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Prediction of Far-Field Subsurface Radionuclide Dispersion Coefficients from Hydraulic Conductivity Measurements

A Multidimensional Stochastic Theory with Application to Fractured Rocks

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ABSTRACT

A multidimensional stochastic theory is presented for far-field dispersion due to the spatial variability of hydraulic conductivities. We use a second-order perturbation approach to relate the far-field velocity vector, $\underline{V}$, and dispersion tensor, $\underline{D}$, to the mean and covariance of the local seepage velocity vector, $\underline{v}$, and the local dispersion tensor, $\underline{d}$. We find that, in general, $\underline{V}$ is not necessarily equal to the ensemble mean of $\underline{v}$, $\underline{\mu}$, and that $\underline{D}$ is a second-rank symmetric tensor. In the particular case where $\nabla \cdot \underline{v} = 0$ (e.g., incompressible fluid in a rigid porous medium of uniform effective porosity), $\underline{V}$ becomes equal to $\underline{\mu}$, and our expressions for $\underline{D}$ simplify to those presented by Gelhar and Axness [1983]. We further extend a conclusion of these authors, that as the Peclet number, ν, increases, $\underline{D}$ becomes asymptotically linear in $|\underline{\mu}|$, by showing that it holds for arbitrary velocity covariance functions. Finally, we derive expressions for $\underline{D}$ as a function of ν for situations where the logarithm of hydraulic conductivity fits a spherical covariance or semivariogram function, as is often the case. These expressions are applied to log hydraulic conductivity data from packer tests conducted in seven boreholes penetrating fractured granites near Oracle, southern Arizona.

TABLE OF CONTENTS

List of Figure Captions

Page

PREFACE

Radionuclides released to the subsurface environment from a radioactive waste repository will be transported and spread through the host rock by groundwater. The average distance traveled by such radionuclides in a given time is determined by the groundwater seepage velocity. The degree to which a plume of radionuclides spreads about its center of gravity is controlled by the dispersion coefficient of the flow field, which in turn depends on the seepage velocity as well as the dispersivity of the host rock. Recent studies have shown that dispersivity is not a constant property of the host rock but increases as the plume moves away from the respository. If the seepage velocity field is statistically homogeneous, the dispersivity tends to a constant "far-field" value as the distance between the plume and the respository increases. Under these conditions, transport in the far field can be modeled by the classical advection-dispersion equation based on an analogy to Fick's law of diffusion.

Most existing subsurface transport models are based on the Fickian adection-dispersion equation. To use these models one must know, among other parameters, the far field dispersivity of the host rock. Unfortunately, this dispersivity cannot be measured directly by tracer tests in low-permeability rocks. The reason is that, in such rocks, one may have to wait very long before the tracer moves far enough from its source for the dispersivity to become constant. To overcome this difficulty, we propose a method to estimate the far field dispersivity of a rock mass indirectly from measurements of hydraulic conductivity. The latter parameter can be obtained with relative ease by packer tests.

Our method of predicting the dispersivity parameter is based on a stochastic theory akin to that developed by others for turbulent diffusion. The theory shows that dispersivity is a second-rank symmetric tensor which can be related to a dimensionless Peclet number. The Peclet number is proportional to the mean seepage velocity, the correlation length of the hydraulic conductivities, and inversely proportional to the near field longitudinal dispersion coefficient. Near field dispersion coefficients can be determined by tracer tests in closely spaced wells. Our theory shows that for large Peclet numbers, the far field dispersivity tensor is independent of these dimensionless numbers.

The formulae developed in this study have been applied to fractured granitic rocks near Oracle, southern Arizona. We believe that the same formuale should also be applicable to other fractured rocks. The U.S. Nuclear Regulatory Commission may be asked to approve applications for licensing subsurface high-level nuclear waste repositories in low-permeability fractured rocks. The formulae and theory developed herein should be of practical help to the NRC in support of such license applications.

1. INTRODUCTION

Subsurface solute transport has traditionally been described by the convection-dispersion equation [Scheidegger, 1954; Bear, 1972; Fried, 1975]

$$\frac{\partial c}{\partial t} = (\nabla \cdot \underline{d} \nabla - \nabla \cdot \underline{v})c \quad ; \qquad c(\underline{x}, o) = c_o(\underline{x}) \tag{1}$$

where $c(\underline{x},t)$ is concentration, $\underline{x}$ is position vector, t is time, $\underline{d}$ is hydrodynamic dispersion tensor, $\underline{v}(\underline{x})$ is seepage velocity vector, and ∇ is gradient operator (all symbols are defined in Appendix A). This equation is derived from mass balance considerations and the assumption that the dispersive mass flux, $\underline{J}_d$, obeys Fick's first law,

$$\underline{J}_d = - \underline{d} \nabla c \tag{2}$$

The hydrodynamic dispersion tensor is believed to have principal directions parallel and normal to the seepage velocity vector, $\underline{v}$. The principal value of $\underline{d}$ parallel to $\underline{v}$, d_L, is called "longitudinal dispersion coefficient." Normal to $\underline{v}$, $\underline{d}$ is often taken to be isotropic and represented by the "transverse dispersion coefficient," d_T. These two coefficients are usually expressed as

$$\begin{aligned} d_L &= d_m + a_L \, |\underline{v}| \\ d_T &= d_m + a_T \, |\underline{v}| \end{aligned} \tag{3}$$

where d_m is the coefficient of subsurface molecular diffusion (generally smaller than the equivalent coefficient in the pore fluid), a_L is "longitudinal dispersivity," and a_T is "transverse dispersivity."

Certain aspects of this theoretical model have been confirmed by small-scale laboratory experiments on relatively uniform granular materials [Bear, 1972; Fried, 1975; Klotz et al., 1980]. These experiments further suggest that a_L and a_T are velocity dependent: when $|\underline{v}|$ tends to zero, so do a_L and a_T, whereas when $|\underline{v}|$ becomes large, the dispersivities approach constant values.

Attempts to apply the same model to large-scale laboratory and field tracer experiments have led to several difficulties. One difficulty is that a_L and a_T seem to vary with the scale of the experiment. Whereas in the laboratory a_L ranges from 10^{-4}m to 10^{-1}m for relatively uniform fine to coarse-grained soils and up to almost 1 m for coarse gravel [Bear, 1961; Lawson and Elrick, 1972; Klotz et al., 1980], in field tracer experiments a_L varies from 10^{-2} m to 10 m, and may on occasion exceed 10^2 m [Lallemand-Barrés and Peaudecerf, 1978; Anderson, 1979; Pickens and Grisak, 1981a]. When a_L is obtained by matching the output of computer models based on (1) with documented histories of aquifer pollution on a regional scale, its value ranges from less than 10 m to more than 100 m [Anderson, 1979]. Another difficulty is that, in a given tracer experiment, a_L and a_T appear to grow with distance of the sampling point from the source [Martin, 1971; Peaudecerf and Sauty, 1978; Sudicky and Cherry, 1979; Dieulin et al., 1980; Silliman and Simpson, 1983]. I phenomenon and treating a_L as a constant may lead to able conclusion that a concentration plume could spre exceeding that predicted by molecular diffusion alone Simpson, 1978].

The difficulty with the classical Fickian model is th scale. One promising way to deal with this scale eff age velocity as a stochastic process. Assume that, o satisfies (1), but the seepage velocity, $\underline{v}(\underline{x})$, varies tion to another due to aquifer heterogeneity. Then c dependent random function: as time (and thus distanc increases, the characteristics of the plume change. expand but, more importantly, its outline becomes inc solute concentration evolves from an initially irregu which is quite regular.

Our problem is reminiscent of scale-dependent random used to describe phenomena in other fields of physics mediate relevance to subsurface transport is work don lent diffusion. On the local scale, turbulent diffus equation having the same mathematical form as (1). L constant, second-rank, symmetric, positive-semidefini weakly stationary stochastic process. We can then wr

$$\underline{v}(\underline{x}) = \underline{\mu} + \varepsilon\, \underline{u}(\underline{x})$$

where $\underline{\mu}$ is the mean velocity vector, $\underline{u}(\underline{x})$ is a weakly zero mean, and ε is a dimensionless parameter measuri velocity fluctuations. Then it has been proven that, ases, the concentration tends asymptotically to a Fick by

$$\frac{\partial C}{\partial \tau} = (\nabla \cdot \underline{D} \nabla - \nabla \cdot \underline{V}) C \quad ; \quad C(\underline{X},0) = c_0(\underline{X})$$

where $C(\underline{X},\tau)$ is the concentration at a large distance after the passage of a long time, τ, $\underline{D}$ is an effectiv $\underline{V}$ is an effective velocity vector, the latter two bei $\bar{c}(\underline{x},t)$ tends asymptotically to $C(\underline{X},\tau)$ have been provi of zero concentration at infinite distances from the cases: (a) for the case of convection-dominated (i.e. diffusion in 1, 2, and 3 spatial dimensions by Kesten and (b) for the case of incompressible (i.e., $\nabla \cdot \underline{v} = 0$ 3 spatial dimensions by Papanicolaou and Pironeau [19 parameter ε is scaled to zero as time gets large.

The assumptions underlying these proofs appear to be valid not only for turbulent diffusion, but also for certain cases of subsurface transport as suggested by the experimental results of Martin [1971], Peaudecerf and Sauty [1978], Sudicky and Cherry [1979], Sudicky et al. [1983] and Silliman and Simpson [1983]. In these large scale laboratory and field tracer experiments a_L and a_T increase with sampling distance from the source. However, the dispersivities tend asymptotically to constant values as this distance increases, implying an asymptotic tendency toward Fickian behavior. The experiment of Sudicky et al. provides an exceptionally vivid illustration of this tendency by showing how the outlines of two three-dimensional plumes change with time from irregular shapes to near-perfect Gaussian distributions.

If we accept the existing mathematical proofs and experimental evidence that the concentration field tends asymptotically toward Fickian behavior, what remains is to develop (a) a model for the early non-Fickian regime and (b) expressions for the effective parameters $\underline{V}$ and $\underline{D}$. Attempts to deal with the first problem in connection with subsurface transport have been reported by various authors including Gelhar et al. [1979], Matheron and de Marsily [1980], Dieulin et al. [1981] and Dagan [1982]. However, Pickens and Grisak [1981b, p. 1701] found that "for systems that exhibit a constant (asymptotic) dispersivity at large times or mean travel distances, the importance of scale-dependent dispersion at early times or short travel distances...[is] minimal in long-term prediction of solute transport." This, together with our primary interest in regional dispersion, has led us to focus on the second problem of determining $\underline{V}$ and $\underline{D}$.

A solution to the latter problem for the case of purely convective turbulent diffusion, where $\underline{d}$ is identically equal to zero, has been given by Roberts [1961]. Gelhar et al. [1979] and Matheron and de Marsily [1980] have considered the highly specialized case of subsurface transport in layered media. The velocity fields in such media are in fact so special that they violate the conclusions of Kesten and Papanicolaou [1979] and Papanicolaou and Pironeau [1980] unless a very strong condition is fulfilled: the covariance function of $\underline{v}$ exhibits a so-called "hole effect." An interesting work on two-and three-dimensional subsurface transport where $\underline{d}$ is very small compared to $\underline{D}$ has been published by Dagan [1982]. More recently, Gelhar and Axness [1983] have presented a comprehensive stochastic theory of dispersion in statistically anisotropic three-dimensional porous media.

In this paper we outline a second-order perturbation theory that relates $\underline{V}$ and $\underline{D}$ to the mean and covariance of the seepage velocity vector, $\underline{v}$, and to the local dispersion tensor, $\underline{d}$. Our perturbation expansion is in the spirit of Kubo [1963] and its mathematical details can be found in the Ph.D. dissertation of Winter [1982] or the paper of Winter et al. [1983]. The theory applies in an arbitrary number of spatial dimensions and under a variety of flow conditions. We find that, in general, $\underline{V}$ is not necessarily the same as $\underline{\mu}$ (in the one dimensional case, $\underline{V}$ is less than $\underline{\mu}$), and $\underline{D}$ is a second-rank symmetric tensor. Only in the particular case where $\nabla \cdot \underline{v} = 0$ (e.g., incompressible fluid in a rigid porous medium of uniform effective porosity) are $\underline{V}$ and $\underline{\mu}$ equal. In this latter case, our expressions for $\underline{D}$ simplify to those presented by Gelhar and Axness [1983].

Suppose that the x_1 coordinate is oriented parallel to $\underline{\mu}$ and define a Peclet number, ν, as

$$\nu = \frac{\mu_1 \ L}{d_{11}}$$

where L is some characteristic length. Gelhar and Axness [1983] were able to show for two specific velocity covariance functions that when $\nabla \cdot \underline{v} = 0$, $\underline{D}$ becomes asymptotically linear in μ_1 as ν increases. We show that their conclusion holds true for all velocity covariance functions, and their corresponding expression for the asymptotic dispersivity has universal validity under the above conditions.

Bakr et al. [1978] and Gelhar and Axness [1983] have derived expressions relating the spectrum of $\underline{v}$ to the spectrum of the log-hydraulic conductivity, K, for statistically isotropic and anisotropic situations, respectively. These expressions make it possible to write $\underline{V}$ and $\underline{D}$ as functions of the mean log-hydraulic conductivity and its covariance (or spectrum). In practice, the spatial variability of K is often analyzed by means of geostatistical methods involving semivariograms. Experience to date has shown that many semivariograms of log K fit a so-called "spherical" model. We therefore conclude our paper by deriving expressions for $\underline{D}$ in terms of a spherical semivariogram or covariance and applying these expressions to packer test data from fractured granites near Oracle in southern Arizona.

2. CENTRAL LIMIT THEOREM

In the following two sections we describe our approach to calculating the effective velocity and dispersion coefficients, $\underline{V}$ and $\underline{D}$. The final forms of these coefficients are given in equations (36)-(40) below.

Three key ideas lie behind our estimates of $\underline{V}$ and $\underline{D}$: averaging the small-scale concentration, c, over the distribution of the local seepage velocity, $\underline{v}$; rescaling time and space in (1); and applying the semigroup approach to the rescaled transport equation. There is an intimate connection between transport equations like (1) and stochastic "diffusion" processes. The latter are processes describing the position of a solute particle whose concentration is given by functions like $c(\underline{x},t)$. In fact, the fundamental solution (Green's function) of (1) is the transition (probability) density of the following stochastic diffusion process [Gihman and Skorohod, 1972]

$$\underline{X}'(t) = \underline{\mu} + \varepsilon\, \underline{u}[\underline{X}(t)] + \underline{b}\, \underline{w}'(t) \qquad (7)$$

where $\underline{X}(t)$ is the particle position at time t, $\underline{b}^2 = 2\underline{d}$, $\underline{w}(t)$ is a standard Wiener process, and the prime indicates differentiation with respect to time.

Since (1) is a stochastic equation due to the randomness of $\underline{u}$, we can consider the (ensemble) mean of the local concentration, $\bar{c}(\underline{x},t)$. Although $\bar{c}$ does not generally satisfy (1) or (5), we proceed on the assumption that, as time increases, $\bar{c}$ tends asymptotically to the solution of (5). The rationale for this assumption is based on the limit theorems of Kesten and Papanicolaou [1979] and Papanicolaou and Pironeau [1980] together with the experimental evidence cited in the introduction.

In order to compare the asymptotic behaviors of (1) and (5), we first rescale the variables τ and $\underline{X}$ in (5) by means of a positive scalar, λ, such that $\tau_\lambda = \tau/\lambda$ and $\underline{X}_\lambda = (\underline{X}-\underline{V}\tau)/\sqrt{\lambda}$, and the convective term vanishes. Thus, upon defining the modified concentration $C_\lambda(\underline{X}_\lambda,\tau_\lambda) = C(\underline{X},\tau)$, (5) takes the form

$$\frac{\partial C_\lambda}{\partial \tau_\lambda} = \nabla_\lambda \cdot (\underline{D}\nabla_\lambda C_\lambda) \quad ; \quad C_\lambda(\underline{X}_\lambda,0) = c_o(\sqrt{\lambda}\underline{X}_\lambda) \tag{8}$$

where ∇_λ is the gradient operator with respect to $\underline{X}_\lambda$. In the limit as $\lambda\to\infty$, this becomes

$$\frac{\partial C_\infty}{\partial \tau_\infty} = \nabla_\infty \cdot (\underline{D}\nabla_\infty C_\infty) \quad ; \quad C_\infty(\underline{X}_\infty,0) = \lim_{\lambda\to\infty} c_o(\sqrt{\lambda}\underline{X}_\lambda) \tag{9}$$

The fundamental solution of (9) is a Gaussian density function, $f(\underline{X}_\infty)$, with zero mean and covariance $2\,\underline{D}\,\tau_\infty$. Equivalently, the random position vector

$$\frac{\underline{X}(\lambda\tau_\lambda) - \lambda\tau_\lambda\underline{V}}{\sqrt{\lambda}} \tag{10}$$

has a density which approaches $f(\underline{X}_\infty)$ as $\lambda\to\infty$. In other words, (10) satisfies a central limit theorem as λ, and thereby τ, become large.

