Hydrodynamic Dispersion Coefficients in a Porous Medium with Parallel Fractures

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ABSTRACT

The results form the application of the method of homogenization for the transport of solute in a porous medium with microscale pores and the rock matrix are applied to examine the dispersion characteristics of a solute in a porous rock matrix with parallel fractures including the retardation in the rock matrix and the decay effects. By using the solutions to a boundary value problem the effective macroscale dispersion coefficients (longitudinal and transverse) are examined for various parameters such as the fracture porosity, the rock matrix porosity, and the retardation. The transverse dispersivity is essentially of diffusion type and shows minor variation with the fracture porosity and the matrix porosity. The longitudinal dispersivity increases with the flow intensity (Peclet number) and the retardation except for very low retardation coefficients. It is also shown that the longitudinal dispersivity decreases with the fracture porosity and the matrix porosity.

INTRODUCTION

The dispersion of solute matter in a rock medium is important from the viewpoints of the management and the safety regard of the underground disposal of the nuclear wastes. Rock formations are typically characterized by the existence of fracture networks in which the ground water is transported and the rock matrix which is composed of solid phase and immobile water. If a solute matter is released in a rock medium, it migrates with the flowing fluid in the fracture. The fluid flow is usually very slow and is in the laminar flow regime.

A released solute matter experiences not only diffusion in the rock matrix but also hydrodynamic dispersion in the fracture caused by the non-uniform fluid velocity distribution (Taylor dispersion). The solute in the rock matrix diffuses through the immobile water and also is sorbed onto the solid phase. Under the local equilibrium condition the solute is partitioned between the solids and the immobile water. This is effectively accounted for by the retardation coefficient of the rock matrix. The solute in the fracture while being transported by the flowing fluid experiences dispersion and interacts with the immobile water in the rock matrix through diffusion on the interface between the fracture and the rock matrix.

Studies on the behavior of radionuclides in a porous rock medium are mostly focused on the analysis in the individual fracture with the interaction with the surrounding host rock matrix including the distribution of the solute concentration in the fracture and the neighboring rock matrix[1-9].

From the viewpoint of the management of the underground repository and the environmental concerns over the rock domain it is necessary to assess and examine the behavior of the released contaminant on a larger macroscale including the spreading characteristics in the rock media with fractures.

In this study, the derivation of the macroscale governing equation for solute transport in a saturated porous rock medium is briefly mentioned. Also a boundary value problem is defined which can be used to determine the dispersion coefficients. The medium is composed of pore space (Ω_f) and the rock matrix (Ω_m) which is further composed of the solid phase and the immobile water. The theoretical frame for deriving the effective relations on the macroscale is the method of homogenization which is known to be highly effective in the treatment of the heterogeneous medium. An explicit expression for calculating the dispersion coefficients on the macroscale is given.

The results are applied to the transport of a solute matter in a porous rock medium with parallel fractures of uniform spacing. Using the approximate solutions to the microcell boundary value problem the longitudinal and transverse dispersion coefficients are calculated for various choices of the fracture porosity, the rock matrix porosity, the retardation coefficients and the flow intensity. The effects of the parameters on the dispersion coefficients are examined.

THE GOVERNING RELATIONS ON THE MICROSCALE

The porous medium is assumed to be composed of the matrix (Ω_m) in which the solid rock phase and immobile water exist and the fluid phase(Ω_f) through which the pore water flows. It is assumed that the porous medium is saturated by water so that Ω_f is occupied by water(assumed to be incompressible).

