific storage is often estimated from aquifer tests and the analysis of the test data does not require the use of the expressions for S_s. Furthermore, the error in the estimation of Ss and K from field data may be so large that misleading assumptions may not play any critical role in the analysis of groundwater flow.

Bibliography on Geostatistical and Stochastic Methods Related to Groundwater-Hydrology

Ababou, R. and L.W. Gelhar, Three-dimensional groundwater flow in random media: Direct simulation versus spectral theory, EOS, 68(44), Nov. 3, 1987.

Ahlstrom, S.W., 1975, Modeling the transport of selected rationuclides in subsurface water systems using the discrete-parcel-random-walk approach, Trans. Am. Geophys. Union, V56(12), 979

Ahlstrom, S.W. and H.P. Foote, 1976, Transport modeling in the environment using the discrete-parcel-walk approach, NTIS Accession No. BNWLSA-5528

Alpay, O.A., 1972, A practical approach to defining reservoir hereogeneity, J. Petrol. Technol., V20(7), 841-848

Anderson, M.P., 1979, Using models to simulate the movement of contaminants through groundwater flow systems, Crit. Rev. in Env. Controls 9(2):97-156

Andersson, J. and A.M. Shapiro, 1983, Stochastic analysis of one-dimensional steady state unsaturated flow: a comparison of Monte Carlo and perturbation methods, Water Resour. Res., 19(1), 121 133

Arya, A., T.A. Hewett, R. Larson, and L.W. Lake, 1985, Dispersion and reservoir heterogeneity, Society of Petroleum Engineers, SPE14364, Presented at the 60th Annual Technical Conference of the Society of Petroleum Engineers, Las Vegas, Nevada, Sept. 22-25

Bachmat, Y., 1969, Hydrodynamic dispersion in a saturated homogeneous porous medium at low Peclet numbers and nonhomogeneous solution, Water Resour. Res., V5(1), 139-143

Bachmat, Y., 1972, Spatial macroscopization of processes in heterogeneous systems, Israel J. of Technology, V10(5), 391

Bachmat, Y., 1976, Annual operation of a coastal groundwater basin at a prescribed reliability level, J. Hydrol., V31 (1-2), 97-118

Bachmat, Y. and J. Bear, 1964, The general equations of hydrodynamic dispersion in homogeneous isotropic porous mediums, J. Geophy. Res. V69(12), 2561-2567

Bakr, A.A., Stochastic analysis of the effect of spatial variations in hydraulic conductivity on groundwater flow, Ph.D. dissertation, New Mexico Institute of Mining and Technology, Socorro, July 1976

Bakr, A.A., L.W. Gelhar, A.L. Gutjahr, and J.R. MacMillan, 1978, Stochastic analysis of spatial variability in subsurface flows, 1, Comparison of one- and three-dimensional flows, Water Resour. Res., V14(2), 263-271

Barrenblat, G.E., I.P. Zheltov, and J.N. Kochina, 1960, Basic Concepts in the theory of homogeneous liquids in fissured rocks, J. Appl. Math. Mech. USSR, 24 (5):1286-1303

Bastin, G., Stochastic parameter estimation of a steady-state groundwater flow model,

Paper presented at the Congress on Simulation of Systems, Sorrento, Italy, September 24-28, 1979

Batchelor, G.K., 1974, Transport properties of two-phase materials with random structure, Annu. Rev. Fluid Mech., V6, 227-257

Bathala, C.T., A.R. Rao, and J.A. Spooner, 1977, Application of linear systems analysis to ground water evaluation studies, Tech. Rep. No. 91, Water Resour. Res. Center, Purdue Univ., West Lafayette, Indiana, 128

Bathala, C.T., A.R. Rao, and J.A. Spooner, 1977, Stochastic- models for groundwater levels using causal relationships, Abstract in Hydraulics in the Coastal Zone, ASCE, New York, p. 211

Bathala, C.T., J.A. Spooner, and A.R. Rao, 1976, Regional aquifer evaluation studies with stochastic inputs, Tech. Rep. No. 72, Purdue Univ., Water Resour. Res. Center, West Lafayette, Indiana

Bear, J., 1961, On the tensor form of dispersion in porous media, J. Geophys. Res., V66(4), 1185-1197

Bear, J., 1961, Some experiments in dispersion, J. Geophys. Res., V66(8), 2455-2468

Bear, J., 1972, Dynamics of fluids in porous media, 764 p., American Elsevier, New York

Bear, J., 1979, Hydraulics of Groundwater, 569 pp., McGraw-Hill, New York

Bear, J. and Y. Bachmat, 1967, A generalized thoery on hydrodynamic dispersion in porous media, Int. Assn Sci. Hydrol Symp., Haifa, Publ. 72, 7-16, March 1967

Bellomo, N. and R. Monaco, 1979, Mathematical models for the time-evolution of stochastic systems in two-phase flow, Appl. Math Modeling, V3(1), 41-44
Bennion, D.W., and J.C. Griffiths, 1966, A stochastic model for predicting variations in reservoir rock properties, Trans. AIME, No. 237, Part 2, 9-16

Bennion, D.W., and J.C. Griffiths, A stochastic model for predicting variations in reservoir rock properties, Trans. AIME, No. 237, Part 2, 9-16, 1966.

Beran, M.J., 1957, Dispersion of soluble matter in flow through granular media, J. Chem. Phys., V27, 270-274

Beran, M.J., 1968, Statistical continuum theories, Interscience, New York

Betson, R.P., J.M. Boggs, S.C. Young, L.W. Gelhar, 1985, Design of a field experiment to investigate groundwater saturated zone transport processes, Interim rpt, RP2485-05, 104pp., Elecr. Power, Res. Inst., Palo Alto, CA

Bhattacharya, R.N., V.K. Gupta, and G. Sposito, 1976, Markovian stochastic basis for tranport of water through unsaturated soil, Soil Sci. Soc. Am. J., V40(3), 465-467

Bhattacharya, R.N., V.K. Gupta, and G. Sposito, 1976, On the stochastic foundations

of the theory of water flow through unsaturated soil, Water Resour. Res., V12(3), 503-512

Bhattacharya, R.N., V.K. Gupta, and G. Sposito, 1976, Physical interpretation of soil-water diffusivity in terms of theory of Markov-processes, Soil Sci., V121(5) 313-314

Bhattacharya, R.N., V.K. Gupta, 1979, Statistical-theory of solute transport in porous media, SIAM J. on Applied Math., V37(3), 485-498

Bibby, R. and D.K. Sunada, 1971, Statistcal error analysis of a numerical model of confined groundwater flow, in Stochastic Hydraulics: Proc. First Int. Symp. on Stochastic Hydraul., C.L. Chiu, ed., 591-612, 1971, School of Engineering, University of Pittsburgh, Pittsburgh, Pennsylvania

Black, T.C. and D.L. Freyberg, 1987, Stochastic modeling of vertically averaged concentration uncertainity in a perfectly stratified aquifer, Water Resour. Res. 23(6): 997-1004

Bogardi, I. and L. Duckstein, Design of a foundation subject of random groundwater levels, in Hydraulic Engineering for Improved Water Mangement, Proc. 17th Congress of Int. Assn for Hydraul. Res., 15-19 August 1977, Vol 6, 383-389

Bogardi, I., L. Duckstein, A. Schmieder, and F. Szidarovszky, 1980, Stochastic forecasting of minewater inrushes, Adv. in Water Resour., V3(1), 3-8

Bonano, E.J. and R.M. Cranwell, 1988, Treatment of uncertainties in the performance assessment of geologic high-level radioactive waste repositories, Math. Geol., 20(5), 543-565

Bonano, E.J., L.R. Shipers, A.L. Gutjahr, 1987, Stochastic analysis of contaminant transport in porous media: analysis of a two-member ratio nuclide chain, Water Resour. Res. 23(6):1063-1078

Boreli, M., M. Radojkovic, and S. Jovic, Some fundamental problems of underground water pollution, in Hydraulic Engineering for Improved Water Management, Proc. 17th Congress of Int. Assn for Hydraul. Res., 15-19 August 1977, Vol 6, 714-717

Bouwer, H., 1969, Planning and interpreting soil permeability measurements, J. Irr Drain Div., ASCE, V95(3), 391-402

Bras, R.L. and I. Rodriguez-Iturbe, 1985, Random functions and hydrology, Addison-Wesley publishing company, 559pp.

