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PROBLEMS ARISING IN APPLICATIONS OF COUNTERFLOW DIFFERENCE SCHEMES IN ENGINEERING CALCULATIONS OF CONTAMINATION OF SHALLOW RESERVOIRS

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Results of a numerical investigation of the stability and errors in the solution obtained with the use of counterflow difference schemes applied to modeling of transfer of suspended substances and solutes in a movable aqueous medium are discussed. Recommendations regarding the proper choice of schemes in engineering calculations are presented.

The development of a mathematical model of the ecosystem of natural reservoirs includes the problem of development of the model of the transfer of suspended substances and solutes in a movable aqueous medium. The hydrodynamics of deep lakes has been investigated in detail by Filatov [1, 2]. A one-dimensional model of the diffusion process considered over the reservoir's depth has been presented by Kolodochka [3]. Of special interest is the study of the ecosystem of shallow reservoirs such as, e.g., the Azov sea [4, 5], the Balkhash lake, and fish breeding ponds. Linear dimensions of these reservoirs substantially exceed their depth, and therefore the "shallow water" equations [6] are applicable to the description of hydrological processes taking place in reservoirs of this type.

The so-called counterflow difference scheme, which is easy-to-implement, is portable, and is highly stable in calculations [7], is the most widespread among engineers solving problems of this type.

At the same time, the problem of the conservative character of the scheme [8] and its sensitivity to the value of the substance decay coefficient in applications of the scheme to closed reservoirs is of extreme importance. This is connected with the use of the boundary condition of the second kind in the calculation of contamination in closed reservoirs, which leads, at the zero decay coefficient, to the spatial degeneracy of the difference operator [9] and emergence of a system of equations not having a unique solution. Bochev [10] has shown how to avoid this difficulty.

The objective of the present work was to present recommendations for engineers on the use of different variants of the approximation of convective terms proposed in [5] for evaluation of their impact on the conservative character of the scheme, and to investigate the effect of the degree of inexplicitness on the stability (i.e., either only diagonal elements or the entire Laplace operator are considered for the $(n+1)$th layer).

We considered the reservoir described by the region Ω (the water region of the reservoir) and the depth array $H(x, y)$, $x, y \in \Omega$, where flows are excited only by the wind and the horizontal dimensions of the reservoir are assumed to exceed substantially the vertical ones (the "shallow water" model).

The concentration equation

$$u\frac{\partial s}{\partial x} + v\frac{\partial s}{\partial y} = K\left(\frac{\partial^2 s}{\partial x^2} + \frac{\partial^2 s}{\partial y^2}\right) - \mu s + f(x, y, t) \tag{1}$$

has been considered in the region Ω with boundary conditions on the boundary $\partial\Omega$

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TABLE 1. Relative Errors (%) for Schemes I-IV

μ	Initial value, s = const	Relative error, %			
		I	II	III	IV
0.1	0.0	431	431	0.30	0.28
	0.5	170	170	0.30	0.28
	1.0	89.7	89.7	0.30	0.29
0.01	0.0	431	431	0.9	0.4
	0.5	170	170	0.5	0.3
	1.0	89.7	89.7	0.5	0.3
0.001	0.0	431	431	9.1	3.4
	0.5	170	170	3.7	2.0
	1.0	89.7	89.7	3.7	2.0
0.0001	0.0	431	431	89.7	33.8
	0.5	170	170	36.7	20.1
	1.0	89.7	89.7	36.7	20.1

TABLE 2. Number of Iterations n and Residual Weight δ of Substances for Schemes I-IV

K	Time step, τ	I		II		III		IV	
		δ	n	δ	n	δ	n	δ	n
100	1000	99.1	438	100	451	99.1	338	100	348
	10,000	99.1	115	100	118	98.8	36	100	37
	50,000	99.1	59	100	60	97.5	9	100	9
10	1000	91.0	1710	100	2062	91.0	1663	100	2007
	10,000	91.0	211	100	253	90.7	167	100	202
	50,000	91.0	69	100	82	89.5	34	100	41
1	1000	55.1	5026	100	8400	55.1	5014	100	8382
	10,000	55.1	515	100	861	55.0	503	100	842
	50,000	55.1	113	100	190	54.8	102	100	172
0.1	1000	23.2	9778	100	18,743	23.2	9776	100	18,738
	10,000	23.2	979	100	1878	23.5	977	100	1874
	50,000	23.2	197	100	379	23.1	195	100	375

TABLE 3. Computation Time T and Number of Steps n Required for Convergence of the Solution for Schemes I-IV

K	I		II		III		IV	
	n	T	n	T	n	T	n	T
1	5026	77.0	8400	178.0	5014	225.8	8382	388.1
10	1710	25.0	2062	43.0	1663	75.6	2007	93.2
100	438	6.7	451	9.4	338	15.2	348	16.1

$$\frac{\partial s}{\partial n} = \frac{1}{K}(\bar{n}, \bar{q}) \cdot s\,, \tag{2}$$

where s is the concentration of the substance, $\bar{q} = \{u, v\}$ is the velocity vector, K is the diffusion coefficient, μ is the substance decay coefficient, $\bar{n}$ is the external normal to the surface, and $f(x, y, t)$ is the function describing the source within the region.

