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Models for environmental monitoring of the territory in the presence of concentrated sources of pollutant emissions

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Abstract. We consider models of the convection-diffusion-reaction for a substance emitted into the atmosphere by a concentrated source (stationary or moving) taking into account its decomposition into atmospheric components and gravitational sedimentation. We consider atmospheric characteristics (wind and diffusion) to be given. For example, we can take average climatic values of diffusion coefficients and air mass velocity according to the wind rose. The problem is solved in a bounded area with a known initial distribution of the impurity. One or another type of boundary conditions is selected in accordance with the content of the problem under study. If the source is an object moving at a certain speed, the problem is reduced to a series of problems with a stationary source. We use discrete approximations and a computational algorithm based on the splitting method, calculations are carried out for model territories and problem parameters. We can use the proposed models for environmental monitoring of regions and conducting environmental assessments of existing sources of pollutant emissions.

1 Introduction

Large quantities of gaseous and aerosol impurities emitted into the atmosphere, as well as mineral fertilizers introduced into the soil undergo changes in the dispersion process and change natural cycles. The threat of local and mesoscale environmental pollution requires the development of methods for modeling the transfer of pollutants. The study of the mechanisms and patterns of impurities migration in air, water and soil is extremely relevant for the development of environmental protection measures, monitoring and forecasting of pollution, and environmental assessment of technological projects.

Many products of the chemical industry, agriculture, transport, etc., belong to the so-called persistent chemical substances, the study into various aspects of the transfer of which has received close attention since the end of the last century [1-2]. In practice, various models for the migration of impurities emitted into the air and water environment are used

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[3]. For numerical modeling of such problems, finite difference methods and the finite element method are widely used.

The complexity and multiparametric nature of the propagation processes of impurities in a turbulent atmosphere makes the air quality forecasting models cumbersome and demanding for computing resources [8]. As an alternative, one could use the simplified models for the operative calculation of the spatial-temporal impurities distribution in the atmospheric layer, allowing assessing the state of the environment and calculating the distribution of the pollutant.

In the work, we consider concentrated stationary and moving sources with a constant speed as sources of primary emission. Models for a moving source also allow us to evaluate the efficiency of field treatment using specialized drones.

2 Materials and methods

In this paper, we consider a model of migration for a gaseous or aerosol impurities coming from a concentrated source, taking into account a number of physical mechanisms responsible for the evolution of the substance in the environment. We consider both stationary and moving emission sources.

2.1 Model of migration for a multicomponent substance

The model is considered in a Cartesian coordinate system. The main equation of transport for a multicomponent substance is written as:

$$\frac{\partial \varphi_j}{\partial t} + \operatorname{div}\left(\varphi_j \mathbf{a} - \boldsymbol{\mu}\operatorname{grad}\left(\varphi_j\right)\right) + \left(\mathbf{B}\boldsymbol{\varphi}\right)_j = f_j\left(\mathbf{x},t\right), \; j = \overline{1,n}. \tag{1}$$

In (1) the following designations are adopted: $\boldsymbol{\varphi}(\mathbf{x},t) = \{\varphi_1,\ldots,\varphi_n\}$ – concentrations of the substance elements, $\mathbf{x} = (x_1, x_2, x_3)$, $\mathbf{a} = (u, \upsilon, w - w_{gj})$, u, υ, w are air flow velocities, w_{gj} is value of the gravitational sedimentation velocity of the *j*-th substance. The wind characteristics of the atmosphere are determined from the equations of hydrothermodynamics [3], but in some cases the speeds of air masses can be considered given. In this paper, the vertical profiles of the wind speed components are considered to be given. The operator $\mathbf{B}$ describes the transformation reactions of impurities. For conservative impurities, the elements of the diagonal matrix $\mathbf{B} = \|\sigma_{mn}\|$ ($\sigma_{mn} = 0,\; m \neq n$) characterize the degradation rates of its components. If the transformations of a complex substance in the atmosphere are described only by means of effective degradation coefficients, we arrive at *n* disconnected initial-boundary value problems for the components of the impurity $\varphi_j(\mathbf{x},t)$, $j = \overline{1,n}$. In system (1), we introduce the diffusion tensor $\boldsymbol{\mu} = \|\mu_{mn}\|$, $m,n = \overline{1,3}$, however, in the following, only its diagonal elements ($\mu_{mn} = 0,\; m \neq n$),which characterize the intensity of turbulent exchange in the direction of the axes of the selected Cartesian coordinate system, are taken into account. In the right part of system (1), the functions f_j specify the locations and powers of emission sources for the *j*-th component of the impurity $\mathbf{f} = \{f_1,\ldots,f_n\}$.

