WATER RESOURCES RESEARCH, VOL. 26, NO. 6, PAGES 1197–1208, JUNE 1990

Effective Hydraulic Conductivity for Gradually Varying Flow

PETER K. KITANIDIS

Department of Civil Engineering, Stanford University, Stanford, California

Consider the problem of flow in a porous medium with hydraulic conductivity which fluctuates locally about a mean value. The flow is unsteady but gradually or slowly varying, i.e., the correlation length of head fluctuations is considerably larger than the correlation length of hydraulic-conductivity fluctuations. The equations which must be satisfied by the effective conductivity tensor are derived under general conditions using a method of volume averaging and spatial moments. The generality of the derived equations is shown by replicating some known results.

1. THE PROBLEM

Consider transient flow in a saturated porous medium. In the absence of sources or sinks, the governing equation is given by

$$\nabla \cdot (\mathbf{K}\nabla\phi) = S\frac{\partial\phi}{\partial t} \tag{1}$$

where ϕ is the piezometric head $[L]$; S is the specific storage coefficient $[L^{-1}]$, which in this analysis will be assumed constant; $\mathbf{K}$ is the hydraulic conductivity $[L/T]$, a symmetric and positive definite second-order tensor (positive definite meaning that the conductivity is positive in every direction); and t denotes time $[T]$. To keep the analysis simple, assume that the boundary condition is that

$$\phi(\mathbf{x}, t) = 0 \qquad \text{for very large } \mathbf{x} \tag{2}$$

and the initial condition is that of a "slug injection"

$$\phi(\mathbf{x}, 0) = \delta(\mathbf{x} - \mathbf{x}') \tag{3}$$

where δ is a Dirac delta function. That is, a "unit volume" increase in the piezometric head was introduced at time 0 at location $\mathbf{x}'$. A point of clarification: In these equations, ϕ should be interpreted as the head above a background level, ϕ_b, which satisfies the governing equation (1) and is subject to prescribed steady boundary conditions. For example, $\phi_b(x_1, x_2, x_3, t) = Jx_1 + c$, where J is slope and c is a constant. However, the background head is of no importance in this analysis. (A reviewer has suggested that ϕ can be seen as the drawdown resulting from a unit-volume slug withdrawal.)

If $\mathbf{K}$ were constant in space, the head would be represented by the following smoothly varying function:

$$\phi(\mathbf{x}, t; \mathbf{x}') = (2\pi)^{-3/2}|2\mathbf{D}t|^{-1/2} \cdot \exp\left[-(\mathbf{x} - \mathbf{x}')\mathbf{D}^{-1}(\mathbf{x} - \mathbf{x}')/4t\right] \tag{4}$$

where $\mathbf{D} = \mathbf{K}/S$; $\mathbf{D}^{-1}$ is the inverse of $\mathbf{D}$; and $|\mathbf{D}|$ is the determinant of $\mathbf{D}$. Equation (4) is valid for three-dimensional flow.

Note that our discussion is not limited by the assumed boundary and initial condition, (2)–(3). If the initial head were not $\delta(\mathbf{x} - \mathbf{x}')$ but an arbitrary function $\phi_0(\mathbf{x})$ then, by the principle of superposition, the solution would have been

$$\phi(\mathbf{x}, t; \mathbf{x}') = \int_{V_\infty} (2\pi)^{-3/2}|2\mathbf{D}t|^{-1/2} \cdot \exp\left[-(\mathbf{x} - \mathbf{x}')\mathbf{D}^{-1}(\mathbf{x} - \mathbf{x}')/4t\right]\phi_0(\mathbf{x}')\, d\mathbf{x}' \tag{5}$$

where V_∞ signifies the entire space.

The point is that by solving for the initial condition (3), the solution can be found for an arbitrary initial condition. Thus the results of this work are not limited to radially diverging or converging flows.

Physically, the solution indicates that a bell-shaped mound is formed and spreads out. The net rate of spreading can be quantified by the rate of increase of

$$\Delta(t) = \int (\mathbf{x} - \mathbf{x}')(\mathbf{x} - \mathbf{x}')\phi(\mathbf{x}, t; \mathbf{x}')\, d\mathbf{x} \tag{6}$$

where $\Delta(t)$ is the average of ϕ at time t weighted by the square distance in each direction. It is known as a spatial moment and is equal to $2\mathbf{D}t$ if $\mathbf{K}$ is constant (as can be verified from (4)). It is worthwhile to note that the relation $\mathbf{D} = \frac{1}{2}(d\Delta/dt)$ will be used later to define the effective conductivity of a heterogeneous medium.

In most cases, $\mathbf{K}$ is not the same everywhere. In principle, one could derive the solution to the governing equation which now has variable coefficients. This is far from a trivial task. Solutions are commonly obtained using numerical methods which cannot easily handle large- and small-scale variability. Another difficulty is that the solution would depend on both $\mathbf{x}$ and $\mathbf{x}'$ instead of only on the difference $\mathbf{x} - \mathbf{x}'$, so that it is needed to solve for many starting points. Finally, it is doubtful that one may specify with precision the value of the parameters at every point.

In many practical situations, one is mainly concerned with the net rate at which the pressure mound spreads, which can be quantified by the rate of increase of Δ, and there is little interest in obtaining the detailed picture of the head as it varies from one point to the next. The question is thus the following: Can the medium be represented by an equivalent homogeneous medium with effective hydraulic conductivity that correctly simulates the net rate of flow? And if so, how can the effective hydraulic conductivity be calculated?

For the sake of illustration, consider one-dimensional flow with periodic $D = K/S$. Figures 1–4 depict the head function at four different times. The head function obtained with the

Paper number 89WR03742.
0043-1397/90/89WR-03742$05.00

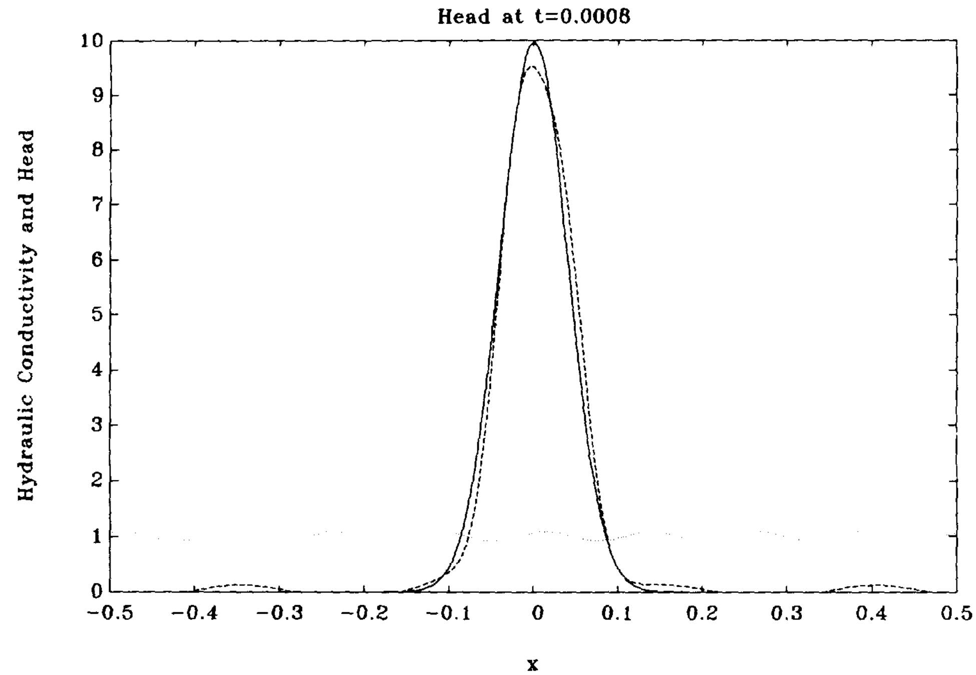

Fig. 1. Head at t = 0.0008. The dashed curve is the actual head, the solid curve is the head if the mean value of the hydraulic conductivity were used, and the dotted curve is the value of the hydraulic conductivity.

average D is also plotted, for comparison purposes. At early times (t = 0.0008 and t = 0.004) the head function depends critically on the conductivity at or near the point of injection. As time passes (t = 0.02 and especially t = 0.1), the mound spreads over an area many times the scale of conductivity fluctuations. Locally, the head still depends on the conductivity, as the head gradient must be steeper in areas of low conductivity and milder in areas of high. However, one can see in Figure 4 that if one is willing to disregard the local effects, by averaging over a scale equal to the scale of conductivity fluctuations, then a nearly bell-shaped function will be obtained. In this sense, it may be possible to represent the actual locally heterogeneous medium by an equivalent homogeneous one.