The basic governing equations on the microscale are summarized as follows. In Ω_f the fluid flow is governed by the conservation laws of mass and momentum and the transport of solute is governed by the masss conservation:

$$\nabla \cdot \mathbf{u} = 0$$

$$\rho_f \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \mu_f \nabla^2 \mathbf{u}$$

$$\frac{\partial c_f}{\partial t} + \mathbf{u} \cdot \nabla c_f = D_f \nabla^2 c_f - \lambda c_f$$

where $\mathbf{u}$ and c_f are the fluid velocity and the solute concentration([M/L^3]) in the fluid, and ρ_f and μ_f are the density and absolute viscosity of the fluid. Also D_f and λ are the diffusivity and decay coefficient of the solute respectively. In Ω_m, the solute mass conservation is governed by

$$\frac{\partial c_m}{\partial t} + \lambda c_m = \phi D_f \nabla^2 c_w$$

where

$$c_m = (1-\phi)\rho_s c_s + \phi c_w$$

is the solute concentration in the rock matrix([M/L^3]). The symbols c_s and c_w are the solute concentration in the solid per unit mass of solid([M/M]) whose density is ρ_s and the solute concentration in the immobile water inside the rock matrix ([M/L^3]). The symbol ϕ is the porosity of the rock matrix. Under the condition of local equilibrium between the solid and immobile water, it becomes $c_s = K_d\, c_w$ with K_d ([L^3 /M]) being the distribution coefficient. The above equation then becomes

$$R_m \frac{\partial c_w}{\partial t} + \lambda R_m c_w = D_f \nabla^2 c_w$$

where R_m =1+ ρ_s K_d (1-ϕ)/ϕ is the retardation coefficient.

On the interface boundary(Γ), the fluid velocity vanishes and the solute concentration and the solute flux are continuous:

$$\mathbf{u} = 0$$
$$c_f = c_w$$
$$D_f \nabla c_f \cdot \mathbf{N} = \phi D_f \nabla c_w \cdot \mathbf{N}$$

THE GOVERNING RELATIONS ON THE MACROSCALE

The process of deriving the macroscale governing equations is briefly summarized [11]. Two basic assumptions are introduced in the method of homogenization. First there exists a scale disparity so that there are two vastly different length scales: the microscale *l* and the macroscale *l'*. Second all the variables and material properties including the medium structure are *l* -periodic. The latter assumption is not very restrictive because the distribution and arrangement in the microscale cell of size *l* are quite arbitrary.

Normalization

Let *l* and *l'* be the length scales on the microscale and macroscale. They are related by

$$\frac{\ell}{\ell'} = \epsilon \ll 1$$

Also let *P'* and c_0 be the pressure drop over the macroscale and the reference concentration. The following normalization is introduced:

$$x = \ell x^*, t = t^* \ell'^2 / D_f, c_f = c_0 c_f^*, c_w = c_0 c_w^*$$
$$p = P' p^*, \mathbf{u} = U \mathbf{u}^* = \frac{P' \ell^2}{\mu_f \ell'} \mathbf{u}^*$$

The governing conditions in the dimensionless variables are omitted.

Dimensionless Parameters

Typical values of the physical parameters are[1, 2, 10].

$$\nu_f = \mu_f / \rho_f = O(10^{-6} m^2/s), \quad D_f = O(10^{-9} m^2/s), \quad \lambda = O(10^{-10} - 10^{-14} s^{-1})$$

where $\nu_f = \mu_f / \rho_f$ is the kinematic viscosity of the fluid. In view of the fact that the fluid flow is very slow and the fracture aperture is in the range of 0.1 - 1 *mm*, the following dimensionless parameters are defined and their orders of magnitude are also indicated:

Reynolds Number: $Re = U\ell/\nu_f = O(\epsilon)$

Peclet Number : $Pe = U\ell/D_f = O(\epsilon),\ \Lambda = \lambda\ell^2/\epsilon^2 D_f = O(1)$

Multiple Scale Analysis

From now on the discussion is for dimensionless quantities.

The fast and slow spatial coordinates are introduced and the derivatives are expanded accordingly:

$$\mathbf{x},\quad \mathbf{x}' = \epsilon\mathbf{x}\quad ;\qquad \frac{\partial}{\partial x_i} \to \frac{\partial}{\partial x_i} + \epsilon\frac{\partial}{\partial x_i'}$$

The dependent variables are expanded in perturbation series:

$$f = f^{(0)} + \epsilon f^{(1)} + \epsilon^2 f^{(2)} + \cdots;\qquad f = \{\mathbf{u}, p, c_f, c_w\}$$

At successive orders of ϵ, the following results are obtained.