We now turn to (1) and treat $\underline{u}$ for a moment as a given (i.e., nonrandom) function. If we define $t_\lambda = t/\lambda$, $\underline{x}_\lambda = \underline{x}/\sqrt{\lambda}$, and $c_\lambda(\underline{x}_\lambda, t_\lambda) = c(\underline{x},t)$, then (1) takes on the modified form

$$\frac{\partial c_\lambda}{\partial t_\lambda} = \nabla_\lambda \cdot (\underline{d}\nabla_\lambda c_\lambda) - \sqrt{\lambda}\, \nabla_\lambda \cdot \{[\underline{\mu}+\varepsilon\, \underline{u}(\sqrt{\lambda}\underline{x}_\lambda)]c_\lambda\} \quad ; \tag{11}$$
$$c_\lambda(\underline{x}_\lambda,0) = c_o(\sqrt{\lambda}\underline{x}_\lambda) \quad .$$

Since $\underline{u}$ is given, $c_\lambda(\underline{x}_\lambda,t_\lambda)$ can be viewed as the conditional density of the position process $\underline{X}_\lambda(t_\lambda) = \underline{X}(\lambda t_\lambda)/\sqrt{\lambda}$. On the other hand the translated process, $\underline{X}_\lambda(t_\lambda) - \sqrt{\lambda}t_\lambda\underline{V}$, has a conditional density, $f_\lambda(\underline{x}_\lambda|\underline{u})$, given by

$$f_\lambda(\underline{x}_\lambda|\underline{u}) = c_\lambda(\underline{x}_\lambda + \sqrt{\lambda}t_\lambda\underline{V},\ t_\lambda) \quad . \tag{12}$$

Let us, for clarity of notation, replace t_λ, $\underline{x}_\lambda$, and ∇_λ by t, $\underline{x}$, and ∇, respectively. To obtain the marginal density, $f_\lambda(\underline{x})$, from $f_\lambda(\underline{x}|\underline{u})$, we recall that

$$\begin{aligned} f_\lambda(\underline{x}) &= \int f_\lambda(\underline{x},\ \underline{u})\ d\underline{u} = \int f_\lambda(\underline{x}|\underline{u})\ f(\underline{u})d\underline{u} \\ &= E_u[f_\lambda(\underline{x}|\underline{u})] \end{aligned} \tag{13}$$

where $f_\lambda(\underline{x},\ \underline{u})$ is the joint density of $\underline{X}_\lambda(t)$ and $\underline{u}$, $f(\underline{u})$ is the marginal density of $\underline{u}$, and E_u represents expectation over $\underline{u}$.

Our objective is to exploit the limit assumption

$$\lim_{\lambda\to\infty} f_\lambda(\underline{x}) = f(\underline{x}) \tag{14}$$

to calculate $\underline{V}$ and $\underline{D}$. According to (13), this is the same as

$$\lim_{\lambda\to\infty} E_u[f_\lambda(\underline{x}|\underline{u})] = f(\underline{x}) \tag{15}$$

An equivalent form of (14) - (15), which we prefer to use below, is

$$\lim_{\lambda\to\infty} E_{\underline{X}_\lambda}[g(X_\lambda - \sqrt{\lambda}t_\lambda\underline{V})] = E_{\underline{X}_\infty}[g(\underline{X}_\infty)] \tag{16}$$

where g is an arbitrary function and $\underline{X}_\infty$ has the density $f(\underline{x})$.

To apply (16) we return to (11). The fundamental solution of the latter equation is equal to the conditional transition density of $\underline{X}(\lambda t)/\sqrt{\lambda}$ for a given $\underline{u}$, which we designate by $p_u(s,\underline{y};t,\underline{x})$. The product $p_u(s,\underline{y};t,\underline{x})\ d\underline{x}$ is the probability that a particle starting at $\underline{y}$ at time s<t has reached a small volume centered on $\underline{x}$ at time t. It is important to note that p_u is also the fundamental solution to the formal adjoint of (11), i.e.,

$$\frac{\partial p_u}{\partial s} = [-\nabla\cdot\underline{d}\nabla - \sqrt{\lambda}\ [\underline{\nu} + \varepsilon\ \underline{u}(\sqrt{\lambda}\underline{y})]\cdot\nabla]p_u \quad = -L_\lambda p_u \tag{17}$$

where $-L_\lambda$ is the differential operator in the middle expression acting on the variable y. The interested reader should consult a standard text on stochastic differential equations, e.g. Gihman and Skorohod [1972], for details.

Define an integral operator with kernel $p_u(s,\underline{y};t,\underline{x})$ on an arbitrary function, h, as

$$P_u(s,t)h = \int_{R^k} p_u(s,\underline{y};t,\underline{x})\ h(\underline{x})d\underline{x} \tag{18}$$

where R^k is the k-dimensional Euclidean space. Since p_u is the transition density of a diffusion process, the operators P_u form a continuous semigroup, the backwards semigroup of p_u [Feller, 1966]. We use these operators because they are conveniently represented by exponentials. To help see this, observe that if (18) is differentiated with respect to s, and the arbitrary h is ignored, then formally

$$\frac{\partial}{\partial s} P_u = - L_\lambda\ P_u \tag{19}$$

Because p_u approaches a Dirac delta function when s approaches t,

$$P_u = e^{-(s-t)L_\lambda} \tag{20}$$

Armed with (18)-(20) we return to the limit assumption (16) which, by virtue of (13) and (12), can be represented as

$$\begin{aligned} E_{\underline{X}_\lambda}[g(\underline{X}_\lambda-\sqrt{\lambda}t_\lambda\underline{V})] &= \int_{R^k} g(\underline{x})\ E_u[f_\lambda(\underline{x}|\underline{u})]d\underline{x} \\ &= \int_{R^k} g(\underline{x})\ E_u[c_\lambda(\underline{x}+\sqrt{\lambda}t\underline{V},t)]d\underline{x} \\ &= \int_{R^k} g(\underline{z}-\sqrt{\lambda}t\underline{V})\ E_u[c_\lambda(\underline{z},t)]d\underline{z} \end{aligned} \tag{21}$$

But the solution of (11) is given by the convolution of its fundamental solution with the initial condition, i.e.,

$$c_\lambda(\underline{z},t) = \int_{R^k} p_u(0,\underline{y};t,\underline{z})\ c_o(\sqrt{\lambda}\underline{y})d\underline{y} \tag{22}$$

On the other hand, translation by $-\sqrt{\lambda}t\underline{V}$ is equivalent to application of the operator $e^{-\sqrt{\lambda}t\underline{V}\cdot\nabla}$. Thus

$$E_{\underline{X}_\lambda}[g(\underline{X}_\lambda)] = \int_{R^k} e^{-\sqrt{\lambda}t\underline{V}\cdot\nabla} g(\underline{z}) \quad E_u[\int_{R^k} p_u(0,\underline{y};t,\underline{z})\ c_o(\sqrt{\lambda}\underline{y})d\underline{y}]d\underline{z}$$

$$= \int_{R^k} c_o(\sqrt{\lambda}\underline{y})\ E_u[\int_{R^k} p_u(0,\underline{y};t,\underline{z})e^{-\sqrt{\lambda}t\underline{V}\cdot\nabla}g(\underline{z})d\underline{z}]\ d\underline{y}$$

$$= \int_{R^k} c_o(\sqrt{\lambda}\underline{y})\ E_u[\ e^{tL_\lambda}\ \ e^{-\sqrt{\lambda}t\underline{V}\cdot\nabla}g]\ d\underline{y} \tag{23}$$

Similarly the asymptotic density, $f(\underline{x})$, satisfies (9). Upon replacing τ_∞, $\underline{X}_\infty$, and ∇_∞ by t, $\underline{x}$, and ∇, we can write the backwards semigroup corresponding to (9) as

$$P(s,t) = e^{-(s-t)\ \nabla\cdot\underline{D}\nabla} \tag{24}$$

Thus, in analogy to (23), we have

$$E_{\underline{X}_\infty}\ [g(\underline{X}_\infty)] = \int_{R^k} C_\infty(\underline{y},0)\ e^{t(\nabla\cdot\underline{D}\nabla)} g(\underline{y})d\underline{y} \tag{25}$$

From $\lim_{\lambda\to\infty} c_o(\sqrt{\lambda}\underline{y}) = C_\infty(\underline{y},o)$ in (9) it is clear that (16) is satisfied only

if

$$\lim_{\lambda\to\infty} E_u[\ e^{tL_\lambda}\ e^{-t\sqrt{\lambda}\ \underline{V}\cdot\nabla}] = e^{t(\nabla\cdot\underline{D}\nabla)} \quad . \tag{26}$$

Because L_λ has random and nonrandom parts, we write it as $L_\lambda = A + \varepsilon B$ where the nonramdom part is

$$A = \nabla\cdot\underline{d}\nabla + \sqrt{\lambda}\underline{\mu}\cdot\nabla \tag{27}$$

and the random part is

$$B = \sqrt{\lambda}\ \underline{u}(\sqrt{\lambda}\underline{x})\cdot\nabla \tag{28}$$

Thus (26) becomes

$$\lim_{\lambda\to\infty} E_u \left[e^{t(A+\varepsilon B)} e^{-\sqrt{\lambda} t \underline{V}\cdot\nabla} \right] = e^{t(\nabla\cdot\underline{D}\nabla)} \tag{29}$$

Equation 29 is the starting point for the next section. It is the mathematical equivalent of the assumption that the solution of (1) converges to that of (5) as time increases.

3. EFFECTIVE COEFFICIENTS

3.1 General Case

Our approach is to derive perturbation expansions for $\underline{V}$ and $\underline{D}$ in powers of ε,

$$\underline{V}(\varepsilon) = \underline{V}_0 + \varepsilon\underline{V}_1 + \varepsilon^2\underline{V}_2 + \ldots \; , \; \underline{D}(\varepsilon) = \underline{D}_0 + \varepsilon\underline{D}_1 + \varepsilon^2\underline{D}_2 + \ldots \tag{30}$$

with $\underline{\mu}$, $\underline{u}$ and $\underline{d}$ given. We obtain our expansions by writing the terms in (29) as series in ε. We use the standard expansion [Hille and Phillips, 1957]

$$e^{t(A+\varepsilon B)} = e^{tA} + \varepsilon \int_0^t e^{(t-t_1)A} B\, e^{t_1 A} dt_1$$

$$+ \varepsilon^2 \int_0^t \int_0^{t_1} e^{(t-t_1)A} B\, e^{(t_1-t_2)A} B\, e^{t_2 A} dt_2 dt_1 + \ldots \tag{31}$$

together with the expansions following from (30),

$$e^{-\sqrt{\lambda} t(\underline{V}\cdot\nabla)} = [1 - \varepsilon\sqrt{\lambda} t \underline{V}_1\cdot\nabla - \varepsilon^2\sqrt{\lambda} t\underline{V}_2\cdot\nabla + \frac{1}{2}\varepsilon^2 \lambda t^2 (\underline{V}_1\cdot\nabla)^2$$

$$+ \ldots] \, e^{-\sqrt{\lambda} t(\underline{V}_0\cdot\nabla)} \tag{32}$$

$$e^{t(\nabla\cdot\underline{D}\nabla)} = [1 + \varepsilon t(\nabla\cdot\underline{D}_1\nabla) + \varepsilon^2 t\,(\nabla\cdot\underline{D}_2\nabla)$$

$$+ \frac{1}{2}\varepsilon^2 t^2 (\nabla\cdot\underline{D}_1\nabla)^2 + \ldots] \, e^{t(\nabla\cdot\underline{D}_0\nabla)} \tag{33}$$

Substituting (31) - (33) into (29) and taking limits term by term we find that $\underline{V}_0 = \underline{\mu}$, $\underline{V}_1 = 0$, $\underline{D}_0 = \underline{d}$, and $\underline{D}_1 = 0$. The second order terms are obtained from

$$\lim_{\lambda\to\infty} \{-\sqrt{\lambda}t\underline{V}_2\cdot\nabla + \int_0^t\int_0^{t_1} e^{(t-t_1)A}E_u[Be^{(t_1-t_2)A}B]e^{(t_2-t)A}dt_2dt_1\}$$

$$= t\nabla\cdot\underline{D}_2\nabla \tag{34}$$

Details of the derivation are given in Appendices B and C.

The second order terms, $\varepsilon^2\underline{V}_2$ and $\varepsilon^2\underline{D}_2$, are expressed in terms of the velocity covariance function

$$\rho_{nm}(\underline{x}-\underline{y}) = E[v_n(\underline{x})v_m(\underline{y})] - \mu^2 \tag{35}$$

or its Fourier transform (the "cross-power spectrum")

$$\hat{\rho}_{nm}(\underline{\xi}) = \int_{R^k} e^{i\underline{\xi}\cdot\underline{x}}\,\rho_{nm}(\underline{x})\,d\underline{x}$$

where $i = \sqrt{-1}$. With this notation, the second order approximation of $\underline{V}$ is given by

$$\underline{V} = \underline{\mu} + \underline{V}^* \tag{36}$$

where

$$V_n^* = (2\pi)^{-k}\sum_{m=1}^{k}\int_{R^k}\frac{i\,\xi_m\,\hat{\rho}_{nm}(\underline{\xi})}{F(\underline{\xi})}\,d\underline{\xi}\;;\; n = 1,\ldots,k\;;\; k > 1 \tag{37}$$

and $F(\underline{\xi}) = \underline{\xi}\cdot\underline{d}\,\underline{\xi} - i\underline{\mu}\cdot\underline{\xi}$. The second order approximation of $\underline{D}$ is given by

$$\underline{D} = \underline{d} + \underline{D}^* \tag{38}$$

where

$$\underline{D}^* = (\underline{D}^{(i)} + \underline{D}^{(i)T} + \underline{D}^{(ii)} + \underline{D}^{(ii)T})$$

and

$$D_{nm}^{(i)} = \frac{1}{2} (2\pi)^{-k} \int_{R^k} \frac{1}{F(\underline{\xi})} \hat{\rho}_{nm}(\underline{\xi})\, d\underline{\xi} \quad ; \quad k>2 \tag{39}$$

$$D_{nm}^{(i)} = \frac{d}{4\pi} \int_{-\infty}^{\infty} \frac{\hat{\rho}(\xi)d\xi}{d^2\xi^2+\mu^2} + \frac{1}{4|\mu|} \int_{-\infty}^{\infty} \rho(x)\, dx \; ; \; k = 1 \; ; \; n = m = 1$$

$$D_{nm}^{(ii)} = - (2\pi)^{-k} \sum_{p=1}^{k} \sum_{r=1}^{k} \int_{R^k} \frac{\xi_p\, \rho_{pm}(\underline{\xi})\, d_{nr}\, \xi_r}{[F(\underline{\xi})]^2}\, d\underline{\xi} \tag{40}$$

T indicating transpose. Clearly, $\underline{D}^*$ is a second rank symmetric tensor. It can be shown that if the elements of $\hat{\underline{\rho}}$ are bounded at the origin and integrable (e.g., if $\underline{\rho}$ is integrable and continuous) then (37) is well defined (i.e., requires no regularizations in the integral for k>2) whenever $\underline{d}$ is positive definite and for k=1 whenever $\mu \neq 0$. Similarly, (39) and (40) are well defined for k>3 whenever $\underline{d}$ is positive definite, for k=2 whenever $\underline{d}$ is positive definite and $\underline{\mu} \neq 0$, and for k=1 whenever $u \neq 0$. In some cases (37), (39) and (40) are well defined even if these conditions are not met so long as $\hat{\underline{\rho}}$ satisfies a more stringent condition. For instance, if $\nabla \cdot \underline{v}=0$ then $\underline{D}^{(ii)}$ vanishes and, in R^2, we can allow $\underline{\mu} = 0$ if $\hat{\underline{\rho}}(0) = 0$. Of course this requires that the matrix valued function $\underline{\rho}$ itsel be not positive semidefinite over some spatial region. Such a hole effect has been investigated by Gelhar et al. [1979] and Matheron and de Marsily [1980], and similar conditions on $\underline{\rho}$ have been obtained. In most realistic cases, however, no such strong conditions on $\underline{\rho}$ are required.

In one-dimension, the evenness and positivity of $\rho(\xi)$ imply that

$$V^* = - \frac{\mu}{2\pi} \int_{-\infty}^{\infty} \frac{\hat{\rho}(\xi)}{d^2\xi^2+\mu^2}\, d\xi < 0 \tag{41}$$

Thus for $\mu > 0$, $V < \mu$ (to second order). When local dispersion is small, i.e., $d = 0$, this simply reflects the difference between the arithmetic mean (μ) and harmonic mean (V) of the velocity. On the other hand, in the special case $\nabla \cdot \underline{v}=0$ for k>1, $\underline{V}^* = 0$ and $\underline{V} = \underline{\mu}$ (again to second order). We return to this point in the next section. Both of these effects are known to be valid, not just to second order but exactly [S.R.S. Varadhan, personal communication].

When $\nabla \cdot \underline{v} \neq 0$, equations 38-40 indicate that the sign of $\underline{D}^*$ depends on the specific form of $\hat{\underline{\rho}}(\underline{\xi})$. For instance in the one-dimensional case

$$D^* = \frac{1}{2|\mu|}\hat{\rho}(0) + \frac{1}{2\pi|\mu|}\int_{-\infty}^{\infty} \frac{3-\xi^2}{(\xi^2+1)^2}\,\hat{\rho}\left(\frac{|\mu|\xi}{d}\right) d\xi$$

which could be positive or negative.

3.2 Case where $\nabla . v = 0$

In the special case where $\nabla \cdot \underline{v} = 0$ (e.g., incompressible fluid in a rigid porous medium of uniform effective porosity) our results simplify considerably. These simplifications follow from the fact that $\nabla \cdot \underline{v} = 0$ implies

$$E[\, v_n(0) \sum_{m=1}^{k} \frac{\partial}{\partial x_m} v_m(\underline{x})] = \sum_{m=1}^{k} \frac{\partial}{\partial x_m} \rho_{mn}(\underline{x}) = 0 \tag{42}$$

Since the Fourier transform of the middle term in (42) is $\sum_{m=1}^{k} (-i\xi_m)\hat{\rho}_{mn}(\underline{\xi})$, $\nabla \cdot \underline{v} = 0$ requires that

$$\sum_{m=1}^{k} (-i\xi_m)\,\hat{\rho}_{mn}(\underline{\xi}) = 0 \tag{43}$$

Applying (43) to (36) - (40) it is obvious that $\underline{V}^* = 0$ and $\underline{D}^{(ii)} = 0$. Thus we have the result quoted in the last section,

$$\underline{V} = \underline{\mu} \tag{44}$$

Additionally, since $\hat{\underline{\rho}}$ is even, $\underline{D}^*$ for k>1 can be expressed as

$$D^*_{nm} = \frac{1}{2}(2\pi)^{-k} \int_{R^k} \frac{\underline{\xi}\cdot \underline{d}\underline{\xi}}{(\underline{\xi}\cdot \underline{d}\underline{\xi})^2 + (\underline{\mu}.\underline{\xi})^2}\, [\hat{\rho}_{nm}(\underline{\xi}) + \hat{\rho}_{mn}(\underline{\xi})] d\underline{\xi} \tag{45}$$

This is equivalent to equation 22' of Gelhar and Axness (1983).

