On Dispersion in Laminar Flow Through Porous Media

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Dispersion of a tracer in fluid flow through a porous medium has been extensively studied [for example, (*2*) to (*11*)]. The present communication seeks to relate the recent work of Whitaker (*11*) to the traditional treatment of the dispersion equation. Some anomalies in Whitaker's results are revealed and discussed.

The usual model for dispersion (*2, 3, 6, 5, 9, 10*) is based on random walk and cell mixing mechanisms and leads quite naturally to an equation identical to the diffusion equation with the molecular diffusion coefficient replaced by a dispersion coefficient. In a general anisotropic porous medium, previous workers (*2, 3, 7,* and *10*) are in agreement that the dispersion coefficient is a second-order tensor. In a system of rectangular Cartesian coordinates, the equation is written as

$$\frac{\partial c}{\partial t} + v_i \left(\frac{\partial c}{\partial x_i} \right) = \frac{\partial}{\partial x_j} \left(D_{jk} \frac{\partial c}{\partial x_k} \right) \tag{1}$$

Summation convention applies; in the forthcoming, attentention is restricted to a rectangular Cartesian frame.

Equation (1) is applicable to laminar or turbulent flows; D_{jk} is an experimentally measured parameter which is a characteristic of the porous medium and is also a function of the velocity of fluid flow. As such, Equation (1) agrees with experimental data remarkably well (*4, 5, 8*) for both laminar and turbulent flows. It is not, however, based on the fundamental transport equations. The possibility of analyzing dispersion in turbulent flows via the transport equations seems to be remote. However, the important problem of dispersion in laminar flow should be amenable to such an analysis. Whitaker (*11*) took such an approach by volume averaging the transport equations in a general porous medium. Making certain assumptions regarding the functional dependence of the dispersion vector $\overline{\psi}_i$, he obtained [Whitaker's Equation (62) in dimensional form]

$$\frac{\partial \overline{c}}{\partial t} + \overline{v}_i \left(\frac{\partial \overline{c}}{\partial x_i} \right) = \frac{\partial}{\partial x_j} \left[\mathcal{D} \left(\frac{\partial \overline{c}}{\partial x_j} + R\tau_j \right) \right] + \frac{\partial}{\partial x_j} \left[\left(A^{I}_{jik} \overline{v}_i + A^{II}_{jilk} \overline{v}_i \overline{v}_l + A^{III}_{jilk} \overline{v}_i \frac{\partial \overline{c}}{\partial x_l} \right) \frac{\partial \overline{c}}{\partial x_k} \right] \tag{2}$$

where the tensors $\mathbf{A}^I$, $\mathbf{A}^{II}$, and $\mathbf{A}^{III}$ are completely symmetric and are functions of the structure of the porous medium and the transport properties such as viscosity, density, etc., of the fluid filling the medium. They may also be weak functions of time. Equation (2) holds for the concentration distribution of the dispersing species for a particular flow field $\mathbf{v}$ of the fluid in the porous medium. The present work seeks to relate Equations (1) and (2) and also to examine in some detail Equation (2) and some of its implications.

REDUCTION OF EQUATION (2) TO DIFFUSION EQUATION FORM

Whitaker (*11*) [Equations (A5) through (A9)] shows that the first term on the right-hand side of Equation (1) may be approximated as an effective diffusion coefficient (which depends on the tortuosity). This enables Equation (2) to be written as

$$\frac{\partial \overline{c}}{\partial t} + \overline{v}_i \frac{\partial \overline{c}}{\partial x_i} = \frac{\partial}{\partial x_j} \left[\left\{ \mathcal{D} \left(\delta_{jk} + R B^{I}_{jk} \right) + A^{I}_{jik} \overline{v}_i + A^{II}_{jilk} \overline{v}_i \overline{v}_l + A^{III}_{jilk} \overline{v}_i \frac{\partial \overline{c}}{\partial x_l} \right\} \frac{\partial \overline{c}}{\partial x_k} \right] \tag{3}$$

