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COMPUTER MODELING OF HARMFUL IMPURITIES TRANSFER

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Abstract. The paper considers solutions to the ecology problems, which set is formulated from cause-effect relationships. According to the adopted model, the equation’s coefficients for the harmful impurities transfer are attributed to the causal features of the process. Herein, the setting of cause-and-effect links is the goal of the ecology’s direct problems. Along with direct methods of mathematical modeling of harmful impurities transfer in the atmosphere from pollution sources, the paper considers the formulation and methods of solving inverse problems, which essence is to estimate the input parameters based on actual information about the modeled system, known from the experiment. Based on the research results, a software package was developed to implement the solution of the coefficient inverse problems of ecology using the mathematical modeling method.

Keywords: mathematical model, inverse methods, harmful impurities, ecology, software package.

Introduction. An essential task now is to forecast changes in ecological systems under natural and anthropogenic factors. Theoretical studies of such phenomena are based on well-known models of continuum mechanics [1]. In mathematical terms, these are multidimensional nonlinear differential equations that include a series of input parameters. Along with direct methods of mathematical modeling of harmful impurities transfer in the atmosphere from pollution sources, the paper considers the formulation and methods of solving inverse problems, which essence is to estimate the input parameters based on actual information about the modeled system, known from the experiment [2, 3]. Currently, various combinations of programs became widespread, which are often called packages or complexes of programs. This paper considers an applied software package (ASP) designed for processing by reverse methods of environmental experiments. The main goal pursued during the ASP designing is to provide significant assistance to the researcher at all stages of processing an environmental experiment by reverse methods on a PC.

Identification of harmful impurities transfer by reverse methods. To solve the inverse problems of the environment dynamics, we apply the equation's simplest approximation for the harmful impurities transfer [1]:

$$u\frac{\partial\phi}{\partial t} + \sigma\phi = D_x\frac{\partial^2\phi}{\partial x^2} + Q\delta(x - x_0), \qquad (1)$$

on a line in an infinite environment $-\propto < x < \propto$, wherein Q is the power of a point source emitting aerosol into the atmosphere; $\delta(x - x_0)$ is Dirac function. Here, the assumption that the sought-for solution is limited in the entire domain of definition should be applied as the boundary conditions. It is advisable to reduce the problem (1) to an equivalent form without further analysis without the delta function. Integrating (3.2) at the point $\mathrm{x} = \mathrm{x}_0$, we get an important relation:

$$D\frac{\partial\phi}{\partial x_{|x_o}} - D\frac{\partial\phi}{\partial x_{|x_o}} + Q = 0, \qquad (2)$$

Two areas can now be considered: $-\propto < x \le x_0,\ x_0 \le x < \propto$. Denoting the corresponding solutions through the functions φ^- u φ^+, consider two tasks:

$$\left.\begin{aligned} &D\frac{\partial^2\phi^-}{\partial x^2} - u\frac{\partial\phi^-}{\partial x} - \sigma\phi^- = 0 \\ &\phi^-_{|x\to-\propto} = 0 \end{aligned}\right\}, \quad (3)$$

$$\left.\begin{aligned} &D\frac{\partial^2\phi^+}{\partial x^2} - u\frac{\partial\phi^+}{\partial x} - \sigma\phi^+ = 0 \\ &\phi^+_{|x\to\propto} = 0 \end{aligned}\right\}, \quad (4)$$

Assuming the sought solution to be continuous at all points of the considered region, including and $x = x_0$, we arrive at the second condition:

$$\phi^+_{|x=x_0} = \phi^-_{|x=x^+} \quad (5)$$

It is easy to verify that the solutions of problems (3), (4) are connected by applying relations (2) and (5).

It is obvious that the following form [1] represents both solutions:

$$\left.\begin{aligned} &\phi^+ = C_+ \, exp\left\{-\left(\sqrt{\frac{\sigma}{D} + \frac{u^2}{4D}} - \frac{u}{2D}\right)(x - x_0)\right\}, x \geq x_0 \\ &\phi^- = C_- \, exp\left\{-\left(\sqrt{\frac{\sigma}{D} + \frac{u^2}{4D}} - \frac{u}{2D}\right)(x - x_0)\right\}, x \leq x_0 \end{aligned}\right\}, \quad (6)$$

where C_+, C_- are integration constants. Substitution (6) into relation (3), (4), transformed to the form:

$$\left.\begin{aligned} &D\frac{\partial\phi^+}{\partial x}_{|x=x_0} - D\frac{\partial\phi^-}{\partial x}_{|x=x_0} + Q = 0 \\ &\phi^+_{|x=x_0} = \phi^-_{|x=x_0} \end{aligned}\right\}, \quad (7)$$

