

NUMERICAL SIMULATION OF SURFACE WATER POLLUTION

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We propose a numerical model for admixture transport in rivers based on solutions of equations of the shallow water theory and semi-empirical equation of turbulent diffusion. The results of numerical experiments obtained for a concrete area of Angara river are presented.

In monographs 1 to 3 one may find a review of the mathematical modeling methods for simulating pollution of the hydrosphere.

When studying pollution of the water basins, one may use a semi-empirical equation of the turbulent diffusion. It is important to note that the network of hydrologic observations available now does not provide data sufficient for making accurate determination of the velocity field and turbulent diffusion coefficients.

In this paper hydrologic characteristics are obtained by solving equations of shallow water theory⁴ using a parametrization of the influence of bottom friction and taking into account horizontal turbulent exchange

$$\begin{aligned} \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} &= -g \frac{\partial(h + \delta)}{\partial x} + \\ &+ lv + \frac{\partial}{\partial x} k_x \frac{\partial u}{\partial x} + \frac{\partial}{\partial y} k_y \frac{\partial u}{\partial y} - \frac{ru |\mathbf{v}|}{h}, \\ \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} &= -g \frac{\partial(h + \delta)}{\partial y} - \\ &- lv + \frac{\partial}{\partial x} k_x \frac{\partial v}{\partial x} + \frac{\partial}{\partial y} k_y \frac{\partial v}{\partial y} - \frac{rv |\mathbf{v}|}{h}, \quad (1) \\ \frac{\partial h}{\partial t} + \frac{\partial uh}{\partial x} + \frac{\partial vh}{\partial y} &= 0, \quad |\mathbf{v}| = \sqrt{u^2 + v^2}, \end{aligned}$$

where t is time, u and v are the components of the velocity vector of water motion along the Cartesian axes x and y , g is the acceleration of gravity; h is the basin depth; $l = 2\omega \sin\varphi$ is the Coriolis parameter, ω is the angular velocity of the Earth's rotation, φ is the latitude; k_x and k_y are the coefficients of turbulent exchange along the coordinate axes x and y , respectively; $\delta(x, y)$ is the function describing the bottom relief; r is the coefficient of bottom friction.

The system of partial differential equations (1) is solved under the following initial conditions:

$$\begin{aligned} u(x, y, 0) &= u^0(x, y), \quad v(x, y, 0) = v^0(x, y), \\ h(x, y, 0) &= h^0(x, y). \end{aligned}$$

The contour of the integration domain consists of a solid part and open boundaries. The condition of sticking is set on the solid part of the contour. The values of unknown functions or their derivatives (depending on the direction of the flow velocity) are set on the open boundaries.

According to the solution method proposed, using the equation of discontinuity, let us transform the system of equations (1) to the following form:

$$\begin{aligned} \frac{\partial U}{\partial t} + \frac{1}{2} u \frac{\partial U}{\partial x} + \frac{1}{2} \frac{\partial u U}{\partial x} + \frac{1}{2} v \frac{\partial U}{\partial y} + \frac{1}{2} \frac{\partial v U}{\partial y} &= \\ = -gH \frac{\partial(h + \delta)}{\partial x} + lV + \frac{\partial}{\partial x} k_x \frac{\partial U}{\partial x} + \frac{\partial}{\partial y} k_y \frac{\partial U}{\partial y} - \frac{rU |\mathbf{v}|}{h}, \\ \frac{\partial V}{\partial t} + \frac{1}{2} u \frac{\partial V}{\partial x} + \frac{1}{2} \frac{\partial u V}{\partial x} + \frac{1}{2} v \frac{\partial V}{\partial y} + \frac{1}{2} \frac{\partial v V}{\partial y} &= \\ = -gH \frac{\partial(h + \delta)}{\partial y} - lU + \frac{\partial}{\partial x} k_x \frac{\partial V}{\partial x} + \frac{\partial}{\partial y} k_y \frac{\partial V}{\partial y} - \frac{rV |\mathbf{v}|}{h}, \quad (2) \end{aligned}$$

$$\frac{\partial h}{\partial t} + \frac{\partial HU}{\partial x} + \frac{\partial HV}{\partial y} = 0.$$

Here, the following designations are introduced: $H = \sqrt{h}$, $U = Hu$, $V = Hv$.

The system of equations (2) is integrated numerically in the Cartesian coordinate system by the method of virtual domains⁵ that enables one to take into account an arbitrary relief of a basin's bottom.

To make equations (2) discrete in time, the Krank-Nikolson scheme and two-cycle component splitting method⁵ were used.

Let us construct a grid with the nodal points at

$$x_i = i\Delta x, \quad y_j = j\Delta y, \quad i = \overline{1, I}, \quad j = \overline{1, J}.$$

We also use auxiliary points $x_{i+1/2}$, $y_{j+1/2}$ positioned in the middle points of the basic intervals.

