

MULTIPHASE MEDIA APPROACH – A KEY TO MODELLING IN ENVIRONMENTAL MECHANICS. DESCRIPTION OF SOLUTE TRANSPORT PHENOMENA IN POROUS MEDIA ¹

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A description of solute migration through porous media is presented. It is assumed that transport of contaminants may be considered as an effect of the two processes: advection and dispersion. The advective transport is attributed to an average motion of the solution through the porous skeleton. The dispersive transport results from molecular diffusion and mechanical mixing. In the paper the Fickian as well as Non-Fickian dispersion is considered.

Key words: porous media, transport of contaminants, advection

1. Introduction

For the past few decades substantial research into contaminant migration in geologic deposits has been conducted. The greatest challenge the scientists dealing with hydrology and related disciplines of environmental mechanics are being confronted at present is to develop the ability to predict, at a reasonable degree of certainty, the spatial and temporal distribution of ground-water contaminants that might result from people activities. Therefore, the research efforts are directed toward studies the development of an improved understanding of the processes of solute migration through porous media are of great importance. These studies comprise a proper theoretical description of

¹Lecture was presented during the TEMPUS Intensive Course on "Environmental Mechanics", Mierki, September 10-12, 1996, Poland

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solute migration through geologic materials, laboratory and field observations of transport processes, and incorporation of the theoretical descriptions into predictive mathematical models for predicting the future spatial distribution of contaminants in ground-water systems. When considering the transport of contaminants we usually deal with the media composed of solid porous skeleton and an immiscible fluid penetrating pores. Such a porous skeleton and a pore fluid constitute phases of separated (individual) material volumes. Moreover, each phase can be considered as consisting of several components continuously distributed (at the molecular level) within the volume of that phase. Transport of contaminants may be controlled by several mechanisms: advection, diffusion and sorption of chemicals and mechanical deformation of the porous skeleton. Adequate approach to modeling of the above coupled phenomena consists in the description based on the theory of multiphase-multicomponent media (see e.g. Bedford and Drumheller, 1983) formulated on the macroscopic scale which is most important for almost all engineering applications. In the first part of the paper main features of description of the solute transport are discussed. Most of this part is based on the results given by Gillham and Cherry (1982), Bear (1972) and Hassanizadeh (1995).

2. Description of the solute transport

A description of the solute transport processes most widely used is the macroscopic (average) approach (Bear, 1972; Bear and Bachmat [2]). The parameters assumed in this approach have deterministic physical representations and comparison of the model performance with experimental results can provide an improved understanding of the transport processes.

On the pore scale of description, solute transport results from physical and chemical processes occurring within the pores and at the solid-solution interfaces. Equations valid on the pore scale are acceptable for describing the migration process on this scale, however, solutions to these equations are not available due to very complex boundary conditions and because of the our inability to measure the respective transport parameters on the pore scale. Therefore, in the statistical approach a procedure of spatial averaging is used to replace the pore-scale of description with the macroscopic scale where the quantities defined at a point represent the average of micro-effects in the vicinity of the point (called the Representative Elementary Volume (REV), see Fig.1). A description of the spatial averaging procedure has been developed

by several researchers (e.g. Bear, 1972; Hassanizadeh, 1995; Hassanizadeh and Gray, 1979; Nigmatulin, 1979; Whitaker, 1969).