get $C_+ = C_- = C$. Ultimate values of the constants have the following form

$$C_+ = C_- = C = \frac{Q}{\sqrt{4\sigma D + u^2}} \quad (8)$$

As a result, we have a solution to the problem in an analytical form

$$\phi(x) = C * \begin{Bmatrix} exp\left\{-\left(\sqrt{\frac{\sigma}{D}+\frac{u^2}{4D}}-\frac{u}{2D}\right)(x-x_0)\right\}, x \geq x_0 \\ exp\left\{-\left(\sqrt{\frac{\sigma}{D}+\frac{u^2}{4D}}-\frac{u}{2D}\right)(x-x_0)\right\}, x \leq x_0 \end{Bmatrix}, \qquad (9)$$

Fig. 2 demonstrates the change nature in function $\varphi(x)$ for the given input data. The simulation analysis shows that for $u > 0$ left (for $x = x_0$) part of the exhibitor is pressed against $x = x_0$, and the right one, on the contrary, spreads, which characterizes the substance drift by the wind with simultaneous diffusion.

Herein the solution to problems from cause-effect links should be attributed to the direct problems of ecology. Indeed, if the parameters:

$$\{D,\ u, \sigma,\ x_0,\ Q\},\ \in\ R, \qquad (10)$$

then, herein, the solution to any direct problem (9) is determined as a function of the spatial coordinate and as a function of the input parameters *R* (10). Therefore, from cause-effect links, each direct problem within the limits of the adopted structure (9) can be compared with some *R*-set of i*nverse problems*. Thus, any inverse problem solution from this class is finding such control that implements the goal for which the functional on the solutions of the controlled system (9) takes the least possible value. Herein, the solution of one or another inverse problem can be implemented by the method developed in [4 – 6]. Let us now consider some applied problems, which solutions can be obtained applying model (9) by inverse methods.

The following values were used as input parameters of the model:

– *U* is speed (*m/s*);

– D_b is diffusion coefficient ($m \cdot m/s$);

– *G* is absorption coefficient (*1/s*);

– *Q* is source power (*kg/s*).

Several computational experiments were carried out. Fig. 1 – 4 shows the simulation results.

Application package work illustration. When the executable file of the application package is launched, a splash screen with the name "Environmental task (Fig. 1) is displayed. Here, in an interactive mode, input data and modes of the output of computed information on the developed model are entered.

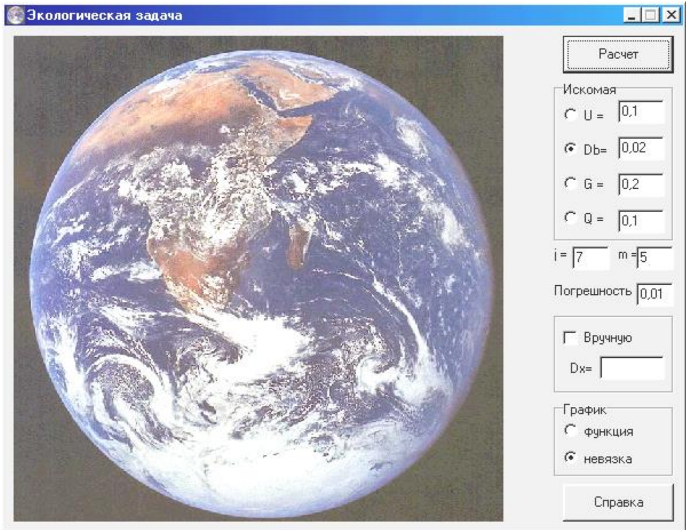

Fig. 1 Application package splash screen

Fig. 2 depicts the solution to the direct problem of ecology. Here, for the mathematical modeling mode implementation, it is possible to enter the appropriate initial conditions. Information output is implemented as a graphical dependency illustrating the function change $\varphi(x)$ nature with the given input data. Here, the graph's right side is blurred, characterizing the substance drift by the wind with simultaneous diffusion.