The determination of the effective or macroscopic conductivity is a difficult problem. In one-dimensional flow, it is

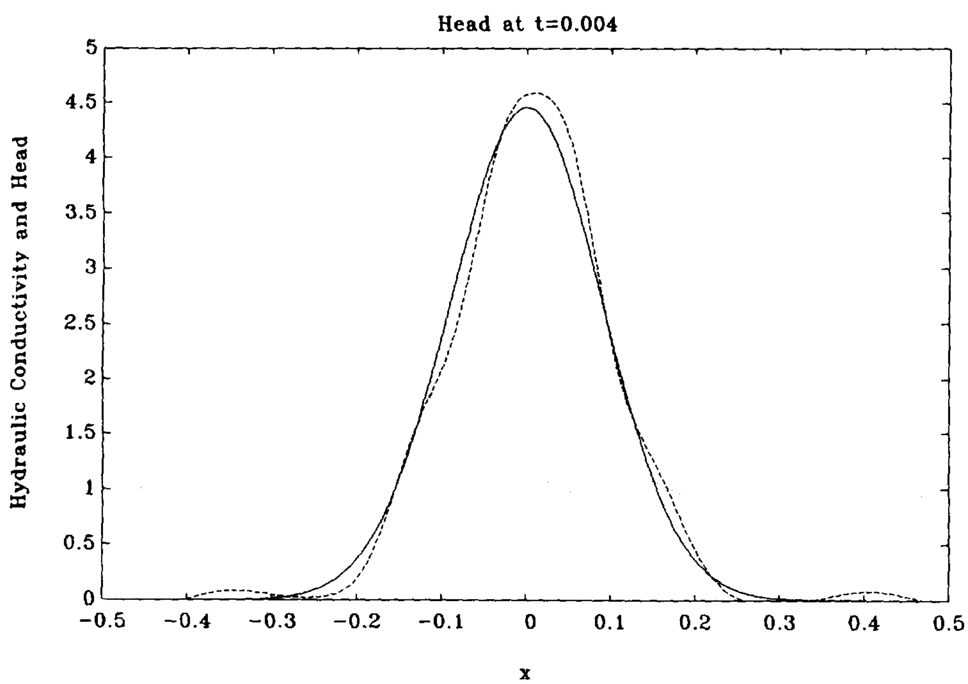

Fig. 2. Head at t = 0.004. The dashed curve is the actual head, the solid curve is the head if the mean value of the hydraulic conductivity were used, and the dotted curve is the value of the hydraulic conductivity.

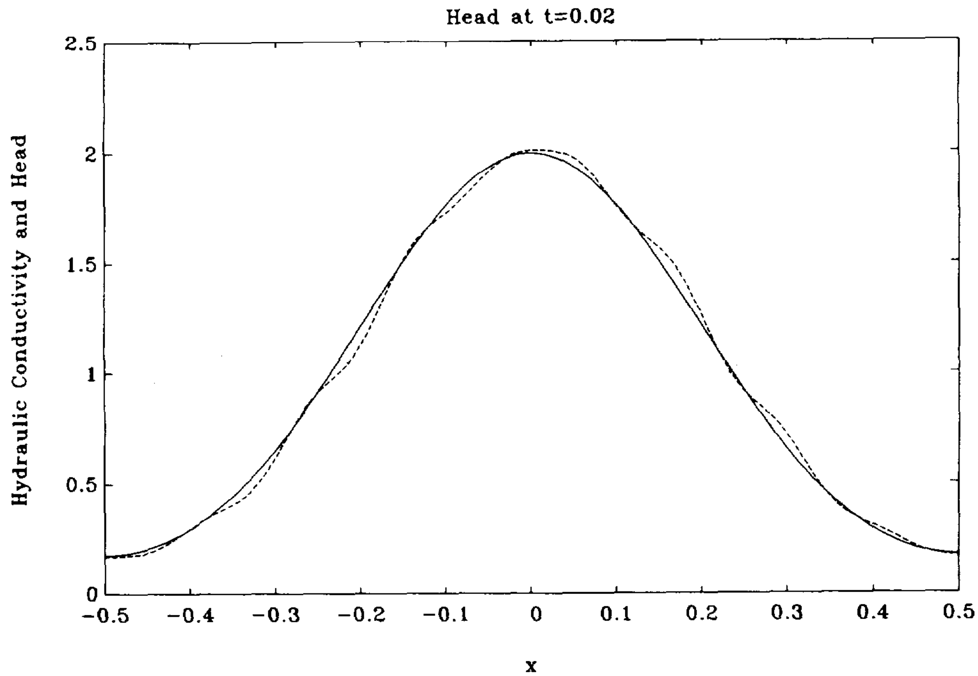

Fig. 3. Head at $t = 0.02$. The dashed curve is the actual head, the solid curve is the head if the mean value of the hydraulic conductivity were used, and the dotted curve is the value of the hydraulic conductivity.

known to be the harmonic mean of the local conductivity, but in higher dimensions of interest in applications an answer is not easily obtained.

This problem has been addressed in the literature, and a number of useful approaches have been suggested. Pioneering works include *Warren and Price* [1961] and *Matheron* [1967] who also refers to *Schwydler* [1962]. Most of the approaches have dealt with locally isotropic medium, i.e., **K** is diagonal with elements $K(\mathbf{x})$. *Gelhar* [1976] and *Gutjahr et al.* [1978] linearized the relation between K and ϕ in uniform steady flow by neglecting products of perturbations of K and ϕ. Then, by using the ensemble average of the discharge, they determined an effective hydraulic conductivity matrix. This analysis requires only the covariance function of $K(\mathbf{x})$. Among other interesting results, they found that for three-dimensional flow in a medium with the same integral scale

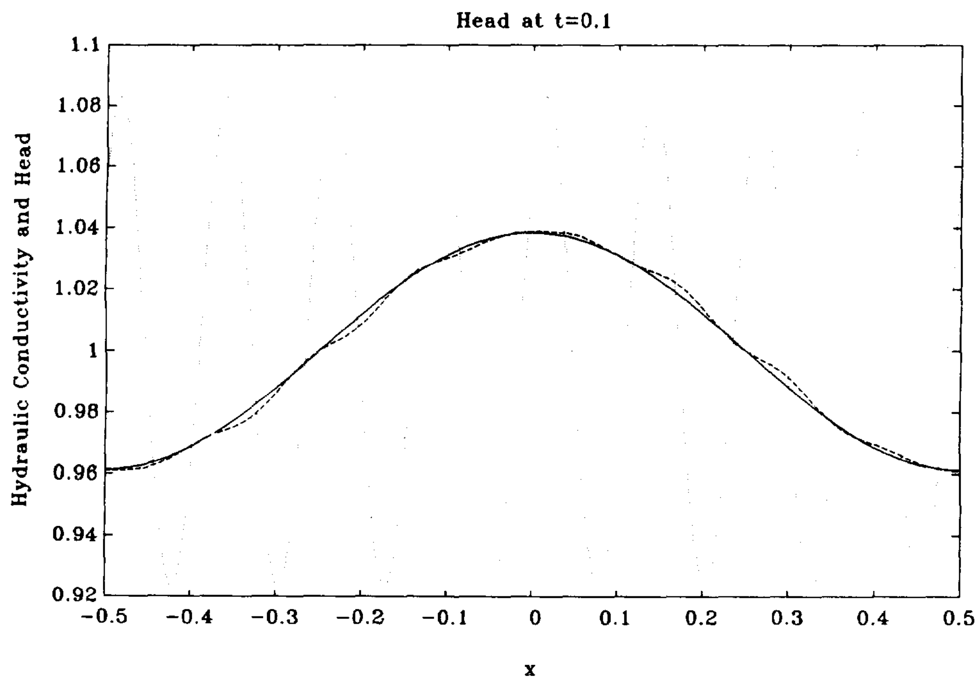

Fig. 4. Head at $t = 0.1$. The dashed curve is the actual head, the solid curve is the head if the mean value of the hydraulic conductivity were used, and the dotted curve is the value of the hydraulic conductivity.

(correlation length) in each direction, the effective hydraulic conductivity is $(1 + \sigma_Y^2/6)$ times the geometric mean, where σ_Y^2 is the variance of the logarithm of K. The result is accurate to the first order of σ_Y^2. The perturbation method is powerful and appealing, but its validity is predicted on small values of σ_Y^2.

Analysis for large-variance cases is considerably more difficult. A common approach uses numerical models [e.g., *Freeze*, 1975; *Desbarats*, 1987]. *Smith and Freeze* [1979] have used straightforward Monte Carlo simulations with a numerical groundwater flow model. Among other results, their numerical experiments have indicated that the effective transmissivity for isotropic (two-dimensional) Gaussian log conductivity is given by the geometric mean. *Dagan* [1979, 1981] has applied the method of the embedding matrix to derive bounds on the effective conductivity and a self-consistent approximation for its approximate calculation. This analysis, which is in the best tradition of statistical mechanics, is not limited by the assumption of small fluctuations but assumes a particular spatial structure and uses only information from the volume fraction of each conductivity value. The results of Dagan's papers agree with the results of the perturbation methods of Gelhar, Gutjahr, and others to the first order of σ_Y^2.

Most of the previously mentioned works focused on steady flow problems. *Dagan* [1982] dealt with the unsteady flow problem in macroscopically uniform flow using the small-perturbation approximation. Among other results, he estimated the "relaxation time" which must elapse after some change in the system so that an effective conductivity can be defined.

In this work, a new approach is proposed. The derived equations are as general as in any other currently available method. An advantage of the derivation is that it is based on volume averaging and makes use of engineering calculus. In this paper the governing equations will be derived and will be verified through application to some problems for which solutions are currently available.

2. FORMULATION AND DEFINITION OF MOMENTS

In the derivation, it will be convenient to take advantage of the mathematical formalism of periodic media, previously used in the determination of solute dispersion in variable-velocity media [*Brenner*, 1980*b*, 1982*b*; *Bhattacharya*, 1985; *Gupta and Bhattacharya*, 1986]. Of course, a periodic medium, is only a conceptual or mathematical model of a formation whose parameters fluctuate about an average value. It is premature to discuss its applicability, which can only be appreciated after results have been obtained and subjected to sensitivity analysis. Suffice it to say that the results of the present analysis will be shown to include the results of the stochastic small-perturbation method. (The key results are summarized in section 5.)

