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In order to integrate the task, an implicit finite-difference scheme and an algorithm with the second order of approximation in terms of time and space variables were developed with the help of which numerical calculations can be carried out on a computer system, on the basis of which it is possible to investigate and predict the ecological state of the industrial region under consideration. To investigate the adequacy of the developed mathematical apparatus, computational experiments were carried out on a computer, the results of which were compared with full-scale data of a real production facility located in the Tashkent region of Uzbekistan.

Topics

Development of a Mathematical Model of Aerosol Particles' Distribution Process in the Surface Layer of the Atmosphere taking into Account the Earth's Heterogeneous Surface

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Abstract. In this paper, a mathematical model, a numerical algorithm for the process of transfer and diffusion of harmful substances, is developed, which takes into account the wind speed in three directions and the rate of deposition of aerosol particles on the underlying surface, as well as the capture of particles by vegetation elements, which play a significant role in the dynamics of the object of study.

In order to integrate the task, an implicit finite-difference scheme and an algorithm with the second order of approximation in terms of time and space variables were developed with the help of which numerical calculations can be carried out on a computer system, on the basis of which it is possible to investigate and predict the ecological state of the industrial region under consideration. To investigate the adequacy of the developed mathematical apparatus, computational experiments were carried out on a computer, the results of which were compared with full-scale data of a real production facility located in the Tashkent region of Uzbekistan.

INTRODUCTION

The environmental task (as a set of issues of environmental protection and rational use of natural resources), which is a global problem, affects the interests of the entire population of our planet and the interests of every person living on Earth. The pace of development of civilization and its impact on natural resources has led to the fact that the control and management of the environment have become the most urgent problems of our time. At present, attention to the study of atmospheric pollution has increased considerably. The nature of these studies has also changed substantially. The problem of environmental protection is extremely science-intensive and is located at the intersection of a number of areas of physics, chemistry and mathematics. It requires a large amount of theoretical and experimental research aimed at monitoring and predicting the state of the surface layer of the atmosphere and the earth's underlying surface.

To solve such problems, it is necessary to develop mathematical models (MM) and efficient algorithms based on numerical methods, using which one can conduct computational experiments (CE) on computer systems (CS).

As we know, methods of mathematical modeling become an important tool for analyzing the management of the development of complex systems, since when solving problems on the aircraft, a certain technological chain has developed: the object of study - a physical model - a mathematical model - a numerical algorithm - a program - calculation for the aircraft, comparison with experimental and other data. Mathematical part of the instrument or computational part of this chain: mathematical model - numerical algorithm - software tool for conducting computational experiments (CE) on the aircraft.

The tasks of modeling the transfer and diffusion of harmful substances are studied in scientific schools created under the guidance of foreign scientists J.W. Deardorff, M.Germano, U.Piomelli, L.C.Berselli, G.S. Winckelmans, W.C. Reynolds, T. Iversen., T.E. Nordeng, R.Lange, M Pekar, G.I. Marchuk, V.V. Penenko, A.E. Aloyan, M.E. Berlyand, Yu.A. Anokhin, A.Kh. Ostromogilsky, L.T. Matveev, V.P. Dymnikov, I.E. Naats, I.A. Kibel, L.N. Gutman and others.

It should be noted that research is being conducted by these scientists and their colleagues in leading research centers and they have obtained significant results of a fundamental and applied nature. In particular, in the work [1], a hydrodynamic model of the long-range transport of aerosol particles in the surface layer of the atmosphere is proposed, where the main physical and mechanical properties and process factors are considered.

In works [2, 3], the process of transfer of harmful substances is studied emitted from production facilities in the atmosphere, and the main criteria for the danger of air pollution are formulated. The concept of the maximum allowable concentration of a harmful substance in the atmospheric air of industrial regions is given by the authors of the article and the concept of especially dangerous air pollution is also considered, and the values of concentrations at different levels of danger are set.

The paper [4] proposes a model for the dispersion of pollutants in the air based on the Gaussian plume, which takes into account the transport of pollutants emitted from open sources. The paper presents numerical experiments illustrating the validity of the computational base. The author of the article conducted numerical experiments in two parts in order to solve the problem. An example of advection-diffusion equations with an exact solution is given in the first part. The effectiveness of discontinuous Galerkin methods is checked. The second part discusses the experiment with the area of consideration for uneven terrain.

The authors of the work [5] developed a model, a numerical algorithm, and a software tool for research, forecasting, and monitoring, as well as for assessing the ecological state of the atmosphere and the underlying surface of the region under consideration by passive and active impurities, which take into account the main parameters and disturbances affecting the object as a whole. To determine the velocities of aerosol particles under the action of an air flow, a system of nonlinear differential equations in partial derivatives was obtained, which involves the basic physical and mechanical properties of aerosol particles, which play an important role in the process under consideration.