At ϵ, $c_f{}^{(0)} = c^{(0)}$ (**x'**, t) and $c_w{}^{(0)} = c^{(0)}$ (**x'**, t) are independent of the microscale.

The first order correction terms are expressed as

$$c_f^{(1)} = \mathbf{M}^f \cdot \nabla c^{(0)} + < c_f^{(1)} >$$
$$c_w^{(1)} = \mathbf{M}^w \cdot \nabla c^{(0)} + < c_w^{(1)} >$$

where $< c_f{}^{(1)} >$ and $< c_w{}^{(1)} >$ are the microcell (Ω) averages defined as

$$< f >= \frac{1}{\Omega}\int_\Omega f d\Omega$$

The vector functions $\mathbf{M}^f$ and $\mathbf{M}^w$ must satisfy the following boundary value problem.

$$\begin{aligned}
Pe\left(\tilde{u}_i^{(0)}\delta_{ij} + u_i{}^{(0)}\nabla_i M_j^f\right) &= \nabla^2 M_j^f && \text{in} \quad \Omega_f \\
-PeLw'\frac{R_m}{n + (1-n)\phi R_m} < u_i{}^{(0)} > \delta_{ij} &= \nabla^2 M_j^w && \text{in} \quad \Omega_m \\
M_j^f &= M_j^w && \text{on} \quad \Gamma \\
\left(\delta_{ij} + \nabla_i M_j^f\right) N_i &= \phi\left(\delta_{ij} + \nabla_i M_j^w\right) N_i && \text{on} \quad \Gamma \\
< M_j^f > = < M_j^w > &= 0
\end{aligned}$$

where

$$\tilde{u}_i^{(0)} = u_i{}^{(0)} - \frac{1}{n + (1-n)\phi R_m} < u_i{}^{(0)} >$$

The Governing Equation on the Macroscale

Adding the governing equations at O(ϵ) and O(ϵ^2), the macroscale solute transport equation becomes

$$E\frac{\partial c^{(0)}}{\partial t} + Pe < \mathbf{u} > \cdot\nabla' c^{(0)} + E\Lambda c^{(0)} = \nabla' \cdot (\mathbf{D} \cdot \nabla' c^{(0)})$$

in which $E = n + (1-n)\phi R_m$

and $\mathbf{u} = \mathbf{u}^{(0)} + \epsilon\,\mathbf{u}^{(1)}$ and **D** is the dispersion coefficient tensor given by

$$\mathbf{D} = [n + (1-n)\phi]\,\mathbf{I} + < \nabla \mathbf{M}^f > + \phi < \nabla \mathbf{M}^w > - Pe < \mathbf{u}^{(0)} \mathbf{M}^f >$$

DISPERSION IN A ROCK MEDIUM WITH PARALLEL FRACTURES

As a model porous medium a rock with parallel fractures with uniform spacing is chosen. The distance between the centerlines of two neighboring fractures is l and the fracture aperture is w as shown in Fig. 1. The unit microcell is chosen as a square with side length of l. It is assumed that $w << l$ so that the medium porosity is very small: $n = \delta = w / l << 1$. Taking this into account a coordinate transformation is introduced as

$$\xi = x/\delta, \quad \eta = z \quad ; \qquad \delta = \bar{w}/\ell \ll 1$$

so that $-l/2 < x < l/2$ and $0 < z < l$ are transformed to $-1/(2\delta) < \xi < 1/2\delta$ and $0 < \eta < 1$ respectively. The fracture domain is for $-1/2 < \xi < 1/2$, and the rock matrix is for $-1/(2\delta) < -1/2$ and $1/2 < \xi < 1/(2\delta)$. In this case, δ is equal to the medium porosity n.