Since $\underline{d}$ and $\hat{\underline{\rho}} + \hat{\underline{\rho}}^T$ are positive semidefinite matrices, so too is the matrix with elements (45). Thus, $\underline{D}^*$ is a symmetric positive semidefinite tensor, implying that $\underline{D} > \underline{d}$ in the sense that $\underline{D} - \underline{d}$ is positive semidefinite.

Similarly in the one-dimensional case

$$D^* = \frac{d}{2\pi}\int_{-\infty}^{\infty} \frac{\hat{\rho}(\xi)}{d^2\xi^2 + \mu^2} d\xi + \frac{1}{2|\mu|}\hat{\rho}(o) \tag{46}$$

which is positive because $\rho(\xi)$ is positive. This explains why dispersion on a large scale is often greater than on a local scale.

Using relationships between the spectra of log hydraulic conductivity and local velocity obtained by Gelhar and Axness [1983], equation 45 can be written in a form which depends only on properties of the medium. For a locally isotropic but statistically anisotropic medium,

$$D^*_{nm} = (2\pi)^{-k} \int_{R^k} \frac{\underline{\xi}\cdot\underline{d}\underline{\xi}}{(\underline{\xi}\cdot\underline{d}\underline{\xi})^2 + (\underline{\mu}\cdot\underline{\xi})^2} G_{nm}(\underline{\xi})\, \hat{\rho}_Y(\underline{\xi})\, d\underline{\xi} \tag{47}$$

where $\hat{\rho}_Y(\underline{\xi})$ is the spectrum of log conductivity, $Y = \log_{10}K$, and

$$G_{nm}(\underline{\xi}) = \left(\frac{K_g}{\phi_e}\right)^2 \sum_{p=1}^{k} \sum_{r=1}^{k} J_p J_r \left(\delta_{np} - \frac{\xi_n\xi_p}{|\underline{\xi}|^2}\right)\left(\delta_{rm} - \frac{\xi_r\xi_m}{|\underline{\xi}|^2}\right) \tag{48}$$

K_g being the geometric mean of hydraulic conductivity, ϕ_e the effective (kinematic) porosity, J the mean hydraulic gradient, and δ_{ij} Kronecker's delta. Equation 47 follows from (45) by

$$\frac{1}{2}\left[\hat{\rho}_{nm}(\underline{\xi}) + \hat{\rho}_{mn}(\underline{\xi})\right] = G_{nm}(\underline{\xi})\, \hat{\rho}_Y(\underline{\xi}) \tag{49}$$

after Gelhar and Axness [1983]. When hydraulic conductivity is statistically isotropic, Bakr et al. [1978] had earlier shown that

$$G_{nm}(\underline{\xi}) = \frac{\mu_1^2}{\gamma^2}\left(\delta_{n1} - \frac{\xi_1\xi_n}{|\underline{\xi}|^2}\right)\left(\delta_{m1} - \frac{\xi_1\xi_m}{|\underline{\xi}|^2}\right) \tag{50}$$

when the coordinate system has been rotated so that ξ_1 coincides with $\underline{\mu}$. Here $\gamma \cong 1 + \sigma_Y^2/6$, σ_Y^2 being the log conductivity variance.

For the remainder of this paper we will treat the case $\nabla\cdot\underline{v} = 0$. In subsurface hydrology this corresponds either to steady state flow of an incompressible fluid in a medium with uniform effective porosity, or transient flow if the medium is additionally rigid. When these conditions are violated, one must use (36)-(40) instead of (44)-(47). On the other hand, (40) shows that another sufficient condition for $\underline{D}^{(ii)}$ (but not $\underline{V}^*$) to vanish is $\underline{d} = 0$. When this happens and the effective porosity, $\phi_e(\underline{x})$, is variable (while the rest of the above conditions hold), mass conservation requires $\nabla\cdot(\phi_e\underline{v}) = 0$, and the equation

$$\frac{\partial}{\partial t}(\phi_e c) = \nabla \cdot (\phi_e \underline{v} c) \tag{51}$$

reduces to (1) with $\underline{d} = 0$. Hence the standard results from the literature of turbulence [e.g., Kesten and Papanicolaou, 1979], which are identical to our (36)-(40) with $\underline{d} = 0$, apply to this case. Note that when $\underline{d} = 0$ one can compute $\underline{D}^*$ from (45)-(47), but (44) does not hold unless $\nabla \cdot \underline{v} = 0$, and the effective velocity, $\underline{V}$, is generally different than $\underline{\mu}$.

3.3 Behavior at large Peclet numbers

Let us orient ξ_1 parallel to $\underline{\mu}$ so that $\mu_1 = |\underline{\mu}|$ and $\mu_2 = \mu_3 = 0$, and define a dimensionless Peclet number, ν, as

$$\nu = \frac{\mu_1 L}{d_{11}} \tag{52}$$

where L is some characteristic length. One-dimensional experiments suggest that D_{11}/d_{11} tends to 1 as $\nu \to 0$, and becomes proportional to ν when the latter is large [e.g., Bear, 1979]. This is equivalent to saying that, for small ν, D^*_{11} tends to zero, whereas for large ν it tends to $\alpha_L|\mu|$ where α_L, the asymptotic longitudinal dispersivity, is a constant. Furthermore, experiments indicate that there is a smooth variation in D_{11} as ν takes on different values. In this section we investigate the behavior of $\underline{D}$ by writing (45) in terms of ν and formally taking the limits as $\nu \to 0$ and $\nu \to \infty$. Since the behavior of $\underline{D}$ depends on the form of $\hat{\underline{\rho}}(\underline{\xi})$ for intermediate values of ν, we defer consideration of such values until the next section. There we employ (47), rewritten as a function of ν, for a particular $\rho_Y(\underline{x})$ arising from the widely used spherical semivariogram of log hydraulic conductivities.

In the case we now consider, $\hat{\underline{\rho}}$ is symmetric and k = 3, so that (45) can be be written as

$$D^*_{nm} = (2\pi)^{-3} \int_{R^3} \frac{\underline{\xi} \cdot \underline{d\xi}}{(\underline{\xi} \cdot \underline{d\xi})^2 + (\underline{\mu} \cdot \underline{\xi})^2} \hat{\rho}_{nm}(\underline{\xi})\, d\underline{\xi}$$

$$= (2\pi)^{-3} \int_{R^3} \hat{H}(\underline{\xi})\, \hat{\rho}_{nm}(\underline{\xi})\, d\underline{\xi} \tag{53}$$

where $\hat{H}(\underline{\xi})$ is just the term in brackets in the first line. By standard Fourier transform arguments--Parseval's theorem-- (53) can be written in terms of the inverse transforms of $\hat{H}$ and $\hat{\rho}_{nm}$,

$$D^*_{nm} = \int_{R^3} H(\underline{x})\, \rho_{nm}(\underline{x})\, d\underline{x} \tag{54}$$

In Appendix D we show that

$$H(\underline{x}) = \frac{1}{2\pi\sqrt{\det(\underline{d})}} \frac{e^{\underline{d}^{-1/2}\underline{\mu}\cdot\underline{d}^{-1/2}\underline{x}} \cdot e^{-\kappa|\underline{d}^{-1/2}\underline{x}|}}{|\underline{d}^{-1/2}\underline{x}|} \tag{55}$$

where $\kappa = |\underline{d}^{-1/2}\underline{\mu}|$ and $\underline{d}^{-1/2}$ is the positive definite matrix square root of $\underline{d}^{-1}$.

Following conventional practice, we assume that $\underline{d}$ is diagonal when $\underline{\mu}$ is parallel to x_1. Then

$$D^*_{nm} = \alpha_{nm}(\nu)\ |\underline{\mu}| \tag{56}$$

where α_{nm} is a second rank symmetric positive semidefinite "dispersivity" tensor given by

$$\alpha_{nm}(\nu) = \frac{L\nu}{2\pi} \int_{R^3} \frac{e^{\nu(z_1 - |\underline{z}|)}}{|\underline{z}|} \beta^2_{nm}(Lz_1,\ L\sqrt{d_{22}/d_{11}}\ z_2,\ L\sqrt{d_{33}/d_{11}}\ z_3)\ d\underline{z} \tag{57}$$

Here $z_1 = x_1/L$, $z_2 = x_2\sqrt{d_{11}/d_{22}}/L$, $z_3 = x_3\sqrt{d_{11}/d_{33}}/L$, and $\beta^2_{nm} = \rho_{nm}/|\underline{\mu}|^2$, i.e., β_{nm} can be viewed as a coefficient of variation of the seepage velocity field, $\underline{v}$.

Since ν, $\underline{z}$ and $\underline{\beta}$ are dimensionless, $\underline{\alpha}$ has dimensions of length, like L. It is intuitively appealing and mathematically convenient to take L as some measure of the correlation length of the log hydraulic conductivity, Y. Thus, L is an intrinsic property of the medium, provided only that the fluid properties are constant. Equations 49-50 show that, in a statistically isotropic medium, $\underline{\beta}$ depends only on σ_Y and ρ_Y, so that it also is an intrinsic medium property. Consequently, $\underline{\alpha}$ in a given statistically isotropic medium is only a function of the Peclet number, ν. On the other hand, (48)-(49) show that in a statistically anisotropic medium $\underline{\alpha}$ is additionally dependent on the direction of the mean hydraulic gradient, $\underline{J}$, though not on the magnitude of this gradient.

As expected, (57) shows that $\alpha_{nm}(\nu)\to 0$ as $\nu\to 0$; thus $\underline{D}\to\underline{d}$ for dispersion dominated transport. Next we observe that $\alpha_{nm}(\nu)\to$ constant as $\nu\to\infty$ for arbitrary $\underline{\beta}$. Appendix E demonstrates that

$$\begin{aligned} \delta_\nu(\underline{z}) &= \frac{\nu}{2\pi}\frac{e^{\nu(z_1-|\underline{z}|)}}{|\underline{z}|} \to \delta(z_2,z_3) && \text{as } \nu\to\infty \text{ when } z_1 > 0 \\ \delta_\nu(\underline{z}) &\to 0 && \text{as } \nu\to\infty \text{ when } z_1 < 0 \end{aligned} \tag{58}$$

That is, $\delta_\nu(\underline{z})$ approaches a delta function concentrated on the $z_1>0$ axis. Hence, from (57)-(58), $\alpha_{nm}(\nu) \to \alpha_{nm}$ where

$$\alpha_{nm} = \int_0^\infty \beta_{nm}{}^2(x_1,0,0)\, dx_1 \tag{59}$$

which clearly is a constant, depending only on the medium when the latter is statistically isotropic, and additionally on the mean hydraulic gradient direction when the medium is statistically anisotropic.

Interesting features of (59) emerge when (48)-(50) are used to represent $\hat{\rho}_{\ell k}$. It follows from (48) that $\rho_{nm}(x_1,0,0)$--and thus $\beta^2_{nm}(x_1,0,0)$--is even in x_1. Therefore

$$\begin{aligned}
\alpha_{nm} &= \frac{1}{2} \int_{-\infty}^{\infty} \beta^2_{nm}\,(x_1,0,0)\, dx_1 \\
&= \frac{1}{2} \int_{R^3} \beta^2_{nm}(x_1,x_2,x_3)\, \delta(x_2,x_3)\, d\underline{x} \\
&= \frac{1}{2(2\pi)^2} \int_{R^3} \hat{\beta}^2_{nm}(\xi_1,\xi_2,\xi_3)\, \delta(\xi_1)\, d\underline{\xi} \\
&= \frac{1}{2(2\pi)^2} \int_{R^2} \hat{\beta}^2_{nm}(0,\xi_2,\xi_3)\, d\xi_2 d\xi_3 \quad ,
\end{aligned} \tag{60}$$

where we use the fact that $2\pi\delta(\xi_1)$ is the Fourier transform of $\delta(x_2,x_3)$. Since

$$\hat{\beta}^2_{nm}\,(0,\xi_2,\xi_3) = \frac{1}{\gamma^2}\, \delta_{1n}\delta_{1m}\, \hat{\rho}_Y(0,\xi_2,\xi_3), \tag{61}$$

$$\alpha_{nm} = \begin{cases} \dfrac{1}{2\gamma^2(2\pi)^2} \displaystyle\int_{R^2} \hat{\rho}_Y(0,\xi_2,\xi_3)\, d\xi_2 d\xi_3 & ; \quad n=m=1 \\ 0 & ; \quad n\neq 1 \text{ or } m\neq 1 \end{cases} \tag{62}$$

Hence for large Peclet numbers the only nonzero component of $\underline{D}^*$ is D^*_{11}, an effect noted earlier by Gelhar and Axness [1983] for a special form of ρ_Y corresponding to an exponential covariance. On the other hand, when the log conductivity is statistically anisotropic, $G_{nm}(0,\eta_2,\eta_3)$ can be nonzero even when $n \neq 1$, $m \neq 1$. Thus $\beta^2_{nm}(0,\eta_2,\eta_3)$ is also nonzero and (61) indicates that $\alpha_{nm} \neq 0$ in general. This implies that $\underline{D}$ has components $D_{nm} \neq 0$ so that even for convection dominated transport the principal directions of $\underline{D}$ do not coincide with $\underline{\mu}$, the mean velocity vector, unless the latter is parallel to a principal direction of effective hydraulic conductivity. This result, too, has been observed by Gelhar and Axness for a particular $\hat{\rho}_Y$, in this case the transform of a modified exponential covariance.

3.4 Formulae for log hydraulic conductivity with spherical covariance or semivariogram

For extreme values of ν, the behavior of $\underline{\alpha}$ is affected by the actual form of $\hat{\underline{\rho}}$ in only a minor way. However, the form of the spectrum has a more pronounced effect on $\underline{\alpha}$ for intermediate ν. Experience with geostatistics has shown that log hydraulic conductivity as well as log transmissivity are often characterized by a spherical semivariogram function [e.g., Neuman 1983; Jones et al., 1983]. It is therefore of interest to calculate a dispersivity tensor, $\underline{\alpha}$, for the corresponding spherical covariance function in three dimensions. For simplicity, we shall assume that this latter function is isotropic,

$$\rho_Y(|\underline{x}|) = \begin{cases} \sigma_Y^2\left(1 - \dfrac{3|\underline{x}|}{2L} + \dfrac{|\underline{x}|^3}{2L^3}\right) ; & 0<|\underline{x}|<L \\ 0 ; & |\underline{x}|>L \end{cases} \tag{63}$$

and refer to L as the "range" of the covariance function. On the other hand, the local dispersion tensor, $\underline{d}$, will be allowed to remain anisotropic with its principal axes parallel and normal to the direction of flow. Thus, when $\underline{\mu}$ coincides with ξ_1, this tensor takes the form

$$\underline{d} = \begin{matrix} d_L & 0 & 0 \\ 0 & d_T & 0 \\ 0 & 0 & d_T \end{matrix} \tag{64}$$

where d_L and d_T are the longitudinal and transverse local dispersion coefficients, respectively.

Our aim is to express $\underline{\alpha}$ as a function of the Peclet number, $\nu = \mu_1 L/d_L$, for ν ranging from 0 to ∞. To accomplish this, we rewrite $\underline{D}^*$ in terms of ν. From (45),

$$D^*_{nm} = \frac{1}{8\pi^3} A_{nm} \tag{65}$$

where

$$A_{nm} = \int_{R^3} \frac{\underline{\xi}\cdot d\underline{\xi}}{(\underline{\xi}\cdot d\underline{\xi})^2 + |\mu|^2 |\xi|^2} \hat{\rho}_{nm}(\underline{\xi})\, d\underline{\xi}$$

Upon letting $\eta_1 = L\xi_1$, $\eta_2 = L\sqrt{d_T/d_L}\,\xi_2$, and $\eta_3 = L\sqrt{d_T/d_L}\,\xi_3$, A_{nm} takes the form

$$A_{nm} = \frac{1}{Ld_T} \int_{R^3} \frac{\underline{\eta}\cdot\underline{\eta}}{(\underline{\eta}\cdot\underline{\eta})^2 + \nu^2\eta_1^2} \hat{\rho}_{nm}(L^{-1}\eta_1, L^{-1}q\eta_2, L^{-1}q\eta_3)\, d\underline{\eta} \tag{66}$$

where $q = \sqrt{d_L/d_T}$.

Since $\hat{\rho}_{nm}$ is an odd function of at least one of its variables when $n \neq m$ (see equation 50), $A_{nm} = 0$ for $n \neq m$, and $\underline{D}^*$ for a statistically isotropic log hydraulic conductivity field is thus a diagonal tensor. Furthermore, $D^*_{22} = D^*_{33}$ and our problem therefore reduces to that of analyzing A_{11} and A_{22}.

