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Double-Relaxation Solute Transport in Porous Media

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ABSTRACT: In the paper a problem of double relaxing solute transport in a porous medium is considered. On the basis of mass balance equation and the double relaxing Fick's law a solute transport equation is derived. The equation is numerically solved and the influence of the relaxation parameters on solute transport characteristics is established.

KEYWORDS: Filtration; mathematical model; porous media; relaxation; suspension; solute transport;

I. INTRODUCTION

In recent times the intensity of studies of anomalous phenomena at diffusion and dispersion of particles in porous media has significantly increased. One of the original works, where violation of classical Fickian diffusion law was indicated is [1]. In [1] the mass solute flow is given by a sum two members - the classic Fick's diffusion and relaxation term. At the transport of solute or other suspended fine particles in porous media breakthrough curves can be non-Gaussian with considerable tailing effect [2, 3, 4]. A Non-Fickian generalized theory dispersion is proposed in [5]. A general equation, from which equations containing different derivatives of the mass dispersion flow with respect to time can be obtained in particular cases, was derived and stochastic models described by integrodifferential equation in which the dispersion tensor increases asymptotically with time and as a function of the space coordinate, were proposed.

In [6] it is found that low-concentration-gradient experiments can be simulated satisfactorily using the Fickian-type dispersion equation. However, calculated breakthrough curves for high-concentration-gradient experiments deviate substantially from the measured curves. It appears that a satisfactory fit to high-concentration-gradient data can be obtained only if the value of longitudinal dispersivity is reduced by a factor of three. Using the non-linear theory, however, it is possible to simulate both low- and high-concentration-gradient experiments with a unique set of parameter values. Fick's law expresses the proportionality of solute flux with respect to concentration gradient. Similar relations are given by Darcy's law for the fluid flow in porous media[7]. In [8] with using an inertial Fick's law hyperbolic solute transport equation is derived. It was shown that such a hyperbolic description is valid, but for transient solute flows with very short characteristic times.

In [9] the problem of the macroscopic simulation of the motion of a viscous fluid and mass transport in a porous medium is considered under the assumption that the mass transport can locally be described by the Fick relaxation law. Several cases determined by the local inertia number of the mass flow and the Pēclet number are investigated. The macroscopic transport models are analyzed and compared with well-known phenomenological models.

It is well known that the flow of aqueous polymeric fluids through porous media plays important role in enhanced oil recovery processes [10]. We can note [11] that the in situ rheology of the fluid does not explicitly depend upon the bulk rheology of the aqueous polymer solution. For polymeric solutions, the apparent viscosity is a function of flow rate through the porous medium and flow rate may be interrelated with the fluid memory in the pore network [12].

Formation of tailing in breakthrough curves, i.e. non-Gaussian concentration profiles investigated also in [2, 3] that explicitly demonstrates the violation of classical Fick's law. Statistical approach to model anomalous dispersion in porous media is used in [13, 14]. Models are presented by integrodifferential equations in which the dispersion tensor is asymptotically increases with time and is a function of the space coordinate.



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Some hypotetic filtration laws for homogeneous liquids in porous media, that take into account the relaxation of the pressure gradient and the velocity of filtration are given in [15,16]. On the basis of these models non-steady filtration equations are derived that makes enable to determine pressure distribution and other filtration characteristics. In this paper principal model approaches and methodology used in these works for filtration processes we attempt to adapt for solute transport problems. First, for double-relaxation Fick's law that includes both the relaxation of solute mass flow and concentration gradient, we derive a solute transport equation and pose an initial-boundary problem. Then we numerically solve the problem. Next we present some results and their short analysis.

II. DERIVATION OF TRANSPORT EQUATION AND FORMULATION OF THE PROBLEM

The mass balance of the solute in the one-dimensional case is expressed by the equation

$$m\frac{\partial c}{\partial t} + \frac{\partial F}{\partial x} = 0, \tag{1}$$

where m - the porosity of the medium, c - the concentration of solute dissolved in the filtrated liquid, F - the total solute mass flow, consisting of the convection (F_c) and diffusion (F_d) flows, $F = F_c + F_d$, t - time, x - space coordinate.

Convective flow has the following form [7]

$$F_c = v_f c = vmc , \qquad (2)$$

where v_f – filtration velocity, v – the physical fluid velocity.

The diffusion law with double-relaxation we write as

$$F_d + \lambda_1 \frac{\partial F_d}{\partial t} = -Dm \left(1 + \lambda_2 \frac{\partial}{\partial t} \right) \frac{\partial c}{\partial x},\tag{3}$$

where λ_1, λ_2 – the relaxation times, D – diffusion coefficient, which we take as a constant.

