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
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 knowl-
edge (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 hydrolog-
ical 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 step 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 pro-
cess, 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 de-
scribed by the three-dimensional equation of turbid diffusion of non-conservative substances [1,4–6]:

\[ \frac{\partial \Phi}{\partial t} = \frac{\partial}{\partial x} \left(K_x \frac{\partial \Phi}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_y \frac{\partial \Phi}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_z \frac{\partial \Phi}{\partial z} \right) - V_x \frac{\partial \Phi}{\partial x} - V_y \frac{\partial \Phi}{\partial y} - u \frac{\partial \Phi}{\partial z} + f(t,x,y,z), \]  

(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 aver-
eged current of the flow, the axis \( y \) is perpendicular to the free sur-
face and is directed downwards; the axis \( z \) is directed across the flow); \( K_x, K_y, K_z \) are the coefficients of turbulent diffusion; \( V_x, V_y \) and \( V_z \) are the time-averaged components of the speed of the river flow; \( u \) is sedimentation velocity; \( k(\Phi) \) is the term describing the

non-conservatism of pollutants (very often there is used a simple approximation of this dependence \( k(\Phi) \equiv k - \Phi \), where \( k \) is the coef-
icient of non-conservatism); \( f(t,x,y,z) \) is the capacity of the pollu-
tion sources. Generally \( K_x, K_y, K_z, V_x, V_y, V_z, k(\Phi) \) coefficients are the functions of space points and time [3.5].

The following models are realized: (1) a one-dimensional model \((m=1)\); (2) a two-dimensional model \((m=2)\); (3) a three-dimen-
sional 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 \( \xi \) and \( \eta \).

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

\[ f(t,r) = \sum_{j=1}^{n} F_j(t) \cdot \delta(r - r_j); \quad F_j(t) = p_j(t) \cdot S_j(t), \]  

(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; \( r \) and \( s \) are parameters of time and space, respectively.

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

\[ s = \Phi(t,r) \cdot P_0 / P, \]  

(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 \( t \geq 0 \) 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:

\[ 0 \leq x \leq 3 \]  
\[ \eta_j(x) \leq y \leq \eta_l(x) \quad (m \geq 2) \]  
\[ 0 \leq z \leq H(x,y) \quad (m = 3), \]

where \( \eta_j(x), \eta_l(x), H(x,y) \) are the given functions. Using the classical boundary conditions, we have \( 0 \leq 2L \); otherwise \( 3 = L + l \) (L is the length of the considered section of the river). The functions \( \eta_j(x) \) 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 val-
ues 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 \( x = 3 \), 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:

\[ \Phi(0,t) = S_0; \quad \Phi(t,r)_{r=0} = \sigma \]  
\[ (S_0, \sigma = \text{const}) \]

(1.4)

The boundary conditions at the end of the considered section may be classical or non-classical. The classical condi-
tions have the following form:
The problem of 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 lines and the bottom of the river is carried out in the package: explicit, clearly implicit and symmetric. The symmetric schemes are realized in the package. In particular, at \( m = 3 \), there should be

\[
\frac{\partial \Phi(t, r)}{\partial z} \bigg|_{z=0} = 0
\]

To solve Eqs. (1.1) and (1.4) or (1.1) and (1.5) in reference to the concentration \( \Phi(t, x, y, z) \) and their particular one- and two-dimensional cases, the difference schemes are realized in the package: explicit, clearly implicit and symmetric. The symmetric scheme provides the accuracy of the \( r^0 \) order; for all other schemes, the accuracy of the \( r \) order is reached. At certain values of the parameters of the difference schemes, their stability is guaranteed at any values of spatial and time grid steps [8].

Thus there are some problems related to the methods of solution of various problems which the practical realization, the accuracy, and the time of obtaining of the results depend on. In particular: (a) an analytical description of the bank or the spatial region for which the diffusion equations and boundary conditions are obtained, i.e. the analytical description of the plan of the river and the bottom of the river; (b) an analytical description of the dependence of the concentration coefficients on spatial coordinates; (c) an analytical description of the dependence of inhomogeneous terms of the diffusion equation, i.e. of the capacities of pollution sources, on spatial coordinates and time; (d) a correct choice of ratios between spatial steps of the grid, and also between them and the step of digitization of time in the difference scheme.