Bresler, E., H. Bielorai, and A. Laufer, 1979, Field test of solution flow models in a herogeneous irrigated cropped soil, Water Resour. Res., V15(3), 645-652

Bresler, E. and G. Dagan, 1979, Solute dispersion in unsaturated heterogeneous soil at field scale, 2. Applications, Soil Sci. Soc. Am. J. 43:467-472

Broadbent, S.R. and J.M. Hammersley, 1957, Percolation processes, crystals and mazes, Proc. Cambridge Phil. Soc., V53, 629-641

Brown, M.C., 1973, Mass balance and spectral analysis applied to karst hydraulic networks, Water Resources Res., V9(3), 749-752

Bulnes, A.C., 1946, An application of statistical methods to core analysis data of dolomitic limestone, Trans. AIME, 165, 223-240

Burrough, P.A., 1983a, Multiscale sources of spatial variation in soil, I: The application of fractal concepts to nested levels of soil variation, J. Soil Science, 34, 577-597

Burrough, P.A., 1983b, Multiscale sources of spatial variation in soil, II: A non-Brownian fractal model and its application in soil survey, J. Soil Science, 34, 599-620

Butler, Jr., J.J., Pumping tests in nonuniform aquifers: a deterministic/stochastic analysis, Ph.D. dissertation, Stanford University, Stanford, CA., 220 pp., December 1986

Butler, S.S. and D.L. Gundlach, 1972, Discharge and travel time for nonuniform groundwater conduits, Trans. Am. Geophys. Union, V53(11), 980 Buyevich, Y.A., A.I. Lenov, and V.M. Safrai, 1969, Variations in filtration velocity due to random large scale fluctuations in porosity, J. Fluid Mech., V37(2), 371-381

Byers, E. and D.B. Stephens, 1983, Statistical and stochastic analysis of hydraulic conductivity and particle size in a fluivial sand, Soil Sci Soc Am J., 47:1072-1081

Carnahan, C.L., 1976, Nonequilibrium thermodynamics of groundwater flow systems--symmetry properties of phenomenological coefficients and conservations of hydrodynamic dispersion, J. Hydrol, V31(1-2), 125-150

Carrera, J. and S.P. Neuman, 1986, Estimation of aquifer parameters under transient and steady state conditions, 1. Maximum likelihood method incorporating prior information, Water Resour. Res. 22(2):199-210

Carrera, J. and S.P. Neuman, 1986, Estimation of aquifer parameters under transient and steady state conditions, 2. Uniqueness, stability, and solution algorithms, Water Resour. Res. 22(2):211-227

Carrera, J. and S.P. Neuman, 1986, Estimation of aquifer parameters under transient and steady state conditions, 3. Application to synthetic and field data, Water Resour. Res. 22(2):228-242

Cavazza, S., 1964, Relationship between rainfall intensity and groundwater movement in subfluvial aquifers, in General Assembly of Berkeley, August 1963, Int. Assn Sci. Hydrol. Publ. No. 64, 390-401

Chander, S., P.N. Kapoor, and S.K. Goyal, 1981, Aquifer parameter estimation using Kalman filters, J. Irrigation and Drainage Div., ASCE, V107(IR1), 25-33

Charbeneau, R.J., and H-D. Yeh, 1979, Conditional simulation of groundwater flow fields with emphasis on regional dispersion, Trans. Am. Geophys. Union, V60(46), 821

Chaudhari, N.M. and A.E. Scheidegger, 1965, Statistical mechanics of certain hyrodynamic dispersion phenomena, Can. J. Phys., V43(10), 1776-1794

Chirlin, G.R. and G. Dagan, 1980, Theoretical head variograms for steady flow in statiscally homogeneous aquifers, Water Resour. Res., V16(6), 1001-1015

Chirlin, G.R. and E.F. Wood, 1979, Some theoretical and practical problems in variogram estimation and application, Trans Am. Geophys. Union, V60(46), 820 Chow, V.T. and S.J. Kareliotis, 1970, Analysis of stochastic hydrological systems, Water Resour. Res., V6(6), 1569-1582

Chu, S.T., 1977, Water table response to a sequence of recharges, Water Resour. Res., V13(4), 739-742

Clapp, R.B., G.M. Hornberger, and B.J. Cosby, 1981, Estimating spatial variability in soil moisture with a dynamic cmodel and Monte-Carlo simulation, Trans. Am. Geophys. Union, V62(17), 287

Clifton, P.M., and S.P. Neuman, 1982, Effects of kriging and inverse modeling on conditional simulation of the Avra Valley aquifer in southern Arizona, Water Resour. Res., 18, 1215-1234

Clifton, P.M., B. Sagar, and R.G. Baca, 1985, Stochastic groundwater traveltime modeling using a Monte Carlo technique, In International Association of Hydrogeologists Memoires: Hydrogeology of Rocks of Low Permeability, Tucson, Arizona, 17(1), 319-329

Codell, R., Draft generic position on groundwater travel time, Div. of Waste Manag., Office of Nuclear Material Safety and Safeguards, U.S. Nuclear Regulatory Commisssion, June 30, 1986

Cole, C.R. and H.P. Foote, Use of a multigrid technique to study effects of limited sampling of heterogeneity on transport prediction, Presented at the National Water Well Association Conference, Solving Ground Water Problems with Models, Denver, Colorado, February 10-12, 1987

Cooley, R.L., 1979, A method of estimating parameters and assessing reliability for models of steady-state groundwater flow, 2. Application of statistical analysis, Water Resour. Res., V15(3), 603-617

Cooley, R.L., J.W. Fordham, and J.A. Westphal, 1973, Some applications of statistical methods to groundwater flow system analysis, Tech. Rept. Series H-W, Hydrology and Water Resources Pub. No. 14, 53 p., Desert Research Institute, University of Nevada, Reno, Nevada

Csanady, G.T., 1973, Turbulent diffusion in the environment, D. Reidel Publishing Co., 248 pp.

Cushman, J.H., 1983, Volume averaging, probabilistic averaging, and ergodicity, Adv. Water Resour. 6:182-184

Cushman, J.H., 1984, On unifying the concepts of scale, instrumentation, and stochastics in the development of multiphase transport theory, Water Resour. Res. 20( ): 1668-1676

Cushman, J.H., 1986, On measurement, scale, and scaling, Water Resour. Res. 22:129-134

Cushman, J.H., 1987, More on stochastic models, Water Resour. Res. 23(4):750-752

Dagan, G., 1967, Hydrodynamic dispersion in a nonhomogeneous porous column, J. Geophys. Res., V72(4), 4075-4080

Dagan, G., 1976, Comment on "A stochastic-cnceptual analysis of one-dimensional groundwater flow in nonuniform homogeneous media" by R.A. Freeze, Water Resour. Res., V12(3), p 567

Dagan, G., 1979, Generalization of Darcy law for nonuniform flows, Water Resour. Res., V15(1), 1-7

Dagan, G., 1979, Models of groundwater flow in statistically homogeneous porous formations, Water Resour. Res., V15(1), 47-63

Dagan, G., 1980, Correction, Water Resour. Res., V16(1), 255, to: Models of groundwater flow in statistically homogenous porous formations, Water Resour. Res., 15(1), 1979

Dagan, G., 1981, Analysis of flow through heterogeneous random aquifers by the method of embedding matrix, 1, Steady flow, Water Resour Res., V17(1), 107-121

Dagan, G., Solute transport in heterogeneous porous formation, J. Fluid Mech., 145, 151-177, 1984.

Dagan, G., 1986, Statistical theory of groundwater flow: pore - to laboratory -, laboratory - to formation, and formation - to regional scale, Water Resour. Res. 22(9):1205-1345

Dagan, G., 1987, Theory of solute transport by groundwater, Ann. Rev. Fluid Mech., 19, 183-215

Dagan, G. and E. Bresler, 1979, Solute-dispersion in unsaturated heterogeheous soil at field scale, 1. theory, Soil Sci. Soc. Am. J., V43(3), 461-467

Davidson, M.R. and B.L. Dickson, 1986, A porous flow model for steady state transport of radium in groundwater, Water Resour. Res. 22(1):34-44

Davis, J.C., 1973, Statistics and Data Analysis in Geology, 550 pp., John Wiley and Sons, Inc., New York

Debouche, Ch., S. Gaspar, and L. Sine, 1974, Diffusivite de l'eau dans un milieu non sature heterogene, J. Hydrol. V22(1-2), 35-51

DeJosselin de Jong, G., 1958, Longitudinal and transverse diffusion in granular deposits, Trans. Am. Geophys. Union, V39(1), 67-74

DeJosselin de Jong, G., 1972, The tensor characteristics of the dispersion coefficient in anisotropic porous media, in Fundamentals of Transport Phenomena in Porous Media, Elsevier, Amsterdam, 1972, 259-267

DeJosselin de Jong, G. and M.J. Bossen, 1961, Discussion of paper by Jacob Bear "On the tensor form of dispersion in porous media", J. Geophys. Res., V66(10), 3623-3624

Delhomme, J.P., 1978, Kriging in the hydrosciences, Adv. in Water Resour., V1(5), 251-266

Delhomme, J.P., 1979, Kriging under boundary conditions, Trans. Am. Geophy., Union, V60(46), 820

Delhomme, J.P., 1979, Spatial variability and uncertainty in groundwater flow parameters: A geostatistical approach, Water Resour. Res., V15(2), 269-280

De Marsily, G., 1984, Spatial variability of properties in porous media: a stochastic approach, in Fundamentals of Transport in Porous Media, J. Bear, Y. Corapcioglu (eds.), Nijhoff, Dordrecht, pp. 721-769