In more general form instead of diffusion coefficient one can use dispersion coefficient that depends on filtration velocity distribution [7].

Equation (1), taking into account (2), (3) becomes

$$m\frac{\partial c}{\partial t} + vm\frac{\partial c}{\partial x} + \frac{\partial F_d}{\partial x} = 0.$$
(4)

Differentiating (3) with respect *x*, we have

$$\left(1 + \lambda_1 \frac{\partial}{\partial t}\right) \frac{\partial F_d}{\partial x} = -mD \left(1 + \lambda_2 \frac{\partial}{\partial t}\right) \frac{\partial^2 c}{\partial x^2}.$$
(5)

From (4) and (5) we obtain

$$\left(1+\lambda_1\frac{\partial}{\partial t}\right)\left(\frac{\partial c}{\partial t}+v\frac{\partial c}{\partial x}\right)=D\left(1+\lambda_2\frac{\partial}{\partial t}\right)\frac{\partial^2 c}{\partial x^2}$$

or

$$\frac{\partial c}{\partial t} + \lambda_1 \frac{\partial^2 c}{\partial t^2} + v \frac{\partial c}{\partial x} + v \lambda_1 \frac{\partial^2 c}{\partial t \partial x} = D \frac{\partial^2 c}{\partial x^2} + \lambda_2 D \frac{\partial^3 c}{\partial t \partial x^2}.$$
(6)

In order to assess the relaxation effects on the solute transport characteristics we pose the following simple problem. Let in the semi infinite porous medium initially filled with pure (without solut) fluid since t > 0 inflows liquid with constant concentration of solute c_0 .

Then the initial and boundary conditions take the from

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$$c(0, x) = 0, \ \frac{\partial c(0, x)}{\partial t} = 0, \ 0 \le x < \infty$$
, (7)

$$c(t,0) = c_0, \ c(t,\infty) = 0.$$
 (8)

III. NUMERICAL SOLUTION OF THE PROBLEM

To solve the problem (6) - (8) we apply the method of finite differences [17]. In the area $\Omega\{(t, x), 0 \le t \le T, x \ge 0\}$ we introduce the following grid

$$\omega_{\tau h} = \left\{ (t_j, x_i), t_j = \tau j, x_i = ih, \ \tau = \frac{T}{J}, i = 0, 1, \dots, j = \overline{0, J} \right\},\$$

where τ , h - steps with respect t and x, respectively. Numerical solution for the concentration on the grid ω_{th} we denote as c_i^j , and solute diffusion flow rate F_d as F_i^j .

We approximate equation (6), using the implicit finite difference scheme on the grid $\omega_{h\tau}$ in the form

$$\frac{c_{i}^{j+1} - c_{i}^{j}}{\tau} + v \frac{c_{i}^{j+1} - c_{i-1}^{j+1}}{h} + \lambda_{1} \frac{c_{i}^{j+1} - 2c_{i}^{j} + c_{i}^{j-1}}{\tau^{2}} + v \lambda_{1} \frac{c_{i}^{j+1} - c_{i-1}^{j+1} - c_{i}^{j} + c_{i-1}^{j}}{\tau h} = D \frac{c_{i-1}^{j+1} - 2c_{i}^{j+1} + c_{i+1}^{j+1} - 2c_{i}^{j+1} - c_{i-1}^{j} + 2c_{i}^{j} - c_{i+1}^{j}}{\tau h}.$$
(9)

The initial and boundary conditions (7), (8) are approximated as

$$c_i^0 = 0, \quad \frac{c_i^1 - c_i^0}{\tau} = 0, \quad i = 0, 1, ...,$$
 (10)

$$c_0^{j+1} = c_0, \quad c_I^{j+1} = 0, \quad j = 0, 1, \dots J$$
 (11)

Finite difference scheme (8) leads to the system of linear algebraic equations

$$Ac_{i-1}^{j+1} - Bc_i^{j+1} + Ec_{i+1}^{j+1} = -G_i^j, \qquad i = \overline{1, I-1}, \ j = \overline{0, J-1},$$
(12)

where

$$\begin{split} A &= -vh\tau^2 - vh\lambda_1\tau - D\tau^2 - D\lambda_2\tau ,\\ B &= -h^2\tau - vh\tau^2 - \lambda_1h^2 - vh\tau\lambda_1 - 2D\tau^2 - 2D\lambda_2\tau ,\\ E &= -D\tau^2 - D\lambda_2\tau ,\\ G_i^{\,j} &= (-h^2\tau - 2\lambda_1h^2 - \lambda_1vh\tau - 2D\lambda_2\tau)c_i^{\,j} + D\lambda_2\tau c_{i+1}^{\,j} + \\ &+ (\lambda_1vh\tau + D\lambda_2\tau)c_{i-1}^{\,j} + \lambda_1h^2c_i^{\,j-1}, \end{split}$$

I – enough large integer.

