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Mathematical Modelling as the Basis of the Information System for Monitoring the Aquatic Environment

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Abstract. During the project preparation of the construction of the facility, an analysis of the environmental situation at the construction site and adjacent territories, including on water bodies, is carried out. Mathematical modelling of processes in water bodies for monitoring their condition has been performed. Water resources of the region are a complex system of interconnected water bodies that interact with each other and have different characteristics. Analysis of the features of the distribution of pollutants in the aquatic environment of the ecological landscape showed that mathematical modelling should be carried out in three main directions, taking into account the nature of the mass transfer of the substance: diffusion; diffusion-convective; predominantly convective. For each type of mass transfer a mathematical model is created: one-dimensional, two-dimensional or three-dimensional. Under conditions of one-dimensional diffusion, when mass transfer occurs in one predominant direction, two options are considered: 1) diffusion from a point source with a known limited amount of matter; 2) diffusion from a permanently operating source with a known rate of outflow of matter. Both these problems are described by the well-known diffusion equation, but their input and boundary conditions are essentially different. The problem of two-dimensional diffusion was solved for the case when contamination occurs on a certain, rather small part of the boundary of a wide reservoir from a source with constant density. The case of three-dimensional spherical diffusion is considered on the example of the solution of the actual problem, when the source of pollution of constant power is at the origin (in the depth of the reservoir). The problem of non-stationary convective diffusion was solved by the example of a flat reservoir with a weak water current, when the simulated region is a wide two-dimensional channel, on the small part of the boundary of which there is a source of a passive impurity. In this case, the known impurity transport equation was used. We used to systematize the potential ecological situation and built the appropriate mathematical models that allowed us to obtain quantitative algorithms for solving the problems of monitoring and developing the components of the information system for calculating the concentrations of pollutants in the water system in the region.

1. Introduction

External influences of a natural-climatic or technogenic nature can cause a variety of changes in construction objects both at the stage of construction and operation. This leads to the need to analyze the environmental situation on the construction site and adjacent areas, including water bodies, during the preparation of the construction project.

The aim of the work is to perform mathematical modelling of water bodies with different properties to create an information system for monitoring their status.

Experimental studies of water objects are associated with certain difficulties. Firstly, this is due to the long duration of the processes of convection and diffusion. The complexity is both the observation of the experiment itself and the analysis of the results from the measurements obtained. Secondly, the high cost of experimental installations is an important factor, especially in the study of long-range areas. In addition, experiments on water bodies are in most cases inadmissible.

As a result, the methods of mathematical modelling play a decisive role in the analysis and prediction of the processes of transport of substances in the aquatic environment.

2. Modelling of transfer of impurity in water objects

Water resources of the region represent difficult system of the reservoirs interconnected and which are interacting among themselves and having different characteristics.

The analysis of subject domain – an ecological condition of regional water resources – showed need of creation of the information system capable to process dynamically changing characteristics of the studied object and to solve a problem with semistructured data, with possibility of expansion of structure of data without change of all system.

Quality of water in reservoirs depends on processes of formation of sewage, processes of self-cleaning and sources of pollution.

The content of the polluting substances in water objects is regulated by their maximum permissible concentration (MPC).

As a result of the operation of the information system, the concentration of pollutants in the given region of the studied reservoir must be calculated at a given time and the value obtained is compared with the MPC. Based on this calculation, recommendations can be made on the possibility of using water for a particular purpose or cleaning it.

2.1. Mathematical modelling of diffusion and convection processes

The analysis of features of distribution of pollutants in water environments of an ecological landscape showed that mathematical modelling needs to be conducted in three main directions, taking into account character of a mass transfer of substance: the diffusive; the simultaneous diffusive and convective; the mainly convective. For each type of transfer of impurity, the mathematical model is created: one-dimensional, two-dimensional or three-dimensional.