Taking the Fourier transform of ρ_Y and rearranging leads to

$$\hat{\rho}_Y(|\underline{\xi}|) = -4\pi \frac{L^2\sigma_Y^2}{|\underline{\xi}|} \Big[\frac{12}{L^5|\underline{\xi}|^5} \left(\cos L|\underline{\xi}| - 1 + \frac{L^2|\underline{\xi}|^2}{2!} - \frac{L^4|\underline{\xi}|^4}{4!}\right)$$

$$+ \frac{12}{L^4|\underline{\xi}|^4} \left(\sin L|\underline{\xi}| - L|\underline{\xi}| + \frac{L^3|\underline{\xi}|^3}{3!}\right)$$

$$- \frac{3}{L^3|\underline{\xi}|^3} \left(\cos L|\underline{\xi}| - 1 + \frac{L^2|\underline{\xi}|^2}{2!}\right)\Big] \tag{67}$$

Note that (67) is well defined even if $|\underline{\xi}| = 0$.

Substituting (50) and (67) into (66) and converting to spherical coordinates gives

$$A_{nn} = -\frac{16\sigma_Y^2 |\mu|^2 L^2 2\pi}{\gamma^2 d_T} \int_0^{\pi/2} \frac{1}{R^2(\theta)} f_n^2(\theta) \left[I_1(\theta) + I_2(\theta) + I_3(\theta)\right] \sin\theta\, d\theta \tag{68}$$

where

$$f_n^2(\theta) = \begin{cases} (\pi/2)\left(1 - \dfrac{\cos^2\theta}{R^2(\theta)}\right)^2 & ; \quad n = 1 \\ (\pi/4)\left(\dfrac{q\cos\theta\sin\theta}{R^2(\theta)}\right)^2 & ; \quad n = 2 \end{cases}$$

$$R(\theta) = \sqrt{\cos^2\theta + q^2\sin^2\theta} \quad ,$$

$$I_1(\theta) = \frac{12}{R^3}\int_0^{\infty} \frac{\sin Rr - Rr + R^3r^3/3!}{r^3(r^2 + \nu^2\cos^2\theta)}\,dr$$

$$= \pi/2\ \frac{12}{R^3}\left(\frac{e^{-\nu R\cos\theta} - 1 + \nu R\cos\theta - \nu^2R^2\cos^2\theta/2! + \nu^3R^3\cos^3\theta/3!}{\nu^4\cos^4\theta}\right)$$

$$I_2 = -\frac{3}{R^2}\int_0^{\infty} \frac{\cos Rr - 1 + R^2r^2/2!}{r^2(r^2+\nu^2\cos^2\theta)}\,dr$$

$$= \pi/2\ \frac{3}{R^2}\left(\frac{e^{-\nu R\cos\theta} - 1 + \nu R\cos\theta - \nu^2R^2\cos^2\theta/2}{\nu^3\cos^3\theta}\right)$$

$$I_3 = \frac{12}{R^4}\int_0^{\infty} \frac{\cos Rr - 1 + R^2r^2/2! - R^4r^4/4!}{r^4(r^2 + \nu^2\cos^2\theta)}\,dr$$

$$= \frac{\pi}{2}\,\frac{12}{R^4}\left(\frac{e^{-\nu R\cos\theta} - 1 + \nu R\cos\theta - \nu^2R^2\cos^2\theta/2! + \nu^3R^3\cos^3\theta/3! - \nu^4R^4\cos^4\theta/4!}{\nu^5\cos^5\theta}\right)$$

The expressions for I_1, I_2, I_3 are obtained by standard methods of contour integration (details are given in Appendix F). Each is well defined even when $\theta = \pi/2$. When local dispersion is isotropic, $q = 1$, $R(\theta) \equiv 1$, and (68) is greatly simplified. In any event (68) can be simplified by letting $u = \cos\theta$,

$$A_{nn} = -\frac{16\sigma_\gamma^2\mu_1{}^2L^2\, 2\pi}{\gamma^2 d_T}\int_0^1 \frac{1}{R^2(u)}\; f_n^2(u)[I_1(u)+I_2(u)+I_3(u))]\,du$$

$$= -\frac{16\sigma_\gamma^2\mu_1{}^2L^2}{\gamma^2 d_T}\; 2\pi\; B_n \tag{69}$$

Series representations for dispersivities can be derived from (69) by expanding I_1, I_2, I_3, summing term-by-term, and then integrating. For $n = 1$,

$$B_1 = \frac{\pi}{2}\int_0^1 \frac{1}{R^2(u)}\left(1 - \frac{u^2}{R^2(u)}\right)^2 [I_1(u) + I_2(u) + I_3(u)]\,du$$

$$= -\frac{3\pi^2}{4}\sum_{m=0}^{\infty}(-1)^m\frac{(m+1)(m+4)}{(m+5)!}\,\beta_m\,\nu^m \quad ,$$

where

$$\beta_m = \int_0^1 \left(1 - \frac{u^2}{R^2(u)}\right)^2 u^m R^{m-1}(u)\,du.$$

Thus,

$$\alpha_{11}(\nu) = \frac{3\sigma_\gamma^2 L q^2}{\gamma^2}\sum_{m=0}^{\infty}(-1)^m\frac{(m+1)(m+4)}{(m+5)!}\,\beta_m\nu^{m+1} \tag{70}$$

If dispersion is locally isotropic, $R(u) = \sqrt{q^2-(q^2-1)u^2} = 1$ and

$$\beta_m = \frac{8}{(m+1)(m+3)(m+5)}$$

In that case

$$\alpha_{11}(\nu) = \frac{24\sigma_\gamma^2 L}{\gamma^2}\sum_{m=0}^{\infty}(-1)^m\frac{(m+4)}{(m+3)(m+5)(m+5)!}\,\nu^{m+1} \tag{71}$$

Equations (70) and (71) are useful for intermediate values of ν, but not for large values of ν. Happily, the fact that

$$\hat{\delta}_\nu(\underline{n}) = \nu \frac{\underline{n}\cdot\underline{n}}{(\underline{n}\cdot\underline{n})^2 + \nu^2 n_1{}^2}$$

is the Fourier transform of the delta sequence (58) and can be used to obtain an expression for α_{11} at large ν. Using (62), we obtain

$$\lim_{\nu\to\infty} \alpha_{11}(\nu) = \frac{L^{-2}}{2(2\pi)^2\gamma^2} \int_{R^2} \hat{\rho}_Y(0,L^{-1}n_2,L^{-1}n_3)dn_2dn_3 \quad . \tag{72}$$

The limit in (72) can be easily evaluated by applying (67) with $n_1 = 0$ and changing to polar coordinates:

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \hat{\rho}_Y(0,L^{-1}n_2, L^{-1}n_3)\ dn_2dn_3$$

$$= -8\pi^2\sigma_Y^2L^2 \int_0^\infty [\frac{12}{r^4}(\sin r - r + \frac{r^3}{3!}) + \frac{12}{r^5}(\cos r - 1 + \frac{r^2}{2!} - \frac{r^4}{4!})$$

$$\cdot \frac{3}{r^3}(\cos r - 1 + \frac{r^2}{2!})]dr = -3\pi^2\sigma_Y^2L^3.$$

Thus, for $\nu\to\infty$,

$$\alpha_{11} = \frac{3\sigma_Y{}^2L}{8\gamma^2} \tag{73}$$

Since (73) does not depend on q, d_T, or d_L, it is clear that the asymptotic longitudinal dispersivity is not affected by local anisotropy in dispersion. Gelhar and Axness [1983] have noted the same when the covariance of log hydraulic conductivity is exponential, in which case

$$\alpha_{11} = \frac{\sigma_Y{}^2L_e}{\gamma^2}$$

where L_e is the distance at which the covariance is $\sigma_Y^2 e^{-1}$.

For intermediate values of ν, the analysis of $\alpha_{22}(\nu)$ is similar to that of $\alpha_{11}(\nu)$. The relevant integral is

$$B_2 = \frac{\pi}{4} q^2 \int_0^1 \frac{u^2(1-u^2)}{R^6(u)} [\, I_1(u)+I_2(u)+I_3(u)] \, du$$

$$= -\frac{3\pi^2}{8} q^2 \sum_{m=0}^{\infty} (-1)^m \frac{(m+1)(m+4)}{(m+5)!} X_m \nu^m \tag{74}$$

where

$$X_m = \int_0^1 (1-u^2)\, u^{m+2} R^{m-5}(u)\, du$$

Thus in general

$$\alpha_{22}(\nu) = \frac{3\sigma_Y^2 L q^4}{2\gamma^2} \sum_{m=0}^{\infty} (-1)^m \frac{(m+1)(m+4)}{(m+5)!} \nu^{m+1} X_m. \tag{75}$$

When local dispersion is isotropic, X_m reduces to

$$X_m = \frac{2}{(m+3)(m+5)}$$

so that

$$\alpha_{22}(\nu) = \frac{3\sigma_Y^2 L q^4}{\gamma^2} \sum_{m=0}^{\infty} (-1)^m \frac{(m+1)(m+4)}{(m+3)\ (m+5)\ (m+5)!} \nu^{m+1} \tag{76}$$

As before, (75) and (76) are good for intermediate values, but not very helpful in the analysis of $\alpha_{22}(\nu)$ for large ν. Furthermore, the line of reasoning which led to (73) is not enlightening, since it only serves to show that $\alpha_{22}(\nu)\to 0$ as $\nu\to\infty$. That suggests that $\alpha_{22}(\nu) = O(\nu^{-\lambda})$ for some $\lambda>0$, and not much more. The problem is to find λ.

The relevant integral is

$$B_2 = \frac{\pi}{4} q^2 \int_0^1 \frac{u^2(1-u^2)}{R^6(u)} [I_1(u)+I_2(u)+I_3(u)]\, du$$

$$= \frac{-\pi^2}{8\nu^2} q^2 \int_0^1 \frac{1-u^2}{R^7(u)}\, du + o(\nu^{-2}). \qquad (77)$$

The second line follows from the first by a lengthy calculation given in Appendix G. The notation, $o(\nu^{-2})$, signifies terms which go to zero as $\nu\to\infty$ faster than ν^{-2}.

To evaluate the integral in (77), let $c^2 = q^2-1$, $u = \frac{\alpha}{c} \sin\theta$, and $\Psi = \sin^{-1}c/q$. Then

$$\int_0^1 \frac{1-u^2}{R^7(u)}\, du = \int_0^1 \frac{1-u^2}{(q^2-c^2u^2)^3 \sqrt{q^2-c^2u^2}}\, du$$

$$= \frac{1}{q^6 c} \int_0^{\Psi} \frac{1-(q/c)^2 \sin^2\theta}{\cos^6\theta}\, d\theta$$

$$= \frac{2}{15q^6} (q^2+4) \qquad (78)$$

Thus

$$\alpha_{22} = \frac{\sigma_\gamma^2 \mu_1 L^2 q^2}{2\gamma^2 d_T} \left[\frac{2}{15q^6} (q^2+4)\nu^{-2} + o(\nu^{-2})\right]$$

$$= \frac{\sigma_\gamma^2 L}{15\gamma^2} \left(1 + \frac{4}{q^2}\right)\nu^{-1} + o(\nu^{-1})$$

and asymptotically

$$\alpha_{22} = \frac{\sigma_Y^2 L}{15\gamma^2} \quad (1 + \frac{4d_T}{d_L}) \quad \frac{1}{\nu} \quad . \tag{79}$$

When local dispersion is isotropic

$$\alpha_{22} = \frac{\sigma_Y^2 L}{3\gamma^2} \quad \frac{1}{\nu} \tag{80}$$

and on the other hand when $d_L >> d_T$.

$$\alpha_{22} = \frac{\sigma_Y^2 L}{15\gamma^2} \frac{1}{\nu} \tag{81}$$

4. APPLICATION TO FRACTURED ROCKS AT ORACLE, SOUTHERN ARIZONA

Some of the results developed in this paper have been applied to log hydraulic conductivity data obtained by packer tests from fractured granitic rocks near Oracle, southern Arizona. Details about the site and the packer tests can be found in the reports of Jones et al. [1983] and Hsieh et al. [1983]. Over a hundred test data have been analyzed from seven boreholes arranged in the pattern shown in Fig. 1 (no data are available from borehole H8). In each test, the distance between the packers was 13 feet, i.e., the measured log hydraulic conductivities are averages over 13 foot depth intervals. The tested intervals cover a range of depths from about 60 to 250 feet in most of the boreholes.

Fig. 2 shows two spherical semivariograms fitted to sample semivariograms obtained from the Oracle data. One of these semivariograms represents the horizontal direction, the other represents the vertical. The parameters σ_Y and L of the two semivariograms were determined by cross-validation with the aid of kriging [see Jones et al., 1983, for details]. While both semivariograms have the same "sill," σ_Y^2 = 0.83, their ranges vary from L = 30 feet in the horizontal direction to L = 60 feet in the vertical direction. Despite this apparent statistical anisotropy, the data can also be fitted with almost equal justification to an isotropic semivariogram (averaged over all directions) with σ_Y^2 = 0.83 and L = 30 feet. It is this latter semivariogram, illustrated in Fig. 3, that we will utilize for our example below.

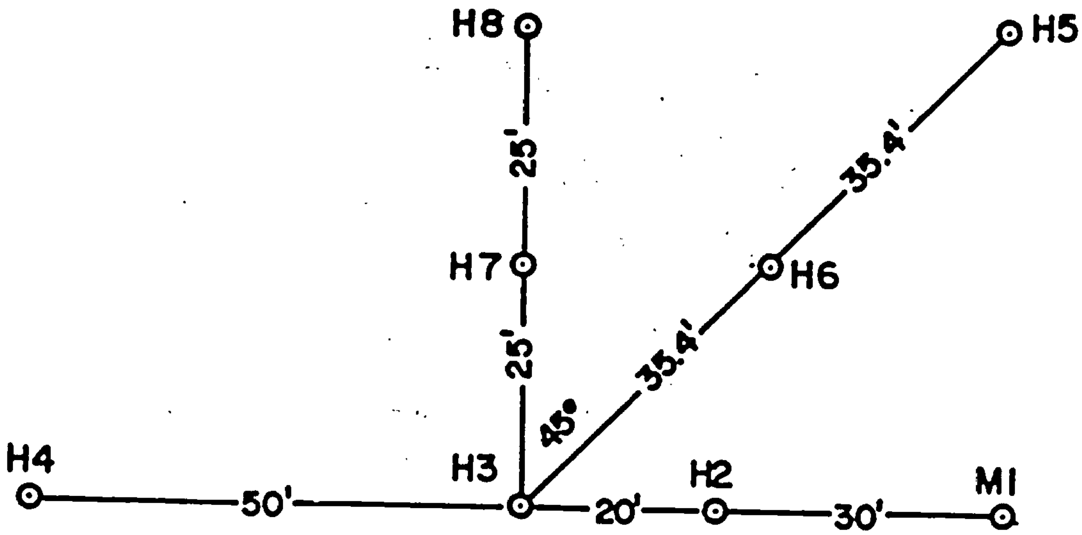

Figure 1. Location of boreholes at Oracle site (after Jones et al., 1983).

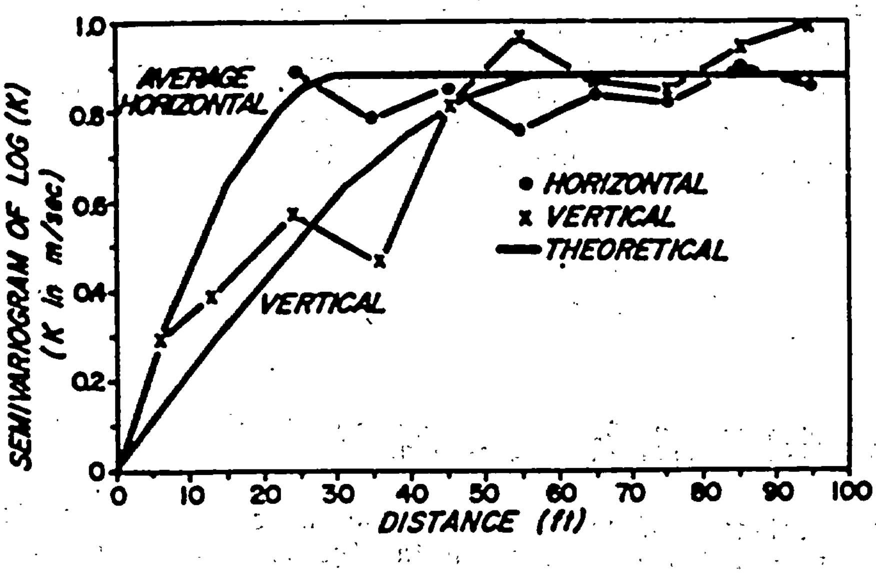

Figure 2. Horizontal and vertical semivariograms of log hydraulic conductivity at Oracle site. Smooth curves represent spherical models fitted to the data (after Jones et al., 1983).

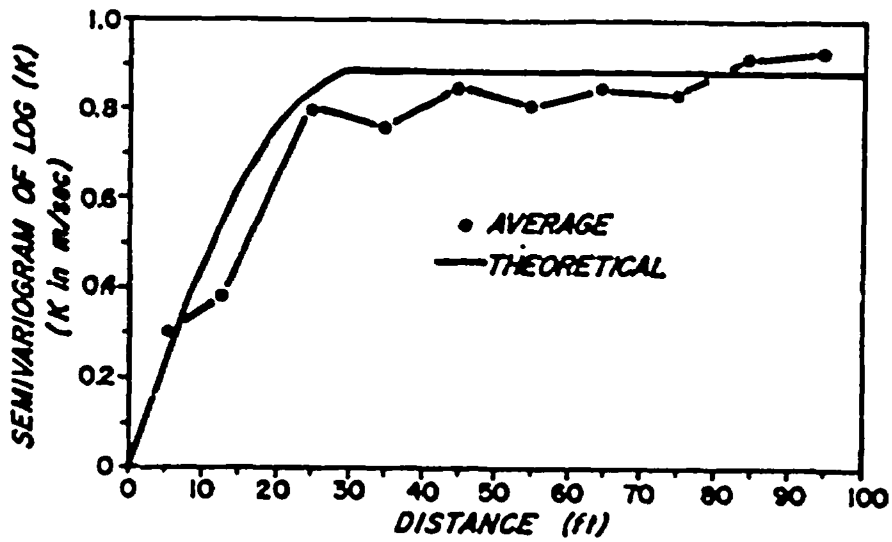

Figure 3. Average (isotropic) semivariogram of log hydraulic conductivity at Oracle site. Smooth curve represents spherical model fitted to the data (after Jones et al., 1983).