Brief descriptions of the methods of solution of the problems which are realized in the offered package are given below.

3. Solution of the problems of practical implementation of the difference schemes

3.1. Description of river banks by splines

The problem of the analytical description of plane or spatial region for which the diffusion equations and boundary conditions are investigated is solved [9]. This region represents the part of the channel of the river filled with water in the considered section. The interpolation by splines is used for the analytical description of the plane curve, represented in the form of a sequence of distinct points with given Cartesian coordinates. Such a sequence, in particular, could be one of the river bank lines. The construction algorithms for splines of two types of the simplest explicit form which ensure continuous dependence of the tangent vector of the curve on its parameter are realized in the package. In particular, the river bottom is described by polynomial splines, and the river banks are described by trigonometrical splines.

3.2. Optimum choice of time and spatial steps of digitization

Let's consider the issues of optimum choice of the steps of digitization of the algorithm at practical realization of difference schemes [10]. The requirements of reduction of the time and the errors of calculation as much as possible are considered as criteria of optimality. The offered algorithm is suitable for the case when the function describing the polluting substances transport in water has got the derivatives up to the fourth order inclusive.

The total number of nodal points \( N \) in the difference schemes determines the time necessary for realization of the algorithm; the accuracy of the obtained result depends on it. Naturally, there arises the question: how to select the numbers \( n_1, \ldots, n_m \) at the given value of \( N \) so that the algorithm should be somewhat optimum.

This problem is solved in the following way [11]: at the given values of total nodal points \( N \), there are determined such values of spatial steps of the grid along coordinate axes \( h_1, \ldots, h_m \) for which the upper bound of the module of the residual takes on the minimum value:

\[
\sum_{k=1}^{m} \rho_k h_k^2 \rightarrow \min,
\]

where \( \rho_k \) is the error of approximation of the equation along the \( k \)th coordinate \( (k = 1, \ldots, m) \).

The solution of this optimization problem is determined by the formula:

\[
h_k^* = \frac{1}{\rho_k} \left( \frac{1}{\rho_1 \cdots \rho_m} \right)^{1/m} (k = 1, \ldots, m).
\]

The problem of optimum choice of the value of the parameter \( \tau \) at given spatial steps of the grid is solved in the following way: at the given value of upper bound of the module of the residual of the equation which is equal to \( e \), there are determined such values of \( \tau \) and \( N \) for which the time of calculation takes on the minimum value:

\[
N^2/\tau \rightarrow \min,
\]

\[
\rho_1 \tau^2 + PN^{-2/m} = e = \text{const}.
\]

where \( \rho_1 \) is the error of approximation of the equation by the time coordinate; \( \kappa \) is the constant dependent on the algorithm of solution of the sets of linear equations, usually \( \kappa = 1 \); \( e \) is the given value of the upper bound of the module of the equation residual.

The solution of this optimization problem is determined by the formula:

\[
N = \left( \frac{\rho_1 + 1/m}{\kappa e} \right)^{m/2}; \quad \tau^2 = \frac{e}{\rho_1 / \left( 1 + km \right)}; \quad \rho_1 h_1^* = \cdots = \rho_m h_m^* = \kappa \rho_1 \rho^2 = \frac{\kappa e}{1 + km}.
\]

The main difficulty for practical realization of the described scheme of optimization is connected with the necessity in estimation of the upper bound of partial derivatives of the function \( \Phi(t, r) \) with respect to the spatial coordinates in terms of which parameters \( \rho_1 \) and \( \rho_m \) are expressed without solving the diffusion equation.

3.3. Estimation of derivatives of the unknown function

As noted above, for practical realization of the described optimization schemes, it is necessary to estimate somehow the upper bounds of the modules of partial derivatives of the unknown function with respect to independent variables without solving the initial task.

It should be borne in mind that the derivatives of these functions can be estimated up to the common constant multiplier.