De Marsily, G., G. Lauedan, M. Boucher, G. Fasanino, 1984, Interpretation of intereference tests in a well field using geostatistical techniques to fit the permeability distribution in a reservoir model, in Geostatistics for Natural Resources Characterization, Proc. NATO-ASI, Berly et al. (eds.) Part 2, Reidel Pub. Co. Dordrecht, The Netherlands

De Marsily, G., 1985, Flow and transport in fractured rocks: connectivity and scale effect, Mem. Int. Assoc. Hydrogeol. 17:267-277

De Marsily, G., 1986, Quantitative Hydrogeology: Groundwater Hydrogeology for Engineers, 440 pp., Academic Press, Inc., Orlando, Florida

Dendrou, B.A., E.N. Houstis, and S.A. Dendrou, 1979, Site selection using a kriging-FEM scheme, Trans. Am. Geophys. Union, V60(46), 821

Desbarats, A.J., 1987, Numerical estimation of effective permeability in sand-shale formations, Water Resour. Res. 23(2):273-286 Dettinger, M.D. and J.L. Wilson, 1981, First-order analysis of uncertainty in numerical models of groundwater flow, 1. Mathematical description, Water Resour. Res. 17:149-161

Devary, J.L. and P.G. Doctor, 1982, Pore velocity estimation uncertainties, Water Resour. Res. 18(4):1157-1164

Dievlin, A., G. Matheson, G. de Marsily, 1981, Growth of the dispersion coefficient with the mean travelled distance in porous media, Sci. Total Env. 21:319-328

Domenico, P.A. and G.A. Robbins, 1984, A dispersion scale effect in model calibrations and field tracer experiments, J. Hydrol. 70:132-

Dooge, J.C.I., Scale problems in hydrology, Kisiel Memorial Lecture at Department of Hydrology and Water Resources, University of Arizona, Tucson, Arizona, February 19, 1986

Dracup, J.A., O.E. Drummond, and P.R. Westlake, 1978, Kalman filtering of water well fluctuations, in Applications of Kalman Filter to Hydrology, Hydraulics, and Water Resouces, C.L. Chiu, ed., Stochastic Hydraulics Program,

University of Pittsburg, Pennsylvania, 693-275

Driscoll, F.G., 1986, Groundwater and Wells, 1089 pp., Johnson Division, St. Paul, Minnesota

Duerbaum, H.J. and K. Trippler, 1972, Comparison of statistical and deterministric approaches in the determinationof hydrological parameters of aquifers, in Proc. Int. Symp. on Uncertainties in Hydrologic and Water Resource Systems, Vol. 3, 3.3-1-3.3-20, Department of Hydrol. and Water Resour., University of Arizona, Tucson

Duffy, C.J. and L.W. Gelhar, 1986, A frequency domain analysis of groundwater quality fluctuations: interpretations of field data, Water Resour. Res. 22(7):1115-1128

Duffy, C.J. and J. Harrison, 1987, The statistical structure and filter characteristics of tritium fluctuations in fractured basalt, Water Resour. Res. 23(5):894-902

Dullien, F.A.L., 1979, orous media-fluid transport and pore structure, 396 p., Academic Press, New York, NY

Elgizawi, M.G., 1974, Use of cross-correlation techniques for determining the relationship between groundwater levels and sources in the Nile delta area, in Mathematical Models in Hydrology, Proc. of the Warsaw Symp., July 1971, Int. Assn Hydrol. Sci. Publ. No. 100, 319-325

Elsworth, D., A boundary element-finite element procedure for porous and fractured media flow, Water Resour. Res., 23(4), 551-560, 1987

Eriksson, G., 1970, Cross-spectrum analysis of groundwater levels in an esker, Nord. Hydrol., V1(4), 245-259

Eriksson, G., 1970, Groundwater time-series: An exercise in stochastic hydrology, Nord. Hydrol. V1(3), 181-205

Fara, H.D., and A.E. Scheidegger, 1961, Statistical geometry of porous media, J. Geophys. Res., V66(10), 3279-3284

Ferrandon, J., 1948, Lew lois de l'ecoulement de filtration, Le Genie Civil, V 125, 24-28

Ferraund, L.A. P.C.D. Milly, G.F. Pinder, 1986, Dual-gamma attenuation for the determination of porous medium saturation with respect to three fluids, Water Resour. Res. 22(12):1657-1663

Fischer, H.B.,E.J. List, R.C.Y. Koh, J. Imberger, N.H. Brooks, 1979, Mixing in inland and coastal waters, Academic press, 483 pp.

Flores, W., E.Z., A.L. Gutjarh, and L.W. Gelhar, 1978, A stochastic model of the operation of a stream-aquifer system, Water Resour. Res., V14(1), 30-38

Fogg, G.E., 1986, Groundwater flow and sand body interconnectedness in a thick multiple-aquifer system, Water Resour. Res. 22(5):679-694

Freeze, R.A., 1971, Three-dimensional, transient, saturated-unsaturated flow in a goundwater basin, Water Resour. Res., 7(2), 347-366

Freeze, R.A., 1975, A stochastic-conceptual analysis of one- dimentional groundwater flow innonuniform homogeneous media, Water Resourc. Res., V11(5), 725-741

Freeze,, R.A., L.W. Gelhar,and T. Maddock, 1978, Geostatistical concepts and stochastic methods in hydrogeology, Geology, V6(5), 297-298

Freyberg, D.L., 1986, A natural gradient experiment of solute transport in a sand aquifer 2. Spatial moments and the advection and dispersion of nonreactive tracers, Water Resour. Res., 22, 2031-2046

Fried, J.J. and M.A. Combarnous, 1971, Dispersionin porous media, in Advances in Hydroscience, V 7, 169-282

Frisch, H.L., and J.M. Hammersley, 1963, Percolation processes and related topics, J. Soc. Ind. Appl. Math., V11(4), 894-918

Gambolati, G., 1979, Kriging in the environmental applications: results and shortcomings, Trans. Am. Geophys. Union, V60(45), 821

Gambolati, G. and G. Volpi, 1979, A conceptual deterministic analysis of the Kriging technique inhydrology, Water Resour, Res., V15(3), 625-629

Gambolati, G. and G. Volpi, 1979, Groundwater countour mapping in Venice by stochastic interpolators, 1, Theory, Water Resour, Res., V15(2), 281-290

Ganoulis, J. and C. Thirriot, 1973, Sur un modele probabiliste de l'equilibre capillaire en milieu poreux C. R. Acad. Sc. Paris, T. 276, Ser. A, 1573-76

Ganoulis, J. and C. Thirriot, 1977, Stochastic study of the entrance of a non-wetting fluid in a pourous medium, under the influence of capillarity in "Hydraulic probems solved by stochastic methods", Proc. 2e Int. IAHR Symp. on Stochastic Hydraulics, Lund, Sweden, Aug. 2-4, 1976,Water Res. Publ., pp 22.1-22.18, Fort Collins, Colorado 80522

Gannon, John M., and T.-C.J. Yeh, Numerical analysis of the effects of heterogeneities on dispersion, in prep 1988.

Garabedian, S.P., Large-scale dispersive transport in aquifers: field experiments and reactive transport theory, PhD. dissertation, Massachusetts Institute of Technology, Cambridge, Massachusetts, July 1987

Gavalas, G.T., P.C. Shah, and J.H. Seinfeld, 1976, Reservoir history matching by Bayesian estimation, Soc. Petrol. Eng. J., V16(6), 337-350

Gelhar, L.W., 1974, Stochastic analysis of phreatic aquifers, Water Resour. Res., V10(3), 539-545

Gelhar, L.W., 1976, Effects of hydraulic conductivity variations on groundwater flows, in Hydraulic Problems Solved by Stochastic Methods, Proc. Second Int. IAHR Symp on Stochas- tic Hydraulics, Lund, Sweden, 409, 429,Water Resourc. Publications, Fort Collins, CO

Gelhar, L.W., A.A. Bakr, A.L. Gutjahr, and J.R. McMillan, Comments on stochastic conceptual analysis of one-dimensional groundwater flow in a non-unifrom homogeneous medium by Freeze, R.A., Water Resour. Res. 13(2), 477-480, 1977.

Gelhar, L.W., A.L. Gutjahr, and R.L. Naff, Stochastic analysis of macrodispersion in a stratified aquifer, Water Resour. Res., 15, 1387-1397, 1979.

Gelhar, L.W., 1984, Stochastic analysis of flow in heterogeneous porous media in Fundamentals of Transport Pheonmena in Porous Media, J. Bear and M.Y. Corapcioglau (eds.), Martinus Nijhoff Publishers, Dordrecht, The Netherlands

Gelhar, L.W., 1986, Stochastic subsurface hydrology: from theory to applications, Water Resour. Res. 22(9):1355-1455

Gelhar, L.W., 1988, Response to O.E. Meinzer Award, GSA Bulletin, July, p. 948.