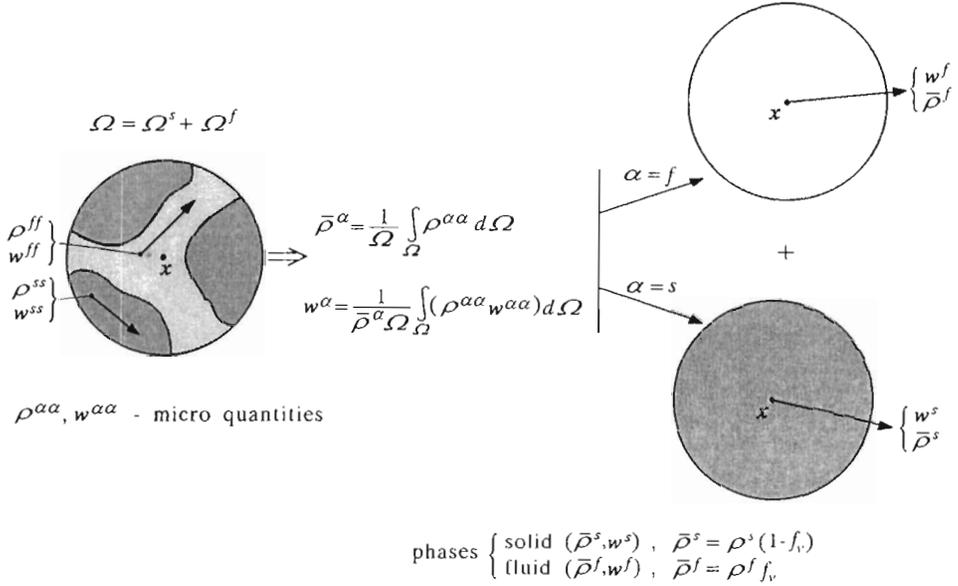


Fig. 1. Volume averaging procedure

The fundamental macroscopic equation governing the spreading of solutes in a porous medium can be derived by considering the mass conservation equation of a movable pore-fluid phase treated as a multi-component mixture. We briefly recall the basic steps of derivation of such an equation using the volume averaging nomenclature.

Let us consider a porous medium composed of non-deformable porous skeleton (of homogeneous and isotropic pore structure) saturated with a multi-component fluid (solution). The fluid phase consists of N miscible components which may, in general, interact chemically with each other (on the molecular level). If Ω represents the REV volume being a sum of the solid skeleton volume Ω^s and the fluid volume Ω^f , i.e.

$$\Omega = \Omega^s + \Omega^f \tag{2.1}$$

one can define the macroscopic mass concentration of species which is the mass of species β per unit volume of the solution

$$c^\beta = \frac{M^\beta}{\Omega^f} \quad \beta = 1, \dots, N \tag{2.2}$$

and this definition is based on the fact that the fluid components are miscible and they all are distributed over the same volume Ω^f . Then, the total mass of fluid phase in Ω per its volume Ω^f is

$$\rho^f = \frac{M^f}{\Omega^f} = \frac{\sum_{\beta} M^{\beta}}{\Omega^f} = \sum_{\beta} c^{\beta} \quad (2.3)$$

and ρ^f is called the effective fluid (solution) density, while its partial density is

$$\bar{\rho}^f = \rho^f f_v = f_v \sum_{\beta} c^{\beta} \quad (2.4)$$

where f_v is the volume porosity defined as

$$f_v = \frac{\Omega^f}{\Omega} \quad (2.5)$$

In a considered solution the various chemical species β are moving at different mass average velocities \mathbf{v}^{β} in the stationary coordinate system. For each chemically active species the macroscopic mass continuity equation has the form

$$\frac{\partial f_v c^{\beta}}{\partial t} + \nabla \cdot (f_v c^{\beta} \mathbf{v}^{\beta}) = f_v g^{\beta} \quad \beta = 1, \dots, N \quad (2.6)$$

where the reaction term g^{β} represents the rate of creation of the component mass β from chemical reactions and should satisfy the following equation

$$\sum_{\beta} f_v g^{\beta} = 0 \quad (2.7)$$

In practical problems of contaminant transport in porous media one is interested in the mean motion of fluid phase (solution) and the diffusive motion of $N - 1$ components with respect to the mean motion. Thus, using the local mass average solution velocity

$$\mathbf{v}^f = \frac{1}{f_v \rho^f} \sum_{\beta} c^{\beta} \mathbf{v}^{\beta} \quad (2.8)$$

and the diffusive velocity for the β component

$$\mathbf{u}^{\beta} = \mathbf{v}^{\beta} - \mathbf{v}^f \quad (2.9)$$

Eq (2.6) may be replaced by the continuity equation for the solution

$$\frac{\partial (f_v \rho^f)}{\partial t} + \nabla \cdot (f_v \rho^f \mathbf{v}^f) = 0 \quad (2.10)$$

and the continuity equation for the $N - 1$ β components

$$\frac{\partial(f_v c^\beta)}{\partial t} + \nabla \cdot \mathbf{j}_{adv} + \nabla \cdot \mathbf{j}^\beta = f_v g^\beta \quad (2.11)$$

where

$$\mathbf{j}_{adv} = f_v c^\beta \mathbf{v}^f \quad (2.12)$$

represents the mean mass flux of the species β and

$$\mathbf{j}^\beta = f_v c^\beta \mathbf{u}^\beta \quad (2.13)$$

is the diffusive-dispersive mass flux of the species β that should satisfy the condition

$$\sum_{\beta} \mathbf{j}^\beta = 0$$

Eq (2.11) allows one to consider the solute transport as the net effect of the two processes: advection and dispersion.

To discuss characteristic features of these processes we confine our considerations to the two-component chemically inert solution; i.e., water (w) and a contaminant (c) soluble in water. In this case, $g^\beta = 0$, $c^1 \equiv c^w$, $c^2 \equiv c^c \equiv c$, and c is the solute concentration.

