Winter, C. Larrabee

ASYMPTOTIC PROPERTIES OF MASS TRANSPORT IN RANDOM POROUS MEDIA

The University of Arizona PH.D. 1982

ASYMPTOTIC PROPERTIES OF MASS TRANSPORT IN RANDOM POROUS MEDIA

by

C. Larrabee Winter

A Dissertation Submitted to the Faculty of the

PROGRAM IN APPLIED MATHEMATICS

In Partial Fulfillment of the Requirements
For the Degree of

DOCTOR OF PHILOSOPHY

In the Graduate College

THE UNIVERSITY OF ARIZONA

1 9 8 2

THE UNIVERSITY OF ARIZONA
GRADUATE COLLEGE

As members of the Final Examination Committee, we certify that we have read the dissertation prepared by C. Larrabee Winter

entitled Asymptotic Properties of Mass Transport in Random Porous Media

and recommend that it be accepted as fulfilling the dissertation requirement for the Degree of Doctor of Philosophy.

Charles M. Newman	Date August 3, 1982
R N Bhattacharya by T Lattech	Date 8/3/82
Larry Wright by T Lattech	Date 8/3/82
	Date
	Date

Final approval and acceptance of this dissertation is contingent upon the candidate's submission of the final copy of the dissertation to the Graduate College.

I hereby certify that I have read this dissertation prepared under my direction and recommend that it be accepted as fulfilling the dissertation requirement.

Charles M. Newman
Dissertation Director

Date August 3, 1982

STATEMENT BY AUTHOR

This dissertation has been submitted in partial fulfillment of requirements for an advanced degree at the University of Arizona and is deposited in the University Library to be made available to borrowers under the rules of the Library.

Brief quotations from this dissertation are allowable without special permission, provided that accurate acknowledgment of source is made. Requests for permission for extended quotation from or reproduction of this manuscript in whole or in part may be granted by the head of the major department or the Dean of the Graduate College when in his judgment the proposed use of the material is in the interests of scholarship. In all other instances, however, permission must be obtained from the author.

SIGNED: C. Larrabee Winter

ACKNOWLEDGMENTS

It is conventional to begin a dissertation by thanking advisors, spouses, and friends without whose patience, etc. the work could not have been completed. I suspect that this is so because it is so often true.

Certainly I could not have done this work without the advice and assistance of my advisors, Dr. S. P. Neuman and Dr. C. M. Newman. I will always be grateful for their generosity.

My wife, Becky, employed a lively sense of humor and the resources of love to tame a savage mathematician. I am happy that she proved so fine a trainer.

TABLE OF CONTENTS

ABSTRACT

Suppose $C(x,t)$ is the concentration at position x in R^d and time $t > 0$ of a solute which is diffusing in some medium. If on a local scale the dispersion of the solute is governed by a constant dispersion matrix, $1/2(\delta^2)$, and a random velocity field, $V(x)$, then C satisfies a convection-diffusion equation with random coefficients,

$$\frac{\partial C}{\partial t} = \{ \frac{1}{2} \nabla \cdot \delta^2 \nabla - \nabla \cdot V(x) \} C, \; C(x,0) = c_0(x) \qquad (1).$$

Usually $V(x)$ is taken to be $\mu + \varepsilon U(x)$ where $\mu \in R^d$, $U(x)$ is a given stationary random field with mean zero, and $\varepsilon > 0$ is a dimensionless parameter which measures the variability of $V(x)$.

Hydrological experiments suggest that on a regional scale the diffusion is classically Fickian with effective diffusion matrix $D(\varepsilon)$ and drift velocity $\alpha(\varepsilon)$. Thus for large scales

$$\frac{\partial \tilde{c}}{\partial \tau} = \{ \frac{1}{2} \nabla \cdot D \nabla - \alpha \cdot \nabla \} \tilde{c}, \; \tilde{c}(\chi,0) = c_0(\chi) \qquad (2)$$

is satisfied by the solute concentration. Here τ and χ are respectively time and space measured on large scales. It is natural to investigate the relation of the large scale coefficients D and α to the statistical properties of $V(x)$.

To relate (1) to (2) -- and thus to approximate $D(\varepsilon)$ and $\alpha(\varepsilon)$ -- it is necessary to rescale t and x and average over the distribution of

V. It can then be shown that the transition form (1) to (2) is equivalent to

$$\lim_{n\to\infty} E_U\, e^{t(A+\varepsilon B_U)}\, e^{-t\sqrt{n}\alpha\cdot\nabla} = e^{t(\nabla\cdot D\nabla)/2} \qquad (3)$$

where $A = (\nabla\cdot\delta^2\nabla)/2 + \sqrt{n}\mu\cdot\nabla$ and $B_U = \sqrt{n}U(\sqrt{n}x)\cdot\nabla$. By expanding each side of (3) estimates of $D(\varepsilon)$ and $\alpha(\varepsilon)$ can be obtained. The estimates have the form

$$D = \delta^2 + \varepsilon^2 D_2,\ \alpha = \mu + \varepsilon^2\alpha_2 \qquad (4).$$

Both D_2 and α_2 depend on the power spectrum of U. Analysis shows that in at least the case of incompressible fluids D_2 is positive definite. In one dimensional transport $\alpha_2 < 0$, hence $\alpha_k < \mu_k$ through second order.

CHAPTER ONE

INTRODUCTION

Consider a pollutant which is intoduced abruptly in the midst of a large porous medium saturated with water. The pollutant might, for instance, be high-level radioactive waste and the medium a mass of fractured rock. Water flowing through the medium will carry the pollutant downstream and as the pollutant migrates it will spread. The spreading, or dispersion, of a pollutant through a porous medium is caused by variations within the fluid velocity field and by diffusion down concentration gradients.

It is well established that the coefficient of dispersion, a parameter describing the spread of pollutants in hydrological formations, varies significantly with the scale of observation (Theis, 1962; Morgan, Kamison, and Stevenson, 1962; Theis, 1963; Fried, 1972). Dispersivities determined by intermediate scale field tests are generally larger than those obtained in laboratory experiments but smaller than those required in computer models which reproduce the behavior of pollution plumes observed on a regional scale. Because in most cases the time required to determine regional scale dispersivities is long, it is desireable to estimate these parameters from intermediate scale hydrological field tests.

In this dissertation I derive expressions for the regional scale dispersivities and velocities of a pollutant from properties which can in principle be determined from intermediate scale experiments. To do so I treat the medium's intermediate scale velocity field as a weakly stationary random field. When the fluid's mean head gradient is constant this is a reasonable assumption. Next I describe the intermediate scale transport of the pollutant by a convection-diffusion equation with a random velocity coefficient. I then suppose that the pollutant's concentration converges to a solution of Fick's equation as time, and thus the scale of observation, increases. Although not every hydrologically significant porous medium satisfies these conditions, many do.

The methods used in this dissertation are not limited to the application just described. They apply as well to the transport of solute by a compressible fluid with a weakly stationary velocity field. Moreover the medium need not be porous; the method easily extends to a description of turbulent diffusion in a gas.

The method can also be used to estimate intermediate scale dispersivities and velocities from values obtained in laboratory experiments. It is independent of the initial scale of observation, and instead relates results obtained on a fine scale to estimates derived for a grosser scale. It only requires that the assumptions of this dissertation be met, in particular that the pollutant concentration on the greater scale be approximately Fickian. I will emphasize this by referring to the fine scale as the macroscopic and the gross as the megascopic. I indicate absolute scales by terms which are specific to them, e.g. regional.

In the remainder of this chapter I outline the model used in this dissertation to describe mass transport in a random medium. A brief review of attempts to derive such models from fundamental physical considerations follows. In the next chapter I consider in more detail papers by Kesten and Papanicolaou (1979), Gelhar, Gutjahr, and Naff (1979), Matheron and de Marsily (1980), and Gelhar and Axness (1981). Those papers derive asymptotic dispersion and drift coefficients for important special cases.

In the third chapter I analyse the general case outlined above and obtain integral expressions whose limits are the megascopic dispersivities and drifts. The analysis which leads to these expressions is formal in the sense that certain nontrivial facts about the expansion and convergence of semigroups of operators are assumed without proof. The integral expressions depend on the covariances between components of the macroscopic velocity field, on the mean of that field, and on the macroscopic dispersivity matrix. By naively taking the point-wise limits of the integrals I obtain estimates for the megascopic dispersivities and drifts. Those estimates are correct for media of two or more dimensions.

In the fourth chapter, however, the limits are derived through a rigorous dominated convergence argument, and it becomes clear that the naive limits for a one dimensional medium are incorrect. On the other hand, for media of more than one dimension, the limits taken by arguing from dominated convergence agree with the naive limits.

In the fifth chapter I give the results for the general case in equations (5.3) - (5.13) and indicate that the megascopic coefficient of dispersion is greater than (or at least equal to) the macroscopic coefficient. This result is consistent with experiment. I also show that equations (5.3) - (5.13) agree with those obtained by others in special cases. Finally I note that my results are in accord with an important empirical relationship: when plotted against Peclet number, the ratio of megascopic to macroscopic dispersivity shows qualitative agreement with experimental results.

Model

Suppose that a pollutant is injected into the flow field of a porous medium at some initial time, say t=0, and that there are no other sources, nor are there sinks, within the medium. Because of macroscopic velocity variations, the drift and spread of the pollutant may initially be irregular. With time, however, mixing induced by hydrodynamic dispersion on the macroscopic scale coupled with a tendency for the effect of velocity fluctuations to cancel as the volume occupied and traversed by the pollutant increases will smooth the outline of the pollution plume. The pollutant may eventually drift and spread regularly (Skibtzke, 1964).

This asymptotic behavior is consistent with the supposition that the pollutant's concentration tends to be governed by Fick's law after the passage of a long time. That is to say that the concentration converges to the solution of a megascopic convection-diffusion equation,

$$\frac{\partial \tilde{c}}{\partial \tau} = \frac{1}{2} \nabla \cdot D \, \nabla \tilde{c} - \alpha \cdot \nabla \tilde{c} \qquad (1.1)$$

with initial condition $\tilde{c}(x,0) = c_0(x)$. Here $\tilde{c}(x,\tau)$ is the megascopic concentration, τ is time measured on a megascopic scale, x is a point in the d dimensional medium, $\alpha \in R^d$ is the megascopic velocity at which the pollutant is convected, and D/2 is the megascopic d x d dispersion matrix. In probability literature D would be called the diffusion matrix.

Since the elements of α and D are constants, the solution to equation (1.1) is the convolution of c (x) with a Gaussian function,

$$(2\pi\tau)^{-d/2} \det(D)^{-1/2} e^{-(x-\alpha\tau)D^{-1}(x-\alpha\tau)/2}$$

with mean $\alpha\tau$ and covariance $D\tau$. Thus $\alpha\tau$ is the uniform displacement of the plume's center of mass and $D\tau$ describes the spread of the plume about its center.

Because the time required to establish a Fickian regime may be long, experimental determination of α and D is often impractical. It is, therefore, important to estimate these quantities from field scale properties. The results of hydrological experiments suggest that pollutant concentration can be described on the field scale by a convection-diffusion equation,

$$\frac{\partial C}{\partial t} = \frac{1}{2} \nabla \cdot \delta^2 \nabla C - \nabla \cdot VC \qquad (1.2)$$

with initial concentration $C(x,0) = c_0(x)$. Here $t \ll \tau$, so the distance travelled by the pollutant is much smaller than that required for equation (1.1) to hold.

The macroscopic pollutant concentration is C(x,t). Note that here and below I use capitalization to indicate that a variable is random. The term $\delta^2/2$, the macroscopic dispersion tensor, is a coefficient which in porous media includes effects of two smaller scale phenomena: molecular diffusion and mechanical dispersion (Bear, 1979). The latter is spreading of pollutant caused by velocity variations within and among the pores of the medium.

In the hydrological application of equation (1.2) the term V is the groundwater seepage velocity. It is the velocity of groundwater through a small section of the medium and its properties can in principle be determined by field experiment. More generally V is the macroscopic solute velocity. In steady flow it is a function of position alone and fluctuates due to spatial variations in properties of the porous medium and in the hydraulic gradient. Because of the complexity of the medium, experiments to completely determine these variations are impossible and the best that can be hoped is to determine statistical properties of V(x).

In flow through a large mass of more or less homogeneous material, for instance a uniformly fractured granite, V(x) can be taken to be a weakly stationary random field. Note that to rigorously show that a pollutant's concentration converges to a Fickian concentration it is probably necessary to assume that the intermediate scale velocity is strongly stationary. Certainly that is the case in the theory of turbulent diffusion (Kesten and Papanicolaou, 1979). Weak stationarity suffices, however, to obtain formal expressions for asymptotic drift and dispersion coefficients.

In such a field the mean is the same at every point,

$$E[V(x)] = \mu \quad (1.3)$$

for every x, and the covariance is a matrix depending on the displacement, x-y,

$$E_V[V(x)V(y)] = \rho_V(x-y) \quad (1.4)$$

but not on the actual location of the points x and y. The notation $E_V[\cdot]$ denotes the operation of taking mathematical expectation with respect to the random variable V.

Hence, the velocity field can be represented as

$$V(x) = \mu + \varepsilon U(x) \quad (1.5)$$

where ε is a number (soon to be presumed small) and U(x) is a weakly stationary random field with mean zero. Then

$$\rho_V(x-y) = \varepsilon^2 \rho(x-y) \quad (1.6)$$

where ρ is the covariance of U(x).

The restrictions on U(x) are fairly weak, allowing for example the velocity field to be anisotropic. It is, however, necessary that

$$\lim_{\|r\| \to \infty} \rho_{\ell j}(r) = 0 \quad (1.7)$$

where $r \in R^d$, $\|r\|$ is the norm of r, and ρ is the ℓj^{th} element in ρ.

For a given realization of the U(x) process, equation (1.2) is the Fokker-Planck equation of a diffusion process (Gihman and Skorohod, 1972). If C(x,t) is normalized so that the total mass is one, then C(x,t) is the probability density of a particle of pollutant conditioned on the given realization of U(x). The particle trajectories are described by the stochastic differential equation,

$$X'(\tilde{t}) = \mu + \varepsilon\, U(X(\tilde{t})) + \delta W'(\tilde{t}) \tag{1.8}$$

where δ is a dxd positive definite matrix and $W(\tilde{t})$ is a Wiener process. For convenience t is replaced by $\tilde{t}$ in (1.8).

Since the solution of (1.1) is the convolution of the initial condition with a Gaussian function, the assumption that C converges (in a sense yet to be defined) to $\tilde{c}$ amounts to assuming that the density of X(t) satisfies a central limit theorem.

If time in equation (1.8) is scaled by letting

$$\tilde{t} = nt \tag{1.9}$$

the limit assumption amounts to assuming that the random variable, $X_n(t)$, defined by

$$X_n^*(t) = \frac{X(nt) - nt\alpha}{\sqrt{n}} \tag{1.10}$$

has a density $f_n^*(x;t)$ which, as n becomes large, approaches a normal density, f(x;t), with zero drift and covariance Dt.

The object is to exploit the limit assumption

$$\lim_{n\to\infty} f_n^*(x) = f(x) \tag{1.11}$$

to approximate D and α. Note that the dependence of f_n^* and f on t is suppressed here and in the sequel. An equivalent form of the limit assumption --the form I will actually use --is

$$\lim_{n\to\infty} E_{X_n^*} [g(X^*)] = E_X [g(X)] \qquad (1.12)$$

where g(x) is arbitrary and X is the random variable which has f as its density.

Marginal densities such as f_n^* are not physically obtainable. After all the density about which there is information is C(x,t), and it is conditioned on a realization of the macroscopic velocity field. From this It would seem that convergence for almost every realization of U is appropriate. Note, however that a marginal density is the average of conditional densities

$$\begin{aligned} f_n^* &= \int f_n^*(x,u)du \\ &= \int f_n^*(x|u)f(u)du \\ &= E_U [f_n^*(x|u)] \end{aligned} \qquad (1.13)$$

where $f_n^*(x,u)$ is the joint density of X_n and U, f(u) is the marginal density of U and $f_n^*(x|u)$ is the conditional density of X^* given U. Thus f_n^* can be obtained by averaging over a family of macroscopic velocity fields. In taking the expectation I exploit the idea that in a large homogeneous medium the volume sampled in a field experiment is replicated many times.

For given U = u the conditional density, $f_n^*(x|u)$, is the density of a diffusion process which is translated by $\sqrt{n}\alpha t$. Let $C_n(x,t)$ be the density of $X(nt)/\sqrt{n}$ for given u. Then $C_n(x,t)$ satisfies the convection-diffusion equation,

$$\frac{\partial C_n}{\partial t} = \frac{1}{2}\nabla\cdot\delta^2\nabla C_n - \sqrt{n}\nabla\cdot(\mu + \varepsilon u(\sqrt{n}\ x))C_n \tag{1.14a}$$

$$C_n(x,0) = C_0(\sqrt{n}\ x) \tag{1.14b}$$

and

$$f_n^*(x|u) = C_n(x+\sqrt{n}\alpha t,t) \tag{1.15}$$

Since U = u is given, $C_n(x,t)$ is the density of a diffusion process. Thus equation (1.14) has the transition density of the diffusion process, $p_U(s,y;t,x)$, as its fundamental solution (Gihman and Skorohod, 1972). The product $p_U(s,y;t,x)dx$ is the probability that a particle at the point y at time s<t will have reached a small volume centered around x at time t. Because p_U is the fundamental solution of (1.14),

$$C_n(x,t) = \int_{R^d} p_U(s,y;t,x)\ C_0(\sqrt{n}\ y)\ dy \tag{1.16}$$

It is important to note that p is also the fundamental solution to the formal adjoint of equation (1.14a),

$$\frac{\partial p_U}{\partial s} = -\frac{1}{2}\nabla\cdot\delta^2\nabla p_U - \sqrt{n}(\mu + \varepsilon u(\sqrt{n}\ y)\cdot\nabla p_U$$

$$= -L_n p_U \tag{1.17}$$

where $-L_n$ is the differential operator in the middle equation.