The work [6] discusses the development of a mathematical model for the process of propagation of aerosol particles in the atmospheric surface layer. The proposed mathematical model serves to solve the problems of monitoring and forecasting the ecological state of the environment of industrial regions. Computational experiments were carried out on a computer in order to check the adequacy of the developed mathematical apparatus, the results of which were compared with field data of a real production facility located in the Bukhara region of Uzbekistan.

The article [7] developed a model of the process of distribution of industrial emissions in the atmosphere, taking into consideration the settling rate of fine particles, which is described using a multidimensional partial differential equation with appropriate initial and boundary conditions.

Although the above works obtained significant results of a fundamental and applied nature, they do not consider the spread of harmful substances, considering the heterogeneity and roughness of the earth's surface: vegetation cover, forest belt, high-rise residential and industrial facilities.

STATEMENT OF THE PROBLEM

Considering the above, in order to study the process of transfer and diffusion of aerosol particles in the atmosphere, involving the essential parameters - the components of the wind speed in directions, respectively, as well as the orography of the area under consideration, we consider the MM, which describes based on the law of hydromechanics:

$$\frac{\partial\theta}{\partial t} + u\frac{\partial\theta}{\partial x} + v\frac{\partial\theta}{\partial y} + (w - w_g)\frac{\partial\theta}{\partial z} + \sigma\theta + \alpha\theta = \mu\frac{\partial^2\theta}{\partial x^2} + \mu\frac{\partial^2\theta}{\partial y^2} + \frac{\partial}{\partial z}\left(\kappa\frac{\partial\theta}{\partial z}\right) + \delta Q; \tag{1}$$

with the corresponding initial and boundary conditions:

$$\left. \boldsymbol{\theta} \right|_{t=0} = \boldsymbol{\theta}^0; \tag{2}$$

$$-\mu \left. \frac{\partial \theta}{\partial x} \right|_{x=0} = \xi \left(\theta_E - \theta \right); \left. \mu \frac{\partial \theta}{\partial x} \right|_{x=Lx} = \xi \left(\theta_E - \theta \right); \tag{3}$$

$$-\mu \left. \frac{\partial \theta}{\partial y} \right|_{y=0} = \xi \left(\theta_E - \theta \right); \left. \mu \frac{\partial \theta}{\partial y} \right|_{y=L_y} = \xi \left(\theta_E - \theta \right); \tag{4}$$

$$-\kappa \frac{\partial \theta}{\partial z}\Big|_{z=0} = (\beta \theta - f_0); \kappa \frac{\partial \theta}{\partial z}\Big|_{z=H_z} = \xi (\theta_E - \theta).$$
⁽⁵⁾

Where θ is the concentration of harmful substances in the atmosphere; *t* is time; θ^0 is the primary concentration of harmful substances in the atmosphere; θ_E is the concentration entering through the boundaries of the area under consideration; w_g is the particle settling rate; σ is a coefficient of absorption of harmful substances in the atmosphere;

 $\alpha(z)$ is the coefficient characterizing the capture of particles by vegetation elements; μ, κ are the diffusion and turbulence coefficients; Q is the power of the source; δ is the Dirac delta-function; ξ is the mass transfer coefficient across the calculation boundaries; β is the coefficient of interaction of particles with the underlying surface; f_0 is the stationary source of emission of harmful substances from the underlying surface of the earth.

Since the task is described by multidimensional partial differential equations, it is difficult to obtain an analytical solution.

For the numerical solution of problem (1)-(5), the area of variation of the required variable (concentration of harmful substances), taking into account the boundary conditions, will be covered with a square grid with a step Δx ; Δy ; Δz :

$$\Omega_{xyzt} = \left\{ (x_i = i\Delta x, y_j = j\Delta y, z_k = k\Delta z, \tau_n = n\Delta t); \\ i = \overline{1, N_x}; \ j = \overline{1, M_y}, \ k = \overline{1, L_z}, \ n = \overline{0, N_t}, \ \Delta t = \frac{1}{N_t} \right\}$$