One of the ways of solution of this problem consists in the following: for some values of the parameters \( h_k \) and \( \tau \) (at solving the
Such sources can be named parameter. It means that the point sources are replaced by ex-

\[ u(x,t) = \frac{1}{\sqrt{2\pi t}} e^{-\frac{x^2}{2t}} \]

plot of this function together with the axis of abscissas forms an

diffusion equation), the values of the function \( \Phi \) are determined as

the first approximation, then, by means of the numerical differenti-

ation operations, the required derivatives are determined, and the

values of the desired parameters are calculated. After that, using these values, there are determined new values of the func-

\( \Phi \) and so on until the difference between the neighbouring cal-

culated values of the function are less than the given value. At

solving the diffusion equation, it is possible to use the explicit

scheme at the first stage. Then it is necessary to determine the values

of the sought for function with higher accuracy.

In this case, for calculation of the unknown function values, there is applied the iteration method similar to the one used in

work [1] for calculation of the multidimensional integral by the

Monte-Carlo method.

It is known that the operations of numerical differentiation are not stable, but this should not prevent the realization of the offered

method since it requires only rough estimates of unknown deriva-

tives.

An obvious drawback of this method is the necessity in perfor-

mance of a plenty of additional actions. Though, due to the capa-

bilities of modern personal computers, it is negligible at solving the partic-

ular tasks.

3.4. The effect of smoothness of the inhomogeneous part of the

diffusion equation on the accuracy of the results

The inhomogeneous parts of diffusion equation (1.1) realized in the

package contain the impulse functions, which are linear combina-

tions of Dirac’s deltas-functions (see (1.2)). These functions

and their derivatives are not bounded. Therefore the difference

schemes of the solution of diffusion equations are not correct in the

vicinities of pollution source localization points.

For elimination of this drawback, it is necessary to consider a model, in which the delta function \( \delta(x-a) \) is replaced by the bounded numerical function \( D(u, x - a) \), where \( u \) is the additional parameter. It means that the point sources are replaced by ex-

 tended ones, the capacity of each of which has the maximum cor-

 responding to the capacity of the source at the point of its location.

Such sources can be named quasi-point sources.

The function \( D(u, x) \) should satisfy the following requirements:

it reaches the maximum value proportional to \( 1/u \) at the point

\( x = 0 \); it tends to zero at \( x \rightarrow \pm \infty \); its integral between the limits

\( -\infty \) and \( +\infty \) is equal to unit; its plot represents a bell-shaped curve. The width of such curve is naturally defined as the width

of the rectangle which height is equal to the ordinate of the peak

of the curve, and its area is equal to the area of the figure limited

by the curve and the axis of abscissas. Thus, the parameter \( u \)

characterizes the width of the plot of the function \( D(u, x) \), i.e. the sizes

of the source. At \( u \rightarrow 0 \), the function \( D(u, x) \) tends to \( \delta(x) \).

One of the elementary continuous functional dependences which may be used for setting the function \( D(u, x) \) is the trapezoid de-

pendence:

\[
D(u, x) = \begin{cases} 
\frac{1}{u} & \text{at } t < 1 - s \\
\frac{(1 + s - t)(2us)}{1 - s \leq t \leq 1 + s} & \\
0 & \text{at } t > 1 + s 
\end{cases}
\]

where \( t = 2|x/u|; s \) is any real parameter from the interval \((0, 1)\). The plot of this function together with the axis of abscissas forms an

isosceles trapezium, the top and bottom bases of which have the lengths equal to \( u(1-s) \) and \( u(1+s) \), respectively, and the height

of which is equal to \( 1/u \). The less is value \( s \), the less this trapezium differs from a rectangle.

Besides the trapezoid dependence, in the developed software

package the following dependences are offered to the user’s choice:

(1) Gaussian

\[
D(u, x) = \frac{1}{u\sqrt{2\pi}} e^{-\frac{u^2}{2}}
\]

(2) Lorentzian

\[
D(u, x) = \frac{2}{\pi u(1 + (x/u)^2)}
\]

In fact, the function \( D(u, x) \) defined by one of the latter relations plays the part of a smoothing function, which allows us to

transform any function from \( L^2 \) into an infinitely differentiable function by means of the operation of convolution [10,11].

