The Adsorbed Solute Transport with Diffusion Effects

Khuzhayorov B* and Mustofokulov Z1
1Department of Radio electronica, Jizzakh Polytechnic Institute, Jizzakh, Uzbekistan
2Department of Mathematical Modelling, Samarkand State University, Samarkand, Uzbekistan

Abstract

In this paper the solute transport in a fractured-porous medium is considered with equilibrium adsorption. One of the basis of numerical results an influence of adsorption on solute transport characteristics is estimated.

Keywords: Convective diffusion; Equilibrium adsorption; Fractured-porous media; Porous block; Relative mass transfer; Solute transport

Introduction

The problem of solute transport in fractured-porous media is encountered under various hydrogeological and ecological processes. A large number of papers have been devoted to the hydrodynamic modeling of the solute transport processes in a porous medium (PM) [1-6]. As a porous medium with a stagnant zone and certain degree of convention, can be considered as a fractured-porous medium (FPM) with a low permeability of porous blocks. In such FPM, liquid in porous blocks is considered to be stationary, and the system of fractures along which the liquid moves is regarded as a transit pore [7-9].

Objects and Methods of Investigation

In this paper, using the model approach [3-6], the motion of a dispersed liquid and the adsorbed solute transport into a FPM are examined taking into account the convective diffusion and dispersion effects. The main attention is paid to longitudinal convective diffusion in fracture and its effect on the adsorption of solute.

In order to investigate the solute transport in such media, we consider an element of a FPM consisting of a single fracture and an adjacent porous block (Figure 1). A fracture is a semi-infinite one-dimensional object, so that the solute distribution and the fluid flow along its cross-section are considered as a homogeneous. In such case, the second fracture measurement, i.e. its thickness is not taken into account. The porous block occupies the first quarter of the plane Figure 1. Thus, the region \( R \{ 0 \leq x < \infty, 0 \leq y < \infty \} \) is considered.

In a fracture there is a convective-diffusion solute transport and in a porous block only a diffusion one. Both in fracture and in porous block, the solute can be adsorbed during the transport process.

The liquid in fracture flows at a given constant rate. At the end (x=0) of fracture, the liquid is supplemented by solute with concentration \( c_0 \). Initially, the fracture and the porous block are considered to be filled with pure (without substance) liquid.

The fracture is modeled as a one-dimensional object, so the distribution of concentration along its cross-section is not considered. In fracture, the coefficient of convective diffusion \( D'f \) must be considered as:

\[
D'_f = D' + \eta \frac{w}{\rho}
\]

where \( D' \) is the coefficient of molecular diffusion of the solute (liquid), \( \eta \) the scattering coefficient, \( \frac{w}{\rho} \) the physical velocity of the fluid. In fracture, the fluid velocity and the speed of filtration coincide, because \( \theta=1 \). Then, we have \( D''f = D' + \eta \nu \), where \( \nu \) is the velocity of the fluid.

The balance equation of the solute transport process and the fluid flow in a FPM with convective diffusion and adsorption can be written as:

\[
b \left( \frac{\partial c_f}{\partial t} + \rho \frac{\partial c_f}{\partial x} + v \frac{\partial c_f}{\partial x} \right) = h D'_f \frac{\partial^2 c_f}{\partial x^2} + \theta_m \frac{\partial c_m}{\partial y}, \quad 0 \leq x < \infty, \quad (1)
\]

\[
\frac{\partial c_m}{\partial t} + \frac{\rho}{\theta_m} \frac{\partial c_m}{\partial x} = D''m \frac{\partial^2 c_m}{\partial y^2}, \quad 0 \leq y < \infty \quad (2)
\]

where \( c_f(x,t) \) is the solute concentration in fracture, \( m^3/m^3 \); \( c_m(x,y) \) the concentration in a matrix, \( m^3/m^3 \); \( c_s(x,y) \) the concentration of the adsorbed solute in fracture, \( m^3/kg \); \( c_m(x,y) \) the concentration of adsorbed matter in a matrix, \( m^3/kg \); \( D''m \) - effective diffusion coefficient in a matrix, \( m^2/s \); \( \rho \) is the density of saturated medium, \( kg/m^3 \); \( b \) the fracture width; \( m \); \( \theta_m \) the matrix porosity coefficient, \( t \) - time, \( s \).

We solve the system in eqns.(1) and (2) with the equilibrium adsorption (Henry isotherm):

\[
c = c_0 e^{-k_s}, \quad k_s = c_f(x,y) / c_m(x,y)
\]

*Corresponding author: Khuzhayorov B, Professor, Department of Mathematical Modelling, Samarkand State University, Samarkand, Uzbekistan, Tel: 998 66 2391140; E-mail: taylanov@yandex.com