Gelhar, L.W. and C.L. Axness, 1983, Three-dimensional stochastic analysis of macrodispersion in aquifers, Water Resour. Res., 19(1), 161-180

Gelhar, L.W., A.A. Bakr, A.L. Gutjahr, and J.R. MacMillan, 1977, Comments on "A stochastic-conceptual analysis of one- dimensional groundwater flow in nonuniform homogeneous media" by R.A. Freeze, Water Resourc. Res., V13(2), 477-479

Gelhar, L.W. and M.S. Collins, 1971, General analysis of longitudinal dispersion in nonuniform flow, Water Resour. Res., V7(6), 1511-1521

Gelhar, L.W., G.W. Gross, and C.J. Duffy, 1979, Stochastic methods of analyzing groundwater recharge, in the Hydrology of Areas of Low Precipitation, Proc. of Canberra Symp., Int. Assn Hydrol Sci Publ No. 128, 313-321

Gelhar, L.W., A.L. Gutjahr, and R.L. Naff, 1979, Stochastic analysis of macrodispersion in a stratified aquifer, Water Resour. Res., V15(6), 1387-1397

Gelhar, L.W., P.Y. Ko, H.H. Kwai, and J.L. Wilson, 1974, Stochastic modelling of groundwater systems, 313 p., Rep. 189, R.M. Parsons Lab for Water Resour. and Hydrodynamics, Massachusetts Institute of Technology, Cambridge, Massachusetts

Gelhar, L.W., J.L. Wilson, and A.L. Gutjahr, 1979, Comments on "Simulation of groundwater flow and mass transport under uncertainty" by D.H. Tang and G.F. Pinder, Adv. in Water Resourc., 2(2), 101

Gillham, R.W., E.A. Sudicky, J.A. Cherry, E.O. Frind, 1984, An advection-diffusion concept for solute transport in heterogeneous unconsolidated geological deposits, Water Resour. Res. 20(3):369-378

Golden, J.M., 1980, Percolation theory and models of unsaturated porous media, Water Resour. Res., V16(1), 201-109

Greenkorn, R.A. and D.P. Kessler, 1969, Dispersion in heterogeneous nonuniform anisotropic porous media, Ind. Eng. Chem., V61(9), 14-32

Gupta, V.K. and R.N. Bhattacharya, 1986, Solute dispersion in multidimensional periodic saturated media, Water Resour. Res. 22(2):156-164

Gutjahr, A.L., Kriging in stochastic hydrology: Assessing the worth of data, paper presented at the Chapman Conference on Spatial Variability in Hydrologic Modeling, AGU, Fort Collins, Colorado, July 1981

Gutjahr, A.L. and L.W. Gelhar, 1981, Stochastic models of subsurface flow: Infinite versus finite domains and stationarity, Water Resour. Res., V17(2), 337-350

Gutjahr, A.L., E.J. Bonano, R.M. Cranwell, 1985, Treatment of parameter uncertainties in modeling contaminant transport in geologic media: stochastic models versus determination models with statistical parameter sampling, in Proc. Int's Assoc. Hydraulic Research Symp. in the Stochastic Approach to Subsurface Flow, G. de Marsily (ed.), Montvillargenne, France, June 3-6, 1985, pp. 332-350

Gutjahr, A.L., L.W. Gelhar, A.A. Bakr, and J.R. MacMillan, 1978, Stochastic analysis of spatial variability in subsurface flows, 2, Evaluation and application, Water Resourc. Res., V14(5), 953-960

Gutjahr, A.L., D. McKay, and J.L. Wilson, Fast Fourier transform methods for random field generation, EOS, 68(44), Nov. 3, 1987.

Guven, O., F.J. Molz, J.G. Melville, 1984, An analysis of dispersion in a stratifed aquifer, Water Resour. Res. 20: 1337-1354

Guven, O., F.J. Molz, J.G. Melville, 1986, Comment on "an advection-diffusion concept for solute transport in heterogeneous unconsolidated geological deposit" by Gillham et al., Water Resour. Res. 22(1):89-91

Guven, O. and F.J. Molz, 1986, Deterministic and stochastic analysis of dispersion in an unbounded stratified porous medium, Water Resour. Res. 22(11):1565-1574

Haldorsen, H.H. and L.W. Lake, 1982, A new approach to shale management in field scale simulation models, Paper presented at the 57th Annual Technical Conference, Soc. Pet. Eng., New Orleans, Sept. 26-29

Haring, R.E. and R.A. Greenkorn, 1970, A statistical model of a porous medium with nonuniform pores, AIChE J., V16(3), 447-483

Harleman, D.R.F. and R.R. Rumer, 1963, Longitudinal and lateral dispersion in an isotropic porous medium, F. Fluid Mech., V16(3), 385-394

Heller, J.P., 1972, Observations of mixing and diffusion in porous media, Proc. Second Int Symp on Fund of Trans Phen in Porpous Media, Int. Assn' Hydraulic Res., 1-26, University of Guelph, Guelph, Ontario, Canada

Hewett, T.A., Fractal distributions of reservoir heterogeneity and their influence on fluid transport, Society of Petroleum Engineers, SPE15386, Presented at the 61st Annual Technical Conference of the Society of Petroleum Engineers, New Orlans, Louisiana, October 5-8, 1986

Hoeksema, R.J. and P.K. Kitanidis, 1984, An application of the geostatistical approach

to the inverse problem in two- dimensional groundwater modeling, Water Resour. Res. 19(3):677-690

Hoeksema, R.J. and P.K. Kitanidis, 1985, Analysis of the spatial structure of properties of selected aquifers, Water Resour. Res. 21, 563-572

Horton, R., M.C. Thompson, J.F. McBride, 1987, Method of estimating the travel time of noninteracting solutes through compacted soil material, Soil Sci. Soc. Am. J. 51(1):48-53

Huang, C. and D.D. Evans, 1985, A 3-dimensional computer model to simulate fluid flow and contaminant transport through a rock fracture system, NUREG/CR-4042, U.S. Nuclear Regulatory Commission, 108 pp.

Hubbert, M.K., 1940, The theory of groundwater motion, J. of Geol., 48, 785-944

Huyakorn, P.S., B.H. Lester, and C.R. Faust, 1983a, Finite element techniques of modeling groundwater flow in fractured aquifers, Water Resour. Res., 19(4), 1019-1035

Huyakorn, P.S., B.H. Lester, and J.W. Mercer, 1983b, An efficient finite element technique for modeling transport in fractured porous media, 1, Single Species Transport, Water Resour. Res., 19(3):841-854

Huyakorn, P.S., B.H. Lester and J.W. Mercer, 1983c, An efficent finite element technique for modeling transport in fractured porous media, 2, Nuclide decay chain transport, Water Resour. Res., 19(3), 841-854

Ilyin, N.I., and others, 1971, tsenka tochnosti opredeleniya vodopronitsayemosti gornykh porod, Moscow, Nedra

Iwasa, Y. and H. Takeuchi, 1971, Dispersive characteristics of flows through porous media, in Stochastic Hydraulics, C.L. Chiu, ed., School of Engineering, University of Pittsburg, 613-631

Jackson, R.E., 1973, Evapotranspiration of groundwater, Scientific Series No. 17, Department of the Environment, Inland Waters Directorate, Ottawa, Canada, 40p.

Jackson, R.E., 1974, Time-series analysis of groundwater hydrographs from surficial deposits on Canadian shield, Can. J. Earth Sci., V11(1), 177-188.

Jackson, R.E., J.A. Gilliland and K. Adamowski, 1973, Time series analysis of the hydrologic regimen of a groundwater recharge area, Water Resour. Res., V9(5), 1411-1419

Javandel, I., and P.A., 1969, Witherspoon, A method of analyzing transient fluid flow in multilayered aquifers, Water Resour. Res., 5(4), 1969

Jenkins, G.M. and D.G. Watts, 1968, Spectral Analysis and its Applications, 525 pp., Holden-Day, Inc., San Francisco

Jensen, J.L., D.V. Hinkley, L.W. Lake, 1987, A statistical study of reservoir permeability: distributions, correlations and averages, Soc. Petr. Eng.,

Formation Evaluation, December, pp. 461-468. Journel, A.G., and CH.J. Huijbregts, 1978, Mining Geostatistics, 600 pp., Academic Press, London

Journel, A.G., and CH.J. Huijbregts, 600 pp., Mining Geostatistics, Academic Press, London, 1978.