Advective transport is attributed to the mean motion of the solution through the porous skeleton and the advective solute flux reads

$$\mathbf{j}_{adv} = f_v c \mathbf{v}^f$$

that represents the mass of solute crossing a unit area of porous medium perpendicular to the mean flow direction. The dispersive mass flux

$$\mathbf{j} = f_v c \mathbf{u}$$

results from the two processes, i.e., molecular diffusion and mechanical mixing. Diffusion is the effect of the thermal motion of molecules resulting in a net flux \mathbf{j}_d of solute directed towards the low-concentration zone. It is usually assumed that the diffusion flux in a porous medium has the Fickian form

$$\mathbf{j}_d = -f_v D_d \text{grad } c \quad (2.14)$$

where \mathbf{j}_d represents the mass of solute per unit area of porous medium per unit time and D_d is the effective molecular diffusion coefficient. The coefficient D_d is generally smaller than the diffusion coefficient in free solution D_o , due to the tortuous diffusion path-way within a porous medium and the presence

of the solution – solid interface, (see Bear, 1972; Perkins and Johnston, 1963). These coefficients are related by the equation

$$D_d = D_o \tau \quad (2.15)$$

where τ is the tortuosity (in general can be a second order tensor). The mechanical mixing component of the dispersive flux results from relative velocity variations within the porous medium being produced by the following three microscopic mechanisms (Gillham and Cherry, 1982), Fig.2:

- The pore velocity distribution associated with the flow of viscous fluid through a pore
- Variations in velocity as a result of different pore geometry
- Fluctuations in the stream lines with respect to the mean flow direction.

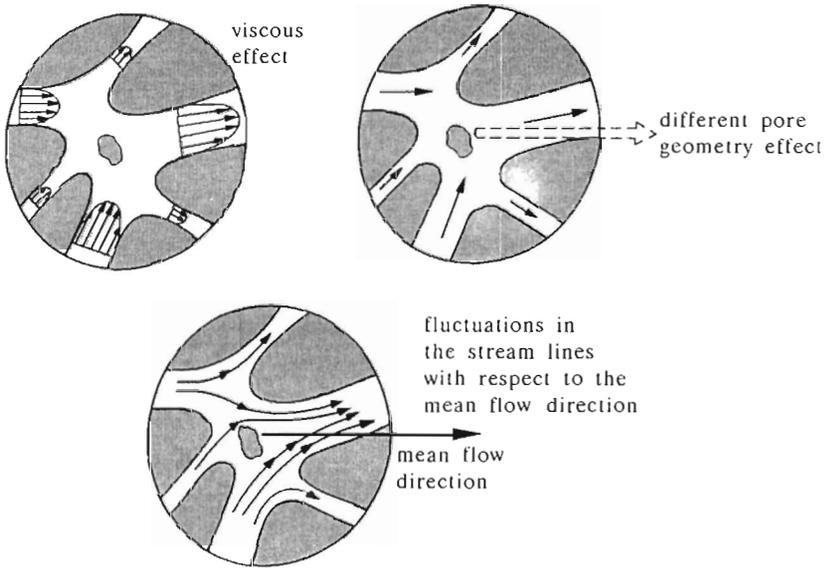


Fig. 2. Microscopic mechanism of mechanical mixing

On the macroscopic scale, the mechanical mixing component of the solute flux is commonly represented by the concentration gradient

$$\mathbf{j}_m = -f_v D_m \text{grad } c \quad (2.16)$$

where D_m is the coefficient of mechanical dispersion.

The total dispersive flux of the solute is

$$\mathbf{j} = \mathbf{j}_d + \mathbf{j}_m = -f_v D \text{grad } c \quad (2.17)$$

where D is the coefficient of dispersion defined as

$$D = D_d + D_m \quad (2.18)$$

Substituting the advective and dispersive flux components into the mass conservation equation (2.11) yield

$$\frac{\partial(f_v c)}{\partial t} = \nabla \cdot (f_v D \nabla c) - \nabla \cdot (f_v c \mathbf{v}^f) \quad (2.19)$$

which is fairly general and valid for the systems with variable porosity f_v and variable coefficient of the dispersion D . When the fluid is assumed to be incompressible and the porous medium is rigid and homogeneous, (the porosity $f_v = \text{const}$) the above equation takes on the form

$$\frac{\partial c}{\partial t} = \nabla \cdot (D \text{grad } c) - \mathbf{v}^f \cdot \text{grad } c \quad (2.20)$$

This is the advective-dispersion equation for solute transport describing the concentration profiles in a binary diffusing system moving through a rigid porous medium.