For brevity of the further treatment, let us designate

$$\Psi_{i,j} = \Psi(x_i, y_j, t_n), \quad t_n = n \Delta t \quad (n = 0, 1, \dots);$$

$$\begin{aligned}
 (A_1 \psi)_{i,j} &= \frac{u_{i+1/2,j}^n \psi_{i+1,j} - u_{i-1/2,j}^n \psi_{i-1,j}}{2\Delta x} - \\
 &- \frac{k_{x_{i+1/2,j}}^n (\psi_{i+1,j} - \psi_{i,j})}{\Delta x^2} - \frac{k_{x_{i-1/2,j}}^n (\psi_{i,j} - \psi_{i-1,j})}{\Delta x^2}; \\
 (A_2 \psi)_{i,j} &= \frac{v_{i,j+1/2}^n \psi_{i,j+1} - v_{i,j-1/2}^n \psi_{i,j-1}}{2\Delta y} - \\
 &- \frac{k_{y_{i,j+1/2}}^n (\psi_{i,j+1} - \psi_{i,j})}{\Delta y^2} - \frac{k_{y_{i,j-1/2}}^n (\psi_{i,j} - \psi_{i,j-1})}{\Delta y^2}; \\
 (B_1 h)_{i,j} &= gH_{i,j}^n \frac{h_{i+1,j} + \delta_{i+1,j} - h_{i-1,j} - \delta_{i-1,j}}{2\Delta x}; \\
 (B_2 h)_{i,j} &= gH_{i,j}^n \frac{h_{i,j+1} + \delta_{i,j+1} - h_{i,j-1} - \delta_{i,j-1}}{2\Delta y}; \\
 (D_1 U)_{i,j} &= \frac{H_{i+1,j}^n U_{i+1,j} - H_{i-1,j}^n U_{i-1,j}}{2\Delta x}; \\
 (D_2 V)_{i,j} &= \frac{H_{i,j+1}^n V_{i,j+1} - H_{i,j-1}^n V_{i,j-1}}{2\Delta y}; \\
 (K\psi)_{i,j} &= \frac{1}{2} l_{i,j} \psi_{i,j}; \quad (\varphi\psi)_{i,j} = \frac{1}{2} \frac{r|\mathbf{v}_{i,j}^n| \psi_{i,j}}{h_{i,j}^n},
 \end{aligned}$$

where ψ is one of the functions of the problem considered; Δt is the step in time.

Then, we introduce the matrix operators

$$\begin{aligned}
 M_1 &= \begin{vmatrix} A_1 + \varphi & -K & B_1 \\ K & A_1 + \varphi & 0 \\ D_1 & 0 & 0 \end{vmatrix}, \\
 M_2 &= \begin{vmatrix} A_2 + \varphi & -K & 0 \\ K & A_2 + \varphi & B_2 \\ 0 & D_2 & 0 \end{vmatrix}.
 \end{aligned}$$

As a result, the finite-difference analogs of the system of equations (2) can be written in the form

$$\begin{aligned}
 \left(E + \frac{\Delta t}{2} M_1^n\right) N^{n-1/2} &= \left(E - \frac{\Delta t}{2} M_1^n\right) N^{n-1}; \\
 \left(E + \frac{\Delta t}{2} M_2^n\right) N^n &= \left(E - \frac{\Delta t}{2} M_2^n\right) N^{n-1/2}; \\
 \left(E + \frac{\Delta t}{2} M_2^n\right) N^{n+1/2} &= \left(E - \frac{\Delta t}{2} M_2^n\right) N^n; \\
 \left(E + \frac{\Delta t}{2} M_1^n\right) N^{n+1} &= \left(E - \frac{\Delta t}{2} M_1^n\right) N^{n+1/2};
 \end{aligned}$$

where $N = \begin{vmatrix} U \\ V \\ h \end{vmatrix}$, E is the unit matrix.

The finite-difference scheme used for component splitting has the second-order approximation with respect to Δx and Δy , and the first-order one with respect to Δt . It conserves mass and full energy of the

system.⁶ The system of equations (3) can be solved by the method of matrix factorization.⁷

To simulate admixture transport in a basin, let us consider the equation of transport and diffusion of a passive admixture for the case of shallow waters⁴

$$\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x} + v \frac{\partial C}{\partial y} = \frac{\partial}{\partial x} k_x \frac{\partial C}{\partial x} + \frac{\partial}{\partial y} k_y \frac{\partial C}{\partial y} + F, \quad (3)$$

where $F(x, y, t)$ is the function describing distribution and power of substance sources considered.

Since no detailed observational data are available, we assume C to be the background distribution. The conditions of the second kind are set at the boundaries. We assume that admixture flows through solid basin's boundaries are absent.

Using the equation of discontinuity, let us transform the Eq. (3) to the following form

$$\begin{aligned}
 \frac{\partial S}{\partial t} + \frac{1}{2} u \frac{\partial S}{\partial x} + \frac{1}{2} \frac{\partial uS}{\partial x} + \frac{1}{2} v \frac{\partial S}{\partial y} + \frac{1}{2} \frac{\partial vS}{\partial y} = \\
 = \frac{\partial}{\partial x} k_x \frac{\partial S}{\partial x} + \frac{\partial}{\partial y} k_y \frac{\partial S}{\partial y} + f, \quad (4)
 \end{aligned}$$

where $S = CH$, $f = FH$.

