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COMPUTATIONAL SCHEMES FOR THE PROCESSES OF CONVECTIVE-DIFFUSION TRANSPORT OF WATER-SOLUBLE COMPOUNDS

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We have developed and tested computational schemes for a one-dimensional equation of convective-diffusion transport of water-soluble compounds providing results satisfactory for practical purposes for various forms of the initial concentration profile and relations between the convective-diffusion transport parameters.

Keywords: *convection, diffusion, water-soluble compounds, computational scheme, numerical dispersion.*

Introduction. To estimate the propagation of mineral water-soluble pollutants in the environment (radionuclides, heavy metals, sodium and potassium chlorides), it is necessary to develop forecast methods based on mathematical models of convective-diffusion transport of water-soluble compounds in soils and grounds. To describe the processes of transport taking into account the diffusion and convective mechanisms, the convective-diffusion equation is used. The wide variety of factors and the nonlinearity of mathematical models permit realizing such models only with the help of modern computer aids by developing computational schemes and appropriate software.

The specific features of the numerical solution of the convective diffusion equation are connected with the taking into account of the convection and its dominance over the process of diffusion transport. The dominance of convection over diffusion and the sharp change in the concentration in the calculation domain are responsible for the instability of computational schemes and inadequacy of obtained results.

The investigation of different computational schemes using finite differences on the basis of the general theory of stability of difference schemes does not permit estimating in full measure the accuracy and convergence of their concrete variants. Therefore, to check the adequacy of results obtained by numerical-solution methods for convection-diffusion problems, testing of these methods by means of standard solutions of corresponding problems is widely used.

Method of Investigation. The given investigation was carried out by testing the numerical-solution methods for convective diffusion problems by means of standard analytical solutions or numerical methods that have passed a test on standard solutions. One of the most widely known analytical solutions for a semibounded medium with homogeneous initial conditions, with a constant velocity of the filtration flow, and a constant concentration of the water-soluble compound on the bounded surface of the medium is the solution of the form [1]

$$C(x,\tau) = \frac{C_{\text{in}} - C_0}{2}\left[\operatorname{erfc}\left(\frac{x - V\tau}{2\sqrt{D\tau}}\right) + \exp\left(\frac{Vx}{D}\right)\operatorname{erfc}\left(\frac{x + V\tau}{2\sqrt{D\tau}}\right)\right]. \tag{1}$$

This equation becomes much simpler when the time τ at which $V\tau > 4(D\tau)^{-0.5}$ is attained; then the concentration distribution is described with the help of the function

$$C(x,\tau) = \left(\frac{C_{\text{in}} - C_0}{2}\right)\operatorname{erfc}\left(\frac{x - V\tau}{2\sqrt{D\tau}}\right). \tag{2}$$

The given analytical solution permits estimating the error with which the computational scheme approximates the exact solution in the corresponding formulation.

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Using the transform $(x - V\tau)$, convective diffusion problems can be reduced to pure diffusion transport problems for which the analytical and numerical methods have been developed in more detail. Such an approach is noted in A. V. Luikov's reference book "Heat and Mass Transfer" with reference to the source [2]. The main condition for legitimacy of such transform is a sufficient distance of the investigated portion from the boundaries of the integration region of the convective diffusion equation, i.e., the theoretical problem must be considered in an unbounded region. Practically, the testing range should be at a distance from the integration region exceeding the size of the diffusion perturbation zone ξ_d determined on the basis of the relation

$$\xi_d > (12D\tau)^{-0.5} . \tag{3}$$

For example, in the formulation of the problem for a semibounded medium with a constant velocity of the filtration flow and a shift of the region of a constant maximum concentration for a distance determined by condition (3), the exact analytical solution will be described by Eq. (2) from the initial instant of time. From this equation it is seen that such a distribution of the concentration of the water-soluble compound corresponds to the diffusion distribution in a stagnant medium with a shift by $V\tau$.

Likewise, problems with a localized initial distribution in the form of certain profiles or any arbitrary distribution can be solved. In such cases, the analytical solution for the corresponding diffusion problem in a stagnant medium is shifted by $V\tau$ or by $V\tau/\Delta x$ of the zones. In the absence of the analytical solution, one can obtain by the numerical method a fairly exact solution of the diffusion problem in a stagnant medium. Then one can shift it in the spatial coordinates by $V\tau$ or from the very beginning shift the initial distribution of the concentration by the same value and then calculate the concentration distribution for the time τ with account for the diffusion transport.

