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MATHEMATICAL MODEL OF DEGRADING SOLUTE TRANSPORT IN A TWO-ZONE POROUS MEDIUM

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Abstract

In the paper a mathematical model of the degrading solute transport in a porous medium, consisting of active and passive zones, taking into account the multistage adsorption kinetics is compiled. Based on this model, the solute transport problem was formulated and numerically solved using finite difference method. The effect of changes in the kinetics of adsorption on transport characteristics was analyzed. It is shown that in profiles of concentration two zones are formed: one is before "charging" and the other is after. In these zones, transport and adsorption characteristics have different rates of change.

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1. Introduction

In recent decades, the problem of solute transport in porous media has been the subject of many studies. Such processes play an important role in various fields, in particular, in the field of environmental protection, ecology, substance migration can directly contribute to the deterioration of groundwater resources [1]. Migration of contaminants such as bacteria, viruses, pesticides, metals, radioactive elements, etc. can serve as pollution. Most of the research to date on pesticide degradation has focused on empirically characterizing the degradation kinetics of these chemicals [2,3]. Adsorption of pesticides has been found to increase or decrease the rate of microbial degradation in soil, depending on the presence or absence of pre-adsorbed pesticide [4].

Formulation of the problem

A two-zone porous medium with active and passive zones is considered. Transport equation in medium [5]

$$\frac{\partial(\theta c)}{\partial t} = -\operatorname{div} J_s - \frac{\partial c_a}{\partial t} - \frac{\partial c_p}{\partial t} - \theta\lambda_e c, \tag{1}$$

$$J_s = -\theta D \nabla c + \vec{w} c, \tag{2}$$

where c is volume concentration, c_a is the concentration of the adsorbed substance in the active zone, c_p is the concentration of the adsorbed substance in the passive zone, J_s is the flux density of the substance, θ is porosity, λ_e is the decomposition coefficient (decomposition) of the first order, $\vec{w}$ is the filtration rate. Substitution of (2) in (1) will give

$$\frac{\partial(\theta c)}{\partial t} + \operatorname{div}(\vec{w} c) = \operatorname{div}(\theta D \nabla c) - \frac{\partial c_a}{\partial t} - \frac{\partial c_p}{\partial t} - \theta\lambda_e c. \tag{3}$$

In the one-dimensional case from (3) we have

$$\frac{\partial(\theta c)}{\partial t} + \frac{\partial}{\partial x}(w_x c) = \frac{\partial}{\partial x}\left(\theta D \frac{\partial c}{\partial x}\right) - \frac{\partial c_a}{\partial t} - \frac{\partial c_p}{\partial t} - \theta\lambda_e c, \tag{4}$$

where w_x is the coordinate of the filtration rate along the axis x.

If the medium is homogeneous, i.e. $\theta = \text{const}$, the filtration rate is constant, the coefficient of hydrodynamic dispersion is constant from (4) we have

$$\frac{\partial c}{\partial t} + v_x \frac{\partial c}{\partial x} = D \frac{\partial^2 c}{\partial x^2} - \frac{1}{\theta}\frac{\partial c_a}{\partial t} - \frac{1}{\theta}\frac{\partial c_p}{\partial t} - \lambda_e c, \tag{5}$$

where $v_x = \frac{w_x}{\theta}$ is the component of the physical velocity of the liquid.

For concentration in the active zone, we accept the following kinetic equations

$$\frac{\partial c_a}{\partial t} = \beta_a \left(c - \frac{c_a}{c_{a0}} c_0 \right) - \lambda_{ea} c_a, \tag{6}$$

where β_a is a coefficient characterizing the intensity of adsorption of a substance in the active zone, c_{a0} is the limiting concentration upon reaching which, i.e. at $c_a = c_{a0}$, and when $c = c_0$ adsorption of the substance in the active zone stops, λ_{ea} is the decay coefficient of the adsorbed substance in the active zone. Here instead of (6) we use following multistage kinetics [6]-[9]:

$$\frac{\partial c_a}{\partial t} = \begin{cases} \beta_{ar} c - \lambda_{ea} c_a, & 0 < c_a \le c_{ar}, \\ \beta_{aa} c - \beta_{ad} c_a - \lambda_{ea} c_a, & c_{ar} < c_a < c_{a0}, \\ 0, & c_a = c_{a0}, \end{cases} \tag{7}$$

where $\beta_{ar}, \beta_{aa}, \beta_{ad}$ are kinetic parameters, c_{ar} is maximum concentration at which the charging effect ends.