Julian, P.R., 1967, Variance spectrum analysis, Water Resourc. Res., V3(3), 831-845

Kasansky, A.B., 1974, A statistical filtration model for the inseepage of melt water into frozen ground, in Mathematical Models in Hydrology, Proc. of the Warsaw Symp., July 1971, Int. Assn Hydrol. Sci. Publ. No. 100, 241-245. Discussion by S. Dyck, Publ No. 102, 1175-1176

Kazemi, H., M.S. Seth, and G.W. Thomas, 1969, The interpretation of interference tests in naturally fractured reservoirs with uniform fracture distribution, Soc. Pet. Eng. J., Dec., 463-472

Kilbury, R.K., T.C. Rasmussen, D.V. Evans, A.W. Warrick, 1986, Water and air intake of surface exposed rock fractures in situ, Water Resour. Res. 22(10):1431-1443

Kipp, K.C., K.G. Stollenwerk, D.B. Grove, 1986, Groundwater transport of strontium 90 in a glacial outwash environment, Water Resour. Res. 22(4):519-530

Kiremidjian, A.S. and P. Kruger, 1979, A stochastic model of radionuclide migration from natural and engineered repositories, in Scientific Basis for Nuclear Waste Management, V 2, 779-785

Kitanidis, P.K., 1986, Comment on "Stochastic modeling of groundwater flow by unconditional and conditional probabilities: the inverse problem" by G. Dagan, Water Resour. Res. 22(6):984-986

Kitanidis, P.K., 1986, Parameter uncertainty in estimation of spatial functions: Boysian analysis, Water Resour. Res. 22(4):499-507

Kitanidis, P.K., and E.G. Vomvoris, 1983, A geostatistical approach to the inverse problem in groundwater modeliling (steady-state) and one-dimensional simulations, Water Resour. Res., 19(3), 677-690

Koval, E.J., 1963, A method for predicting the performance of unstable miscible displacement in heterogeneous media, Soc. Petrol Eng. J. V392), 145-154

Kriz, H., 1972, Statistical processing of long-term observations of groundwaters, J. Hydrol., V16(1), 17-37

Labadie, J.W. and D.R. Hampton, 1979, Estimation of hydrogeologic parameters for optimal groundwater basin development, in Mathematical Programming with Data Perturbations, A.V. Fiacco, ed., Lecture Notest in Pure and Applied mathematics, Marcel Dekker, Inc., New York sched. pub. date, 1981

Larson, R.G., L.E. Scriven, and H.T. Davis, 1981, Percolation theory of two phase flow inporous media, Chem. Eng. Sci., V36, 57-73

Lau, L.K., W.J. Kaufman, and D.K. Todd, 1959, Dispersion of a water tracer in

radial laminar flow through porous media, Inst. Eng. Research Rept 93-5, University of California, Berkeley, 78 p.

Law, A.G., 1974, Stochastic analysis of groundwater level time series in the western United States, Hydrology Paper No. 68, Colorado State University, Fort Collins, CO

Law, J., 1944, A statistical approach to the interstitial heterogeneity of sand reservoirs, Trans AIME, v. 155, 202-222

Liao, K.H. and A.E. Scheidegger, 1968, A computer model for some branching-type phenomena in hydrology, Bull. Int. Assn. Sci. Hydrol., V13(1), 5-13

Liao, K.H. and A.E. Scheidegger, 1969, Branching-type models of flow through porous media, Bull Int Assn Sci Hydrol, V14(4), 137-145

Liao, K.H. and A.E. Scheidegger, 1970, Statistical models of flow through porous media, Pure and Appl. Geophys., V83(6), 74-81

Lippmann, M.J., 1974, Two-dimensional stochastic model of a heterogeneous geologic system, Ph.D. thesis, 135 p., University of California, Berkelye, University Microfilms order no 75-5810

Lippmann, M.J., and P.A. Witherspoon, 1974, Stochastic model to simulate cross sections of layered heterogeneous groundwater systems, Trans. Am. Geophys. Union, V55(12), 1118.

Lumley, J.L., and H.A. Panofsky, 1964, The Structure of Atmospheric Turbulence, John Wiley, New York

Maddock, T., III, 1974, The operation of a stream-aquifer sytem under stochastic demand,s Water Resour. Res., V10(1), 1-10

Maddock, T., III, 1976, A drawdown prediction model based on regression analysis, Water Resour. Res., V12(4), 818-822

Mandel, S. and Z. Weinberger, 1972, Analysis of a network-model for dispersive flow, J. Hydrol., V16(2), 147-157

Mandelbrot, B.B., 1967, How long is the coastline of Great Britain? Statistical self-similarity and fractional dimension, Science, 155, 636-638

Mandelbrot, B.B., 1983, The Fractal Geometry of Nature, 468 pp., W.H. Freeman, San Francisco, California

Mantoglou, A., and J.L. Wilson, 1982, The turning bands method for simulation of random fields using line generation by a spectral method, Water Resour. Res., 18(5), 1379-1394

Mantoglou, A., and L.W. Gelhar, 1987a, Stochastic modeling of large-scale transient unsaturated flow systems, Water Resour, Res., 23(1), 37-46

Mantoglou, A., and L.W. Gelhar, 1987b, Capillary tension head variance, mean soil moistsure content, and effctive specific soil moisture capacity of transient

unsaturated flow in stratified soils, Water Resour. Res., 23(1), 47-56

Mantoglou, A. and L.W. Gelhar, 1987c, Effective hydraulic conductivities of transient unsaturated flow in stratified soils, Water Resour. Res., 23(1), 57-68

Marle, C., 1967, Ecoulements polyphasiques en milieu poreux, Rev. Inst. Fr. Pet, 22(10), 1471-1509

Marle, C., P. Simandoux, J. Pacsirsky, and C. Gaulier, 1967, Etude du deplacement de fluides miscibles en milieu poreux startifie, Rev. Inst. Francais Petrole, V2292), 272-294

Massman, J. and R.A. Freeze, 1987, Groundwater contamination from waste management site: the interaction between risk-based engineering design and regulatory policy, 1. Methodology, Water Resour. Res. 23(2):351-367

Massman, J. and R.A. Freeze, 1987, Groundwater contamination from waste management sites: the interaction between risk-based engineering design and regulatory policy, 2. Results, Water Resour. Res. 23(2):368-380

Matheron, G., 1967, Composition des permeabilities en milieu poreux heterogene methode de Schwydler et regles de ponderation, Rev. Inst. Francais Petrole, V 22, 443-466

Matheron, G., 1967, Elements pour une theorie des milieux poreux, Masson et Cie, Paris.

Matheron, G., 1973, The intrinsic random functions and their applications, Advan. Appl. Probab., 5, 438-468

Matheron, G., and G. de Marsily, 1980, Is transport in porous media always diffusive? A counter example, Water Resour. Res., 16(5), 901-917

McLaughlin, D., 1978, Potential applications of Kalman filtering concepts to gorundwater basin management, in Applications of Kalman Filter to Hydrology, Hydraulics, and Water Resources, C.L. Chiu, ed., Stochastic Hydraulics Program, University of Pittsburg, Pennsylvania, 639-655

McLaughlin, D. 1979, Application of kriging to a groundwater plume mapping problem, Trans, Am. Geophys. Union, V60(46), 820

McMillan, W.D., 1966, Theoretical analysis of groundwater basin operations, Contrib. 114, 167 p., University of California, Water Resour. Center, Berkeley, California

Mercado, A., 1967, The spreading pattern of injected waters in a permeable stratified aquifer, Symp. of Haifa, Artificial Recharge and mangement of Aquifers, IASH Publ. 72, 23-36, Int Assn Hydrol Sci., Gentbrugge, Belgium

Mizell, S.A., A.L. Gutjahr, and L.W. Gelhar, 1982, Stochastic analysis of spatial variability in two-dimensional steady groundwater flow assuming stationary and non-stationary heads, Water Resour. Res., 19, 1853-1867

Moench, A.F., 1984, Double-porosity models for a fissured groundwater reservoir

with fracture skin, Water Resour. Res., 20(7), 831-846

Moltyaner, G.L., 1985, Stochastic versus determinate: a case study, in Proc. Int'l Assoc. Hydraulic Research Symp. on The Stochastic Approach to Subsurface Flow, G. de Marsily (ed.), Montuillargenne, France, June 3-6, pp. 362-364

Molz, F.J., O. Guven, J.G. Melville, R.D. Crocker, K.T. Matteson, 1986, Performance, analysis and simulation of a two-well tracer test at the Mobile site, Water Resour. Res. 22(7):1031-1037

Morel-Seytoux, H.J., 1976, Water resources planning (an illustration on management of surface and groundwaters), in Stochastic Approaches to Water Resources, Vol 1., H.W. Shen, ed., pp 10-1-10-61

Moreno, L. and A. Rasmuson, 1986, Contaminant transport through a fractured porous rock: impact of the inlet boundary condition on the concentration profile in a rock matrix, Water Resour. Res. 22(12):1728-1730

Morrison, P., and P. Morrison, 1982, Powers of Ten, Scientific American Books, New York

Musy, A. and L. Duckstein, 1976, Bayesian approach to tile drain design, J. Irr. Drain Div., ASCE, V102(3), 317-334

Naff, R.L. and A.V. Vecchia, 1986, Stochastic analysis of three- dimensional flow in a bounded domain, Water Resour. Res. 22(5):695-704

Naff, R.L. and A.V. Vecchia, 1987, Depth-averaging effects on hydraulic head for media with stochastic hydraulic conductivity, Water Resour. Res. 23(4):5612-570

Nelson, R.W., 1964, Stream functions for three-dimentional flow in heterogeneous porous media, in General Assembly of Berkeley, August 1963, Int. Assn. Sci. Hydrol. Publ. No. 64, 290-297

Nelson, R.W., 1966, Flow in heterogeneous porous mediums, 1, Darcian-type description of two-phase systems, Water Resour. Res. V2(3), 487-495

Neretnieks, I., 1985, Transport in fractured rocks, Mem. Int. Assoc. Hydrogeol., 17:301-318

Neuman, S.P., 1979, Statistical characterization of aquifer heterogeneities: An overview, Recent Trends in Hydrogeology, Geol. Soc. Am. Spec. Pap., in press

Neuman, S.P., 1980, Statistical analysis and stochastic modeling of the Cortaro aquifer in southern Arizona, Trans. Am. Geophys. Union, V61(46), 952

Neuman, S.P., 1980, A statistical approach to the inverse problem of aquifer hydrology, 3, Improved solution method and added perspetive, Water Resour. Res., V16(2), 331-346

Neuman, S.P., 1982, Statistical characterization of aquifer heterogeneitics: an overview, in Recent Trends in Hydrogeology (T.N. Narasimham, ed.), Spec.