3. Discussion

There are several limitation imposed on the analysis presented above leading to the advective-dispersion equation (2.20):

- Contaminant are soluble in water and chemically inert
- The coefficients of molecular diffusion and mechanical mixing are additive
- The fluid is incompressible and its physical properties are independent of solute concentration.

The effects of advection and dispersion for one-dimensional solute transport are shown schematically in Fig.3. It is seen that a plane profile of solute

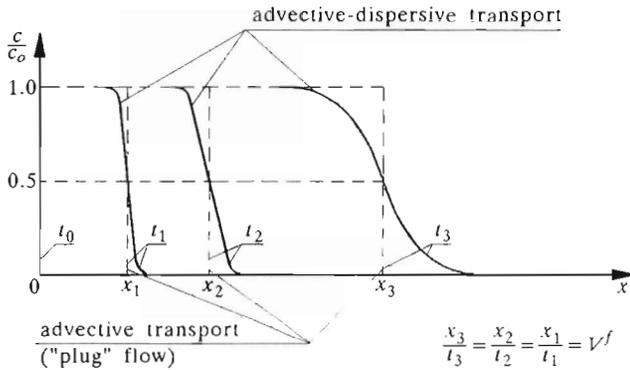


Fig. 3. Scheme of the advective and dispersive solute transport processes

front due to advection alone is strongly influenced by the dispersion phenomena and as the transport process goes on the profile becomes more dispersed.

The applicability of the advection-dispersion model is usually verified from the column experiment by one-dimensional miscible-displacement measurement. In such an experiment a column (of soil) is initially saturated with water. Water is displaced with a solution of concentration c_0 .

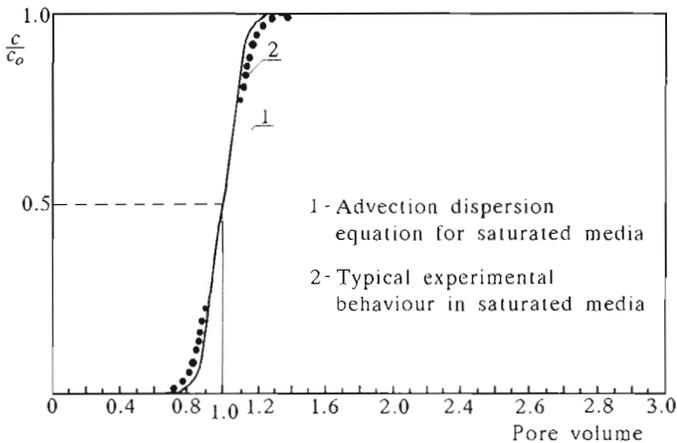


Fig. 4. Typical deviations from the breakthrough curve saturated porous media predicted by the advective-dispersion solute transport model

The concentration history of the column effluent is generally represented by the breakthrough curve graph of dimensionless concentration (c_0/c) versus dimensionless time represented by the number of pore volumes, see Fig.4.

4. The effect of mean velocity on dispersion coefficients. Experimental observations

A rigorous analysis of Eq (2.20) shows (for homogeneous media) the dispersive coefficient to be the second order tensor (Bear, 1972; Hassanizadeh, 1996). This tensor is considered to be the following function of mean flow velocity

$$\mathbf{D} = (D_\alpha + \alpha_T |\mathbf{v}^f|) \mathbf{I} + (\alpha_L - \alpha_T) \frac{\mathbf{v}^f \otimes \mathbf{v}^f}{|\mathbf{v}^f|} \quad (4.1)$$

where α_T and α_L are the transversal and longitudinal dispersivities [Sch], respectively, \mathbf{I} is the unit tensor. Its principal values are

$$D_L = D_d + \alpha_L |\mathbf{v}^f| \quad D_T = D_d + \alpha_T |\mathbf{v}^f|$$

and represent the longitudinal and transverse dispersion coefficients, respectively.

Laboratory experiments have provided a considerable amount of information on the nature of the dispersion process, such as the influence of velocity on the components of dispersion tensor (see Perkins and Johnston, 1963; Rose, 1973). Empirical results have proved that the dispersion coefficients are strongly dependent on the solution velocity v^f as well as on the geometrical properties of the pore/grain structure represented by a characteristic length, generally taken to be the mean grain diameter d . The empirical formulae for the longitudinal and transverse dispersion coefficients expressed in terms of the molecular diffusion coefficient D_o and the Peclet number Pe defined as $v^f d/D_o$, are suggested in the following form (cf Perkins and Johnston, 1963)

$$\frac{D_L}{D_o} = \frac{D_d}{D_o} + 1.75 \frac{v^f d}{D_o} \quad (4.2)$$

the corresponding 1D equation is

$$\frac{\partial C}{\partial t} = D_L \frac{\partial^2 c}{\partial x^2} - v^f \frac{\partial c}{\partial x}$$

and

$$\frac{D_T}{D_o} = \frac{D_d}{D_o} + 0.55 \frac{v^f d}{D_o} \quad (4.3)$$

the corresponding 2D equation is

$$\frac{\partial C}{\partial t} = D_L \frac{\partial^2 c}{\partial x^2} + D_T \frac{\partial^2 c}{\partial y^2} - v^f \frac{\partial c}{\partial x}$$

