Journal of Engineering Physics and Thermophysics, Vol. 70, No. 2, 1997

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

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UDC 532.546

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 ($(c_{\text{im}})'_z = 0$, $(c_{\text{im}})''_{zz}) = 0$.

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

$$dM_i = 2\pi r 2h \frac{\partial\,(m_i s_i \rho_i c_i)}{\partial t}\, dr dt\,,$$

and changes in the amount of material due to convection

$$dM_{1i} = -\,Q_i \frac{\partial\,(m_i s_i \rho_i c_i)}{\partial r}\, dr dt\,,$$

diffusion

$$dM_{2i} = 2\pi r 2h D_i \frac{1}{r}\frac{\partial}{\partial r}\left(r \frac{\partial\,(m_i s_i \rho_i c_i)}{\partial r}\right) dr dt\,,$$

Sterlitamak Pedagogical Institute, Russia. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 71, No. 2, pp. 205-210, March-April, 1997. Original article submitted May 5, 1995.

the diffusive flow through planes of the bed $z = h$ and $z = -h$

$$dM_{3i} = 2\pi r \left[D_{1i} \frac{\partial (m_{1i} s_{1i} \rho_{1i} c_{1i})}{\partial z} \bigg|_{z=h} - D_{2i} \frac{\partial (m_{2i} s_{2i} \rho_{2i} c_{2i})}{\partial z} \bigg|_{z=-h} \right] drdt,$$

mass exchange between the porous skeleton and liquid

$$dM_{4i} = -2\pi r 2h \frac{\partial (m_{si} s_{si} \rho_{si} c_{si})}{\partial t} drdt$$

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

$$\frac{\partial (m_i s_i \rho_i c_i)}{\partial t} = D_i \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial (m_i s_i \rho_i c_i)}{\partial r} \right) - \frac{Q_i}{4\pi h r} \frac{\partial (m_i s_i \rho_i c_i)}{\partial r} +$$

$$+ \frac{D_{1i}}{2h} \frac{\partial (m_{1i} s_{1i} \rho_{1i} c_{1i})}{\partial z} \bigg|_{z=h} - \frac{D_{2i}}{2h} \frac{\partial (m_{2i} s_{2i} \rho_{2i} c_{2i})}{\partial z} \bigg|_{z=-h} - \frac{\partial (m_{si} s_{si} \rho_{si} c_{si})}{\partial t} + q_i. \quad (1)$$

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

$$\delta_{1i} = \frac{D_{1i} m_{1i} s_{1i} \rho_{1i}}{2 m_i s_i \rho_i h}; \quad \delta_{2i} = \frac{D_{2i} m_{2i} s_{2i} \rho_{2i}}{2 m_i s_i \rho_i h}; \quad B_i = \frac{Q_i}{4\pi h}$$

Eq. (1) takes the form

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

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^{-5} 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

$$\frac{\partial c}{\partial t} = D \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial c}{\partial r} \right) - \frac{B}{r} \frac{\partial c}{\partial r} + \delta_1 \frac{\partial c_1}{\partial z} \bigg|_{z=h} - \delta_2 \frac{\partial c_2}{\partial z} \bigg|_{z=-h}. \quad (3)$$

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

$$\frac{\partial c}{\partial t} = -\frac{B}{r} \frac{\partial c}{\partial r} + \delta_1 \frac{\partial c_1}{\partial z} \bigg|_{z=h} - \delta_2 \frac{\partial c_2}{\partial z} \bigg|_{z=-h}. \quad (4)$$

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 the bed to the medium surrounding the bed is observed and in this medium the harmful impurity is dissipated only by diffusion. With the assumption that the physicochemical properties of the surrounding rocks are equal, i.e., $D_1 = D_2$, $c_1 = c_2$, $\delta = \delta_1 + \delta_2$, we consider diffusion in the half space $z > 0$. The plane $z = 0$ is assumed to be a boundary of the bed.