Consider unsteady flow in a formation with constant specific storage S and conductivity $\mathbf{K}$ which varies periodically in all directions (see Figure 5) and is differentiable. Define the periodic "diffusion matrix" $\mathbf{D} = \mathbf{K}/S$. Let l_i be the period in direction i. That is,

$$\mathbf{D}(X_1, X_2, X_3) = \mathbf{D}(X_1 + m_1 l_1, X_2 + m_2 l_2, X_3 + m_3 l_3) \tag{7}$$

where $\mathbf{D} = (\mathbf{d}_1, \mathbf{d}_2, \mathbf{d}_3)$ is the symmetric diffusion matrix, consisting of three vectors; $\mathbf{X} = (X_1, X_2, X_3)$ are the spatial

Variable Hydraulic Conductivity

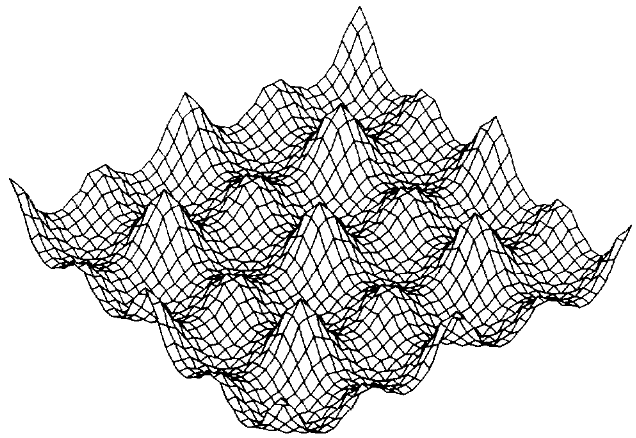

Fig. 5. An example of a two-dimensional periodic hydraulic conductivity. A group of four elements is shown.

coordinates in a Cartesian coordinate system, and m_1, m_2, and m_3 are integers (positive, negative, or zero). The analysis will be carried out for a three-dimensional flow field, but the result can be easily reduced to apply to one- or two-dimensional flow.

In the introduction, it was mentioned that in the search for effective parameters, local variability must be averaged out. Consider the superimposition of a rectangular grid with spacing l_i in direction i. The grid subdivides the domain into elements, rectangular parallelepipeds with lengths of sides l_1, l_2, and l_3. Assuming that the origin of the universal coordinate system coincides with the center of an element, the coordinates of the center of any element are $(n_1 l_1, n_2 l_2, n_3 l_3)$ where $n_1, n_2, n_3 = \cdots, -2, -1, 0, 1, 2, \cdots$. Consequently, each element is identified with a triplet of integers (n_1, n_2, n_3), or $\mathbf{n}$,

For the sake of convenience, a system of local coordinates (x_1, x_2, x_3) will be introduced for each element. The origin of this Cartesian system is at the center of the element and the three axes are parallel to the axes of the universal system. Now each point with $\mathbf{X} = (X_1, X_2, X_3)$ can be represented as $(\mathbf{n}, \mathbf{x}) = (n_1, n_2, n_3, x_1, x_2, x_3)$ where $\mathbf{n} = (n_1, n_2, n_3)$ specifies the element and $\mathbf{x} = (x_1, x_2, x_3)$ specifies the location within the element. The relation between universal and local coordinates is given by

$$X_i = n_i l_i + x_i \qquad i = 1, 2, 3 \tag{8}$$

where in this work n_1, n_2, n_3 are always integers and x_1, x_2, and x_3 always satisfy the conditions $-l_1/2 \le x_1 \le l_1/2$, $-l_2/2 \le x_2 \le l_2/2$, and $-l_3/2 \le x_3 \le l_3/2$.

$\mathbf{D}$ at local coordinate $\mathbf{x}$ is the same for all elements. Thus one may suppress the dependence of the diffusion on the number of the element and show only the dependence on the local coordinates

$$\mathbf{D}(n_1, n_2, n_3, x_1, x_2, x_3) = \mathbf{D}(x_1, x_2, x_3) \tag{9}$$

where the following conditions are due to continuity

$$\mathbf{D}(l_1/2, x_2, x_3) = \mathbf{D}(-l_1/2, x_2, x_3) \tag{10a}$$

$$\mathbf{D}(x_1, l_2/2, x_3) = \mathbf{D}(x_1, -l_2/2, x_3) \tag{10b}$$

$$\mathbf{D}(x_1, x_2, l_3/2) = \mathbf{D}(x_1, x_2, -l_3/2) \tag{10c}$$

The same conditions hold for the gradient of $\mathbf{D}$.

Let $\phi(X_1, X_2, X_3, t)$ or $\phi(n_1, n_2, n_3, x_1, x_2, x_3, t)$ be the head. As already mentioned, it is convenient and involves no loss of generality, to consider the case of point injection of unit volume so that from continuity,

$$\int \phi(\mathbf{X}, t)\, d\mathbf{X} = 1 \tag{11}$$

Within each element, the governing equation is

$$\frac{\partial \phi}{\partial t} - \nabla \cdot (\mathbf{D}\nabla\phi) = 0 \tag{12}$$

where ∇ is the vector differential operator $\nabla = (\partial/\partial x_1, \partial/\partial x_2, \partial/\partial x_3)^T$, with respect to the local coordinates. Equation (12) has assumed that $\mathbf{D}$ is not affected by ϕ (i.e., the resistance to flow does not depend on the value of the head) and that no water is added or subtracted after the initial time.

Equation (12) is satisfied in the interior of each element. At the interface of two adjacent elements, it is required that the head and the flux be the same no matter what system of local coordinates they are calculated in. These conditions mean that the head and its gradient must satisfy

$$\phi(n_1, n_2, n_3, l_1/2, x_2, x_3, t) = \phi(n_1 + 1, n_2, n_3, -l_1/2, x_2, x_3, t) \tag{13a}$$

$$\phi(n_1, n_2, n_3, x_1, l_2/2, x_3, t) = \phi(n_1, n_2 + 1, n_3, x_1, -l_2/2, x_3, t) \tag{13b}$$

$$\phi(n_1, n_2, n_3, x_1, x_2, l_3/2, t) = \phi(n_1, n_2, n_3 + 1, x_1, x_2, -l_3/2, t) \tag{13c}$$

and exactly the same conditions must be satisfied if in (13a)–(13c) ϕ is substituted by $\partial\phi/\partial x_i$, $i = 1, 2, 3$.

Finally, the head (above the background value) at very large distances from the origin vanishes:

$$\phi(n_1, n_2, n_3, x_1, x_2, x_3, t) = 0 \quad \text{as } n_1, n_2, n_3 \to \pm\infty \tag{14}$$

It is assumed that the rate of decrease of ϕ to zero is such that spatial moments can be defined.

A method similar to the method of moments originally proposed by *Aris* [1956] for the determination of dispersion and subsequently generalized by *Brenner* [1980a, b] will be followed. Among other applications, this method has been applied in transport problems in stratified porous media [*Güven et al.*, 1984; *Valocchi*, 1989]. In this approach, two types of moments, local and global, are introduced.

Local moments depend on the vector of local coordinates as well as on time. The zeroth-order moment is a scalar defined as the sum of head at all points with local coordinates $\mathbf{x}$,

$$a(\mathbf{x}, t) = \sum_{\mathbf{n}} \phi(\mathbf{n}, \mathbf{x}, t) \tag{15}$$

where by $\sum_{\mathbf{n}}$ denote the triple summation $\sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} \sum_{n_3=-\infty}^{\infty}$. The $a(\mathbf{x}, t)$ represents the distribution of the volume with respect to local coordinates. More precisely, $a(\mathbf{x}, t)\, d\mathbf{x}$ is the water volume which at time t is contained in small cubes $d\mathbf{x}$ about local coordinates $\mathbf{x}$, for all elements.

The first moment is a three-dimensional vector $\mathbf{b}(\mathbf{x}, t)$ whose ith element is defined as follows:

$$b_i = [\mathbf{b}(\mathbf{x}, t)]_i = \sum_{\mathbf{n}} (n_i l_i)\phi(\mathbf{n}, \mathbf{x}, t) \tag{16}$$

For example,

$$b_1 = l_1 \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} \sum_{n_3=-\infty}^{\infty} n_1 \phi(n_1, n_2, n_3, x_1, x_2, x_3, t) \tag{17}$$

The second moment is a 3×3 symmetric matrix whose ijth element is defined as follows:

$$C_{ij} = [\mathbf{C}(\mathbf{x}, t)]_{ij} = \sum_{\mathbf{n}} (n_i l_i)(n_j l_j)\phi(\mathbf{n}, \mathbf{x}, t) \tag{18}$$

For example,

$$C_{11} = l_1^2 \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} \sum_{n_3=-\infty}^{\infty} n_1^2 \cdot \phi(n_1, n_2, n_3, x_1, x_2, x_3, t) \tag{19}$$

$$C_{12} = l_1 l_2 \sum_{n_1=-\infty}^{\infty} \sum_{n_2=-\infty}^{\infty} \sum_{n_3=-\infty}^{\infty} n_1 n_2 \cdot \phi(n_1, n_2, n_3, x_1, x_2, x_3, t) \tag{20}$$

and so on. Higher moments could be defined in a similar way but they will not be required in this analysis.