Active impurities $(\varphi_1, \varphi_2, \ldots, \varphi_n)$ as a result of chemical reactions with atmospheric air compounds can form chains of chemical substances $\varphi_i = \varphi_{i0} \to \varphi_{i1} \to \varphi_{i2} \ldots \to \varphi_{im_i}$. In this case, system (1) should be supplemented with $\sum_i m_i$ new equations.

The problem under consideration gives a solution within a given area that satisfies system:

$$\frac{\partial \varphi_j}{\partial t} + \operatorname{div}(\varphi_j \mathbf{a}) - \sum_{k=1}^{3} \frac{\partial}{\partial x_k}\left(\mu_{kk} \frac{\partial \varphi_j}{\partial x_k}\right) + \sigma_j \varphi_j = f_j(\mathbf{x}, t), \; j = \overline{1, n}, \tag{2}$$

And the given initial and boundary conditions for each component of the impurity. System (2) is solved in the area $D_t = D \times [t_j, t_{j+1}]$ for $D = \{-X < x_1 < X, -Y < x_2 < Y, h < x_3 < H\}$. Boundary conditions may vary depending on the studied problem. Thus, conditions for the impurity concentration to reach its background values or impermeability conditions may be specified on the upper face and side surfaces of D [3].

For a heterogeneous underlying surface, mixed boundary conditions can be set, taking into account the ability of different regions to reflect or accumulate pollutants. The general form of such conditions for each of the heterogeneous regions can be represented as:

$$\left.\left(\mu_3 \frac{\partial \varphi}{\partial x_3} - \vartheta_l \varphi\right)\right|_{x_3=0} = q_l(x_1, x_2, t), \; (x_1, x_2) \in \Sigma_l \;, \; l = \overline{1, L}.$$

Here the parameter ϑ_l is determined by the properties of the region according to the land use categories: forest, swamp, water surface, etc.

Solution (2) is sought in the interval $t \in [0, T]$ on the set of non-negative solutions that satisfy the formulated boundary conditions. Numerical modeling based on the use of difference schemes. The computational algorithms used to solve the problem are based on the process splitting method. To construct stable difference schemes of the second order of approximation in *t*, we used the Crank–Nicholson scheme.

2.2 The moving source model

Unmanned agricultural aviation is currently effectively used in crop production, including for spraying pesticides to combat pests and diseases. We considered the convection-diffusion problem of a single-component aerosol emitted by a moving concentrated source, simulating an agricultural drone, in a three-dimensional domain.

For a moving concentrated source, we reduce the function $\mathbf{f}(\mathbf{x}, t)$, which specifies its location and intensity, to a difference form $\mathbf{f}_k^j = \mathbf{f}(x_k, \tau_j)$, where $x_k = x_k(\tau_j)$, so that the problem can be represented as a series of problems with a stationary source. Solving each of these problems and using the condition of continuity for concentration $\boldsymbol{\varphi}$, we obtain a solution to the problem for a moving source.

In the software implementation of the task for a single-component impurity, all parameters specific to a particular run (area size, number of partitions, diffusion coefficients, etc.) are specified at the beginning of the module as constants, from which the associated parameters (partition grid, partition step, etc.) are then calculated. Before the start of the time cycle, the values of the matrix elements and the function *f* are calculated at the initial moment of time, taking into account the initial and boundary conditions. Then, for each value t_j from the time grid created according to the input parameters, the above values are calculated again, since the source is moving.

3 The results of solving certain model problems

For the grid area D_τ^h we constructed the discrete approximations and the computational algorithm scheme using the process splitting method [3]. The system of linear equations of the difference evolutionary problem is solved by the tridiagonal matrix algorithm. As a result, we obtained the values of the spatiotemporal distribution for the substance.

The implemented numerical models allow us to predict the intensity of substance dispersion for various sets of parameter values that are significant for practice. The results of computational experiments based on the described models are presented in Figures 1, 2 and 3.

With specific cartographic and technological reference, the developed models are applicable for analyzing the environmental situation in a region and can become one of the tools for environmental assessment. The authors used a digital model of the region built at the Kuban University [12], where information about the value of the pollutant concentration is graphically displayed in the form of a point layer. Figure 1 shows the level lines for the horizontal section of the concentration field of a single-component pollutant for a given time step (2 h after the start of the simulation) for different model data at an altitude of 300 m and two different point sources located at altitudes of 200 m (left) and 100 m (right), grid parameters: $\tau = 600$ s, $\Delta x_j = 2000$ m $(j = 1, 2)$, $\Delta x_3 = 100$ m.