Pap. Geol. Soc. Amer. v. 189, pp. 81-102, Boulder, CO

Neuman, S.P., 1984, Role of geostatistics in subsurface hydrology in Geostatistics for Natural Resources Characterization, Proc. NATO-ASI, Verly, G., David, M., Journel, A.G., and Marechal, A. (eds.), Part 1, pp. 781-817, Reidel, Dordrecth, The Netherlands

Neuman, S.P., Stochastic continuum representation of fractured rock permeability as an alternative to the REV and fracture network concepts, 533-561, 28th U.S. symposium on rock mechanics, Tucson, Arizona, 29 June -1 July, 1987.

Neuman, S.P., and S. Yakowitz, 1979, A statistical approach to the inverse problem of aquifer hydrology, 1, Theory, Water Resour. Res., V15(4), 845-860

Neuman, S.P., G.E. Fogg, and E.A. Jacobson, 1980, A statistical approach to the inverse probelm of aquifer hydrology: 2. Case study, Water Resour. Res., V16(1), 33-58

Neuman, S.P., C.L. Winter, C.M. Newman, 1987, Stochastic theory of field-scale fickian dispersion in anisotropic porous media, Water Resour. Res. 23(3):453-466

Neuzil, C.E., 1986, Groundwater flow in low-permeability environments, Water Resour. Res. 22(8):1163-1195

Nielsen, D.R., 1979, Analyzing the spatial variability of soil parameters infield soils, Trans. Am. Geophys. Union, V60(32), 583-584

Nielsen, D.R., J.W. Biggar, and K.T. Erh, 1973, Spatial variability of field measured soil-water properties, Hilgardia, V. 42:215-260

Nielsen, D.R., J. W. Biggar, and C.S. Simmons, 1979, Analysis of water and solute movement in field soils, Trans. Am. Geophys. Union, V60(7), 113

Nikolaevskii, V.N., 1959, Convective diffusion in porous media, Prikl, Matem. Mekhan, V23(6), 1042-1050

Olbrisch, H-D., 1977, Modeling of groundwater recharge according to infiltration measurements by lysimeters, in Hydraulic Engineering for Improved Water Management, Proc. 17th Congress of Int. Assn for Hydraul Res., 15-19 August 1977, Vol 6, 718-722

Osborn, J.F., 1966, The prediction fo piezometric groundwater levels in observation wells based on prior occurrences, Water Resour. Res., V2(1), 139-144 Oster, C.A., A.G. Gibbs, and D.H. Tang, 1981, Analysis of a numerical solution to the one-dimentional stochastic convection equation, Adv. in Water Resour., V4(1), 2-8

Parker, J.C., and K.A. Albrecht, 1987, Sample volume effects on solute transport predictions, Water Resour. Res. 23(12): 2293-2301

Parsons, A.M., E.D. Mattson, D.B. Stephens, K. Flamigan, K. Black, 1988, Field simulation of waste impoundment seepage in the vadose zone, Proc. Focus on Groundwater Issues, Conf. Nat. Water Well Assoc., March 23-35,

Albuquerque. Peck, A.J., R.J. Luxmoore, and J.L. Stolzy, 1977, Effects of spatial variability of soil hydraulic properties in water budget modeling, Water Resour. Res., V13(2), 348-354

Perkins, T.K. and O.E. Johnston, 1963, A review of diffusion and dispersion in porous media, Soc. Petrol. Eng. J., V3(1), 70-84f

Philip, J.R., 1967, Sorption and infiltration in heterogeneous media, Aust. J. Soil Res., V5, 1-10Peters, R.R., J.H. Gauthier, and A.L. Dudley, The effect of percolation rate on water-travel time in deep, partially saturated zones, Sandia Report, SAND85-0854, 1986

Philip, J.R., 1980, Field heterogeneity: Some basic issues, Water Resour. Res., V16(2), 443-448

Philip, J.R., 1984, Travel times from buried and surface infiltration point sources, Water Resour. Res. 20( ): 990-994

Pickens, J.F. and G.E. Grisak, 1981, Modeling of scale-dependent dispersion in hydrogeologic systems, Water Resour. Res. 17(6):1701-1711

Pickens, J.F. and G.E. Grisak, 1981, Scale-dependent dispersion in a stratified granular aquifer, Water Resour. Res. 17: 1191-1211

Pimentel, K.D., 1978, Asymptotic estimation error growth applied to monitoring, in Applications of Kalman Filter to Hydrology, Hydraulics, and Water Resources, C.L. Chiu, ed., Stochastic Hydraulics Program, University of Pittsburg, Pennsylvania, 681-691

Pimentel, K.D., J.V. Candy, S.G. Azevedo, and T.A. Doerr, 1980, Simplified ground-water flow modeling: An application of Kalman filter based identification, NTIS Accession No. UCRL- 82649.

Pollock, D.W., 1986, Simulation of fluid flow and energy transport processes associated with high-level radioactive waste disposal in unsaturated alluvium, Water Resour. Res. 22(5):765-777

Poreh, M., 1965, The dispersivitytensor inisotropic and axisymmetric mediums, J. Geophys. Res., V70(16), 3909-3914

Prager, S., 1961, Viscous flow through porous media, Phys Fluids, V4(12), 1477-1482

Raats, P.A.C., 1975, Continuum interpretation of discrete, structured and probabilistic models for transport of solutes in prous media, Trans. Am. Geophys. Union, V56(12), 978

Rao, A.R., R.G.S. Rao, and R.L. Kashyap, 1975, Stochastic models for groundwater levels, Tech. Rep. No. 67, Water Resour. Res. Center, Purdue Univ.,West Lafayette, Indiana

Rao, P.S.C, P.V. Rao, J.M. Davidson, 1977, Estimation of the spatial variability of soil-water flux, Soil Sci. Soc. Am. J. 41:1208-1209

Rao, P.V., K.M. Portier, and P.S.C. Rao, 1981, A stochastic approach for describing

convective-dispersive solute transport in saturated porous media. Water Resour. Res., V17, in press

Rasmuson, A. and I. Neretnieks, 1986, Radionuclide migration in strongly fissured zones: the sensitivity to some assumptions and parameters, Water Resour. Res. 22(4):559-569

Rasmuson, A. and I. Neretnieks, 1986, Radionuclide transport in fast channels in crystaline rock, Water Resour. Res. 22(8):1247-1256

Rasmussen, T.C., 1987, Computer simulation of steady fluid flow and solute transport through three-dimensional networks of variably saturated, discrete fractures, in Evans, D.D. and T.J. Nicholson (Eds.), Flow and Transport Through Unsaturated Fractured Rock, AGU Geophysical Monograph 42, 107-114

Remson, I. and J.R. Randolph, 1958, Application of statistical methods to the analysis of groundwater levels, Trans. Am. Geophys. union, V39(1), 75-83

Rifai, E.M.N., W.J. Kaufman, and D.K. Todd, 1956, Dispersion phenomena in laminar flow through porous media, Progr. Report 3, Sanitary Eng. Research Lab., University of California, Berkeley, 156 p.

