PHYSICO-MATHEMATICAL MODELS OF HETERODIFFUSION IN A LAYER

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We obtain and study the solution of vertical diffusion problems for a dopant applying different model approximations. We establish the area of applicability of models of diffusion with two migration paths, with and without consideration of the mutual transitions of dopant particles, and diffusion in a medium with traps.

In solving applied problems connected with the estimation of the safety of ground water from surface pollution it is necessary to apply certain imaginative models of the process of redistribution of a dopant in the upper layers of soil. Such model approaches must take sufficient account of the influence of the structure of the medium on the kinetics of transport of pollutant particles. In particular, the diffusion of a dopant with different intensities occurs in a pore water solution and in adsorbed layers of water on the skeleton of the soil and is accompanied by processes of mutual transition of particles between the different migration paths (heterodiffusion of dopants) [1–4]. In this situation the particles of the dopant also pass from the adsorbed layers of water into the region of monocrystals of soil that form the skeleton. In the region of monocrystals the coefficients of diffusion are several orders smaller than in the adsorbed layers of water, so that in macroscopic description the region of monocrystals can be regarded as a trap for dopant particles [5].

In the present paper we find and study the solutions of problems involving diffusion of dopants in a layer of soil in the presence of a point source on one of its surfaces, applying different models. We establish the area of applicability of heterodiffusion models by two paths with and without consideration of the mutual interchange of particles and also diffusion in a medium with traps.

We shall consider a porous medium (an aerated layer of soil), an arbitrarily chosen small region of which always contains, in addition to the particles that form the base components (the skeleton, a porous solution) dopant particles of a single type in three physically different states. We denote by $C_1$ the concentration of dopant particles migrating in the pore water solution, by $C_2$ the concentration of particles diffusing in the adsorbed layers of the water, and by $C_3$ the concentration of pollutants in the region of the skeleton (traps). A quantitative description of the heterodiffusion processes in such bodies basically reduces to solving coupled boundary-value problems that can be written in dimensionless form by introducing the quantities $\tau = k_2 t$, and $\xi = (k_2/D_1)^{1/2} x$, where $k_2$ is a coefficient of dimension $[\ell^1]$, $t$ is time, and $x$ is a coordinate (the $Ox$-axis is perpendicular to the surface of the layer). We recall following the relations from the models proposed in practice [4, 5].

In the models of noninteracting diffusion fluxes the migration of the dopant occurs over two paths without taking account of the transitions between the two and is described by the differential equations

$$\frac{\partial C_1}{\partial \tau} = \frac{\partial^2 C_1}{\partial \xi^2}, \quad \frac{\partial C_2}{\partial \tau} = d \frac{\partial^2 C_2}{\partial \xi^2},$$

where $d = D_2/D_1$, and $D_1$ and $D_2$ are respectively the coefficients of diffusion of the dopant in the porous solution and in the adsorbed layers of water. For each equation the initial and boundary conditions are stated independently.

In the model of heterodiffusion by two paths we take account of the transitions of particles from one migration path to the other and determine the functions $C_1(\tau, \xi)$ and $C_2(\tau, \xi)$ from a system of two coupled differential equations

$$\frac{\partial C_1}{\partial \tau} = \frac{\partial^2 C_1}{\partial \xi^2} + d_1 \frac{\partial^2 C_2}{\partial \xi^2} - a C_1 + C_2,$$

where $d_1 = D_3/D_1$, $d_2 = D_4/D_1$, $a = k_1/k_2$, $D_3$ and $D_4$ are the transverse diffusion coefficients, $k_1$ is the coefficient of transition intensity of dopant particles from the porous solution into the adsorbed layers of water, and $k_2$ is the coefficient of transition in the opposite direction.

The model of diffusion in a medium with traps describes diffusion of dopant in a pore water solution with penetration of particles into the region of the skeleton of the soil:

\[
\frac{\partial C_1}{\partial \tau} = \frac{\partial^2 C_1}{\partial \xi^2} - aC_1 + a_1C_3, \quad \frac{\partial C_3}{\partial \tau} = aC_1 - a_1C_3,
\]

where $a_1 = k_3/k_2$, and $k_3$ is the coefficient of intensity of transition of the dopant into the traps.

A comprehensive view of diffusion in a porous solution and in adsorbed layers of water in the presence of particles in the region of monocrystals of soil taking account of mutual transitions between these states (the model of heterodiffusion with traps) reduces to finding the concentration functions $C_1(\tau, \xi)$, $C_2(\tau, \xi)$, and $C_3(\tau, \xi)$ from a system of three coupled differential equations

\[
\begin{align*}
\frac{\partial C_1}{\partial \tau} &= \frac{\partial^2 C_1}{\partial \xi^2} + a_2 \frac{\partial^2 C_2}{\partial \xi^2} - aC_1 + C_2, \\
\frac{\partial C_2}{\partial \tau} &= d_2 \frac{\partial^2 C_1}{\partial \xi^2} + d \frac{\partial^2 C_2}{\partial \xi^2} + aC_1 - (1 + a_2)C_2 + a_1C_3, \\
\frac{\partial C_3}{\partial \tau} &= a_2C_2 - a_1C_3.
\end{align*}
\]

Here $a_2 = k_4/k_2$, and $k_4$ is the coefficient of intensity of transition of particles from the traps to the adsorbed layers of water.

We shall assume that at the initial instant of time $\tau = 0$ a point source of dopant particles of power $Q$ is acting on the soil surface $\xi = 0$, and that the particles are distributed among the different states as follows:

\[
C_1(0, \xi) = \gamma Q\delta(\xi), \quad C_2(0, \xi) = (1 - \gamma)Q\delta(\xi), \quad C_3(0, \xi) = 0,
\]

where $\gamma$ is a certain positive parameter ($0 \leq \gamma \leq 1$) that determines the surface distribution of dopant particles between the rapid and slow migration paths. For $\tau > 0$ we take the conditions of mass isolation as boundary conditions:

\[
\left. \frac{\partial C_1}{\partial \xi} \right|_{\xi=0} = \left. \frac{\partial C_2}{\partial \xi} \right|_{\xi=0} = \left. \frac{\partial C_1}{\partial \xi} \right|_{\xi=\xi_0} = \left. \frac{\partial C_2}{\partial \xi} \right|_{\xi=\xi_0} = 0,
\]

where $\xi_0$ is the dimensionless thickness of the layer.

The systems of differential equations (1)--(4) admit closed-form solutions. We recall the expressions for the total concentrations $C(\tau, \xi) = \sum_i C_i(\tau, \xi)$.

For the set of equations (1) we have

\[
C(\tau, \xi) = \frac{Q}{\xi_0} \left\{ 1 + 2 \sum_{n=1}^{\infty} \cos y_n \xi \left[ \gamma e^{-y_2^2 \tau} + (1 - \gamma) e^{-y_1^2 \tau} \right] \right\}.
\]

We write the complete solution for the system (2) as follows:

\[
C(\tau, \xi) = \frac{Q}{\xi_0} \left\{ 1 + 2 \sum_{n=1}^{\infty} \cos y_n \xi \left[ (s_1 + P^*) e^{s_1 \tau} - (s_2 + P^*) e^{s_2 \tau} \right] \right\}.
\]