Fig. 4 shows a logarithmic plot of $\alpha_{11}(\nu)$ versus ν as obtained from the isotropic semivariogram of the Oracle test data by means of (71). The horizontal line labeled $\nu = \infty$ represents the asymptotic value of α_{11} (= 7.2 feet) as computed from (73). It is of some interest to note that this asymptotic value seems to be reached at approximately $\nu = 100$. The same data can be replotted as D_{11}/d_{11} versus ν based on the relationship

$$\frac{D_{11}}{d_{11}} = 1 + \frac{\alpha_{11}\,\nu}{L} \tag{82}$$

as shown in Fig. 5. The reader may do well to compare the resulting curve with Fig. 7-4(a) in Bear [1979].

The variation of $\alpha_{22}(\nu)$ with ν for the case of isotropic local dispersion ($d_L = d_T$ and $q = 1$) is shown in Fig. 6, based on (76). The straight line labeled $\nu = \infty$ represents the asymptotic value of α_{22} (= $6.4\nu^{-1}$ feet) as computed from (80). Fig. 7 shows (D_{22}/d_{22} -1) versus ν as computed from

$$\frac{D_{22}}{d_{22}} = 1 + \frac{\alpha_{22}\ \nu}{L}\ q^2$$

for $q^2 = 1$ (a plot of D_{22}/d_{22} versus ν would be essentially a horizontal line with $D_{22}/d_{22} = 1.0$). The horizontal line labeled $\nu = \infty$ corresponds to the asymp-totic value of α_{22}. The behavior of α_{33} and D_{33}/d_{33} is identical to that of α_{22} and D_{22}/d_{22}.

Figure 8 shows the ratio between α_{11} and α_{22} for isotropic local dispersion ($q = \sqrt{d_L/d_T} = 1$). This curve does not depend on σ_Y^2 or L and is thus valid not only for the Oracle site, but for any rock whose log hydraulic conduc-tivity is characterized by a spherical covariance function. Note that for $\nu < 1$, $\alpha_{11}/\alpha_{22} = 8.00$, whereas for $\nu > 100$, $\alpha_{11}/\alpha_{22} = 1.12\ \nu$.

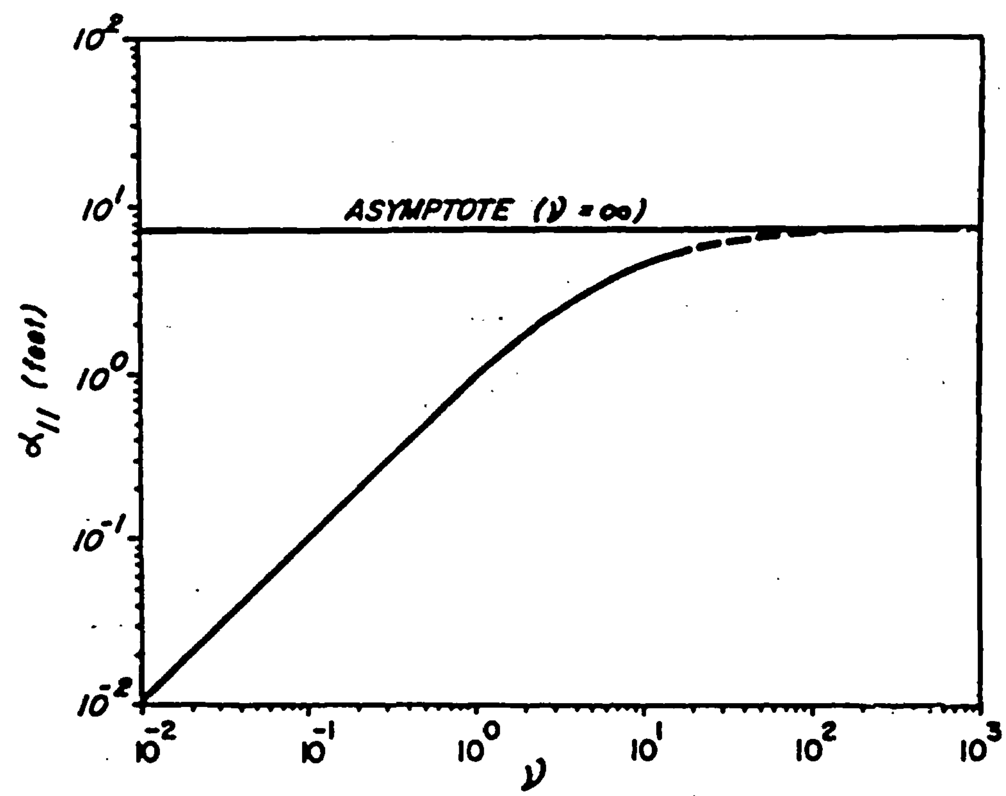

Figure 4 Variation of α_{11} with ν for fractured granite near Oracle. The straight line labeled $\nu = \infty$ represents asymptotic behavior.

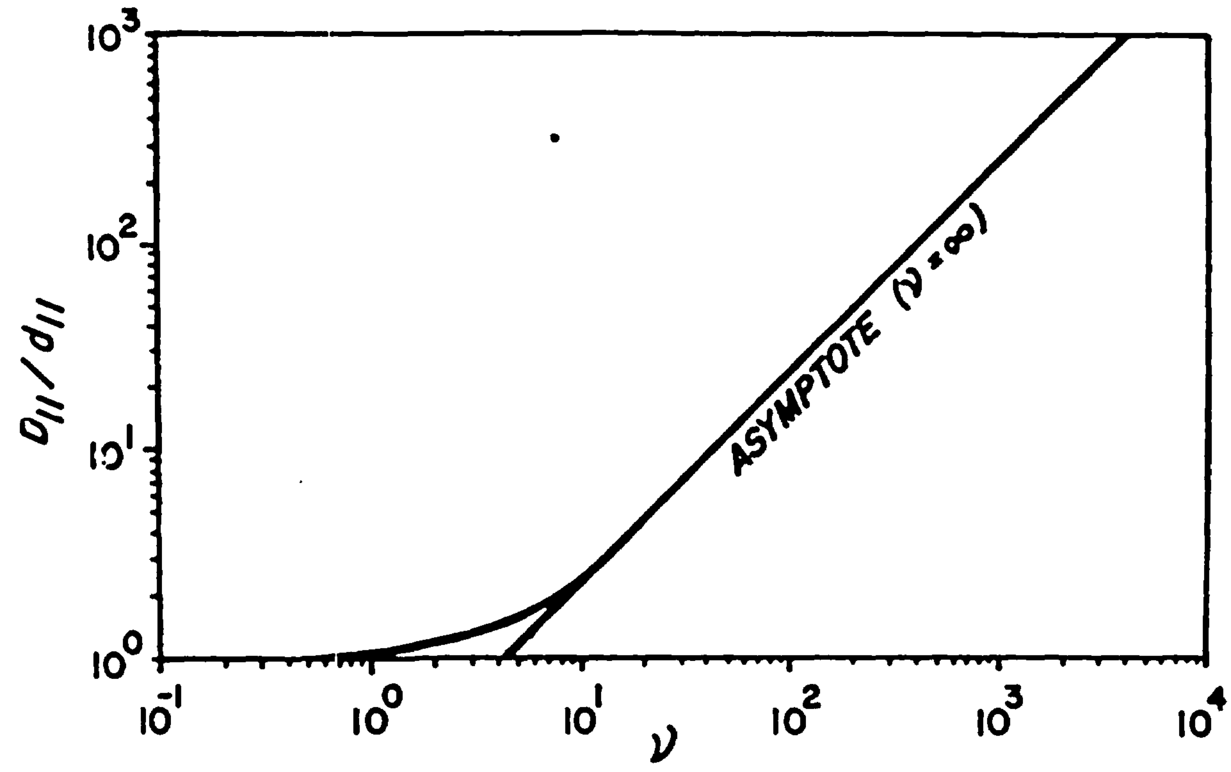

Fig. 5. Variation of D_{11}/d_{11} with ν for fractured granite near Oracle. The straight line labeled $\nu = \infty$ represents asymptotic behavior.

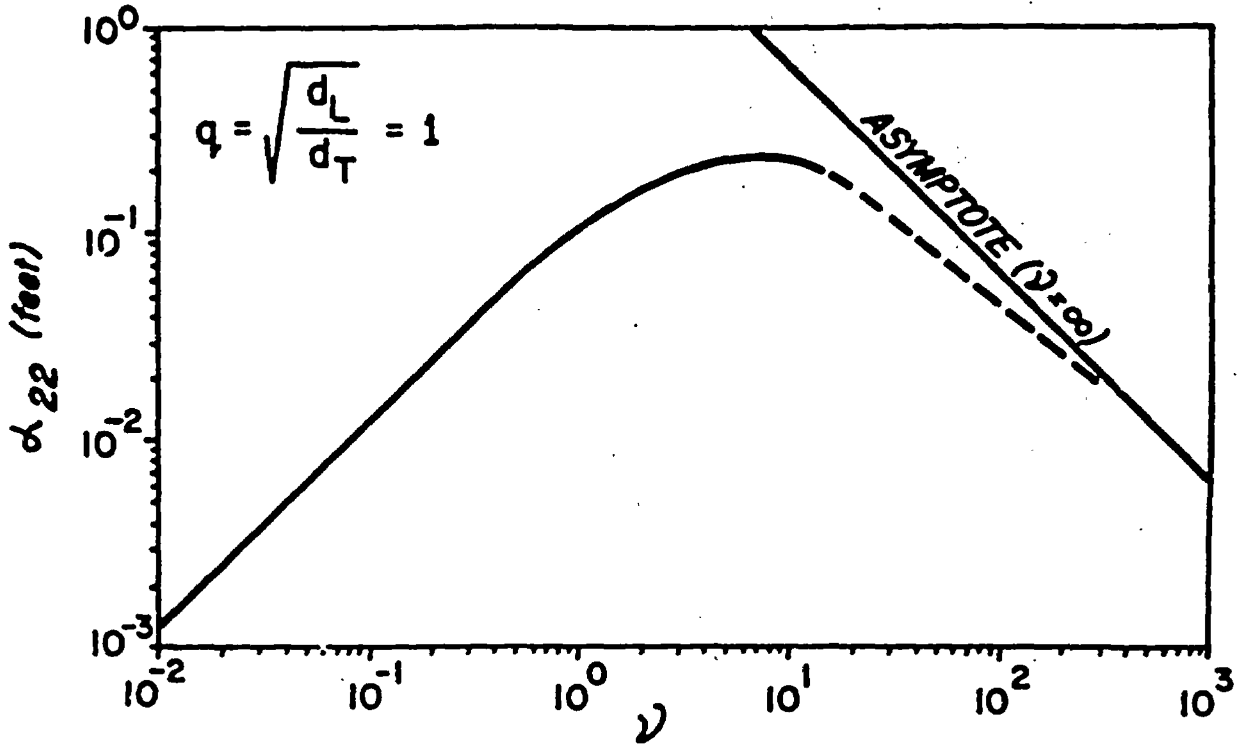

Figure 6. Variation of α_{22} with ν for fractured granite near Oracle when $d_L = d_T$ ($q = 1$). The straight line labeled $\nu = \infty$ represents asymptotic behavior.

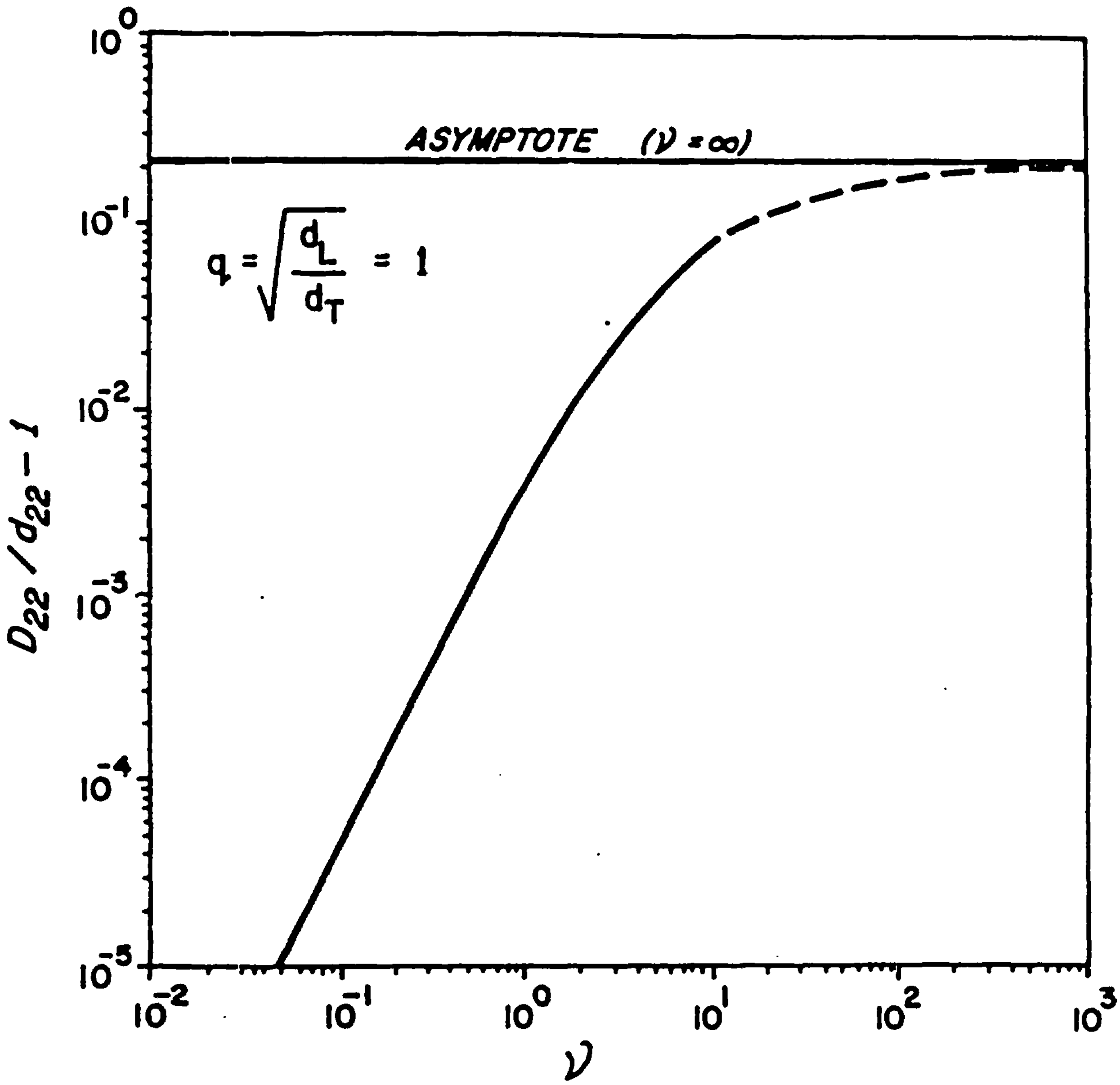

Figure 7. Variation of $(D_{22}/d_{22} - 1)$ with ν for fractured granite near Oracle when $d_L = d_T$ ($q = 1$). The straight line labeled $\nu = \infty$ represents asymptotic behavior.

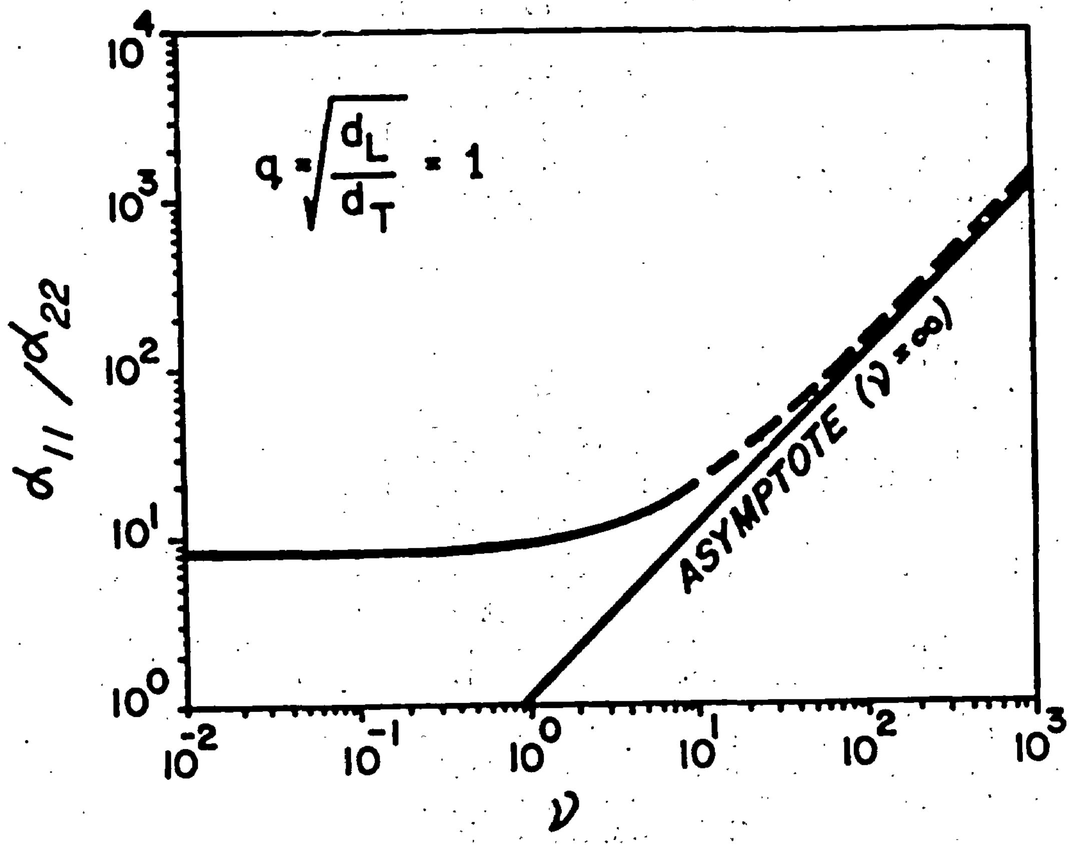

Figure 8. Variation of α_{11}/α_{22} with ν when $d_L = d_T$. The straight line labeled $\nu = \infty$ represents asymptotic behavior.