The kinetics of adsorption in the passive zone is taken as in [6]-[9],

$$\frac{\partial c_p}{\partial t} = \beta_n \left(c_p \right) c - \lambda_{ep} c_p, \tag{8}$$

where $\beta_p = \alpha \left(c_p \right) \beta_{p0}$,

$$\alpha \left(c_p \right) = \begin{cases} 1, & c_p \le c_{p1}, \\ \frac{c_{p1}}{c_p}, & c_{p1} < c_p < c_{p0}, \\ 0, & c_p = c_{p0}, \end{cases} \tag{9}$$

where c_{p1} is the maximum concentration at which the “aging“ effect begins, λ_{ep} - the coefficient of decomposition (decomposition) of the deposited substance in the passive zone.

Taking into account (9), we write equation (8) in the form

$$\frac{\partial c_p}{\partial t} = \begin{cases} \beta_{p0} c - \lambda_{ep} c_p, & 0 < c_p \le c_{p1} \\ \frac{\beta_{p0} c_{p1} c}{c_p} - \lambda_{ep} c_p, & c_{p1} < c_p \le c_{p0}, \\ 0, & c_p = c_{p0}. \end{cases} \tag{10}$$

The system of equations (5), (7), (10) is solved under the conditions

$$c(0,x)=0, c_a(0,x)=0, c_p(0,x)=0 \qquad (11)$$

$$c(t,0)=c_0, c(t,\infty)=0 \qquad (12)$$

where $c_0=$ const.

Numerical solution

To solve problem (5), (7), (10)-(12), we apply the finite difference method [10-17]. In the area $D=\{0\le x<\infty, 0\le t\le T\}$, let us introduce the net $\omega_{h\tau}$, where T is the maximum time during which the process is studied. To do this, we divide the interval $[0,\infty)$ step by step h and $[0,T]$ in J parts with steps τ. As a result we have a net

$$\omega_{h\tau}=\{(x_i,t_j)\,,\ x_i=ih,\ i=0,1,\dots,$$

$$t_j=j\tau,\ j=0,1,\dots,J,\quad \tau=T/J\}\,.$$

Instead of the functions $c(t,x), c_a(t,x), c_p(t,x)$ we consider the net functions whose values in nodes (x_i,t_j) accordingly, we denote by $c_i^j\cdot c_{a,i}^j\cdot c_{\mathrm{p},i}^j$.

Equation (1) is approximated on a net $\omega_{h\tau}$ in the following form

$$\frac{c_i^{j+1}-c_i^j}{\tau}+v_x\frac{c_i^{j+1}-c_{i-1}^{j+1}}{h}=D\frac{c_{i+1}^{j+1}-2c_i^{j+1}+c_{i-1}^{j+1}}{h^2}-\frac{1}{\theta}\frac{c_{a,i}^{j+1}-c_{a,i}^j}{\tau}-\frac{1}{\theta}\frac{c_{p,i}^{j+1}-c_{p,i}^j}{\tau}-\lambda_e c_i^j. \qquad (13)$$

The difference scheme for equations (7) and (10) will look like:

$$\frac{c_{a,i}^{j+1}-c_{a,i}^j}{\tau}=\begin{cases}\beta_{ar}vc_i^j-\lambda_{ea}c_{a,i}^j, & 0<c_{a,i}^j\le c_{ar},\\ \beta_{aa}vc_i^j-\beta_{ad}c_{a,i}^j-\lambda_{ea}c_{a,i}^j, & c_{ar}<c_{a,i}^j<c_{a0},\\ 0, & c_{a,i}^j=c_{a0};\end{cases} \qquad (14)$$

$$\frac{c_{p,i}^{j+1}-c_{p,i}^j}{\tau}=\begin{cases}\beta_{p0}c_i^j-\lambda_{ep}c_{p,i}^j, & 0<c_{p,i}^j\le c_{p1},\\ \frac{\beta_{p0}c_{p1}c_i^j}{c_{p,i}^j}-\lambda_{ep}c_{p,i}^j & c_{p1}<c_{p,i}^j<c_{p0},\\ 0, & c_{p,i}^j=c_{p0}.\end{cases} \qquad (15)$$

