NUMERICAL METHOD OF SOLVING A CERTAIN PROBLEM ON CONVECTIVE DIFFUSION IN A MOVING LIQUID

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A numerical method of solving a system of two second-order parabolic partial differential equations describing the diffusion of matter in a moving liquid is described.

1. Formulation of the Problem

We consider the following problem on convective diffusion in a moving liquid medium: the concentration of conservative impurities (ions of Na, Cl, and so on) equals zero at the initial moment of time $t = t_0$ along a segment of length l of a channel along which a liquid is flowing from left to right; on the left boundary of the segment there is a certain source of contamination which introduces into the moving liquid impurities of concentration S₁. Given sources of contamination, each with its own mode of operation, are prescribed along the entire length of the segment. We assume that on the right boundary of the segment the impurity concentration reaches the value S₂. It is required to determine the impurity content at time t along the entire length of the segment. This problem is described by a system of equations consisting of the St. Venant equations and equations of convective-diffusion type:

$$\frac{\partial w}{\partial t} + \frac{\partial Q}{\partial x} = p(x, t), \tag{1.1}$$

$$\frac{\partial (wv)}{\partial t} + \frac{\partial (Qv)}{\partial x} = -gw\left(\frac{\partial y}{\partial x} + \frac{v[v]}{c^2 R}\right), \qquad (1.2)$$

$$\frac{\partial (S\omega)}{\partial t} + \frac{\partial (SQ)}{\partial x} = \frac{\partial}{\partial x} \left(E\omega \frac{\partial S}{\partial x} \right) + f(x, t)$$
(1.3)

together with the conditions

$$S_{x=0} = S_1(t), \ y_{x=0} = y_1(t),$$
 (1.4)

$$S|_{x=l} = S_2(t), \ y|_{x=l} = y_2(t),$$
 (1.5)

$$S_{t=0} = S_0(x), \ y_{t=0} = y_0(x).$$
 (1.6)

We note that problems of this sort are encountered in the study of the motion of conservative impurities in river systems. Thus, the system of equations (1.1)-(1.3) forms an essential part of the mathematical model of water quality developed by Vasil'ev [1]. In order to describe the processes occurring in the water medium due to the dumping into it of industrial and domestic effluents, this model utilizes the St. Venant equations and equations describing the balance of the various impurities, oxygen, and heat. As a result, this model permits determination of the content of the various impurities, oxygen, and heat along the entire length of the river system at any moment of time as a function of the hydrologic conditions of the river system and for any sources of contamination.

In the present paper we investigate the quality of the water in a flow system using the chamber model, a simplification of the model of [1]. Essentially, in the chamber model the river or river system is divided up into individual chambers (parts of the river channel) in which all the characteristics of the flow and of the quality of the water are taken to be constant. The chamber model has been used [2,5-7] to calculate the hydro-logic characteristics of rivers. We shall utilize the chamber model to calculate the motion of impurities in water. Like Vasil'ev's model [1], the chamber model is one-dimensional.

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Fig.1. Propagation of contamination from a single continuously acting source [1) t = 10; 20; 30; 40; 40; 50; 60; 60].

Fig.2. Contamination wave from source operating for a short time [1) t = 10; 2) 20; 3) 30; 4) 50; 5) 70; 6) 80].

We carry out a few manipulations on Eqs. (1.1)-(1.3) contradicting the sense of the problem: expand the differentiation operators on the left side of (1.2) and set the inertial terms $\partial v/\partial t$, $v\partial v/\partial x$ equal to zero (we assume that they are small for the plains-type rivers that we shall be considering). Then, utilizing the continuity equation $\partial w/\partial t + \partial Q/\partial x = p$, we obtain in place of (1.1)-(1.3) a system of equations of the form

$$\frac{\partial w}{\partial t} + \frac{\partial Q}{\partial x} = p(x, t), \tag{1.7}$$