If the pollution sources do not operate continuously, but they

operate for a limited interval of time \([0, T]\), then the capacity of each source should be smoothed not only by spatial coordinates, but also by time. It means that this function should be proportional to \( A(v, t - T) \), where \( v \) is the additional parameter, and \( A(v, t) \) is the function satisfying the following conditions: at \( t \rightarrow -\infty \) it tends to unit, and at \( t \rightarrow +\infty \) to zero. Its plot represents a quasi-stepped curve, which steepness is maximum at \( t = 0 \), and this maximum

value of the steepness is proportional to \( 1/v \). The parameter \( v \) char-

acterizes the time of diminution of the function of discharge. At \( v \rightarrow 0 \), the function \( A(v, x) \) tends to \( 1 - \theta(x) \), where \( \theta(x) \) is Heavi-

side’s stepped function. In the developed software package, it is

possible to choose an explicit form of the function \( A(v, x) \) from the following types:

(1) Gaussian

\[
A(v, x) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-v^2/2} dt;
\]

(2) Lorentzian

\[
A(v, x) = \frac{1}{2} - \frac{1}{\pi} \arctan(t/v);
\]

As the computation results show, the smoother are the func-

tions of discharge, the more accurate are the results of solution of the equations in the vicinities of the points of discharge. For gi-

ven types of functions \( D(u, x) \) and \( V(v, t) \), the accuracy of the re-

sults increases as the values of parameters \( u \) and \( v \) increase.

4. Study of the efficiency of the developed methods and

algorithms

A complex of the programs of numerical realization of the tasks of

distribution of pollution in streams consists of three basic parts: (1) the program of realization of one-dimensional tasks; (2) the program of realization of two-dimensional tasks; (3) the program of realization of three-dimensional tasks.

The programs are basically developed on the basis of finite-dif-

ference algorithms. Analytical methods are used in some concrete

tasks of particular character.

The basic program modules used in all three parts are the fol-

lowing: (1) the program of realization of the double-sweep method–factorization method; (2) the program of the solution of two-

dimensional and three-dimensional implicit finite-difference equa-

tions, which has been created on the basis of the Gauss–Seidel iter-

ation method.

The test of a complex of programs was carried out by using the

specially selected test tasks. The numerical experiments were car-

ried out with the purpose of revealing the mechanical mistakes in

algorithmization and programming, the stability concerning the

initial data, the accuracy of obtained results and the time of com-

putation, for comparison of different algorithms, etc.
Particular attention was given to the realization of computing experiments in the cases of polluting sources of a special type (point or distributed sources), oscillations in the solutions of the equations at singularities in initial data, etc. The numerical experiments have shown that:

1. In the case of classical one-dimensional tasks, the purely implicit scheme and the Crank–Nicolson scheme exhibited certain computing qualities; in the case of special loadings, it is preferable to use the purely implicit scheme, and in the case of the smooth initial data – the Crank–Nicolson scheme.
2. In the case of nonclassical boundary conditions (non-local conditions), the finite-difference algorithms exhibited the same qualities as in the classical case.
3. In the two-dimensional case, the experiments were carried out on the basis of the schemes of decomposition of parallel counting and the two-dimensional implicit scheme, and also the two-dimensional Crank–Nicolson scheme; the scheme of decomposition looks more preferable by the time of the calculation. It should be noted that the property of parallelization of the schemes of decomposition was not applied at counting; in the case of smooth initial data, the Crank–Nicolson algorithm with the use of iteration Gauss–Seidel process showed better quality by accuracy, which reasonably corresponds to theoretical research.
4. In the case of non-classical two-dimensional tasks, the experiments were carried out only with the use of the schemes of decomposition; in this case, all theoretical preconditions concerning the algorithms used proved to be true.

Being compared, the three-dimensional algorithms showed the same properties and qualities as the corresponding two-dimensional algorithms. Naturally, three-dimensionality of the task affected the possibility of increasing the accuracy of calculation; a similar assertion is true also in the case of non-classical (non-local) initial boundary value problems.