Robbins, G.A. and P.A. Domenico, 1985, Determining dispersion coefficients and sources of model-dependent scaling, J. Hydrol. 75:195-211

Rockaway, J.D., Jr., 1970, Trend-surface analysis of ground- water fluctuations, Ground Water, May-June 1970, 29-36

Ross, B. and C.M. Kopllik, 1978, A statistical approach to modeling transport of pollutants in ground water, J. Int. Assn. Math Geology, V10(6), 657-672

Ross, B. and C.M. Koplik, 1979, A new numerical method for solving the solute transport equation, Water Resour. Res., V15(4), 949-955

Ross, B., 1986, Dispersion in fractal fracture networks, Water Resour. Res. 22(5):823-827

Russo, D. and E. Bresler, 1980, Field determinations of soil hydraulic properties for statistical analyses, Soil Sci. Soc. Am. J., V44(4), 697-702

Russo, D. and E. Bresler, 1980, Scaling soil hydraulic properties of heterogeneous field, Soil Sci Soc Am J., V44(4), 681-684

Saffman, P.G., 1959, A theory of dispersion in a porous medium, J. Fluid Mech., V6(3), 321-349

Saffman, P.G., 1960, Dispersion due to molecular diffusion and macroscopic mixing inflow through a network of capillaries, J. Fluid Mech., V7(2), 194-208

Sager, B., 1978, Analysis of dynamic aquifers with stochastic forcing function, Water Resour. Res., V14(2), 207-216

Sager, B., 1978, Galerkin finite element procedure for analyzing flow through random media, Water Resour. Res., V14(6), 1035- 1044

Sager, B., 1979, Solution of lineraized Boussineq equation with stochastic boundaries and recharge, Water Resour. Res. V15(3), 618-624

Sagar, B. and C.C. Kiesiel, 1972, Limits of deterministic predictability of saturated flow equations, in Proc. Second Int. Symp. on Fund of Trans. Phen. in Porous Media, V 1, 194-205, Int. Assn Hydraul. Res., University of Guelph, Guelph, Ontario, Canada

Sager, B. and C. Preller, 1980, Stochastic model of water table under drainage, J. Irr. Drain. Div., ASCE, V106(3), 189-202

Sager, B. and S.R. Singh, 1979, Aquifer diffusivity from noisy boundary data, J. Hydraul. Div., ASCE, V105(8), 943-954

Scheidegger, A.E., 1954, Statistical hydrodynamics in porous media, J. Appl Phy., V25(8), 994-1001

Scheidegger, A.E., 1958, The random-walk model with autocorrelation of flow through porous media, Can. J. Phys., V36, 649-658

Scheidegger, A.E., 1959, Statistical approach to miscible displacement in porous media, Can. Mining Met. Bull., V 52(561), 26-30

Scheidegger, A.E., 1960, The physics of flow through porous media, revised edition, University of Toronto Press, Toronto, Ontario, Canada

Scheidegger, A.E., 1961, General theory of dispersion in porous media, J. Geophys. Res., V66(10), 3273-3278

Scheidegger, A.E., 1961, On the statistical properties of some transport equations, Can. J. Phys., V39(11), 1573-1582

Scheidegger, A.E., 1964, Statistical hydrodynamics in porous media, Advan. Hydrosci., V1, 161-181, V.T. Chow, ed., Academic Press, New York, NY

Scheidegger, A.E., 1967, Solitary dispersion, Can. J. Phys., V45(5), 1783-1789

Scheidegger, A.E., 1974, The physics of flow through porous media, 3rd ed., University of Toronto Press, Toronto, Ontario, Canada

Scheidegger, A.E., and N.M. Chandhari, 1964, Some statistical properties of certain geophysical transport equations, Pure and Appl. Geophys., V59(3), 45

Schmidtke, K., E.A. McBean, and J.F. Sykes, 1980, Stochastic estimation of states in unconfined aquifers subject to artificial recharge, Trans. Am. Geophys. Union, V61(46), 954

Schwartz, F.W., 1977, Macroscopic dispersion in porous media: The controlling factors, Water Resour. Res., V13(4), 743-752

Schwartz, F.W., L. Smith, and A.S. Crowe, 1983, A stochastic analysis of macroscopic dispersion in fractured media, Water Resour. Res., 19,1253-1265

Schwydler, M.I., 1962, Flow inheterogeheous media (in Russian), Izv. Akad. Nauk

SSSR Mekh Zhidk. Gaza., V 3, 185

Shapiro, A. M., and J. Andersson, 1983, Steady-state fluid response in fractured rock: A boundary element solution for a coupled, discrete fracture continuum model, Water Resour. Res. 19(4), 959-969

Shih, S.F., 1973, Modified Monte Carlo application to groundwater movement--the simultaneity procedures, Water Resour. Res., V9(4), 1029-1038

Shvidler, M.I., 1975, Dispersion of a filtration stream in a medium with random in homogeneities, Sov. Phys. Doklady, V20(3), 171-173

Siddiqui, S.H. and R.R. Parizek, 1974, An application of parametric statistical tests to well-yield data from carbonates of central Pennsylvania, J. Hydrol., V21(1),1-14

Simmons, C.S., 1982, A stochastic-convective ensemble method for representing dispersive transport in groundwater, EPRI, Palo Alto CA, Tech. Rept. CS-2558, RP 1406-1

Simmons, C.S., 1982, A stochastic-convective transport representation of dispersion in one-dimensional porous media systems, Water Resour. Res. 18(4):1193-1214

Simmons, C.S., D.R. Nielsen and J.W. Biggar, 1979, Scaling of field-measured soil-water properties, Hilgardia, V47(4), 77-173

Simpson, E.S., 1962, Transverse dispersion in liquid flow through porous media, USGS Prof. Paper 411-C, Washington, D.C.

Simpson, E.S., 1970, On the dispersivity of real aquifers, Trans. Am. Geophys. Union, V51(4), 284

Sitar, N., J.D. Cawlfield, A. Der Kiureghian, 1987, First-order reliability approach to stochastic analysis of flow and contaminant transport, Water Resour. Res. 23(5):794-804

Skagius, K. and I. Neretnieks, 1986, Porosities and diffusivities of some nonsorbing species in crystalline rocks, Water Resour. Res. 22(3):389-398

Smith, D.V., 1972, Comments on "A chance-constrained approach to the conjunctive use of surface waters and groundwaters" by G.H. Nieswand and M.L. Granstrom, Water Resour. Res., V8(6), 1621-1622. Nieswand, G.H. and M.L. Granstrom, 1972, Reply, Water Resourc. Res., V8(6), 1623-1625

Smith, L. and R.A. Freeze, 1979a, Stochastic analysis of steady state groundwater flow in a bounded domain, 1, One- dimensional simulations, Water Resour. Res., V15(3), 521-528

Smith, L. and R.A. Freeze, 1979b, Stochastic analysis of steady state groundwater flow in a bounded domain, 2, Two- dimensional simulations, Water Resour. Res., V15(6), 1543-1559

Smith, L. and F.W. Schwartz, 1980, Role of laboratory-scale measurements in mass-transport modeling, Trans. Am. Geophys. Union, V61(17), 232

Smith, L. and F.W. Schwartz, 1980, Mass transport, 1. A stochastic analysis of macroscopic dispersion, Water Resour. Res. 16:303-313

Smith, L., F.W. Schwartz, 1981a, Mass transport, 2. Analysis of uncertanity in prediction, Water Resour. Res. 17(2): 351-369

Smith, L. and F.W. Schwartz, 1981b, Mass transport, 3. Role of hydraulic conductivity in prediction, Water Resour. Res., 17(5), 1463-1479

Smith, L., 1981, Spatial variability of flow parameters in a stratified sand, Int. J. Math. Geol., V13(1), 1-21

Smith, R.E., 1976, Effects of random variation in soil parameters relating to infiltration patterns, Trans. Am. Geophys. Union, V57(12), 914

Snyder, W.M. and L.E. Asmussen, 1972, Subsurface hydrograph analysis by convolution, J. Irr. Drain. Div., ASCE, V98(3), 405-418,Smith,R.E., 1973, Discussion, V99(3), 404-406

Sposito, G., 1981, The statistical mechanical theory of groundwater flow, Water Resour. Res., V 17, in press

Sposito, G., W.A. Jury, V.K. Gupta, 1986, Fundamental problems in the stochastic convection-dispersion model of solute transport in aquifers and field soils, Water Resour. Res. 22(1):77-88

Sposito, G., P.J. Sullivan, and V.K. Gupta, 1977, Experimental test of Langevin equation as a model for waterflow through unsaturated soil, SoilSci. Soc. Am. J., V41(4), 820-822

Stephens, D.B., L.W. Gelhar, S. Young, 1984, Field experiment to evaluate dispersion in unsaturated media (Abs.) EOS, 65(16):106.

Strecker, E.W., W.-S. Chaurd, D.P. Lettenmaier, 1986, Parameter identification of ground-water contamination transport model, Groundwater 24(1):56-62

Sudicky, E.A., 1986, A natural gradient experiment on solute transport in a sand aquifer: spatial variability of hydraulic conductivity and its role in the dispersion process, Water Resour. Res., 22, 2069-2082

Sunada, D.K., 1976, Statistical applications in groundwater systems, in Stochastic Approaches to Water Resources, Vol. 2, H.W. Shen, ed., pp 20-1-20-17Taylor, G.I., Diffusion by continuous movements, Proc. London. Math. Soc. Ser. A20, 196-211, 1922

Tang, D.H. and G.F. Pinder, 1977, Simulation of groundwater flow and mass transport under uncertainty, Adv. in Water Resources 1(1):25-30

Tang, D.H., and G.F. Pinder, 1979, Analysis of mass transport with uncertain physical parameters, Water Resourc. Res., V15(5), 1147-1155

Tang, D.H., F.W. Schwartz, L. Smith, 1982, Stochastic modeling of mass transport in a random velocity field, Water Resour. Res. 18( ):231-244

Taylor, G. I., Diffusion by continuous movements, Proc. London. Math. Soc. Ser. A20, 196-211, 1922.

Taylor, G.I., Dispersion of soluble matter in solvent flowing slowly through a tube, Proc. London. Math. Soc. Ser. A219, 186-203, 1953.

