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Transport in structured porous media

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1 INTRODUCTION

Aggregates, cracks, channels left behind by decayed roots, and by animals, and layering often have a large influence on the transport of water and of solutes in soils. Physico-mathematical models for transport in soils with such structures usually are based on a distribution of water and/or solutes among a mobile and a stagnant phase, roughly corresponding to networks of large and of small pores. For any constituent the combined balances of mass for the mobile and stagnant phases can be written as

$$\frac{\partial \rho_m}{\partial t} + \frac{\partial \rho_s}{\partial t} = - \nabla \cdot \underset{\sim}{F} , \qquad (1)$$

where t is the time, ∇ is the vector differential operator, ρ_m is the mass of the constituent in the mobile phase per unit bulk volume (including the volume occupied by the solid phase of the porous material), ρ_s is the mass of the constituent in the stagnant phase per unit bulk volume, and $\underset{\sim}{F}$ is the flux of the constituent in the mobile phase. Important further ingredients in these models are the mechanisms of transport in the mobile phase and the nature of the storage capacities of the phases and the associated mechanisms of exchange between the phases.

2 MECHANISMS OF TRANSPORT IN THE MOBILE PHASE

In the literature the transport is often assumed to be either purely convective or purely diffusive, but sometimes it is assumed to be simultaneously convective and diffusive. Purely convective transport has been assumed to describe mass transport in packed beds (Klinkenberg 1948) and soils (Gardner and Brooks 1957; Raats 1973); it also appears in mathematically related theories for heat exchangers (Nusselt 1911; Anzelius 1926) and for transport of sediment (Einstein 1936; Polya 1937). Purely diffusive transport occurs in theories describing the influence of tides along coasts and in rivers on water levels in adjoining aquifer systems (Steggewentz 1933; van der Kamp 1973), transport of water and oil in structured porous media (Barenblatt and Zheltov 1960; Barenblatt et al. 1960; Raats 1969; Streltsova 1976), secondary consolidation in soil mechanics (Taylor and Merchant 1940; Gibson and Lo 1961) and in mathematically related theories describing heat transfer in media with two temperatures (Maxwell 1867; Chen and Gurtin 1968). Simultaneous convective and diffusive transport has been used to describe transport of solutes in packed beds (Lapidus and Amundson 1952) and soils (see Bolt 1979 and Van Genuchten and Cleary 1979 for reviews). In the context of this paper, no special complications arise from assuming simultaneous convective and diffusive transport. For definiteness, all equations will be written for a solute dissolved in water, but the results are easily adaptable to any entity, including solutes, water and heat, and to either purely convective or purely diffusive transport. Thus the flux $\underset{\sim}{F}$ is assumed to be given by

$$\underset{\sim}{F} = \theta_m \underset{\sim}{v} c - D_m \nabla c, \qquad (2)$$

where θ_m is the volumetric water content of the mobile phase, $\underset{\sim}{v}$ is the velocity of the water in the mobile phase, c is the concentration of the solute in the mobile

phase, and D_m is the dispersion coefficient associated with the mobile phase.

3 SOME SIMPLE CAPACITY RELATIONSHIPS

The bulk density ρ_m and the concentration c are assumed to be related by

$$\rho_m = (\theta_m + k)\, c, \tag{3}$$

where k describes instantaneous, linear adsorption. A vanishing storage capacity in the mobile phase ($\theta_m + k \to 0$) represents an important special case (e.g., Anzelius 1926; Steggewentz 1933; Polya 1937; Raats 1969, 1973). Introducing equations (2) and (3) into equation (1) and using the mass balance for water in the mobile phase (assuming there is no exchange of water between the mobile and stagnant phases),

$$\frac{\partial \theta_m}{\partial t} = -\nabla\cdot(\theta_m \underline{v}), \tag{4}$$

gives

$$M = -\frac{\partial \rho_s}{\partial t}, \tag{5}$$

where the mobile phase operator M is given by

$$M = (\theta_m + k)\frac{\partial c}{\partial t} + \theta_m \underline{v}\cdot\nabla c - D_m \nabla^2 c. \tag{6}$$

The main concern of this paper is the exchange between the mobile and stagnant phases, accounted for by the term $\partial\rho_s/\partial t$ in equations (1) and (5). In most papers cited above the rate of exchange is assumed to be given by an expression of the form

$$\frac{\partial \rho_s}{\partial t} = -\alpha\,(\rho_s - \kappa\,\rho_m), \tag{7}$$

where α is an exchange constant, and κ is the capacity ratio of the stagnant and mobile phases at equilibrium. Equation (7) is tantamount to assuming that the two phases are separated by a membrane with conductance α and that the phases themselves are perfectly mixed. If the time rates of change are very slow, then the equivalent conductance model given by equation (7) reduces to the equilibrium model given by

$$\rho_s = \kappa\,\rho_m,$$

$$\text{or}\quad \frac{\partial \rho_s}{\partial t} = \kappa\frac{\partial \rho_m}{\partial t} = \kappa\,(\theta_m + k)\frac{\partial c}{\partial t}. \tag{8}$$

Some studies suggest that the effect of structure upon transport of solute can be represented by an equivalent dispersion coefficient D_e proportional to v^2 (Passioura 1971):

$$\frac{\partial \rho_s}{\partial t} = \kappa\,(\theta_m + k)\frac{\partial c}{\partial t} - D_e\frac{\partial^2 c}{\partial x^2}. \tag{9}$$

In this paper the exchange among the phases will be treated as a full-fledged diffusion process. As a result, equation (5) will become a linear, partial integro-differential equation. It will be shown that, by using Laplace transforms, this equation can be converted to a partial differential equation in which derivatives with respect to time of all orders occur. The equilibrium, equivalent conductance, and equivalent dispersion models, given by equations (8), (7), and (9) respectively, will be shown to be approximations of such partial differential equations.