5. Capabilities of the package

It is possible to input and to edit the initial data describing geographical, geometrical and hydrological specific features of the simulated section of the river, the condition and the specific features of pollution of the river, the number and names of the parameters of pollution, the types of models and restrictions, the ways of assignment of these data in the package. There is a possibility of choosing the language of dialogue with the package, the conditions of realization of computation, the desirable accuracy of computation, the type and format of display of the results of computation. At any stage of working with the package, there is a possibility of getting the help about the methods realized in the package, the capabilities and specific features of the package, parameters of tasks and received results.

The choice of these possibilities is carried out by means of appropriate options from the commands of the main menu of the package. The main menu includes the following commands and options (see Fig. 5.1): File (Page setup, Printer setup, Exit), Tools (Language, Model, Save options, Autosave), Coordinates (Type of coordinates, Banks and bottom, Flow velocity, List of objects, Objects, Convert files), Water parameters (List of substances, Upper cross-section, Capacities of sources, Coefficients of diffusion, Coefficient of non-conservation, Coefficient of decreasing), Run (Accuracy, Calculations) and Help (Contents, Algorithms). The desirable language of dialogue with the package and the type of diffusion equation are selected directly from two pull-down lists. The description of purposes and capabilities of these options is given below.

### 5.1 Input and editing of the initial data

The input of information necessary for operation of the package is performed in the form of separate constants, tables or the choice of the appropriate line from the pull-down. Let’s adduce the substantial description of this information.

**The data, which are not represented as tables.** In the list given below, some parameters are common for all sections of the river, and some are specific for the chosen section; the latter are marked by the sign “d” in square brackets. The parameters marked by the sign “n” in square brackets are not saved in files.

- Type of model – one-dimensional, two-dimensional or three-dimensional. It is selected from the drop-down list displayed directly on the main toolbar or by selection of the option “Model” from the command “Tools” (see Fig. 5.2).
- The indicator determining the method of the numerical solution of two-dimensional and three-dimensional diffusion equations – by means of iteration algorithm or by representation of the sought-for solution as a linear combination of the solutions of one-dimensional equations (see Fig. 5.2).
- The number of sections of the river which can be considered in the package (see Fig. 5.2).
- The number of polluting substances in the available list (see Fig. 5.2).
- The indicator determining the type of coordinates (Cartesian or curvilinear), which are listed in the tables “Banks and bottom” and “Objects”. It is switched by means of the option “Type of coordinates” (see Fig. 5.3).
- The parameters determining the accuracy of calculations at solving the diffusion equations. They include the total number of nodal points, the number of nodal points along the axis Y (for the two-dimensional and three-dimensional models), the number of nodal points along the axis Z (for the three-dimensional model) and the factor, determining the step of time discretization, i.e. the factor, which the value accepted by default is multiplied by. These parameters are entered by means of execution of the option “Accuracy” from the command “Run” of the menu of the main form (see Fig. 5.4).
- The number of the considered section. It is entered by execution of the option “Calculations” from the command “Run” of the menu of the main form (see Fig. 5.4).
- The number of polluting sources within the considered section [d]. It is entered by means of the option “List of objects” from the command “Coordinates” of the menu of the main form (see Fig. 5.3. The format of input is of the form shown in Fig. 5.5.
The indicator determining whether the diffusion equations for the considered section will be solved under nonclassical boundary conditions \([d]\). It is switched by means of the option "Calculations" from the command "Run" of menu of the main form (see Fig. 5.4). The format of input is of the form shown in Fig. 5.6.

The indicator determining whether the given boundary conditions in the upper cross-section of the section will be taken into account at solving the diffusion equations or these boundary conditions will be taken equal to zero \([d, n]\) (see Fig. 5.6).

The indicator determining whether the given initial conditions will be taken into account at solving of the diffusion equations or these initial conditions will be taken equal to zero \([d, n]\) (see Fig. 5.6).

The polluting substance from the available list the concentration of which will be determined \([d, n]\) (see Fig. 5.6).