Global moments are defined from the integral of local moments over the local coordinates. That is,

$$\alpha(t) = \int_V a(\mathbf{x}, t)\, d\mathbf{x} \tag{21}$$

$$\beta(t) = \int_V \mathbf{b}(\mathbf{x}, t)\, d\mathbf{x} \tag{22}$$

$$\Gamma(t) = \int_V \mathbf{C}(\mathbf{x}, t)\, d\mathbf{x} \tag{23}$$

where V is the volume of an element.

Consider the physical meaning of the global moments. For each element $\mathbf{n}$, define $\bar{\phi}$ as

$$\bar{\phi}(\mathbf{n}, t) = \int_V \phi(\mathbf{n}, \mathbf{x}, t)\, d\mathbf{x} \tag{24}$$

This is the volume of water in element $\mathbf{n}$ at time t. If this volume is assumed located at the center of the element, then α, β, Γ are the spatial moments. The zero moment, α, represents the total volume and is equal to 1 at all times (see (11)). The first moment, $\beta(t)$, is the vector of coordinates of the centroid (center of mass) of the mound and can be written

$$\beta(t) = \sum_{\mathbf{n}} \bar{\phi}(\mathbf{n}, t)\mathbf{X}(\mathbf{n}) \tag{25}$$

where $\mathbf{X}(\mathbf{n})$ is the vector of global coordinates of the center of element $\mathbf{n}$.

The second moment is the matrix of the mean square displacements about the origin of the global coordinate system and can be written as

$$\Gamma(t) = \sum_{\mathbf{n}} \bar{\phi}(\mathbf{n}, t)\mathbf{X}(\mathbf{n})\mathbf{X}(\mathbf{n})^T \tag{26}$$

To measure the spreading of the mound about its center, define the central second global moment

$$\Delta(t) = \sum_{\mathbf{n}} \bar{\phi}(\mathbf{n}, t)[\mathbf{X}(\mathbf{n}) - \beta(t)][\mathbf{X}(\mathbf{n}) - \beta(t)]^T = \Gamma(t) - \beta(t)\beta(t)^T \tag{27}$$

Thus the global moments are defined for head after averaging within each element.

3. Equations Satisfied by the Local Moments

First off, obtain the equations satisfied by the local moments. For fixed $\mathbf{x}$, summation over all elements gives:

$$\sum_{\mathbf{n}} \left[\frac{\partial \phi}{\partial t} - \nabla \cdot (\mathbf{D}\nabla\phi)\right] = 0 \tag{28}$$

Since $\mathbf{D}$ does not depend on $\mathbf{n}$ and ∇ is with respect to local coordinates,

$$\frac{\partial}{\partial t}\left[\sum_{\mathbf{n}} \phi(\mathbf{n}, \mathbf{x}, t)\right] - \nabla \cdot \left[\mathbf{D}\nabla \sum_{\mathbf{n}} \phi(\mathbf{n}, \mathbf{x}, t)\right] = 0 \tag{29}$$

$$\frac{\partial a}{\partial t} - \nabla \cdot (\mathbf{D}\nabla a) = 0 \tag{30}$$

where $a(\mathbf{x}, t)$ satisfies partial differential equation (30) and the following boundary conditions:

$$a(l_1/2, x_2, x_3, t) = a(-l_1/2, x_2, x_3, t) \tag{31a}$$

$$a(x_1, l_2/2, x_3, t) = a(x_1, -l_2/2, x_3, t) \tag{31b}$$

$$a(x_1, x_2, l_3/2, t) = a(x_1, x_2, -l_3/2, t) \tag{31c}$$

$$\left.\frac{\partial a}{\partial x_i}\right|_{l_1/2, x_2, x_3, t} = \left.\frac{\partial a}{\partial x_i}\right|_{-l_1/2, x_2, x_3, t} \tag{32a}$$

$$\left.\frac{\partial a}{\partial x_i}\right|_{x_1, l_2/2, x_3, t} = \left.\frac{\partial a}{\partial x_i}\right|_{x_1, -l_2/2, x_3, t} \tag{32b}$$

$$\left.\frac{\partial a}{\partial x_i}\right|_{x_1, x_2, l_3/2, t} = \left.\frac{\partial a}{\partial x_i}\right|_{x_1, x_2, -l_3/2, t} \tag{32c}$$

where $i = 1, 2, 3$. These conditions are obtained through summation of (13*a*)–(13*c*) over $\mathbf{n}$.

To determine the equation satisfied by the components of the first local moment, a similar procedure will be followed. For the first component, b_1 satisfies exactly the same form of a differential equation as a:

$$\frac{\partial b_1}{\partial t} - \nabla \cdot (\mathbf{D}\nabla b_1) = 0 \tag{33}$$

but with different boundary conditions:

$$b_1(l_1/2, x_2, x_3, t) = b_1(-l_1/2, x_2, x_3, t) - a(-l_1/2, x_2, x_3, t)l_1 \tag{34a}$$

$$b_1(x_1, l_2/2, x_3, t) = b_1(x_1, -l_2/2, x_3, t) \tag{34b}$$

$$b_1(x_1, x_2, l_3/2, t) = b_1(x_1, x_2, -l_3/2, t) \tag{34c}$$

$$\left.\frac{\partial b_1}{\partial x_i}\right|_{l_1/2, x_2, x_3, t} = \left.\frac{\partial b_1}{\partial x_i}\right|_{-l_1/2, x_2, x_3, t} - \left.\frac{\partial a}{\partial x_i}\right|_{-l_1/2, x_2, x_3, t} l_1 \tag{35a}$$

$$\left.\frac{\partial b_1}{\partial x_i}\right|_{x_1, l_2/2, x_3, t} = \left.\frac{\partial b_1}{\partial x_i}\right|_{x_1, -l_2/2, x_3, t} \tag{35b}$$

$$\left.\frac{\partial b_1}{\partial x_i}\right|_{x_1, x_2, l_3/2, t} = \left.\frac{\partial b_1}{\partial x_i}\right|_{x_1, x_2, -l_3/2, t} \tag{35c}$$

By analogy, obtain the partial differential equation and the boundary conditions which must be satisfied by b_2 and b_3.

Now consider the second local moment. Each of its elements, C_{ij}, satisfies

$$\frac{\partial C_{ij}}{\partial t} - \nabla \cdot (\mathbf{D}\nabla C_{ij}) = 0 \tag{36}$$

with given boundary conditions. Consider, first, the case of C_{11}.

$$C_{11}(l_1/2, x_2, x_3, t) = C_{11}(-l_1/2, x_2, x_3, t) - 2b_1(-l_1/2, x_2, x_3, t)l_1 + a(-l_1/2, x_2, x_3, t)l_1^2 \tag{37a}$$

$$C_{11}(x_1, l_2/2, x_3, t) = C_{11}(x_1, -l_2/2, x_3, t) \tag{37b}$$

$$C_{11}(x_1, x_2, l_3/2, t) = C_{11}(x_1, x_2, -l_3/2, t) \tag{37c}$$

$$\left.\frac{\partial C_{11}}{\partial x_i}\right|_{l_1/2, x_2, x_3, t} = \left.\frac{\partial C_{11}}{\partial x_i}\right|_{-l_1/2, x_2, x_3, t} - 2\left.\frac{\partial b_1}{\partial x_i}\right|_{-l_1/2, x_2, x_3, t} l_1 + \left.\frac{\partial a}{\partial x_i}\right|_{-l_1/2, x_2, x_3, t} l_1^2 \tag{38a}$$

$$\left.\frac{\partial C_{11}}{\partial x_i}\right|_{x_1, l_2/2, x_3, t} = \left.\frac{\partial C_{11}}{\partial x_i}\right|_{x_1, -l_2/2, x_3, t} \tag{38b}$$

$$\left.\frac{\partial C_{11}}{\partial x_i}\right|_{x_1, x_2, l_3/2, t} = \left.\frac{\partial C_{11}}{\partial x_i}\right|_{x_1, x_2, -l_3/2, t} \tag{38c}$$

By analogy, obtain the boundary value problems for the other diagonal elements.

The boundary conditions for C_{12} are

$$C_{12}(l_1/2, x_2, x_3, t) = C_{12}(-l_1/2, x_2, x_3, t) - b_2(-l_1/2, x_2, x_3, t)l_1 \tag{39a}$$

$$C_{12}(x_1, l_2/2, x_3, t) = C_{12}(x_1, -l_2/2, x_3, t) - b_1(x_1, -l_2/2, x_3, t)l_2 \tag{39b}$$

$$C_{12}(x_1, x_2, l_3/2, t) = C_{12}(x_1, x_2, -l_3/2, t) \tag{39c}$$

$$\left.\frac{\partial C_{12}}{\partial x_i}\right|_{l_1/2, x_2, x_3, t} = \left.\frac{\partial C_{12}}{\partial x_i}\right|_{-l_1/2, x_2, x_3, t} - \left.\frac{\partial b_2}{\partial x_i}\right|_{-l_1/2, x_2, x_3, t} l_1 \tag{40a}$$

$$\left.\frac{\partial C_{12}}{\partial x_i}\right|_{x_1,l_2/2,x_3,t} = \left.\frac{\partial C_{12}}{\partial x_i}\right|_{x_1,-l_2/2,x_3,t} - \left.\frac{\partial b_1}{\partial x_i}\right|_{x_1,-l_2/2,x_3,t} l_2 \quad (40b)$$

$$\left.\frac{\partial C_{12}}{\partial x_i}\right|_{x_1,x_2,l_3/2,t} = \left.\frac{\partial C_{12}}{\partial x_i}\right|_{x_1,x_2,-l_3/2,t} \quad (40c)$$

and similarly for all other off-diagonal elements of the second-moment matrix C.