In the literature sources, classical solutions of diffusion-type problems on the basis of which standard solutions of convective-diffusion transport problems can be constructed are known [3]. At a strongly localized initial distribution of the water-soluble compound, when the localization coordinate, the total quantity of the substance M_0 per unit area in the plane $x = x_0$, and the linear velocity of the filtration flow V are known, a solution of the form

$$C(x, \tau) = \frac{M_0}{2(\pi D\tau)^{0.5}\rho_{\tilde{a}}} \exp\left[-\frac{(x - V\tau - x_0)^2}{4D\tau}\right] \tag{4}$$

can be used.

If the initial distribution of the concentration of the water-soluble compound is given by the function $C_0(x)$, then the solution of this problem in the general form

$$C(x, \tau) = \frac{1}{\sqrt{4\pi D\tau}} \int_{-\infty}^{+\infty} C_0(\eta) \exp\left[-\frac{(x - V\tau - \eta)^2}{4D\tau}\right] d\eta \tag{5}$$

is known.

In a particular case, at a uniform initial distribution of the concentration C_0 of the water-soluble compound in a layer bound by coordinates x_1 and x_2, i.e., in the form of a rectangle, let us give the standard solution in a moving medium as

$$C(x, \tau) = \frac{1}{2} C_0 \left[\operatorname{erf}\left(\frac{x - V\tau - x_1}{2\sqrt{D\tau}}\right) + \operatorname{erf}\left(\frac{-(x - V\tau - x_2)}{2\sqrt{D\tau}}\right)\right] . \tag{6}$$

To estimate the known and new computational schemes, we have developed an applied program that makes it possible to perform computing experiments by varying the initial concentration profiles, the input parameters of convective diffusion problems, and the parameters of the computational schemes. The developed interface permits entering such parameters as the filtration-flow velocity, the diffusion coefficient, the coordinate step, the time-integration step, the finite computing time, the region number, the initial distribution profiles, and the standard solution parameters. The output parameters are represented by graphic and tabular information on the distribution of the standard and calculated concentrations by which the error of the tested computational scheme is estimated. Norms are determined in accordance with the formulas

$$||C||_{\max} = \max |C_{ci} - C_{sti}| \ , \quad 0 \le i \le N \ ; \tag{7}$$

$$||C||_{s} = \Delta x \sum_{i=0}^{N} |C_{ci} - C_{sti}| \ . \tag{8}$$

These norms comply with the basic norms used in comparing various computational schemes in [4–6]. Moreover, to check the conservativeness of computational schemes, the concentration balance throughout the calculation region was calculated:

$$M_t = \Delta x \rho_g \sum_{i=0}^{N} C_{ci} \ . \tag{9}$$

Computational Schemes. The convective term in the convective diffusion equation can be approximated by either the central-difference scheme or schemes with one-sided differences. However, the central-difference scheme, independent of the time step in fulfilling the condition $V\Delta x < D$, is absolutely unstable. To avoid instability at a relatively small diffusion coefficient, it is necessary to resort to a strong fining of the mesh, which markedly increases the computing time. What is more, the computational schemes based on central differences can in no way be used in the absence of diffusion transport. The scheme with "forward" differences is absolutely unstable. Therefore, for approximation one usually uses the "backward" difference.

There exist combined computational schemes [7] using one-sided differences for approximating the derivative $\partial C/\partial x$ and calculating the change in the concentration $\Delta C_i(V)$ by the formula

$$\Delta C_i (V) = \begin{cases} \dfrac{C_{i-1} - C_i}{\Delta x} V\Delta\tau \ , & V \ge 0 \ , \\ \dfrac{C_i - C_{i+1}}{\Delta x} V\Delta\tau \ , & V < 0 \ . \end{cases} \tag{10}$$

Testing of the backward-difference scheme has shown that in approximating numerical dispersion D_f arises, which, depending on the linear velocity of the filtration flow and the coordinate and time integration steps is determined by the following relation:

$$D_f = 0.5V (\Delta x - \Delta\tau V) \ , \tag{11}$$

i.e., the calculated diffusion coefficient will be larger than the real one by the D_f value. From relation (11) it follows that at a time integration step $\Delta\tau$ corresponding to the time in which the filtration covers the distance Δx, the numerical dispersion will be equal to zero. However, it is not always possible to realize such a condition, since the filtration-flow velocity may depend on the coordinate and time and the integration step may be determined by other conditions.