The tensor A^{III}_{jilk} is given by

$$A^{III}_{jilk} = \left. \frac{\partial^3 \overline{\psi}_j}{\partial \overline{v}_i \, \partial \left(\frac{\partial \overline{c}}{\partial x_l} \right) \partial \left(\frac{\partial \overline{c}}{\partial x_k} \right)} \right|_{\overline{v}_i = 0,\ \frac{\partial \overline{c}}{\partial x_l} = 0,\ \frac{\partial \overline{c}}{\partial x_k} = 0} \tag{4}$$

and may be assumed negligible from an intuitive standpoint. It involves a second partial of $\overline{\psi}_j$ with respect to the concentration gradient, which variable does not affect dispersion greatly. The predominant variable affecting dispersion is the velocity vector, and hence the tensors $\mathbf{A}^I$ and $\mathbf{A}^{II}$ are retained. They are given by

$$A^{I}_{jik} = \left. \frac{\partial^2 \overline{\psi}_j}{\partial \overline{v}_i \, \partial \left(\frac{\partial \overline{c}}{\partial x_k} \right)} \right|_{\overline{v}_i = 0,\ \frac{\partial \overline{c}}{\partial x_k} = 0} \tag{5}$$

and

$$A^{II}_{jilk} = \left. \frac{\partial^3 \overline{\psi}_j}{\partial \overline{v}_i \, \partial \overline{v}_l \, \partial \left(\frac{\partial \overline{c}}{\partial x_k} \right)} \right|_{\overline{v}_i = 0,\ \overline{v}_l = 0,\ \frac{\partial \overline{c}}{\partial x_k} = 0} \tag{6}$$

Under the above assumption, the equation for the concentration field [Equation (3)] may be written

$$\frac{\partial \bar{c}}{\partial t} + \bar{v}_i \frac{\partial \bar{c}}{\partial x_i} = \frac{\partial}{\partial x_j}\left[D_{jk} \frac{\partial \bar{c}}{\partial x_k} \right] \qquad (7)$$

where the dispersion tensor D_{jk} is defined by

$$D_{jk} = \mathcal{D}(\delta_{jk} + R\overset{I}{B}_{jk}) + \overset{I}{A}_{jik}\,\bar{v}_i + \overset{II}{A}_{jilk}\,\bar{v}_i\,\bar{v}_l \qquad (8)$$

Equation (7) is identical to the usual form of the dispersion equation.

DISPERSION TENSOR

Asymptotic Effects

It is of interest to examine the effect of the magnitude of the fluid velocity on the dispersion tensor.

As is apparent from Equation (8), at low velocities the diffusion term dominates:

$$\text{As} \quad \bar{v}_i \to 0; \; D_{jk} = \mathcal{D}(\delta_{jk} + RB^I{}_{jk}) = \mathcal{D}_{\text{eff}} \qquad (9)$$

The diffusion coefficient in the presence of the porous medium is thus given by $\mathcal{D}_{\text{eff}}$ which is the molecular diffusion coefficient multiplied by the factor $(\delta_{jk} + RB^I{}_{jk})$ and has a lower numerical value than the molecular diffusion coefficient. This is a tortuosity effect reflected in the tensor $B^I{}_{jk}$. Media of different tortuosities yield different effective diffusion coefficients. This is substantiated by experimental investigations (8).

At higher velocities, the diffusion term becomes less important, so that

$$D_{jk} \approx \overset{I}{A}_{jik}\,\bar{v}_i + \overset{II}{A}_{jilk}\,\bar{v}_i\,\bar{v}_l \qquad (10)$$

and we enter the regime where dispersion occurs predominantly because of varying fluid velocity. It is interesting that Equation (10) predicts no direct influence of tortuosity on the dispersion tensor. The effect of the structure of the medium is accounted for by the tensors $\mathbf{A}^I$ and $\mathbf{A}^{II}$. This is also supported by experimental data (8).

Thus, Equation (8) correctly predicts that at low velocities, molecular diffusion dominates, and the tortuosity of the medium has a direct effect on diffusion. At higher velocities, dispersion occurs mainly by convection, and the tortuosity of the medium is unimportant.

Velocity Dependence

Several attempts have been made in the past to describe the velocity dependence of the dispersion tensor for velocities high enough so that molecular diffusion may be neglected. Using geometrical arguments, Bear (2) derived a relation between the dispersion tensor and the displacements of a tracer particle in an isotropic porous medium. De Jong and Bossen (3) extended Bear's analysis to arrive at the following result for a uniform velocity field in an isotropic porous medium:

$$D_{jk} = a_{jklm} \frac{v_l v_m}{|\mathbf{v}|} \qquad (11)$$

These authors showed that the tensor a has only two distinct components (for isotropic media). A result identical to Equation (11) was obtained by Nikolaevskii (7) who derived it by analogy with diffusion in a homogeneous isotropic turbulent flow. Nikolaevskii considered an expression of the form of Equation (10) but eliminated $\mathbf{A}^I$ since he was considering an isotropic medium. Scheidegger (*10*), however, stated that Equation (11) could also apply to an anisotropic medium, with the tensor a having in general thirty-six distinct components.