In this case the mathematical statement of the problem has the form:

$$\frac{\partial c_1}{\partial t} = a \frac{\partial^2 c_1}{\partial z^2}, \quad t > 0, \quad z > 0;$$

$$\frac{\partial c}{\partial t} = -\frac{B}{r}\frac{\partial c}{\partial r} + \delta \left.\frac{\partial c_1}{\partial z}\right|_{z=0}, \quad r > 0, \quad t > 0;$$

$$c_1|_{z\to\infty} = 0; \quad c_1|_{t=0} = 0; \quad c|_{r=r_0} = c_0; \quad c = c_1|_{z=0}; \quad c|_{t=0} = 0.$$

With the use of the Laplace–Carson transformation, it is possible to obtain solution of the system in the space of the transforms

$$C^{t} = c_0 \exp\left(-\frac{r^2 - r_0^2}{2B} p\right) \exp\left(-\sqrt{p/a}\left(\frac{(r^2 - r_0^2)\,\delta}{2B} + z\right)\right).$$

Inversion of the transform makes it possible to restore the initial concentration distribution function in the environment

$$c_1 = c_0 \operatorname{erfc}\left(\frac{(r^2 - r_0^2)\,\delta + 2Bz}{\sqrt{8aB\,[2Bt - (r^2 - r_0^2)]}}\right) I\left(t - \frac{r^2 - r_0^2}{2B}\right).$$

Inclusion of the difference in the physicochemical properties of the surrounding rocks leads to consideration of the impurity distribution in the half-spaces $z > h$ and $z < -h$:

$$\frac{\partial c_1}{\partial t} = a_1 \frac{\partial^2 c_1}{\partial z^2}, \quad t > 0, \quad z > h;$$

$$\frac{\partial c_2}{\partial t} = a_2 \frac{\partial^2 c_2}{\partial z^2}, \quad t > 0, \quad z < -h;$$

$$\frac{\partial c}{\partial t} = -\frac{B}{r}\frac{\partial c}{\partial r} + \delta_1 \left.\frac{\partial c_1}{\partial z}\right|_{z=h} - \delta_2 \left.\frac{\partial c_2}{\partial z}\right|_{z=-h}, \quad r > 0, \quad t > 0, \quad |z| < h;$$

$$c_1|_{|z|\to\infty} = 0; \quad c_1|_{t=0} = 0; \quad c_2|_{|z|\to\infty} = 0; \quad c_2|_{t=0} = 0;$$

$$c|_{r=r_0} = c_0; \quad c = c_1|_{z=h} = c_2|_{z=-h}; \quad c|_{t=0} = 0.$$

The concentration distribution function in the transforms has the form

$$C_1^{t} = c_0 \exp\left(-\frac{r^2 - r_0^2}{2B} p\right) \exp\left(-\left[\frac{r^2 - r_0^2}{2B}\left(\frac{\delta_1}{\sqrt{a_1}} + \frac{\delta_2}{\sqrt{a_2}}\right) + \frac{z - h}{\sqrt{a_1}}\right]\sqrt{p}\right);$$

$$C_2^t = c_0 \exp\left(-\frac{r^2 - r_0^2}{2B} p\right) \exp\left(-\left[\frac{r^2 - r_0^2}{2B}\left(\frac{\delta_1}{\sqrt{a_1}} + \frac{\delta_2}{\sqrt{a_2}}\right) - \frac{z+h}{\sqrt{a_2}}\right]\sqrt{p}\right).$$

The obtained analytical solutions are written as

$$c_1 = c_0 \operatorname{erfc}\left(\frac{(r^2 - r_0^2)(\delta_1 \sqrt{a_2} + \delta_2 \sqrt{a_1}) + 2B\sqrt{a_2}(z-h)}{\sqrt{8a_1 a_2 B\,[2Bt - (r^2 - r_0^2)]}}\right) I\left(t - \frac{r^2 - r_0^2}{2B}\right);$$

$$c_2 = c_0 \operatorname{erfc}\left(\frac{(r^2 - r_0^2)(\delta_1 \sqrt{a_2} + \delta_2 \sqrt{a_1}) - 2B\sqrt{a_1}(z+h)}{\sqrt{8a_1 a_2 B\,[2Bt - (r^2 - r_0^2)]}}\right) I\left(t - \frac{r^2 - r_0^2}{2B}\right).$$

Inclusion of radial diffusion makes the problem more complicated. If the physicochemical properties of the rock surrounding the bed are assumed to be identical, for the half space $z > 0$ we obtain the system of equations

$$\frac{\partial c_1}{\partial t} = a\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c_1}{\partial r}\right) + \frac{\partial^2 c_1}{\partial z^2}\right], \quad r > 0, \quad t > 0, \quad z > 0;$$

$$\frac{\partial c}{\partial t} = -\frac{B}{r}\frac{\partial c}{\partial r} + \delta \left.\frac{\partial c_1}{\partial z}\right|_{z=0}, \quad r > 0, \quad t > 0;$$

$$\lim_{z+r\to\infty} c_1 = 0; \quad c_1|_{t=0} = 0; \quad c|_{r=0} = c_0; \quad c = c_1|_{z=0}; \quad c|_{t=0} = 0.$$