The list of polluting sources which are considered to be operating at solving the diffusion equations. At solving of these equations, the capacities of other sources are considered equal to zero \([d, n]\) (see Fig. 5.6).

The type of functions of spatial distribution of sources \(D(u, x)\). This function can be trapezoidal, Gaussian or Lorentzian (see Item 3.4).

The type of function of discharge \(A(v, x)\), determining the character of attenuation of capacities of the sources. This function can be stepwise, equal to the function of normal distribution or equal to the function of Cauchy distribution (see Item 3.4).
Relative sizes of sources, i.e. the ratio between the parameter \( u \) and the spatial step used in the difference scheme grid along the corresponding coordinate axis (see Item 3.4).

Relative duration of recession of the function of discharge, i.e. the ratio between the parameter \( v \) and the duration of operation of the source (see Item 3.4).

Below the number of polluting substances from the available list common for all sections is designated by \( M \), and the number of polluting sources from the list corresponding to the considered section is designated by \( R \).

The data given in the table “Banks and bottom” (Fig. 5.3). Each of these parameters corresponds to some cross-section of the river with number \( j \): \( j = 1, \ldots, N \):

- \( z_l \) – the longitudinal coordinate;
- \( \eta_l \) – the cross coordinate of the point of the left bank;
- \( z_r, \eta_r \) – the cross coordinate of the point of the right bank;
- \( x_l, y_l \) – the horizontal Cartesian coordinates of the point of the left bank;
- \( x_r, y_r \) – the horizontal Cartesian coordinates of the point of the right bank;
- \( h_l(k = 1, \ldots, m_h) \) – the depth of the river at the point with cross coordinate \( \eta_l = \eta_l - \eta_r \cdot k/(m_h + 1) \).

Here \( N \) is the number of cross-sections; \( m_h \) is the number of equidistant points of the bottom in the cross-section. For each cross-section the value \( w_l = \eta_l - \eta_r \) represents the width of the river.

We have used the spline-interpolation for the functions \( \eta_l(\zeta) \) and \( \eta_r(\zeta) \), determining the cross coordinates of the points of bank lines of the river for the given \( \zeta \)-coordinate, and the polynomial interpolation for the function \( H(\zeta, \eta) \), determining the depth of the river at the point with the given horizontal coordinates at the specified value of \( \zeta \).

Depending on the type of coordinates chosen by the user for data input – Cartesian or curvilinear, the following parameters are consistently entered in columns of this table: \( T_l, x_l \), or \( z_l, \eta_l \) (for the two-dimensional and three-dimensional models), \( z_l \) (for the three-dimensional model). The format of input is similar to the format of input of curvilinear coordinates.

The data given in the table “Capacity of sources” (Fig. 5.8). The first column of the table contains the number of the source and its name; the second column contains water flow rate \( q_j \) of the \( j \)-th source of pollution; other columns contain concentration \( s_j \) of polluting substances discharged into the river water by the \( j \)-th source; \( j = 1, \ldots, R; k = 1, \ldots, M \). The format of input is similar to the format of input of curvilinear coordinates.

The data given in the tables “Coefficients of diffusion”, “Coefficients of non-conservatism”, “Coefficient of decreasing” (Fig. 5.8). Each of the following parameters corresponds to one of the polluting substances with number \( j = 1, \ldots, M \):

- \( K_x, K_y, K_z \) are the coefficients of turbulent diffusion in the upper cross-section;
- \( K'_{x}, K'_{y}, K'_{z} \) are the coefficients of turbulent diffusion in the lower cross-section;
- \( K_j \) is the coefficient of non-conservatism in the upper cross-section;
- \( K'_j \) is the coefficient of non-conservatism in the lower cross-section;

The data given in the table “Flow velocity” (Fig. 5.3). The quantity \( V_j \) is the speed of the water flow in the cross-section with number \( j = 1, \ldots, N \). The format of input is similar to the format of input of curvilinear coordinates.

The linear interpolation is used in the package to describe the dependence of the water rate \( P(r) = E(r) \cdot n(r) \) on the \( \zeta \)-coordinate.