For fixed $U = u$ define an integral operator with kernel $p_U(s,y;t,x)$,

$$P_U(s,t)\, g = \int_{R^d} p_U(s,y;t,x)\, g(x)\, dx \qquad (1.19)$$

where g is arbitrary. Since p_U is the transition density of a diffusion process, the operators $P_U(s,t)$ form a continuous semigroup, the backwards semigroup of p_U (Feller, 1966). Because, furthermore, the operator L_n is independent of t, P_U is stationary, i.e. $P_U(s,t) = P_U(s-t)$.

It is a fact that these operators can be represented as exponentials. To help see this note that if (1.19) is differentiated with respect to s -- and the arbitrary g is ignored -- then formally,

$$\frac{\partial P_U}{\partial s} = -L_n P_U \qquad (1.20).$$

Since P behaves like a δ function when s=t,

$$P_U = e^{-(s-t)L_n} \qquad (1.21).$$

On the other hand the asymptotic density, $f(x) = C(x,t)$, satisfies the heat equation,

$$\frac{\partial c}{\partial t} = \frac{1}{2} \nabla \cdot D \nabla c \qquad (1.22)$$

with initial condition $c(x,0) = c_\infty(x) = \lim c_0(\sqrt{n}\,x)$. The fundamental solution of the heat equation is a Gaussian transition density, $p(s,y;t,x)$ with mean zero and covariance Dt. Since p is the transition density of a diffusion process, it has a corresponding backwards semi-group,

$$P(s,t) = e^{-[(s-t)\nabla\cdot D\nabla]/2} \tag{1.23}$$

If I return to the limit assumption (1.1), I find that its terms can be represented as

$$E_{X_n^*}[\ g(X_n^*)\ ] = \int_{R^d} dx\ g(x)\ E_U[\ f^*(x|u)\ ]$$

$$= \int_{R^d} dx\ g(x)\ E_U[\ C_n(x+\sqrt{n}\alpha t,t)\ ]$$

$$= \int_{R^d} d\xi\ g(\xi-\sqrt{n}\alpha t)\ E_U[\ C_n(\xi,t)\ ] \tag{1.24}$$

by change of variables. But

$$C_n(\xi,t) = \int_{R^d} p_U(0,y;t,\xi)\ c_0(\sqrt{n}y)\ dy \tag{1.25}$$

and since translation by $\sqrt{n}\alpha t$ is equivalent to the application of the operator $e^{-t\sqrt{n}\alpha\cdot\nabla}$,

$$E_{X_n^*}[\ g(X_n^*)\ ] = \int_{R^d} d\xi\ e^{-t\sqrt{n}\alpha\cdot\nabla} g(\xi) E_U[\int_{R^d} dy\ p_U(0,y;t,\xi) c_0(\sqrt{n}y)$$

$$= \int_{R^d} dy\ c_0(\sqrt{n}y)\ E_U[\int_{R^d} d\xi\ p_U(0,y;t,\xi) e^{-t\sqrt{n}\alpha\cdot\nabla} g(\xi)$$

$$= \int_{R^d} dy\ c_0(\sqrt{n}y)\ E_U[e^{tL_n}\ e^{-t\sqrt{n}\alpha\cdot\nabla} g] \tag{1.26}$$

Similarly

$$E_X[\ g(X)\ ] = \int_{R^d} dy\ c_\infty(y)\ e^{t/2(\nabla\cdot D\ \nabla)} \tag{1.27}$$

Since $\lim c_0(\sqrt{n}y) = c_\infty(y)$, it is clear that I have (1.1) just when

$$\lim_{n\to\infty} E_U[\, e^{tL_n} e^{-t\sqrt{n}\alpha\cdot\nabla} \,] = e^{t/2(\nabla\cdot D\,\nabla)} \tag{1.28}$$

From a mathematical point of view equation (1.28) is the starting point for the rest of the analysis. It is equivalent to the assumption that the solution to (1.2) converges to that of (1.1). To estimate $\alpha(\varepsilon)$ and $D(\varepsilon)$ I expand each side of (1.28) in terms of ε. Let

$$A = \frac{1}{2}\nabla\cdot\delta^2\nabla + \sqrt{n}\mu\cdot\nabla \tag{1.29}$$

and

$$B_U = \sqrt{n}\; U(\sqrt{n}x)\cdot\nabla \tag{1.30}.$$

Next substitute B_U for B in the following formula

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

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

$$+ \dots \tag{1.31}.$$

When B is almost surely bounded in operator norm, the formula is correct (Hille and Phillips, 1957). Since the analysis in this dissertation is formal, I will not analyse conditions on U which would assure the applicability of (1.31). That the substitution is not straightforward is clear from the fact that B_U is unbounded.

Suppose that

$$\alpha(\varepsilon) = \alpha_0 + \alpha_1\varepsilon + \alpha_2\varepsilon^2 + \ldots \qquad (1.32)$$

$$D(\varepsilon) = D_0 + D_1\varepsilon + D_2\varepsilon^2 + \ldots \qquad (1.33).$$

Then by expanding each side of (1.28) in powers of ε and supposing that the limit is valid term by term, I can in principle derive formal expressions for any D_n or α_n, $n = 0, 1, 2, \ldots$. In this dissertation, however, I will be content to approximate D and α through terms of second order.

Review

Both the applicability of equations (1.1) and (1.2) to the problem of pollutant dispersion in a porous medium and the convergence of the solution of (1.2) to that of (1.1) are assumed in this dissertation. The assumptions are, as noted earlier, consistent with experimental results. No attempt to derive them from fundamental considerations is made here. Considerable effort has, however, been devoted to doing so.

Fried and Combarnous (1971) and Sposito, Gupta, and Bhattacharya (1979) have critically reviewed theories which attempt to derive a governing convection-diffusion equation on intermediate scales from pore scale considerations. Sposito, Gupta, and Bhattacharya (1979) divide these attempts into three classes. The most straightforward are those which elaborate on Taylor's description of dispersion in capillary tubes (Taylor 1953 and 1954). The medium is idealized as either a fixed or random bundle of capillaries, some fluid mechanical description of solute transport in a capillary is applied to each capillary and the result is averaged over an intermediate volume to obtain a macroscopic convection-diffusion equation (e.g.,Saffman 1959 and 1960, Whitaker, 1967; Bear and Bachmat, 1967). These theories have been criticized by Sposito, Gupta, and Bhattacharya (1979) for depending upon a misapplication of ergodicity, having no dynamical basis, requiring an artificial model of the medium, or leading to a governing equation which is not a convection-diffusion equation.

A second class of models treats either the motion of a solute molecule or the solute concentration in a small portion of the medium as a Markov process. In the former case (for instance Beran 1968 and Todorovic 1975) some form of the central limit theorem is invoked to show that the probability density function of a molecule tends to a Gaussian density after many time steps. Thus the concentration of pollutant obeys a convection-diffusion equation at intermediate scales. Most such theories lack " ... a specification of the velocity process in terms of molecular dynamics." (Sposito, Gupta, and Bhattacharya, 1979) Recently, however, Bhattacharya and Gupta (1979) have derived a pore level convection-diffusion equation by following a molecule of solute which randomly collides with the medium. Its velocity between collisions is governed by a Langevin equation. Theories which treat solute concentration as a Markov process (e.g. Chaudhari and Scheidegger, 1965) do not lead to a macroscopic convection-diffusion equation.

The last class of theories treated by Sposito, Gupta, and Bhattacharya (1979) depend upon an analogy between mass and heat transport. Of course heat transport obeys a convection-diffusion equation. Thus to, the extent that the analogy is apt, a similar equation can be used to describe mass transport. Such theories, however, propose no physical basis for the presumed connection between the two kinds of transport.

Given equation (1.2) several have tried to derive equation (1.1). The greater part of this work has been undertaken by fluid dynamicists and has been applied to dispersion in turbulent media. Thus it has been natural to suppose the macroscopic fluid velocity to be a random field. The paradigm for the fluid dynamical problem is the dispersion of smoke in the atmosphere. Because in such a problem variations in the velocity field contribute much more to the dispersion of a pollutant than does molecular diffusion, it has also been natural for fluid dynamicists to take $\delta = 0$ in (1.2). Many investigators (e.g. Taylor, 1921; Roberts, 1961; Kraichnan, 1970; and Monin and Yaglom, 1971) have treated this problem with varying degrees of rigor. Perhaps the most thorough have been Kesten and Papanicolaou (1979) who have proved a central limit theorem for the case of turbulent diffusion in a homogeneous velocity field.

Since the velocity of fluid in a porous medium is generally much lower than the velocity of a turbulent gas, the influence of molecular diffusion (or, more properly, the coefficient of hydrodynamic dispersion) is not always negligible in hydrological problems. In the case of low permeability media, for instance the rocks suggested as repositories for nuclear waste, the effect of hydrodynamic dispersivity may be as great as the effect of seepage velocity. Hence in Chapters 3 and 4 I retain the term δ in my calculations and later indicate that the results are consistent with Kesten and Papanicolaou (1979) when $\delta = 0$.

This is a good time to emphasize a subtle point: the coefficient $\delta^2/2$ has slightly different meanings in hydrological and turbulent diffusion. In the literature of turbulence it is simply the coefficient of molecular diffusion. Hence, when molecular diffusion is negligible, $\delta^2/2$ is zero, i.e. $\delta = 0$. In hydrology, on the other hand, it is the coefficient of hydrodynamic dispersion and includes micro-mechanical as well as thermal effects. Thus even when the thermal effect of molecular diffusion is negligible, variations in the pore-scale velocity field can cause sufficient mechanical dispersion for $\delta^2/2$ to be nonzero.

Note that the pore scale is much smaller than any scale which qualifies as macroscopic in the discussion which follows. Variations in the macroscopic velocity field are the result of variations in hydraulic conductivity (Gutjahr et al., 1978; Bakr et al., 1978) and, perhaps, variations in head gradient, both of which are macroscopic quantities. Thus the velocity variations which affect hydrodynamic dispersion are not the same as variations in the macroscopic field. Hydrodynamic dispersion is independent of fluctuations in the latter field.

Several groups of hydrologists have obtained values for D in special cases of passage from equation (1.2) with $\delta \neq 0$ to (1.1). Gelhar et al. (1979), Matheron and de Marsily (1980), and Gelhar and Axness (1981) have been most prominent among them. Others who have worked in this area are Dieulin et al. (1981) and Dagan (in press). Gelhar et al. (1979) and Matheron and de Marsily (1980) have considered special cases of the problem in two dimensional media. The former have investigated dispersion in a stratified aquifer, a porous medium in which the seepage velocity is strictly horizontal and varies only with depth in the medium.

They have also calculated dispersion coefficients for times intermediate between the macroscopic and megascopic scales. From their expression for the megascopic dispersion matrix, D, it is clear that in this case the solution to (1.2) converges to that of (1.1) only if the velocity field satisfies a very restrictive condition: the covariance of the horizontal component -- the only nonzero component -- must be negative over some interval(s). This requirement has become known as the "hole effect".

Matheron and de Marsily (1980) have analysed the same case via a different method and have obtained the same result. They have, however, also found that if there is any systematic tilt to the flow field away from the horizontal, the condition of negative velocity covariances is unnecessary.

After the results reported in this dissertation were obtained it came to my attention that Gelhar and Axness (1981) had derived large scale dispersion matrices for general three dimensional porous media by a completely different method from mine. They assume that the fluid is incompressible and that the concentration is locally stationary. With these assumptions they show that the mean concentration is asymptotically Fickian and derive an approximation for the megascopic dispersion coefficient which agrees with mine. When, however, the fluid is compressible, additional terms appear in the approximation of the megascopic dispersion coefficient which, because of the problem they treat, Gelhar and Axness (1981) do not find. Furthermore, the asymptotic drift of a pollutant in a compressible fluid is not identical to macroscopic velocity and must be corrected. Still the approximation of Gelhar and Axness (1981) is correct for incompressible fluids through terms of second order and represents a considerable advance in the hydrological theory of mass transport.

CHAPTER 2

SPECIAL CASES

Since the asymptotic drift and dispersion coefficients derived by Kesten and Papanicolaou (1979), Gelhar et al. (1979), Matheron and de Marsily (1980), and Gelhar and Axness (1981) are obtained for special cases of the problem I investigate, it will prove instructive to consider their work in detail. Later I compare their results to mine and find that the two sets agree.

Turbulent Diffusion

If I consider C(x,t) in equation (1.2) to be the probability density function for the position of a solute particle, then as already noted the trajectory of a particle can be described by the stochastic differential equation

$$X'(t) = \mu + \varepsilon\ U(X(t)) + \delta\ W'(t) \qquad (2.1)$$

with terms defined as in equation (1.8). When the mean macroscopic velocity, μ, is large, the effect of macroscopic dispersion can be neglected and (2.1) reduces to

$$X'(t) = \mu + \varepsilon\ U(X(t)) \qquad (2.2),$$

the turbulent diffusion case treated by Kesten and Papanicolaou (1979).

By scaling time in terms of the magnitude of variability about mean seepage velocity, $t = \tau\varepsilon^{-2}$, and defining a centered position process

$$X_\varepsilon(\tau) = X(\tau\varepsilon^{-2}) - \tau\varepsilon^{-2}\mu \qquad (2.3),$$

Kesten and Papanicolaou (1979) deduce expressions for the asymptotic drift and dispersion coefficients in the limit $\varepsilon\to 0$. They are able to do so because when $\delta = 0$, the asymptotic covariance matrix, $D\tau$, is well-behaved in this scaling: suppose that D can be formally expanded as

$$D(\varepsilon;\delta) = \delta + \varepsilon^2 D_2(\delta) + O(\varepsilon^3) \qquad (2.4).$$

Then in Kesten and Papanicolaou's (1979) scaling

$$D(\varepsilon;0)t = D(\varepsilon;0)\tau\varepsilon^{-2} = D_2(0)\tau + O(\varepsilon) \to D_2(0)\tau \qquad (2.5)$$

as $\varepsilon\to 0$.

Earlier papers (e.g. Roberts, 1961) have given formal asymptotic drift and dispersion coefficients for the turbulent diffusion case. Kesten and Papanicolaou (1979) derive slightly more general formal asymptotic coefficients; in the notation of this dissertation they are,

$$(\alpha_2(0))_j = \int_0^\infty \sum_{k=1}^{d} E[\, U_k(x) \frac{\partial}{\partial x_k} U_j(x+t\mu) \,]\, dt \qquad (2.6)$$

and

$$(D_2(0))_{kj} = 1/2 \{ \int_0^\infty E[\, U_k(x)U_j(x+t\mu) \,]\, dt + \int_0^\infty E[\, U_k(x+t\mu)U_j(x) \,]\, dt \} \qquad (2.7)$$

where d is the number of dimensions, $(\alpha_2(0))_j$ is the j^{th} element in $\alpha_2(0)$

and $(D_2(0))_{\ell j}$ the ℓj^{th} element in $D_2(0)$. When, furthermore, $U(x)$ is strictly stationary and satisfies other technical assumptions, Kesten and Papanicolaou (1979) prove the convergence of C to c as a limit theorem.

For strictly isotropic $U(x)$ the expressions (2.6) and (2.7) have a simple form,

$$(\alpha_2)_j = \sum_{k=1}^{d} \int_0^\infty \frac{\partial}{\partial \tau_k} \rho_{kj}(\|\tilde{t}\|)\, dt$$

$$= -\sum_{k=1}^{d} (\mu_k/\|\mu\|)\, \rho_{kj}(0) \qquad (2.8)$$

and

$$(D_2)_{kj} = \int_{-\infty}^{\infty} \rho_{kj}(\|\tilde{t}\|)\, dt$$

$$= \|\mu\|^{-1} \int_{-\infty}^{\infty} \rho_{kj}(t)\, dt \qquad (2.9)$$

where $\tilde{t} = \mu t$. Note that if the elements of $U(x)$ are uncorrelated, then $(\alpha_2)_j < 0$. Since, as I will later show, the α_1 vector is zero, this indicates that, for an isotropic velocity field with uncorrelated elements, the long-term progress of the pollutant is less than (or, perhaps, equal to) the local seepage velocity.

Before leaving the case $\delta = 0$ it is important to note that Kesten and Papanicolaou's (1979) limit, $\varepsilon \to 0$ simultaneously with $t \to \infty$, is not the only one possible. If, in particular, t is not scaled in terms of ε, it is possible to treat velocity fields with relatively large variability about the mean. With such a scaling terms of $O(\varepsilon^3)$ will remain in the expansions of $\alpha(0)$ and $D(0)$ even after the limit $t \to \infty$ has been taken. In Chapters 3 and 4 I will take just such a limit. I will not, however, calculate terms of any order greater than ε^2 in the approximations given there.

Of course higher order terms are useful in determining the accuracy of approximations through terms of order ε^2. While in general such terms are difficult to obtain, an expression for $\alpha(0)$ -- and thus terms of all orders in its expansion -- can be determined relatively easily in a particular case of a one dimensional diffusion. The case requires that $\delta = 0$ and $U(x)$ be stationary with certain mixing properties such as ergodicity.

To begin, consider equation (2.2) in one dimension and note that $\Phi(x)$ can be found such that

$$\Phi(x) = \int_0^x \frac{dx'}{\mu + \varepsilon U(x')} \tag{2.10}$$

where it is assumed that V is bounded away from zero.

Thus the process X(t) is determined by

$$X(t) = \Phi(X(t)) \tag{2.11}$$

Let

$$\phi_U(x) = \frac{1}{\mu + \varepsilon U(x)} \tag{2.12}$$

Then from the ergodicity of U(x),

$$\lim_{x\to\infty} \frac{\Phi(x)}{x} = \lim_{x\to\infty} \frac{1}{x} \int_0^x \phi_U(x')\, dx'$$

$$= E[\, \phi_U(x)\,] \tag{2.13}$$

But

$$E[\phi(x)] = E[\frac{1}{\mu + \varepsilon U(x)}]$$

$$= \frac{1}{\mu} E[\sum_{n=0}^{\infty} (-1)^n \frac{(\varepsilon U(x))^n}{\mu^n}$$

$$= \frac{1}{\mu} (1 + \frac{\varepsilon^2}{\mu 2} M_2 - \frac{\varepsilon^3}{\mu 3} M_3 + \ldots)$$

$$= \beta \qquad (2.14)$$

where M_k is the k^{th} moment of U(x), a constant by stationarity, and $M_1 = 0$ by definition.