To avoid numerical dispersion in using one-sided differences approximating the concentration gradient of water-soluble compounds, it is suggested to introduce into the computational scheme buffer-exchange parameters that make it possible to introduce for a certain period of time a delay of the change in the concentration caused by the convective change in the concentration at the elementary volume boundary. This is realized as follows. From the side of feeding the convective flow to the node i, a buffer zone, for which the change in the concentration ΔC_{bi} is calculated, is introduced into the convective transport equation. The convective component of the concentration change in the node i with account for the concentration in the buffer zones is calculated analogously to the computational schemes with the use of one-sided differences (10):

$$\Delta C_{\mathrm{b}i} = \begin{cases} \dfrac{(C_{i-1} - C_{\mathrm{b}i-1}) - (C_i - C_{\mathrm{b}i})}{\Delta x} \Delta x_{\mathrm{b}i} \,, & V > 0 \,, \\ \dfrac{(C_i - C_{\mathrm{b}i}) - (C_{i+1} - C_{\mathrm{b}i+1})}{\Delta x} \Delta x_{\mathrm{b}i} \,, & V < 0 \,, \\ 0 \,, \quad V = 0 \,, \end{cases} \tag{12}$$

where $\Delta x_{\mathrm{b}i} = V\Delta\tau$. As the concentration in a buffer zone undergoes an increment, the concentration due to the convective transport in the corresponding node remains unaltered. Simultaneously with a change in the concentration in the buffer zone its width changes as

$$\Delta x_{\mathrm{b}i} = x_{\mathrm{b}i} + \Delta x_{\mathrm{b}i} \,. \tag{13}$$

When the parameter $x_{\mathrm{b}i}$ reaches the Δx value, the values of $C_{\mathrm{b}i}$ and $x_{\mathrm{b}i}$ are equated to zero. Thus, the procedure of concentration-change transfer from the buffer zone to the corresponding node is repeated with a period equal to the time in which the filtration flow covers the distance Δx between adjacent nodes.

The concentration change in the node i is calculated with account for the concentration change in the corresponding buffer zone for the convective component, as well as with account for the diffusion transfer according to the classical explicit scheme:

$$\Delta C_i = \Delta C_{\mathrm{b}i} + D\left(C_{i-1} - 2C_i + C_{i+1}\right)\frac{\Delta\tau}{\Delta x^2} \,. \tag{14}$$

The legitimacy of such an approach has been checked by test calculations using standard solutions. In so doing, the filtration flow velocity, the time step, the diffusion coefficient, and the initial distribution of the concentration were varied. The test data have shown a highly satisfactory agreement between the results obtained with the use of the computational scheme with a buffer zone and those obtained by standard solutions; the discrepancy between the data did not exceed 1% of the range of change in the concentration of the water-soluble compound in the computational domain.

It should be noted that the buffer-exchange computational scheme has disadvantages. The chief disadvantages are its limited applications at a sharply changing velocity of the filtration flow and in taking into account the kinetics of exchange of water-soluble compounds between the pore solution and the solid phase of soils. The computational scheme with a one-sided backward difference and buffer exchange can be used in the range of its applicability as a standard computational scheme for testing other schemes.

Analysis of the literature sources on the topic of the investigation shows that today the search for optimal computational schemes for the convective-diffusion equation is urgent. Worthy of notice along these lines are the works of researchers from the M. V. Keldysh Institute of Mathematics, Russian Academy of Sciences, [4–6], in which they have analyzed and tested more than 20 computational schemes for convective transport. In so doing, they considered the equations of pure convective transport in the absence of diffusion. The results of these investigations show that despite the wide variety of computational schemes for the convective transport equation, it is impossible to choose from them such a scheme that would be universal for any initial distributions of concentrations.

