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COMPUTER SCIENCE

THE ENVIRONMENT DYNAMICS IDENTIFICATION BASED ON THE MODULAR COMPUTING COMPLEX

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ABSTRACT

The research aims at covering the mathematical modeling issues of multidimensional applied problems of ecology based on the application of a modular computing complex. The problem of modeling air pollution processes is solved by mathematical models that adequately describe fundamental processes. That reveals issues such as a detailed analysis of the atmosphere of the city or industrial area, short-term forecast of air quality in the region, assessment of long-term air purification programs, optimal emission management, transboundary transfer, etc. At the same time, the formulation and methods of solving problems of environmental dynamics identification are considered, which essence is to estimate the input parameters based on the factual information about the modeled system known from the experiment.

In these studies, the multidimensional equation of harmful impurities transfer was reduced to a sequence of schemes involving unknown values in a single direction, alternately in the longitudinal, transverse and vertical. The implicit schemes lead to systems of algebraic linear equations with a three-diagonal structure. Thus, the methodological basis of the difference splitting schemes provides the economic and sustainable implementation of numerical models by the scalar runs method. That approach focuses on the fact that the greatest effect of a parallel processor is achieved when it is used to perform matrix computations of linear algebra.

In order to analyze the feasibility of mathematical models, a package of applications was developed to compute the transfer of harmful impurities. A solution to several applied problems for the identification of the environmental dynamics is given.

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Analysis of the current research state to make mathematical models of the atmosphere dynamics. The basis of atmosphere dynamics' modern models is the laws of conservation of mass and energy, which along with the laws of thermodynamics; describe the processes of the atmosphere, ocean, and their interaction [1]. In mathematical terms, those are systems of multidimensional nonlinear differential equations [2 – 4]. Those systems include some input parameters known from the experiment with the specified error. The input parameters here usually mean the coefficients of the equations, the initial fields, the features of the integration domain, etc. In each case, it is possible to describe with some reliability some acceptable set of input parameters and the results of processing the measurement data to assess the system's state under consideration.

In this regard, it is notable that the solution of any particular class problem is defined as a function of the coordinates of space and time and as a function of input parameters.

Thus, to evaluate the validity of the obtained solution in the space of input parameters, it is necessary to study the behavior of the corresponding object by variations on their admissible set.

The mathematical models' sensitivity theory that considers these issues was developed in optimal control theory and identification of different systems [5]. The formulation and methods of solving inverse problems, which are its basis, estimate the input parameters from the factual information about the modeled system.

Some input parameters for ecology and environmental protection problems (power of pollution sources, turbulent diffusion coefficients, etc.) can be determined only from experimental data. Hence, to process the experimental data of the problems under consideration, it is appropriate to solve inverse problems [6].

The mathematical formulation of the research problem. Emission sources of various pollutants characterize the mathematical model of pollution transfer during technical equipment operation. The exhaust devices run contaminants removal from the working area of the equipment in the premises. The greatest effect from the exhaust devices is achieved when the ventilation outflow of polluted air can be placed close to the pollution source.

The simplest scheme of pollutant emission during the technological equipment operation, as a rule, is replaced by point sources, or a system of point sources that are characterized by a given intensity and time of emission. Thus, adequate to the entire process, a physical model is built, where the whole process of pollution transfer by technological equipment is a system of point sources of a given location, intensity, and mode of operation.

Modeling the harmful impurities transfer against the background of atmospheric processes plays a significant role in this problem study. Suppose the model structure is given and determined by a system of nonlinear differential equations of environmental mechanics. Then the state of the natural environment is described by a vector of indicators, one of which is the concentration level of harmful substances in the air basin.

Mathematically, this problem is formulated as follows. The amount of pollution per unit volume of air is denoted by Φ $\left[kg/m^3\right]$. The pollution source is presented as the point sources:

$$\vartheta_i(t)\delta(r-r_i), \quad (1)$$

where $\delta(r-r_i)$ is Dirac delta function; $\vartheta_i(t)$ is the intensity of pollution sources. Possible environmental pollution is presented as a system of n point sources:

$$\sum_{i=1}^{N}\vartheta_i\delta(r-r_i). \quad (2)$$

Under such conditions, the differential equation for the harmful impurities transfer are presented as follows:

$$\frac{\partial\Phi}{\partial t}+U_x\frac{\partial\Phi}{\partial x}+U_y\frac{\partial\Phi}{\partial y}+U_z\frac{\partial\Phi}{\partial z}+\delta\Phi=\mu\left(U_x\frac{\partial^2\Phi}{\partial x^2}+U_y\frac{\partial^2\Phi}{\partial y^2}+U_z\frac{\partial^2\Phi}{\partial z^2}\right)+P(x,y,z), \quad (3)$$

where $\{U_x, U_y, U_z\}$ are velocity vector components $\left[m/s\right]$; σ is the coefficient of spontaneous decay of particles, $\left[1/s\right]$; μ is the turbulent diffusion coefficient, m^2/s; $P(x,y,z)$ is a set of point sources modeled by relations (1), or (2).