5. RELEVANCE TO NRC LICENSING OF HIGH-LEVEL RADIOACTIVE WASTE REPOSITORIES

In licensing high-level radioactive waste (HLW) disposal, NRC will be responsible for implementing the Environmental Protection Agency's (EPA) radiological standard for HLW, Part 191 of Title 40 of the Code of Federal Regulations (40 CFR 191). This standard was published as a Notice of Proposed Rulemaking (NPR) on page 58196 of Volume 47 of the Federal Register (47 FR 58196). As the regulatory vehicle for implementing 40 CFR 191, NRC has published procedural and technical criteria for its high-level waste rule 10 CFR 60. The procedural criteria were published as a final rule in the Code of Federal Regulations. The technical criteria was published as an NPR in 46 FR 35280. NRC is currently preparing a final rule for 10 CFR 60 which contains modifications to both the procedural and technical criteria. To clarify what needs to be done to comply with 10 CFR 60, NRC is planning to publish some regulatory guides. One such guide, on the preparation of site characterization reports, was published. The Department of Energy (DOE), the sole licensee for HLW disposal, published an NPR on guidelines for disposal of HLW, 10 CFR 960 (48 FR 5670).

In ¶60.21 of 10 CFR 60, item (6) states that a license application must include "a description of site characterization work actually conducted by DOE at all sites considered in the application." Item (c) states that a Safety Analysis Report must be submitted including "a description and analysis of the site at which the proposed geologic repository operations is to be located ... the assessment shall contain an analysis of the geology, geophysics, hydrology, ..." and other aspects of the site. The NRC Regulatory Guide 4.17 for the preparation of site characterization report states specifically that hydrological evaluation of a site must include "information on hydraulic characteristics of the matrix and fluid for each principal hydrogeologic unit" and "the method of determination (¶5.9.2). Among these hydraulic characteristics are "intrinsic permeability" and "hydraulic conductivity." The Guide further requires "a discussion of statistical parameters" including "range, and mean values." If this requirement is fulfilled, there should be enough data to perform the statistical analyses (described in this report) necessary for the computation of far-field dispersivities.

That such dispersivity values are needed is evident from the requirement of the NRC Regulatory Guide 4.17 to characterize "radionuclide transport factors" (¶5.9.4). Furthermore, the EPA takes the attitude that despite (Section 191.13 of 47 FR 58196) "significant uncertainties in the analytical models used to assess the long-term performance of geologic repositories," (Section 191.15)" a vital part of [the EPA standard] implementation will be the use of adequate models...to relate appropriate site and engineering data to projected performance." Some of these models will include dispersivity parameters to predict the effect of hydrodynamic spread on the concentration of radionuclides at various points along their flow paths. The larger is this spread, the earlier will the radionuclides arrive at designated points along their flow paths, and the smaller will be their concentration. Since both the arrival time and the concentration decrease with increasing dispersivities, it is important to estimate the correct values of these parameters as accurately as possible: neither by overestimating nor by underestimating the dispersivities will the models be taking a conservative approach to the assessment of risk posed by subsurface radionuclide migration.

In this report, we propose a method to estimate dispersivities in the far field based on measurements of hydraulic conductivities. Since such measurements must be performed as an integral part of every site characterization, the data required for our proposed calculations should be readily available. What remains is to analyze these data statistically and insert the resulting statistical parameters into appropriate formulae to compute dispersivities, as described in Chapter 4.

6. REFERENCES

1. Anderson, M., Modelling of groundwater flow systems as they relate to the movement of contaminants, C.R.C. Critical Rev. Environ. Control, 9, 97-156, 1979.

2. Bakr, A. A., L. W. Gelhar, A. L. Gutjahr, and J. R. McMillan, Stochastic analysis of spatial variability in subsurface flows, 1, Comparison of one- and three-dimensional flows, Water Resour. Res., 14(2), 263-271, 1978.

3. Bear, J., Some experiments in dispersion, Jour. Geophys. Res., 66, 2455-2467, 1961.

4. Bear, J., Dynamics of Fluids in Porous Media, Amer. Elsevier, New York, 1972.

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

6. Dagan, G., Stochastic modeling of groundwater flow by unconditional and conditional probabilities, 2, The solute transport, Water Res. Res., 18(4), 835-848, 1982.

7. Dieulin, A., G. Matheron, G. de Marsily, and B. Beaudoin, Time dependence of an "equivalent dispersion coefficient" for transport in porous media, Proc. Euromech Symposium, published by A. A. Balkema, Rotterdam, The Netherlands, 1981.

8. Feller, W., An Introduction to Probability Theory and its Applications, Vol. 2, John Wiley & Sons, New York, 1966.

9. Fried, J. J., Groundwater Pollution, Elsevier, Amsterdam, 1975.

10. Gelhar, L. W., A. L. Gutjahr, and R. L. Naff, Stochastic analysis of macro-dispersion in a stratified aquifer, Water Resour. Res., 15(6), 1387-1397, 1979.

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

12. Gihman, I. I. and A. V. Skorohod, Stochastic Differential Equations, Springer-Verlag, Berlin, 1972.

13. Hille, E. and R. S. Phillips, Functional Analysis and Semigroups, American Mathematical Society Colloquium Publications Vol. XXXI, American Mathematical Society, Providence, Rhode Island, 1957

14. Hsieh, P. A., S. P. Neuman, and E. S. Simpson, Pressure testing of fractured rocks: A methodology employing three-dimensional cross-hole tests, NUREG/CR-3213 Rep., 176 pp. U. S. Nuclear Reg. Comm., 1983.

15. Jones, J. W., E. S. Simpson, S. P. Neuman, and W. S. Keys, Field and theoretical investigation of fractured crystalline rock near Oracle, Southern Arizona, NUREG/CR-3736, Nuclear Regulatory Commission, to be published in June 1984.

16. Kesten, H. and G. Papanicolaou, A limit theorem for turbulent diffusion, Comm. Math. Phys., 65(2), 97-128, 1979.

17. Klotz, D., K.-P. Seiler, H. Moser, and F. Neumaier, Dispersivity and velocity relationship from laboratory and field experiments, Jour. Hydrology, 45(3/4), 169-184, 1980.

18. Kubo, R., Stochastic Liouville equations, Jour. Math. Phys., 4, 174-183, 1963.

19. Lallemand-Barrés, A. and P. Peaudecerf, Recherche des relations entre la valeur de la dispersivité macroscopique d'un milieu aquifere, ses autres caractéristiques et les conditions de mesure, Bull. Bur. Rech. Geol. Min. 2nd Series, Section III, (4), 277-284, 1978.

20. Lawson, D. E. and D. E. Elrick, A new method for determining and interpreting dispersion coefficients in porous media, Proc. Sec. Symp. on Fundamentals of Transport Phenomena in Porous Media, Univ. of Guelph, Guelph, Ontario, Canada, 753-777, 1972.

21. de Marsily, G., de L'identification des systemes hydrogeologiques, I. Synthese, Doctorates Sciences, Université Pierre et Marie Curie (Paris VI), Paris, 1978.

22. Martin, J. M., Deplacements miscibles dans des milieux poreux naturels de grande extension, Rev. Inst. Franc. Petrole, 26, 1065-1075, 1971.

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

24. Neuman, S. P., Role of geostatistics in subsurface hydrology, Invited tutorial, Proc. NATO Workshop on Geostatistics, Lake Tahoe, Calif., Sept. 1983 (in press).

25. Papanicolaou, G. and O. Pironeau, On the asymptotic behavior of motions in random flows, in Stochastic Nonlinear Systems in Physics, Chemistry and Biology, L. Arnold and R. Lefever, ed., Springer-Verlag, Berlin, 36-41, 1981.

26. Peaudecerf, P. and J.-P. Sauty, Application of a mathematical model to the characterization of dispersion effects of groundwater quality, Prog. Water Technol., 10(5/6), 443-454, 1978.

27. Pickens, J. F. and G. E. Grisak, Scale-dependent dispersion in a stratified granular aquifer, Water Resour. Res., 17(4), 1191-1211, 1981a.

28. Pickens, J. F. and G. E. Grisak, Modeling of scale-dependent dispersion in Hydrogeologic systems, Water Resour. Res., 17(6), 1701-1711, 1981b.

29. Roberts, P. H., Analytical theory of turbulent diffusion, Jour. Fluid. Mech., 11, 257-283, 1961.

30. Sauty, J.-P., Contribution à l'identification des paramètres de dispersion dans les aquifères par l'interprétation des experiences de tracage, D. Ing. Thesis, Univ. Sci. et Med. de Grenoble, France, 1977.

31. Scheidegger, A. E., Statistical hydrodynamics in porous media, Jour. Appl. Phys., 25, 994-1001, 1954.

32. Silliman, S. E. and E. S. Simpson, Laboratory evidence of the scale effect in solute transport, unpublished manuscript., 1983.

33. Simpson, E. S., A note on the structure of the dispersion coefficient, Abstracts and Program, Geol. Soc. Am., 10(7), 493, 1978.

34. Spohn, H., Kinetic equations from Hamiltonian dynamics: Markovian limits, Rev. Modern Phys., 53(3), 569-615, 1980.

35. Sudicky, E. A. and J. A. Cherry, Field observations of tracer dispersion under natural flow conditions in an unconfined sandy aquifer, Water Pollut. Res. Can., 14, 1-17, 1979.

36. Sudicky, E. A., J. A. Cherry, and E. O. Frind, Migration of contaminants in groundwater at a landfill, 4. A natural-gradient dispersion test, Jour. Hydrology, 63 (1/2), 81-108, 1983.

37. Varadhan, S. R. S., Courant Institute of Mathematical Sciences, New York University, New York.

38. Winter, C. L., Asymptotic properties of mass transport in random porous media, Ph.D. dissertation, Univ. Arizona, Tucson, Arizona, 1982.

39. Winter, C. L., C. M. Newman, and S. P. Neuman, A perturbation expansion for diffusion in a random velocity field, SIAM Jour. Appl. Math., (in press) 1983.

APPENDIX A: NOMENCLATURE

Symbol		Description	Dimensions
$\underline{a}$		Local dispersivity tensor	L
a_L		Local longitudinal dispersivity	L
a_T		Local transverse dispersivity	L
C		Far-field concentration	ML^{-3}
c		Local concentration	ML^{-3}
c_o		Initial concentration	ML^{-3}
$\underline{D}$		Far-field dispersion tensor	L^2T^{-1}
$\underline{D}^*$	=	$\underline{D} - \underline{d}$	L^2T^{-1}
$\underline{d}$		Local dispersion tensor	L^2T^{-1}
d_L		Local longitudinal dispersion coefficient	L^2T^{-1}
d_T		Local transverse dispersion coefficient	L^2T^{-1}
d_m		Molecular diffusion coefficient	L^2T^{-1}
$\underline{J}_d$		Local dispersive mass flux	$ML^{-2}T^{-1}$
K		Hydraulic conductivity	LT^{-1}
K_g		Geometric mean hydraulic conductivity	LT^{-1}
k		Dimension of Euclidean space	-
L		Correlation length of Y, or range of semivariogram of Y	L
q	=	$\sqrt{d_L/d_T}$	-
R		Euclidean space	L^k
t		Time	T
$\underline{u}$		Weakly stationary zero mean velocity process	LT^{-1}
$\underline{V}$		Far-field effective seepage velocity vector	LT^{-1}
$\underline{V}^*$	=	$\underline{V} - \underline{\mu}$	LT^{-1}

$\underline{v}$		Local seepage velocity vector	LT^{-1}
X		Lagrangian position vector	L
$\underline{x}$		Eulerian position vector	L
Y	=	Log K	-
$\underline{\alpha}$		Far-field dispersivity tensor	L
α_L		Far-field logitudinal dispersivity	L
α_T		Far-field transverse dispersivity	L
β_{nm}^2	=	$\rho_{nm}/\lvert\underline{\mu}\rvert^2$	-
γ	=	$1 + \sigma_Y^2/6$	-
λ		Positive scaling factor	-
ε		Perturbation parameter	-
$\underline{\mu}$	=	$E(\underline{v})$, mean seepage velocity	LT^{-1}
ν	=	$\mu_1 L/d_{11}$ when $\underline{\mu} = (\mu_1, 0, 0)$, Peclet number	-
$\underline{\rho}$		tensorial covariance function of $\underline{v}$	L^2T^{-2}
$\hat{\underline{\rho}}$		Fourier transform of $\underline{\rho}$	$L^{2+k}T^{-2}$
ρ_Y		Covariance function of Y	-
$\hat{\rho}_Y$		Fourier transform of ρ_Y	L^k
σ_Y^2		variance of Y	-
τ		Large-scale time	T
ϕ_e		effective (kinematic) porosity	-
$\underline{\xi}$		Fourier transform variable (vector)	L^{-1}
$\underline{\chi}$		Large-scale Eulerian positive vector	L
∇		Gradient operator	L^{-1}

APPENDIX B: PERTURBATION EXPANSIONS

To simplify the integral in (34) let $K_s(\underline{y}-\underline{x})$ denote the kernel of e^{sA} and substitute $\underline{\delta} = 4\underline{d}$. Then applying e^{sA} to an arbitrary function, g, is equivalent to convolving K_s and g,

$$e^{sA}g = (2\pi)^{-k/2} \int_{R^k} \frac{e^{-(\underline{x}-\underline{y}-\sqrt{k}\underline{\mu}s)^t \underline{\delta}^{-1}(\underline{x}-\underline{y}-\sqrt{k}\underline{\mu}s)/s}}{\sqrt{\det(\underline{\delta})s}} \, g(\underline{x}) \, d\underline{x}$$

$$= \int_{R^k} K_s(\underline{y}-\underline{x}) \, g(\underline{x}) \, d\underline{x} \tag{B1}$$

Hence

$$E[Be^{sA}Bg] = E[\sqrt{\lambda}\underline{u}(\sqrt{\lambda}\underline{y})\cdot\nabla\int_{R^k} K_s(\underline{y}-\underline{x})(\sqrt{\lambda}\underline{u}(\sqrt{\lambda}\underline{x})\cdot \nabla g(\underline{x}))d\underline{x}]$$

$$= \lambda \sum_{\ell=1}^{k} \sum_{j=1}^{k} \int_{R^k} E[u_\ell(\sqrt{\lambda}\underline{y})u_j(\sqrt{\lambda}\underline{x})] \, (\frac{\partial}{\partial y_\ell} K_s(\underline{y}-\underline{x})\frac{\partial}{\partial x_j} g(\underline{x}))d\underline{x}$$

$$= \lambda \sum_{\ell=1}^{k} \sum_{j=1}^{k} \int_{R^k} \rho_{\ell j} \, [\sqrt{\lambda}(\underline{y}-\underline{x})] \frac{\partial}{\partial y_\ell} K_s(\underline{y}-\underline{x}) \, \frac{\partial}{\partial x_j} g(\underline{x}) \, d\underline{x} \, . \tag{B2}$$

The integral in (B2) is just the convolution of a new function, $K^s_{\ell j}(\underline{z}) = \rho_{\ell j}(\sqrt{\lambda}\underline{z})\frac{\partial}{\partial z_\ell} K_s(\underline{z})$, with $\frac{\partial}{\partial z_j} g(\underline{z})$.

The Fourier transform of $K^s_{\ell j} * \frac{\partial}{\partial z_j} g$ is $(-i\xi_j)\hat{K}^s_{\ell j}\hat{g}$, where the star symbol indicates convolution. Using standard results from the theory of Fourier transforms

$$\hat{K}^s_{\ell j} = \rho_{\ell j}(\sqrt{\lambda}\underline{z}) \frac{\partial}{\partial z_\ell} K_s(\underline{z})$$

$$= (2\pi)^{-k} \rho_{\ell j}(\sqrt{\lambda}\underline{z}) * \frac{\partial}{\partial z_\ell} \hat{K}_s(\underline{z}). \tag{B3}$$

But the transform of $\rho_{\ell j}(\sqrt{\lambda}\underline{z})$ is $\lambda^{-k/2}\, \hat{\rho}_{\ell j}(\underline{\eta}/\sqrt{\lambda})$, where $\underline{\eta}$ is the transform variable, and K_s is Gaussian with Fourier transform $\hat{K}_s(\underline{\eta}) = e^{s\hat{A}(\underline{\eta})}$. The operator A has the Fourier transform $\hat{A} = -(\underline{\eta}\cdot \underline{d\eta}) - i\sqrt{\lambda}\underline{\mu}\cdot\underline{\eta}$. Hence

$$\hat{K}^s_{\ell j} = (-i)(2\pi\sqrt{\lambda})^{-k} \int_{R^k} \hat{\rho}_{\ell j}(\underline{\eta}/\sqrt{\lambda})(\xi'_\ell - \eta_\ell)\hat{K}_s(\underline{\xi}'-\underline{\eta})\, d\underline{\eta}$$

$$= (-i)(2\pi)^{-k} \int_{R^k} \hat{\rho}_{\ell j}(\underline{\xi})\; (\xi'_\ell - \sqrt{\lambda}\xi_\ell)\; \hat{K}_s(\underline{\xi}'-\sqrt{\lambda}\underline{\xi})\; d\underline{\xi}$$

$$= \frac{(-i)e^{s\hat{A}(\underline{\xi}')}}{(2\pi)^k} \int_{R^k} (\xi'_\ell - \sqrt{\lambda}\xi_\ell)\, e^{-s\lambda F_\lambda(\underline{\xi};\underline{\xi}')} \hat{\rho}_{\ell j}(\underline{\xi})\; d\underline{\xi}\,, \tag{B4}$$

since

$$\hat{A}(\underline{\xi}'-\sqrt{\lambda}\underline{\xi}) = (-\underline{\xi}'\cdot\underline{d\xi}' - i\sqrt{\lambda}\underline{\mu}.\underline{\xi}') - \lambda(\underline{\xi}\cdot\underline{d\xi} - \frac{2}{\sqrt{\lambda}}\underline{\xi}'\cdot\underline{d\xi} - i\underline{\mu}\cdot\underline{\xi})$$

$$= \hat{A}(\underline{\xi}') - \lambda F_\lambda(\underline{\xi};\underline{\xi}'), \tag{B5}$$

where F_λ is defined by the second equality of (B5).