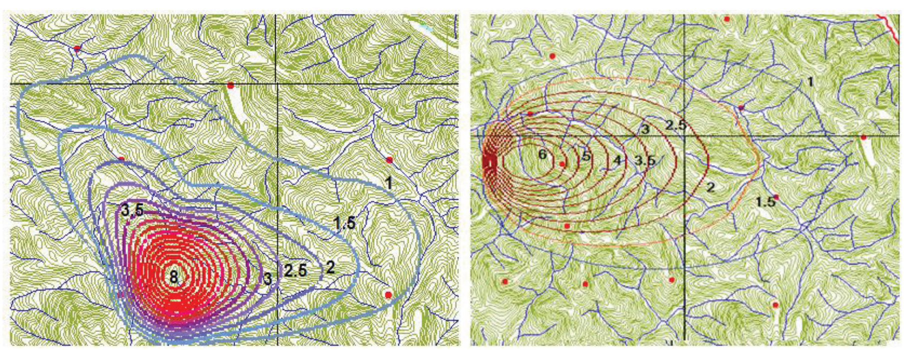

Fig. 1. Examples of the cartographic reference for the results for various model parameters in a digital model of the region.

Figure 2 shows pollution levels in navigation mode, which has less detail.

The implemented models can be supplemented with reactions between the impurity components according to system (1). They allow calculation of concentrations and distributions of substances at given heights in given areas by varying the location of sources and emission powers. They can be used in regional monitoring systems, as they provide the opportunity to study the influence of various factors on the environmental situation of given territories, predicting both the overall picture of pollution by various substances and the contribution of individual radiation sources.

Figure 3 illustrates the process of dispersion for a single-component impurity at the height of a source moving at a constant speed ($u_1 = 1, \upsilon_1 = 1$) and emitting a precipitating impurity over 20 time steps.

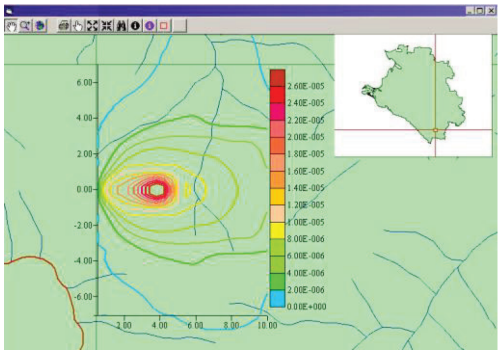

Fig. 2. Pollutant distribution in the system navigation window.

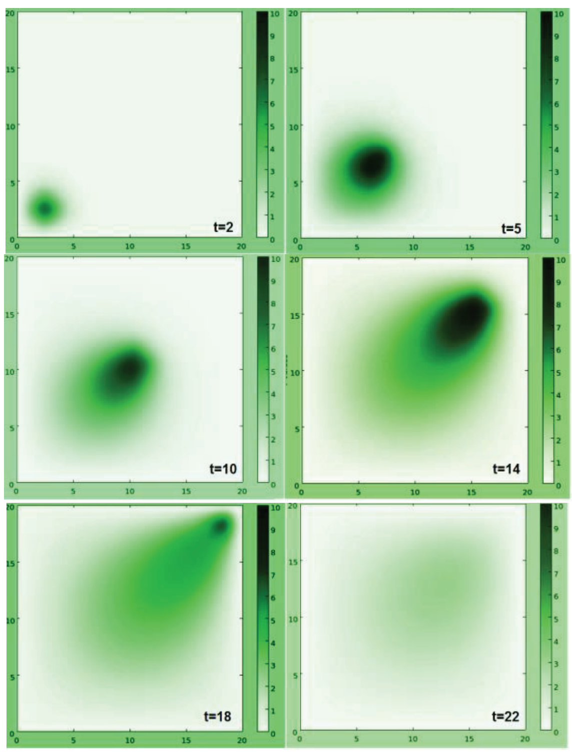

Fig. 3. Concentration of an impurity at the height of a source moving at a constant speed, emitting an impurity over 20 time steps.

4 Conclusion

The development of methods for mathematical modeling of the spread for pollutants emitted into the air and water environment is relevant in connection with the growing scale of anthropogenic impact on nature.

In this paper we consider models of convection-diffusion-reaction for a substance emitted into the atmosphere by a concentrated source (stationary or moving), taking into account its decomposition into atmospheric components and gravitational sedimentation. Atmospheric characteristics (wind and diffusion) are considered given. For example, average climatic values of diffusion coefficients and air mass velocity can be taken according to the wind rose. The problem is solved in a bounded area with a known initial distribution of the impurity. One or another type of boundary conditions is selected in accordance with the content of the problem being studied.

If the source is represented by an object moving at a certain speed, the problem is reduced to a series of problems with a stationary source.

We selected discrete approximations and a computational algorithm scheme based on the splitting method and performed calculations for model areas and task parameters.

The described models can be integrated into an environmental geographic information system used in environmental protection, resource management, land use planning, etc. Environmental organizations can use such models in air quality analysis and water quality monitoring systems.

The equations considered in the work are the basis for describing mathematical models of processes of various natures (diffusion of an electrically charged impurity in a solid, heat transfer, etc.) The approach developed in the work can also be applied to the study of mantle convection problems, interest in which is currently extremely high.

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