Equation (1) is divided into three directions in time Δt and approximated along the direction of the Ox axis and we get:

$$\begin{split} \frac{\theta_{i,j,k}^{n+1/3} - \theta_{i,j,k}^{n}}{\Delta t/3} + \begin{pmatrix} u - |u| \\ 2 \end{pmatrix} \frac{\theta_{i+1,j,k}^{n+1/3} - \theta_{i,j,k}^{n+1/3}}{\Delta x} + \begin{pmatrix} u + |u| \\ 2 \end{pmatrix} \frac{\theta_{i,j,k}^{n+1/3} - \theta_{i-1,j,k}^{n+1/3}}{\Delta x} + \\ &+ \begin{pmatrix} \frac{(v - |v|)}{2} \end{pmatrix} \frac{\theta_{i,j+1,k}^{n} - \theta_{i,j,k}^{n}}{\Delta y} + \begin{pmatrix} \frac{(v + |v|)}{2} \end{pmatrix} \frac{\theta_{i,j,k}^{n} - \theta_{i,j-1,k}^{n}}{\Delta y} + \\ &+ \begin{pmatrix} \frac{(w - w_{g}^{n+1/3}) - |w - w_{g}^{n+1/3}}{2} \\ \frac{(w - w_{g}^{n+1/3}) + |w - w_{g}^{n+1/3}}{2} \end{pmatrix} \frac{\theta_{i,j,k-1}^{n} - \theta_{i,j,k}^{n}}{\Delta z} + \\ &+ \begin{pmatrix} \frac{(w - w_{g}^{n+1/3}) + |w - w_{g}^{n+1/3}}{2} \\ \frac{(w - w_{g}^{n+1/3}) + |w - w_{g}^{n+1/3}}{2} \end{pmatrix} \frac{\theta_{i,j,k-1}^{n} - \theta_{i,j,k-1}^{n}}{\Delta z} + \\ &+ \sigma \theta_{i,j,k}^{n+1/3} + \alpha \theta_{i,j,k}^{n+1/3} = \mu \frac{\theta_{i+1,j,k}^{n+1/3} - 2\theta_{i,j,k}^{n+1/3} + \theta_{i-1,j,k}^{n+1/3}}{\Delta x^{2}} + \mu \frac{\theta_{i,j+1,k}^{n} - 2\theta_{i,j,k}^{n} + \theta_{i,j-1,k}^{n}}{\Delta y^{2}} + \\ &+ \frac{\kappa_{k+0.5} \theta_{i,j,k+1}^{n} - (\kappa_{k+0.5} + \kappa_{k-0.5}) \theta_{i,j,k}^{n} + \kappa_{k-0.5} \theta_{i,j,k-1}^{n}}{\Delta z^{2}} + \frac{1}{3} \delta_{i,j,k} Q. \end{split}$$

To simplify the equation above, we introduce the following notation:

$$\begin{split} a_{i,j,k} &= -\frac{(u+|u|)\Delta x + 2\mu}{2\Delta x^2}, \ b_{i,j,k} = -\frac{1}{\Delta t/3} - \frac{|u|}{\Delta x} - \sigma - \alpha - \frac{2\mu}{\Delta x^2}, \ c_{i,j,k} = \frac{(u-|u|)\Delta x - 2\mu}{2\Delta x^2}, \\ d_{i,j,k} &= -\frac{\theta_{i,j,k}^n}{\Delta t/3} + \left(\frac{v-|v|}{2}\right) \frac{\theta_{i,j+1,k}^n - \theta_{i,j,k}^n}{\Delta y} + \left(\frac{v+|v|}{2}\right) \frac{\theta_{i,j,k}^n - \theta_{i,j-1,k}^n}{\Delta y} + \\ &+ \left(\frac{\left(\frac{(w-w_g^{n+1/3})}{2}\right) - \left|w-w_g^{n+1/3}\right|}{2}\right) \frac{\theta_{i,j,k}^n - \theta_{i,j,k-1}^n}{\Delta z} - \mu \frac{\theta_{i,j+1,k}^n - 2\theta_{i,j,k}^n + \theta_{i,j-1,k}^n}{\Delta y^2} - \\ &- \frac{\kappa_{k+0,5}\theta_{i,j,k+1}^n - (\kappa_{k+0,5} + \kappa_{k-0,5})\theta_{i,j,k}^n + \kappa_{k-0,5}\theta_{i,j,k-1}^n}{\Delta z^2} - \frac{1}{3}\delta_{i,j,k}Q. \end{split}$$

As a result, we obtain a tridiagonal system of linear algebraic equations (SLAE):

$$a_{i,j,k}\theta_{i-1,j,k}^{n+1/3} - b_{i,j,k}\theta_{i,j,k}^{n+1/3} + c_{i,j,k}\theta_{i+1,j,k}^{n+1/3} = -d_{i,j,k}.$$
(6)