Thus the transform of $E[Be^{sA}B]$ is

$$\lambda(2\pi)^{-k} \sum_{\ell,j} (i\xi'_j)e^{s\hat{A}(\underline{\xi})} \int_{R^k} i(\xi'_\ell - \sqrt{\lambda}\xi_\ell)e^{-s\lambda F_\lambda(\underline{\xi};\underline{\xi}')})\hat{\rho}_{\ell j}(\underline{\xi})\; d\underline{\xi}\,, \tag{B6}$$

and the requirement (34) becomes

$$\lim_{\lambda\to\infty} \lambda(2\pi)^{-k} \sum_{\ell,j} \int_{R^k} \{[-i(\xi'_\ell - \sqrt{\lambda}\xi_\ell)\,\hat{\rho}_{\ell j}(\underline{\xi})]$$

$$[-i\xi'_j \int_0^t \int_0^{t_1} e^{-(t_1-t_2)\lambda F_\lambda(\underline{\xi};\underline{\xi}')} dt_2 dt_1]\}\, d\underline{\xi}$$

$$-t\sqrt{\lambda}\underline{V_2}\cdot(-i\underline{\xi}') = t \sum_{\ell,j} (D_2)_{\ell j}\, (-i\xi'_\ell)(-i\xi'_j)\ . \qquad \text{(B7)}$$

The expression on the left of (B7) can be simplified by letting

$$G_\lambda(\underline{\xi};\underline{\xi}') = \frac{\lambda}{t} \int_0^t \int_0^{t_1} e^{-(t_1-t_2)\lambda F_\lambda(\underline{\xi};\underline{\xi}')} dt_2 dt_1$$

$$= \lambda t\, \frac{(e^{-\lambda t F_\lambda} - 1 + \lambda t F_\lambda)}{\lambda^2 t^2 F_\lambda{}^2} \qquad \text{(B8)}$$

Then dividing (B7) by t the requirement becomes, in the limit as $\lambda \to \infty$,

$$(2\pi)^{-k} \sum_{\ell,j} (-i\xi_j{}')(-i\xi'_\ell) \int_{R^k} \hat{\rho}_{\ell j}(\underline{\xi})\, G_\lambda(\underline{\xi};\underline{\xi}')\, d\underline{\xi}$$

$$+ (2\pi)^{-k} \sum_{\ell,j} (-i\xi_j{}') \int_{R^k} \sqrt{\lambda}\, (i\xi_\ell)\, \hat{\rho}_{\ell j}(\underline{\xi})\, G_\lambda(\underline{\xi};\underline{\xi}') d\underline{\xi} + \sqrt{\lambda}\, \underline{V_2}\cdot(i\underline{\xi}')$$

$$= (2\pi)^{-k} \sum_{\ell,j} (i\xi_j{}')(i\xi'_\ell) \int_{R^k} \hat{\rho}_{\ell j}(\underline{\xi})\, G_\lambda(\underline{\xi};\underline{\xi}')\, d\underline{\xi}$$

$$+ \sqrt{\lambda} \sum_j (-i\xi_j{}')\, \{[(2\pi)^{-k} \sum_\ell \int_{R^k} (i\xi_\ell)\, \hat{\rho}_{\ell j}(\underline{\xi})\, G_\lambda(\underline{\xi};\underline{\xi}')\, d\underline{\xi}] - (\underline{V_2})_j\}$$

$$+ \sum_{\ell,j} (\underline{D_2})_{\ell j}\, (i\xi'_\ell)\, (i\xi'_j)\ . \qquad \text{(B9)}$$

Hence, it would suffice to have

$$(i)\ \frac{1}{2}(2\pi)^{-k}\int_{R^k}\hat{\rho}_{\ell j}(\underline{\xi})\ G_\lambda(\underline{\xi};\underline{\xi}')\ d\underline{\xi} \to D_{\ell j}^{(i)} \tag{B10}$$

$$(ii)\ \frac{1}{2}\sqrt{\lambda}\ \{(2\pi)^{-k}\int_{R^k}\ [\sum_{\ell}(i\xi_\ell)\hat{\rho}_{\ell j}(\underline{\xi})]\ G_\lambda(\underline{\xi};\underline{\xi}')\ d\underline{\xi} - (\underline{V_2})_j\}$$

$$\to \sum_{\ell} D_{\ell j}^{(ii)}(-i\xi'_\ell) \tag{B11}$$

where the ℓjth component of $\underline{D_2}$ is

$$(\underline{D_2})_{\ell j} = D_{\ell j}^{(i)} + D_{j\ell}^{(i)} + D_{\ell j}^{(ii)} + D_{j\ell}^{(ii)}\ . \tag{B12}$$

From (B11) it is clear that we should also have

$$(iii)\ \ (2\pi)^{-k}\int_{R^k}[\sum_{\ell}\ (i\xi_\ell)\hat{\rho}_{\ell j}(\underline{\xi})]\ G_\lambda(\underline{\xi};\underline{\xi}')\ d\underline{\xi}\ \to (\underline{V_2})_j\ , \tag{B13}$$

$(\underline{V_2})_j$ being the jth component of $\underline{V_2}$.

It is convenient to put conditions (ii) and (iii) somewhat differently. It would also suffice if

$$(ii)'\ \frac{1}{2}\sqrt{\lambda}\ (2\pi)^{-k}[\int_{R^k}\ (i\xi_m)\ \hat{\rho}_{mj}(\underline{\xi})\ G_\lambda(\underline{\xi};\underline{\xi}')\ d\underline{\xi} - V_{mj}]$$

$$\to \sum_{\ell=1}^{k} D_{\ell jm}^{(ii)}\ (-i\xi'_\ell)\ , \tag{B14}$$

$$(iii)'\ \frac{1}{2}(2\pi)^{-k}\int_{R^k}(i\xi_m)\ \hat{\rho}_{mj}(\underline{\xi})\ G_\lambda(\underline{\xi};\underline{\xi}')\ d\underline{\xi}\ \to\ V_{mj}\ , \tag{B15}$$

where

$$(\underline{V}_2)_j = \sum_m V_{mj} \quad , \tag{B16}$$

$$D_{\ell j}^{(ii)} = \sum_m D_{\ell jm}^{(ii)} \quad . \tag{B17}$$

From (i), (ii)', and (iii)' it is clear that if there are generalized functions, $\tilde{D}(\underline{\xi})$, $\tilde{A}_m(\underline{\xi})$, $\tilde{\tilde{D}}_{m\ell}(\underline{\xi})$ which, in the sense of generalized functions on R^k, satisfy

$$\text{(i)"} \; 4 \; G_\lambda(\underline{\xi};\underline{\xi}') \to \tilde{D}(\underline{\xi}) \; , \tag{B18}$$

$$\text{(ii)"} \; 4 \sqrt{\lambda} \; [(i\xi_m) \; G_\lambda(\underline{\xi}.\underline{\xi}') - \tilde{A}_m(\underline{\xi})] \to \sum_\ell \tilde{\tilde{D}}_{m\ell}(\underline{\xi})(-i\xi_\ell') \quad , \tag{B19}$$

$$\text{(iii)"} \quad (i\xi_m) \; G_\lambda(\underline{\xi};\underline{\xi}') \to \tilde{A}_m(\underline{\xi}) \; , \tag{B20}$$

then

$$D_{\ell j}^{(i)} = \frac{1}{2} (2\pi)^{-k} \int_{R^k} \tilde{D}(\underline{\xi}) \; \hat{\rho}_{\ell j}(\underline{\xi}) \; d\underline{\xi} \quad , \tag{B21}$$

$$V_{mj} = (2\pi)^{-k} \int_{R^k} \tilde{A}_m(\underline{\xi}) \hat{\rho}_{mj}(\underline{\xi}) \; d\underline{\xi} \quad , \tag{B22}$$

$$D_{\ell jm}^{(ii)} = \frac{1}{2} (2\pi)^{-k} \int_{R^k} \tilde{\tilde{D}}_{\ell m}(\underline{\xi}) \hat{\rho}_{mj}(\underline{\xi}) \; d\underline{\xi} \quad , \tag{B23}$$

In our other paper (Winter, Newman, and Neuman, 1983) we find such generalized limits. In this paper we apply those limits in equations (36) - (40) where we give the large-scale velocity and dispersion coefficients.

APPENDIX C: GENERALIZED LIMITS

We can determine the limits (B18)-(B20) by applying dominated convergence arguments. The final results are

$$\tilde{D}(\underline{\xi}) = \begin{cases} 1/F(\underline{\xi}) & , k \geq 2 \\ \dfrac{\gamma}{\gamma^2\xi^2+\mu^2} + \dfrac{\pi}{|\mu|}\,\delta(\xi) & , k = 1 \end{cases} \tag{C1}$$

$$\tilde{A}_m(\underline{\xi}) = i\xi_m/F(\underline{\xi}) \tag{C2}$$

$$\tilde{\tilde{D}}_{m\ell} = -\,2\sum_{n=1}^{k} \xi_m d_{\ell n}\xi_n/[F(\underline{\xi})]^2. \tag{C3}$$

When these limits are substituted into (B21)-(B23), they yield (36)-(40).

Although it may at first seem unnecessarily rigorous to apply dominated convergence to so formal a perturbation analysis, by doing so we obtain the δ function regularization of (C1) when $k = 1$, which does not appear in the naive limit, and we show that no other "hidden regularizations" appear in the other expressions.

Consider (B18) first. Since $\underline{\xi}'$ is a parameter we can define a sphere centered on the origin,

$$A_\lambda = \{\, \underline{\xi} \in R^k : |\underline{\xi}\cdot\underline{d\xi}| < (16\lambda^{-1})|\underline{\xi}'\cdot\underline{d\xi}'|\}, \tag{C4}$$

and a function

$$\overline{G}_\lambda = \begin{cases} G_\lambda & \underline{\xi} \in A_\lambda \\ 0 & \underline{\xi} \in A_\lambda \end{cases} . \tag{C5}$$

Suppose $\phi(\underline{\xi})$ is a bounded function which approaches zero "fast enough" at ∞. Then

$$\int_{R^k} G_\lambda\phi(\underline{\xi})d\underline{\xi} = \int_{R^k} \overline{G}_\lambda\phi(\underline{\xi})d\underline{\xi} + \int_{A_\lambda} G_\lambda\phi(\underline{\xi})d\underline{\xi}\ . \tag{C6}$$

Our strategy (for $k \neq 1$) is to take the limit inside the first integral on the right by dominated convergence and to show that the second integral converges to zero.

It can be shown (Winter, Newman, and Neuman, 1983) that there is a positive constant, K, such that

$$|\overline{G}_\lambda \phi| < K \frac{|\phi|}{|F|} \tag{C7}$$

where $F(\underline{\xi})$ has been defined following (37). When $k > 3$, it can easily be seen that $|F|^{-1}$ is integrable near the origin even if $\mu = 0$. If $k = 2$ and $\underline{\mu} \neq 0$, rotating the coordinate system so that one axis coincides with $\underline{\mu}$ shows that the integrability of $|F|^{-1}$ near the origin follows from that of $[(x^2+y^2)^2 + x^2]^{-1/2}$. A change to polar coordinates shows that the latter is integrable near the origin.

Hence if $k > 2$, $\overline{G}_\lambda \phi$ is dominated by an integrable function. Since F^{-1} is the pointwise limit of G_λ,

$$\lim_{\lambda \to \infty} \int_{R^k} \overline{G}_\lambda \phi \, d\underline{\xi} = \int_{R^k} \frac{\phi}{F} \, d\underline{\xi}. \tag{C8}$$

To see that the rightmost integral of (C6) converges to zero, observe that $|G_\lambda| = O(\lambda)$ when $\underline{\xi} \varepsilon A_\lambda$ since $\mathrm{Re}(\lambda F_\lambda) = O(1)$. Thus

$$\int_{A_\lambda} G_\lambda \phi \, d\underline{\xi} = O(\lambda) \int_{A_\lambda} d\underline{\xi} = O(\lambda^{-(k-2)/2}). \tag{C9}$$

If $k > 3$, the integral clearly approaches zero as $\lambda \to \infty$.

To determine the case $k = 2$, we define

$$B = \{\underline{\xi}: |\underline{\mu} \cdot \underline{\xi}| < 2(\underline{\xi} \cdot \underline{d\xi})/\sqrt{3}\} \tag{C10}$$

Of course we can determine the behavior of the integral over A_λ by analyzing integrals over A_λ B and A_λ $\tilde{B}$ separately where $\tilde{B}$ denotes the complement of B.

First suppose $\xi \varepsilon A_\lambda$ $\tilde{B}$. From Winter, Newman, and Neuman (1983),

$$\int_{A_\lambda \tilde{B}} G_\lambda \phi \, d\underline{\xi} < \int_{A_\lambda \tilde{B}} K \frac{|\phi|}{|F|} \, d\underline{\xi}. \tag{C11}$$

As we have indicated in discussing (C3), the integral on the right of (C11) exists in every region of R^k $(k > 2)$ so long as $\underline{\mu} \neq 0$. In the case of (C11), however, the integral tends to zero because A_λ (thus $A_\lambda \; \bar{B}$) approaches {0} as $\lambda \to \infty$.

There remains only the region $A_\lambda \; B$ in R^2 for which it will be enough to show that

$$\lambda \int_{A_\lambda \quad B} d\underline{\xi} \to 0. \tag{C12}$$

Since in R^2 we require $\underline{\mu} \neq 0$, we can suppose without loss of generality that $\underline{\mu} = (\mu_1, 0)$ with $\mu_1 \neq 0$. Then

$$A_\lambda \quad B \quad \{\underline{\xi} \in R^2 : \xi_1 = O(\lambda^{-1}) \text{ and } \xi_2 = O(\lambda^{-1/2})\} \tag{C13}$$

and thus

$$\lambda \int_{A_\lambda \quad B} d\underline{\xi} = O(\lambda^{-1/2}). \tag{C14}$$

Using (C8), (C9), (C11) and (C14) we find that for $k > 2$,

$$\lim_{\lambda \to \infty} \int_{R^k} G_\lambda \phi \, d\underline{\xi} = \int_{R^k} \frac{\phi}{F} \, d\underline{\xi} \tag{C15}$$

which gives (C1) for $k > 2$.

For $k = 1$ the case is different. Let $\gamma = d$, and suppose that $\mu > 0$, then

$$F_\lambda(\xi;\xi') = \gamma \xi^{2} - \frac{2\gamma}{\sqrt{\lambda}}(\xi'\xi) - i\mu\xi$$

$$= \frac{1}{\lambda}(a_\lambda + ib_\lambda) \tag{C16}$$

where $a_\lambda = \gamma(\lambda\xi^2 - 2\sqrt{\lambda}\,\xi'\xi)$ and $b_\lambda = -\lambda\mu\xi$. Thus,

$$G_\lambda = \lambda t \, \frac{e^{-(a_\lambda + ib_\lambda)t} - 1 + (a_\lambda + ib_\lambda)t}{(a_\lambda + ib_\lambda)^2 t^2}. \tag{C17}$$

Now $G_\lambda \to 1/F(\xi)$ and the bound $|e^{-z}-1| < k|z|$ for Re $z > 0$ and some $k > 0$ shows that this convergence is uniform in compact subsets of some small complex strip, $0 < \text{Im}\, \xi < \varepsilon$, since Re$F > 0$ there. It follows that

$$\lim_{\lambda \to \infty} \int_{-\infty}^{\infty} G_\lambda \phi \, d\xi = \lim_{\varepsilon \to 0+} \int_{-\infty}^{\infty} \frac{1}{F(\xi + i\varepsilon)} \phi(\xi) \, d\xi. \tag{C18}$$

The right hand side of (C18) has the standard representation

$$P\int_{-\infty}^{\infty} \frac{\phi(\xi)}{F(\xi)} \, d\xi - \frac{\pi i}{F'(0)} \phi(0) , \tag{C19}$$

where P denotes the principal part. The calculation for the case $\mu < 0$ is the same except that the contour is deformed into the lower half plane. By substituting ρ for ϕ and using the fact that $\hat{\rho}$ is even, we obtain (C1) for $k = 1$.