4. Equations for Rates of Change of the Global Moments and Results for Gradual Flow

Rates of Change of Global Moments

From (30),

$$\int_V \left[\frac{\partial a}{\partial t} - \nabla \cdot (\mathbf{D}\nabla a)\right] d\mathbf{x} = 0 \quad (41)$$

Integrating each term and applying the divergence theorem,

$$\frac{\partial \alpha}{\partial t} = \int_V \nabla \cdot (\mathbf{D}\nabla a)\, d\mathbf{x} = \int_S (\mathbf{D}\nabla a) \cdot \boldsymbol{\eta}\, dS \quad (42)$$

where S is the surface which surrounds the parallelepipedal element, $\boldsymbol{\eta}$ is a unit vector normal to the surface and pointed outward, and dS is an infinitesimal area on the surface which surrounds the element. Because of symmetry in $\mathbf{D}$ and ∇a on the boundary, this integral vanishes and obtains the anticipated result

$$\frac{d\alpha}{dt} = 0 \quad (43)$$

In a similar fashion the rate of increase of β_1, the first element of the first moment, is

$$\frac{d\beta_1}{dt} = \int_S (\mathbf{D}\nabla b_1) \cdot \boldsymbol{\eta}\, dS = \int_{-l_2/2}^{l_2/2}\int_{-l_3/2}^{l_3/2} \sum_{i=1}^{3} D_{1i} \cdot \left(\left.\frac{\partial b_1}{\partial x_i}\right|_{l_1/2,x_2,x_3,t} - \left.\frac{\partial b_1}{\partial x_i}\right|_{-l_1/2,x_2,x_3,t}\right) dx_2\, dx_3$$

$$= -l_1 \int_{-l_2/2}^{l_2/2}\int_{-l_3/2}^{l_3/2} \mathbf{d}_1 \cdot \nabla a\Big|_{-l_1/2,x_2,x_3,t} dx_2\, dx_3 \quad (44a)$$

where $\mathbf{d}_1$ is the vector formed by the first column of the symmetric diffusion matrix $\mathbf{D}$.

Similarly, for the other components,

$$\frac{d\beta_2}{dt} = -l_2 \int_{-l_1/2}^{l_1/2}\int_{-l_3/2}^{l_3/2} \mathbf{d}_2 \cdot \nabla a\Big|_{x_1,-l_2/2,x_3,t} dx_1\, dx_3 \quad (44b)$$

$$\frac{d\beta_3}{dt} = -l_3 \int_{-l_1/2}^{l_1/2}\int_{-l_2/2}^{l_2/2} \mathbf{d}_3 \cdot \nabla a\Big|_{x_1,x_2,-l_3/2,t} dx_1\, dx_2 \quad (44c)$$

What is particularly interesting is that the rate of increase of the first global moment depends only on the zero local moment. The same is true in the analysis of the problem examined in the classical works of *Taylor* [1953] and *Aris* [1956].

Consider now the second moment. The rate of increase of Γ_{11} is

$$\frac{d\Gamma_{11}}{dt} = \int_S (\mathbf{D}\nabla C_{11}) \cdot \boldsymbol{\eta}\, dS = \int_{-l_2/2}^{l_2/2}\int_{-l_3/2}^{l_3/2} \sum_{i=1}^{3} D_{1i} \cdot \left(\left.\frac{\partial C_{11}}{\partial x_i}\right|_{l_1/2,x_2,x_3,t} - \left.\frac{\partial C_{11}}{\partial x_i}\right|_{-l_1/2,x_2,x_3,t}\right) dx_2\, dx_3$$

$$= \int_{-l_2/2}^{l_2/2}\int_{-l_3/2}^{l_3/2} \mathbf{d}_1 \cdot \nabla(-2b_1 l_1 + a l_1^2)\Big|_{-l_1/2,x_2,x_3,t} dx_2\, dx_3 \quad (45)$$

and similarly for Γ_{22} and Γ_{33}.

For rate of increase of Γ_{12},

$$\frac{d\Gamma_{12}}{dt} = \int_S (\mathbf{D}\nabla C_{12}) \cdot \boldsymbol{\eta}\, dS = \int_{-l_2/2}^{l_2/2}\int_{-l_3/2}^{l_3/2} \sum_{i=1}^{3} D_{1i} \cdot \left(\left.\frac{\partial C_{12}}{\partial x_i}\right|_{l_1/2,x_2,x_3,t} - \left.\frac{\partial C_{12}}{\partial x_i}\right|_{-l_1/2,x_2,x_3,t}\right) dx_2\, dx_3$$

$$+ \int_{-l_1/2}^{l_1/2}\int_{-l_3/2}^{l_3/2} \sum_{i=1}^{3} D_{2i} \cdot \left(\left.\frac{\partial C_{12}}{\partial x_i}\right|_{x_1,l_2/2,x_3,t} - \left.\frac{\partial C_{12}}{\partial x_i}\right|_{x_1,-l_2/2,x_3,t}\right) dx_1\, dx_3$$

$$= -l_1 \int_{-l_2/2}^{l_2/2}\int_{-l_3/2}^{l_3/2} \mathbf{d}_1 \cdot \nabla b_2\Big|_{-l_1/2,x_2,x_3,t} dx_2\, dx_3 - l_2 \int_{-l_1/2}^{l_1/2}\int_{-l_3/2}^{l_3/2} \mathbf{d}_2 \cdot \nabla b_1\Big|_{x_1,-l_2/2,x_3,t} dx_1\, dx_3 \quad (46)$$

In a similar fashion, obtain the equations for all other elements.

Results for Gradually Varied Flow

As the mound spreads, the distribution $a(\mathbf{x}, t)$ gradually becomes more uniform. One may show (see appendix), that the "large-time" solution to the boundary value problem of (30)–(32) is

$$a(\mathbf{x}, t) = \frac{1}{l_1 l_2 l_3} + T(\mathbf{x}, t) \simeq \frac{1}{l_1 l_2 l_3} \quad (47)$$

where the transient term $T(\mathbf{x}, t)$ decays exponentially with time and is negligible once t exceeds a relaxation time $\bar{l}^2/\bar{D}$, where $\bar{l}$ is the periodicity and $\bar{D}$ is a typical value of the diffusion. Thus the distribution of water volume over the local coordinates is uniform. Note that this is the essence of what will be referred to as "gradually varying" flow.

Once the steady state value of $a(\mathbf{x}, t)$ is determined, the rate of change of β can be calculated from (44) and (47):

$$\frac{d\beta_i}{dt} = 0 \tag{48}$$

Thus after the mound has spread enough to sample all conductivities, its centroid ceases to move.

The first local moment can now be determined from the solution of a boundary value problem, equations (33) through (35). Starting with b_1, one may verify that for gradually varying flow

$$b_1(x_1, x_2, x_3) = \{\text{const} - x_1 + g_1(x_1, x_2, x_3)\}/l_1 l_2 l_3 \tag{49}$$

where g is a function of local spatial coordinates which satisfies the differential equation

$$\nabla \cdot (\mathbf{D}\nabla g_1) = \nabla \cdot \mathbf{d}_1 \tag{50}$$

where, as already mentioned, $\mathbf{d}_1$ is the first column of the spatially variable $\mathbf{D}$, subject to the symmetric boundary conditions:

$$g_1(l_1/2, x_2, x_3) = g_1(-l_1/2, x_2, x_3) \tag{51a}$$

$$g_1(x_1, l_2/2, x_3) = g_1(x_1, -l_2/2, x_3) \tag{51b}$$

$$g_1(x_1, x_2, l_3/2) = g_1(x_1, x_2, -l_3/2) \tag{51c}$$

$$\left.\frac{\partial g_1}{\partial x_i}\right|_{l_1/2, x_2, x_3} = \left.\frac{\partial g_1}{\partial x_i}\right|_{-l_1/2, x_2, x_3} \tag{52a}$$

$$\left.\frac{\partial g_1}{\partial x_i}\right|_{x_1, l_2/2, x_3} = \left.\frac{\partial g_1}{\partial x_i}\right|_{x_1, -l_2/2, x_3} \tag{52b}$$

$$\left.\frac{\partial g_1}{\partial x_i}\right|_{x_1, x_2, l_3/2} = \left.\frac{\partial g_1}{\partial x_i}\right|_{x_1, x_2, -l_3/2} \tag{52c}$$

The rate of increase of Γ_{11} may be written as follows

$$\frac{d\Gamma_{11}}{dt} = -2\int_{\mathbf{V}} \mathbf{d}_1 \cdot \nabla b_1 \, d\mathbf{x} \tag{53}$$

after substituting areal by volume averages, which can be shown to be appropriate under gradually varying flow conditions. Then, from the definition of the second central moment and substituting in terms of g_1,

$$\frac{d\Gamma_{11}}{dt} = -\frac{2}{l_1 l_2 l_3}\int_{\mathbf{V}} \mathbf{d}_1 \cdot \nabla(-x_1 + g_1)\, d\mathbf{x}$$

$$= -\frac{2}{l_1 l_2 l_3}\int_{\mathbf{V}} \mathbf{d}_1 \cdot \nabla g_1 \, d\mathbf{x} + 2\bar{D}_{11} \tag{54}$$

where $\bar{D}_{11}$ is the spatial average of D_{11} ($\bar{D}_{11} = (1/V)\int_{\mathbf{V}} D_{11}(\mathbf{x})\, d\mathbf{x}$). However,

$$\frac{d\Delta_{ij}}{dt} = \frac{d\Gamma_{ij}}{dt} - \beta_i \frac{d\beta_j}{dt} - \beta_j \frac{d\beta_i}{dt} = \frac{d\Gamma_{ij}}{dt}$$

$$= -\frac{2}{l_1 l_2 l_3}\int_{\mathbf{V}} \mathbf{d}_1 \cdot \nabla g_1 \, d\mathbf{x} + 2\bar{D}_{11} \tag{55}$$

and similarly for the other elements. In general, the result is

$$D^e_{ij} = \frac{1}{2}\frac{d\Delta_{ij}}{dt} = -\frac{1}{2 l_1 l_2 l_3}\int_{\mathbf{V}} [\mathbf{d}_i \cdot \nabla g_j + \mathbf{d}_j \cdot \nabla g_i]\, d\mathbf{x} + \bar{D}_{ij} \tag{56}$$

where the three-dimensional matrix $\mathbf{D}^e$ is the effective diffusion matrix. Since the specific storage is assumed constant, we can substitute hydraulic conductivities for diffusivities.