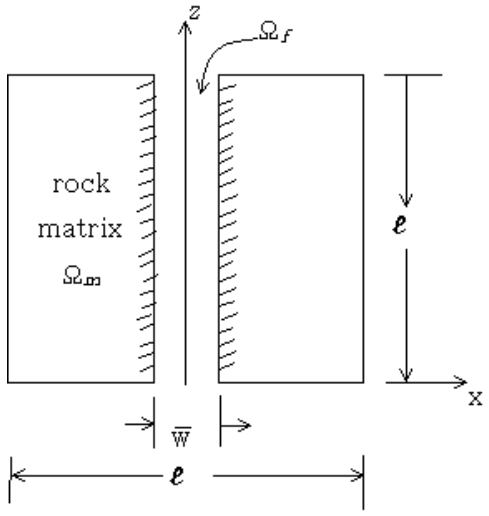

Fig. 1. A sample rock medium with a straight fracture.

Rewriting the microcell boundary value problem defined earlier in ξ and η, expanding $\mathbf{M}^f = (M^f_x, M^f_z)$ and $\mathbf{M}^w = (M^w_x, M^w_z)$ in perturbation series in δ, and solving the reduced problems

$$M_x^f = -\frac{\delta(1-\delta)(1-\phi)}{1-\delta(1-\phi)}\xi + O(\delta^2), \qquad -1/2 < \xi < 1/2$$

$$M_x^w = \frac{\delta(1-\phi)(\delta\xi \pm 1/2)}{1-\delta(1-\phi)} + O(\delta^2), \qquad 1/2 < \mp\xi < 1/2\delta$$

$$M_z^f = M_z^w = M_z = \frac{b-c}{a}\left[\frac{1}{2} - \frac{1}{a} + \frac{e^{a\eta}}{e^a - 1} - \eta\right] + O(\delta^2)$$

where

$$a = Pe < u_z^{(0)} >$$

$$b = Pe < \tilde{u}_z^{(0)} >$$

$$c = Pe < u_z^{(0)} > (1-\delta)$$

The symmetric longitudinal and transverse dispersion coefficients are then given as

$$D_{zz}^s = [\delta + \phi(1-\delta)]\left[1 + \frac{(b-c)^2}{2a^2}\frac{(a-2)e^a + (a+2)}{e^a - 1}\right]$$

$$D_{xx}^s = \delta + (1-\delta)\phi + (1+\phi)\left[\frac{\delta(1-\delta)(1-\phi)}{1-\delta(1-\phi)}\right]^2 - 2\frac{\delta(1-\delta)(1-\phi)[\phi + \delta(1-\phi)]}{1-\delta(1-\phi)}$$

It is noted that the dispersion effect, flow-enhanced diffusion, is reflected in D_{zz}^s via the factors *a*, *b* and *c*. On the other hand, the transverse dispersion coefficient D_{zz}^s is due to combined effects of the diffusion in the fracture and the diffusion in the immobile fluid inside the rock matrix.

RESULTS AND DISCUSSIONS

Variations of the longitudinal and transverse dispersion coefficients are examined for a few geometrical characteristics and the retardation coefficient of the rock medium.

The fracture aperture varies typically from 0.1 to 2*mm* whereas the fracture spacing varies from 0.3 to 1*m*. In this study, the following values of rock porosity δ are chosen as [7-8]

$\delta = (n) = 0.001, 0.005, 0.01, 0.05$

The rock matrix porosity values are chosen as[4, 7, 8]

$\phi = 0.01, 0.1, 0.2, 0.3$

Transverse Dispersion Coefficient

Due to the blockage of the rock matrix the transverse dispersion is essentially of diffusive nature in a medium with parallel fractures.

The effects of varying the rock matrix porosity are shown in Fig. 2(a) for various values of the fracture porosity and the effects of varying the fracture porosity are shown in Fig. 2(b).

