STUDY OF SPACE-TIME IMPURITY DISTRIBUTIONS USING A "LUMPED-CAPACITANCE" SCHEME

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New problems of convective diffusion are considered in a "lumped-capacitance" approximation. Analytical solutions are obtained for cases of axisymmetric radial flow of liquids with impurities. Results of calculations as applied to ecology have revealed trends in the distributions of harmful impurities in groundwater flows.

Exacerbation of the ecological situation makes it necessary to solve some important problems of engineering physics connected with the development of simplified mathematical models for integration of measured concentrations of harmful impurities and for calculation of their space-time distributions.

Impurity concentrations change as a result of such processes as diffusion, convective mass transfer, etc. Theoretical studies of convective diffusion lead to a system of equations including continuity, Navier-Stokes, and energy equations, and the equation of state of the impurity. It is very difficult to imagine a general system of equations in a specific statement. Therefore, various kinds of simplifying assumptions are used for solution of such problems. One-dimensional problems of convective diffusion are solved most easily [1-3].

In what follows we consider two-dimensional axisymmetric problems in a cylindrical coordinate system that describe impurity propagation in a horizontal bed with a flow of water or some other liquid with impurities and in the environment. For simplification of convective diffusion problems we used the lumped-capacitance method that was developed earlier for thermal-physics problems. The essence of the method consists in isolation of areas with slightly changing concentrations along one or several coordinates and substitution of average values of the unknown parameter for this parameter in these areas. For the concentration of a compound in a bed and in the rocks surrounding it, the condition of equality is postulated at the contact area. In the present case it is assumed that in liquid flow in a porous medium the impurity concentration \( c_{im} \) depends only on the horizontal distance \( r \) and is independent of the vertical coordinate \( z \) \((c_{im})_z = 0, (c_{im})_{zz} = 0\).

In the problems it is assumed that the concentrations of impurities in the porous skeleton of the medium and in the incompressible solution that saturates the medium are equal [4-6].

The equation of mass balance of the impurity in the part of the bed located between two cylindrical coaxial surfaces \( r - r + dr, 2h \) in height, contains the increment of the amount of material in the volume element considered

\[
\frac{dM_1}{dt} = 2\pi r_2h \frac{\partial}{\partial t} \left( m_s \rho c_i \right) dr dt,
\]

and changes in the amount of material due to convection

\[
\frac{dM_{1i}}{dt} = -Q_i \frac{\partial}{\partial r} \left( m_s \rho c_i \right) dr dt,
\]

diffusion

\[
\frac{dM_{2i}}{dt} = 2\pi r_2 h D_i \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial}{\partial r} \left( m_s \rho c_i \right) \right) dr dt,
\]


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the diffusive flow through planes of the bed \( z = h \) and \( z = -h \)

\[
dM_{3i} = 2\pi r \left[ D_{1i} \frac{\partial}{\partial z} \left( m_1 s_{1i} \rho_1 c_{1i} \right) \bigg|_{z=h} - D_{2i} \frac{\partial}{\partial z} \left( m_2 s_{2i} \rho_2 c_{2i} \right) \bigg|_{z=-h} \right] dr dt,
\]

mass exchange between the porous skeleton and liquid

\[
dM_{4i} = -2\pi r \left( s_{si} \rho_s c_{si} \right) \frac{\partial}{\partial t} + Q_i \left( m_i s_i \rho_i c_i \right) + \frac{Q_i \partial}{\partial t} \left( m_i s_i \rho_i c_i \right) + q_i.
\]

and the presence of concentration sources. Finally, we obtain an equation for description of the impurity concentration in liquid flow in a porous medium:

\[
\frac{\partial}{\partial t} \left( m_i s_i \rho_i c_i \right) = D_{1i} \frac{1}{\partial r} \left( \frac{\partial}{\partial r} \left( m_i s_i \rho_i c_i \right) \right) - \frac{Q_i}{4\pi hr} \frac{\partial}{\partial r} \left( m_i s_i \rho_i c_i \right) + \\
\frac{D_{1i}}{2h} \frac{\partial}{\partial z} \left( m_i s_i \rho_i c_i \right) \bigg|_{z=h} - \frac{D_{2i}}{2h} \frac{\partial}{\partial z} \left( m_i s_i \rho_i c_i \right) \bigg|_{z=-h} - \frac{Q_i}{4\pi hr} \frac{\partial}{\partial r} \left( m_i s_i \rho_i c_i \right) + q_i.
\]

(1)

It is assumed that the densities of the \( i \)-th component in the bed, medium, and skeleton, the porosity, saturation, and the diffusion coefficients are constant and that there are no concentration sources. With the notation

\[
\delta_{1i} = \frac{D_{1i} m_{1i} s_{1i} \rho_{1i}}{2m_{si} \rho_{si} h} ; \quad \delta_{2i} = \frac{D_{2i} m_{2i} s_{2i} \rho_{2i}}{2m_{si} \rho_{si} h} ; \quad B_i = \frac{Q_i}{4\pi hr},
\]

Eq. (1) takes the form

\[
\frac{\partial c_i}{\partial t} = D_i \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial c_i}{\partial r} \right) - B_i \frac{\partial c_i}{\partial r} + \delta_{1i} \frac{\partial c_i}{\partial z} \bigg|_{z=h} - \delta_{2i} \frac{\partial c_i}{\partial z} \bigg|_{z=-h} - \frac{m_{si} s_{si} \rho_{si} c_{si}}{m_{si} \rho_i} \frac{\partial c_i}{\partial t}.
\]

(2)

We will only consider problems for a single impurity species \( (m_0 = m, m_1 = 1 - m, s_1 = 1) \). The last term in Eq. (2) describes adsorption of the impurity on the porous skeleton. Its contribution is thoroughly investigated in [4]. In what follows, for simplicity it is assumed that mass exchange between the skeleton and liquid is rather rapid. This assumption is satisfied at low liquid velocities. In the case of a single impurity, its concentrations in the porous skeleton and in the liquid are assumed to be equal. Indeed, in real porous clay beds, the contact surface area is \( 10^5 \) m\(^2\) per 1 m\(^3\). If we imagine this surface to be rolled as a thin layer, its thickness will be \( 10^{-7} \) m. According to the Fourier number \(Dt/h^2 = 1\), it is possible to estimate the time of mass exchange between the liquid and porous skeleton. The diffusion coefficients for liquids in liquid media are of the order of magnitude of \( 10^{-9} \) m\(^2\)/sec, and, consequently, the order of magnitude of \( t \) is 0.1 sec. As one can see, mass exchange between the liquid and skeleton occurs rather rapidly. In view of the above, Eq. (2) is written as

\[
\frac{\partial c}{\partial t} = D \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial c}{\partial r} \right) - B \frac{\partial c}{\partial r} + \delta_1 \frac{\partial c}{\partial z} \bigg|_{z=h} - \delta_2 \frac{\partial c}{\partial z} \bigg|_{z=-h}.
\]

(3)

With radial diffusion along the coordinate \( r \) neglected at high liquid velocities in the bed, Eq. (3) is transformed to the form

\[
\frac{\partial c}{\partial t} = - \frac{B}{r} \frac{\partial c}{\partial r} + \delta_1 \frac{\partial c}{\partial z} \bigg|_{z=h} - \delta_2 \frac{\partial c}{\partial z} \bigg|_{z=-h}.
\]

(4)

Now, we consider some concrete problems. Let water with an impurity whose concentration is equal at any point in a selected cross-section penetrate into an infinitely long horizontal bed. A constant concentration \( c_0 \) of the impurity is maintained in the liquid entering the bed at \( r = r_0 \). A diffusive impurity flow through the boundaries of