4 DIFFUSIVE EXCHANGE BETWEEN PHASES

I will sketch the theory for the simplest type of structured medium, namely one in which the mobile, stagnant and inert phases occur in layers (Fig. 1).

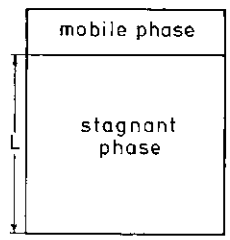

Fig. 1. Layered structure.

The exchange among the phases can then be treated as a one-dimensional diffusion process over distance L, with an effective diffusion coefficient D within the stagnant phase. The ratio L^2/D is the characteristic time of the exchange process and can be used to define a dimensionless time t^* by

$$t^* = \frac{D}{L^2} t. \qquad (10)$$

Using Duhamel's theorem, the concentration c in the mobile phase can be shown to satisfy (Skopp and Warrick 1974):

$$M = - (\theta_m + k) \kappa \frac{D}{L^2} \int_0^{t^*} \frac{\partial c}{\partial t^*} (\underset{\sim}{x}, \tau^*) \sum_{n=0}^{\infty} 2 \exp - \beta_n^2 (t^* - \tau^*) \, d\tau^*, \qquad (11)$$

where

$$\tau^* = \frac{D}{L^2} \tau \qquad (12)$$

denotes instants in the past, and

$$\beta_n = \frac{(2n + 1)\pi}{2} \qquad (13)$$

denotes a geometry factor. The combination $L^2/(D\beta_n^2)$ represent a discrete spectrum of relaxation times. The sum

$$\sum_{n=0}^{\infty} 2 \exp - \beta_n^2 (t^* - \tau^*) \qquad (14)$$

describes the memory of the stagnant phase for changes of concentration at the boundary between the mobile and stagnant phases. Fig. 2 shows successive terms of this sum.

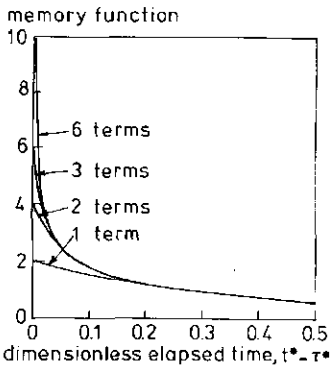

Fig. 2. The memory function.

Taking the Laplace transform of the relaxation integral form (11) of the transport equation gives

$$\bar{M} = - \sum_{n=0}^{\infty} \frac{2}{s^* + \beta_n} (\theta_m + k) \kappa \bar{sc}, \qquad (15)$$

where $\bar{M}$ is the Laplace transform of the mobile phase operator,

$$\bar{M} = (\theta_m + k) \bar{sc} + \theta_m \underset{\sim}{v} \cdot \nabla \bar{c} - D_m \nabla^2 \bar{c}, \qquad (16)$$

and

$$s^* = (L^2/D)s. \qquad (17)$$

The infinite series in equation (15) can be expressed in terms of a tanh function:

$$\bar{M} = - (s^*)^{-\frac{1}{2}} \tanh (s^*)^{\frac{1}{2}} (\theta_m + k) \kappa \bar{sc} \qquad (18)$$

The tanh function can in turn be expanded in another infinite series:

$$\bar{M} = - \{1 - \tfrac{1}{3} s^* + \bar{R}_1\} (\theta_m + k) \kappa \bar{sc} \qquad (19)$$

where the remainder $\bar{R}_1$ is given by

$$\bar{R}_1 = \frac{2}{15} (s^*)^2 - \frac{7}{315} (s^*)^3 + \ldots . \qquad (20)$$

Inversion of the Laplace transforms in equations (19) and (20) gives the first differential form of the transport equation:

$$M = - \{1 - \frac{1}{3} \frac{L^2}{D} \frac{\partial}{\partial t} + R_1\} (\theta_m + k) \kappa \frac{\partial c}{\partial t}, \qquad (21)$$

where the remainder R_1 is given by

$$R_1 = \frac{2}{15} \{\frac{L^2}{D}\}^2 \frac{\partial^2}{\partial t^2} - \frac{7}{315} \{\frac{L^2}{D}\}^3 \frac{\partial^3}{\partial t^3} + \ldots . \qquad (22)$$