$$Q = -\psi(x, y) \sqrt{\left| \frac{\partial y}{\partial x} \right|} \operatorname{sign} \frac{\partial y}{\partial x} , \qquad (1.8)$$

$$w \frac{\partial S}{\partial t} + Q \frac{\partial S}{\partial x} = \frac{\partial}{\partial x} \left(Ew \operatorname{sign} \frac{\partial y}{\partial x} \cdot \frac{\partial S}{\partial x} \right) + f(x, t)$$
(1.9)

with the same boundary conditions as before. Here $\psi = cwR^{1/2}$, and as in [1] we take the coefficient of longitudinal dispersion E in the form $E = \alpha Rvc^{-1}$, where $\alpha = const$. In the future, instead of the Chézy coefficient c, we shall use the Strickler roughness coefficient k given by $c = kR^{1/6}$.

2. Description of the Numerical Method

We consider the system of equations (1.7)-(1.9) in the region $D = (0 \le x \le l, 0 \le t \le T)$ with given initial and boundary conditions (1.4)-(1.6). Equation (1.1) has been studied by Baklanovskaya and Chechel' [2], who described a numerical method of computing the approximate solution and who showed that the latter converged toward the exact solution when the number of steps in x and in t was allowed to increase without limit. For Eq. (1.1) we shall employ the same scheme as in [2]; for Eq. (1.3) we shall utilize an implicit scheme of the first order of accuracy in x and t, namely: we divide the investigated stretch of river into chambers and number them going downstream. Let h_i be the length of the i-th chamber (i = 1, 2, ..., N) and τ , the step in time, i.e., $t_n = n\tau$. The difference equations corresponding to system (1.7)-(1.9) we write in the form

$$\frac{w_i^{n+1} - w_i^n}{\tau} = \frac{1}{h_i} \left(Q_{ii-1}^{n+1} + Q_{ii+1}^{n+1} \right) + p_i^{n+1} \left(x, t \right), \tag{2.1}$$

$$Q_{ij}^{n+1} = \frac{(\psi_i^{n+1} + \psi_j^{n+1})}{2} \sqrt{\frac{|y_j^{n+1} - y_i^{n+1}|}{h_i}} \operatorname{sign}(y_j - y_i), \qquad (2.2)$$

$$\frac{w_{i}^{n+1} - \frac{(S_{i}^{n+1} - S_{i}^{n})}{\tau} + \gamma Q_{i-1i}^{n+1} - \frac{(S_{i}^{n+1} - S_{i-1}^{n-1})}{h_{i}} + \delta Q_{ii+1}^{n+1} - \frac{(S_{i+1}^{n+1} - S_{i}^{n+1})}{h_{i}}}{h_{i}} - \frac{(\varphi_{i+1}^{n+1} + \varphi_{i-1}^{n+1})}{2} \cdot \frac{(S_{i+1}^{n+1} - S_{i-1}^{n+1})}{h_{i}} + f_{i}^{n+1} (x, t),$$

$$(2.3)$$

where $\gamma = 1$, $\delta = 0$, if sign $\partial y/\partial x = +1$ and $\gamma = 0$, $\delta = 1$, if sign $\partial y/\partial x = 1$; Q_{ij}^n is the amount of water passing

at time t_n from chamber j to chamber i; $\varphi_i^{n+1} = \alpha R_i (n+1)^{5/6} Q_i^{n+1} k_i^{-1}$; $\alpha = 20.2 \cdot 3600 \sqrt{g}$. The boundary conditions are approximated in the following manner:

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Fig. 3. Propagation of contamination from two sources [1) t = 1; 2) 3; 3) 10; 4) 30; 5) 50], t, h; x, km; S, mg/liter.

$$y_{i0} = y_0 (x_{av}), \ S_{i0} = S_0 (x_{av}), \ x_{i-1} \le x_{av} \le x_i,$$
$$y_{1n} = y_1 (t_n), \ S_{1n} = S_1 (t_n),$$
$$y_{Nn} = y_2 (t_n), \ S_{Nn} = S_2 (t_n).$$

We consider a river with a rectangular channel, so that

$$w_i^n = \beta_i (y_i^n - y_{3i}^n), \ R_i^n = w_i^n (\beta_i + 2 [y_i^n - y_{3i}^n])^{-1}$$
.