Thirriot, C., R. Gaudu, and j. Valiantzas, 1979, Microscopic and macroscopic aspects of heterogeneity in porous media, Trans., Am. Geophys. Union,V60(7), 116-117

Todorovic, P., 1970, A stochastic model of longitudinal diffusion in porous media, Water Resour. Res.,V6(1), 211-222

Todorovic, P.N., 1971, A stochastic model of lateral diffusion in a porous medium, in Stochastic Hydraulics, C.L. Chiu, ed., School of Engineering, University of Pittsburg, 632-653

Todorovic, P., 1975, A stochastic model of dispersion in a porous medium, Water Resourc. Res., V11(2), 348-354

Tomkoria, B.N. and A.E. Scheidegger, 1967, A complete thermo- dynamic analogy for transport processes, Can., J. Phys., V45(11), 3569-3587

Torelli, L. and A.E. Scheidegger,1971, A review of the stochastic approach to flow through porous media, in Stochastic Hydraulics, C.L. Chiu, ed., School of Engineering, University of Pittsburg, 644-666.

Torelli, L. and A.E. Scheidegger, 1972, Three-dimensional branching-type models of flow through porous media, J. Hydrol. V15(1), 23-35

Torelli, L., 1972, Computer simultaion of the dispersion phenomena occurring during flow through porous media, using a random maze model, Pure and Appl. Geophys. V96(4), 75-88

Torelli, L. and P. Tomasi, 1977, Interpolation and trend analysis, two geohydrological applications, J. Int. Ass'n for Math. Geol., V995), 529-542

van Genuchten, M.T., A closed-form equation for predicting the hydraulic conductivity of unsaturated soils, Soil Sci. Soc. Am. J., 44, 892-898, 1980.

Vomvoris, E.G., and L.W. Gelhar, Stochastic prediction of dispersive contaminant transport, U.S. Department of Commerce National Technical Information Service, Cooperative Agreement, CR-811135-01-2, Dec., 1986.

Vanmarke, E. 1983, Random fields: analysis and synthesis, MIT Press, Cambridge, MA

Vauclin, M., Imbernon, J., Vachaud, G. and C. Danceete, 1983, Description experimentale et modelisation stochastique des transferts par la mise en echelle des proprietes hydrodynamiques. In: Isotope and radiation techniques in Soil Physics and irrigation studies 1983, IAEA, Vienne 1983

Vauclin, M., 1983, Methods d'etude de la variabilite spatiale des proprietes d' un sol, Variabilite spatiale des processus de transfert dans les sols, Avignon, 24-25

Juin 1982 Ed. INRA Publ. 1983 (Les Colloques de l' INRA, no 15). Vetier, A., 1978, Covariance function of a stochastic process, Periodica Polytech., Electr. Eng., V22(2-3), 85-89

Volpi, G. and G. Gambolati, 1978, On the use of main trend for the kriging technique in hydrology, Adv. in Water Resour., V1(6), 345-349

Wagner, B.J. and S.M. Gorelick, 1986, A statistical methodology for estimating transport parameters: theory and applications to one-dimensional advective-dispersive systems, Water Resour. Res. 22(8):1303-1315

Wang, J.S.Y., and T.N. Narasimhan, Hydrologic mechanisms governing fluid flow in a partially saturated, fractured, porous medium, Water Resour. Res., 21(12), 1861-1874, 1985.

Warren, J.E., and H.S. Price, Flow in heterogeneous porous media, Society of Petroleum Engineers Journal, 1, 153-169, 1961.

Warren, J.E., and P.J. Root, Behavior of naturally fractured reservoirs, Society of Petroleum Engineers Journal, 9, 245-255, 1963.

Warren, J.E., and F.F. Skiba, Macroscopic dispersion, Trans AIME, 231, 215-230, 1964.

Warren, J.E., F.F. Skiba, and H.S. Price, An evaluation of the significance of permeability measurements, Journal Petroleum Technology, 13, 739-744, 1961.

Warrick, A.W., G.J. Mullen, and D.R. Nielsen, 1977, Scaling field-measured soil hydraulic properties using a similar media concept, Water Resour. Res., V13(2), 355-362

Wen-Sen, C., E.W. Strecker, D.P. Lettenmaier, 1987, An evaluation of data requirements for groundwater contaminant transport modeling, Water Resour. Res. 23(3): 408-424

Wheatcraft, S.W. and S.W. Tyler, An explanation of scale- dependent dispersivity in heterogeneous aquifers using concepts of fractal geometry, Water Resour. Res., 24(4), 525-532, 1988.

Wierenga, P.J., L.W. Gelhar, C.S. Simmons, G.W.Gee, T.J. Nicholson, 1986, Validation of stochastical flow and transport models for unsaturated soil: a comprehensive field study, U.S. Nuc. Reg. Comm. Report NUREG/CR-4622.

Williams, D., Geostatistical analysis and inverse modeling of the Upper Santa Cruz Basin, Arizona, Master Thesis, Univ. of Arizona, pp149, 1987.

Williams, R.E., Comment on "Statistical theory of groundwater flow and transport: Pore to Laboratory, Laboratory to Formation, and Formation to Regional Scale" by Gedeon Dagan, Water Resour. Res., 24(7), 1197-1200, 1988.

Williams, R.E., Comment on "Double-porosity models for a fissured groundwater reservoir with fracture skin" by Allen F. Moench, Water Resour. Res., 21(6), 889-891, 1985.

Wilson, J.L., and L.W. Gelhar, 1974, Dispersive mixing in a partially saturated porous medium, 353 p., Rep. 191, R.M. Parsons Lab. for Water Resour. and Hydrodynamics, Massachusetts Institute of Technology, Cambridge

Wilson, J.L., P.K. Kitanidis, and M.D. Dettinger, 1978, State and parameter estimation in groundwater models, in Applications of Kalman Filter to Hydrology, Hydraulics, and Water Resources, C.L. Chin, ed., Stochastic Hydraulics Program, University of Pittsburg, 657-679

Wilson, J.L., 1979, Piezometric head prediction: Conditional simulation vs. first-order analysis, Trans. Am. Geophys. union, V60(46), 820.

Wilson, J.L., 1981, The unified approach to groundwater modeling, Trans. Am. Geophys. Union, V62(17), 281

Winter, C.L., C.M. Newman, and S.P. Neuman, A perturbation expansion for diffusion in a random velocity field, SIAM J. Appl. Math, 44(2), 411-424, 1984.

Wood, E.F., 1981, The unified approach to groundwater modeling, Trans. Am. Geophys. Union, V62(17), 281

Wu, T.H., S.K. Vyas, and N.Y. Change, 1973, Probabilistic analysis of seepage, J. Soil Mech. Found. Div.,ASCE, V99(4), 323-240

Yakowitz, S., 1976, Model-free statistical methods for water table prediction, Water Resour. Res., V12(5), 836-844

Yakowitz, S. and L. Duckstein, 1980, Instability in aquifer identification: Theory and case studies, Water Resour. Res., V1696), 1045-1064

Yeh, T.-C.J., L.W. Gelhar, A.L. Gutjahr, 1985a, Stochastic analysis of unsaturated flow in heterogeneous soils, 1, Statistically isotropic media, Water Resour. Res., 21(4), 447-456

Yeh, T.-C.J., L. W. Gelhar and A.L. Gutjahr, 1985b, Stochastic analysis of unsaturated flow in heterogeneous soils, 2, Statistically anisotropic media with variable alpha, Water Resour. Res., 21(4), 457-464

Yeh, T.-C.J., L.W. Gelhar and A.L. Gutjahr, 1985c, Stochastic analysis of unsaturated flow in heterogeneous soils, 3, Observations and applications, Water Resour. Res., 21(4), 465-472

Yeh, T.-C.J., L.W. Gelhar, A.L. Gutjahr, 1986, Correction to "Stochastic analysis of unsaturated flow in heterogeneous soils, 1 and 2", Water Resour. Res. 22(5):843

Yeh, T.-C.J., 1987, Comment on "modeling of scale dependent dispersion in hydrogeologic systems" by J.F. Pickens and G.E. Grisak, Water Resour. Res. 23(3):522

Yeh, W.W.-G., 1986, Review of parameter identification procedures in groundwater hydrology: the inverse problem, Water Resour. Res. 22(2):95-108

Yoon, Y.S. and W. W-G. Yeh, 1979, Identification of aquifer parameters with the kriging technique, Trans. Am. Geophys. Union, V60(46), 821.

Zal'tsberg, E.A., 1975, Application of the theory of stationary random functions to hydrogeologic forecasting, Soviet Hydrology-Selected papers, 1975, No. 4, 216-219

Zaporozec, A., 1980, Statistical analysis as a tool in evaluating the effect of drought on shallow ground-water levels, Trans. Am. Geophys. Union, V61(17), 229-230 Zhang, Y., 1982, Double Porosity Model and its Finite Element Solution for the flow in Fractured-Karst Rocks, Hydrogeology and Engineering Geology, 4.