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The Coefficients of Dispersion and Dispersivity in Anisotropic Porous Media

by

JACOB BEAR & LEONID FEL

Technion-Israel Institute of Technology, Haifa, Israel

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❖BACKGROUND

Since the early 60's, almost all research on (solute) dispersion has been limited to isotropic porous media. For such media, the components of the dispersivity tensor have been shown to depend only on two material moduli, referred to as longitudinal and transversal dispersivities. Based on the works of Robertson (1948) and Batchelor (1946}, a study of the dispersivity for axially symmetric porous medium was conducted by Poreh (1965), leading to the conclusion that four material moduli are required to describe all components of the dispersivity coefficient, a_{ijkl}. In the last four decades, to our best knowledge, no theoretical work based on the inner symmetry of a_{ijkl} and external symmetry of porous media has been undertaken.

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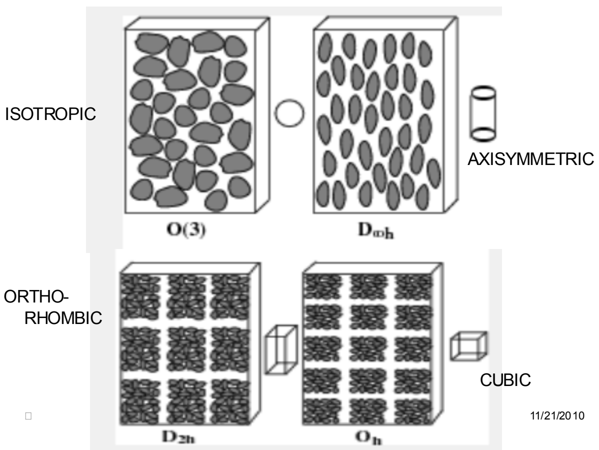
❖ISOTROPIC and ANISOTROPIC POROUS MEDIA



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❖OBJECTIVE OF PRESENTATION

To discuss the coefficients of dispersion and dispersivity in anisotropic porous media, focusing on axially symmetric porous media, e.g., a stratified porous medium. We show that in such a medium, the dispersivity is governed by six independent moduli which have to satisfy certain constraints. We also show that at least two independent experiments are required in order to obtain the values of these moduli for any 3D porous medium domain.

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- We are considering the transport of a chemical species, at concentration c, in a phase occupying the void space (or part of it) in a porous medium (pm) domain.
- The total flux of that species (mass per unit area of porous Medium per unit time) is the sum of fluxes by advection, Dispersion and diffusion. Here we focus on DISPERSION.
- The dispersive flux, $\mathbf{J}$, is assumed to be expressed by a *Fickian-type* law:

$$J_i = -D_{ij}\frac{\partial c}{\partial x_j}, \qquad i,j \equiv x,y,z, \quad \text{or} \quad i,j \equiv 1,2,3,$$

D_{ij} = dispersion coefficient, a 2nd rank tensor that relates the vector $\mathbf{J}$ to the vector ∇c.

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- In thermodynamics, the rate of *entropy production* $\dot{S}$ is related to the thermodynamic driving force $\mathbf{X}$ and to the *thermodynamic flux*, $\mathbf{Y}$, called "conjugate Flux and Force", by

$$\dot{S} = \mathbf{X}\cdot\mathbf{Y}$$

- With $\mathbf{Y} = \chi\mathbf{J}$, and $\mathbf{X} = -\chi\,\nabla c$, we have:

$$\dot{S} = \chi\left[\left(-D_{ij}\frac{\partial c}{\partial x_j}\right)\right]\times\chi\left[\left(-\frac{\partial c}{\partial x_i}\right)\right] = \chi^2 D_{ij}\frac{\partial c}{\partial x_j}\frac{\partial c}{\partial x_i} > 0,$$

χ depends on the transported extensive property.

- Hence:
  1. The matrix D_{ij} is positive definite.
  2. The matrix D_{ij} is symmetric, i.e., $D_{ij} = D_{ji}$

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- The above conclusions are also valid for k_{ij}, $\mathcal{D}^*_{ij}$, λ^*_{ij}

However, D_{ij} depends also on the velocity, $\mathbf{V}$ (and not only on the diffusive coefficient and the geometry of the phase in the void space).

- The coefficient of dispersion D_{ij} is related to the dispersivity, a_{ijkl} by:

$$D_{ij} = a_{ijkl}\frac{V_k V_l}{V}, \qquad V = |\mathbf{V}|,\ \mathbf{V} = (V_1, V_2, V_3)$$

- The coefficient a_{ijkl} is a 4th rank tensor, with the following properties:

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1. From the requirement that the rate of entropy production, $\dot{S}$ expressed as

$$\dot{S} = Y_i X_i = \chi\left(-D_{ij}\frac{\partial c}{\partial x_j}\right)\times\chi\left(-\frac{\partial c}{\partial x_i}\right) = \chi^2 a_{ijkl}\frac{V_k V_l}{V}\frac{\partial c}{\partial x_j}\frac{\partial c}{\partial x_i} \geq 0,$$

be positive definite, it follows that a_{ijkl} is also positive definite.