The data given in the table “Objects” (Fig. 5.3). Each of the following parameters corresponds to one of the pollution sources with number \( j = 1, \ldots, R \):

- \( T_j \) is the duration of operation;
- \( z_l, \eta_l \) are the longitudinal and cross curvilinear coordinates;
- \( x_l, y_l \) are the horizontal Cartesian coordinates;
- \( z_l \) is the depth.

Depending on the type of coordinates chosen by the user for data input – Cartesian or curvilinear, the following parameters are consistently entered in columns of this table: \( T_j, x_j \) or \( z_j, \eta_j \) (for the two-dimensional and three-dimensional models), \( z_j \) (for the three-dimensional model). The format of input is similar to the format of input of curvilinear coordinates.
• $l$ is the length of self-cleaning;
• $q$ is the coefficient of self-cleaning.

The format of input is similar to the format of input of curvilinear coordinates.

The linear interpolation for dependence of parameters $K_0(r), K_0(r), K_0(r), K(r)$ on coordinate $\zeta$, is used in the package.

5.2. Working language

The working language of the package is the language in which all text messages will be displayed. A list of languages is determined by the existence of files-dictionaries, serving for translation of the messages from English, in the main directory. The user can add new or to remove the existing files-dictionaries (their total number should not exceed 16).

For translation of text messages by the program, in the main directory, there should be a file with the name coinciding with the name of chosen language (Russian, Georgian, etc.) and having the extension .dic (for example georgian.dic), containing a dictionary of translated lines, and also a file with the same name and with extension .add (for example georgian.add). For representation of the help information in the chosen language, in the main directory there should also be a file with the same name and with extension .hlp (for example georgian.hlp) or a file with the same name and with extension .pdf (for example georgian.pdf), containing this information.

The working language can be chosen from the list on the ToolBar or by means of the option of the main menu Language (see Fig. 5.2). In the first case, accessible languages are those for which there are both files – with extensions .dic and .add. In the second case, the presence only of the file with extension .dic is enough; thus the auxiliary file with extension .add is created by pressing the button Create.

The file-dictionary with extension .dic can be created or changed as it is described in Help of the package. At each change in this file, it is also necessary to create the corresponding file with extension .add in the way described above.

5.3. Parameters of the package

The change in the value of each parameter is carried out with the help of standard Windows components which allow editing the text, choosing the line from the list, setting the indicator, etc.

At working with each form containing the main menu, the assignment of parameters is carried out with the help of commands of the main menu from the groups File, Tools and Parameters. Most important parameters could also be determined with the help of the components located on the ToolBar.

It is possible to split the parameters used in the package into several groups, which are considered below.

The main parameters of the package which are not used in calculations:

- Sizes of pages for printing out; they are changed with the help of the option File/Pagesetup (see Fig. 5.9);
- Working language (see Item 5.2);
- Working directory is the directory where data files are looked up at choosing them; it changes at each change of a folder in standard dialogue windows for opening and saving the files.

These parameters are read from the files mdinare.num and mdinare.str at running of the package. The option of the menu Save options records the values of parameters changed during the operation of the package in this file. The item of the menu Autosave contains the indicator which, in the switched-on state, provides the record of changed values of parameters in the files mdinare.num and mdinare.str at exiting the package.

The parameters of the package which are used in calculations and are not represented as tables: they are the parameters listed in Item 5.1. The parameters which are not marked by the sign ‘n’ in this list, as well as some parameters of the previous group, are read from the file mdinare.num and can be saved in this file.

The type of the model, the type of the algorithm, the number of sections of the river and the number of polluting substances are changed by means of the option of the menu Tools/Model in the main form of the program.

The type of coordinates is changed by means of the option of the menu Coordinates/Typeofcoordinates in the main form of the program.

The number of polluting sources in each section is changed at editing the tables List of objects.

The parameters determining the accuracy of calculations are changed by means of the option of the menu Parameters/Accuracy in the form of the task “Calculations”; the parameter $n$ also is changed by means of the option of the menu Run/Accuracy in the main form of the program.