We transform the difference schemes (13), (14), (15) and get

$$Ac_{i-1}^{j+1}-Bc_i^{j+1}+Ec_{i+1}^{j+1}=F, \qquad (16)$$

where $F = (h^2 - \lambda_e) c_i^j - \frac{1}{\theta}\frac{c_{a,i}^{j+1} - c_{a,i}^j}{\tau} - \frac{1}{\theta}\frac{c_{p,i}^{j+1} - c_{p,i}^j}{\tau}$, $A = h\tau v_x + D\tau$, $B = h^2 + v_x h\tau + 2D\tau, E = D\tau$,

$$c_{a,i}^{j+1} = \begin{cases} c_{a,i}^j + \tau\left(\beta_{ar}\nu c_i^j - \lambda_{ea} c_{a,i}^j\right), & 0 < c_{a,i}^j \le c_{ar}, \\ c_{a,i}^j + \tau\left(\beta_{aa}\nu c_i^j - \beta_{ad} c_{a,i}^j - \lambda_{ea} c_{a,i}^j\right), & c_{ar} < c_{a,i}^j < c_{a0}, \\ c_{a,i}^j, & c_{a,i}^j = c_{a0}, \end{cases} \tag{17}$$

$$c_{p,i}^{j+1} = \begin{cases} c_{p,i}^j + \tau\left(\beta_{p0} c_i^j - \lambda_{ep} c_{p,i}^j\right), & 0 < c_{p,i}^j \le c_{p1}, \\ c_{p,i}^j + \tau\left(\frac{\beta_{p0} c_{p1} c_i^j}{c_{p,i}^j} - \lambda_{ep} c_{p,i}^j\right), & c_{p1} < c_{p,i}^j < c_{p0}, \\ c_{p,i}^j, & c_{p,i}^j = c_{p0}. \end{cases} \tag{18}$$

The initial and boundary conditions (10), (11) are also presented in mesh form:

$$\begin{aligned} &c_{a,i}^j = 0, i = \overline{0, I}, j = 0, \\ &c_{p,i}^j = 0, i = \overline{0, I}, j = 0, \\ &c_i^j = 0, i = \overline{0, I}, j = 0, \\ &c_i^j = c_0, i = 0, j = \overline{0, J}, \end{aligned} \tag{19}$$

where I is a sufficiently large number for which $c_I^j = 0$.

Results and discussion

In Figure 1 three concentration fields $(c/c_0, c_a, c_p)$ are given, it can be seen from the graphs that over time, all three concentrations gradually penetrate into the inner side of the porous medium. In particular, if at $t = 3000s$ the concentration of the substance has reached the estimated distance 0.37 m (Fig. 1.a), at $t = 6000$ s it can be seen that it has exceeded 0.4 m and at $t = 9000$ s almost approached substance concentration reached about 0.5 m (Fig.1.a).

Concentrations of adsorbed substances in active and passive zones are also pushed into the environment with a slight delay compared to the distribution of substance concentration. At $t = 3000s$ it can be seen that both concentrations c_a and c_p have not reached their saturation value (Fig. 1.b and 1.c). In this case, the adsorbed substance in the active zone was about 65% of its maximum value, while in the passive zone, this indicator was around 80%. At $t = 6000s$ it can be seen that the adsorbed substance reached its maximum value in both zones (Fig. 1.b and 1.c).

At this time the saturation in the passive zone is more widespread than in the active zone. At $t = 9000$ s this situation continued.

Figure 2 shows the solutions for the case where the value of da c_{p1} is increased from $3 \cdot 10^{-3}$ to $.5 \cdot 10^{-3}$. That is at $t = 3000$ s it can be seen that the concentration of adsorbed substance c_p has reached its maximum value (Fig. 2.b). This is explained by the fact that increasing the value of c_{p1} increases the adsorption process in the passive zone. Acceleration of adsorption in the passive zone, in turn, leads to a slight decrease in the concentrations of the solute transport and the adsorbed substance in the active zone.