The transverse dispersion coefficient increases, as shown in Fig. 2(a), with the matrix porosity due to increased diffusion from the fracture into the surrounding matrix for larger matrix porosity. The increasing trend with the matrix porosity is quite linear. In Fig. 2(b), the variations of the transverse dispersion coefficient with the fracture porosity are shown over the chosen range. Except very small matrix porosity the variation is small. For $\phi = 0.01$ the variation is quite large because of relatively large fluid content in the fracture as compared with the amount of the fluid in the rock matrix.

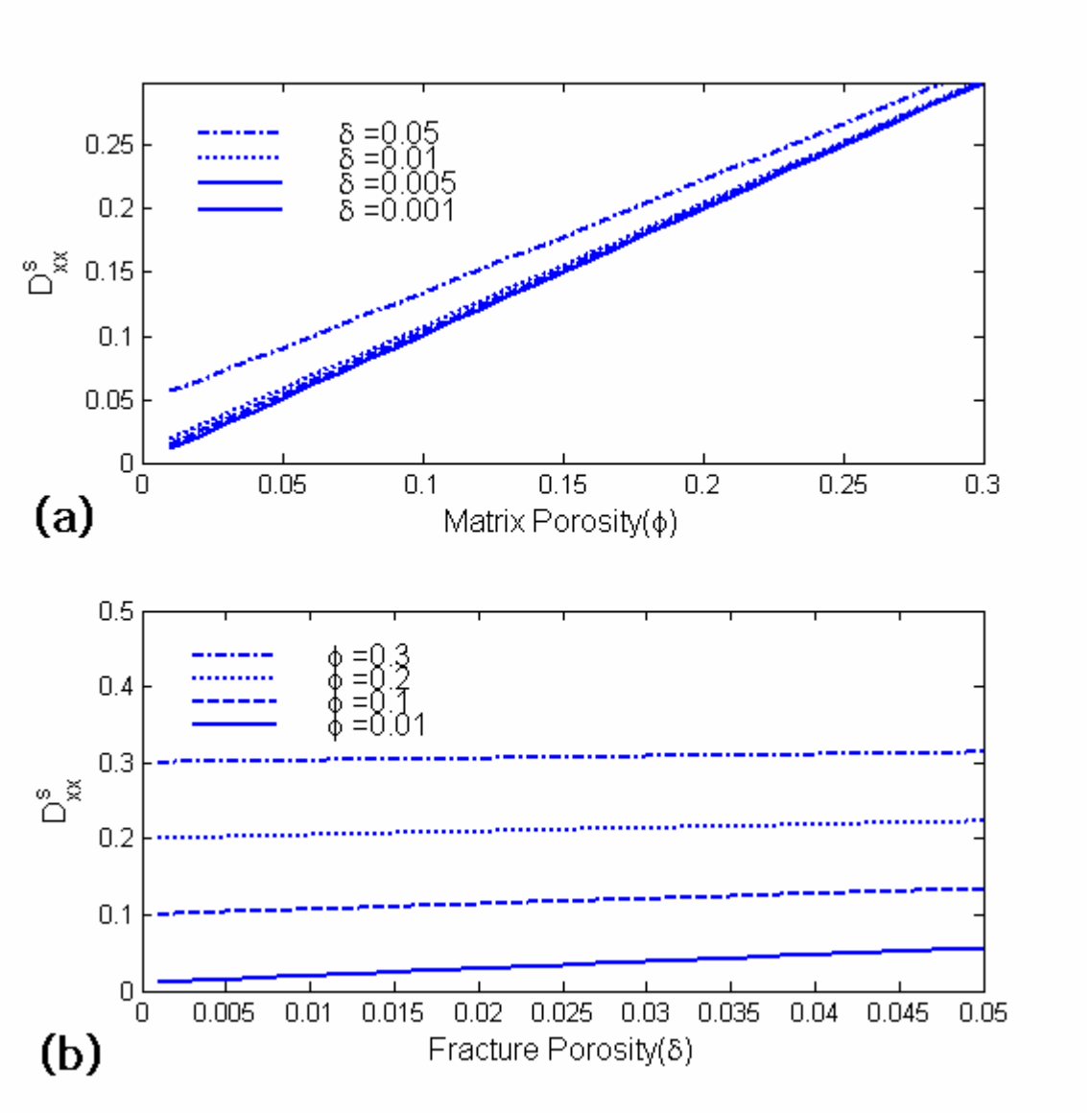

Fig. 2. Variations of the transverse dispersion coefficient with (a) the matrix porosity and (b) the fracture porosity.