From Equation (10) we observe that for the general porous medium, the dispersion coefficient depends on velocity in a more complex fashion than indicated by Equation (11). It is necessary to incorporate a third-order tensor as well as one of fourth order. Equation (10) is completely consistent with Nikolaevskii's development. As noted above, Nikolaevskii argued that the geometrical dispersivity tensor must be of even rank, since the medium he considered was isotropic. For anisotropic media, these arguments clearly do not apply. No conflict with Bear's work occurs, since he considered only isotropic media. A reappraisal of the work of Bear, de Jong, Nikolaevskii, and Scheidegger appears to show that Equation (11) is not valid for anisotropic materials; rather Equation (10), where the A tensors are not necessarily completely symmetric, should be used. We may come to the above conclusion without agreeing with Whitaker's assumptions, although his work certainly led us to it.

For the case of isotropic porous media, the tensors $\mathbf{A}^I$ and $\mathbf{A}^{II}$ must be isotropic. Hence, $\mathbf{A}^I = 0$, and $\mathbf{A}^{II}$ is given by a linear combination of the Kronecker deltas (*1*). Since $\mathbf{A}^{II}$ is completely symmetric, Equation (10) reduces to

$$D_{jk} = A^{II}\,(\delta_{ji}\delta_{lk} + \delta_{jl}\delta_{ik} + \delta_{jk}\delta_{il})\,\bar{v}_i\,\bar{v}_l \qquad (12)$$

which is similar to Equation (11) in agreement with Bear and Nikolaevskii. There is one striking difference. The results of Bear and Nikolaevskii show that a has two distinct components; Equation (12) shows that $\mathbf{A}^{II}$ has only one distinct component.

The significance of this difference is best shown by considering a one-dimensional uniform velocity field in an isotropic porous medium as shown below.

Longitudinal and Transverse Dispersion Coefficients

Performing the indicated contractions in Equation (12), we get

$$D_{jk} = A^{II}\,(2\bar{v}_j\,\bar{v}_k + \delta_{jk}\,|\mathbf{v}|^2) \qquad (13)$$

If one-dimensional flow is considered in a rectangular Cartesian coordinate frame such that

$$\bar{v}_1 = u, \; \bar{v}_2 = \bar{v}_3 = 0 \qquad (14)$$

then Equation (13) reduces to

$$\left.\begin{aligned} D_{11} &= 3\;A^{II}\;u^2 \\ D_{22} &= D_{33} = A^{II}\;u^2 \\ D_{ij} &= 0 \qquad i \neq j \end{aligned}\right\} \qquad (15)$$

Hence

$$D_{22} = D_{33} = \frac{1}{3} D_{11} \qquad (16)$$

We obtain the result that the longitudinal dispersion coefficient D_{11} (that is, in the direction of flow) is three times the transverse dispersion coefficient (that is, perpendicular to the flow).

It should be noted that previous workers (*2, 4, 5*) have always considered the usual dispersion equation in such a flow field to contain two independent parameters, characterizing the dispersion as

$$\frac{\partial \bar{c}}{\partial t} + \bar{v}_1 \frac{\partial \bar{c}}{\partial x_1} = D_L \frac{\partial^2 \bar{c}}{\partial x_1^2} + D_T \frac{\partial^2 \bar{c}}{\partial x_2^2} + D_T \frac{\partial^2 \bar{c}}{\partial x_3^2} \qquad (17)$$

Experimental measurements have always been made (*3, 5*) by using Equation (17) as the model. The results of these experiments show that the ratio D_L/D_T varies from a lower value of about 3 to a high value of about 60. This ratio of longitudinal to transverse dispersion coefficients is found by these workers to be actually a function of the velocity of flow. The results of Whitaker's analysis are clearly at variance with these observations but do give the correct lower limit for a homogeneous, uniform, isotropic medium.

A possible explanation is that it is necessary to consider higher-order terms in the expansion of $\overline{\psi}_i$, the dispersion vector [Whitaker's Equation (60)]. This would indicate that no relation between the longitudinal and transverse coefficients could be derived.

Another explanation that could be advanced is that some of the assumptions inherent in the derivation of Equation (2) are invalid. One such assumption is that

$$\overline{\psi}_i = 0 \quad \text{when} \quad \frac{\partial \overline{c}}{\partial x_i} = 0 \tag{18}$$

which is Whitaker's Equation (52). As he points out, there are no theoretical arguments to support it. We, therefore, consider the effect of relaxing this assumption. This is done below. However, it is found that although a correction is introduced into Equation (7) in the form of an additional term, this term vanishes for uniform flow in an isotropic medium. Thus, this is not the source of the anomaly represented by Equation (16). The other assumptions inherent in Whitaker's work are more reasonable. It does not appear that they contribute to Equation (16). In any case, a reappraisal of his analysis seems necessary.