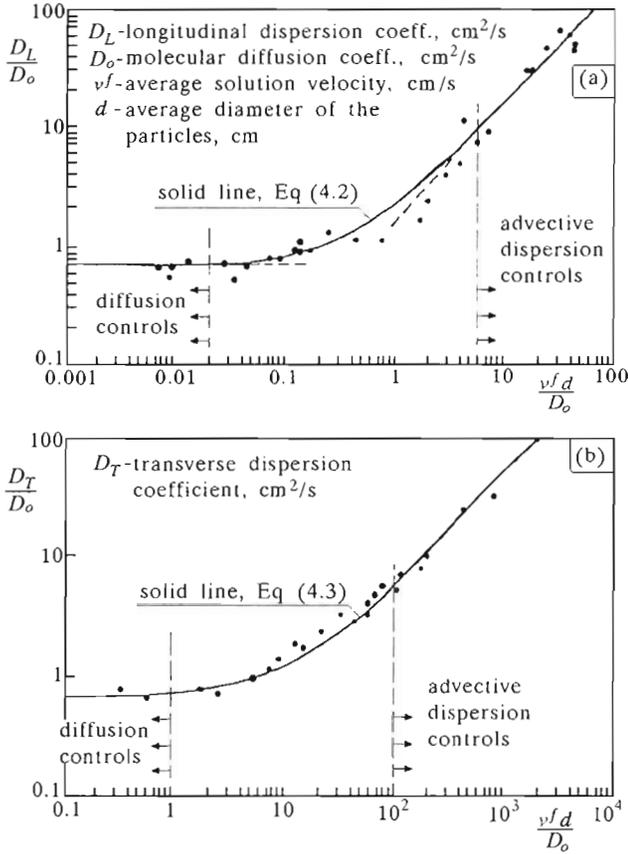


Fig. 5. Graphs of the dimensionless dispersion coefficient versus the Peclet number, V_d/D_o . (a) D_L/D_o versus Pe , (b) D_T/D_o versus Pe (after Perkins and Johnston, 1963)

Eqs (4.2) and (4.3) suggest that, in general, at low Peclet numbers the dispersion coefficient has a constant value being equal to the value of effective diffusion coefficient of the tracer in the porous medium. In such a case molecular diffusion controls the dispersion process. At a high solution velocity (large Peclet number) the mechanical mixing processes predominate. At intermediate values of Pe (of different range for D_L and D_T) both diffusion and mechanical mixing play a significant role in the dispersion process. The graphs of dimensionless dispersion coefficients D_L/D_o and D_T/D_o versus the Peclet number are shown in Fig.5. Eqs (4.2) and (4.3) suggest the more

general relationship between the dispersion coefficients and \mathbf{v}^f

$$D_L = D_o + \alpha_L |\mathbf{v}^f|^m \quad D_T = D_o + \alpha_T |\mathbf{v}^f|^n \quad (4.4)$$

where m and n are empirical constants and for practical purposes when the mechanical mixing is a dominant dispersive process (Bear, 1972)

$$m = n \cong 1$$

then

$$D_L = \alpha_L |\mathbf{v}^f| \quad D_T = \alpha_T |\mathbf{v}^f| \quad (4.5)$$

5. Description of the Non-Fickian dispersion from the equation of motion for a solute

The advection-dispersion equation (2.19) with the dispersion tensor (4.1) has been shown to give satisfactory results for homogeneous permeable media. In the case of small scale or large scale heterogeneities in the permeable matrix the deviations occur from the so-called Fickian dispersion behaviour. This problem was discussed by Scheidegger (1958), Tompson (1988), Strack (1992) and recently by Hassanizadeh (1996).

Commonly, two kinds of deviations from the Fickian behaviour are considered. The first kind regards dependence of the dispersive tensor on flow velocity. This deviation, however, is often considered not to be important in practical situations. A more serious shortcoming is that the values of longitudinal and transversal dispersivities often increase with the distance (and/or time) approaching some asymptotic values (Matheron and De Marsily, 1980; Dagan, 1989). In this case the linear relationship between the dispersive mass flux \mathbf{j} and the solute concentration gradient no longer holds. Here, a generalized relationship for the Non-Fickian dispersion flux is shown, which is derived from the equation of motion for a solute (Hassanizadeh, 1996).