2. Permutation in indices: $a_{ijkl} = a_{ijlk}$, $a_{ijkl} = a_{jukl}$

- Hence, a_{ijkl} has 36 independent components and $2^6 - 1 = 63$ constraints should be satisfied.

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❖ISOTROPIC porous media:

$$a_{ijkl} = a_T\delta_{ij}\delta_{kl} + \frac{a_L - a_T}{2}\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right)$$

$$D_{im} = a_T V\delta_{im} + (a_L - a_T)\frac{V_i V_m}{V}$$

a_L Longitudinal dispersivity

a_T Transversal dispersivity

➢Special case : Uniform horizontal flow:

$$V_1 = V, V_2 = V_3 = 0, \qquad D_{ij} = \begin{pmatrix} a_L & 0 & 0 \\ 0 & a_T & 0 \\ 0 & 0 & a_T \end{pmatrix}$$

The matrix is positive if $a_L, a_T \geq 0.$

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❖ANISOTROPIC POROUS MEDIUM, WITH UNIAXIAL SYMMETRY (Transverse isotropy)

➢For this case, with $\mathbf{e}$ (comp. e_i), indicating the axis of symmetry, there exist six independent moduli, a_i

The dispersivity & dispersion are expressed as;

$$a_{ijkl} = a_1\,\delta_{ij}\delta_{kl} + \frac{a_2}{2}\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}\right) + a_3\,e_ie_j\delta_{kl} + a_4\,e_ke_l\delta_{ij}$$

$$+\frac{a_5}{2}(e_ie_k\delta_{jl} + e_je_k\delta_{il} + e_ie_l\delta_{jk} + e_je_l\delta_{ik}) + a_6\,e_ie_je_ke_l.$$

$$VD_{ij} = a_1V^2\delta_{ij} + a_2V_iV_j + a_3\mathbf{V}^2e_ie_j + a_4(\mathbf{e}.\mathbf{V})^2\delta_{ij}$$

$$+ a_5(\mathbf{e}.\mathbf{V})(V_ie_j + e_iV_j) + a_6(\mathbf{e}.\mathbf{V})^2e_ie_j,$$

where $(\mathbf{e}\mathbf{V})$ denotes a scalar product of the two vectors,

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➢The a_i 's, $1 \leq i \leq 6$, are the dispersivity moduli, which satisfy the six inequalities:

$$a_1 + a_2 + a_3 + a_4 + 2a_5 + a_6 > 0\,, \quad a_1 > 0\,,$$
$$a_1 + a_2 > 0\,, \quad a_1 + a_3 > 0\,, \quad a_1 + a_4 > 0,$$
$$a_1^2 + a_1(3a_2 + a_3 + a_4 + 2a_5 + a_6)$$
$$+2a_2(a_3 + a_4 + a_6) > 2a_5^2.$$

➢Example 1: Axis of symmetry--- z
Uniform flow in the $e_3 (\equiv z)$ -direction:

Then: $\mathrm{e}_1 = \mathrm{e}_2 = 0, \mathrm{e}_3 = 1, \quad \mathrm{V}_1 = \mathrm{V}_2 = 0, \mathrm{V}_3 = V.$

$$D_{ij} = \begin{pmatrix} a_{TH}^v & 0 & 0 \\ 0 & a_{TH}^v & 0 \\ 0 & 0 & a_{LV}^v \end{pmatrix} V, \qquad \begin{aligned} a_{TH}^v &= a_1 + a_4 \\ a_{LV}^v &= a_1 + a_2 + a_3 + a_4 + 2a_5 + a_6 \end{aligned}$$

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a_{TH}^v = transverse dispersivity in the horizontal direction when flow is along vertical axis of symmetry

a_{LV}^v = longitudinal dispersivity in the vertical direction when flow is normal to vertical axis of symmetry

➢Example 2: Axis of symmetry---z.
Uniform flow in the x-direction

$$\mathrm{e}_1 = \mathrm{e}_2 = 0, \mathrm{e}_3 = 1, \quad \mathrm{V}_1 = \mathrm{V}, \mathrm{V}_2 = \mathrm{V}_3 = 0$$

$$D_{ij} = \begin{pmatrix} a_{LH}^H & 0 & 0 \\ 0 & a_{TH}^H & 0 \\ 0 & 0 & a_{TV}^H \end{pmatrix} V, \; a_{LH}^H = a_1 + a_2,\; a_{TH}^H = a_1,\; a_{TV}^H = a_1 + a_3.$$

a_{TH}^H a_{TV}^H = transverse dispersivities in the horizontal and in the vertical directions when flow is horizontal.

a_{LH}^H = longitudinal dispersivity in the horizontal direction when flow is horizontal.