For solution of the formulated problem, apart from the Laplace–Carson transformation, Hunkel transformation in r is also used. The inverse a Hunkel transformation makes it possible to obtain the concentration distribution function in the space of the transforms

$$C^t = c_0 \int_0^\infty \frac{Bs}{\delta} J_0(sr) \exp\left(-\sqrt{s^2 + p/a}\,(z + B/\delta) + B/\delta\sqrt{p/a}\right) \times$$

$$\times \left(\sqrt{s^2 + p/a} + p/\delta\right)^{(Bp-\delta^2)/\delta^2} \left(\sqrt{p/a} + p/\delta\right)^{-Bp/\delta^2} ds.$$

It is very difficult to find the integral of this equation, but it is possible to obtain its particular solution at $p \to 0$, which corresponds to a steady-state concentration distribution. Assuming $p = 0$, we obtain the distribution function in the environment

$$c = \frac{c_0 B}{\delta}\int_0^\infty J_0(sr)\exp\left(-s\,(z + B/\delta)\right) ds = \frac{c_0 B}{\sqrt{(B + \delta z)^2 + r^2\delta^2}}.$$

Consideration of the differences in the physicochemical properties of the surrounding rocks with allowance for radial diffusion in the plane perpendicular to the z-axis leads to the problem:

$$\frac{\partial c_1}{\partial t} = a_1\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c_1}{\partial r}\right) + \frac{\partial^2 c_1}{\partial z^2}\right], \quad r > 0, \quad t > 0, \quad z > h;$$

$$\frac{\partial c_2}{\partial t} = a_2\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial c_2}{\partial r}\right) + \frac{\partial^2 c_2}{\partial z^2}\right], \quad r > 0, \quad t > 0, \quad z < -h;$$

$$\frac{\partial c}{\partial t} = -\frac{B}{r}\frac{\partial c}{\partial r} + \delta_1 \frac{\partial c_1}{\partial z}\bigg|_{z=h} - \delta_2 \frac{\partial c_2}{\partial z}\bigg|_{z=-h}, \quad r > 0, \quad t > 0, \quad |z| < h;$$

$$\lim_{|z|+r\to\infty} c_1 = 0; \quad c_1|_{t=0} = 0; \quad \lim_{|z|+r\to\infty} c_2 = 0; \quad c_2|_{t=0} = 0;$$

$$c|_{r=0} = c_0; \quad c = c_1|_{z=h} = c_2|_{z=-h}; \quad c|_{t=0} = 0.$$

For transformed functions in the half-spaces $z > h$ and $z < -h$, the following expressions are obtained:

$$C_1^t = c_0 \int_0^\infty J_0(sr) \exp\left(-\sqrt{s^2 + p/a_1}\,(z-h)\right) \times$$

$$\times \exp\left(-\int_0^s \frac{Bsds}{p + \delta_1\sqrt{s^2 + p/a_1} + \delta_2\sqrt{s^2 + p/a_2}}\right) \times$$

$$\times \frac{Bs}{p + \delta_1\sqrt{s^2 + p/a_1} + \delta_2\sqrt{s^2 + p/a_2}}\,ds;$$

$$C_2^t = c_0 \int_0^\infty J_0(sr) \exp\left(\sqrt{s^2 + p/a_2}\,(z+h)\right) \times$$

$$\times \exp\left(-\int_0^s \frac{Bsds}{p + \delta_1\sqrt{s^2 + p/a_1} + \delta_2\sqrt{s^2 + p/a_2}}\right) \times$$

$$\times \frac{Bs}{p + \delta_1\sqrt{s^2 + p/a_1} + \delta_2\sqrt{s^2 + p/a_2}}\,ds.$$

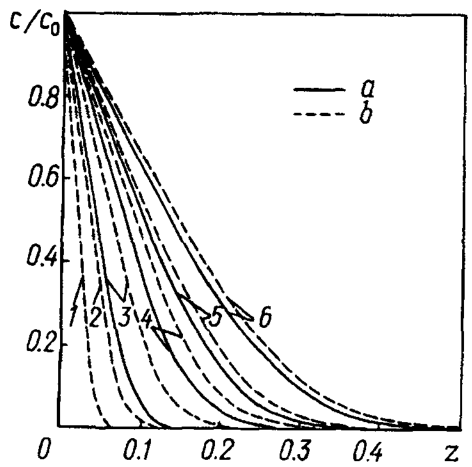
It is difficult to find this integral, however a particular solution for $p \to 0$ can be given. Concentrations in half-spaces $z > h$ and $z < -h$ are expressed as:

$$c_1 = \frac{c_0 B}{\sqrt{[B + (\delta_1 + \delta_2)(z - h)]^2 + r^2(\delta_1 + \delta_2)^2}};$$

$$c_2 = \frac{c_0 B}{\sqrt{[B - (\delta_1 + \delta_2)(z + h)]^2 + r^2(\delta_1 + \delta_2)^2}}.$$