In the conditions of one-dimensional diffusion when the mass transfer occurs in one prevailing direction, two options are considered: 1) diffusion from a dot source with known limited amount of substance; 2) diffusion from a constant source with a known speed of the expiration of substance. Both of these tasks are described by the known equation of diffusion [1], however their entry and boundary conditions are significantly various.

Concentration change on various surfaces of the spheres described by r radius from the center of a source for some model substance is convenient to present eventually in the form of the surface constructed in a mathematical MATLAB package (figure 1).

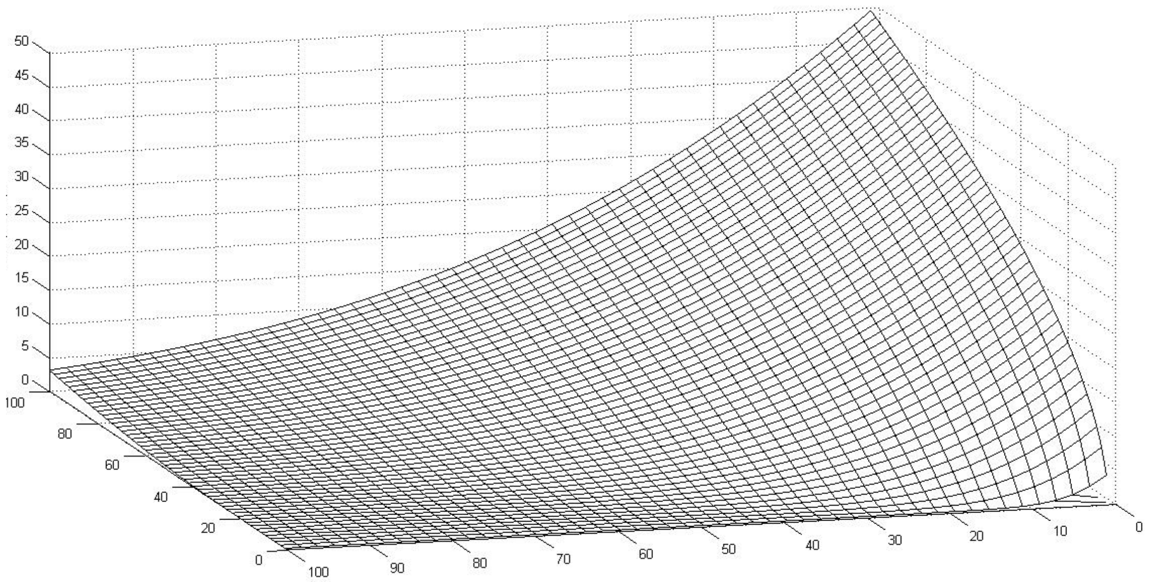

Figure 1. Example of diffusion from a source of constant pollution

Solutions of these tasks are found by means of Poisson's integral $C(x,t) = C_0[1-\Phi(z)]$, $z = \frac{x}{2\sqrt{Dt}}$, and functions of a source $C(x,t) = \sqrt{\frac{D}{\pi}} \cdot \int_0^t \frac{P(\tau)}{\sqrt{t-\tau}} \cdot e^{-\frac{x^2}{4D(t-\tau)}} d\tau.$ Here $\Phi(z) = \frac{2}{\sqrt{\pi}} \int_0^z e^{-\alpha^2} d\alpha$ – function of mistakes [2].

The problem of two-dimensional diffusion was solved for a case when pollution comes on some, rather small site of border of a wide reservoir (figure 2) from density source $p = \text{const}$:

$$\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2}\right); \quad C(x,y,0) = 0; \quad \left.\frac{\partial C}{\partial y}\right|_{y=0} = \begin{cases} p & \text{при } x \in [-a, a], \\ 0 & \text{при } x \notin [-a, a], \end{cases}$$

$$C(x,0)\big|_{-a \le x \le a} = C_0, \ C(x,y)\big|_{y=\infty} = 0, \ C(x,y)\big|_{x=\pm\infty} = 0.$$