Let us construct a rectangular grid G with steps h_1 and h_2 along the Ox and Oy axes, respectively, within the region Ω. We consider the following approximation of Eq. (1) on the grid G in the node (i, y):

$$L_p^1{}^n s_{i,j} + L_p^2{}^n s_{i,j} = K\left(\frac{s_{i+1,j}^{n+\alpha} - 2s_{i,j}^{n+1} + s_{i-1,j}^{n+\alpha}}{h_1^2} + \frac{s_{i,j+1}^{n+\alpha} - 2s_{i,j}^{n+1} + s_{i,j-1}^{n+\alpha}}{h_2^2}\right) - \mu s_{i,j}^{n+1} + f_{i,j}^n\,,\quad p = 1, 2\,, \tag{3}$$

where $L_p^{1,2}{}^n s_{i,j}$ is the approximation of convection terms by counterflow differences [7] along x and y, respectively, having the following form:

$$L_1^1{}^n s_{i,j}\, s_{i,j} = \begin{cases} u_{i,j}\dfrac{s_{i,j} - s_{i-1,j}}{h_1}\,, & u_{i,j} \geq 0\,, \\ u_{i,j}\dfrac{s_{i+1,j} - s_{i,j}}{h_1}\,, & u_{i,j} < 0\,; \end{cases} \tag{4}$$

$$L_2^1 s_{i,j} = \frac{U_R S_R - U_L S_L}{h_1}\,,\quad U_R = u_{i+1,j}\,,\quad U_L = u_{i,j}\,;$$

$$S_R = \begin{cases} s_{i,j}\,, & U_L \geq 0\,, \\ s_{i+1,j}\,, & U_L < 0\,, \end{cases} \quad S_L = \begin{cases} s_{i-1,j}\,, & U_R \geq 0\,, \\ s_{i,j}\,, & U_R < 0\,. \end{cases} \tag{5}$$

A similar approximation is used for L_p^2; n denotes the iteration number.

The boundary condition (2) was approximated in the following manner:

$$S|_{\partial\Omega} = S_B\left(1 + \frac{h_1}{K}(u \cdot \cos(\bar{n}, \bar{x}) + v \cdot \sin(\bar{n}, \bar{x}))\right)\,, \tag{6}$$

where $S|_{\partial\Omega}$ is the concentration on the boundary, S_B is the concentration in an internal point of the grid G situated at the smallest distance from the boundary, and x is the positively directed unit vector of the Ox axis.

In what follows, we consider four variants of the scheme (3): (I) $p = 1$, $\alpha = 0$, (II) $p = 2$, $\alpha = 0$, (III) $p = 1$, $\alpha = 1$, and (IV) $p = 2$, $\alpha = 1$.

In schemes I and II, only diagonal elements are considered on the $(n+1)$th layer, whereas in schemes III and IV the entire Laplace operator is taken into consideration. The term characterizing decay of the substance is taken from the $(n+1)$th layer. In this case, a standard subroutine from the LINPACK mathematical package is used for the inversion of the symmetrical positive-definite matrix. The problem under consideration was solved by the settlement method.

The problem of propagation of a substance within a closed square $[0, 1] \times [0, 1]$ with constant depth and known stationary circulatory flow with changing velocity signs was used as a model problem. The step along the spatial coordinates was $h_1 = h_2 = 0.125$; the reservoir's depth was $h = 0.5$. Since the region of calculations is closed, the boundary condition (2) takes the form

$$\frac{\partial s}{\partial n} = 0\,, \tag{7}$$

i.e., it becomes a Neumann-type condition and assumes the absence of transfer of the substance through the boundary.

At the first stage of the investigation, we compared the accuracy of numerical and analytical solutions. The latter was given by the function

$$s(x, y) = \frac{x^2 + y^2}{2} - \frac{x^3 + y^3}{3}, \tag{8}$$

satisfying the boundary condition (7). Then (8) was substituted into (1) and values of $f(x, y)$ were calculated in each point of the grid, which was followed by the solution of Eq. (3), and the relative error was evaluated for different starting data of the iteration method (s = const) and different values of μ. Results of this test are presented in Table 1.

At the same time, it should be noted that all schemes yielded the exact solution when being tested with problem (1) with boundary conditions of the first kind.

The second test checked the conservative character of schemes and their stability with respect to the value of the diffusion coefficient, and was used for evaluation of the number of iterations necessary to achieve the given accuracy ε. The solution was considered as converged if the condition

$$\| s \|_C = \max_{i,j} |s_{i,j}^{n+1} - s_{i,j}^{n}| < \varepsilon\tau .$$

was satisfied on the space C of continuous functions. The conservative character was checked against the residual substance weight δ over the entire region Ω. At the initial instant, 100 weight units of the substance were introduced into the region.

A δ-function localized in the center of the region was taken as the initial condition. Results of the test are presented in Table 2.

Table 3 presents the computation time T (sec) and the number of steps n required to obtain the converged solution obtained on an IBM AT 486DX2-66 personal computer for different values of k at $\tau = 1000$, $\mu = 0$, and $\varepsilon = 10^{-7}$.

The computations make it possible to draw the following conclusions:

1. When approximating correction terms, one should use formulas (5) preserving the conservative character of the problem (schemes II and IV).

2. In the case of calculation of contamination with conservative or almost conservative substances ($\mu < 0.01$), one should employ the special method of computation proposed in [10] and scheme IV.

3. When diffusion coefficients are of the order of $O(1)$ or smaller, it is more advisable to use scheme IV, which makes it possible to perform stable computations with a larger time step.

4. Despite the fact that scheme IV requires a longer computation time and is more involved in implementation, results of its applications make us recommend this scheme for use in applications.

5. The following method of choosing the finite-difference scheme for engineering computations of the contamination spread in shallow reservoirs can be recommended: if boundary conditions of the first kind are set up on the boundary of the region or a portion of it, the use of the scheme II is advisable; if the condition of the second kind is set up on the entire boundary of the region, scheme IV should be used.

It should be noted that completely explicit schemes where all values of s_{ij} in (3) are taken from the nth layer are almost unconditionally unstable, since computations can be carried out only if $\tau/h < 2 \cdot 10^{-4}$.

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