Longitudinal Dispersion Coefficient

The longitudinal dispersion coefficient is directly influenced by the flow intensity because the parameters *a*, *b* and *c* are proportional to the Peclet number. The range of the Peclet number has been chosen up to 10.

In view of the fact that the retardation coefficient varies over a wide range, the values 1, 10, 100, 100 were chosen.

The variations of the longitudinal dispersion coefficient with Peclet number for a few fracture porosity values and the smallest of the rock porosity 0.01 are shown in Fig. 3(a) for the same set of retardation coefficients. First the dispersion coefficient increases with Peclet number as a result of increased velocity gradient in the fracture for larger Peclet number. Second it increases with the retardation coefficient. It is due to increased sorption onto the rock matrix for larger retardation thereby contributing to the longitudinal spreading of the solute matter.

It is noted that the increasing trend of the longitudinal dispersion coefficient increases with the fracture porosity for relatively larger values of retardation coefficients (10 and larger) whereas it decreases with the fracture porosity for the retardation coefficient of 1. This implies that the two different patterns of the longitudinal dispersion are separated at a retardation coefficient value somewhere between 1 and 10. As the fracture porosity increases the nonuniformity of the velocity(velocity shear) in the pore decreases for a fixed Peclet number and the Taylor dispersion is reduced which in turn causes a decrease of the longitudinal dispersion. On the other hand, the retardation causes an increase of dispersion. When the retardation coefficient is large, the dispersion is dominated by retardation. But if the retardation coefficient is low, the dispersion is dominantly affected by Taylor dispersion and hence decreases with increasing fracture porosity.

The variations of the longitudinal dispersion coefficient with Peclet number for the rock porosity of 0.1 are shown in Fig. 3(b). As compared with Fig. 3(a), it is seen that the longitudinal dispersion coefficient becomes noticeably smaller. The rock matrix in Fig. 3(b) has the fluid content 10 times larger than that in Fig. 3(a). It was shown earlier in Fig. 2(a) that the transverse dispersion increases with the rock porosity. This has the effect of decreasing the longitudinal dispersion as is shown in Fig. 3(b). The same remarks made in Fig. 3(a) apply here.

The same types of variations are shown in Fig. 4 (a) and (b) for the rock porosity values of 0.2 and 0.3. It is observed again that the longitudinal dispersion coefficient decreases with increasing rock porosity. The opposite trends with the rock porosity for high and low retardation coefficients are also seen.