The system of equations (11) we solve by the Tomas' algorithm [17].

In accordance with (3) we define the solute flow rate. With $F_d(0,x)=0$ we have

$$F_{d}(t,x) = -\frac{mDe^{-t/\lambda_{1}}}{\lambda_{1}} \int_{0}^{t} e^{\xi/\lambda_{1}} \left(1 + \lambda_{2}\frac{\partial}{\partial t}\right) \frac{\partial c(\xi,x)}{\partial x} d\xi .$$
(13)

The $F_d(t,x)$ can be determined by calculating the integral (13) at the known concentration distribution c(t,x).

We can also directly discretizaze equation (5) on the grid.

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So, equation (3) is approximated as

$$F_{i}^{j+1} + \lambda_{1} \frac{F_{i}^{j+1} - F_{i}^{j}}{\tau} = -mD \frac{c_{i+1}^{j+1} - c_{i}^{j+1}}{h} - mD\lambda_{2} \frac{c_{i}^{j+1} - c_{i}^{j} - c_{i-1}^{j+1} + c_{i-1}^{j}}{th},$$

from which F_i^{j+1} is determined

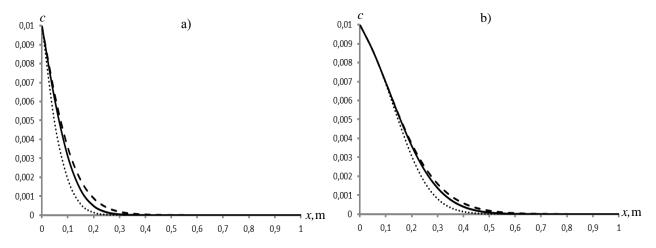
$$F_{i}^{j+1} = \frac{\lambda_{1}}{\tau + \lambda_{1}} F_{i}^{j} - \frac{mD\tau}{\tau + \lambda_{1}} \frac{c_{i+1}^{j+1} - c_{i}^{j+1}}{h} - \frac{mD\lambda_{2}}{\tau + \lambda_{1}} \frac{c_{i}^{j+1} - c_{i}^{j} - c_{i-1}^{j+1} + c_{i-1}^{j}}{h}.$$
 (14)

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Since $\frac{\lambda_1}{\tau + \lambda_1} < 1$, the finite difference scheme (14) is stable. At known c_i^j, c_i^{j+1} from (14) we find $F_i^{j+1}, j = 0, 1, ..., J - 1$. At the lowest grid layer j = 0 we have $F_i^0 = 0, i = 1, 2, ...$

IV. RESULTS

In the calculations the following initial values of parameters are used: $c_0 = 0,01$, m = 0,3 and the various $v, D, \lambda_1, \lambda_2$. Some results of numerical calculations are shown in Fig. 1 - 4. With the increasing of λ_1 at given λ_2 the development of concentration profiles is delayed. It can be seen from the figures that in the transition period, the duration of which is determined by the relaxation times, the concentration profiles lag behind the corresponding profiles without taking into account the relaxation. With increasing of λ_2 at the given λ_1 the development of concentration profiles intensifies (Fig.2). In this case also at large times we can observe the weakening of relaxation phenomena. Comparison of two cases shows that influences of λ_1 and λ_2 on concentration profiles are quite opposite. Joint influences of two relaxation parameters on solute transport characteristics are determined by dominant values of λ_1 at different points x and for different values of relaxation times is shown in Fig. 3, 4. Results indicate non-monotonous dependences of F_d at given points. The character of relaxation parameters influences on F_d is same as for concentrations. We can see decreasing dynamics of F_d for large times. It occurs due to decreasing of concentration gradients for large times at a given points of the area. On the basis of presented results we can conclude that the relaxation character of diffusion law considerably alters all solute transport characteristics.