The task is solved by means of Fourier's transformation [2]:

$$C(x,y,t) = \frac{P}{\left(2\sqrt{D\pi}\right)^3} \int_0^t \int_{-a}^{a} \left[\frac{1}{(t-\tau)^{3/2}}\right] \cdot \mathrm{e}^{-\frac{(x-\xi)^2+y^2}{4D(t-\tau)}} d\xi d\tau. \tag{1}$$

The case of three-dimensional spherical diffusion is considered on the example of the solution of an actual task when the source of pollution is at the beginning of coordinates (in the depth of a reservoir) and produces in unit of time a substance quantity q=const. The equation of spatial diffusion in spherical system of coordinates: $\frac{\partial C}{\partial t} = D\left(\frac{\partial^2 C}{\partial r^2} + \frac{2}{r}\frac{\partial C}{\partial r}\right)$, where r – the radius of the sphere described round a source of a pollutant [1].

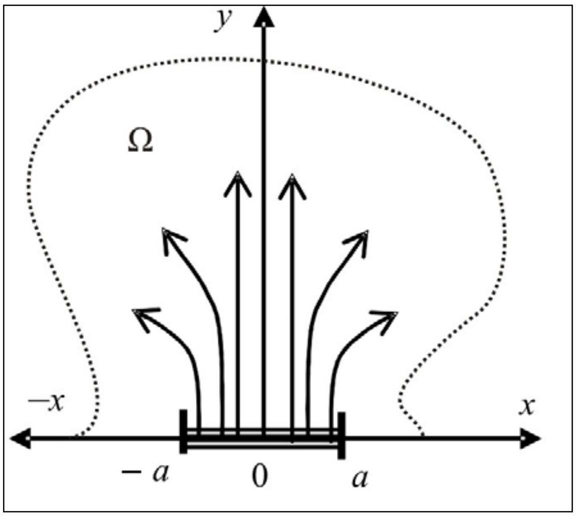

Figure 2. The source of pollution is on reservoir border

Using replacement $V(r,t)=r\cdot C(r,t)$, we will receive the equation $\frac{\partial V}{\partial t}=D\frac{\partial^2 V}{\partial r^2}$ with an entry condition $V(r,0)=0$. We will describe the sphere of S_ε of radius ε round the beginning of coordinates ($r = 0$). Amount of the substance passing through the sphere: $\iint\limits_{S_\varepsilon}\frac{\partial C}{\partial N}d\sigma$. We will pass to a limit $\lim\limits_{\varepsilon\to 0}\left[-\iint\limits_{S_\varepsilon}\frac{\partial C}{\partial N}d\sigma\right]=q$ or $-\frac{\partial C}{\partial N}\cdot 4\pi\varepsilon^2\to q$. And therefore, $C\to q/4\pi\varepsilon$, and a boundary condition $V=q/4\pi=V_0$ at $r = 0$. The solution of this equation can be written down in the following look: $V(r,t)=V_0\left[1-\Phi\left(x/2\sqrt{Dt}\right)\right]$, and therefore,

$$C(r,t)=\frac{2q}{4\pi r\sqrt{\pi}}\cdot\int\limits_{\frac{r}{2\sqrt{Dt}}}^{\infty}e^{-\alpha^2}d\alpha. \tag{2}$$

The problem of non-stationary convective diffusion was solved on the example of a flat reservoir with a weak current of water when the modelled area represents the wide two-dimensional channel on which some rather small piece of border there is a source of passive impurity (figure 3). In this case the known equation of transfer of impurity was used: where x both y – longitudinal and cross coordinates of rather water stream; ρ – impurity density; u and v – average speeds of a stream in the directions x and y [1].

In this case the known equation of transfer of impurity was used:

$$\frac{\partial}{\partial x}(\rho uC)+\frac{\partial}{\partial y}(\rho vC)=\frac{\partial}{\partial x}\left(D\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(D\frac{\partial C}{\partial y}\right), \tag{3}$$

where x – the coordinate, longitudinal in relation to a water stream; coordinate of y is directed across a water stream; ρ – impurity density; u and v – average speeds of a stream in the directions x and y [1].