We consider a porous medium saturated with water containing a reacting solute. For both the components water (w) and solute (l) we have the equations of mass balance

$$\frac{\partial(f_v c^w)}{\partial t} + \nabla \cdot (f_v c^w \mathbf{v}^w) = f_v c^w g^w \quad (5.1)$$

$$\frac{\partial(f_v c^l)}{\partial t} + \nabla \cdot (f_v c^l \mathbf{v}^l) = f_v c^l g^l$$

the equations of momentum balance

$$\begin{aligned} \frac{\partial(f_v c^w \mathbf{v}^w)}{\partial t} + \nabla \cdot (f_v c^w \mathbf{v}^w \otimes \mathbf{v}^w) &= \nabla \cdot \boldsymbol{\sigma}^w + f_v c^w \mathbf{g} + f_v c^w (\mathbf{r}^w + g^w \mathbf{v}^w) \\ \frac{\partial(f_v c^l \mathbf{v}^l)}{\partial t} + \nabla \cdot (f_v c^l \mathbf{v}^l \otimes \mathbf{v}^l) &= \nabla \cdot \boldsymbol{\sigma}^l + f_v c^l \mathbf{g} + f_v c^l (\mathbf{r}^l + g^l \mathbf{v}^l) \end{aligned} \quad (5.2)$$

respectively, where

- $c^\beta, \boldsymbol{\sigma}^\beta$ – mass concentration and the stress tensor of the β component
- \mathbf{g} – gravity vector
- g^β – rate of exchange of mass of the β component with other components and the solid phase
- \mathbf{r}^β – force exerted on the β component by all other components and the solid phase.

Combining Eqs (5.1) and (5.2) we obtain the equation of relative momentum balance for the solute in the following form

$$\begin{aligned} f_v c^l \frac{\partial(\mathbf{v}^l - \mathbf{v}^w)}{\partial t} + f_v c^l (\mathbf{v}^l \cdot \nabla \mathbf{v}^l - \mathbf{v}^w \cdot \nabla \mathbf{v}^w) &= \\ = (\nabla \cdot \boldsymbol{\sigma}^l - \frac{c^l}{c^w} \nabla \cdot \boldsymbol{\sigma}^w) + f_v c^l (\mathbf{r}^l - \mathbf{r}^w) \end{aligned} \quad (5.3)$$

We focus our attention on the case when the solute concentration is low, so that the fluid phase density will not be affected by changes in the solute concentration. Then, one can write

$$\frac{c^l}{\rho^f} \ll 1 \quad \Rightarrow \quad \rho^f \approx \rho^w \quad (5.4)$$

and the relation

$$\rho^f \mathbf{v}^f = c^l \mathbf{v}^l + c^w \mathbf{v}^w \quad (5.5)$$

yields

$$\mathbf{v}^f \approx \mathbf{v}^w \quad (5.6)$$

Also, the relative solute velocity \mathbf{u}^l , and the dispersive mass flux \mathbf{j} , we can defined as

$$\begin{aligned} \mathbf{u}^l &= \mathbf{v}^l - \mathbf{v}^f \cong \mathbf{v}^l - \mathbf{v}^w \\ \mathbf{j} &= f_v c^l \mathbf{u}^l = f_v c^l (\mathbf{v}^l - \mathbf{v}^w) \end{aligned} \quad (5.7)$$

Basing on these definitions and assumptions, Eq (5.3) may be rearranged to obtain the following equation of motion for the solute

$$\begin{aligned} \frac{\partial \mathbf{j}}{\partial t} + \mathbf{v}^f \cdot \nabla \mathbf{j} + \mathbf{j} \cdot \nabla \mathbf{v}^f + \nabla \cdot \left(\frac{\mathbf{j} \otimes \mathbf{j}}{f_v c^l} \right) + \mathbf{j} (\nabla \cdot \mathbf{v}^f) = \\ = \nabla \cdot \left(\boldsymbol{\sigma}^l - \frac{c^l}{c^w} \boldsymbol{\sigma}^w \right) + f_v c^l (\boldsymbol{\tau}^l - \boldsymbol{\tau}^w) + \boldsymbol{\sigma}^w \cdot \nabla \left(\frac{c^l}{c^w} \right) + \mathbf{j} g^l \end{aligned} \quad (5.8)$$