Application of the "lumped-capacitance" approach to problems of convective diffusion gives analytical formulas for space-time concentration distributions of harmful impurities in the cases of complicated geometries for which visible solutions could not be constructed earlier. These formulas were used to calculate concentration distributions and graphs are presented for acetone dissolved in water surrounded by argillaceous beds. The program is written in Turbo Pascal for IBM-compatible PCs. We investigated the impurity concentration distribution functions in a water flow $c = c(r)$ at $z = 0$ and in surrounding clays $c = c(z)$ for different times. The calculations were carried out for liquid discharges $Q = 5$, 10, 25, and 50 m^3/day and for flow thicknesses $h = 1$, 5, and 10 m.

The vertical distribution $c = c(r)$ is plotted for three distances from the concentration source $r = 0.1$, 0.5, and 1 m. As can be seen from Fig. 1, for long periods of time the space-time distributions almost coincide, i.e., the liquid discharge and the flow thickness do not have a marked effect on diffusion. The space-time concentration distributions depend on these quantities only over short time periods. As time passes, at $z = 0$ for the various distances r the concentration of acetone tends to the limiting value c_0.



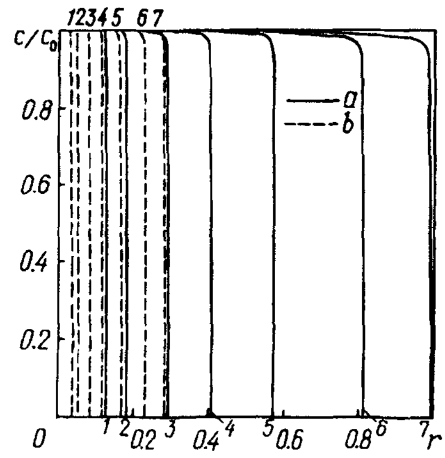


Fig. 1. Plot of impurity concentration versus coordinate z for fixed distance from source ($r = 1$ m): 1) 50 h, 2) 100, 3) 250, 4) 500, 5) 750, 6) 1250; a) liquid discharge $Q = 5$ m^3/day, thickness of bed $h = 5$ m; b) 50 and 10. z, m.

Fig. 2. Radial impurity concentration distributions for various times: 1) 0.1 h, 3) 0.2, 3) 0.5, 4) 1, 5) 2, 6) 4, 7) 6; a) liquid discharge $Q = 25$ m^3/day, thickness of bed $h = 1$ m; b) 10 and 5. r, m.

Plots of the radial concentration distribution $c = c(r)$ are given in Fig. 2. One can see from the figure that as time passes, the impurity front moves from the coordinate origin at a velocity that depends on Q and h. The front is smeared due to diffusion mass transfer to the medium surrounding the flow. From calculations it is possible to estimate the radial dimension of the region of the front in which a noticeable contribution of mass transfer is observed. For example, for $t = 6$ h at distance $r = 1$ m, the length of the zone is 0.2 m and smearing occurs at a distance of 0.1 m with changes in the concentration by at most 0.9 of c_0. As time passes, the front becomes more and more smeared due to diffusive flow to the surrounding medium.

Analytical formulas for the concentrations of harmful impurities obtained by the "lumped-capacitance" scheme can be used to plot the space-time distribution functions of the impurity and to solve particular inverse problems. Solution of convective diffusion problems opens new prospects for development of devices for monitoring the conditions of the environment.

NOTATION

m_i, porosity for i-th component of impurity; $m_{si} = 1 - m_i$; s_i, s_{si}, saturation of the bed and porous skeleton with i-th component; ρ_i, ρ_{1i}, ρ_{2i}, ρ_{si}, densities of i-th component in bed, half spaces $z > h$ and $z < -h$, and in the porous skeleton; c_i, c_{1i}, c_{2i}, c_{si}, respective concentrations; D_i, D_{1i}, D_{2i}, diffusion coefficients in bed and half spaces; c_{im}, concentration in liquid flow; Q_i, discharge of i-th component; q_i, density of concentration sources; $J_0(x)$, first-order Bessel function; $a_i = D_i/m_i s_i$; erfc $(x) = (2/\sqrt{\pi})\int_x^\infty \exp(-u^2)du$; $I(t)$, unit Heaviside function.

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