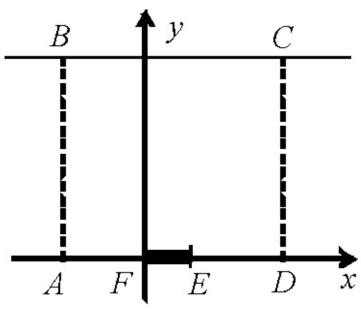

Figure 3. Scheme of settlement area: *AB* and *CD* are strongly removed from *FE* source

Regional conditions are set as follows: 1) we will assume that $C|_{AB} = C|_{CD} = 0$; 2) $\partial C/\partial n = 0$ on the intervals |*BC*|, |*AF*|, |*ED*|; where *n* – direction of an internal normal; 3) on the interval |*FE*| two cases are considered: a) the rate of arrival of pollutants is low: if $|AB| >> |FE|$, it can be assumed $C|_{FE} = \text{const} = C_0$; b) the pollutants under pressure enters the channel *ABCD*: |*AB* | is comparable with |*FE*|, it is possible to consider the speed of intake of impurity of a constant $(\partial C/\partial n)|_{FE} = \text{const} = C_n$.

To solve the equation compiled computational algorithm based on the finite- difference method with a regular square grid with step *h*. The problem is reduced to a system of linear algebraic equations, which is solved using the method of Seidel with a good rate of convergence: $\overline{C}^{n+1} = \overline{D}^{-1}\left(-\overline{M} \cdot \overline{C}^{n} - \overline{N} \cdot \overline{C}^{n} + \bar{f}\right)$, where $\overline{A}$ – the matrix coefficients of the unknown $\overline{C}$; $\bar{f}$ – column vector of free terms; $\overline{C}^{n}$ – vector of unknowns, found on the *n*-th iteration; $\overline{D}$ – a diagonal matrix; $\overline{M}$, $\overline{N}$ – the lower and upper triangular matrices, such that $\overline{A} = \overline{D} + \overline{M} + \overline{N}$.

Convective mechanism is characteristic for the case where pollutants are discharged into the water for a long time and form a uniformly moving stream whose speed matches the speed of the watercourse. Assuming that the change in flow rate is proportional to the length of the watercourse, it is possible to predict the change in the concentration of pollutants in the watercourse.

We made an attempt to systematize the potential environmental situation and build corresponding mathematical models that allowed us to obtain quantitative algorithms for solving the tasks of monitoring and develop the components of the information system for calculating the concentrations of pollutants in the water system in the region [3].

2.2. Development of information system components

The water system area, which is a combination of small rivers, lakes, wetlands and other water bodies through the ground or groundwater flows in a single closed loop, and can be formalized to create a mathematical model of it. An effective means of images and the study of various kinds of water systems are the graphs as a powerful class of objects related to the graphical.

The most obvious and easy to use way to present the regional water system is a weighted directed graph (figure 4), which is defined as the union of two sets.

The vertex set consists of points of possible discharge of pollutants into the water system and check points : recreation , settlements , stations hydrological and hydrochemical monitoring , as well as a change places in the characteristics of reservoirs (relief , flow rate , etc).

A plurality of ribs (the set of edges – arcs) – is homogeneous portions of the object, ie, segments having similar properties (the speed of the river, the shape of the relief, the diffusion coefficient of pollutants, etc.). Thus for vertices and edges of the graph indicate the corresponding weight – the numerical values of the basic parameters of the investigated area (such as the geometric dimensions, water temperature and others.) Or input data for the calculation (e.g., flow rate, an initial concentration of pollutants, etc.).