Information about the atmosphere state, particularly the velocity vector $\{U_x, U_y, U_z\}$ components, for the problems (1) – (3) is the input.

Each specific simulation problem is possible with some probability based on a priori information to describe some good set of input parameters and the results of processing the measurement data to assess the system's initial state. Then the solution of a specific problem is defined as a function of spatial coordinates and time and as a function of input parameters. Hence, to evaluate the obtained solution, it is necessary to study its behavior with the variation of the input data. That is the essence of studying the model sensitivity to variation of input data. However, no less important are the methods of solving inverse problems, which essence includes estimating the input parameters based on the factual information about the modeled system and the information known from the experiment.

Mathematical modeling of the harmful impurities transfer problem. The differential equation for the harmful impurities (3) transfer is highly measurable and non-stationary. Efficient solutions are based on splitting the problem on a time interval $t_{y-1} \le t \le t_y$ on a sequence of simpler problems.

Reducing complex problems to simpler ones is usually possible when the original operator of the problem (3) can be represented as the sum of the simplest operators.

Therefore, considering the specified equation (3) can be shown as:

$$\frac{\partial \Phi}{\partial t} + A\Phi = f \text{ in } DxD_t \,, \tag{4}$$

where the function $A \ge 0$ does not depend on time and is formed as follows:

$$A = A_x + A_y + A_z \,. \tag{5}$$

Applying local-one-dimensional schemes of splitting by spatial variables (x, y, z) for equation (4), we can make the three simplest equations of the following form

for x :

$$\frac{\partial \Phi_1}{\partial t} + U_x \frac{\partial \Phi_1}{\partial x} + \frac{\delta}{3}\Phi_1 = \mu \frac{\partial^2 \Phi_1}{\partial x^2} + \frac{f}{3},$$
$$\Phi_1(x, y, z, t_{y-1}) = \Phi_0(x, y, z), \tag{6}$$

for y :

$$\frac{\partial \Phi_2}{\partial t} + U_y \frac{\partial \Phi_2}{\partial y} + \frac{\delta}{3}\Phi_2 = \mu \frac{\partial^2 \Phi_2}{\partial y^2} + \frac{f}{3},$$
$$\Phi_2(x, y, z, t_{y-1}) = \Phi_1(x, y, z), \tag{7}$$

for z :

$$\frac{\partial \Phi_3}{\partial t} + U_z \frac{\partial \Phi_3}{\partial z} + \frac{\delta}{3}\Phi_3 = \mu \frac{\partial^2 \Phi_3}{\partial z^2} + \frac{f}{3},$$
$$\Phi_3(x, y, z, t_{y-1}) = \Phi_2(x, y, z, t_y). \tag{8}$$

Starting from (6) - (8), the difference splitting scheme can be made in many ways. The implicit schemes lead to making systems of linear algebraic equations (SLAE)

$$C_\Phi Y_{p+1,1} - Y_{p,1} + D_p Y_{p-1,1} = f_{p,1} \,, \tag{9}$$

having a three-diagonal structure ($p = \overline{1{,}2\mathrm{m}-1}$ are network mesh numbers).

In SLAE (9), the $\{C_p, D_p, f_{p,1}\}$ coefficients include information about the equation itself, boundary, and initial conditions.

Consider further a simple and convenient method for solving difference boundary value problems of the form (9). It is one of the variants of excluding the unknown and is called the run method. Then the availability of two vectors is possible E_p and G_p , such that for any $Y_{p,1}$ there is a fair ratio

$$Y_{p,1} = E_p Y_{p+1,1} + G_p \,. \tag{10}$$

Let us lower the index by one p in equation (10), which gives

$$Y_{p-1,1} = E_{p-1} Y_{p,1} + G_{p-1}. \qquad (11)$$

Substituting $Y_{p-1,1}$ from relation (11) in SLAE (9) and solving it relatively $Y_{p,1}$, we obtain the following recurrent relation:

$$Y_{p,1} = \frac{C_p}{1 - D_p E_{p-1}} Y_{p+1,1} + \frac{D_p E_{p-1} - f_{p,1}}{1 - D_p E_{p-1}}. \qquad (12)$$

A comparative analysis of relations (9) and (12) demonstrate that they are both fair to all $Y_{p,1}$. Then we get the system:

$$E_p = \frac{C_p}{1 - D_p E_{p-1}},$$

$$G_p = \frac{D_p E_{p-1} - f_{p,1}}{1 - D_p E_{p-1}} \quad \text{at} \quad p = \overline{1, 2\text{m} - 1}. \qquad (13)$$

From the given conditions on the left border we define E_0 and G_0, then to determine E_p and G_p at all points in the direction of growth p up to $p = 2\text{m} - 1$ one can use the recurrent relation (13). Next, the value is determined from the right boundary condition $Y_{2\text{m},1}$, and equation (11) with known coefficients E_p and G_p is used to compute values $Y_{p,1}$ for $Y_{p+1,1}$, etc., in the descending direction p from $p = 2\text{m} - 1$ to $p = 1$.