In view of the necessity of improving the computational schemes for the convective diffusion equation, we have developed a new scheme based on estimation of the values of concentrations at the right and left boundaries of the elementary cell corresponding to the mesh node of the computational domain. The main idea of the computing algorithm is the choice of concentration values of the water-soluble compound determining the inward and outward flows at the boundaries between nodes. The choice of the concentration at the boundary between nodes $i - 1$ and i at a positive velocity of the filtration flow V and a monotonic decrease in the concentration with increasing node number is determined by the comparison condition

$$C_{1i} = \begin{cases} C_{i-1} \,, \quad C_{i-2} - C_{i-1} - k\,[C_{i-3} - 2C_{i-2} + C_{i-1}] \le C_i - C_{i+1} + k\,[C_i - 2C_{i+1} + C_{i+2}] \,, \\ 0.995C_i + 0.005C_{i-1} \,, \quad C_{i-2} - C_{i-1} - k\,[C_{i-3} - 2C_{i-2} + C_{i-1}] > C_i - C_{i+1} + k\,[C_i - 2C_{i+1} + C_{i+2}] \,. \end{cases} \tag{15}$$

Likewise, the choice of the concentration at the boundary between nodes i and $i + 1$ is determined:

$$C_{2i} = \begin{cases} C_i\,, & C_{i-1} - C_i - k\,[C_{i-2} - 2C_{i-1} + C_i] \le C_{i+1} - C_{i+2} + k\,[C_{i+1} - 2C_{i+2} + C_{i+3}]\,, \\ 0.995C_{i+1} + 0.005C_i\,, & C_{i-1} - C_i - k\,[C_{i-2} - 2C_{i-1} + C_i] > C_{i+1} - C_{i+2} + k\,[C_{i+1} - 2C_{i+2} + C_{i+3}]\,. \end{cases} \tag{16}$$

The concentration change in the node i at a time step $\Delta\tau$ is calculated by the formula

$$\Delta C_i = \left(C_{1i}V - C_{2i}V\right) \frac{\Delta\tau}{\Delta x}\,. \tag{17}$$

At a monotonic increase in the concentration of the water-soluble compound with increasing node number in the comparison operators (15) and (16) the sign changes from "≤" to "≥." The value of the parameter k taking into account the degree of nonlinearity of the concentration change versus the coordinate, depending on the ratio between the diffusion and convective components $D/V\Delta x$, is determined on the basis of the empirical formula

$$k = 0.5\left[1 - \exp\left(-150\frac{D}{V\Delta x}\right)\right] + 0.001\,. \tag{18}$$

According to the above empirical relation, k varies from 0.001 in the absence of diffusion transfer to 0.5 at a value of the diffusion coefficient comparable to the convective transport value.

At a negative velocity of the filtration flow in expressions (15), (16) the direction of the sequence of indices, i.e., from $i+2$ to $i-3$, changes.

At a nonmonotonic change in the concentration in the range of indices from $i-2$ to $i+2$, for the values of C_{1i} and C_{2i}, the values of concentrations corresponding to the backward difference are taken, i.e., for the positive velocity $C_{1i} = C_{i-1}$, $C_{2i} = C_i$.

The complete change in the water-soluble compound concentration with account for the diffusion transfer in a time step is calculated by adding to the convective component calculated by formula (17) the diffusion component determined by the explicit computational scheme

$$\Delta C_i = \left(C_{1i}V - C_{2i}V\right)\frac{\Delta\tau}{\Delta x} + D\left[C_{i-1} - 2C_i + C_{i+1}\right]\frac{\Delta\tau}{\Delta x^2}\,. \tag{19}$$

The computational scheme also permits taking into account by the additive method other changes in the concentration of water-soluble compounds, e.g., the chemical reactions or the sorption exchange with the solid phase of soils.