System (2.1)-(2.3) is solved in the following manner: first, y_i^{n+1} is found from the first equation $(Q_{ij}^{n+1} is determined in the process)$, then the third equation with coefficients taken from the (n+1)-th sheet is solved. We cite the algorithm for calculating S_i^{n+1} , where the expression for Q_{ij}^{n+1} is linearized as in [2]:

$$Q_{ij}^{n+1} = Q_{ij}^{n} + \frac{\partial Q_{ij}}{\partial y_i} \bigg|_{y^n} (y_i^{n+1} - y_i^n) + \frac{\partial Q_{ij}}{\partial y_j} \bigg|_{y^n} (y_j^{n+1} - y_j^n),$$
(2.4)

$$\frac{\partial Q_{ij}}{\partial y_j} = 0.5 \frac{\partial \psi_j}{\partial y_j} \sqrt{\frac{|y_i - y_j|}{h_i}} \operatorname{sign}(y_j - y_i) + \frac{(\psi_i + \psi_j)}{4\sqrt{h_i}\sqrt{|y_j - y_i|}}.$$
(2.5)

Inserting expressions (2.4)-(2.5) into Eq. (1.7) gives an equation for y_i^{n+1} :

$$A_i y_{i+1}^{n+1} - C_i y_i^{n+1} + B_i y_{i-1}^{n+1} = -F_i, (2.6)$$

where the coefficients have the form

$$A_{i} = \tau \frac{\partial Q_{ii+1}}{\partial y_{i+1}} \bigg|_{y^{n}}, \quad B_{i} = \tau \frac{\partial Q_{il-1}}{\partial y_{i-1}} \bigg|_{y^{n}},$$

$$C_{i} = \beta_{i}h_{i} - \tau \bigg(\frac{\partial Q_{ii-1}}{\partial y_{i}} + \frac{\partial Q_{ii+1}}{\partial y_{i}} \bigg) \bigg|_{y^{n}},$$

$$F_{i} = \tau (Q_{ii-1}^{n} + Q_{ii+1}^{n} + p_{i}^{n+1}).$$
(2.7)

After some straightforward manipulations Eq. (2.3) can be brought to a similar equation:

$$A_{i}^{\prime}S_{i+1}^{n+1} - C_{i}^{\prime}S_{i}^{n+1} + B_{i}^{\prime}S_{i-1}^{n+1} = -F_{i}^{\prime},$$
(2.8)

where

$$A_{i}^{\prime} = \frac{\alpha \tau}{h_{i}^{2}} \left[\sqrt{\frac{[y_{i+1}^{n-1} - y_{i}^{n+1}]}{h_{i}}} \cdot \frac{(R_{i+1}^{3/2} \omega_{i+1} + R_{i}^{3/2} \omega_{i})^{n+1}}{2} \right], \qquad (2.9)$$

$$B_{i}^{\prime} = \left[\frac{\alpha \tau}{h_{i}^{2}} \frac{(R_{i-1}^{3/2} \omega_{i-1} + R_{i}^{3/2} \omega_{i})^{n+1}}{2} + \frac{\psi_{i}^{n+1} \tau}{h_{i}} \right] \sqrt{\frac{[y_{i}^{n+1} - y_{i-1}^{n+1}]}{h_{i}}}, \qquad (2.9)$$

$$C_{i}^{\prime} = \omega_{i}^{n+1} + A_{i}^{\prime} + B_{i}^{\prime}, \quad F_{i}^{\prime} = -\omega_{i}^{n+1} S_{i}^{n} - f_{i}^{n+1} \tau.$$

Both equations (2.6) and (2.8) are solved independently by the sweep method with sweep coefficients calculated in the usual manner (see [4], for example). It is shown in [2] that the sweep method for Eq. (2.6) is stable. It follows from the form of (2.9) that the conditions for stability of the sweep $A'_i \ge 0$, $B'_i \ge 0$, $C'_i \ge A'_i + B'_i$ are also satisfied for Eq. (2.8).