Procedure (13) is called direct run, (13) - reverse. On solutions of arbitrary linear system N equations with N unknown exclusion methods usually have to spend arithmetic operations in quantity N^2. This reduction in the number of arithmetic operations for solving SLAE (9) by the run method was achieved by successfully using the specifics of this system.

The difference splitting scheme (6) - (13) is economical and certainly stable. In this sense, it combines the advantages of explicit schemes (explicit schemes do not improve in the number of arithmetic operations) and implicit schemes.

Development of methods for solving multidimensional non-stationary problems of type (1) - (3), associated with splitting methods and provides the economic and sustainable implementation of numerical models (6) - (13) on a PC.

The computer simulation results on a modular computer system. A program was run to assess the mathematical model's feasibility to compute the harmful impurities transfer in the region for areas that represent the shape of a regular rectangular parallelepiped. The computations were performed based on the multiprocessor computing system [7 – 9].

Fig. 1 demonstrates the transfer of harmful impurities concentrations from the ground source of pollution in the form of patterns and isolines in the middle horizontal plane of the parallelepiped when the velocity vector components are identically equal to zero.

Fig. 2 represents the results of modeling the transfer of harmful impurities from two-point sources of pollution at given components of the velocity vector u_x, u_y, different in the direction in the horizontal plane of the region.

For soft boundary conditions in the simulation results for the middle surfaces on the Z coordinate, there are bends of isolines (Fig.2b); the use of the same compiled algorithms based on boundary conditions of the 4th kind allows avoiding them (Fig. 2a). That circumstance also allows considering the specified boundary conditions at the modeling of transfer of impurity against atmospheric processes as transparent.

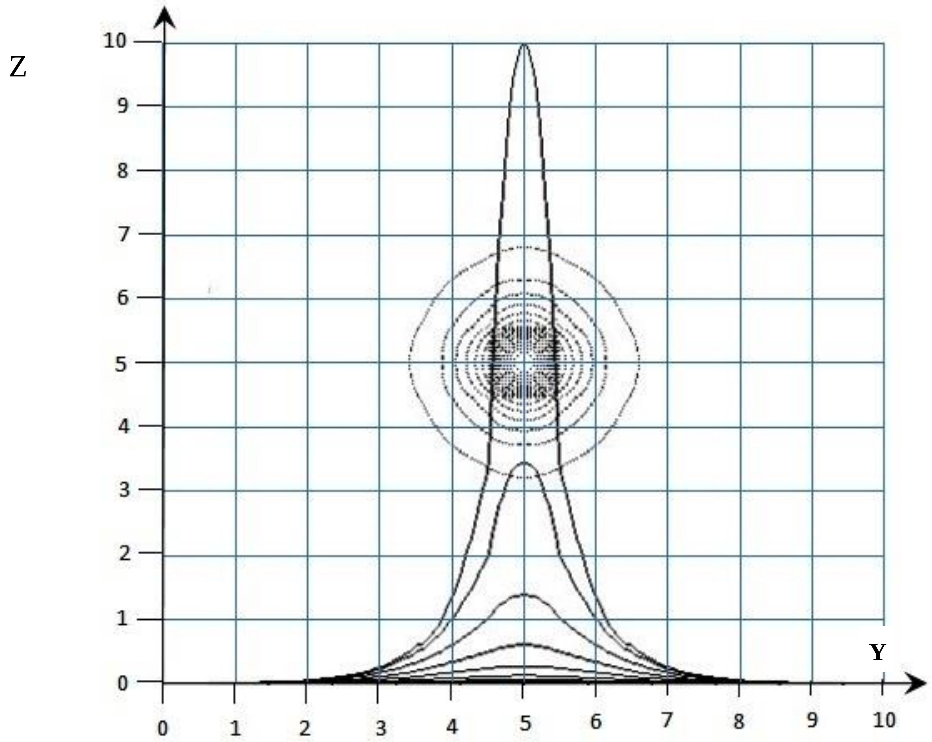

Fig. 1. Concentrations' transfer and the isolines from a point source of contaminants located in middle horizontal plane of parallelepiped's control volume