Figure 3 shows $c/c_0, c_a, c_p$ concentration profiles given for different values of c_{p1} at $t = 9000s$. When value of c_{p1} is reduced to the value of $2 \cdot 10^{-3}$, it can be observed that the process of substance adsorption in the passive zone slowed down, while the substance concentration and the process of substance adsorption in the active zone increased on the contrary (Fig. 3). In general, it can be seen that increasing the value of c_{p1}, increases the adsorption of substance in the passive zone in places closer to the point $x = 0$, and vice versa, starting from the point $x \approx 0.2$, it decreases (Fig. 3.c). In profiles of c/c_0, the opposite is observed.

Figure 4 shows the solutions for the case where the value of c_{a1} is increased from $2 \cdot 10^{-4}$ to $8 \cdot 10^{-4}$. In this case, when the value of c_{a1} is increased, it is observed the presence of areas with two different intensities in the concentration profile of the adsorbed substance c_a (Fig. 4.b). This is explained by the fact that the kinetics equation considered in the active zone is multi-stage. With a further increase in the value of c_{a1}, these different fields are more clearly visible (Fig. 5.b). Increasing the value of c_{a1}, in turn, slows down the process of substance adsorption in the passive zone (Fig. 5.c).

Keeping other parameters of the model unchanged, it can be observed that a slight increase in speed has a significant effect on the process of substance migration (Fig. 6). An increase in speed leads to a proportionally wider spread of both substance concentration and adsorption in both zones.

Conclusion

This paper addresses a solute transport problem in a porous medium with different types zones of adsorption characteristics. The solute is

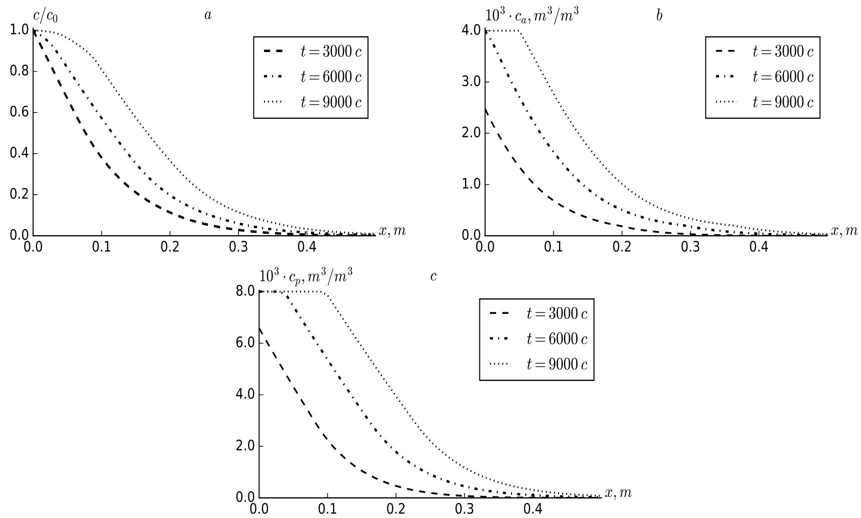

Figure 1. Profiles of changes $c/c_0(a), c_a(b), c_p(c)$, at $c_{p1} = 3 \cdot 10^{-3}$ m^3/m^3 and various time values.

considered as an active substance, incorporating degradation and decay, along with adsorption in active and passive zones of porous media. The degradation coefficients in the transport equations are assumed to be equal in the case of a radioactive solute. Multistage models of kinetic adsorption is examined. The solute transport problem for the one-dimensional case is numerically solved using the finite difference method. It is observed that increasing the value of "aging" parameter leads to increase of the adsorption process in the passive zone. Acceleration of adsorption in the passive zone, in turn, leads to a slight decrease in the concentrations of the solute transport and the adsorbed substance in the active zone. When the value of "charging" parameter for active zone is increased, it is observed the presence of areas with two different intensities in the concentration profile of the adsorbed substance.