Testing and Analysis of the Computational Scheme. In refining the computational scheme, we took into account the features of the numerical approximation of the convective transport processes at various initial concentration profiles. The initial profiles represented localized distributions of the concentration in a region with a width of 40 mesh widths by which the computational domain was split. For the initial profiles, we chose distributions in the forms of a step bounded by horizontal and vertical lines (profile No. 1), a left triangle (profile No. 2), a right triangle (profile No. 3), in the form of the letter "M" (profile No. 4), and a sinusoidal distribution (profile No. 5). Such methods of specifying the initial profiles, according to the terminology used in [4–6], are called the finite initial conditions. Besides the varieties of initial profiles in the calculations, the diffusion coefficient was varied from 0 to a value equal to $10V\Delta x$. At the initial stage of refining the computational scheme for each variety of the initial profile and D, we estimated the computational error by norms corresponding to Eqs. (7) and (8) and made the necessary correction in the computational scheme. Primary consideration was given to the elimination of the scattering of the spatial initial concentration profile in the absence of diffusion on rectangular profiles. Then, when we managed to eliminate the above scattering, we focused on the elimination of the steps on the triangle hypotenuses. Next we took into account the cutting of acute angles in the vertices of triangles and the cutting of the diffusion region in the rectangular profiles at a relatively small diffusion coefficient. Taking into account the foregoing, we refined the computational scheme and obtained the empirical formula (18) for calculating the nonlinearity coefficient k. In so doing, we proceeded from the fact that the computational scheme should yield satisfactory results suitable for practical calculations at various initial profiles and relations between the convective-diffusion transport parameters.

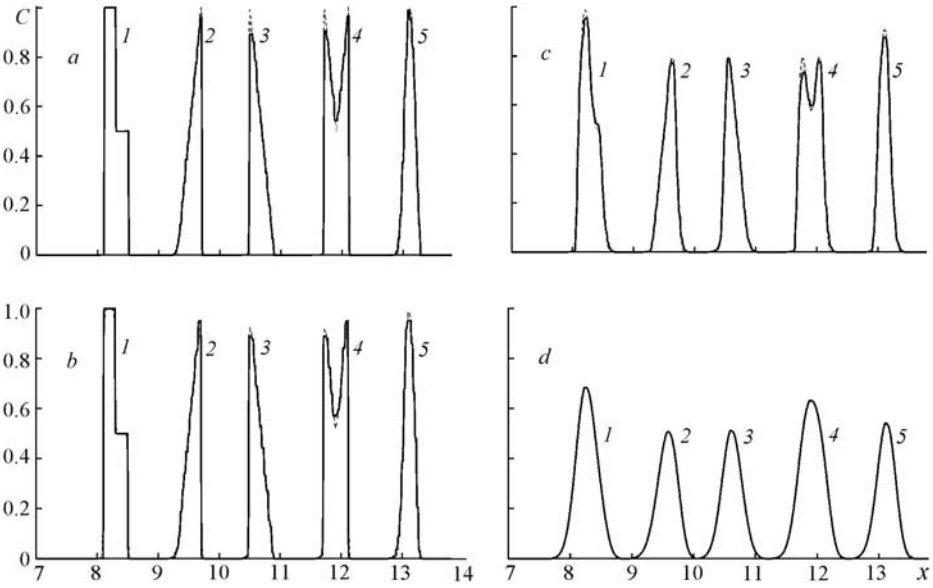

Fig. 1. Change in the concentration profiles in convective-diffusion transport ($V = 10^{-5}$ m/s, $\Delta\tau = 10$ s, $\tau = 800{,}000$ s, $\Delta x = 0.01$ m) at various diffusion coefficients (dotted line — control, solid line — calculation): a) $D = 0$; b) 10^{-10}; c) 10^{-9}; d) 10^{-8}m^2/s.

Upon refining the computational scheme we performed a set of computing experiments at various initial profiles and relations between the convective-diffusion transport parameters. For the input data, we chose parameters corresponding in order of magnitude to the transport of water-soluble compounds in soils and grounds, namely: the filtration-flow velocity $V = 10^{-5}$ m/s, $D = 0$, 10^{-10}, 10^{-9}, 10^{-8} m^2/s, the width of the initial concentration profile of the water-soluble compound equal to 0.4 m, the displacement of the initial concentration region equal to 8 m, or 20 initial profiles. The coordinate grid step was 0.01 m, and the time step was 10 s. It should be noted that the proposed computational scheme yields satisfactory results at a time step corresponding to a value of the Courant number ($\gamma = V\Delta\tau/\Delta x$) of the order of 0.01.