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➢Example 3: $V_1 = 0, V_2 = V_3 = V, e_1 = 1, e_2 = e_3 = 0.$

In this case:

$$D_{11} = 2(a_1 + a_3)V, \qquad D_{22} = D_{33} = (2a_1 + a_2)V,$$
$$D_{23} = a_2V, \qquad D_{12} = D_{31} = 0.$$

Here, we need three moduli: $a_1, a_2, a_3.$

➢Example 4: $V_1 = V_2 = V,\; V_3 = 0,\; e_1 = 1,\; e_2 = e_3 = 0.$
In this case:

$$D_{11} = (2a_1 + a_2 + 2a_3 + a_4 + 2a_5 + a_6)V, \qquad D_{12} = (a_2 + a_5)V,$$
$$D_{22} = (2a_1 + a_2 + a_4)V, \quad D_{33} = (2a_1 + a_4)V, \quad D_{21} = D_{31} = 0.$$

Here, we have three additional moduli: $a_4, a_5, a_6.$

➢Thus, with two experiments, with different setups of $\mathbf{V}$, ***and a known*** $\mathbf{e}$, we can find the six dispersivity moduli.

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❖EXPERIMENTAL DETERMINATION OF DISPERSIVITY MODULI

➢We consider the two 6-dim vectors,

$$\mathbf{D}_6 = (D_{11}, D_{22}, D_{33}, D_{12}, D_{23}, D_{31}),$$
$$\mathbf{a}_6 = (a_1, a_2, a_3, a_4, a_5, a_6)$$

and their transposed counterparts, $\mathbf{D}_6^T, \mathbf{a}_6^T$

➢We can then relate the two vectors by

$$V\mathbf{D}_6^T = \mathbf{a}_6^T\Delta_1(\mathbf{V}.e) = \begin{Bmatrix} \mathbf{V}^2 & V_1^2 & e_1^2\mathbf{V}^2 & (\mathbf{e}.\mathbf{V})^2 & 2(\mathbf{e}.\mathbf{V})e_1V_1 & (\mathbf{e}.\mathbf{V})^2e_1^2 \\ \mathbf{V}^2 & V_2^2 & e_2^2\mathbf{V}^2 & (\mathbf{e}.\mathbf{V})^2 & 2(\mathbf{e}.\mathbf{V})e_2V_2 & (\mathbf{e}.\mathbf{V})^2e_2^2 \\ \mathbf{V}^2 & V_3^2 & e_3^2\mathbf{V}^2 & (\mathbf{e}.\mathbf{V})^2 & 2(\mathbf{e}.\mathbf{V})e_3V_3 & (\mathbf{e}.\mathbf{V})^2e_3^2 \\ 0 & V_1V_2 & e_1e_2\mathbf{V}^2 & 0 & (\mathbf{e}.\mathbf{V})(e_2V_1 + e_1V_2) & (\mathbf{e}.\mathbf{V})^2e_1e_2 \\ 0 & V_2V_3 & e_2e_3\mathbf{V}^2 & 0 & (\mathbf{e}.\mathbf{V})(e_2V_3 + e_3V_2) & (\mathbf{e}.\mathbf{V})^2e_2e_3 \\ 0 & V_3V_1 & e_3e_1\mathbf{V}^2 & 0 & (\mathbf{e}.\mathbf{V})(e_1V_3 + e_3V_1) & (\mathbf{e}.\mathbf{V})^2e_3e_1 \end{Bmatrix}$$

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➢Assume that the symmetry axis, $\mathbf{e}$ is know and so is the velocity $\mathbf{V}$ in a know frame of reference, x_1, x_2, x_3

➢By examining the matrix $\Delta_1(\mathbf{V}.\mathbf{e})$

$$\det\Delta_1(\mathbf{V}.\mathbf{e}) = 0, \quad rank\Delta_1(\mathbf{V}.\mathbf{e}) = 4.$$

➢ With the conclusion that
One cannot get all six dispersivity $\mathbf{a}_i$-moduli from a single experiment.

➢Instead,
Two different experiments are required in order to determine all six $\mathbf{a}_i$-moduli

Example:

1st exp.: $\mathrm{V}_1 = 0, \mathrm{V}_2 = \mathrm{V}_3 = \mathrm{V}$ and $\mathrm{e}_1 = 1, \mathrm{e}_2 = \mathrm{e}_3 = 0.$

➢Then $D_{11} = 2(a_1 + a_3)V, \quad D_{22} = D_{33} = (2a_1 + a_2)V,$

$$D_{23} = a_2V, \quad D_{12} = D_{31} = 0.$$

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➢2nd exp.: $\mathrm{V}_1 = \mathrm{V}_2 = \mathrm{V}, \mathrm{V}_3 = 0,$ and $\mathrm{e}_1 = 1, \mathrm{e}_2 = \mathrm{e}_3 = 0.$

➢Then

$$D_{11} = (2a_1 + a_2 + 2a_3 + a_4 + 2a_5 + a_6)V, \quad D_{12} = (a_2 + a_5)V,$$
$$D_{22} = (2a_1 + a_2 + a_4)V, \quad D_{33} = (2a_1 + a_4)V, \quad D_{23} = D_{31} = 0.$$

The above relationships, obtained from two independent experiments, with different setups of $\mathbf{V}$ and a known $\mathbf{e}$, lead to the 6 a_i-moduli in a 3D domain with uniaxial symmetry.

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