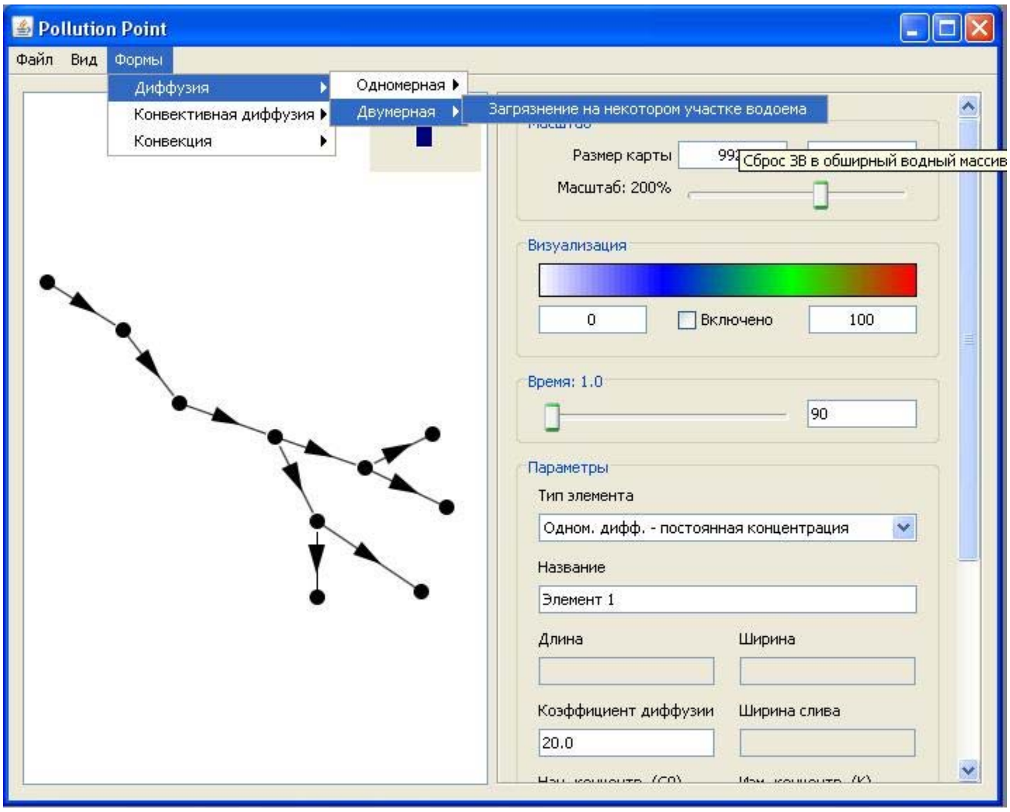

Figure 4. Screen form of the information system for input of initial data

In this information system as a criterion for assessing the potential danger of the effects of pollution on human health was chosen concentration of the pollutant. Obviously, the value of concentration at the outlet of each rib should be automatically transmitted to the input of the next rib. The main difficulty in the design of the algorithm has been in the modelling of branching and merging streams.

Branched flow corresponds to the vertex (node), which has one incoming arc, and several outgoing. In the simplest case, the concentration of pollutants at the entrance of each edge coming out of this summit, can be taken as the concentration of pollutants at the output of the previous edges.

Merging occurs when the vertex of the graph has multiple edges incoming and one outgoing. In general, incoming edges have different properties, and the results of computing the concentration of pollutants in the output is different.

Thus, the impurity concentration C at the confluence of ribs will be determined as a weighted sum of the concentrations at the outlet of the edges C_i, suitable to the vertex:

$$C = \sum_{i=1}^{n} C_i f_i \Big/ \sum_{i=1}^{n} f_i . \tag{4}$$

, where: f_i – value of the water flow in each edge – selected as weighting factors.

A program written in Java, allows you to visualize the water system consisting of various types of bodies of water, and calculate and display the mass transfer processes for the entire system and for individual water bodies, its components.