Thus

$$\lim_{x\to\infty} \frac{\Phi(x)}{x} = \beta \qquad (2.15),$$

which is equivalent to

$$\lim_{t\to\infty} \frac{t}{X(t)} = \beta \qquad (2.16).$$

But

$$\lim_{t\to\infty} \frac{X(t)}{t} = \alpha \qquad (2.17),$$

so clearly

$$\alpha = \frac{1}{\beta}$$

$$= \mu \left(1 - \frac{\varepsilon^2\sigma^2}{\mu^2} + O((\varepsilon/\mu)^3) \right) \qquad (2.18)$$

where $\sigma^2 = M_2$.

Hence if variations in the local seepage velocity are relatively small with respect to the mean local seepage velocity

$$\alpha \cong \mu - \frac{\varepsilon^2\sigma^2}{\mu} = \mu - \sigma_V^2/\mu \qquad (2.19).$$

Here σ_V^2 is the variance of the local velocity, V(x). If the third and higher central moments of V(x) are relatively small with respect to the corresponding power of μ, the approximation is a good one. If, moreover, $U(x)$ is a Gaussian random variable (or, more generally, if U has a density which is even) so that $M_{2k+1} = 0$ for all k, the approximation is even better.

A related, but more difficult, calculation leads to terms of all orders of ε in the expansion of D. It depends on an unpublished proof of the central theorem for $X(t)$. The proof was shown to me by C. Newman and is known to other experts in the field (Papanicolaou, personal communication). Suppose that $\Phi(x)$ satisfies a central limit theorem

$$\frac{\Phi(nx) - n\beta x}{\sqrt{n}} = W_n(x) \to W(x) \quad \text{as } n \to \infty \tag{2.20}$$

where $W(x)$ is a Wiener process with mean zero and variance $\sigma_\Phi^2 x$. The term σ_Φ^2 is the variance of $\Phi(x)$.

Then by invoking an invariance principle it can be shown that

$$\frac{X(nt) - \alpha nt}{\sqrt{n}} = V_n(t) \to \alpha W(\alpha t) \quad \text{as } n \to \infty \tag{2.21}$$

with variance $\alpha^3 \sigma_\Phi^2 t = Dt$.

But

$$\sigma_\Phi^2 = \frac{\varepsilon^2}{\mu^4} \int_{-\infty}^{\infty} \rho(t)\, dt + O(\varepsilon^3/\mu^5) \tag{2.22},$$

so

$$D = \frac{\varepsilon^2}{\mu^2} \int_{-\infty}^{\infty} \rho(t)\, dt + O(\varepsilon^3/\mu^2) \tag{2.23}.$$

The error in estimating D by the first nonzero term in its expansion is not great when ε is small with respect to μ.

Special Cases in Hydrology

The investigation of mass transport in the presence of hydrodynamical dispersion, i.e. transport when $\delta \neq 0$, is more complicated than is the analysis of the usual turbulent transport problem. Note, for instance, that Kesten and Papanicolaou's (1979) scaling cannot be used unless $\delta = 0$. Their expression for D is otherwise undefined in the limit $t \to \infty$. Difficulties such as these have led hydrologists to analyse transport in special cases of porous media.

Stratified Aquifers

Gelhar et al. (1979) have investigated the degenerate case of a two dimensional aquifer with a macroscopic flow field which is 1) a function of only one coordinate, say x_2, and 2) is strictly parallel to the other, x_1. Hence the velocity field can be represented as

$$V_1(x) = \mu + \varepsilon U(x_2) \tag{2.24a}$$

$$V_2(x) = 0 \tag{2.24b}$$

They assume, furthermore, that δ is diagonal. Thus the macroscopic convection-diffusion equation reduces to

$$\frac{\partial C}{\partial t} = \delta_{11} \frac{\partial^2 C}{\partial x_1^2} + \delta_{22} \frac{\partial^2 C}{\partial x_2^2} - \frac{\partial VC}{\partial x_1} \tag{2.25}$$

Gelhar et al. (1979) analyse the dispersion tensor by expressing every term in (2.25) as the sum of a mean plus a random deviation.

$$C(x_1,x_2,t) = \overline{c}(x_1,t) + \varepsilon C'(x_1,x_2,t) \tag{2.26a}$$

$$E[C'] = 0 \quad (2.26b)$$

$$\delta_i = d_i + \varepsilon^2 d_i' \quad (2.26c)$$

$$E[d_i'] = 0 \qquad i = 1, 2 \quad (2.26d)$$

where the primed terms are random. $V_1(x)$ has already been expressed appropriately.

To calculate asymptotic coefficients Gelhar et al. (1979) take the expected value of (2.25), an operation which they assume is equivalent to averaging over x_2. By doing so they obtain a mean equation,

$$\frac{\partial \bar{c}}{\partial t} = \mu_1 \frac{\partial \bar{c}}{\partial x_1} + \varepsilon^2 \frac{\partial}{\partial x_1} E[UC'] + d_1 \frac{\partial^2}{\partial x_1^2} \bar{c} + \varepsilon^2 \frac{\partial}{\partial x_1} E[d'C']$$

$$+ \varepsilon^2 \frac{\partial}{\partial x_2}[d_2' c'] \quad (2.27)$$

Note that if δ is constant ($d_1' = d_2' = 0$), equation (2.27) is strictly one dimensional. Even if it is not, Gelhar et al. (1979) argue from physical principles that the last two terms in (2.27) can be ignored.

Thus the mean equation (which is equivalent to the megascopic equation) is Fickian if

$$E[UC'] = D_1 \frac{\partial \bar{c}}{\partial x_1} \quad (2.28)$$

where D_1 is a constant to be determined. Since the argument which justifies (2.28) is similar to that given in Gelhar and Axness (1981), it is deferred until the latter paper is considered. Suffice it to say that Gelhar et al. (1979) derive the relationship (2.28) for stratified aquifers and find that the asymptotic dispersion coefficient is

$$D_1 = \delta_1 + \frac{\varepsilon^2}{2\pi\delta_2} \int_{-\infty}^{\infty} \frac{\hat{\rho}^1(\xi)}{\xi^2} \, d\xi \qquad (2.29)$$

Of course the integral in (2.29) exists only if

$$\hat{\rho}_1(0) = \int_{-\infty}^{\infty} \rho_1(x)\, dx = 0 \qquad (2.30)$$

As noted earlier, this condition (commonly known as the "hole effect") excludes velocity fields which are positively correlated over every interval. In a perfectly stratified two dimensional aquifer such a velocity field cannot possibly lead to asymptotically Fickian diffusion. Later it will be clear that this result is limited to this special case.

Tilted Aquifers

That the result of Gelhar et al. (1979) is restricted is strongly suggested by the work of Matheron and de Marsily (1980) who show that in any systematically tilted two dimensional flow field condition (2.30) is not necessary.

Using a different analysis Matheron and de Marsily (1980) obtain the same result for perfectly stratified aquifers as Gelhar et al. (1979). They have, however, also investigated dispersion in two dimensional aquifers with tilted velocity fields,

$$V_1(x) = \mu_1 + \varepsilon U(x_2) \qquad (2.31a)$$

$$V_2(x) = \mu_2 \qquad (2.31b)$$

since Matheron and de Marsily (1980) take the hydrodynamic dispersion matrix to be constant and diagonal, the macroscopic convection-diffusion equation is,

$$\frac{\partial C}{\partial t} = \delta_{11} \frac{\partial^2 C}{\partial x_1^2} + \delta_{22} \frac{\partial^2 C}{\partial x_2^2} - \left(\frac{\partial V_1 C}{\partial x_1} + \mu_2 \frac{\partial C}{\partial x_2} \right) \qquad (2.32).$$

The corresponding terms of the megascopic dispersion matrix are

$$D_{11} = \delta_{11} + \frac{\varepsilon^2}{2\pi} \int_{-\infty}^{\infty} \frac{\hat{\rho}1(\xi 2)}{\delta_2 \xi_2^2 - i\mu_2 \xi_2} d\xi_2 \qquad (2.33a)$$

$$D_{22} = \delta_{22} \qquad (2.33b)$$

Here $\rho_1(x)$ is the covariance of $U(x_2)$.

Note that the integrand in the expression for D_{11} is singular only if $\mu_2 = 0$. Of course when $\mu_2 = 0$ this case reduces to a stratified aquifer. Since it must be rare aquifer which has a strictly horizontal flow field, in most cases relatively weak conditions -- for instance, boundedness and approach to zero at ∞ -- on the covariance of the velocity field will suffice to calculate the megascopic dispersion matrix.

As preparation for the asymptotic analysis of mass transport in more general media it is instructive to consider three dimensional analogues of the tilted aquifers treated by Matheron and de Marsily (1980). The aquifers which I now investigate have the property: if an element of the macroscopic velocity field is variable, then it can only depend on coordinates in the direction of which the velocity field is constant.

Typical three dimensional velocity fields with this property are

1) $$V_1(x) = \mu_1 + \varepsilon U_1(x_3) \quad (2.34a)$$

$$V_2(x) = \mu_2 + \varepsilon U_2(x_3) \quad (2.34b)$$

$$V_3(x) = \mu_3 \quad (2.34c)$$

2) $$V_1(x) = \mu_1 + \varepsilon U_1(x_2, x_3) \quad (2.35a)$$

$$V_2(x) = \mu_2 \quad (2.35b)$$

$$V_3(x) = \mu_3 \quad (2.35c)$$

As earlier noted the position process of a particle whose probability density function obeys an equation like (1.2) must satisfy a stochastic differential equation

$$X'(t) = V(X(t)) + \sqrt{2}\,\hat{\delta}\, W'(t) \quad (2.36).$$

In the case I now consider $\hat{\delta}$ is diagonal with constant elements and W(t) is a Wiener vector process with independent elements. Since $\hat{\delta}$ is diagonal so too is $\tilde{\delta} = 2\hat{\delta}^2$. Its $\ell\ell^{th}$ element can be denoted by $\tilde{\delta}_\ell$.

If the probability density function of X(t) converges to the solution of equation (1.1) with a Dirac function as initial condition, the covariance matrix of X(t), $\sigma^2(t)$, converges to Dt. While D is presently undetermined, it can be found by taking

$$\lim_{t\to\infty} \frac{\sigma^2(t)}{t} = D \quad (2.37).$$

When $V_\ell(x)$ is constant, $D_{\ell\ell} = \tilde{\delta}_\ell$. If $V_\ell(x)$ is constant but $V_k(x)$ is not, then (from the independence of U_k, W_k, and W_ℓ) $\sigma^2_{\ell k}(t) = 0$. This implies that $D_{\ell k} = 0$.

To calculate σ^2 (t) when neither $V_\ell(x)$ nor $V_k(x)$ is constant, observe that

$$X_\ell(t) = \mu_\ell t + \varepsilon \int_0^t U_\ell(Z(\tau))\, d\tau + \sqrt{2}\ \hat{\delta}_\ell W_\ell(t) \tag{2.38}$$

and similarly for $X_k(t)$. Because of the condition which defines this special case, $Z(\tau)$ can only be one dimensional when $\ell \neq k$.

For instance in example 1) above

$$Z(\tau) = X_3(\tau) = \mu_3\tau + \sqrt{2}\,\hat{\delta}_3\ W_3(\tau) \tag{2.39}$$

and the covariance matrix is

$$\sigma^2(t) = \begin{matrix} \sigma^2_{11}(t) & \sigma^2_{12}(t) & 0 \\ \sigma^2_{21}(t) & \sigma^2_{22}(t) & 0 \\ 0 & 0 & \tilde{\delta}_3 t \end{matrix} \tag{2.40}$$

Note that $\sigma^2_{12}(t) = \sigma^2_{21}(t)$.

If $Z(\tau)$ is two dimensional, $\sigma^2_{\ell k}(t) = 0$ if $\ell \neq k$. In example 2)

$$Z_1(\tau) = X_2(\tau) = \mu_2\tau + \sqrt{2}\,\hat{\delta}_2\ W_2(\tau) \tag{2.41a}$$

$$Z_2(\tau) = X_3(\tau) = \mu_3\tau + \sqrt{2}\,\hat{\delta}_3\ W_3(\tau) \tag{2.41b}$$

and the covariance matrix is

$$\sigma^2(t) = \begin{matrix} \sigma^2_{11}(t) & 0 & 0 \\ 0 & \tilde{\delta}_2 t & 0 \\ 0 & 0 & \tilde{\delta}_3 t \end{matrix} \tag{2.42}$$

In any event the elements of $Z(\tau)$ have the form

$$Z_j(\tau) = \beta_j\tau + \gamma_j W_j(\tau) \tag{2.43}$$

where β_j and γ_j are respectively elements of μ and $\sqrt{2}\,\hat{\delta}$.

The computation of $\sigma^2_{\ell k}(t)$ is straightforward, if tedious. Of course

$$\sigma^2_{\ell k}(t) = E[X_\ell(t)X_k(t)] - \mu_\ell\mu_k t^2 \tag{2.44}$$

where I use the homogeneity of $U(x)$.

From the definition of $X_\ell(t)$ and $X_k(t)$, as well as the independence among W_ℓ, W_k, U_ℓ, and U_k, it follows that

$$\sigma^2_{\ell k}(t) = 2\,\hat{\delta}_\ell\hat{\delta}_k(\kappa_{\ell k})t + \varepsilon^2\int_0^t\int_0^t E[U_\ell(Z)U_k(Z')]\,d\tau'd\tau \tag{2.45}$$

where $\kappa_{\ell k}$ is 1 if $\ell = k$ and 0 otherwise, $Z = Z(\tau)$ and $Z' = Z(\tau')$.

Because U is homogeneous in space and the elements of Z are independent of each other, the joint probability density function of U_ℓ, U_k, Z and Z' is

$$p(u_\ell,u_k,z,z') = p(u_\ell,u_k)\prod_{j=1} p(z_j,z_j') \tag{2.46}$$

where m is the dimension of Z. Since

$$\rho_{\ell k}(z-z') = \mathrm{Cov}[U_\ell(z)U_k(z')]$$

$$= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} [u_\ell(z)u_k(z')]\ p(u_\ell,u_k)\ du_\ell du_k \ , \qquad (2.47)$$

$$E[U_\ell(Z)U_k(Z')] = \int_{R^m}\int_{R^m} \rho_{\ell k}(z-z')[\prod_{j=1}^{m} p(z_j,z_j')]\ dz'dz \qquad (2.48).$$

Suppose that τ' follows τ, then $p(z_j'|z_j)$ is the transition density for moving from $Z_j(\tau) = z_j$ to $Z_j(\tau') = z_j'$. Of course

$$p(z_j,z_j') = p(z_j'|z_j)p(z_j) \qquad (2.49).$$

Because each z is like a Wiener process with a constant drift,

$$p(z_j'|z_j) = \frac{e^{-(z_j'-z_j-\beta_j(\tau'-\tau))^2/2\gamma_j(\tau'-\tau)}}{[2\pi\gamma\ (\tau'-\tau)]^{1/2}} \qquad (2.50).$$

Thus

$$\int_{R^m} \rho_{\ell k}(z'-z)[\prod_{1}^{m}\ p(z_j'|z_j)\ dz'$$

$$= \int_{R^m} \rho_{\ell k}(r)\ \frac{e^{-\sum(r_j-\beta_j(\tau'-\tau))^2/2\gamma_j(\tau'-\tau)}}{[2\pi(\tau'-\tau)]^{m/2}\ [\Pi\ \gamma^{1/2}]}dr$$

$$= I(\tau'-\tau) \qquad (2.51),$$

letting $r_j = z_j' - z_j$.

Since $I(\tau'-\tau)$ is independent of z,

$$\int_{R^m} I(\tau'-\tau) \prod_{1}^{m} p(z_j)\ dz = I(\tau'-\tau) \qquad (2.52)$$

Hence

$$\sigma_{\ell k}^2(t) = 2\ \hat{\delta}_\ell \hat{\delta}_k(\kappa_{\ell k})t + \int_0^t\int_0^t I(\tau'-\tau)\ d\tau'd\tau \qquad (2.53).$$

To simplify the double integral, note first that it is symmetric with respect to τ' and τ. Thus

$$\int_0^t\int_0^t I(\tau'-\tau)\, d\tau' d\tau = 2\int_0^t\int_\tau^t I(\tau'-\tau)\, d\tau' d\tau \qquad (2.54).$$

Next change variables (let $y = \tau' - \tau$), integrate by parts, and change variables again (let $s = t-\tau$) to derive

$$\int_0^t\int_0^t I(\tau'-\tau)\, d\tau' d\tau = \int_0^t (t-s)\, I(s)\, ds \qquad (2.55).$$

By Parseval's relation

$$I(s) = \frac{\varepsilon^2}{2\pi^m}\int_{R^m} \hat{\rho}_{\ell k}(\xi)\, e^{-Q(\xi)s/2}\, e^{iB(\xi)s}\, d\xi \qquad (2.56)$$

where $B(\xi) = \sum_1^m \beta_j \xi_j$, $Q(\xi) = \sum_1^m \gamma_j \xi_j^2$, and $\hat{\rho}_{\ell k}$ is the Fourier transform of $\rho_{\ell k}$.

Let

$$I^*(t) = \int_0^t (t-s)\, I(s)\, ds$$

$$= \frac{\varepsilon^2}{2\pi^m}\int_{R^m} \hat{\rho}_{\ell k}(\xi)\Big[\int_0^t (t-s)\, e^{-Q(\xi)s/2}\, e^{iB(\xi)s}\, ds\Big]\, d\xi \qquad (2.57)$$

Say $A = Q(\xi) - iB(\xi)$, then

$$\int_0^t (t-s)\, e^{-As}\, ds = \frac{e^{-At} - 1 - At}{A^2} = G_t(\xi) \qquad (2.58).$$

It is clear from equation (2.53) that $\lim \sigma^2(t) = D$ exists only if

$$\lim_{t\to\infty} \frac{I^*(t)}{t} = \frac{\varepsilon^2}{(2\pi)^m} \lim_{t\to\infty} \frac{1}{2} \int_{R^m} \hat{\rho}_{\ell k}(\xi)\, G_t(\xi)\, d\xi \qquad (2.59)$$

exists.