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The problem in eqns. (1) and (9) is solved by the finite differences method in eqn. (9). To do this, in the region \( R \) we construct a grid 
\[
\omega_{h,k} = \left\{ \left( t_i, x_j, y_j \right) \right\}, \quad t_i = \tau k, \quad x_j = h_i, \quad y_j = h_j, \quad k = 0, K, \quad i = 0, 1, \ldots, J = T/J, \quad \tau = T/K ,
\]
where \( h_i \) is the grid spacing in the x direction, \( h_j \) the grid spacing in the y direction, \( \tau \) the grid spacing in time, \( T \) the maximum time during which the process is investigated, \( K \) the number of grid intervals in time. Thus, in eqn. (1) is approximated on the grid \( \partial / \partial t \cup \partial / \partial h_x \) and in eqn. (2) on the grid \( \partial / \partial x \cup \partial / \partial h_y \). To approximate in eqn. (1), we use an implicit ‘anti-flow’ scheme, and for eqn. (2) we use a purely implicit scheme or a scheme with an advance. For Henry isotherms this approximations have the form
\[
\begin{align*}
\frac{\partial c_i}{\partial t} &= \frac{k_j}{h_j} \frac{\partial c_i}{\partial x}, \quad 0 \leq x < \infty, \quad i = 1, 2, \ldots, \\numberofxintervals, \\
\frac{\partial c_i}{\partial y} &= \frac{k_j}{h_j} \frac{\partial c_i}{\partial y}, \quad 0 < y < \infty,
\end{align*}
\]
where \( k_x, k_y \) are the adsorption coefficients in a matrix and fracture, \( \text{m}^2/\text{kg} \).

We assume that there is no solute flow at the boundaries \( x = 0, \infty \) of fracture and matrix. The equilibrium of concentrations \( c_m \) and \( c_i \) is ensured at the boundary. Under these conditions, the initial and boundary conditions have the form:
\[
\begin{align*}
c_i(0, x, y) &= c_{i0}(x, y), \quad x \geq 0, \quad y \geq 0, \\
c_i(t, 0) &= c_i(t, 0), \\
c_i(t, x) &= c_i(0, x, y) = c_{i0}(x, y), \quad t > 0, \quad x \geq 0, \quad y \geq 0, \\
\frac{\partial c_i}{\partial x}(t, x, 0) &= 0, \\
\frac{\partial c_i}{\partial y}(t, x, y) &= 0.
\end{align*}
\]

\( c_{i0}(x, y) \) are the run ratios. Using in eqn. (19) from eqn. (16), whence
\[
\begin{align*}
cf_{i+1} &= c_{f_{i+1}}, \\
cf_{i} &= c_{f_{i}}, \\
cf_{0} &= c_{f_{0}},
\end{align*}
\]
are the grid values of \( c = c_m, c_f \).

For Henry isotherms this concentration and adsorption fronts do not reach the points, with a small \( x \) the solute transport from the fractures into the porous blocks becomes significant. The longitudinal convective diffusion in fracture leads to a smearing of the profiles \( c_i \) which in turn affects the distribution of \( c_f \). In turn, convective diffusion leads to an increase in adsorption in the fracture and the porous block Figure 2b, as well as
The results of calculations of the relative mass transfer $Q$ from a fracture to a porous block are shown in Figure 3a. Analysis of the graphs shows that for a certain value of time the increase in the value of convective diffusion in fracture leads to an increase in $Q$ through $y=0$. Based on the curves in Figure 3a was also estimated cumulative conditional mass transfer $Q_{cum}$ through $y=0$.

For each time point $t$ that characterizes the total mass transfer through $y=0$, a cumulative conditional mass transfer $Q_{cum}$ at a given time $t$ is estimated. In Figure 3b shows graphs of the change $Q_{cum}$ in time $t$. It can be seen that the cumulative conditional mass transfer grows first and then decreases, and a monotonic decrease in its value is observed. At the same time, with an increase in the value of convective diffusion in the fracture $Q_{cum}$, the growth rate is more accelerated.

In Figure 3c, shows the graphs of the total conditional solute transport change through $y=0$ from fracture to porous block versus time.

The graphs show that $Q_{cum}$ increases monotonically with time. In this case, an increase in the value of convective diffusion in the fracture contributes to an increase $Q_{cum}$.

The results of calculations for different values of the velocity of motion $\nu=5 \cdot 10^{-4}$ m/s are shown in Figures 4 and 5. In Figure 4, the surfaces $c/c_0$ are also reflected for two values $\nu$.

On surfaces it can be seen that an increase in the velocity of the fluid in a fracture leads to an increase in the distribution of concentration in the region $R$, which in turn increases the adsorption of the substance.

The nature of the change in the relative mass transfer $Q$ is shown...
in Figure 5a. For $v=2.10^{-3}$ m/s, the relative mass transfer $Q$ is higher in the whole region $x$ than in $v=1.10^{-3}$ m/s and $v=5.10^{-4}$ m/s. This pattern is observed for the cumulative and relative flow from the fracture to the porous block (Figure 5). At the same time, with increasing speed, movement in a fracture leads to an increase in $Q_{cum}$ and $Q_{rel}$.

**Conclusion**

We conclude that an increase of the convective diffusion coefficient leads to an acceleration of the process of the formation of an equilibrium adsorption regime as well as the distribution of concentration in a porous medium. Comparing the data presented, it can be seen that the diffusion rate leads to an increase in the concentration distribution zone, however, higher concentration gradients are formed at the boundary of the fracture and porous block.

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