Then, the finite-difference analogs of Eq. (4) can be written in the form

$$\begin{aligned}
 \left(E + \frac{\Delta t}{2} A_1^n\right) S^{n-1/2} &= \left(E - \frac{\Delta t}{2} A_1^n\right) S^{n-1}; \\
 \left(E + \frac{\Delta t}{2} A_2^n\right) S^n &= \left(E - \frac{\Delta t}{2} A_2^n\right) S^{n-1/2} + \Delta t f; \\
 \left(E + \frac{\Delta t}{2} A_2^n\right) S^{n+1/2} &= \left(E - \frac{\Delta t}{2} A_2^n\right) S^n + \Delta t f; \\
 \left(E + \frac{\Delta t}{2} A_1^n\right) S^{n+1} &= \left(E - \frac{\Delta t}{2} A_1^n\right) S^{n+1/2}.
 \end{aligned}$$

To solve the finite-difference equations numerically we use nonmonotonic sweep.⁸

Let us now describe the results of numerical simulations of the water pollution dynamics for the case of eventual leakage from a pipeline projected across the Angara river at a distance of 34 to 37 km down river from Irkutsk. In this region, the river turns to the left, and its bed is divided by Ashun island. The river depth was taken from the bathymetric map of the scale 1:5000 with the step of 25 m.

Figure 1 presents the flow velocity field calculated using the hydrodynamic model proposed.

Calculations of the river pollution were performed for different types of the gas pipeline damages. The power of the source was assumed to be 0.1 l/s. The break points are chosen in the section where the gas pipeline is planned for construction. The first point is near the right bank of the river, the second one in the middle, and the third one near its left bank. The calculations were performed for liquid

hydrocarbons (fraction close to gasoline) that may present in gas. The maximum permissible concentration of a condensed gas in water must not exceed 0.05 mg/l.

The first series of calculations characterizes water pollution in 90 s during which time the emergency stopcocks should be closed. Since the velocity of water flow is low, near the right bank, the main pollution spot will be near this bank if the leakage is near the right bank also. The highest concentration of the substance is 10 mg/l. In the case of gas pipeline leakage near the left bank or in the middle of the river, the pollution spot is extended along the stream. The highest substance concentration is 4–5 mg/l because the flow velocities near the break points are higher as compared with that in the first case.

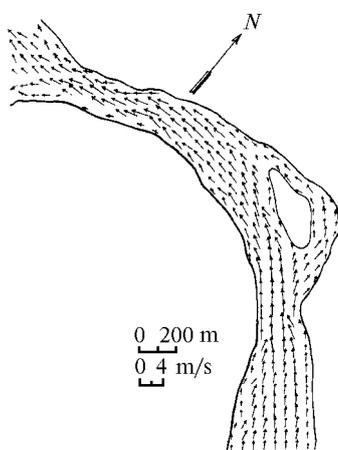


FIG. 1. Surface flows in the area considered .

The next series of calculations has been performed for the same break points but for the case when a stationary point source acts during 30 min (Figs. 2 to 4). The isolines show the pollution distribution in a step of ten maximum permissible concentration levels; the first curve outlines pollution at the level of 1 maximum permissible concentration. In the middle of the river and near its left bank, the admixture propagates faster as compared with that near the right bank.

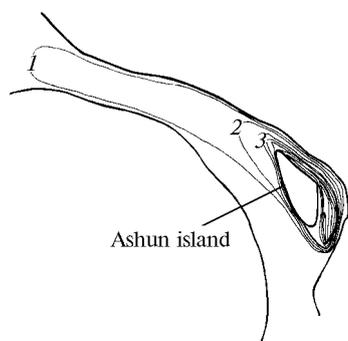


FIG. 2. Water pollution field for the case of gas pipeline break near the right bank.

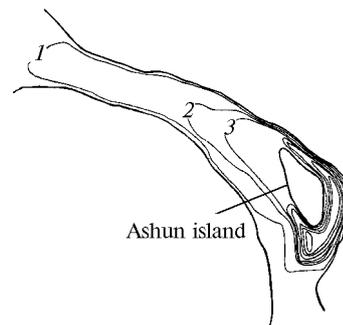


FIG. 3. Water pollution field for the case of gas pipeline break in the middle of the river.

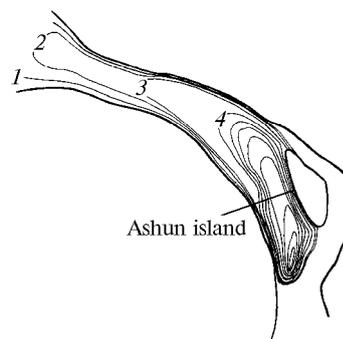


FIG. 4. Water pollution field for the case of gas pipeline break near the left bank.

This is connected with the flow dynamics as the flow velocity is higher in this part of the river. So the admixture can quickly spread down river and threaten the water intake of Angarsk city.

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