In Chapter 4 I give a dominated convergence argument for taking the limit inside the integral in the general case which is analogous to (2.59). From the result obtained in Chapter 4 I have

$$\lim_{t\to\infty} \frac{I^*(t)}{t} = \frac{\varepsilon^2}{(2\pi)^m} \int_{R^m} \frac{\hat{\rho}_{\ell k}(\xi)}{Q(\xi) - iB(\xi)}\, d\xi \qquad (2.60)$$

When $B(\xi) \equiv 0$, that is for the case treated by Gelhar et al. (1979), the integrand is $\hat{\rho}_{\ell k}(\xi)/\sum \gamma\, \xi^2$ which is integrable only if

$$\hat{\rho}_{\ell k}(0) = \int_{R^m} \rho_{\ell k}(x)\, dx = 0 \qquad (2.61).$$

This is exactly Gelhar et al.'s (1979) condition in R^m.

If $B(\xi)$ is not identically zero, consider the cases $m = 1$ and $m = 2$ separately. When $m = 1$,

$$\int_{-\infty}^{\infty} \frac{\hat{\rho}_{\ell k}(\varepsilon)}{\gamma\xi^2 - i\beta\xi}\, d\xi = \int_{-\infty}^{\infty} \hat{\rho}_{\ell k}(\xi)\, \frac{\gamma}{\gamma^2\xi^2 + \beta^2}\, d\xi$$
$$+ i \int_{-\infty}^{\infty} \hat{\rho}_{\ell k}(\xi)\, \frac{\beta}{\xi(\gamma^2\xi^2 + \beta^2)}\, d\xi \qquad (2.62).$$

The first integral on the right obviously exists with very mild assumptions on $\hat{\rho}_{\ell k}$. In Chapter 4 I apply Cauchy's integral formula to the second integral and find that it is $2\pi\hat{\rho}_{\ell k}(0)/\beta$.

Thus

$$\lim_{t\to\infty} \frac{I_2(t)}{t} = \frac{\varepsilon^2}{2\pi}\left[\int_{-\infty}^{\infty} \hat{\rho}_{\ell k}(\xi) \frac{\gamma}{\gamma^2\xi^2+\beta^2}\, d\xi + \frac{2\pi}{\beta}\hat{\rho}_{\ell k}(0) \right] \qquad (2.63).$$

Applying this result to equation (2.53),

$$D_{\ell k} = 2\,\hat{\delta}_\ell \hat{\delta}_k(\kappa_{\ell k}) + \frac{\varepsilon^2}{2\pi}\left[\int_{-\infty}^{\infty} \hat{\rho}_{\ell k}(\xi) \frac{\gamma}{\gamma^2\xi^2+\beta^2}\, d\xi + \frac{2\pi}{\beta}\hat{\rho}_{\ell k}(0) \right] \qquad (2.64).$$

Note that when $\ell \neq k$, $D_{\ell k} = O(\varepsilon^2)$. Thus the matrix, D, is approximately diagonal.

The last case is m = 2 and B not identically zero. Hence either $\beta_1 \neq 0$ or $\beta_2 \neq 0$ or both. When this is so

$$\int_{R^2} \frac{\hat{\rho}_{\ell k}(\xi)}{Q(\xi) - iB(\xi)}\, d\xi \qquad (2.65)$$

exists with no further restrictions on $\rho_{\ell k}(\xi)$. This fact is shown in Chapter 4 in the analysis of the general case. Thus

$$D_{\ell\ell} = \tilde{\delta}_\ell + \frac{\varepsilon^2}{(2\pi)^2} \int_{R^m} \frac{\hat{\rho}_{\ell k}(\xi)}{Q(\xi) - iB(\xi)}\, d\xi \qquad (2.66).$$

Incompressible Three Dimensional Flow

Gelhar and Axness (1981) have investigated the transport of a non-reactive, conservative solute by a homogeneous liquid which saturates a three dimensional porous medium of constant porosity. The liquid is assumed to be incompressible. As they note, their result can be extended to d dimensional porous media where $d > 2$. It does not, however, extend to one dimensional media.

As in the 1979 paper of Gelhar et al., pollutant concentration and fluid velocity are assumed to be composed of deterministic and random parts. The latter are small.

Suppose that the coordinate system has been rotated so that the x_1 axis coincides with the mean fluid velocity vector. Then the concentration and velocity can be written

$$C(x,t) = \overline{c}(x,t) + \varepsilon C'(x,t), \quad E[C'] = 0 \tag{2.67a}$$

$$V(x) = (V_1(x), V_2(x), V_3(x)) \tag{2.67b}$$

$$V_1(x) = \mu + \varepsilon U_1(x) \tag{2.67c}$$

$$V_2(x) = \varepsilon U_2(x), \quad V_3(x) = \varepsilon U_3(x) \tag{2.67d}$$

$$E[U_j(x)] = 0 \quad \text{for } j = 1, 2, 3 \tag{2.67e}$$

The $U_j(x)$ are at least weakly stationary.

With the velocity vector as defined the intermediate scale dispersion matrix is approximately (Naff, 1978 as cited in Gelhar and Axness, 1981)

$$\delta^2/2 = \begin{matrix} \alpha_L\mu & 0 & 0 \\ 0 & \alpha_T\mu & 0 \\ 0 & 0 & \alpha_T\mu \end{matrix} \tag{2.68}$$

where α_L and α_T are constants.

With $\delta^2/2$ diagonal the intermediate scale convection-diffusion equation is

$$\frac{\partial C}{\partial t} = \mu\alpha_j \frac{\partial^2 C}{\partial x_j^2} - \mu \frac{\partial C}{\partial x_1} - \varepsilon U_j \frac{\partial C}{\partial x_j} \tag{2.69}$$

with summation over repeated subscripts.

The mean equation corresponding to (2.69) is

$$\frac{\partial \bar{c}}{\partial t} = \mu\alpha_j \frac{\partial^2 \bar{c}}{\partial x_j^2} - \mu \frac{\partial \bar{c}}{\partial x_1} - \varepsilon^2 E[U_j \frac{\partial C'}{\partial x_j}] \tag{2.70}$$

By subtracting (2.70) from (2.69) the mean removed equation is

$$\varepsilon\frac{\partial C'}{\partial t} = \varepsilon\mu\alpha_j \frac{\partial^2 C'}{\partial x_j^2} - \varepsilon\mu \frac{\partial C'}{\partial x_1} - \varepsilon U_j \frac{\partial \bar{c}}{\partial x_j} - \varepsilon^2[U_j \frac{\partial C'}{\partial x_j} - EU_j \frac{\partial C'}{\partial x_j}] \tag{2.71}$$

If the perturbations are small enough, terms of $O(\varepsilon^2)$ can be neglected in (2.71) which then reduces to

$$\frac{\partial C'}{\partial t} = \mu\alpha_j \frac{\partial^2 C'}{\partial x_j^2} - \mu \frac{\partial C'}{\partial x_1} - U_j \frac{\partial \bar{c}}{\partial x_j} \tag{2.72}$$

The object is to decouple equations (2.70) and (2.72). If $\partial c/\partial x$ is independent of c and if there is some $(D_2)_{\ell j}$ such that

$$E_U[U_j C'] = -(D_2)_{j\ell} \frac{\partial \bar{c}}{\partial x_\ell} \tag{2.73},$$

the equations can be decoupled. Gelhar and Axness (1981) assume that (2.73) holds for large times, an assumption which is equivalent to my assumption that C(x,t) converges to a Fickian regime. Thus (2.70) can be assumed to include $\bar{c}$ alone.

To remove the dependence of (2.72) on $\bar{c}$ recall from the introduction that the problem of estimating D is essentially independent of the initial conditions. Thus the initial conditions can be chosen to suit one's purposes. Suppose that initially $C'(x,0) = 0$ and

$$\bar{c}(x,0) = c_0(x) = \beta \cdot x \tag{2.74}$$

where β is a constant vector. Then using assumption (2.73), equation (2.70) has the solution

$$\bar{c}(x,t) = \beta \cdot (x - \tilde{\mu} t) \tag{2.75}$$

where $\mu = (\mu, 0, 0)$. With this choice of $c_0(x)$ equation (2.72) becomes

$$\frac{\partial C'}{\partial t} = \mu\alpha_j \frac{\partial^2 C'}{\partial x_j^2} - \mu \frac{\partial C'}{\partial x_1} - U_j \beta_j \tag{2.76}$$

Now $(D_2)_{\ell j}$ can be calculated if only $E_U[U_j C']$ can be found. In Fourier transform space equation (2.76) is

$$\frac{\partial \hat{C}'}{\partial t} = -\mu\alpha_\ell \xi_\ell^2 \hat{C}' + i\mu \xi_1 \hat{C}' + \beta_\ell \hat{U}_\ell \tag{2.77}.$$

The solution to (2.77) with $C'(x,0) = 0$ is

$$\hat{C}' = \beta_\ell \hat{U}_\ell \frac{(1 - e^{-\gamma(\xi)t})}{\gamma(\xi)} \to \frac{\beta_\ell \hat{U}_\ell}{\gamma(\xi)} \quad \text{as } t \to \infty \tag{2.78}$$

where $\gamma(\xi) = \mu\alpha_\ell \xi_\ell^2 - i\mu \xi_1$.

By multiplying (2.78) by U and taking the expected value, the cross-spectrum of C' and U_j can be found:

$$\hat{\rho}_{C'U_j}(\xi) = \frac{\beta_\ell}{\gamma(\xi)} \hat{\rho}_{\ell j}(\xi) \tag{2.79}$$

where $\rho_{C'U}$ is the cross-covariance between C' and U_j and $\rho_{\ell j}$ is the covariance of U_j with U_ℓ. Then

$$E_U[C'U_j] = \frac{\beta_\ell}{(2\pi)^3} \int_{R^3} \frac{\hat{\rho}_{\ell j}(\xi)}{\mu\alpha_\ell \xi_\ell^2 - i\mu\xi_1} d\xi \tag{2.80}$$

and, noting that $\beta_\ell = \partial \bar{c}/\partial x_\ell$,

$$(D_2)_{\ell j} = \frac{1}{(2\pi)^3} \int_{R^3} \frac{\hat{\rho}_{\ell j}(\xi)}{\mu\alpha_\ell \xi_\ell^2 - i\mu\xi_1} d\xi \tag{2.81}$$

In Chapter 5 I will return to this result, as well as to those obtained by Kesten and Papanicolaou (1979), Gelhar et al. (1979) and Matheron and de Marsily (1980). There I will show that my approximations of the megascopic drift and dispersion coefficients agree with those obtained in these special cases. The cases investigated by Kesten and Papanicolaou (1979) and Gelhar and Axness (1981) are of course significant in their own right. In fact Kesten and Papanicolaou (1979) give a rigorous second order analysis of the turbulent diffusion problem, while Gelhar and Axness (1981) acheive a formal analysis of the hydrologically important case of transport by an incompressible fluid through a three dimensional medium.

The sequel extends the asymptotic analysis of transport in random flow fields to media of one or more dimensions and to fluids which may be incompressible. The expressions obtained in Chapter 3 can in principle be extended to terms of any order in ε. However, I develop explicit expressions only through second order. In Chapter 4 I give a rigorous limit for the second order terms.

CHAPTER 3

INTEGRAL EXPRESSIONS FOR MEGASCOPIC TRANSPORT COEFFICIENTS

To find expressions for the megascopic coefficients $D(\varepsilon;\delta)$ and $\alpha(\varepsilon;\delta)$ I return to the point of view introduced in Chapter 1. I suppose that a solute is flowing through a d dimensional medium. I further assume that the fluid's macroscopic velocity is a weakly stationary random field with a preffered direction of drift, μ. Since the covariances among elements of the velocity field need only depend on the differences between points, the field may be anisotropic.

In Chapter 1 I noted that the problem of approximating D and α can be formally reduced to expanding the equation

$$\lim_{n\to\infty} E_U e^{t(A+\varepsilon B_U)} e^{-t\sqrt{n}\alpha\cdot\nabla} = e^{t/2(\nabla\cdot D\nabla)} \tag{3.1}$$

in powers of ε and then equating the coefficients of each power. To do so I suppose that D and α can be expanded in ε and that the limit is correct term-by-term. The expressions A and B_U are as defined in chapter 1.

With the assumptions on D and α I can write

$$e^{-t\sqrt{n}\alpha(\varepsilon;\delta)\cdot\nabla} = e^{-t\sqrt{n}\alpha_0\cdot\nabla} - (t\sqrt{n}\alpha_1\cdot\nabla)e^{-t\sqrt{n}\alpha_0\cdot\nabla} \tag{3.2}$$
$$+ \varepsilon^2[(t\sqrt{n}\alpha_1\cdot\nabla)^2 - (t\sqrt{n}\alpha_2\cdot\nabla)]e^{-t\sqrt{n}\alpha_0\cdot\nabla} + \dots$$

and

$$e^{t/2(\nabla\cdot D(\varepsilon;\delta)\nabla)} = e^{t/2(\nabla\cdot D_0\nabla)} + \varepsilon \frac{t}{2}(\nabla\cdot D_1\nabla)e^{t/2(\nabla\cdot D_0\nabla)}$$

$$+ \varepsilon^2 \frac{t}{2}[(\nabla\cdot D_1\nabla) + (\nabla\cdot D_2\nabla)]e^{t/2(\nabla\cdot D_0\nabla)} + \ldots \qquad (3.3)$$

I also assume that the expansion

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

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

$$+ \ldots \qquad (3.4)$$

is correct.

Terms in ε^0

Comparing terms in ε^0 I find

$$E_U[e^{tA} e^{-t\sqrt{n}\alpha_0\cdot\nabla}] = e^{t\sqrt{n}(\mu-\alpha_0)\cdot\nabla + t/2(\nabla\cdot\delta^2\alpha)} \qquad (3.5)$$

$$\to e^{t/2(\nabla\cdot D_0\nabla)} \quad \text{as } n\to\infty$$

where I use the fact that A and $\alpha\cdot\nabla$ commute. The left side of (3.5) converges to the right only if $\alpha_0 = \mu$ and $D_0 = \delta^2$.

Terms in ε^1

The coefficients of ε^1 are nearly as easy to compare, since

$$E_U[(\int_0^t e^{(t-t_1)A} B_U e^{t_1A} dt_1)e^{-t\sqrt{n}\alpha_0\cdot\nabla} - e^{tA}(t\sqrt{n}\alpha_1\cdot\nabla)e^{-t\sqrt{n}\alpha_0\cdot\nabla}] =$$

$$= e^{-tA}(t\sqrt{n}\alpha_1 \cdot \nabla)e^{-t\sqrt{n}\alpha_0 \cdot \nabla}$$

$$= (t\sqrt{n}\alpha_1 \cdot \nabla)e^{t/2(\nabla \cdot \delta^2 \nabla)}$$

$$+ \frac{t}{2}(\nabla \cdot D_1 \nabla)e^{t/2(\nabla \cdot \delta^2 \nabla)} \qquad \text{as } n \to \infty \qquad (3.6)$$

only if $\alpha_1 = 0$ and $D_1 = 0$. The last follows because α and D are constants with respect to n. Thus the different n-dependencies on each side of the limit require the result.

Terms in ε^2

With these results the second order terms become

$$E_U[(\int_0^t \int_0^{t_1} e^{(t-t_1)A} B_U e^{(t_1-t_2)A} B_U e^{t_2A} dt_1dt_2)e^{-t\sqrt{n}\mu \cdot \nabla}$$
$$- e^{tA}(t\sqrt{n}\alpha_2 \cdot \nabla)e^{-t\sqrt{n}\mu \cdot \nabla}]$$

$$= (\int_0^t \int_0^{t_1} e^{(t-t_1)A} E_U[B_U e^{(t_1-t_2)A} B_U] e^{(t_2-t)A} dt_1dt_2)e^{tA} e^{-t\sqrt{n}\mu \cdot \nabla}$$
$$- (t\sqrt{n}\alpha_2 \cdot \nabla)e^{tA} e^{-t\sqrt{n}\mu \cdot \nabla}$$

$$= (\int_0^t \int_0^{t_1} e^{(t-t_1)A} E_U[B_U e^{(t_1-t_2)A} B_U] e^{(t_2-t)A} dt_1dt_2)e^{t/2(\nabla \cdot \delta^2 \nabla)}$$
$$- (t\sqrt{n}\alpha_2 \cdot \nabla)e^{t/2(\nabla \cdot \delta^2 \nabla)}$$

$$+ \frac{t}{2}(\nabla \cdot D_2 \nabla)e^{t/2(\nabla \cdot \delta^2 \nabla)} \qquad \text{as } n \to \infty \qquad (3.7).$$

Here I have again used the commutativity of A and $\mu \cdot \nabla$.

The left side of (3.7) converges to the right only if

$$\int_0^t \int_0^{t_1} e^{(t-t_1)A} E_U[B_U\, e^{(t_1-t_2)A} B_U]\, e^{(t_2-t)A}\, dt_1 dt_2 - (t\sqrt{n}\alpha_2 \cdot \nabla)$$

$$\rightarrow \frac{t}{2}(\nabla \cdot D_2 \nabla) \qquad \text{as } n \rightarrow \infty \qquad (3.8).$$

To simplify the integral in (3.8), let $K_s(y-x)$ denote the kernel of e^{sA}. For arbitrary g,

$$e^{sA} g = (2\pi)^{-d/2} \int_{R^d} \frac{e^{-(x-y-\sqrt{n}\mu s)\delta^{-1}(x-y-\sqrt{n}\mu s)/s}}{(|\delta|s)^{1/2}}\, g(x)\, dx$$

$$= \int_{R^d} K_s(y-x)\, g(x)\, dx \qquad (3.9).$$

Then

$$E_U[B_U e^{sA} B_U g] = E_U[\sqrt{n}U(\sqrt{n}y) \cdot \nabla \int_{R^d} K_s(y-x)(\sqrt{n}U(\sqrt{n}x) \cdot \nabla g(x))\, dx]$$

$$= n \sum_{\ell=1}^{d} \sum_{j=1}^{d} \int_{R^d} E\,[U_\ell(\sqrt{n}y) U_j(\sqrt{n}x)]\, \left(\frac{\partial}{\partial y_\ell} K_s(y-x) \frac{\partial}{\partial x_j} g(x)\right) dx$$

$$= n \sum_1^d \sum_1^d \int_{R^d} \rho_{\ell j}(\sqrt{n}(y-x))\, \frac{\partial}{\partial y_\ell} K_s(y-x) \frac{\partial}{\partial x_j} g(x)\, dx \qquad (3.10).$$

The integral in (3.10) is just the convolution of

$$K^s_{\ell j}(z) = \rho_{\ell j}(\sqrt{n}z) \frac{\partial}{\partial z_\ell} K_s(z) \qquad (3.11)$$

with $\partial g(z)/\partial z_j$.