An alternative form can be derived by using in equation (18) the reciprocal relationship between the tanh and the ctanh functions:

$$(s^*)^{\frac{1}{2}} \operatorname{ctanh} (s^*)^{\frac{1}{2}} \bar{M} = - (\theta_m+k)\kappa s\bar{c}. \quad (23)$$

Expanding the ctanh function in an infinite series gives:

$$\{1 + \tfrac{1}{3} s^* + \bar{R}_2\}\bar{M} = -(\theta_m + k)\kappa s\bar{c}, \quad (24)$$

where the remainder $\bar{R}_2$ is given by

$$\bar{R}_2 = - \tfrac{1}{45} (s^*)^2 + \tfrac{2}{945} (s^*)^3 + \ldots \quad (25)$$

Inversion of the Laplace transforms in equations (24) and (25) gives the second differential form of the transport equation:

$$\{1 + \tfrac{1}{3} \frac{L^2}{D} \frac{\partial}{\partial t} + R_2\} M = - (\theta_m + k) \kappa \frac{\partial c}{\partial t}, \quad (26)$$

where the remainder R_2 is given by

$$R_2 = - \tfrac{1}{45} \{\frac{L^2}{D}\}^2 \frac{\partial^2}{\partial t^2} + \tfrac{2}{945} \{\frac{L^2}{D}\}^3 \frac{\partial^3}{\partial t^3} + \ldots . \quad (27)$$

5 FOUR APPROXIMATIONS

Substituting (6) into (21), neglecting the remainder R_1, and rearranging gives the first approximate differential form of the transport equation:

$$(1 + \kappa) (\theta_m + k) \frac{\partial c}{\partial t} + \theta_m \underset{\sim}{v} \cdot \nabla c - D_m \nabla^2 c = \tfrac{1}{3} \frac{L^2}{D} (\theta_m + k) R \frac{\partial^2 c}{\partial t^2} . \quad (28)$$

Neglecting the right hand side of equation (28) amounts to assuming that the two phases are in equilibrium with each other:

$$(1 + \kappa) (\theta_m + k) \frac{\partial c}{\partial t} + \theta_m \underset{\sim}{v} \cdot \nabla c - D_m \nabla^2 c = 0 \quad (29)$$

The second order time derivative on the right hand side of equation (28) describes the negative "inertia" of the structured medium with regard to changes of concentration.

Substituting (6) into (26), neglecting the remainder R_2, and rearranging, gives the second approximate differential form of the transport equation:

$$(1 + \kappa) (\theta_m + k) \frac{\partial c}{\partial t} + \theta_m \underset{\sim}{v} \cdot \nabla c - D_m \nabla^2 c = - \tfrac{1}{3} \frac{L^2}{D} (\theta_m + k) \frac{\partial^2 c}{\partial t^2} - \tfrac{1}{3} \frac{L^2}{D} \frac{\partial}{\partial t} \{\theta_m \underset{\sim}{v} \cdot \nabla c - D_m \nabla^2 c\}. \quad (30)$$

This form of the transport equation also results if equations (1), (2), and (3) are combined with the equivalent conductance model given by equation (7), provided the conductance α is chosen to be

$$\alpha = \frac{3D}{L^2} . \quad (31)$$

This result is a nice surprise!

The equilibrium equation (29) represents a zeroth-order approximation, while equations (28) and (30) are two alternative first-order approximations. Solving the zeroth-order equation for $\theta_m \underset{\sim}{v} \cdot \nabla c - D_m \nabla^2 c$ and substituting the result in the last term of equation (30) gives equation (28). Thus the right hand sides of equation (28) and (30) are roughly equivalent, as one would hope for two approximations of the same order.

The zeroth-order equation (29) can be used in yet another way to modify the right hand sides of the first order equations (28) and (30). Assuming the flow is one-dimensional and v is constant and neglecting the term accounting for the dispersion, equation (29) reduces to

$$\frac{\partial c}{\partial t} = - \frac{\theta_m v}{(1 + \kappa) (\theta_m + k)} \frac{\partial c}{\partial x} . \quad (32)$$

Substituting the proportional relationship between time and space derivatives implied in equation (32) into the right hand side of equation (28) or of equation (30) gives:

$$(1 + \kappa) (\theta_m + k) \frac{\partial c}{\partial t} + \theta_m v \frac{\partial c}{\partial x} - (D_m + D_e) \frac{\partial^2 c}{\partial x^2} = 0, \quad (33)$$

where the equivalent dispersion coefficient D_e is given by:

$$D_e = \frac{1}{3}\frac{L^2}{D}\frac{\theta_m^2}{(\theta_m + k)^2}\frac{K}{(1 + K)^2}v^2 \qquad (34)$$

This expression for the equivalent dispersion coefficient was also obtained by Passioura (1971; see also Bolt 1979). This result is another nice surprise!

6 CONCLUDING REMARKS

In this paper a variety of linear theories for transport in structured porous media were all shown to have a common basis. The pattern of links between the various theories is similar to that long familiar in linear viscoelasticity (cf., Freudenthal and Geiringer 1958; Leitman and Fisher 1973). The type of analysis presented here for a layered structure can in principle be carried out for any geometry. Results for media with spherical stagnant regions will be presented at the colloquium Euromech 143.

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