The derivation of $\tilde{A}_m$, the limit of $(i\xi_m)G_\lambda$, follows a similar line. In this event, however, the case $k = 1$ is not exceptional. Let A_λ, B and $\bar{G}$ be as before. Then for $\underline{\xi} \in A_\lambda$ the same reasoning which led to (C8) shows that

$$|(i\xi_m)G_\lambda \phi| < |\xi_m| \; |\phi| \frac{K}{|F|} . \tag{C20}$$

If $\underline{d}$ is positive definite the expression on the right is integrable for $k > 2$ even if $\underline{\mu} = 0$. It is also integrable when $k = 1$ so long as $\mu \neq 0$. If, moreover, $\underline{\xi} \in A_\lambda \setminus \tilde{B}$, it can be shown that $|F_\lambda| > (1/2)\; |F|$ and we have (C20) once again. For $\underline{\xi} \in A_\lambda$ we have, by the positive definiteness of $\underline{d}$, that for some constant, $\kappa > 0$, $|\underline{\xi} \cdot \underline{d}\underline{\xi}| > (\kappa \xi_m)^2$ for every m. Hence $|\xi_m| = O(\lambda^{-1/2})$ in A_λ. Since $|G_\lambda \phi| = O(\lambda)$ in A_λ,

$$\int_{A_\lambda \setminus B} |\xi_m| \; |G_\lambda \phi| \; d\underline{\xi} < \int_{A_\lambda} |\xi_m| \; |G_\lambda \phi| \; d\underline{\xi}$$

$$= O(\lambda^{1/2}) \int_{A_\lambda} d\underline{\xi} = O(\lambda^{-(k-1)/2}). \tag{C21}$$

Of course when $k > 2$ the last expression approaches zero as $\lambda \to \infty$. If $k = 1$ and $\underline{\mu} \neq 0$, the def'nition of B requires that $\underline{\xi} = O(\lambda^{-1})$, so

$$\int_{A_\lambda \quad B \quad R^1} d\underline{\xi} = O(\lambda^{-1}). \tag{C22}$$

Thus

$$\int_{A_\lambda \quad B \quad R^1} |\underline{\xi}| \; |G_\lambda \phi| \; d\underline{\xi} = O(\lambda^{-1}\lambda^{-1}\lambda) = O(\lambda^{-1}) \to 0. \tag{C23}$$

Applying dominated convergence,

$$\lim_{\lambda \to \infty} \int_{R^k} (i\xi_m) \; G_\lambda \phi \; d\underline{\xi} = \int_{R^k} \frac{(i\xi_m)}{F} \phi \; d\underline{\xi} \tag{C24}$$

for $k > 2$ (and for $k = 1$ if $\mu \neq 0$) which is just (C1).

The argument leading to (C3) as the limit in (B19) is familiar. Let

$$\overline{H}_\lambda = \begin{cases} \sqrt{\lambda}[i\xi_m G_\lambda - \tilde{A}_m] & \underline{\xi} \in A_\lambda \\ 0 & \underline{\xi} \in A_\lambda \end{cases} \tag{C25}$$

where A_λ is as before. To see that $\overline{H}_\lambda$ is bounded by an integrable function, note that

$$|\overline{H}_\lambda| = |\sqrt{\lambda}(i\xi_m)[G_\lambda - F^{-1}]|$$

$$\leq \sqrt{\lambda}|\xi_m|[|G_\lambda - F_\lambda^{-1}| + |F_\lambda^{-1} - F^{-1}|]. \tag{C26}$$

In Winter, Newman, and Neuman (1983) it is shown that the expression on the right side of the inequality is bounded in $\overline{A}_\lambda$, the complement of A_λ, by an integrable function. $\overline{H}_\lambda$ converges (as a generalized function) to its pointwise limit $2(i\xi_m)(\underline{\xi}' \cdot \underline{d\xi})/F^2$.

Now we need only show that

$$\int_{A_\lambda} \sqrt{\lambda}[i\xi_m G_\lambda - \tilde{A}_m] \; \phi \; d\underline{\xi} \to 0. \tag{C27}$$

For $k > 2$ observe that, when $\underline{\xi} \in A_\lambda$, $|\xi_m| = O(\lambda^{-1/2})$ for any m. Thus.

$$|\sqrt{\lambda}[i\xi_m G_\lambda - \tilde{A}_\ell]| = \sqrt{\lambda}|\xi_m|\ |G_\lambda - F^{-1}|$$

$$< O(1)\ [|G\lambda| + |F^{-1}|]. \tag{C28}$$

In taking the limit we need only consider the terms in brackets in (C28). The integrability of $|F^{-1}|$ implies that

$$\int_{A_\lambda} |F^{-1}|\ \phi\ d\underline{\xi} \to 0 \tag{C29}$$

while the arguments leading to (C8), (C9), (C11), and (C12) establish that

$$\int_{A_\lambda} |G_\lambda|\ |\phi|\ d\underline{\xi} \to 0. \tag{C30}$$

Of course we have (C30) when $k = 2$ only if $\underline{\mu} \neq 0$.

The argument for $k = 1$ is analogous to that used to obtain (C2).

APPENDIX D: DERIVATION OF H(x)

To find $H(\underline{x})$ we note first that

$$\hat{Q}(\underline{\xi}) = \frac{1}{1+\underline{\xi}\cdot\underline{\xi}} = \hat{\phi}(\|\underline{\xi}\|) \tag{D1}$$

is radially symmetric and thus has inverse transform

$$Q(\underline{x}) = \frac{-1}{2\pi r}\,\frac{d}{dr}\,\phi(r) = \frac{1}{4\pi\|\underline{x}\|}\,e^{-\|\underline{x}\|} \tag{D2}$$

where $\phi(r) = \frac{1}{2}e^{-|r|}$ has the one-dimensional Fourier transform $\hat{\phi}(\kappa) = \frac{1}{1+\kappa^2}$, $r = \|\underline{x}\|$ and $\kappa = \|\underline{\xi}\|$. Applying two other standard results from the theory of Fourier transforms, the inverse transform of $\hat{f}(\xi - i\beta)$ is $e^{\beta x}f(x)$ and that of $\hat{f}(\underline{T}\xi)$ is $\frac{1}{\det(\underline{T})}\,f(\underline{T}^{-1}\underline{x})$, so that we obtain (55) from (39).

APPENDIX E: DELTA SEQUENCE

A delta sequence is a sequence of functions, δ_ν, which converges to a delta function. Convergence is in the natural sense: $\delta_\nu \to \delta$ if

$$\lim_{\nu\to\infty} \int \delta_\nu(\underline{z})\, f(\underline{z})\, d\underline{z} = f(0) \tag{E1}$$

for $f(\underline{z})$ arbitrary (up to some technical conditions).

To show that

$$\delta_\nu(\underline{z}) = \frac{\nu\, e^{\nu(z_1 - |\underline{z}|)}}{2\pi |\underline{z}|} \tag{E2}$$

is a delta sequence concentrated on the positive z_1 axis, we must show that (E1) holds in R^2 for fixed $z_1 = b > 0$, b a constant. However, before giving the proof we note that $\delta_\nu(\underline{z})$ defined by (E2) exhibits the kind of behavior classically associated with delta sequences. In particular

$$\delta_\nu(\underline{z}) \to \begin{array}{ll} 0 & \text{if } z_1 < 0 \text{ or } z_2 \neq 0,\ z_3 \neq 0 \\ \infty & \text{if } z_1 > 0 \text{ and } z_2 = z_3 = 0 \end{array}$$

Furthermore

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \delta_\nu(\underline{z})\, dz_2\, dz_3 = 1$$

a fact which we demonstrate in a moment. Thus $\delta_\nu(\underline{z})$ for $z_1 = b$, which we denote by $\delta_\nu(z_2,z_3)$, certainly appears to be a delta sequence.

The argument we give to establish this rigorously is standard. First write $f(b, z_2, z_3) = [f(b, z_2, z_3) - f(b, 0, 0)] + f(b, 0, 0)$ and let $g(z_2, z_3) = f(b, z_2, z_3) - f(b, 0, 0)$. Then

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(b,z_2,z_3)\, \delta_\nu(z_2,z_3)\, dz_2\, dz_3$$

$$= f(b, 0, 0) \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \delta_\nu(z_2,z_3)\, dz_2\, dz_3 + \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} g(z_2,z_3)\delta_\nu(z_2,z_3) dz_2\, dz_3$$

Observe that

$$\int_{R^2} \delta_\nu(z_2,z_3)dz_2\, dz_3 = \int_0^{2\pi} \int_0^{\infty} \frac{\nu\, e^{\nu(b-\sqrt{b^2+r^2})}}{2\pi\sqrt{b^2+r^2}}\, r\, dr\, d\theta$$

$$= \nu e^{\nu b} \int_b^{\infty} e^{-\nu w}\, dw$$

$$= 1$$

demonstrating the fact alluded to above.

The technical conditions we require of $f(\underline{z})$ are that it be 1) bounded and 2) continuous at the origin. Since $f(\underline{z})$ corresponds to $\rho_{nm}(\underline{z})$, these requirements are realistic. The function $g(z_2,z_3)$ is thus bounded and approaches zero at the origin. Our problem is to show that

$$\int_{R^2} g(\underline{y})\, \delta_\nu(\underline{y})\, d\underline{y} \to 0 \text{ as } \nu \to \infty \quad . \tag{E3}$$

This integral can be separated into two: one over an open sphere, Ω, centered on the origin and with radius a; the other the remainder of R^2 denoted by $R^2\text{-}\Omega$. So

$$\int_{R^2} g(\underline{y})\, \delta_\nu(\underline{y})\, d\underline{y} = \int_\Omega g(\underline{y})\, \delta_\nu(\underline{y})\, d\underline{y} + \int_{R^2-\Omega} g(\underline{y})\, \delta_\nu(\underline{y})\, d\underline{y}$$

Let

$$M(\Omega) = \max_{\underline{y}\epsilon\Omega} |g(\underline{y})| \ ,$$

then

$$\int_\Omega g(\underline{y})\, \delta_\nu(\underline{y})\, d\underline{y} < M(\Omega) \int_\Omega \delta_\nu(\underline{y})\, d\underline{y} < M(\Omega) \int_{R^2} \delta_\nu(\underline{y})d\underline{y} = M(\Omega)$$

Since $g(\underline{y})$ is continuous at the origin and $g(0) = 0$, $M(\Omega) \to 0$ as $a \to 0$. Thus for any $\varepsilon > 0$ there is an a so small that the integral over Ω of $g(\underline{y})\delta_\nu(\underline{y})$ is less than $\varepsilon/2$ in absolute value. Since this result is independent of ν, we can consider a to be fixed below.

Letting $M = \max_{\underline{y} \in R^2} |g(\underline{y})|$, we have

$$\int_{R^2-\Omega} g(\underline{y})\delta_\nu(\underline{y})\, d\underline{y} < M\nu e^{\nu b} \int_{\sqrt{a^2+b^2}}^{\infty} e^{-\nu w}\, dw$$

$$= M\, e^{\nu(b - \sqrt{a^2+b^2})}$$

With fixed a we can find N large enough that

$$M\, e^{\nu(b - \sqrt{a^2+b^2})} < \varepsilon/2$$

when $\nu > N$.

The limit (E3) follows immediately and the proof is complete.

APPENDIX F: CONTOUR INTEGRALS

We want to evaluate the integrals

$$J_1 = \int_0^\infty \frac{\sin(Rr) - Rr + R^3r^3/3!}{r^3(r^2 + \nu^2 \cos^2\theta)}\, dr,$$

$$J_2 = \int_0^\infty \frac{\cos(Rr) - 1 + R^2r^2/2!}{r^2(r^2+\nu^2\cos^2\theta)}\, dr,$$

$$J_3 = \int_0^\infty \frac{\cos(Rr) - 1 + R^2r^2/2! - R^4r^4/4!}{r^4(r^2+\nu^2\cos^2\theta)}\, dr.$$

Since the techniques are the same for all three integrals, we demonstrate the method by evaluating J_2. Note that $I_2 = -\frac{3}{R^2} J_2$.

The integrand of J_2 is an even function, thus

$$J_2 = \frac{1}{2} \int_{-\infty}^\infty \frac{\cos(Rr)-1+R^2r^2/2!}{r^2(r^2+b^2)}\, dr = \frac{1}{2} \int_{-\infty}^\infty \frac{e^{iRr}-1-iRr+R^2r^2/2!}{r^2(r^2+b^2)} \qquad \text{(F1)}$$

where we let $b = \nu\cos(\theta)$. We suppose $b > 0$; the $b = 0$ cose can be obtained as a limit. Because J_2 cannot be evaluated by elementary methods, we find it by contour integration in the complex plane. The countour is shown in Figure 8 below.

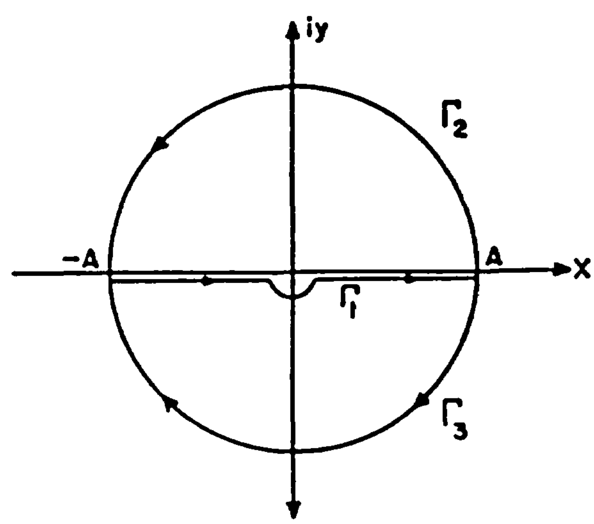

Figure 8 Contour integral in the complex domain

If we write

$$\phi(z) = \frac{e^{iRz} - 1 - iRz + R^2z^2/2!}{z^2(z^2+b^2)}$$

then

$$J_2 = \frac{1}{2} \lim_{A\to\infty} \int_{\Gamma_1} \phi(z)dz = \frac{1}{2} \lim_{A\to\infty} \int_{\Gamma_1+\Gamma_2} \phi(z)dz \qquad \text{(F2)}$$

since on Γ_2,

$$|\phi(z)| < \frac{2 + RA + R^2A^2/2}{A^2(A^2+b^2)} \quad ,$$

and hence $\lim_{A\to\infty} \int_{\Gamma_2} \phi(z)dz = 0$. From ($F_2$) and the Residue Theorem, the integral over $\Gamma_1+\Gamma_2$ is $2\pi i$ times the residue at $z=ib$ (which is the only residue of ϕ in the upper half plane),

$$\frac{e^{-Rb} - 1 + Rb - R^2b^2/2}{(-b^2)(2ib)} \quad .$$

Thus

$$J_2 = -\frac{\pi}{2} \left[\frac{e^{-Rb} - 1 + Rb - R^2b^2/2}{b^3} \right]$$

and

$$I_2 = \frac{3\pi}{2R^2} \left[\frac{e^{-Rb} - 1 + Rb - R^2b^2/2}{b^3} \right] \quad .$$

APPENDIX G: α_{22} FOR LARGE ν

The asymptotic evaluation of

$$B_2 = \frac{\pi}{4}q^2 \int_0^1 \frac{u^2(1-u^2)}{R^6(u)} [\ I_1(u) + I_2(u) + I_3(u)\ ]\, du \qquad \text{(G1)}$$

is simple, if a bit tedious. By separating (G1) into subintegrals and cancelling terms we can write

$$\int_0^1 \frac{u^2(1-u^2)}{R^6(u)} [\ I_1(u) + I_2(u) + I_3(u)\ ]\, du$$

$$= \frac{\pi}{2\nu^2} \int_0^1 \frac{1-u^2}{R^7} [-1+\Psi(\nu Ru)]\, du, \qquad \text{(G2)}$$

where

$$\Psi(x) = 12\ \frac{e^{-x}-1+x}{x^2} + 3\ \frac{e^x-1}{x} + 12\ \frac{e^{-x}-1+x-x^2/2}{x^3} \quad .$$

Now $\Psi(x)$ is a bounded function on $[\ 0,\infty)$ and $\Psi(x) \to 0$ as $x \to \infty$. Thus, as $\nu \to \infty$, $\Psi(\nu Ru) \to 0$ pointwise and is uniformly bounded. It follows by the dominated convergence theorem, since $R^{-7}(1-u^2)$ is integrable on $[0,1]$, that (G2) is asymptotically given by

$$- \frac{\pi}{2\nu^2} \int_0^1 \frac{1-u^2}{R^7(u)}\, du + O(1)$$

which yields (77).

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A multidimensional stochastic theory is presented for far-field dispersion due to the spatial variability of hydraulic conductivities. We use a second-order perturbation approach to relate the far-field velocity vector, $\underline{V}$, and dispersion tensor, $\underline{D}$, to the mean and covariance of the local seepage velocity vector, $\underline{v}$, and the local dispersion tensor, $\underline{d}$. We find that, in general, $\underline{V}$ is not necessarily equal to the ensemble mean of $\underline{v}$, $\underline{\mu}$, and that $\underline{D}$ is a second-rank symmetric tensor. In the particular case where $\nabla \cdot \underline{v} = 0$ (e.g., incompressible fluid in a rigid porous medium of uniform effective porosity), $\underline{V}$ becomes equal to $\underline{\mu}$, and our expressions for $\underline{D}$ simplify to those presented by Gelhar and Axness [1983]. We further extend a conclusion of these authors, that as the Peclet number, ν, increases, $\underline{D}$ becomes asymptotically linear in $|\underline{\mu}|$, by showing that it holds for arbitrary velocity covariance functions. Finally, we derive expressions for $\underline{D}$ as a function of ν for situations where the logarithm of hydraulic conductivity fits a spherical covariance or semivariogram function, as is often the case. These expressions are applied to log hydraulic conductivity data from packer tests conducted in seven boreholes penetrating fractured granites near Oracle, southern Arizona.

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