Under Fourier Transformation

$$K^s_{\ell j} * \frac{\partial}{\partial z_j} \overset{FT}{\rightarrow} (-i\xi'_j)\hat{K}^s_{\ell j} \qquad (3.12)$$

where the symbol $\overset{FT}{\rightarrow}$ indicates Fourier transformation. In this dissertation I denote the Fourier transform of a function, say g, by $\hat{g}$ and use the definition

$$\hat{g}(\xi) = \int_{R^d} g(x)e^{i\xi\cdot x}\, dx \qquad (3.13).$$

Of course many other definitions of the Fourier transform are possible.

Now

$$\hat{K}^s_{\ell j} = \rho_{\ell j}(\sqrt{n}z)\frac{\partial}{\partial z_\ell}K_s(z) = (2\pi)^{-d/2}\, \rho_{\ell j}(\sqrt{n}z)*\frac{\partial}{\partial z_\ell}K_s(z)$$

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

$$= (-i)(2\pi)-d/2\int_{R^d} (\xi'_\ell-\sqrt{n}\xi_\ell)\hat{K}_s(\xi'-\sqrt{n}\xi)\hat{\rho}_{\ell j}(\xi)\, d\xi \qquad (3.14).$$

But K_s is Gaussian with Fourier transform

$$K_s(\zeta) = (2\pi)^{-d/2}e^{s\hat{A}(\zeta)} \qquad (3.15)$$

where $A(\zeta) = -1/2(\zeta\cdot\delta^2\zeta) - i\sqrt{n}\mu\cdot\zeta$. Hence

$$\hat{A}(\xi' - \sqrt{n}\xi) = (\frac{-1}{2}\xi'\cdot\delta^2\xi'-i\sqrt{n}\mu\cdot\xi')$$

$$- n(\frac{1}{2}\xi\cdot\delta^2\xi-\frac{1}{n}\,\xi'\cdot\delta^2\xi-i\mu\cdot\xi) \qquad (3.16)$$

and

$$\hat{K}^s_{\ell j} = \frac{(-i)}{(2\pi)^d}\, e^{s\hat{A}(\xi')}\int_{R^d} (\xi' - \sqrt{n}\xi\ )e^{-snF_n(\varepsilon;\varepsilon')}\,\hat{\rho}_{\ell j}(\xi)\, d\xi \qquad (3.17)$$

where

$$F_n(\xi;\xi') = \frac{1}{2}\xi\cdot\delta^2\xi - \frac{1}{\sqrt{n}}\xi'\cdot\delta^2\xi - i\mu\cdot\xi \quad (3.18)$$

Thus in Fourier transform space

$$E_U[B_U e^{sA} B_U] \overset{FT}{\to} n(2\pi)^{-d}\sum_{\ell,j}(i\xi_j')e^{s\hat{A}(\xi')}\cdot$$
$$\int_{R^d} i(\xi_\ell' - \sqrt{n}\xi_\ell)e^{-snF_n(\xi;\xi')}\hat{\rho}_{\ell j}(\xi)\,d\xi \quad (3.19),$$

and the requirement (3.8) becomes

$$n(2\pi)^{-d}\sum_{\ell,j}\int_{R^d}\{[-i(\xi_\ell' - \sqrt{n}\xi_\ell)\hat{\rho}_{\ell j}(\xi)][-i\xi_j'\int_0^t\int_0^{t_1} e^{-(t_1-t_2)nFn(\xi;\xi')}dt_2dt_1]\}d\xi$$
$$-t\sqrt{n}\alpha_2\circ(-i\xi') \to \frac{t}{2}\sum_{\ell,j}(D_2)_{\ell j}(-i\xi_\ell')(-i\xi_j') \quad \text{as } n\to\infty \quad (3.20).$$

The expression on the left can be simplified by letting

$$G_n(\xi;\xi') = \frac{n}{t}\int_0^t\int_0^{t_1} e^{-(t_1-t_2)nFn(\xi;\xi')}dt_2dt_1$$
$$= nt\,\frac{e^{-ntF_n} - 1 + ntF_n}{n^2t^2F_n^2} \quad (3.20).$$

Then dividing by t the requirement is

$$(2\pi)^{-d}\sum_{\ell,j}(-i\xi_j')(-i\xi_\ell')\int_{R^d}\hat{\rho}_{\ell j}(\xi)G_n(\xi;\xi')\,d\xi$$
$$+ (2\pi)^{-d}\sum_{\ell,j}(-i\xi_j')\int_{R^d}\sqrt{n}\,(i\xi_\ell)\hat{\rho}_{\ell j}(\xi)G_n(\xi;\xi')\,d\xi - \sqrt{n}\alpha_2\cdot(-i\xi')$$

$$= (2\pi)^{-d} \sum_{\ell,j} (i\xi'_j)(i\xi'_\ell) \int_{R^d} \hat{\rho}_{\ell j}(\xi) G_n(\xi;\xi')\, d\xi$$

$$+ \sqrt{n} \sum_\ell (-i\xi_j)\{[(2\pi)^{-d} \sum_j \int_{R^d} (i\xi_\ell)\, \hat{\rho}_{\ell j}(\xi) G_n(\xi;\xi')\, d\xi] - (\alpha_2)_j\}$$

$$\to (1/2) \sum_{\ell,j} (D_2)_{\ell j} (i\xi'_\ell)(i\xi'_j) \quad \text{as } n \to \infty \qquad (3.21).$$

Hence, it would suffice to have

(i) $$(2\pi)^{-d} \int_{R^d} \hat{\rho}_{\ell j}(\xi) G_n(\xi;\xi')\, d\xi \to D^{(i)}_{\ell j} \quad \text{as } n \to \infty \qquad (3.22),$$

(ii) $$(2\pi)^{-d} \int_{R^d} [\sum_\ell (i\xi_\ell) \hat{\rho}_{\ell j}(\xi)]\, G_n(\xi;\xi')\, d\xi \to (\alpha_2)_j \qquad (3.23),$$

as $n \to \infty$

(iii) $$\sqrt{n}\{(2\pi)^{-d} \int_{R^d} [\sum_\ell (i\xi_\ell) \hat{\rho}_{\ell j}(\xi)]\, G_n(\xi;\xi')\, d\xi - (\alpha_2)_j\}$$

$$\to \sum_\ell D^{(ii)}_{\ell j} (-i\xi_\ell) \quad \text{as } n \to \infty \qquad (3.24),$$

where the ℓj^{th} component of D_2 is

$$(D_2)_{\ell j} = D^{(i)}_{\ell j} + D^{(i)}_{j\ell} + D^{(ii)}_{\ell j} + D^{(ii)}_{j\ell} \qquad (3.25)$$

and $(\alpha_2)_j$ is the j^{th} component in the α_2 vector.

It is convenient, however, to put conditions (ii) and (iii) somewhat differently. To determine D_2 and α_2 it would also suffice if

(ii)' $$(2\pi)^{-d} \int_{R^d} (i\xi_\ell) \hat{\rho}_{\ell j}(\xi)\, G_n(\xi;\xi')\, d\xi \to \alpha_{\ell j} \qquad (3.26)$$

as $n \to \infty$, and

(iii)' $$\sqrt{n}\{(2\pi)^{-d}\int_{R^d}(i\xi_m)\hat{\rho}_{mj}(\xi)\,G_n(\xi;\xi')d\xi - \alpha_{mj}\} \to \sum_{\ell=1}^{d} D^{(ii)}_{\ell jm}(i\xi'_\ell) \quad \text{as } n \to \infty \qquad (3.27).$$

With (ii)' and (iii)'

$$(\alpha_2)_j = \sum_\ell \alpha_{\ell j} \qquad (3.28),$$

and

$$D^{(ii)}_{\ell j} = \sum_m D^{(ii)}_{mj\ell} \qquad (3.29).$$

Hence if there are generalized functions, $\tilde{D}(\xi)$, $\tilde{A}_m(\xi)$, $\tilde{\tilde{D}}_{jm}(\xi)$, which in the sense of generalized functions on R^d satisfy

(i)" $$G_n(\xi;\xi') \to \tilde{D}(\xi) \quad \text{as } n \to \infty \qquad (3.30),$$

(ii)" $$(i\xi_m)G_n(\xi;\xi') \to \tilde{A}_m(\xi) \quad \text{as } n \to \infty \qquad (3.31),$$

(iii)" $$\sqrt{n}[(i\xi_m)G_n(\xi;\xi') - \tilde{A}_m(\xi) \to \sum_j \tilde{\tilde{D}}_{jm}(\xi)(i\xi'_j) \quad \text{as } n \to \infty \qquad (3.32).$$

Then

$$D^{(i)}_{\ell j} = (2\pi)^{-d}\int_{R^d} \tilde{D}(\xi)\,\hat{\rho}_{\ell j}(\xi)\,d\xi \qquad (3.33),$$

$$\alpha_{\ell j} = (2\pi)^{-d}\int_{R^d} \tilde{A}_m(\xi)\,\hat{\rho}_{\ell j}(\xi)\,d\xi \qquad (3.34),$$

$$D_{jm}^{(ii)} = (2\pi)^{-d}\int_{R^d} \tilde{\tilde{D}}_{jm}(\xi)\,\hat{\rho}_{\ell j}(\xi)\,d\xi \qquad (3.35).$$

<u>Naive Limits</u>

If I take just the point-wise limits of (i)", (ii)", and (iii)", I find, since $F_n(\xi;\xi') = 1/2(\xi\cdot\delta^2\xi) - n^{-1/2}(\xi'\cdot\delta^2\xi) - i\mu\cdot\xi$, that for (i)"

$$\lim_{n\to\infty} G_n(\xi;\xi') = \lim_{n\to\infty} nt\,\frac{e^{-ntF_n} - 1 + ntF_n}{n^2t^2F_n^2}$$

$$= \lim_{n\to\infty} \frac{1}{F_n}$$

$$= (1/2(\xi\cdot\delta^2\xi) - i\mu\cdot\xi)^{-1}$$

$$= F^{-1}(\xi) \qquad (3.36)$$

Here I let $F(\xi) = (1/2(\xi\cdot\delta^2\xi) - i\mu\cdot\xi)^{-1}$.

From (3.35) it is clear that for (ii)"

$$\lim_{n\to\infty} (i\xi_m)\,Gn(\xi;\xi') = (i\xi_m)(1/2(\xi\cdot\delta^2\xi) - i\mu\cdot\xi)^{-1} \qquad (3.37).$$

Finally for (iii)"

$$\lim_{n\to\infty} \sqrt{n}[(i\xi_m)\,Gn(\xi;\xi') - \tilde{A}_m(\xi)] = (i\xi_m)\lim_{n\to\infty} \sqrt{n}[G_n(\xi;\xi') - F^{-1}] \qquad (3.38)$$

But

$$\sqrt{n}[G_n - F^{-1}] = \sqrt{n}[\,(G_n - F_n^{-1}) + (F_n - F^{-1})\,] \qquad (3.39)$$

and

$$\sqrt{n}(G_n - F_n^{-1}) = \sqrt{n}\ \frac{e^{-ntF_n} - 1}{ntF_n^2}$$

$$= n^{-1/2}\ 0(1/F_n) \to 0 \quad \text{as } n \to \infty \tag{3.40}$$

Also

$$\sqrt{n}\ (F_n^{-1} - F^{-1}) = \sqrt{n}\ [\frac{1}{F - (\xi'\cdot\delta^2\xi)/\sqrt{n}} - \frac{1}{F}]$$

$$= \frac{\sqrt{n}}{F}\ [\frac{(\xi'\cdot\delta^2\xi)/\sqrt{(nF)}}{1 - (\xi'\cdot\delta^2\xi)/\sqrt{(nF)}}]$$

$$\to \frac{\xi'\cdot\delta^2\xi}{F^2} \quad \text{as } n \to \infty \tag{3.41}$$

Hence

$$\lim_{n\to\infty} \sqrt{n}[(i\xi_m)\ Gn(\xi;\xi') - \tilde{A}_m(\xi)] = (i\xi_m)\ \frac{\xi'\cdot\delta^2\xi}{F^2} \tag{3.42}$$

In the next chapter it will be clear that expressions (3.36), (3.37), and (3.42) are correct limits when $d > 2$. For that matter (3.37) and (3.42) are correct when $d=1$.

CHAPTER 4

LIMITS FOR MEGASCOPIC TRANSPORT COEFFICIENTS

In this chapter I apply a dominated convergence argument to take the limits of (i)", (ii)", and (iii)". Hence the treatment given here is rigorous in the sense that if (i)", (ii)", and (iii)" are correct, then so are the limits taken here. Although it may appear unnecessary to take rigorous limits in an analysis which is basically formal, it will become clear that the naive limit of (i)" is incorrect when $d = 1$. In this case the dominated convergence argument leads to an important correction. For that, and other, reasons I treat the one dimensional problem separately.

Because convergence in the sense of generalized functions is required, in this chapter I suppose that $\hat{\rho}_{\ell j}$ is well enough behaved to serve as a test function. To emphasize this point I replace $\hat{\rho}_{\ell j}$ by ϕ. In particular I suppose that ϕ is bounded and approaches zero at infinity. Later, when I return to the stratified medium investigated by Gelhar et al. (1979), I shall emphasize that in their case the unboundedness of ϕ, i.e. $\hat{\rho}$, is the source of the requirement that the covariance of the velocity field be negative over some interval(s).

Limits For $d > 2$

To establish convergence I divide the domain R^d into two regions: one a ball centered around the origin and the other the remainder of R^d. The ball is parameterized by n and shrinks as n increases. By showing that the integrands corresponding to (i)", (ii)" and (iii)" are bounded near the origin, I find that the limit in the sense of generalized functions is the limit in the remainder of R^d. To find the limit I use dominated convergence and note that the remainder of R^d becomes $R^d-\{0\}$ as n increases.

Note that in the definitions (3.18) and (3.20) of respectively $F_n(\xi;\xi')$ and $G_n(\xi;\xi')$ ξ' is a parameter which is effectively fixed. Thus I can define the region

$$A_n = \{ \xi \in R^d \mid \|\delta\xi\| < 4(n^{-1/2})\|\delta\xi'\| \} \quad (4.1),$$

which is a ball centered around the origin.

Limit of (i)"

Let

$$\tilde{G}_n(\xi;\xi') = \begin{cases} G_n(\xi;\xi') & \text{if } \xi \text{ is not in } A_n \\ 0 & \text{if } \xi \text{ is in } A_n \end{cases} \quad (4.2).$$

Then to take the limit of (i)" I have

$$\int_{R^d} G_n(\xi;\xi')\phi(\xi)d\xi = \int_{R^d} \tilde{G}_n(\xi;\xi')\phi(\xi)d\xi + \int_{A_n} G_n(\xi;\xi')\phi(\xi)d\xi \quad (4.3).$$

Consider the first integral on the right and note that for ξ not an element of A_n,

$$|\tilde{G}_n(\xi;\xi')\phi(\xi)| = \left| nt \frac{e^{-ntF_n} - 1 + ntF_n}{n^2 t^2 F_n^2} \right| |\phi|$$

$$< K \frac{|\phi|}{|F_n|} \qquad (4.3)$$

for some constant, K, so long as $Re(F_n) > 0$.

I prove that the last part of (4.3) follows as an aside. Note first that in $R^d - A_n$ I have $Re(F_n) = 1/2(\xi\cdot\delta^2\xi) - n^{-1/2}(\xi'\cdot\delta^2\xi) > 0$: since δ is positive definite,

$$\begin{aligned} n^{-1/2}(\xi'\cdot\delta^2\xi) &= n^{-1/2}(\delta\xi')(\delta\xi) \\ &< n^{-1/2}\|\delta\xi'\| \; \|\delta\xi\| \\ &< 1/4 \; \|\delta\xi\| \\ &< 1/4(\xi\cdot\delta^2\xi) \qquad (4.4). \end{aligned}$$

Hence in $R^d - A_n$

$$Re(F_n) > 1/4(\xi\cdot\delta^2\xi) = 1/2 \; Re(F) > 0 \qquad (4.5).$$

Now to establish (4.3) I need only show that so long as $Re(z)=x>0$,

$$\frac{|e^{-z} - 1 + z|}{|z|^2} = 0(|z|^{-1}) \qquad (4.6).$$

But
$$\frac{|e^{-z} - 1 + z|}{|z|^2} < \frac{1}{|z|} + \frac{|e^{-z} - 1|}{|z|^2} \qquad (4.7).$$

Thus it will suffice to show that

$$|e^{-z} - 1| \leq K|z| \qquad (4.8).$$

This is clearly true when $|z| \geq 2/K$, for then

$$|e^{-z} - 1| \leq e^{-x} + 1 \leq 2 \leq K|z| \qquad (4.9).$$

Even when $|z| < 2/K$,

$$\frac{|e^{-z} - 1|}{|z|^2} \leq \frac{1}{|z|}\left(1 + \frac{|z|}{2} + \frac{|z|^2}{3!} + \ldots\right)$$

$$\leq \frac{1}{|z|}\left(1 + \frac{(2/K)}{2} + \frac{(2/K)^2}{3!} + \ldots\right) \qquad (4.10).$$

Since the sum in (4.10) is absolutely convergent by the ratio test, there is some

$$K' = \sum_{n=0}^{\infty} \frac{(2/K)^n}{(n+1)!} \qquad (4.11)$$

such that for $|z| < 2/K$

$$\frac{|e^{-z} - 1|}{|z|^2} \leq \frac{K'}{|z|} \qquad (4.12).$$

From (4.9) and (4.12)

$$\frac{|e^{-z} - 1|}{|z|^2} = O(|z|^{-1}) \qquad (4.13).$$

To return to the main argument, since $Im(F_n) = Im(F)$, from (4.5) it now follows that $|F_n| > |F|$ and

$$|\tilde{G}_n\phi| < 2K \frac{|\phi|}{|F|} \qquad (4.14).$$

But for $d > 2$ this last expression is integrable if $\mu \neq 0$. To see this, diagonalize the matrix $1/2(\delta^2)$ so that

$$\int_{R^d} \frac{1}{|F(\xi)|} d\xi = \int_{R^d} \frac{1}{|\eta\cdot\Lambda^2\eta - iM\cdot\eta|} d\eta \qquad (4.15).$$

Here $M=P^t\mu$, P is the matrix whose columns are the eigenvectors of $1/2(\delta^2)$ and Λ^2 is the diagonal matrix of eigenvalues of $1/2(\delta^2)$. Since $1/2(\delta^2)$ is positive definite, its eigenvalues are positive.