From the constitutive analysis (Hassanizadeh, 1986), one can suggest

$$\boldsymbol{\sigma}^l - \frac{c^l}{c^w} \boldsymbol{\sigma}^w = - \left[f_v c^l (\boldsymbol{\mu}_*^l - A_*^l) \right] \mathbf{l} \quad (5.9)$$

$$f_v c^l (\boldsymbol{\tau}^l - \boldsymbol{\tau}^w) = \nabla \left[f_v c^l (\boldsymbol{\mu}_*^l - A_*^l) \right] - f_v c^l \nabla \boldsymbol{\mu}_*^l - \boldsymbol{\sigma}^w \cdot \nabla \left(\frac{c^l}{c^w} \right) + f_v c^l \boldsymbol{\tau}_*^l$$

where $\boldsymbol{\mu}_*^l$ and A_*^l stand for the relative chemical potential and the relative Helmholtz free energy of the solute, respectively (both relative to the pure water component), and $\boldsymbol{\tau}_*^l$ is the nonequilibrium component of the resisting force, which is the dissipative force.

After the substitution of Eqs (5.9) into Eq (5.8) the right-hand side (*RHS*) of Eq (5.8) takes form

$$RHS = -f_v c^l \boldsymbol{\mu}_*^l + f_v c^l \boldsymbol{\tau}_*^l + \mathbf{j} g^l \quad (5.10)$$

Since the nonzero resisting force $\boldsymbol{\tau}_*^l$ appears only if the solute moves with respect to the pure water component and the solid phase, with the use of Eqs (5.7) we find

$$\mathbf{v}^l - \mathbf{v}^f \cong \mathbf{v}^l - \mathbf{v}^w = \frac{1}{f_v c^l} \mathbf{j} \quad (5.11)$$

$$\mathbf{v}^l - \mathbf{v}^s = (\mathbf{v}^l - \mathbf{v}^f) + (\mathbf{v}^f - \mathbf{v}^s) = \frac{1}{f_v c^l} \mathbf{j} + \mathbf{u}^f$$

where \mathbf{v}^s is the velocity of the solid phase and \mathbf{u}^f is the relative fluid phase velocity with respect to solid, and the following constitutive relation for $\boldsymbol{\tau}_*^l$ may be proposed

$$\boldsymbol{\tau}_*^l = \boldsymbol{\tau}_*^l(f_v, \rho^f, c^l, \mathbf{j}, \mathbf{u}^f) \quad (5.12)$$

As a first order approximation, we assume that $\boldsymbol{\tau}_*^l$ depends on \mathbf{j} linearly

$$\boldsymbol{\tau}_*^l = -\mathbf{R}(f_v, \rho^f c^l, \mathbf{u}^f) \cdot \mathbf{j} \quad (5.13)$$

where \mathbf{R} is the resistivity tensor which still could be a nonlinear function of \mathbf{u}^f .

After substitution of Eq (5.13) into Eq (5.10) and applying to Eq (5.8) we obtain the governing relationship for the dispersion mass flux \mathbf{j}

$$\begin{aligned} & \left[f_v c^l \mathbf{R} + \nabla \mathbf{v}^f (\nabla \mathbf{v}^f)^l - g^l \mathbf{I} \right] \mathbf{j} = \\ & = f_v c^l \frac{\partial \mu_*^l}{\partial c^l} \nabla c^l \frac{\partial \mathbf{j}}{\partial t} - \mathbf{v}^f \nabla \mathbf{j} - \nabla \left(\frac{\mathbf{j} \otimes \mathbf{j}}{f_v c^l} \right) + \mathbf{j} (\nabla \cdot \mathbf{v}^f) \end{aligned} \tag{5.14}$$

that together with the conservation of mass of solute and the known flow velocity field, forms a determinate set of equations to solve for the solute concentration. Eq (5.14) represents balance of forces and is a fundamental relationship for describing the dynamics of solute dispersion in a porous medium. This equation, however, is too general and for practical problems some simplified forms are needed.

Case1. Fickian dispersion

The simplest equation of dispersion may be obtained by neglecting all the terms of dynamic type and the mass exchange term. In such a case the resulting equation is

$$f_v c^l \mathbf{R} \mathbf{j} = - f_v c^l \frac{\partial \mu_*^l}{\partial c^l} \nabla c^l \tag{5.15}$$

which can be transformed to the Fician form

$$\mathbf{j} = f_v \mathbf{D} \nabla c^l \tag{5.16}$$

where \mathbf{D} is the dispersion tensor given by

$$\mathbf{D} = \frac{1}{f_v} \frac{\partial \mu_*^l}{\partial c^l} \mathbf{R}^{-1} \tag{5.17}$$

that may be a function of the fluid phase relative velocity \mathbf{u} .