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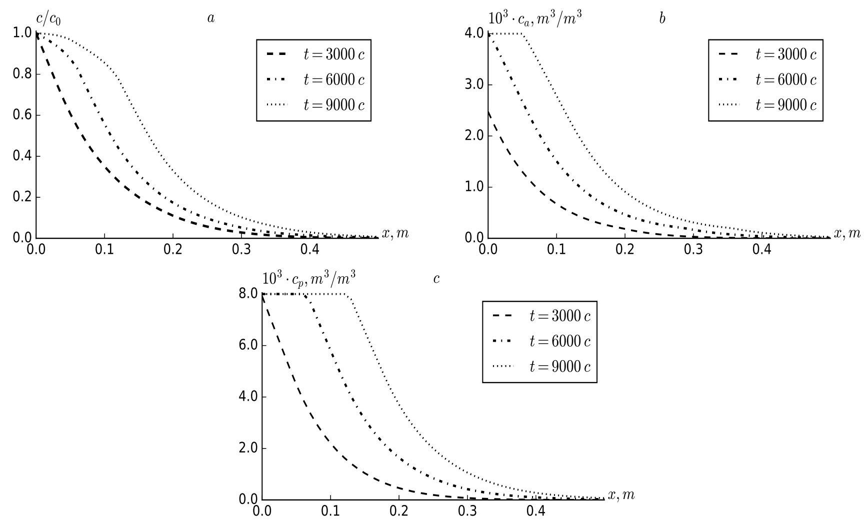

Figure 2. Profiles of changes $c/c_0(a), c_a(b), c_p(c)$, at $c_{p1} = 5 \cdot 10^{-3}$ m^3/m^3 and various time values.

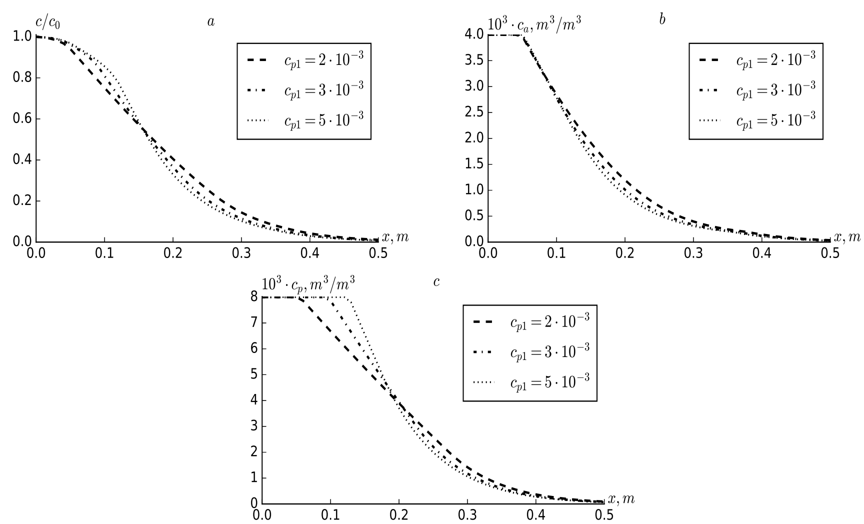

Figure 3. Profiles of changes $c/c_0(a), c_a(b), c_p(c)$, at $t = 9000$c and various values c_{p1}.

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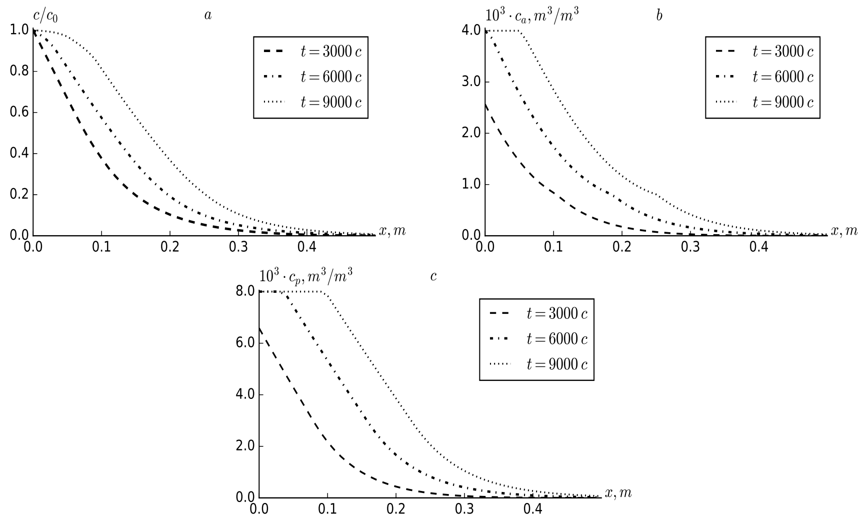