When $d > 3$, the integral on the right of (4.15) exists even if $\mu=0$. This is clear after a change to spherical coordinates. If $d=2$, rotating the coordinate system so that one axis coincides with the vector M yields an integral of the form

$$\int_{R^2} [(x^2+y^2)^2+x^2)]^{-1/2} \, dxdy$$

$$= \int_0^{2\pi}\int_0^{\infty} [r^2+\sin^2\theta]^{-1/2} \, drd\theta$$

$$= \int_0^{2\pi} [\ln(1+\sqrt{1+\sin^2\theta}) - \ln(\sin\theta)] \, d\theta \qquad (4.16a)$$

But

$$\int_0^{2\pi} \ln(1+\sqrt{1+\sin^2\theta}) \, d\theta < \infty \qquad (4.16b)$$

and

$$\int_0^{2\pi} \ln(\sin\theta)\, d\theta = \int_0^{2\pi} \ln(\theta)\, d\theta + \int_0^{2\pi} \ln(\sin\theta/\theta)\, d\theta \tag{4.16c}$$

Now

$$\int_0^{2\pi} \ln(\theta)\, d\theta = \left[\theta \ln\theta - \theta\right]_0^{2\pi} < \infty \tag{4.16d}$$

since $\theta \ln\theta |_{\theta=0} = 0$.

Because $\sin\theta/\theta \to 1$ as $\theta \to 0$,

$$\int_0^{2\pi} \ln(\sin\theta/\theta)\, d\theta < \infty \tag{4.16e}$$

Thus for $d > 2$, $|F(\xi)|^{-1}$ is integrable. Since $|\phi|$ is also integrable, the expression on the right of (4.14) is integrable as well. Note that in Chapter 2 I appealed to this result when I extended the results of Matheron and de Marsily (1980) to three dimensions.

Since $G_n\phi$ is dominated by an integrable function, I can take the limit

$$\int_{R^d} \tilde{G}_n\phi \, d\xi \to \int_{R^d - \{0\}} \frac{\phi}{F}\, d\xi \quad \text{as } n \to \infty$$

$$= \int_{R^d} \frac{\phi}{F}\, d\xi \tag{4.17}$$

The last line follows because the integral of an integrable function is unaffected by the value of the integrand at a single point.

To show that the rightmost integral of (4.3) converges to zero, I begin by writing

$$G_n = nt\,\frac{e^{-z} - 1 + z}{z^2} \qquad (4.18)$$

where $z = ntF_n$. I will show that $|G_n| = O(n)$ when $\xi \in A_n$.

Since $\xi \in A_n$,

$$1/2(\xi'\cdot\delta^2\xi) < \frac{8}{n}\|\delta\xi'\|^2 \qquad (4.19)$$

and

$$n^{-1/2}(\xi'\cdot\delta^2\xi) < \frac{4}{n}\|\delta\xi'\|^2 \qquad (4.20)$$

so $Re(F_n) = O(n^{-1})$. Thus $Re(z) = O(1)$, i.e. there is a constant, K, such that $|Re(z)| < K$.

But

$$\sup_{|Re(z)|<K} \frac{|e^{-z} - 1 + z|}{|z|^2} = \sup_{I_1 \cup I_2} \frac{|e^{-z} - 1 + z|}{|z|^2} \qquad (4.21)$$

where

$$I_1 = \{z|\ |Re(z)|<K \text{ and } |Im(z)|<K\} \qquad (4.22)$$

and

$$I_2 = \{z|\ |Re(z)|<K \text{ and } |Im(z)|>K\} \qquad (4.23).$$

Now

$$\sup_{I_1} \frac{|e^{-z} - 1 + z|}{|z|^2} = \sup_{I_1} \left|\frac{1}{2} + O(z)\right| \qquad (4.24),$$

but the expression on the right is finite, because $|z|$ is bounded in I_1.

On the other hand

$$\sup_{I_2} \frac{|e^{-z} -1 +z|}{|z|^2} < \sup_{I_2} \frac{|e^{-z}|}{|z|^2} + \sup_{I_2} \frac{1}{|z|^2} + \sup_{I_2} \frac{1}{|z|}$$

$$= \frac{e^K}{K^2} + \frac{1}{K^2} + \frac{1}{K} \qquad (4.25)$$

which, since $K \neq 0$, is also finite.

Hence there is K', a constant, such that in A_n

$$\frac{|e^{-z} -1 +z|}{|z|^2} < K' \qquad (4.26).$$

This implies that $|G_n| = O(n)$ in A_n.

It follows that

$$\int_{A_n} G_n\phi \; d\xi = O(n)\int_{A_n} d\xi \qquad (4.27).$$

Since δ^2 is positive definite, $\|\delta\xi\| < 4n^{-1/2} \|\delta\xi'\|$ which implies that $\|\xi\| = O(n^{-1/2})$. Thus

$$\int_{A_n} d\xi < \int_{\{\xi \mid \|\xi\|=O(n^{-1/2})\}} d\xi = O(n^{-d/2}) \qquad (4.28).$$

Then

$$\int_{A_n} G_n\phi \; d\xi = O(n^{-(d-2)/2}) \qquad (4.29).$$

If $d > 3$, then the integral clearly approaches zero as $n \to \infty$. To determine the case $d = 2$, define

$$B = \{\xi \mid |\mu\cdot\xi| < \frac{1}{\sqrt{3}} \xi\cdot\delta^2\xi\} \qquad (4.30).$$

I analyse the cases $\xi \in A_nB$ and $\xi \in A_n\overline{B}$ separately.

First suppose $\xi \in A_n\overline{B}$. Then

$$|\mathrm{Im}(F_n)| = |\mathrm{Im}(F)| = \frac{1}{\sqrt{3}}|\mu\cdot\xi| > \frac{1}{\sqrt{3}}\,\xi\cdot\delta^2\varepsilon = \frac{1}{\sqrt{3}}\,|\mathrm{Re}(F)| \qquad (4.31).$$

Hence

$$\begin{aligned} |F_n|^2 &= |\mathrm{Re}(F_n)|^2 + |\mathrm{Im}(F_n)|^2 \\ &> |\mathrm{Im}(F_n)|^2 \\ &= \frac{1}{4}|\mathrm{Im}(F)|^2 + \frac{3}{4}\,|\mathrm{Im}(F)|^2 \\ &> \frac{1}{4}(|\mathrm{Im}(F)|^2 + |\mathrm{Re}(F)|^2) \\ &= \frac{|F|^2}{4} \end{aligned} \qquad (4.32).$$

Thus

$$\int_{A_n\overline{B}} G_n\phi \; d\xi < \int_{A_n\overline{B}} K\,\frac{|\phi|}{|F|}\, d\xi \qquad (4.33),$$

where, since the integral on the right exists (so long as $\mu\neq 0$), I can take the limit and find that it is zero. This follows because $A_n\overline{B}\to\{0\}$ as $n\to\infty$.

There remains only the region A_nB in R^2. It will be enough to show that

$$n\int_{A_nB} d\xi \to 0 \quad \text{as } n\to\infty \qquad (4.34).$$

Since in R^2 I must have $\mu \neq 0$, I can suppose without loss of generality that $\mu = (\mu_1, 0)$. Because δ is positive definite

$$A_nB < \{\xi \mid \|\xi\| < C_1 n^{-1/2} \text{ and } |\xi_1| < C_2\|\varepsilon\|\}$$

$$= \{\xi \mid (\xi_1^2+\xi_2^2)^{1/2} = O(n^{-1/2}) \text{ and } |\xi_1| < C_2(\xi_1^2+\xi_2^2)\}$$

$$< \{\xi \mid \xi_1^2+\xi_2^2 = O(n^{-1}) \text{ and } |\xi_1| = O(n^{-1})\}$$

$$< \{\xi \mid \xi_1 = O(n^{-1}) \text{ and } \xi_2 = O(n^{-1/2})\} \qquad (4.35).$$

Thus

$$\int_{A_n B} d\xi = O(n^{-3/2}) \qquad (4.36),$$

and

$$n \int_{A_n B} d\xi = O(n^{-1/2}) \to 0 \text{ as } n \to \infty \qquad (4.37).$$

Thus for $d > 3$ I have

$$\tilde{D}(\xi) = [1/2(\xi \cdot \delta^2 \xi) - i\mu \cdot \xi)]^{-1} \qquad (4.38)$$

so long as δ is positive definite. If $\mu \neq 0$, I have the same result in R^2.

Limit For (ii)"

The argument leading to the limit of (ii)" is similar. Let A_n, B, and G be as before. Then for ξ not in A_n,

$$|(i\xi_m)\tilde{G}_n| = |\xi_m| \; |\phi| \; |\tilde{G}_n|$$

$$< |\xi_m| \; |\phi| \; \frac{K}{|F|} \qquad (4.39).$$

Because δ is positive definite, this last expression is integrable for $d > 2$ even if $\mu = 0$. It is also integrable in R^1 so long as $\mu \neq 0$.

If $\xi \in A_n\overline{B}$, then, since $|F_n| > 1/2\ |F|$ in that region, I have (4.3) again. Thus I can take the limit

$$\int_{A_n\overline{B}} i\xi_m G_n\phi\ d\xi \to \int_{\{0\}} \frac{i\xi_m\ \phi}{F}\ d\xi = 0 \qquad (4.40).$$

For $\xi \in A_nB$ recall that by the positive definiteness of δ in that region $\|\delta\xi\|^2 > \xi_m^2$ for any ξ_m. Thus $|\xi_m| = 0(n^{-1/2})$. As I showed when considering (i)", $|G_n\phi| = 0(n)$. Thus

$$\int_{A_nB} |\xi_m|\ |G_n|\ |\phi|\ d\xi = 0(n^{1/2})\int_{A_nB} d\xi$$

$$= 0(n^{-1}) \to 0 \quad \text{as } n \to \infty \qquad (4.41).$$

Hence for $d>2$ -- $d=1$ if $\mu\neq 0$ -- I find

$$\tilde{A}_m = (i\xi_m)[1/2(\xi\cdot\delta^2\xi)-i\mu\cdot\xi)]^{-1} \qquad (4.42).$$

Limit For (iii)"

The argument for the limit in (iii)" is by now familiar. Let,

$$H_n = \begin{cases} \sqrt{n}[i\xi_m G_n - \tilde{A}_m] & \text{if } \xi \text{ is not in } A_n \\ 0 & \text{if } \xi \text{ is in } A_n \end{cases} \qquad (4.43).$$

To show that H_n is bounded by an integrable function, note that

$$H_n = \sqrt{n}(i\xi_m)[G_n - F^{-1}]$$
$$< \sqrt{n}|\xi_m|[|G_n - F_n^{-1}| + |F_n^{-1} + F^{-1}|] \qquad (4.44).$$

For ξ not in A_n,

$$|F_n^{-1} + F^{-1}| = \sqrt{n}\,\frac{|\xi'\cdot\delta^2\xi|}{|F_nF|}$$

$$< 2\sqrt{n}\,\frac{|\xi'\cdot\delta^2\xi|}{|F|^2} \qquad (4.45)$$

since $|F_n| > 1/2|F|$ in this region. Thus

$$\sqrt{n}|\xi_m|\,|F_n^{-1} + F^{-1}| < 2|\xi_m|\,\frac{|\xi'\cdot\delta^2\xi|}{|F|^2} \qquad (4.46).$$

This last expression is integrable. In fact it reduces to the form

$$\int_{\|\xi\|<1} |\xi_m\xi_j|\;|F|^{-2}\,d\xi = \int_{\|\xi\|<1} |\xi_m\xi_j|\;|1/2(\xi\cdot\delta^2\xi) - i\mu\cdot\xi|^{-2}\,d\xi$$

$$< \frac{1}{\lambda}\int_{\|\eta\|<k} |\eta_m\eta_j|\;|\eta\cdot\eta - iM\cdot\eta|^{-2}\,d\eta$$

$$= \frac{1}{\lambda}\int_{\|\eta\|<k} |\eta_m\eta_j|\;(\|\eta\|^4 + (M\cdot\eta)^2)^{-1}\,d\eta$$

$$< \frac{C'}{\lambda}\int_{\|\eta\|<k} \|\eta\|^{-2}\,d\eta$$

$$< C\int_0^k r^{d-3}\,dr \qquad (4.47)$$

C and C' are both constants, λ is the minimum eigenvalue of δ^2, and $r = \|\eta\|$. The last expression in (4.47) is finite for $d > 2$.

Suppose d = 1, then the integral has the form

$$\int_0^1 \frac{\xi^2}{|\gamma\xi^2 - i\mu\xi|^2}\, d\xi = \int_0^1 \frac{\xi^2}{\gamma^2\xi^4 + \mu^2\xi^2}\, d\xi$$

$$= \int_0^1 \frac{1}{\gamma^2\xi^2 + \mu^2}\, d\xi \qquad (4.48)$$

which exists so long as $\mu \neq 0$.

If d = 2, suppose that $\mu \neq 0$ and that the coordinate system has been rotated so that the x_1 axis coincides with M. Then the integral reduces to

$$\int_0^1\int_0^1 \frac{x_j x_m}{(x_1^2 + x_2^2)^2 + x_1^2}\, dx_1 dx_2 \qquad (4.49)$$

Let $x = x_1$ and $y = x_2$. There are three cases to consider:

1) j = m = 1, then

$$\int_0^1\int_0^1 \frac{x_j x_m}{(x_1^2 + x_2^2)^2 + x_1^2}\, dx_1 dx_2 = \int_0^1\int_0^1 \frac{x^2}{(x^2 + y^2)^2 + x^2}\, dxdy$$

$$< \int_0^1 \frac{x^2}{x^4 + x^2}\, dx$$

$$= \int_0^1 \frac{1}{x^2 + 1}\, dx < \infty \qquad (4.49a)$$

2) j = m = 2, then

$$\int_0^1\int_0^1 \frac{x_j x_m}{(x_1^2 + x_2^2)^2 + x_1^2}\, dx_1 dx_2 = \int_0^1\int_0^1 \frac{y^2}{(x^2 + y^2)^2 + x^2}\, dxdy$$

$$< \int_0^1\int_0^1 \frac{y^2}{y^4 + x^2}\, dxdy$$

$$= \int_0^1 \tan^{-1}(y^{-2})\, dy$$

$$< \infty \tag{4.49b}$$

because $\tan^{-1}(\zeta)$ is finite for all ζ.

3) $j \neq m$, then

$$\int_0^1\int_0^1 \frac{x_j x_m}{(x_1^2 + x_2^2)^2 + x_1^2}\, dx_1 dx_2 = \int_0^1\int_0^1 \frac{xy}{(x^2 + y^2)^2 + x^2}\, dxdy$$

$$< \int_0^1\int_0^2 \frac{x}{u^2 + x^2}\, dudx$$

$$= \int_0^1 \tan^{-1}(2/x)\, dx$$

$$< \infty \tag{4.49c}$$

Return to (4.44) and consider

$$\sqrt{n}|\xi_m|E|G_n - F_n^{-1}| = \frac{1}{\sqrt{nt}}|\xi_m|\left| n^2t^2 \frac{e^{-ntFn} - 1}{n^2t^2F_n^2}\right|$$

$$< \frac{1}{\sqrt{nt}}|\xi_m| \frac{C}{|F_n|^2} \tag{4.50}$$

for some constant C.

Since ξ is not in A_n,

$$\|\delta\xi\| > 4n^{-1/2}\|\delta\xi'\| = Kn^{-1/2} \tag{4.51},$$

where $K=4\|\delta\xi'\|$. Thus, noting that $|F_n| > |F|/2$,

$$\frac{1}{\sqrt{n}} \frac{|\xi_m|}{|F_n|^2} < \frac{|\xi_m| \|\delta\xi\|}{K'|F|^2} \qquad (4.52).$$

The expression on the right of (4.52) leads to a bound like (4.47) which is integrable for $d > 1$ if $\mu \neq 0$. Thus on $R^d - A_n$, H_n is bounded by an integrable function. Therefore I can take the limit

$$\int_{R^d - A_n} H_n\phi \; d\xi \to \int_{R^d} \frac{\xi' \cdot \delta^2 \xi \; \phi(\xi)}{F(\xi)^2} \; d\xi \qquad (4.53).$$

To show that

$$\int_{A_n} \sqrt{n}[i\xi_m G_n - \tilde{A}_m] \; \phi \; d\xi \to 0 \quad \text{as } n \to \infty \qquad (4.54),$$

consider that $|\xi_m| = O(n^{-1/2})$ on A_n. Thus

$$\begin{aligned} |\sqrt{n}[i\xi_m G_n - \tilde{A}_m| &= \sqrt{n}|\xi_m| \; |G_n - F^{-1}| \\ &= O(1) \; |G_n - F^{-1}| \\ &< O(1) \; [|G_n| + |F|^{-1}] \end{aligned} \qquad (4.55).$$

As I have shown $|F|^{-1}$ is integrable on A_n and $|G_n| = O(n)$. By the argument given above, $\int_{A_n} = O(n^{-d/2})$ always and, when $d=2$, $\int_{A_n} = O(n^{-3/2})$ if $\mu \neq 0$. The limit (4.50) follows immediately.

Thus when $\mu \neq 0$, I have

$$\tilde{\tilde{D}}_{jm} = [\xi_m \sum_{\ell} \delta^2_{j\ell} \; \xi_{\ell}] \; / \; F^2 \qquad (4.56)$$

Even if $\mu = 0$, this expression is correct for $d > 3$.