The authors developed a database that stores information about the reservoirs in the region, as well as chemical elements and maximum allowable concentrations of pollutants. All units (modules) of information systems are interconnected and represent a set of one-dimensional, two-dimensional and (or) three-dimensional models. Output parameters of the previous module are the input data for the subsequent module.

To illustrate the operation of the information system was carried out computational experiment. To do this chosen portion of the water system, which by the nature of distribution of an impurity can be divided into three parts:

- a one-dimensional diffusion limited concentration of pollutants;
- a one-dimensional diffusion with a permanent source of pollutants;
- two-dimensional diffusion with a permanent source of pollutants (figure 5).

The chosen values of input data: the diffusion coefficient model substance is 20 m^2 / day; initial concentration of 100 g / m^3; the length of the 1st section of 23.6 m.

As shown in figure 5, the results of calculation, the initial concentration of the 2 nd area is 66.03 g / m^3, and for third portion the initial concentration of 10.21 g / m^3, if the length of the 2nd area 28.02m.

At the 3rd section with a width of 50 m the concentration value at a distance of 27.46 m is equal to 0.08 g / m^3. This corresponds to a flow time of 23.75 days.

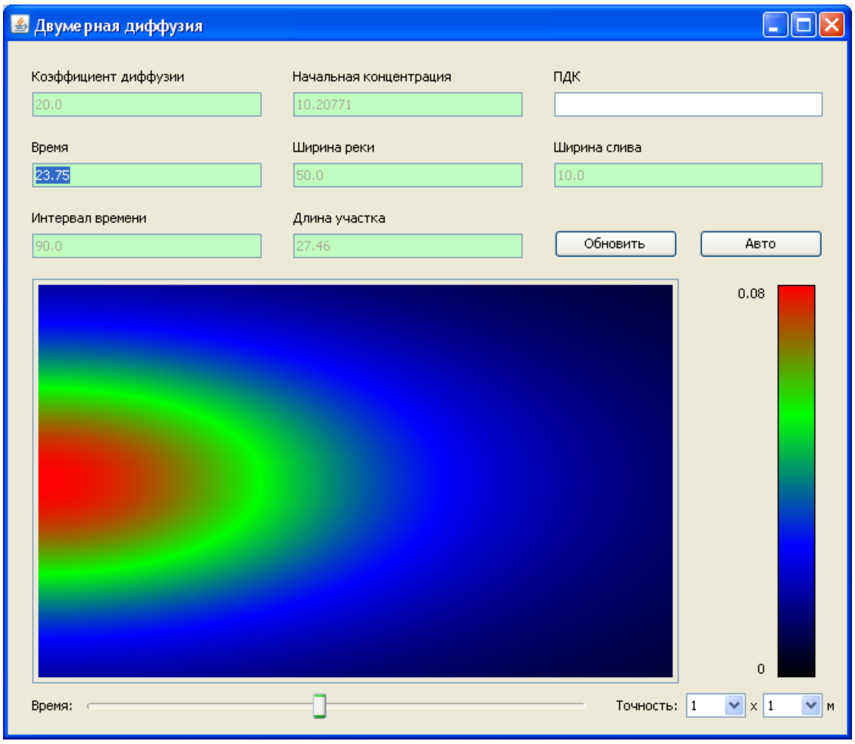

Figure 5. The screen format for the two-dimensional diffusion process

3. Results and discussions

We systematized the potential ecological situation and built the appropriate mathematical models that allowed us to obtain quantitative algorithms for solving the problems of monitoring and developing the components of the information system for calculating the concentrations of pollutants in the water system in the region.

The mathematical models and methods of graphical representation of the water environment of the region studied by the authors were used by the authors in the development of project documentation for the construction of a chemical plant (a chemical weapons destruction plant in Leonidovka settlement) in the Penza region.

4. Conclusions

The information system allows: to calculate the concentration of pollutants at any point in the water system at any point in time; visualize the calculation results in the form of text and graphic formats; save the calculation results in a file; compare the concentration of the substance in the control point with the MPC and to determine the time to reach the maximum allowable concentration.

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