It must be pointed out that the result was derived for a Dirac initial condition $\delta(\mathbf{x} - \mathbf{x}')$. However, an important result is that the rate of change of the global moments for gradually varying flow does not depend on the original location of the input, $\mathbf{x}'$. Consider the case of an arbitrary initial condition $\phi_0(\mathbf{x})$. This can be written as the summation of many Diracs, $\phi_0(\mathbf{x}) = \int_{\mathbf{V}_\infty} \phi_0(\mathbf{x}')\, \delta(\mathbf{x} - \mathbf{x}')\, d\mathbf{x}'$. Using the principle of superposition, one can verify that the analysis is applicable for any initial condition (see *Dagan* [1987] and *Kitanidis* [1988]).

5. KEY RESULTS

In this section we will review the key results of this work and will discuss how the method can be applied in the case of nonperiodic and random media.

Basic Result

The key result of section 4 was that the effective diffusion matrix of the variable-conductivity medium is given by computing a volume integral given by (56). Functions g_i are determined from the partial differential equation

$$\nabla \cdot (\mathbf{D}\nabla g_i) = \nabla \cdot \mathbf{d}_i \tag{57}$$

defined over the elementary volume and subject to symmetric boundary conditions (see, for example, (51) and (52)). Thus the problem reduces to solving a well-defined boundary value problem and carrying out an integration. Even if those have to be performed numerically, this approach is potentially a significant improvement over other numerical methods because (1) all computations are performed within one elementary volume or spatial period; and (2) even though the original problem is an unsteady flow one, the boundary value problem to obtain the effective conductivity involves no time derivatives. Examples of how to apply these equations to find effective conductivities will be presented later.

Extension to Nonperiodic and Random Media

We are ready now to discuss the significance of the periodic assumption. Our discussion will be based on intuitive arguments rather than rigorous mathematical analysis. Consider that $\mathbf{D}$ is not truly periodic but still varies about a mean value $\bar{\mathbf{D}}$ in a "stationary" fashion. (The assumption of stationary variability underlies every attempt to define effective properties.) Despite the fact that the medium is not truly periodic, one can still superimpose a regular grid and apply the methodology using the D values over one of the elements. One can then solve the associated boundary value problems and calculate the integral. If the size of the grid is large enough, it is quite possible that the value of the volume integral of (56) will tend to a constant value. This value will be practically independent of the spacing of the grid and of which element was used in the computation.

There are some deep questions regarding the mathematical conditions under which such a volume integral will indeed converge for a (nonperiodic) stationary medium [see *Koch et al.*, 1989]. It is well beyond the scope of this work to investigate these conditions (except in some special cases to be examined in section 6). Suffice it to say that every effort to define effective macroscopic parameters of a locally heterogeneous medium is predicated on the tacit assumption that convergence can be achieved. The prevailing attitude is that it is of greater practical interest to investigate whether a practically useful result can be obtained for a reasonably small volume of averaging. The thrust of this work was to provide the means for the computation of the effective hydraulic conductivity for a given volume of averaging and variable local hydraulic conductivity.

A related issue is that of stochastic analysis. This work followed a purely deterministic approach, i.e., the local hydraulic conductivity was assumed precisely specified at every point. However, inspection of the final result indicates that a less precise definition of the local properties might be quite sufficient to obtain the desired result. That is, because the final result is in terms of a volume average, the specification of some volume-average properties of the hydraulic conductivity may suffice. Thus a "statistical" specification of the local conductivity may be quite adequate. Further analysis will be required to establish which averages are needed for determination of the effective hydraulic conductivity. An example will be presented when the small-fluctuation case is examined.

6. Some Solutions for Locally Isotropic Medium

In this section, the application of the developed method will be illustrated and at the same time it will be confirmed that the general solution yields the right results for cases for which results are already available. Here the focus is on locally isotropic media,

$$\mathbf{K} = \begin{bmatrix} K & 0 & 0 \\ 0 & K & 0 \\ 0 & 0 & K \end{bmatrix} \tag{58}$$

From this condition and (50), the equation satisfied by g_i is

$$\frac{\partial}{\partial x_1}\left(K\frac{\partial g_i}{\partial x_1}\right) + \frac{\partial}{\partial x_2}\left(K\frac{\partial g_i}{\partial x_2}\right) + \frac{\partial}{\partial x_3}\left(K\frac{\partial g_i}{\partial x_3}\right) = \frac{\partial K}{\partial x_i} \tag{59}$$

and the effective hydraulic conductivity is

$$K_{ij}^e = -\frac{1}{2l_1l_2l_3}\int_V K\left[\frac{\partial g_j}{\partial x_i} + \frac{\partial g_i}{\partial x_j}\right] d\mathbf{x} + \bar{K}\,\delta_{ij} \tag{60}$$

where $\delta_{ij} = 1$, if $i = j$ and $\delta_{ij} = 0$, otherwise. Consider the familiar cases of perfect stratification and of small fluctuations.

Perfect Stratification

Assume that the values of K are constant in directions 1 and 2 and vary only in direction 3. Then, the effective conductivity in x_1 direction is calculated as follows:

$$K\left(\frac{\partial^2 g_1}{\partial x_1^2} + \frac{\partial^2 g_1}{\partial x_2^2}\right) + \frac{\partial}{\partial x_3}\left(K\frac{\partial g_1}{\partial x_3}\right) = 0 \tag{61}$$

The solution depends only on x_3 and $dg_1/dx_3 = \text{const}/K$. Then, from (60),

$$K_{11}^e = \bar{K} \tag{62}$$

and similarly for direction 2, $K_{22}^e = \bar{K}$. This is the well-known result that the effective hydraulic conductivity parallel to the stratification is the arithmetic average for K.

Consider now the direction perpendicular to the stratification. The associated equation for g_3 is

$$K\left(\frac{\partial^2 g_3}{\partial x_1^2} + \frac{\partial^2 g_3}{\partial x_2^2}\right) + \frac{\partial}{\partial x_3}\left(K\frac{\partial g_3}{\partial x_3}\right) = \frac{\partial K}{\partial x_3} \tag{63}$$

g_3 depends only on x_3 and

$$K\frac{dg_3}{dx_3} - K = C_1 \tag{64}$$

where C_1 is a constant. The solution of this differential equation is

$$g_3 = C_1 \int_0^{x_3} \frac{du}{K(u)} + x_3 + C_2 \tag{65}$$

where C_2 is another constant (which does not need to be determined). Because of the boundary conditions for g_3,

$$g_3(l_3) - g_3(0) = C_1 \int_0^{l_3} \frac{du}{K(u)} + l_3 = 0 \tag{66}$$

thus $C_1 = -l_3/\int_0^{l_3} (du/K(u)) = -\overline{K^{-1}}$ where $\overline{K^{-1}}$ is the so-called harmonic mean of K. Then,

$$K_{33}^e = -\frac{1}{l_1l_2l_3}\int_V K\frac{\partial g_3}{\partial x_3}\,d\mathbf{x} + \bar{K} = \overline{K^{-1}} = \left[\frac{1}{l_3}\int_0^{l_3}\frac{du}{K(u)}\right]^{-1} \tag{67}$$

Thus the effective hydraulic conductivity in the direction perpendicular to the stratification is the harmonic mean of the hydraulic conductivity, another well-known result.

Small Variations of Hydraulic Conductivity

A general method of solution can be developed when the fluctuations of K are small.

It is convenient to introduce $Y = \ln(K)$. Then g_i satisfies

$$\frac{\partial Y}{\partial x_1}\frac{\partial g_i}{\partial x_1} + \frac{\partial^2 g_i}{\partial x_1^2} + \frac{\partial Y}{\partial x_2}\frac{\partial g_i}{\partial x_2} + \frac{\partial^2 g_i}{\partial x_2^2} + \frac{\partial Y}{\partial x_3}\frac{\partial g_i}{\partial x_3} + \frac{\partial^2 g_i}{\partial x_3^2} = \frac{\partial Y}{\partial x_i} \tag{68}$$

subject to symmetric boundary conditions.