Limits For d = 1

When d=1 there is no need for subscripts, so I drop them below. Since the bounds (4.39) and (4.46) apply to the one dimensional case (so long as $\mu \neq 0$), the limits (4.42) and (4.56) for A and D are also correct in R^1. Hence, I can express α_2 and $D_2(ii)$ very simply. For the rest of this section I let $\gamma = \delta^2/2$.

To calculte $D_2(i)$ it is convenient to return to condition (i)

$$\text{(i)} \qquad \frac{1}{2\pi}\int_{-\infty}^{\infty} G_n(\xi)\,\hat{\rho}(\xi)\,d\xi \to D_2^i \quad \text{as } n \to \infty \qquad (4.57).$$

Note that in R^1

$$F_n(\xi;\xi') = \gamma\,\xi^2 - \frac{2\gamma(\xi'\xi)}{\sqrt{n}} - i\mu\xi$$

$$= \frac{1}{n}(a_n + ib_n) \qquad (4.58)$$

where $a_n = \gamma(n\xi + 2\sqrt{n}\xi'\xi)$ and $b_n = -n\mu\xi$. Thus

$$F_n(\xi;\xi') = (a_n + ib_n)t \qquad (4.59).$$

With this notation I can write

$$G_n = nt\,\frac{e^{-(a_n+ib_n)t} - 1 + (a_n+ib_n)t}{(a_n+ib_n)^2t^2}$$

$$= \frac{n}{t}(R + I) \qquad (4.60)$$

where

$$R = \frac{(e^{-a_nt}\cos b_nt-1+a_nt)(a_n^2-b_n^2) + 2a_nb_n(b_nt-e^{-a_nt}\sin b_nt)}{(a_n^2+b_n^2)^2} \quad (4.61)$$

$$I = \frac{-(b_nt-e^{-a_nt}\sin b_nt)(a_n^2-b_n^2) - 2a_nb_n(e^{-a_nt}\cos b_nt-1+a_nt)}{(a_n^2+b_n^2)^2} \quad (4.62).$$

Because G_n is finite at zero, I can take the limit of the integral in (i) by first taking the limit of G_n and then integrating. To do so I observe that both a_n and b_n are $0(n)$. Thus in taking the limit, I need only consider terms including n^4. I find that

$$nR \to \frac{\gamma}{\gamma^2\xi^2+\mu^2}\,t \quad (4.63),$$

$$nI \to \frac{-\mu}{\xi(\gamma^2\xi^2+\mu^2)}\,t \quad (4.64).$$

In both (4.63) and (4.64) the limit is taken as $n \to \infty$.

Thus

$$\int_{-\infty}^{\infty} G_n\hat{\rho}\,d\xi \to \gamma\int_{-\infty}^{\infty}\frac{\hat{\rho}(\xi)}{\gamma^2\xi^2+\mu^2}\,d\xi - i\mu\int_{-\infty}^{\infty}\frac{\hat{\rho}(\xi)}{\xi(\gamma^2\xi^2+\mu^2)}\,d\xi$$

$$= \gamma\int_{-\infty}^{\infty}\frac{\hat{\rho}(\xi)}{\gamma^2\xi^2+\mu^2}\,d\xi + \frac{\pi}{\mu}\hat{\rho}(0) \quad (4.65)$$

where I obtain the last line by applying Cauchy's integral formula: consider the contour $C = C_1 + C_2 + C_3 + C_4 + C_5 + C_6 + C_7 + C_8$ where

$$C_1 = \{\xi \mid Re(\xi)=-R \text{ and } Im(\xi)<(\mu/\gamma)^{-1/2}\} \quad (4.66)$$

$$C_2 = \{\xi=re^{i\theta} \mid -R<r<-1/R \text{ and } \theta=0\} \quad (4.67)$$

$$C_2 = \{\xi = (1/R)e^{i\theta} \mid \pi < \theta < 2\pi\} \quad (4.68)$$

$$C_3 = \{\xi = re^{i\theta} \mid 1/R < r < R \text{ and } \theta = 0\} \quad (4.69)$$

$$C_4 = \{\xi = Re^{i\theta} \mid 0 < \theta < \pi\} \quad (4.70)$$

$$C_5 = \{\xi \mid Re(\xi) = R \text{ and } Im(\xi) < (\mu/\gamma)^{-1/2}\} \quad (4.71).$$

The contours C_6, C_7 and C_8 are identical to C_2, C_3 and C_4 respectively except that they run in the opposite direction.

Of course

$$\int_C \frac{\hat{\rho}(z)}{z(\gamma^2 z^2 + \mu^2)} dz = \frac{i2\pi}{\mu^2} \hat{\rho}(0) \quad (4.72).$$

Also

$$\int_{C_2} + \int_{C_3} + \int_{C_4} \to \int_{-\infty}^{\infty} \frac{\hat{\rho}(\xi)}{\xi(\gamma^2 \xi^2 + \mu^2)} d\xi \quad \text{as } R \to \infty \quad (4.73),$$

and

$$\int_{C_6} + \int_{C_7} + \int_{C_8} \to \int_{\infty}^{-\infty} \frac{\hat{\rho}(\xi)}{\xi(\gamma^2 \xi^2 + \mu^2)} d\xi \quad \text{as } R \to \infty \quad (4.74).$$

On the other hand

$$\int_{C_1} = -\int_{C_5} \quad (4.75).$$

Thus

$$\int_C = \int_{C_2} + \int_{C_3} + \int_{C_4} + \int_{C_6} + \int_{C_7} + \int_{C_8}$$

$$= 2\int_{-\infty}^{\infty} \frac{\hat{\rho}(\xi)}{\xi(\gamma^2 \xi^2 + \mu^2)} d\xi \quad (4.76).$$

So

$$D^{(i)} = \frac{\gamma}{2\pi} \int_{-\infty}^{\infty} \frac{\hat{\rho}(\xi)}{\gamma^2 \xi^2 + \mu^2} d\xi + \frac{1}{2\mu} \hat{\rho}(0) \quad (4.77).$$

CHAPTER 5

RESULTS AND APPLICATIONS

In the first section of this chapter I give expressions for megascopic dispersion and drift coefficients in media of one or more dimensions. These expressions are obtained from the limits (4.37), (4.41), and either (4.55) for media of more than one dimension or (4.73) for one dimensional media.

In the following three sections I compare the results (5.3) - (5.15) for the general case to those obtained for turbulent diffusion by Kesten and Papanicolaou (1979), for stratified two dimensional media by Gelher et al. (1979) and for incompressible fluids in three dimensional media by Gelhar and Axness (1981). The agreement between my results and those of Matheron and de Marsily (1980) is so obvious that a demonstration is almost unnecessary. In the other examples, however, such a demonstration sheds new light on the general as well as the special case.

The penultimate section returns to transport in one dimensional media. I show that the theory developed for one dimensional compressible fluids gives a result which, when related to Peclet number, is similar to experimental and theoretical results in hydrology. Hydrologists have found that when the mean flow of water is parallel to one axis, the coefficient of dispersion in that direction is proportional to mean fluid velocity. Of course the hydrological results are for multidimensional media and an incompressible fluid, water. However, my result suggests an approach which should prove useful in the analysis of transport in hydrological systems.

Results

Recall that I have assumed that the macroscopic dispersion matrix matrix, $\delta^2/2$, is positive definite and, when $d < 2$, $\mu \neq 0$. Furthermore, I have supposed that

$$\alpha(\xi;\delta) = \alpha_0(\delta) + \varepsilon\alpha_1(\delta) + \varepsilon^2\alpha_2(\delta) + \ldots \qquad (5.1)$$

and

$$D(\varepsilon;\delta) = D_0(\delta) + \varepsilon D_1(\delta) + \varepsilon^2 D_2(\delta) + \ldots \qquad (5.2)$$

where for each j, $\alpha_j \in R^d$ and for each j, k, and ℓ, $(D_j)_{\ell k}$ is a constant.

I have shown that in R^d $(d > 2)$,

$$\alpha_0 = \mu \qquad (5.3),$$

$$D_0 = \delta^2 \qquad (5.4),$$

$$(\alpha_2)_k = \sum_{m=1}^{d} \alpha_{mk} \qquad (5.5),$$

$$\alpha_{mk} = (2\pi)^{-d} \int_{R^d} \frac{(i\varepsilon_m)\,\hat{\rho}_{mk}(\xi)}{(\xi\cdot\delta^2\xi)/2 - i\mu\cdot\xi}\, d\xi \qquad (5.6),$$

$$(D_2)_{\ell k} = D_{\ell k}^{(i)} + D_{k\ell}^{(i)} + D_{\ell k}^{(ii)} + D_{k\ell}^{(ii)} \qquad (5.7),$$

$$D_{\ell k}^{(i)} = (2\pi)^{-d} \int_{R^d} \frac{\hat{\rho}_{mk}(\xi)}{(\xi\cdot\delta^2\xi)/2 - i\mu\cdot\xi}\, d\xi \qquad (5.8),$$

$$D_{\ell k}^{(ii)} = \sum_{m=1}^{d} D_{\ell km}^{(ii)} \qquad (5.9),$$

$$D^{(ii)}_{\ell km} = (2\pi)^{-d} \int_{R^d} \frac{\xi_m (\sum_n \delta^2_{\ell n}\xi_n)\, \hat{\rho}_{mk}(\xi)}{[(\xi\cdot\delta^2\xi)/2 - i\mu\cdot\xi)]^2}\, d\xi \qquad (5.10),$$

where I have substituted the appropriate element of $\hat{\rho}$ for the function ϕ in equations (4.37), (4.41) and (4.55).

Of course equations (5.3), (5.4), (5.6) and (5.10) carry over directly to R^1. Since they can be simplified, I rewrite (5.6) and (5.10):

$$\alpha_2 = (2\pi)^{-1} \int_{-\infty}^{\infty} \frac{i\varepsilon\, \hat{\rho}(\xi)}{\gamma\xi^2 - i\mu\xi}\, d\xi$$

$$= \frac{-\mu}{(2\pi)} \int_{-\infty}^{\infty} \frac{\rho(\hat{\xi})}{\gamma^2\xi^2 + \mu^2}\, d\xi \qquad (5.11)$$

since $\hat{\rho}$ is even. Once again I have let $\gamma = \delta^2/2$ when $d = 1$. Similarly

$$D^{(ii)} = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{\gamma\,(\gamma^2\xi^2 - \mu^2)\, \hat{\rho}(\xi)}{(\gamma^2\xi^2 + \mu^2)^2}\, d\xi \qquad (5.12).$$

From (4.73) on the other hand

$$D^{(i)} = \frac{\gamma}{2\pi} \int_{-\infty}^{\infty} \frac{\hat{\rho}(\xi)}{\gamma^2\xi^2 + \mu^2}\, d\xi + \frac{1}{2\mu} \int_{-\infty}^{\infty} \rho(x)\, dx \qquad (5.13).$$

A few points are worth noting. First, since the integral in (5.8) can be transformed to

$$\int_{R^d} \frac{\hat{\rho}_{mk}(\xi)}{\eta\cdot\eta - iM_1\eta_1}\, d\xi = \int_{R^d} \frac{\hat{\rho}_{mk}(\eta)}{(\eta\cdot\eta)^2 + (M_1\eta_1)^2}\, d\eta \qquad (5.14),$$

it follows that $D_{mk} \geq 0$. Thus the megascopic coefficient of dispersion is equal to or greater than the macroscopic. This is consistent with hydrological experiments.

Next note that (5.11) shows that in one dimension $\alpha_2 \leq 0$. Thus the megascopic drift is equal to or less than the mean macrsocopic. More generally (5.6) indicates that in d dimensions the megascopic drift is not always identical to the mean macroscopic velocity, μ. When, however, the fluid is incompressible $\alpha_2 = 0$, a fact which I show in the section on incompressible fluids.

Turbulent Diffusion

Since the turbulent diffusion case is defined by $\delta = 0$, equations (5.4) and (5.10) make it clear that $D_0 = 0$ and $D^{(ii)}_{\ell km} = 0$. Furthermore the particle trajectory defined by Kesten and Papanicolaou (1979) in equation (2.3) is centered with mean drift μ. Hence $\alpha_0 = \mu$. Thus, to demonstrate that my results agree with those of Kesten and Papanicolaou (1979), I need only show that (5.6) and (5.8) reduce respectively to (2.6) and (2.7) in the limit $\delta \to 0$.

Consider the integral relevant to (2.6):

$$\int_0^\infty E_U[U_\ell(x)\frac{\partial}{\partial x_\ell} U_j(x+t\mu)]\, dt = \int_0^\infty \frac{\partial}{\partial \tau_\ell} \rho_{\ell j}(\tau)\, d\tau \qquad (5.15)$$

where $\tau = t\mu$ and the right side follows from the stationarity of U(x).

Let

$$h(t\mu) = \frac{\partial}{\partial \tau_\ell} \rho_{\ell j}(\tau) \qquad (5.16)$$

and define a generalized function, $F(x)$, which when applied to an arbitrary function acts in the limit $\delta \to 0$ like a Dirac function on the ray $t\mu$. In particular

$$\lim_{\delta\to 0} \int_{R^d} F(x)\ h(x)\ dx = \int_0^\infty h(t\mu)\ dt \qquad (5.17).$$

Since $h(t\mu) = h(\tau) = \partial/\partial\tau_\ell[\rho_{\ell j}(\tau)]$, $h(x) = \partial/\partial x_\ell[\rho_{\ell j}(x)]$. Thus

$$\int_0^\infty \frac{\partial}{\partial\tau_\ell} \rho_{\ell j}(\tau)\ d\tau = \lim_{\delta\to 0} \int_{R^d} F(x) \frac{\partial}{\partial x_\ell} \rho_{\ell j}(x)\ dx \qquad (5.18).$$

Integrating by parts and noting that $\rho_{\ell j}(x)\big|_{|x_j|=\infty} = 0$,

$$\int_{-\infty}^{\infty} F(x) \frac{\partial}{\partial x_\ell} \rho_{\ell j}(x)\ dx = -\int_{-\infty}^{\infty} \left(\frac{\partial}{\partial x_\ell} F(x)\right) \rho_{\ell j}(x)\ dx_\ell \qquad (5.19).$$

Let $G(x) = -\partial/\partial x_\ell[F(x)]$, then

$$\int_0^\infty \frac{\partial}{\partial\tau_\ell} \rho_{\ell j}(\tau)\ d\tau = \lim_{\delta\to 0} \int_{R^d} G(x)\ \rho_{\ell j}(x)\ dx$$

$$= \lim_{\delta\to 0} \int_{R^d} \hat{G}(\xi)\ \hat{\rho}_{\ell j}(\xi)\ d\xi$$

$$= \lim_{\delta\to 0} \int_{R^d} (i\xi_\ell)\ \hat{F}(\xi)\ \hat{\rho}_{\ell j}(\xi)\ d\xi \qquad (5.20)$$

where I have applied the generalized Parseval formula to obtain the second line from the first (Gel'fand and Shilov, 1964).

To formally determine $\hat{F}(\xi)$ note that

$$\lim_{\delta\to 0} \hat{F}(\xi) = \lim_{\delta\to 0} (2\pi)^{-d/2} \int_{R^d} F(x)\ e^{-i\xi\cdot x}\ dx$$

$$= (2\pi)^{-d/2} \int_0^\infty e^{-i(\xi\cdot\mu)t}\, dt$$

$$= \frac{(2\pi)^{-d/2}}{-i\xi\cdot\mu} \qquad (5.21).$$

Thus

$$\hat{F}(\xi) = \frac{(2\pi)^{-d/2}}{(\xi\cdot\delta^2\xi)/2 - i\xi\cdot\mu} \qquad (5.22)$$

is a suitable Dirac function and

$$\int_0^\infty \frac{\partial}{\partial\tau_\ell} \rho_{\ell j}(\tau)\, d\tau = (2\pi)^{-d} \lim_{\delta\to 0} \int_{R^d} \frac{(i\xi_\ell)\,\hat{\rho}_{\ell j}(\xi)}{(\xi\cdot\delta^2\xi)/2 - i\xi\cdot\mu}\, d\xi \qquad (5.23).$$

The last equation relates the integrals relevant to (2.6) and (5.6).

A similar approach relates (2.7) and (5.8). Since $U(x)$ is weakly stationary,

$$\int_0^\infty E_U[U_\ell(x)U_j(x+t\mu)]\, dt = \int_0^\infty \rho_{\ell j}(t\mu)\, d\tau \qquad (5.24).$$

Hence I can use $F(x) \overset{FT}{\to} \hat{F}(\xi)$ as determined above to find that

$$(D_2)_{\ell j} = (2\pi)^{-d} \lim_{\delta\to 0} \int_{R^d} \frac{\hat{\rho}_{\ell j}(\xi)}{(\xi\cdot\delta^2\xi)/2 - i\xi\cdot\mu}\, d\xi \qquad (5.25).$$

Stratified Two Dimensional Aquifers

Recall that in this case Gelhar et al. (1979) found that

$$D_{11} = \delta_{11}^2 + \frac{\varepsilon^2}{(2\pi)^2(\delta_{22}^2/2)} \int_{-\infty}^{\infty} \frac{\hat{\rho}_{\ell j}(\xi)}{\xi^2}\, d\xi \qquad (5.26).$$

Of course the integrand is finite only if $\hat{\rho}_{\ell j}(0) = 0$.

To derive (5.26) from condition (i) in Chapter 3, note that for this case the covariance matrix of the velocity field has only one non-zero component, $\rho_{11}(x_2)$. Thus from (i) it is clear that

$$D_{12}^{(i)} = D_{21}^{(i)} = D_{22}^{(i)} = 0 \tag{5.27}$$

and, furthermore,

$$\frac{1}{(2\pi)^2} \int_{R^2} G_n(\xi;\xi') \hat{\rho}_{11}(\xi)\, d\xi \to D_{11}^{(i)} \quad \text{as } n \to \infty \tag{5.28}.$$

But

$$\hat{\rho}_{11}(\xi) = (2\pi)^{-d/2} \int_{R^2} \rho_{11}(x_2)\, e^{-i\xi\cdot x}\, dx$$

$$= \hat{\rho}_{11}(\xi_2)\, \delta(\xi_1) \tag{5.29}$$

where $\hat{\rho}_{11}(\xi_2)$ is the power spectrum of $U_1(x_2)$ and $\delta(\cdot)$ is a Dirac function. It is the presence of the latter term which leads to the singularity in the integrand of (5.26). Hence the degeneracy of this case stems from the fact that $\hat{\rho}_{11}$ is a function of a single variable, while the problem is fundamentally two dimensional.