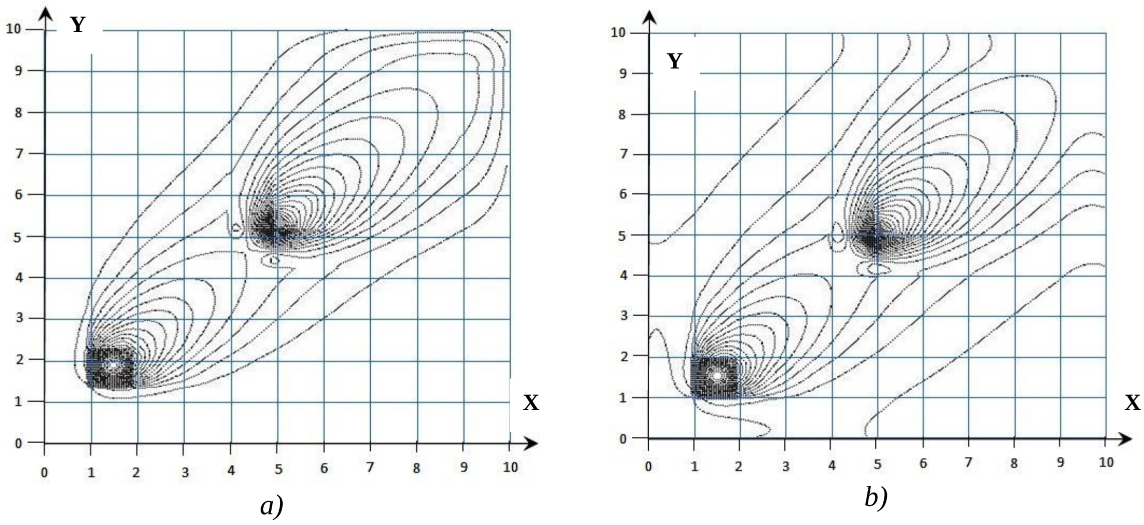

Fig. 2. Solution modeling of a three-dimensional problem under different asymptotic *boundary conditions: a) solution of a three-dimensional problem with asymptotic boundary conditions of the fourth kind; b) solution of a three-dimensional problem with soft boundary conditions of the second kind*

Conclusions. The paper covers the mathematical modeling of applied problems of ecology based on personal computing clusters. With:

1. The rapid development of industry in all countries worldwide posed to humanity an acute problem of environmental protection to preserve the planet's ecological systems. In this regard, environmental science is now forced to deal with problems of previously unknown complexity. New problems require new ways to solve them. Nevertheless, mathematical modeling, computational experiments on parallel cluster systems with a sufficiently complete mathematical content of the phenomena we study form the basis of new scientific research technology, analysis, and forecasting. Today's reality is that due to the development of parallel computing and, especially with the advent of computing clusters, the fundamental problems in the potentially infinite increase in peak performance

of computers disappeared. That opens the way to the widespread use of mathematical modeling, making basic and applied research more effective.

2. This article considers the statement and methods of solving environment dynamics identification problems which essentially consists of an estimation of input parameters on the actual information on the modeled system known from the experiment.

3. The research aims to solve the problem of modeling the air pollution processes by mathematical models that adequately describe the fundamental processes. It can explore issues such as a detailed analysis of the atmosphere of the city or industrial area, short-term forecast of air quality in the region, evaluation of long-term air purification programs, optimal emission management, transboundary transfer, etc.

4. The multidimensional equation of transfer of harmful impurities was reduced to a sequence of schemes involving unknown quantities in a single direction, alternately in the longitudinal, transverse and vertical. The use of implicit schemes leads to systems of linear equations of algebra having a three-diagonal structure. Thus, the methodological basis of the difference splitting schemes provides the economic and sustainable implementation of numerical models by scalar runs. On the other hand, it is known that the greatest effect of a parallel processor is in cases where it is used to perform matrix computations of linear algebra.

5. To analyze the mathematical models' feasibility assessment, a package of applications was developed to compute the harmful impurities transfer. The solution of several applied problems on the identification of environmental dynamics is given.

6. At the present stage of scientific research, a numerical experiment is one of the most important areas in studying the internal aerodynamics of the environment. The information obtained by numerical computations allows correctly comprehending and understanding the physical effects obtained by the experimental method and, in some cases, replacing the physical or field experiment with a machine, as is cheaper. Note that machine experiment is sometimes the only possible way to obtain information about the process under study. Given the further progress in the research methodology of parallel numerical methods and parallel computing systems, we can expect a further and significant increase in numerical computations of environmental aerodynamics problems on more complete mathematical models of atmospheric dynamics shortly.

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