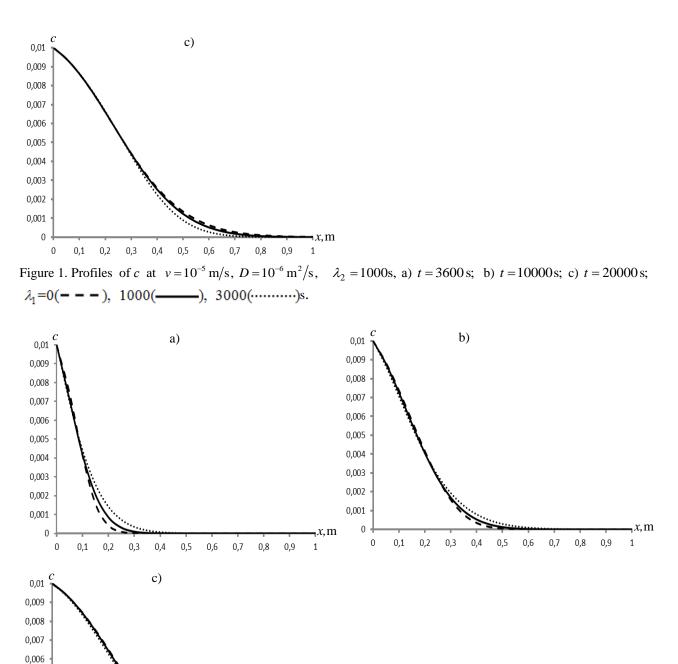




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 $\lambda_{2} = 0(---), 1000(----), 3000(-----) s.$

0,005 0,004 0,003 0,002 0,001

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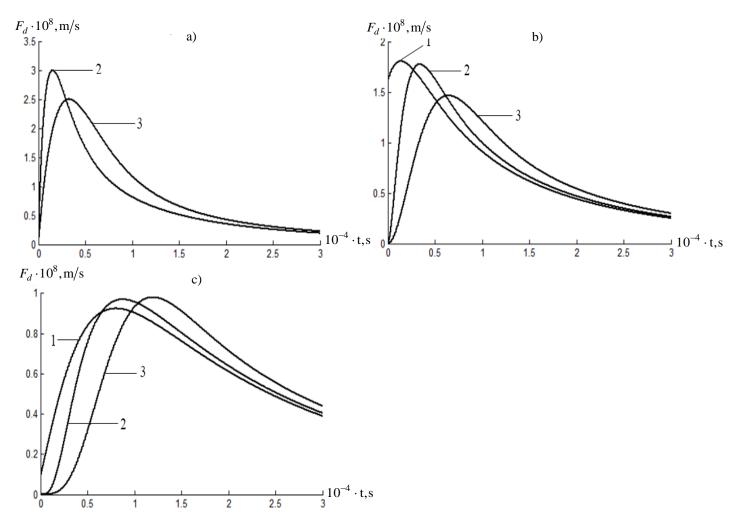
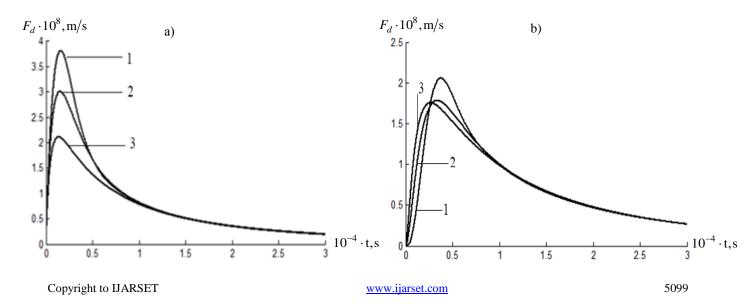


Figure 3. Dynamics of F_d at $\lambda_2 = 1000$ s, $v = 10^{-5}$ m/s, $D = 10^{-6}$ m²/s, x = 0 (a); 0,1m (b); 0,2m (c); $\lambda_1 = 0(1), 1000(2), 3000(3)$ s.





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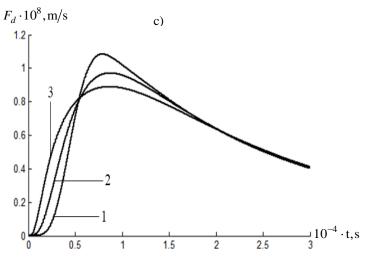


Figure 4. Dynamics of F_d at $\lambda_1 = 1000$ s, $v = 10^{-5}$ m/s, $D = 10^{-6}$ m²/s, x = 0 (a); 0,1m (b); 0,2m (c); $\lambda_2 = 0(1), 1000(2), 3000(3)$ s.

V. CONCLUSION

In this paper a solute transport equation for double-relaxation solute diffusion law is derived. Solute diffusion law takes into account both the relaxation of the diffusion solute flux and concentration gradient. An initial-boundary problem for this equation is posed and numerically solved. On the basis of numerical solutions the influence of relaxation times on solute transport characteristics is studied. It was shown that the relaxation of the solute diffusion mass, λ_1 , leads to delaying of transport characteristics, while the relaxation of solute concentration gradients, λ_2 , leads to the advance distribution of transport characteristics. So, influences of λ_1 and λ_2 on solute transport characteristics are quite opposite. All obtained results show that relaxation behaviour of the diffusion law considerably alters all solute transport characteristics.

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