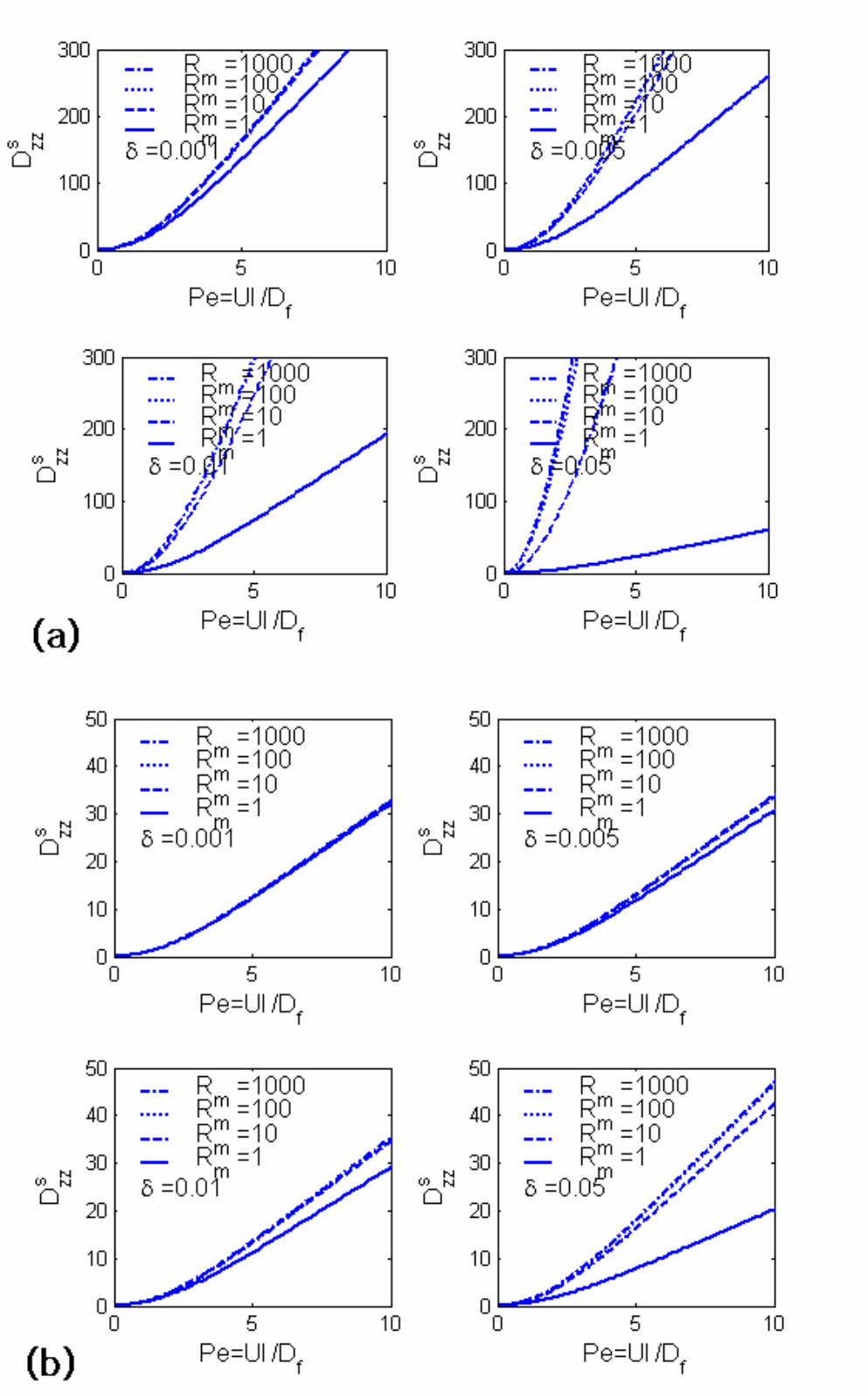

Fig. 3. Variations of the longitudinal dispersion coefficient with Peclet number for various fracture porosity and retardation values for the matrix porosity values of (a) 0.01and (b) 0.1.