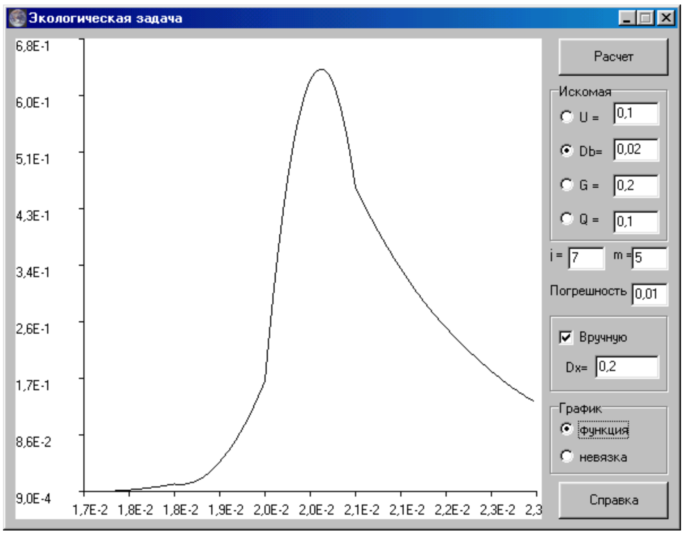

Fig. 2. Graphic interpretation of the ecology direct problem solution

Fig. 3 and Fig. 4 show the graphical dependences of the turbulent diffusion coefficient determination for different modes of input data error.

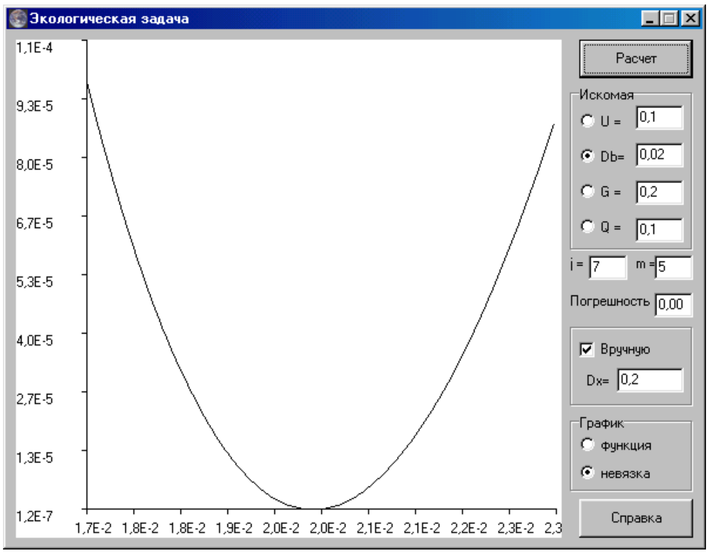

Fig. 3 Graph of changes in the turbulent diffusion coefficient with zero error in the input data

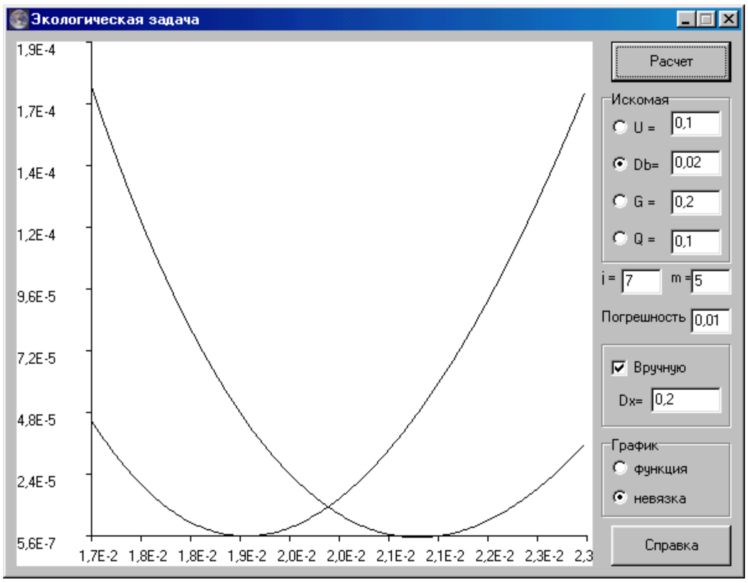

Fig. 4 Graph of changes in the turbulent diffusion coefficient with input data error + 1%

Conclusions. The paper deals with the ecology problems' solution, which set is formulated from cause-effect links. According to the adopted model, the equation's coefficients for harmful impurities transfer in a one-dimensional formulation are attributed to the causal features of the heat exchange process. Herein, the setting of cause-and-effect links is the goal of the ecology's direct problems. The paper presents the results of solving direct problems of ecology. In the above studies, the inverse problem of ecology is solved. The essence of its solution is as follows: according to certain information about atmospheric pollution, it is required to restore the causal features. Herein, one arrives at the formulation of inverse problems of ecology, which belong to the class of Hadamard ill-posed problems.

Currently, various combinations of programs became widespread, which are often called packages or complexes of programs. In this paper, an applied software package (ASP) is developed for processing environmental experiments. The main goal pursued when creating the ASP is to provide substantial assistance to the researcher at all stages of processing an environmental experiment by a PC. The ASP is applicable in planning and processing the results of an environmental experiment.

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