MODIFICATION OF EQUATION (7)

We now consider the effect of relaxing the assumption of Equation (18) so that $\overline{\psi}_i \neq 0$ for $\partial \overline{c}/\partial x_j = 0$. The power series expansion of $\overline{\psi}_i$ [Equation (60) in Whitaker] must also include terms containing only v_i. They were eliminated as a result of this assumption. Insertion of the new expansion results in Equation (19) which is the analogue of Equation (7):

$$\frac{\partial \overline{c}}{\partial t} + \overline{v}_i \frac{\partial \overline{c}}{\partial x_i} = \frac{\partial}{\partial x_j}\left[D_{jk} \frac{\partial \overline{c}}{\partial x_k} \right] - \frac{\partial}{\partial x_j}\left[\overset{I}{F}_{ji}\, \overline{v}_i + \overset{II}{F}_{jik}\, \overline{v}_i \overline{v}_k + \overset{III}{F}_{jikl}\, \overline{v}_i \overline{v}_k \overline{v}_l + \ldots \right] \tag{19}$$

where, for example

$$\overset{II}{F}_{jik} = \left. \frac{\partial^2 \overline{\psi}_j}{\partial \overline{v}_i\, \partial \overline{v}_k} \right|_{\overline{v}_i = \overline{v}_k = 0} \tag{20}$$

These **F** tensors are functions of the structure of the porous media, the transport properties of the fluid, and possibly weak functions of time. The **F** tensors are symmetric in all indexes except the first by virtue of Equation (20), and hence Equation (19) may be written as

$$\frac{\partial \overline{c}}{\partial t} + \overline{v}_i \frac{\partial \overline{c}}{\partial x_i} = \frac{\partial}{\partial x_j}\left[D_{jk} \frac{\partial \overline{c}}{\partial x_k} \right] - \left[\overset{I}{F}_{ji} \frac{\partial \overline{v}_i}{\partial x_j} + 2\overset{II}{F}_{jik}\, \overline{v}_i \frac{\partial \overline{v}_k}{\partial x_j} + 3\overset{II}{F}_{jikl}\, \overline{v}_i \overline{v}_k \frac{\partial \overline{v}_l}{\partial x_j} + \ldots \right] \tag{21}$$

The correction term [the last term on the right-hand side of Equation (21)] is nonzero for an arbitrary flow field in a general anisotropic heterogeneous porous medium. However, for uniform flows it is zero. Hence, for uniform flows we obtain Equation (7) once again.

CONCLUSIONS

1. Whitaker's analysis of dispersion in porous media results in an equation identical to the usual dispersion equation.
2. For anisotropic media, the dispersion tensor is related to the fluid velocity through a tensor of third order as well as one of fourth order. For isotropic materials, only the fourth-order tensor is to be retained. However, Whitaker's analysis indicates (contrary to previous work) that this fourth-order tensor has only one distinct component for such isotropic media.
3. Whitaker's analysis leads to predicting that the longitudinal dispersion coefficient is three times the value of the transverse dispersion coefficient for uniform flow in isotropic materials.

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NOTATION

a_{jklm} = geometrical dispensivity tensor, cm.
$\mathbf{A}^{I,\,II,\,\ldots}$ = tensors defined by Equations (4) to (6)
$\mathbf{B}^{I}$ = tensor defined by Whitaker, Equation (A5)
c = concentration, g. mole/cc.
D_{jk} = dispersion tensor, sq.cm./sec.
D_L = longitudinal dispersion cöefficient, sq.cm./sec.
D_T = transverse dispersion coefficient, sq.cm./sec.
$\mathcal{D}$ = molecular diffusivity, sq.cm./sec.
$\mathbf{F}^{I,\,II,\,\ldots}$ = tensors defined by Equation (20)
R = fluid-solid interfacial area per unit volume, cm.$^{-1}$
t = time, sec.
v_i = velocity vector, cm./sec.
$|\mathbf{v}|$ = magnitude of velocity vector, cm./sec.
x_i = spatial coordinates, cm.
δ_{jk} = Kronecker delta
τ_j = tortuosity vector, g. moles/sq.cm.
$\overline{\psi}_i$ = dispersion vector, g. moles/sq.cm.

Superscripts

— = volume-averaged value

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