The obtained results of the computing experiment are presented in Fig. 1, showing the calculated and control distributions of the concentration for various profiles corresponding to the above profiles and the sequence of their numbering. The results obtained on the basis of the computational scheme with a one-sided backward difference and buffer exchange were used as control distributions.

Analysis of the results presented shows that on the whole the proposed computational scheme provides results satisfactory for practical purposes with various forms of the initial concentration profile and relations between the convective-diffusion transport parameters. It can be noted that the greatest deviations from control data arise primarily on the vertices of triangles, i.e., blunting of the vertices to a width of 3–4 mesh widths occurs. At a relatively small value of the diffusion coefficient of the order of 0.001 of $V\Delta x$, also a cutting of the diffusion region in the rectangular portions of the concentration distribution occurs. The above errors cause no appreciable distortion of the calculated configuration of the distribution of water-soluble compounds. One should focus attention on Fig. 1d, where the diffusion coefficient was $0.1V\Delta x$. In such events, the initial concentration profile after a certain time interval produces no appreciable effect on the current distribution profile. At the same time, it is seen that the total amount of the water-soluble compound in the initial profile determines the concentration-change amplitude. In this case, the concentration distribution in the first approximation will be described by solution (4). Calculations have shown that the proposed scheme can also work at relatively small parameters of convective transport when diffusion dominates.

Conclusions. Computational schemes for the one-dimensional equation of convective-diffusion transport of water-soluble compounds have been developed. It has been shown that the computational scheme with a backward difference and buffer exchange can be used in the range of its applicability as a standard scheme for testing other computational schemes. The computational scheme based on estimation of the values of the concentrations at the right and left boundaries of the elementary cell provides results satisfactory for practical purposes for various forms of the initial concentration profile and relations between the convective-diffusion transport parameters. The given scheme can be recommended for calculating the propagation of water-soluble pollutants (radionuclides, heavy metals, sodium and potassium chlorides) in layers of soils and grounds.

NOTATION

C_{in}, concentration of the solution input into the medium, kg/kg; C_0, initial solution concentration in the medium, kg/kg; C, concentration of the water-soluble compound, kg/kg; C_i, concentration of the water-soluble compound in node i, kg/kg; ΔC_i, concentration change in node i, kg/kg; $\|C\|_{\max}$, maximal deviation, kg/kg; $\|C\|_{\text{s}}$, area of discrepancy between the calculated and standard concentration profiles, kg·m/kg; $C_{\text{b}i}$, concentration of the water-soluble compound in the buffer area i, kg/kg; $\Delta C_{\text{b}i}$, change in the concentration of the water-soluble compound in the buffer area i, kg/kg; $C_{\text{c}i}$, calculated concentration at point i, kg/kg; $C_{\text{st}i}$, standard concentration at point i, kg/kg; C_{1i}, concentration of the water-soluble compound at the boundary between nodes $i-1$ and i, kg/kg; C_{2i}, concentration of the water-soluble compound at the boundary between nodes i and $i+1$, kg/kg; D, diffusion coefficient of the water-soluble compound, m^2/s; D_{f}, numerical dispersion, m^2/s; k, parameter taking into account the degree of nonlinearity of the concentration change from the coordinate; M_0, mass of the water-soluble compound per unit area of the soil layer, kg/m^2; M_{t}, mass of the water-soluble compound throughout the calculation area of the solid layer, kg/m^2; N, number of mesh nodes on the x coordinate; V, linear velocity of the filtration flow, m/s; x, coordinate, m; $x_{\text{b}i}$, width of the buffer area, m; $\Delta x_{\text{b}i}$, change in the width of the buffer area, m; Δx, mesh width on the x coordinate, m; γ, Courant number; η, coordinate integration variable; ξ_{d}, size of the diffusion perturbation zone, m; ρ_{g}, ground density, kg/m^3; $\Delta\tau$, time step, s. Subscripts: in, input; i, calculation node number; 0, initial; 1, boundary between nodes $i-1$ and i; 2, boundary between nodes i and $i+1$; s, area; b, buffer; d, diffusion; f, fictitious; max, maximum; c, calculated. st, standard; g, ground; t, total.

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