Other parameters are changed by means of the option of the menu Parameters/Taskparameters and Parameters/Additional parameters in the form of the task Calculations, and also in the dialogue windows which appear on the screen before running of this task.
The parameters of the package which are used in calculations and are represented as tables: they are sequences of the same elements, which are entered in tables and are saved in separate files (see Item 5.4). The data of the considered type which have been saved in files are used in calculations. The concrete tables of initial data used in the package are described in Item 5.1.

The parameters of setting of the printer are parameters Windows, which, in particular, are used by the package; they are changed by means of the option `File Printer setup` (see Fig. 5.9).

The parameters determining the type of the diagram at representation of computation results (see Item 5.5).

5.4. Data input and editing

The entered data which form sequences of elements of the same type are represented in the form of tables. When there are several editing windows with tables on the screen, different windows correspond to different sections of the river.

There are the possibilities of entering the data which have not been recorded anywhere, reading data from files and saving them in files by means of commands `File New File Open File Save File Save as File Saveall` standard for the text and graphic Windows editors (see Fig. 5.10).

The option `File Send` records the data in a text file. The option `File Print` performs printing of the table.

The data files have quite a simple structure and can be created outside of this package.

The data of the package presented in the form of a table can be entered and edited by means of a mouse and a keyboard. There are the possibilities changing, deleting or adding the symbols into the record of the element; deleting or adding new elements in the necessary place; selecting a block of data; moving or copying the selected block to a new place; removing, writing down in a file or reading the block of the data from the file; printing out both the selected block and all contents of the data file.

There are two operating modes with a table of data – the mode of editing of cells and the operating mode with blocks. In the first mode, it is possible to edit the text in each cell of the table, but it is impossible to select a block from several cells. In the second mode, on the contrary, it is possible to select the block from several cells (for copying, removal, insertion, etc.), but it is impossible to edit the text.

The switching between these modes is carried out by the button `Edit` on the `ToolBar`.

5.5. Realization of computation and representation of the results

The package uses curvilinear coordinates of the points of the river banks and polluting sources at solving the diffusion equations. Therefore, if the user has chosen Cartesian coordinates for data input, all these Cartesian coordinates should be transformed into curvilinear ones. Such transformation is carried out by the

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**Fig. 5.10.**

**Fig. 5.11.**
The algorithms and analytical methods are used at solving the diffusion equation. For realization of two-dimensional and three-dimensional models, one of the two algorithms may be used depending on user’s choice:

1. The classical algorithm in which the difference equation for layers is equivalent to a system of $N$ linear equations for $N$ values of unknown function at nodal points; this system is solved by the iteration method;

2. The algorithm in which the solution of two-dimensional or three-dimensional diffusion equation is represented in the form of a linear combination of solutions of some one-dimensional diffusion equations.

As the experience shows, the second algorithm can be realized by computer much more quickly than the first one.

The method of calculations is also determined by some other parameters listed in Item 5.2.

The results of calculations are displayed in the form of text messages, tables, graphs, etc. For example, the formats of display of computation results as diagrams and tables are shown in Figs. 5.11 and 5.12, respectively.

The results of calculations together with some initial data are split into groups, which are represented on the screen in various windows. By calling the options Print and Send text, the user can select which of the existing groups of data he wants to print or to write down in a file.

In the task Calculations, it is possible to choose the mode of representation of the graph or the table: to represent the graph with a coordinate grid or without it, to increase or to decrease the thickness of lines of a graph, to increase or to decrease the scale of data presentation in the graph, to set the standard or maximum size of the window containing the graph and the table. The parameters determining the view of the screen are changed by means of the command of the menu Parameters/Graphview or by means of some components on the ToolBar.

6. Conclusion

A computer package of realization of mathematical models of propagation of polluting substances in rivers has been created. The package comprises original models, methods and algorithms developed by the authors. The software package is realized for IBM-compatible personal computers according to the generally accepted standard for similar production all over the world. The
consumer can use it as a modern, convenient, simple and reliable tool for resolution the problems he deals with in the considered area. Versatile experimental investigation of the developed software package and the algorithms realized in it have confirmed their high computing, operational and service qualities.

References