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# Software realization problems of mathematical models of pollutants transport in rivers

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ABSTRACT

A software package of realization of mathematical models of pollutants transport in rivers is offered. This package is designed as a up-to-date convenient, reliable tool for specialists of various areas of knowledge such as ecology, hydrology, building, agriculture, biology, ichthyology and so on. It allows us to calculate pollutant concentrations at any point of the river depending on the quantity and the conditions of discharging from several pollution sources. One-, two-, and three-dimensional advection–diffusion mathematical models of river water quality formation both under classical and new, original boundary conditions are realized in the package. New finite-difference schemes of calculation have been developed and the known ones have been improved for these mathematical models. At the same time, a number of important problems which provide practical realization, high accuracy and short time of obtaining the solution by computer have been solved. In particular: (a) the analytical description of plane or spatial region for which the diffusion equations and boundary conditions are investigated, i.e. the analytical description of the bank line and the bottom of the river; (b) the analytical description of dependence of coefficients of the equation on the spatial coordinates; (c) the analytical description of dependence of non-homogeneous parts of the diffusion equation (i.e. the capacities of pollution sources) on the spatial coordinates and on the time; (d) the correct choice of ratios between spatial steps of the grid, and also between them and the step of digitations of time in the difference scheme.



## 1. Introduction

For solving the problems of analysis and control of the environment quality, it is necessary to process operatively big arrays of measurement information about the parameters characterizing its physical, chemical and biological aspects. This is possible to do at a suitable level in accordance with up-to-date requirements only by means of wide application of mathematical methods and computers. For this purpose, it is necessary to create the automated systems and universal advanced software packages, in which self-learning algorithms requiring minimal a priori information and having a capability of adaptation to the most unexpected changes in the investigated object are realized [1].

Among the most topical problems of control of environmental water quality, the task of modeling of polluting substances propagation in water objects should be emphasized.

The theoretical analysis of consequences of water pollution, the economic estimation of damages and, on the basis of these investigations, the development of methodical bases of determination of the efficiency of capital investments in environment protection measures are impossible without the knowledge about the processes of polluting substances propagation. The development of scientifically justified programs of long-term planning of the measures aimed at the reduction of discharges of individual sources, the estimation of ecological perfection of different technologies, the development of methods and means of the control, prognosis and management of the environment quality are indissolubly related to mathematical modeling of the processes of transport and diffusion of harmful admixtures. The mathematical models describing the formation and the development in time of the conditions of environmental objects are used both at designing the monitoring systems at the pre-designing stage (the choice of the system structure and the locations of measurement stations, the spatial-temporary solvability of measuring devices and so on) and during the process of their operation (algorithms of estimation of the object condition, prognosis, emergency pollution sources detection and so on [1]).

## 2. Capabilities of the developed software package

### 2.1. General capabilities

The description of the applied program package created by the authors for realization of mathematical models of pollutants

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transport in rivers is given in the work. It is designed an up-to-date as convenient reliable tool for experts in different fields of knowledge (biology, ichthyology, ecology, hydrology, building, agriculture, etc.), allowing them to calculate the polluting substance concentrations at any point of the river depending on the quantity and the conditions of discharging from several pollution sources. As the mathematical models of water quality formation in the river under the influence of several pollution sources, spatially one-, two- and three-dimensional advective-diffusion models at different initial and boundary conditions (see below) are realized in the package: (a) an advective-diffusion equation with non-local boundary condition at the end of the controlled section with account for the coefficient of natural self-purification of the river; (b) an advective-diffusion equation with boundary condition of full mixing at the end of the controlled section; (c) an advective-diffusion equation ignoring the vertical advection with non-local boundary condition at the end of the controlled section with account for the coefficient of natural self-purification of the river; (d) an advective-diffusion equation ignoring the vertical advection with boundary condition of full mixing at the end of the controlled section; (e) a diffusion equation with non-local boundary condition at the end of the controlled section with account for the coefficient of natural self-purification of the river; (f) a diffusion equation with boundary condition of full mixing at the end of the river controlled section. For the abovementioned mathematical models, there were developed new computation schemes and advanced the known finite-difference ones [2,3].

In the package there are the options of inputting and editing the initial data describing the geographical, geometrical and hydrological features of the simulated section of the river, the condition and the specific features of pollution of the river, the quantity and the name of the pollutant of interest, the types of used models and restrictions, the ways of assignment of these data, etc. There are the options of choosing the language of dialogue with the package, the conditions of computation realization, the desirable accuracy of computation, the type and format of output of the results. At any stage of working with the package, there is an option of help concerning the methods which are realized in the package, the capabilities and specific features of the package, the parameters of tasks and obtained results.

### *2.2. Specific features of mathematical models realized in the package*

Modeling of environmental water pollution is a challenge. This is caused by a great number of factors affecting the pollution process, by a wide variety of pollution types. The models describing the processes of transport, dilution and self-purification of harmful substances in water bodies for a rather small interval of time are realized in the offered package.