Figure 4. Profiles of changes $c/c_0(a), c_a(b), c_p(c)$, at $c_{a1} = 8 \cdot 10^{-4}$ $\mathrm{m}^3/\mathrm{m}^3$ and various time values.

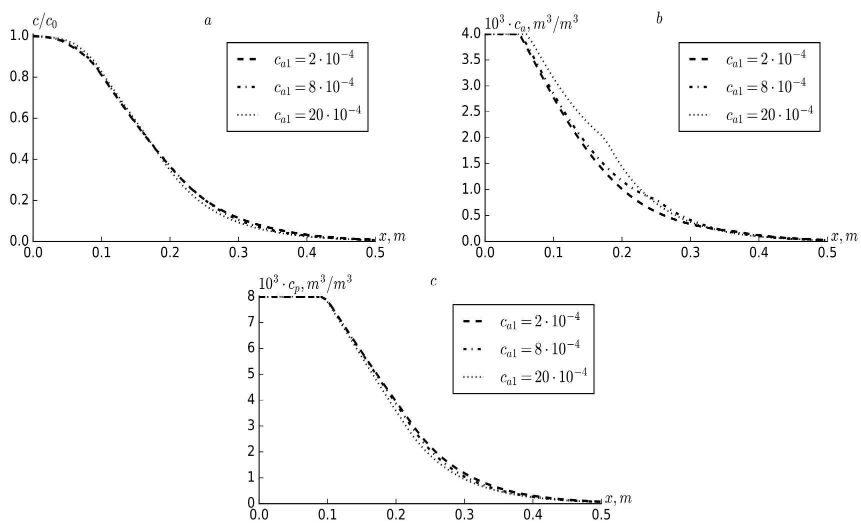

Figure 5. Profiles of changes $c/c_0(a), c_a(b), c_p(c)$, at $t = 9000$c and various values c_{a1}.

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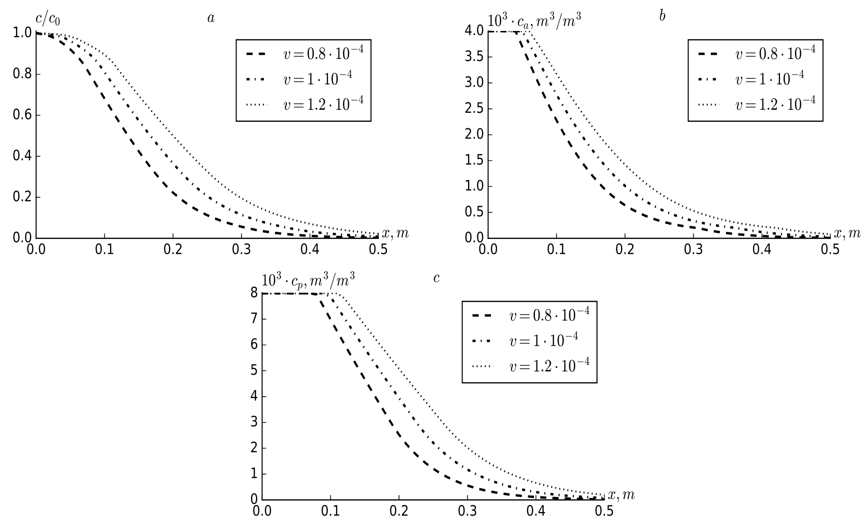

Figure 6. Profiles of changes $c/c_0(a), c_a(b), c_p(c)$, with $t = 9000$ s and various values v.

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