If Y were constant, g_i would also have been equal to a constant value $\bar{g}_i$. Let Y fluctuate slightly about its volume average

$$Y(x) = \bar{Y} + Y'(\mathbf{x}) \tag{69}$$

where $\bar{Y}$ is the volume average of $Y(x)$ and Y' is the local fluctuation about the average. Then, g_i should fluctuate about its mean value

$$g_i(\mathbf{x}) = \bar{g}_i + g_i'(\mathbf{x}) \tag{70}$$

In this analysis, the primed terms are treated as small. Substituting and neglecting products of primed quantities,

$$\frac{\partial^2 g_i'}{\partial x_1^2} + \frac{\partial^2 g_i'}{\partial x_2^2} + \frac{\partial^2 g_i'}{\partial x_3^2} = \frac{\partial Y'}{\partial x_i} \tag{71}$$

which is a linear partial differential equation with constant coefficients. The variable Y' can be expanded into a Fourier series:

$$Y'(\mathbf{x}) = \sum_{\mathbf{k}} \Psi(\mathbf{k}) \exp(j2\pi\mathbf{x}\cdot\mathbf{k}) \tag{72}$$

where $j = (-1)^{1/2}$; $\mathbf{k} = (n_1/l_1, n_2/l_2, n_3/l_3)^T$; n_1, n_2, and n_3 are integers; and $\Sigma_{\mathbf{k}}$ is a triple summation over all k_1, k_2, k_3 (excluding $k_1 = k_2 = k_3 = 0$ since there is no constant term). The vector of wave numbers is $\mathbf{k}$ and $\Psi(\mathbf{k})$ is a Fourier coefficient. The Fourier coefficient can be calculated as a weighted volume average of Y' from the familiar relation

$$\Psi(\mathbf{k}) = \frac{1}{l_1 l_2 l_3} \int_V Y'(\mathbf{x}) \exp(-j2\pi\mathbf{x}\cdot\mathbf{k})\, d\mathbf{x} \tag{73}$$

The solution can also be written in the form

$$g_i(\mathbf{x}) = \sum_{\mathbf{k}} G_i(\mathbf{k}) \exp(j2\pi\mathbf{x}\cdot\mathbf{k}) \tag{74}$$

which automatically satisfies the boundary conditions so that the problem reduces to finding the values of G_i so that (71) is satisfied. Substituting and accounting for the orthogonality of the $\exp(j2\pi\mathbf{x}\cdot\mathbf{k})$ functions,

$$G_i(\mathbf{k}) = -\frac{jk_i}{2\pi k^2}\Psi(\mathbf{k}) \qquad \text{all } \mathbf{k}, \text{ except for } \mathbf{k} = 0 \tag{75}$$

where $k^2 = k_1^2 + k_2^2 + k_3^2$. From this it follows that

$$\frac{\partial g_i}{\partial x_j} = \sum_{\mathbf{k}} \frac{k_i k_j}{k^2} \Psi(\mathbf{k}) \exp(j2\pi\mathbf{x}\cdot\mathbf{k}) \tag{76}$$

From

$$K = \exp(\bar{Y} + Y') \simeq \exp(\bar{Y})[1 + Y' + Y'^2/2 + \cdots] \tag{77}$$

taking volume averages

$$\bar{K} \simeq \exp(\bar{Y})[1 + \sigma_Y^2/2 + \cdots] \tag{78}$$

where $\sigma_Y^2 = (1/l_1 l_2 l_3)\int_V Y'^2\, d\mathbf{x}$. Also note that

$$\frac{1}{l_1 l_2 l_3}\int_V [1 + Y' + \cdots]\left[\frac{\partial g_j}{\partial x_i}\right] d\mathbf{x}$$

$$= \frac{1}{l_1 l_2 l_3}\int_V \left[1 + \sum_{\mathbf{l}} \Psi(\mathbf{l}) \exp(j2\pi\mathbf{x}\cdot\mathbf{l})\right] \cdot \left[\sum_{k} \frac{k_i k_j}{k^2}\Psi(\mathbf{k}) \exp(j2\pi\mathbf{x}\cdot\mathbf{k})\right] d\mathbf{x}$$

$$= \sum_{\mathbf{l}}\sum_{\mathbf{k}} \Psi(\mathbf{l}) \frac{k_i k_j}{k^2} \Psi(\mathbf{k}) \frac{1}{l_1 l_2 l_3}\int_V \exp(j2\pi\mathbf{x}\cdot(\mathbf{l}+\mathbf{k}))\, d\mathbf{x}$$

$$= \sum_{k} \frac{k_i k_j}{k^2}\Psi(-\mathbf{k})\Psi(\mathbf{k}) \tag{79}$$

Using $\Psi(-\mathbf{k}) = \Psi^*(\mathbf{k})$, where the asterisk indicates complex conjugate, and $\Psi(\mathbf{k})\Psi^*(\mathbf{k}) = |\Psi(\mathbf{k})|^2$, the small-perturbation solution is

$$K_{ij}^e = -\exp(\bar{Y}) \sum_{\mathbf{k}} \frac{k_i k_j}{k^2} |\Psi(\mathbf{k})|^2 + \exp(\bar{Y})[1 + \sigma_Y^2/2]\delta_{ij} \tag{80}$$

where $|\Psi(\mathbf{k})|^2$ is known as the power spectrum of the periodic function. If the averaging volume is increased in size, the power spectrum tends to become a function of continuously varying variables. At the limit, the multiple summation may be substituted with a multiple integral:

$$K_{ij}^e = -\exp(\bar{Y}) \int \frac{k_i k_j}{k^2} S(\mathbf{k})\, d\mathbf{k} + \exp(\bar{Y})[1 + \sigma_Y^2/2]\delta_{ij} \tag{81}$$

where $S(\mathbf{k})$ is the power spectral density (i.e., the Fourier transform of the covariance function of the stationary function Y). Equation (80) is suited for numerical computations while (81) lends itself to analytical treatment.

Interestingly enough, (81) is identical to the result of *Gutjahr et al.* [1978] which was obtained with different means and under more restrictive assumptions. Note also that the present analysis followed a purely deterministic volume-averaging approach while Gutjahr et al. followed a stochastic ensemble-averaging approach. It is important to note that at least in this case the result which is applicable to a random medium could be obtained from the result for a periodic medium by taking a limit (the period tending to infinity).

Note that for (1) one-dimensional flow (or for flow perpendicular to perfect stratification), $K^e = -\exp(\bar{Y})\sigma_Y^2 + \exp(\bar{Y})[1 + \sigma_Y^2/2] = \exp(\bar{Y})[1 - \sigma_Y^2/2]$, which is a first-order approximation to the harmonic mean; (2) for two-dimensional flow with isotropic variability, in the sense that $|\Psi(\mathbf{k})| = |\Psi(k)|$, by virtue of symmetry $\Sigma_{\mathbf{k}} (k_i k_i/k^2)|\Psi(\mathbf{k})|^2 = \sigma_Y^2/2$ which means that $K_{11}^e = K_{22}^e = \exp(\bar{Y})$; (3) for three-dimensional flow with isotropic variability, again by virtue of symmetry, $\Sigma_{\mathbf{k}} (k_i k_i/k^2)|\Psi(\mathbf{k})|^2 = \sigma_Y^2/3$, which means that $K_{ii}^e = \exp(\bar{Y})[1 + \sigma_Y^2/6]$. Note that these results, which were derived previously (see, for example, *Gelhar and Axness* [1983] and *Gelhar* [1986]) with other methods, involve no other assumption than the variability is isotropic.

In the small-fluctuation case, it is straightforward to answer the question: what volume averages are needed for the determination of the effective conductivity? From (80) or (81) it is obvious that the effective conductivity depends solely on the power spectrum of the local hydraulic conductivity. The power spectrum is the Fourier transform of the volume-average covariance function, which could be employed instead of the power spectrum for purposes of determination of the effective conductivity. (Incidentally, this conclusion was reached without invoking a "Gaussian-distribution" assumption. However, it is an asymptotic result, predicated on the assumption of small fluctuations of the logarithm of hydraulic conductivity.)

Furthermore, since an explicit expression was obtained, the conditions for covergence of the volume integral of (56) and for existence of effective conductivity are obvious. The power spectrum must be such that the summation of (80) or the integral of (81) must be finite.

7. Concluding Remarks

This work has examined the problem of determining the field scale or effective hydraulic conductivity of a medium with locally variable conductivity. It was shown that the assumptions of steady state and locally uniform flows, which are commonly made in other approaches (an exception being *Dagan* [1982], who studied slowly varying flow), are not essential in the definition or determination of effective parameters. Instead, the essential assumption is that of "gradually varying" flow. That is, that the scale of fluctuations of the head must be large in comparison to the typical length scale of fluctuations of local conductivity so that all values of conductivity are sampled (equation (47)).

An example of when this condition is not satisfied is shortly after the injection of a volume of water at a point. The net rate of spreading depends not on a constant "effective conductivity" but on the value of conductivity in the neighborhood of the injection and varies with time. However, after enough time has elapsed for the mound to spread out over an area larger than the scale of fluctuations of conductivity, the net rate of spreading converges to a constant. The time required for the conductivity to become a constant is given approximately by $\bar{l}^2 S/\bar{K}$, where $\bar{l}$ is the scale of conductivity fluctuations, $\bar{K}$ is a typical value of conductivity, and S is the specific storage coefficient. This result is in general agreement with that of *Dagan* [1982].

Of course, any representation of a locally heterogeneous medium by an equivalent homogeneous medium with an effective conductivity is bound to be incomplete in that the latter cannot describe variability of the head at the scale of local conductivity fluctuations. However, if such variability is deemed unimportant for the application at hand, the concept of the effective conductivity is a useful one.