The diffusion of polluting substances in rivers is most fully described by the three-dimensional equation of turbulent diffusion of non-conservative substances [1,4–6]:

$$\frac{\partial \Phi}{\partial t} = \frac{\partial}{\partial x}\left(K_x \frac{\partial \Phi}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_y \frac{\partial \Phi}{\partial x}\right) + \frac{\partial}{\partial z}\left(K_z \frac{\partial \Phi}{\partial z}\right) - V_x \frac{\partial \Phi}{\partial x} - V_y \frac{\partial \Phi}{\partial y} - V_z \frac{\partial \Phi}{\partial z} - u\frac{\partial \Phi}{\partial y} - k(\Phi) + f(t,x,y,z), \quad (1.1)$$

where $\Phi$ is the time-averaged concentration of non-conservative pollutant; $t$ is the time; $x, y, z$ are the spatial coordinates (the axis $x$ is horizontal and its direction coincides with the direction of averaged current of the flow, the axis $y$ is perpendicular to the free surface and is directed downwards; the axis $z$ is directed across the flow); $K_x, K_y, K_z$ are the coefficients of turbulent diffusion; $V_x, V$ and $V_z$ are the time-averaged components of the speed of the river flow; $u$ is sedimentation velocity; $\kappa(\Phi)$ is the term describing the non-conservatism of pollutants (very often there is used a simple approximation of this dependence $\kappa(\Phi) \equiv k \cdot \Phi$, where $k$ is the coefficient of non-conservatism); $f(t,x,y,z)$ is the capacity of the pollution sources. Generally $K_x, K_y, K_z, V_x, V_y, V_z, \kappa(\Phi)$ coefficients are the functions of space points and time [3,5].

The following models are realized: (1) a one-dimensional model ($m$ = l); (2) a two-dimensional model ($m = 2$); (3) a three-dimensional model ($m = 3$). The three-dimensional model is the exactest. Other models should be considered as special cases of the three-dimensional model. As for their practical use depending on the characteristics of the rivers and the tasks to be solved (see [7]).

If the considered section of the river stretches along the axis of abscissas without deviations, the Cartesian coordinates are used in the design algorithms. If, within the considered section the river is twisting, then horizontal Cartesian coordinates $x$ and $y$ in the equations should be replaced by corresponding curvilinear coordinates, longitudinal and cross coordinates $\zeta$ and $\eta$.

For calculation of the capacities of the pollution sources, we use the following formula:

$$f(t,r) = \sum_{j=1}^{R} F_j(t) \cdot \delta(r - r_j); \quad F_j(t) = p_j(t) \cdot S_j(t), \quad (1.2)$$

where $S_j(t)$ is the concentration of the polluting substance discharged into water by the $j$th source; $r_j$ is the radius-vector of action of the $j$th source; $t$ and $r$ are parameters of time and space, respectively.

The concentration of the polluting substance transported in the river water is determined by the formula:

$$s = \Phi(t,r) \cdot P_0/P, \quad (1.3)$$

where $\Phi(t,r)$ is the solution of diffusion equation (1.1); $P$ is the water rate at the current point; $P_0$ is the water rate in the upper cross-section of the considered section, i.e. at $x = 0$.

The function $\Phi(t,r)$ is determined at $t \geqslant 0$ and $r \in G$, where $G$ is the one-dimensional interval, the plane or spatial region, which the diffusion equation is solved for. This region is determined by means of the following inequalities:

$$0 \leqslant x \leqslant \Im$$
$$\eta_r(x) \leqslant y \leqslant \eta_l(x) \quad (m \geqslant 2);$$
$$0 \leqslant z \leqslant H(x,y) \quad (m = 3),$$

where $\eta_r(x), \eta_l(x)$ and $H(x,y)$ are the given functions. Using the classical boundary conditions, we have $\Im = 2L$; otherwise $\Im = L + l$ ($L$ is the length of the considered section of the river). The functions $\eta_r(x)$ and $\eta_l(x)$ describe the position of the right and left banks of the river on the horizontal plane, respectively. The function $H(x,y)$ describes the position of the river bottom in space, i.e. it determines the values of the water depth at different points.

Thus, it is possible to split the boundary of the region $G$, which we shall designate by $\partial G$, into several parts. Among them, there are upper and lower cross-sections of the river in which $x = 0$ and $x = \Im$, respectively. In the one-dimensional model, they are simply the points which are extremes of the interval $G$. At $m = 2$, the boundary $\partial G$ also contains the river banks, and at $m = 3$, – the side walls (if they exist), the river bottom and the top free surface.

The initial and boundary conditions of the solution to the diffusion equation look like:

$$\Phi(0,r) = S_0; \quad \Phi(t,r)|_{x=0} = \sigma$$

($S_0, \sigma = \text{const}$). The boundary conditions at the end of the considered section may be classical or non-classical. The classical conditions have the following form:

$$\left.\frac{\partial}{\partial x}\Phi(t,r)\right|_{x=\Im} = 0 \quad \text{(condition of complete mixing);} \quad (1.4)$$