Case 2. The effect of mass exchange

Eq (5.14) shows that the dispersive mass flux may be affected by the mass exchange process. Neglecting all the inertial terms in Eq (5.14) we obtain

$$(f_v c^l \mathbf{R} - g^l \mathbf{I}) \mathbf{j} = - f_v c^l \frac{\partial \mu_*^l}{\partial c^l} \nabla c^l \tag{5.18}$$

Next, by virtue of Eq (5.17) Eq (5.18) may be rewritten in the form of Fickian dispersion equation

$$\mathbf{j} = -f_v \mathbf{D}_{nc} \nabla c^l \quad (5.19)$$

where

$$\mathbf{D}_{nc} = (\mathbf{I} - g^l \mathbf{A})^{-1} \mathbf{D} \quad (5.20)$$

is the dispersion coefficient for a non-conservative solute and \mathbf{A} is the dispersion parameter defined by

$$\mathbf{A} = \frac{1}{f_v c^l} \mathbf{R}^{-1} = \left(\frac{\partial \mu_x^l}{\partial c^l} \right)^{-1} \mathbf{D} \quad (5.21)$$

Eq (5.20) indicates that, as compared with conservative solutes, the dispersion tensor for a non-conservative solute may be smaller or larger at a given time, depending on whether the solute mass is created or removed, respectively.

6. Concluding remarks

- Application of the advection-dispersion model with the Fickian dispersion flux to description of the solute transport in porous media requires solution of the dispersion equation (in general nonlinear)

$$\frac{\partial(f_v c)}{\partial t} = \nabla(f_v \mathbf{D} \nabla c - f_v c \mathbf{v}^f)$$

in which the fluid phase mean velocity must be prescribed. The mean velocity distribution can be determined from the solution of the flow equation (Darcy law) (Scheidegger, 1963)

$$\mathbf{v}^f = -\frac{k}{f_v \mu} (\nabla p^f - \rho^f \mathbf{g})$$

where k is the permeability, μ is the fluid viscosity and p^f stands for the (fluid) pore pressure.

In general, the two coupled equations: advection-dispersion equation and flow equation need to be solved. If $\mathbf{v}^f = \text{const}$ the problem becomes the uncoupled one.

- The above analysis of contaminant migration shows that in formulation of the fundamental equation governing the spreading of solutes in a fully saturated porous medium the only exploited balance equation is the equation of mass conservation and dispersion flux of solutes in extended Fick's law diffusion. The applied multiphase approach, even in such a limited range (to derive continuity equation and Darcy flow law) allows one to expose the role of material characteristics of particular phases of a porous medium. The porous (rigid) solid phase is described by the pore structure parameters; porosity f_v and the permeability k from Darcy's law and the tortuosity parameter relating the effective diffusion coefficient D_d and the diffusion coefficient D_o in a free solution. The fluid phase is characterized by the mean flow velocity v^f (satisfying Darcy's law) and the viscosity μ . Moreover the fluid phase is treated as a miscible mixture of water and contaminants soluble in water being described by the solute concentration.
- An extended phase characteristics is needed in the case of nonhomogeneous permeable deposits when the dispersion parameters are functions of a scale and thus various pore structure characteristics and flow conditions corresponding to each scale must be defined.
- An extension of the advective-dispersive model is necessary if contaminants are immiscible in water, the porous material is not fully saturated, or deformations of the skeleton are significant. Then, the model should include the equations of motion for additional phases and/or a deformable skeleton. The theory of multiphase media is a suitable tool for writing such equations having in mind that motions of immiscible phases are kinematically independent. The extended characteristics of the internal structure of the medium will enter through volume fractions and relative permeabilities of the phases.

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Wielofazowy opis ciał jako podstawa modelowania w mechanice środowiska. Opis transportu substancji w ośrodku porowatym

Streszczenie

Przedmiotem pracy jest opis migracji substancji (rozpuszczalnej w cieczy wypełniającej pory) przez ośrodki porowate. Zakłada się, że wypadkowy transport zanieczyszczeń jest złożeniem dwóch procesów: adwekcji i dyspersji. Transport adwekcyjny związany jest ze średnim (makroskopowym) przepływem roztworu przez porowaty szkielet, natomiast efekty dyspersyjne są następstwem molekularnej dyfuzji i mechanicznego mieszania.

W pracy przeanalizowano dyspersję opisaną liniowym prawem Ficka wiążącym strumień transportowanej masy z koncentracją substancji, a także dyspersję gdy liniowe prawo nie obowiązuje.

Manuscript received January 19, 1998; accepted for print March 18, 1998