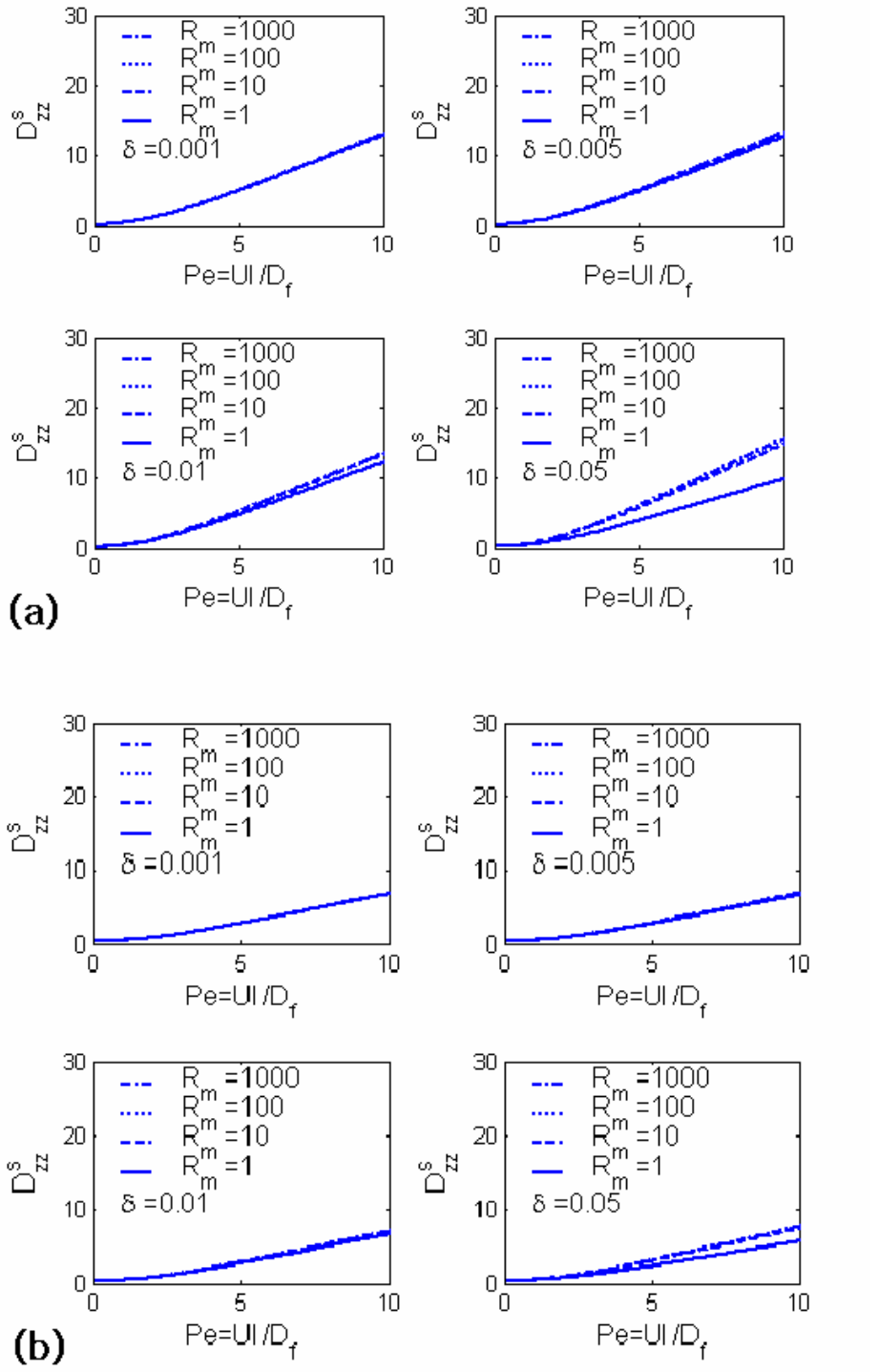

Fig. 4. Variations of the longitudinal dispersion coefficient with Peclet number for various fracture porosity and retardation values for the matrix porosity values of (a) 0.2and (b) 0.3.

CONCLUSIONS

From the present study of the dispersion of a solute in a saturated rock medium which is composed of parallel fractures and porous matrix with solids and immobile fluid the following conclusions are drawn.

1. The transverse dispersion coefficient in the direction normal to the fractures increases with both the fracture porosity and the rock matrix porosity although the changes are minor.

2. The longitudinal dispersion coefficient along the fractures increases with the flow intensity, i.e. the Peclet number.

3. The retardation has the effect of increasing the longitudinal dispersion whereas the fracture porosity causes a decrease of the dispersion. When the retardation is sufficiently large, the longitudinal dispersion increases with increased fracture porosity. But when the retardation is low, the longitudinal dispersion decreases with the fracture porosity.

4. The rock matrix porosity has the effect of decreasing the longitudinal dispersion.

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