To continue, observe that from (5.29) the left side of (5.28) reduces to

$$\frac{1}{(2\pi)^2} \int_{R^2} G_n(0,\xi_2)\, \hat{\rho}_{11}(\xi_2)\, d\xi_2 \tag{5.30}$$

where I have dropped the fixed quantity ξ' from the argument of G_n.

From the definition of G_n

$$G_n(0,\xi_2) = nt\,\frac{e^{-ntH_n(\xi_2)} - 1 + nH_n(\xi_2)}{n^2t^2H_n^2(\xi_2)} \qquad (5.31)$$

where

$$H_n(\xi_2) = F_n(0,\xi_2)$$

$$= \frac{\delta_{22}^2\ \xi_2^2}{2} - \frac{(\delta_{12}^2\ \xi_1' + \delta_{22}^2\ \xi_2')}{\sqrt{n}} \cdot \xi_2$$

$$= \alpha\xi_2^2 - \beta_n\varepsilon_2 \qquad (5.32).$$

Note that, because $\mu = (\mu_1,0)$ in this case, the term $\mu\cdot\xi$ drops out of F_n. In (5.32) I have let $\alpha = \delta_{22}^2/2$ and $\beta = (\delta_{12}^2\xi' + \delta_{22}^2\xi')/\sqrt{n} \to 0$ as $n\to\infty$.

Thus

$$\frac{1}{(2\pi)^2}\int_{R^2} G_n(0,\xi_2)\,\hat{\rho}_{11}(\xi_2)\,d\xi_2 \to$$

$$\frac{1}{(2\pi)^2(\delta_{22}^2/2)}\int_{-\infty}^{\infty}\frac{\hat{\rho}_{11}(\xi_2)}{\xi_2^2}\,d\xi_2 \quad \text{as } n\to\infty \qquad (5.33)$$

from which (5.25) follows immediately.

Next consider condition (ii). In this special case the left side of (ii) is

$$\frac{1}{(2\pi)^2}\int_{R^2} G_n(\xi_1,\xi_2)[i\xi_1\hat{\rho}_{1j}(\xi)+i\xi_2\hat{\rho}_{2j}(\xi)]\,d\xi$$

$$= \begin{cases}\dfrac{1}{(2\pi)^2}\displaystyle\int_{R^2} G_n(\xi_1,\xi_2)[i\xi_1\hat{\rho}_{11}(\xi_2)\delta(\xi_1)]\,d\xi_1 d\xi_2 & \text{if } j = 1\\[2ex] 0 \text{ if } j \neq 1\end{cases} \qquad (5.34)$$

Since

$$\int_{-\infty}^{\infty} G_n(\xi_1,\xi_2)[i\xi_1\hat{\rho}_{11}(\xi_2)\delta(\xi_1)]\, d\xi_1 = 0 \qquad (5.35),$$

$(\alpha_2)_j = 0$ for all j.

From (iii) and this last result $D_{11} = 0$, and my results agree with those of Gelhar et al. (1979).

It is important to note that in the case of a systematically tilted two dimensional porous medium

$$H_n(\xi_2) = \alpha\xi_2^2 - \beta_n\xi_2 - i\mu_2\xi_2 \qquad (5.36).$$

Hence

$$\frac{1}{(2\pi)^2}\int_{-\infty}^{\infty} G_n(0,\xi_2)\,\hat{\rho}_{11}(\xi_2)\, d\xi_2$$

$$+\frac{1}{(2\pi)^2}\int_{-\infty}^{\infty} \frac{\hat{\rho}_{11}(\xi_2)}{(\delta_2^2\ \xi_2^2)/2-i\mu_2\xi_2}\, d\xi_2 \qquad (5.37)$$

which is in accordance with the result obtained by Matheron and de Marsily (1980).

Incompressible Fluids

In the three dimensional case examined by Gelhar and Axness (1981) the fluid is incompressible. Since Gelhar and Axness assume that the medium's porosity is constant, this amounts to assuming that $\nabla\cdot U(x)=0$ for almost every realization of the velocity field. Note, however, that when d=1 the condition $d/dx[U(x)]=0$ requires that U (and thus V, the macroscopic velocity) be a constant. In that case $\rho(x)=0$, so that the megascopic and macroscopic parameters are the same; of course, when V is a constant, the trajectory of a particle is a Brownian process. Hence the parameters are not affected by a change of scale.

Thus in this section I treat media of two or more dimensions. There incompressibility implies that

$$E_U[U_j(y)\nabla\cdot U(x)] = \sum_{m=1}^{d} \frac{\partial}{\partial x_m} \rho_{jm}(y-x) = 0 \qquad (5.38).$$

The Fourier transform of the middle expression in (5.38) must also be zero, i.e.

$$\sum_{m=1}^{d} (-i\xi_m)\, \hat{\rho}_{jm}(\xi) = 0 \qquad (5.39),$$

for all j.

It is clear from (ii) and (iii) Chapter 3 that when the fluid is incompressible

$$(\alpha_2)_j = 0 \qquad (5.40)$$

and

$$(D_2)_{\ell j} = D^{(i)}_{\ell j} + D^{(i)}_{j\ell} \qquad (5.41).$$

Of course the latter equation is the same as (2.8) given by Gelhar and Axness (1981). There is no reason, however, to restrict these results to three dimensional media; they apply as well to any d dimensional medium with $d > 2$.

One Dimensional Transport: Relation of Asymptotic Dispersion to Mean Macroscopic Velocity

Hydrological experiments suggest that the asymptotic longitudinal dispersion coefficient, D_L, is proportional to mean macroscopic velocity, μ, when μ is large (Bear 1972 and 1979). When μ is small, transport is basically a Brownian process with a diffusion coefficient $\sqrt{\delta^2/2} = \sqrt{\gamma}$. Thus for $\mu=0$, $D_L=\gamma$. Previous theoretical work in hydrology (Saffman, 1960; Bear and Bachmat, 1965 and 1966) has accounted for these results. It has not, however, accurately reproduced the results of experiments for intermediate μ.

For such values of μ the relationship between D_L and μ depends on the form of the velocity's covariance. Because earlier work in this area did not rely on the fundamentally random character of the velocity, it proved impossible to account for the variability of D_L with respect to μ.

In this section I treat the case of a compressible fluid moving with mean velocity, μ, through a one dimensional medium. This is not quite the same as the hydrological problem: water is not compressible under ordinary pressures, the hydrological medium is multidimensional, and the megascopic coefficient of longitudinal dispersion, D_L, is not the same as the one dimensional coefficient, D. The case I analyze is, however, significant to hydrologists. It emphasizes the influence that randomness in the velocity field has on fundamental physical properties of transport. Furthermore, it points the way to an analysis of dispersion in hydrologically significant flow fields.

It is convenient to frame this problem in terms of the ratios D/γ and μ/γ. The latter is a pseudo Peclet number with dimension L^{-1}. The Peclet number plays an important role in the hydrological description of mass transport. A dimensionless number, it characterizes the relative influence of macroscopic velocity and dispersion on transport.

While various kinds of Peclet number can be defined, all have the form $(VL)/(L^2/t)$ where V has the dimensions of velocity, L is some characteristic length of the medium and t is time. In hydrology the term corresponding to V is most often mean seepage velocity, μ, and the denominator is ordinarily γ (Fried, 1975). If the effect of variation in characteristic length is not at issue, a pseudo Peclet number, $\lambda = \mu/\gamma$, can be defined. Of course λ has dimension L^{-1}.

Before proceeding note that the following analysis is for $D \cong \gamma + \varepsilon^2 D_2$. When variation in the random velocity field is large, the analysis may break down.

To see that $\gamma + \varepsilon^2 D_2$ behaves in accordance with the results mentioned above, first rewrite $D^{(i)}$ and $D^{(ii)}$ in terms of λ:

$$D^{(i)} = \frac{\lambda}{2\pi\mu} \int_{-\infty}^{\infty} \frac{\hat{\rho}(\xi)}{\xi^2+\lambda^2}\, d\xi + \frac{1}{\mu}\int_{-\infty}^{\infty} \rho(x)\, dx$$

$$= \frac{2}{\pi}\int_{-\infty}^{\infty} e^{-\lambda|x|} \rho(x)\, dx + \frac{1}{\mu}\int_{-\infty}^{\infty} \rho(x)\, dx \qquad (5.41)$$

and

$$D^{(ii)} = \frac{2}{2\mu} \int_{-\infty}^{\infty} \frac{(\xi^2-\lambda^2)\,\hat{\rho}(\xi)}{\gamma(\xi^2+\lambda^2)^2}\, d\xi$$

$$= -\frac{k}{\gamma}\int_{-\infty}^{\infty} e^{-\lambda|x|} |x|\rho(x)\, dx \qquad (5.42)$$

where $k > 0$ is a constant. I have used Parseval's formula to derive the last lines of both (5.41) and (5.42).

Now divide both sides of (5.41) by γ to find,

$$\frac{D^{(i)}}{\gamma} = \frac{1}{2\gamma\mu} \int_{-\infty}^{\infty} e^{-\lambda|x|} \rho(x)\, dx + \frac{1}{\gamma\mu} \int_{-\infty}^{\infty} \rho(x)\, dx$$

$$= \frac{\lambda}{2} \int_{-\infty}^{\infty} e^{-\lambda|x|} \frac{\rho(x)}{\mu^2}\, dx + \lambda \int_{-\infty}^{\infty} \frac{\rho(x)}{\mu^2}\, dx \qquad (5.43).$$

Similarly

$$\frac{D^{(ii)}}{\gamma} = -k\lambda^2 \int_{-\infty}^{\infty} e^{-\lambda|x|} \frac{|x|\rho(x)}{\mu^2}\, dx \qquad (5.44).$$

Since the ratios $D^{(i)}/\gamma$ and $D^{(ii)}/\gamma$ are dimensionless, so should be the right sides of (5.43) and (5.44). To see that this is so note that $\rho(x)$, which is the expectation of the product of two velocities, has dimensions $(L/t)^2$. Hence $\rho(x)/\mu^2$ is dimensionless. Furthermore, λ has dimension L^{-1}, so $\lambda|x|$ is dimensionless. Thus the integrals in (5.43) have dimension L; the product of λ with those integrals is dimensionless. Similarly the integral in (5.44) is like L^2 which when multiplied by λ^2 is dimensionless.

Note that when λ is large

$$\frac{D^{(i)}}{\gamma} \cong \lambda \int_{-\infty}^{\infty} \frac{\rho(x)}{\mu^2}\, dx \qquad (5.45),$$

but

$$\frac{D^{(ii)}}{\gamma} \cong 0 \qquad (5.46).$$

Thus $D/\gamma \propto \lambda L$ as expected. On the other hand, when $\lambda = 0$, $D^{(i)} = D^{(ii)} = 0$. Hence $D/\gamma = 1$, also as expected.

It is clear from (5.43) and (5.44) that D/γ is proportional to some function of λ for intermediate values of λ. The function will depend on the form of $\rho(x)$. This is an important point: it suggests that the form of the covariance plays a significant role in the relation between mean velocity and the coefficient of longitudinal dispersion in hydrological systems. A demonstration, however, awaits further work.

Summary

By treating the macroscopic velocity of a fluid as a weakly stationary random field, I obtained formal expressions for the asymptotic coefficients of dispersion and drift of a solute transported by the fluid. Furthermore, I approximated the asymptotic coefficients by expansions of second order in ε, where ε is related to the variability of the velocity field. Although my analysis is basically formal, in Chapter 4 I rigorously took the limit of the integrals which lead to terms in the expansions of the asymptotic coefficients. By doing so I obtained in one dimensional transport an important correction for the dispersion coefficient.

The results are consistent with experimental results in hydrology. In particular, I find that the megascopic dispersion coefficient is equal to or greater than the macroscopic. Perhaps unexpectedly I find that the megascopic drift of solute is equal to or less than the mean macroscopic velocity in one dimensional problems. The megascopic drift equals mean macroscopic velocity only when the fluid is incompressible.

Of course the result also applies to transport in truly compressible fluids like gases.

In special cases my results reduce to theoretical results obtained by Kesten and Papanicolaou (1979), Gelhar et al. (1979), Matheron and de Marsily (1980) and Gelhar and Axness (1981); the agreement is exact.

When considering my results for one dimensional flows I confirmed that for large values of a pseudo Peclet number, λ, the ratio of the megascopic to macroscopic dispersion is proportional to λ; for small values of λ the ratio is one. At intermediate values the ratio strongly depends on the form of the covariance of the velocity.

LIST OF REFERENCES

Bakr, A. A., Gelhar, L. W., Gutjahr, A. L. and MacMillan, J. R., Stochastic analysis of spatial variability in subsurface flows, 1, comparison of one-and three-dimensional flows, Water Resource Research, 14, 2, 1978.

Bear, J. and Bachmat, Y., A generalized theory of hydrodynamic dispersion in porous media, Proceedings International Association of Science Hydrology Symposium, Haifa, Publication number 72, 1967.

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

Bear. J., Hydraulics of Groundwater, McGraw-Hill International Book Co., New York, 1979.

Beran, N. J., Statistical Continuum Theories, Monographs in Statistical Physics, Interscience, New York, Vol. 9, 1968.

Chaudhari, N. M. and Scheidegger, A. E., Statistical mechanics of certain dispersion phenomena, Canadian Journal of Physics, 43, 1965.

Dieulin, A., Matheron, G., de Marsily, G. and Beaudoin, B., Time dependence of an "equivalent dispersion coefficient" for transport in porous media, Proceedings of Euromech 143, A. A. Balkema, Rotterdam, 1981.

Dagan, G., Stochastic modeling of groundwater flow by unconditional and conditional probabilities part 2: the solute transport, Water Resources Research, 1982 (in press).

Feller, W., An Introduction to Probability Theory and Its Applications, John Wiley and Sons, Inc., New York, 1966.

Fried, J. J. and Combarnous, M. A., Dispersion in porous media, in Advances in Hydroscience, ed. by V. T. Chow, Academic Press, New York, 1971.

Fried, J. J., Miscible pollution of groundwater: a study of methodology, Proceedings of the International Symposium on Modelling Techniques in Water Resource Systems, Vol. 2, ed. by A. K. Biswas, Environment Canada, Ottawa, 1972.

Fried, J. J., Groundwater Pollution, American Elsevier, New York, 1975.

Gel'fand, I. M. and Shilov, G. E., Generalized Functions, Vol. 1, Academic Press, New York, 1964.

Gelhar, L. W., Gutjahr, A. L., and Naff, R. L., Stochastic analysis of macrodispersion in a stratified aquifer, Water Resources Research, Vol. 15(6), 1979.

Gelhar, L. W. and Axness, C. L., Stochastic analysis of macrodispersion in three dimensionally heterogeneous aquifers, Report H-8, Hydrological Research Program, Geophysical Research Center, New Mexico Institute of Mining and Technology, Socorro, 1981.

Hille, E. and Phillips, R., Functional Analysis and Semi-Groups, American Mathematical Society, Providence, 1957.

Kesten, H. and Papanicolaou, G., A limit theorem for turbulent diffusion, Communications in Mathematical Physics 65, 1979.

Matheron, G. and de Marsily, G., Is transport in porous media always diffusive? a counter example, Water Resources Research, Vol. 16, 5, 1980.

Monin, A. S. and Yaglom, A. M., Statistical Fluid Mechanics: Mechanics of Turbulence, Vol. 1, M. I. T. Press, Cambridge, 1971.

Morgan, J. M., Kamison, D. K. and Stevenson, J. D., Proceedings of the Conference on Ground Disposal of Radioactive Wastes, Chalk River, Ontario, ed. by J. M. Morgan, D. K. Kamison and J. D. Stevenson, United States Atomic Energy Commission, TID-7628, 1962.

Naff, R. L., A continuum approach to the study and determination of field longitudinal dispersion coefficients, as cited in L. W. Gelhar and C. L. Axness, Stochastic analysis of macrodispersion in three dimensionally heterogeneous aquifers, Report H-8, Hydrological Research Program, Geophysical Research Center, New Mexico Institute of Mining and Technology, Socorro, 1981.

Papanicolaou, G., Personal communication, Professor, Courant Institute of Applied Mathematics, New York University, New York, 1981.

Roberts, P. H., Analytical theory of turbulent diffusion, Journal of Fluid Mechanics 11, 1961.

Sposito, G., Gupta, V. K. and Bhattacharya, R. N., Foundation theories of solute transport in porous media: a critical review, Advances in Water Resources, Vol. 2, no. 2, 1979.

Saffman, P. G., A theory of dispersion in a porous medium, Journal of Fluid Mechanics, 6, 1959.

Saffman, P. G., Dispersion due to molecular diffusivity and macroscopic mixing in flow through a network of capillaries, Journal of Fluid Mechanics, 7, 1960.

Taylor, G. I., Dispersion of soluble matter in solvent flowing through a tube, 1953, In: The Scientific Papers of Sir Geoffrey Ingram Taylor, Vol. IV, ed. by G. K. Batchelor, Cambridge University Press, Cambridge, 1971.

Taylor, G. I., Conditions under which dispersion of a solute in a stream of solvent can be used to measure molecular diffusion, 1954, In: The Scientific Papers of Sir Geoffrey Ingram Taylor, Vol. IV, ed. by G. K. Batchelor, Cambridge University Press, Cambridge, 1971.

Theis, C. V., Notes on dispersion in fluid flow by geologic features, Proceedings of the Conference on Ground Disposal of Radioactive Wastes, Chalk River, Ontario, ed. by J. M. Morgan, D. K. Kamison and J. D. Stevenson, United States Atomic Energy Commission, TID-7628, 1962.

Theis, C. V., Hydrologic phenomena affecting the use of tracers in timing groundwater flow, In: Radioisotopes in Hydrology, IAEA, Vienna, 1963.

Whitaker, S., Diffusion and dispersion in porous media, Journal of the American Institute of Chemical Engineering, 1967.