3. Solution of Problem by Method Described Above

We consider three types of problem on water quality for the same hydrologic data in each case: width of river constant $\beta_1 = 300$ m; length of river l = 1500 km; variation with x of height of river bed $y_3 = 6 (l-x) l^{-1}$; water level at initial moment of time $y_0 = (y_3 + 3)$ m, water level at left end $y_1 = 9$ m; at the right end water level is also constant $y_2 = 3$ m, although the described method can be used to solve the quality problem when the river is in a state of flood; roughness coefficient k = $120 \cdot 10^3 \text{ m}^{1/3}/\text{h}$. Similar hydrologic data were considered in [3].

<u>Problem 1</u>. At the left boundary (x = 0) of the segment of the river there is a source of contamination releasing continuously into the water an impurity with concentration $S_1 = 100 \text{ mg/liter}$; at the right boundary we assume that the impurity concentration $S|_{x=l} = 0$; at the initial moment of time over the entire stretch of river we have $S|_{t=0} = 0$. There are no more sources of contamination.

<u>Problem 2</u>. A source located at the left boundary introduces contamination up to a time t = 12 h, $S|_{t \le 12} = 100 \text{ mg/liter}$, after which it ceases to operate $S|_{t>12} = 0$; as before, $S|_{x=l} = 0$, $S|_{t=0} = 0$, $f_i(x, t) = 0$.

<u>Problem 3.</u> A source at the left boundary operates continuously: $S|_{X=0} = 100 \text{ mg/liter}$, $S|_{X=l} = 0$, $S|_{t=0} = 0$; at a distance of 60 km there is another source that dumps into the water at time t = 0.1 h impurity of concentration $S|_{X=60} = 80 \text{ mg/liter}$.

For all these problems the computation was carried out with a constant step in the time of $\tau = 0.1$ h and a constant step in distance of h = 600 m. Figure 1 shows the function S(x,t) at various moments of time for Problem 1. It can be seen that the front of the contamination wave propagates as a step with a well-defined shape due to the fact that the diffusion term $\partial(Ew \partial S/\partial x)/\partial x$ is small compared with the term describing hydrodynamic transport $Q \partial S/\partial x$. The effect of diffusion shows up, however, in the smearing out of the front of the contamination wave with time. The continuous release of contaminant of concentration S_1 by a source located at the left boundary results, even after only t = 40 h, in the impurity concentration at a distance of 48 km being equal or approximately equal to that at the point of introduction.

Figure 2 shows the dependence of S(x,t) on distance for various fixed moments of time for Problem 2. Up to a time t = 12 h the graph is the same as for the first problem, but even at t = 20 h the picture has changed greatly: the graph of concentration has a sawtooth shape, and the concentration at the top of the "teeth" does not reach the value S_1 but rapidly decreases with time. The contamination wave eventually completely leaves the investigated zone.

Figure 3 illustrates Problem 3, the propagation of contamination in the case of two sources. The fact that the second source operates only once and is located far from the first (at a distance of 60 km) has the effect that the contaminations from these sources are not superposed on each other; the progress of the contamination from each of the sources can be clearly followed.

NOTATION

S,x,t, impurity concentration, distance along river, and time, respectively; Q,w,v, water flow rate, cross-sectioned area of river, and mean velocity of flow, respectively; y,R, line-of-sight water level and hydraulic radius; c,E, Chézy coefficient and coefficient of longitudinal dispersion; p, f, on-route influx of water per unit length and strength of source of contamination; y_3 , β , ordinate of river bottom and width of river channel; g, acceleration due to gravity.

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