Key results of this analysis are two equations which must be solved for the numerical determination of the effective conductivity. The validity of the approach was verified by comparison with the results of cases for which results are currently available.

Appendix

Consider (30) and the periodic boundary conditions (31a)–(32c). We will investigate the large-time behavior of the solution to this problem.

The solution is necessarily of the form

$$a(x_1, x_2, x_3, t) = \sum_{k_1=-\infty}^{\infty} \sum_{k_2=-\infty}^{\infty} \sum_{k_3=-\infty}^{\infty} A(k_1, k_2, k_3, t) \cdot e^{j2\pi(k_1x_1/l_1 + k_2x_2/l_2 + k_3x_3/l_3)} \tag{A1}$$

because the complex exponentials form a complete orthogonal basis for functions defined over an elementary volume and having periodic boundary conditions.

Integrating (A1) over V,

$$\int_V a(\mathbf{x}, t)\, d\mathbf{x} = l_1l_2l_3A(0, 0, 0, t) \tag{A2}$$

which should be 1 because of the initial condition, (3), and continuity. Thus

$$A(0, 0, 0, t) = \frac{1}{l_1l_2l_3} \tag{A3}$$

The other (generally complex) coefficients are found by substituting in (30)

$$\frac{\partial a}{\partial t} - \sum_m \frac{\partial}{\partial x_m} \sum_n \left(D_{mn} \frac{\partial a}{\partial x_n}\right) = 0 \tag{A4}$$

yielding

$$\sum_{k_1=-\infty}^{\infty} \sum_{k_2=-\infty}^{\infty} \sum_{k_3=-\infty}^{\infty} \left\{\frac{\partial A}{\partial t} - j2\pi \sum_m \sum_n \frac{\partial D_{mn}}{\partial x_m} \frac{k_n}{l_n} + 4\pi^2 \sum_m \sum_n D_{mn} \frac{k_mk_n}{l_ml_n}\right\} e^{j2\pi(k_1x_1/l_1 + k_2x_2/l_2 + k_3x_3/l_3)} = 0 \tag{A5}$$

From (A5), again because the complex exponentials are a complete basis, the bracketed expressions must vanish for every (k_1, k_2, k_3):

$$\frac{\partial A}{\partial t} - j2\pi \sum_m \sum_n \frac{\partial D_{mn}}{\partial x_m} \frac{k_n}{l_n} A + 4\pi^2 \sum_m \sum_n D_{mn} \frac{k_mk_n}{l_ml_n} A = 0 \qquad \text{for every } (k_1, k_2, k_3) \tag{A6}$$

The solution of this first-order linear equation is

$$A(k_1, k_2, k_3, t) = A(k_1, k_2, k_3, 0) \cdot \exp\left[j2\pi \sum_m \sum_n \frac{\partial D_{mn}}{\partial x_m} \frac{k_n}{l_n} t\right] \cdot \exp\left[-4\pi^2 \sum_m \sum_n D_{mn} \frac{k_mk_n}{l_ml_n} t\right] \tag{A7}$$

Taking absolute values,

$$|A(k_1, k_2, k_3, t)| = |A(k_1, k_2, k_3, 0)| \cdot \exp\left[-4\pi^2 \sum_m \sum_n D_{mn} \frac{k_mk_n}{l_ml_n} t\right] \tag{A8}$$

$\mathbf{D}$ is positive definite which means that $\Sigma_m \Sigma_n D_{mn} (k_mk_n/l_ml_n) > 0$ except in the special case that $k_1 = k_2 = k_3 = 0$. Thus all terms except for the constant one decay exponentially (the high-frequency components vanishing the fastest) and

$$a(\mathbf{x}, t) \simeq \frac{1}{l_1l_2l_3} \qquad \text{when } t \gg \left[\sum_m \sum_n D_{mn} \frac{k_mk_n}{l_ml_n}\right]^{-1} \qquad \text{for all } (k_1, k_2, k_3) \tag{A9}$$

We may define the relaxation time as the maximum value of $[\Sigma_m \Sigma_n D_{mn} (k_mk_n/l_ml_n)]^{-1}$. An estimate of the relaxation time is $\bar{l}^2/\bar{D}$, where $\bar{l}$ is a length characteristic of the periodicity and $\bar{D}$ is typical diffusion value. This result is essentially the same with that of *Dagan* [1982] who followed a different methodology. Using Dagan's results, it can be shown that the relaxation time can be quite short. For example, it is of the order of minutes or hours for three-dimensional flow in relatively permeable formations with conductivity correlation lengths of the order of a few meters.

Acknowledgments. This work has been supported by the National Science Foundation under grant EET 87-16585 and the Office of Research and Development, U.S. EPA, under agreement R-815738-01-0. The content of this article does not necessarily represent the views of the agencies. Sincere thanks to anonymous reviewers and to G. Dagan for useful suggestions.

REFERENCES

Aris, R., On the dispersion of a solute in a fluid flowing through a tube, *Proc. R. Soc. London, Ser. A*, *235*, 67–77, 1956.

Bhattacharya, R. N., A central limit theorem for diffusions with periodic coefficients, *Ann. Probability*, *13*(2), 385–396, 1985.

Brenner, H., A general theory of Taylor dispersion phenomena, *Physicochem. Hydrodyn.*, *1*, 91–123, 1980*a*.

Brenner, H., Dispersion resulting from flow through spatially periodic porous media, *Philos. Trans. R. Soc. London, Ser. A*, *297*(1498), 81–133, 1980*b*.

Brenner, H., A general theory of Taylor dispersion phenomena, II, An extension, *Physicochem. Hydrodyn.*, *3*(2), 139–157, 1982*a*.

Brenner, H., Dispersion resulting from flow through spatially periodic porous media, II, Surface and interparticle transport, *Philos. Trans. R. Soc. London, Ser. A*, *307*(1498), 149–200, 1982*b*.

Dagan, G., Models of groundwater flow in statistically homogeneous porous formations, *Water Resour. Res.*, *15*(1), 47–63, 1979.

Dagan, G., Analysis of flow through heterogeneous random aquifers by the method of embedding matrix, 1, Steady flow, *Water Resour. Res.*, *17*(1), 107–121, 1981.

Dagan, G., Analysis of flow through heterogeneous random aquifers, 1, Unsteady flow in confined formations, *Water Resour. Res.*, *18*(5), 1571–1585, 1982.

Dagan, G., Solute transport in groundwater, *Annu. Rev. Fluid Mech.*, *19*, 183–215, 1987.

Desbarats, A. J., Numerical estimation of effective permeability in sand-shale formations, *Water Resour. Res.*, *23*(2), 273–286, 1987.

Freeze, R. A., A stochastic conceptual analysis of one-dimensional groundwater flow in nonuniform homogeneous media, *Water Resour. Res.*, *11*(5), 725–741, 1975.

Gelhar, L. W., Effects of hydraulic conductivity variations on groundwater flows, in *International Symposium on Stochastic Hydraulics*, pp. 409–429, Int. Assoc. for Hydraul. Res., Lund, Sweden, 1976.

Gelhar, L. W., Stochastic subsurface hydrology from theory to applications, *Water Resour. Res.*, *22*(9), 135S–145S, 1986.

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

Gupta, V. K., and R. N. Bhattacharya, Solute dispersion in multidimensional periodic saturated porous media, *Water Resour. Res.*, *22*(2), 156–164, 1986.

Gutjahr, A. L., L. W. Gelhar, A. D. Bakr, and J. R. MacMillan, Stochastic analysis of spatial variability in subsurface flows, 2, Evaluation and applications, *Water Resour. Res.*, *14*(5), 953–959, 1978.

Güvan, O., F. J. Molz, and J. G. Melville, An analysis of dispersion in a stratified aquifer, *Water Resour. Res.*, *20*(10), 1337–1354, 1984.

Kitanidis, P. K., Prediction by the method of moments of transport in heterogeneous formations, *J. Hydrol.*, *102*, 453–473, 1988.

Koch, D. L., R. G. Cox, H. Brenner, and J. F. Brady, The effect of order on dispersion in porous media, *J. Fluid Mech.*, *200*, 173–188, 1989.

Matheron, G., *Elements Pour une Theorie des Millieux Poreux*, Masson et Cie, Paris, 1967.

Schwydler, M. I., Flow in heterogeneous media (in Russian), *Izv. Akad. Nauk SSSR Mech.*, *3*, 185–190, 1962.

Smith, L., and R. A. Freeze, Stochastic analysis of steady state groundwater flow in an unbounded domain, 2, Two-dimensional simulations, *Water Resour. Res.*, *15*(6), 1543–1559, 1979.

Taylor, G. I., Dispersion of soluble matter in solvent flowing slowly through a tube, *Proc. R. Soc. London Ser. A*, *219*, 186–203, 1953.

Valocchi, A. J., Spatial moment analysis of the transport of kinetically adsorbing solutes through stratified aquifers, *Water Resour. Res.*, *25*(2), 273–279, 1989.

Warren, J. E., and H. S. Price, Flow in heterogeneous porous media, *Soc. Pet. Eng. J.*, *1*, 153–167, 1961.

P. K. Kitanidis, Department of Civil Engineering, Terman Engineering Center, Stanford University, Stanford, CA 94305.

(Received June 26, 1989;
revised October 20, 1989;
accepted December 11, 1989.)