In the boundary condition (3) we use the approximation of the second order of accuracy, and for x=0 we have

$$-\mu \frac{-3\theta_{0,j,k}^{n+1/3} + 4\theta_{1,j,k}^{n+1/3} - \theta_{2,j,k}^{n+1/3}}{2\Delta x} = \xi \theta_E - \xi \theta_{0,j,k}^{n+1/3}$$

or

$$3\mu\theta_{0,j,k}^{n+1/3} - 4\mu\theta_{1,j,k}^{n+1/3} + \mu\theta_{2,j,k}^{n+1/3} = 2\Delta x\xi\theta_E - 2\Delta x\xi\theta_{0,j,k}^{n+1/3}.$$
(7)

From the resulting tridiagonal system of linear algebraic equations for x=1 we have

$$a_{1,j,k}\boldsymbol{\theta}_{0,j,k}^{n+1/3} - b_{1,j,k}\boldsymbol{\theta}_{1,j,k}^{n+1/3} + c_{1,j,k}\boldsymbol{\theta}_{2,j,k}^{n+1/3} = -d_{1,j,k}$$

and find $\theta_{2,j,k}^{n+1/3}$ like this:

$$\boldsymbol{\theta}_{2,j,k}^{n+1/3} = -\frac{a_{1,j,k}}{c_{1,j,k}} \boldsymbol{\theta}_{0,j,k}^{n+1/3} + \frac{b_{1,j,k}}{c_{1,j,k}} \boldsymbol{\theta}_{1,j,k}^{n+1/3} - \frac{d_{1,j,k}}{c_{1,j,k}} \tag{8}$$

Equation (8) is substituted $\theta_{2, j, k}^{n+1/3}$ in (7)

$$3\mu\theta_{0,j,k}^{n+1/3} - 4\mu\theta_{1,j,k}^{n+1/3} - \mu\frac{a_{1,j,k}}{c_{1,j,k}}\theta_{0,j,k}^{n+1/3} + \mu\frac{b_{1,j,k}}{c_{1,j,k}}\theta_{1,j,k}^{n+1/3} - \mu\frac{d_{1,j,k}}{c_{1,j,k}} = 2\Delta x\xi\theta_E - 2\Delta x\xi\theta_{0,j,k}^{n+1/3};$$

and found $\theta_{0,j,k}^{n+1/3}$ in the following form:

$$\theta_{0,j,k}^{n+1/3} = \frac{4\mu c_{1,j,k} - b_{1,j,k}\mu}{3\mu c_{1,j,k} - a_{1,j,k}\mu + 2\Delta x\xi} \theta_{1,j,k}^{n+1/3} + \frac{\mu d_{1,j,k} + 2\Delta x\xi c_{1,j,k}\theta_E}{3\mu c_{1,j,k} - a_{1,j,k}\mu + 2\Delta x\xi}.$$
(9)

Using the above formulas (9), we find the values of the sweep coefficients $\alpha_{0,j,k}$ and $\beta_{0,j,k}$:

$$\alpha_{0,j,k} = \frac{4\mu c_{1,j,k} - b_{1,j,k}\mu}{3\mu c_{1,j,k} - a_{1,j,k}\mu + 2\Delta x\xi}; \ \beta_{0,j,k} = \frac{\mu d_{1,j,k} + 2\Delta x\xi c_{1,j,k}\theta_E}{3\mu c_{1,j,k} - a_{1,j,k}\mu + 2\Delta x\xi}.$$
(10)

Similarly, using the above actions for the boundary condition (3), for $x = L_x$ we obtain

$$\mu \frac{\theta_{N-2,j,k}^{n+1/3} - 4\theta_{N-1,j,k}^{n+1/3} + 3\theta_{N,j,k}^{n+1/3}}{2\Delta x} = \xi \theta_E - \xi \theta_{N,j,k}^{n+1/3}$$

or

$$\mu \theta_{N-2,j,k}^{n+1/3} - 4\mu \theta_{N-1,j,k}^{n+1/3} + 3\mu \theta_{N,j,k}^{n+1/3} = 2\Delta x \xi \theta_E - 2\Delta x \xi \theta_{N,j,k}^{n+1/3}.$$
(11)

Sequentially applying the sweep method for N-1 and N-2, we find $\theta_{N-1,j,k}^{n+1/3}$ and $\theta_{N-2,j,k}^{n+1/3}$:

$$\boldsymbol{\theta}_{N-1,j,k}^{n+1/3} = \alpha_{N-1,j,k} \boldsymbol{\theta}_{N,j,k}^{n+1/3} + \beta_{N-1,j,k};$$
(12)

$$\theta_{N-2,j,k}^{n+1/3} = \alpha_{N-2,j,k} \theta_{N-1,j,k}^{n+1/3} + \beta_{N-2,j,k} = = \alpha_{N-2,j,k} \left(\alpha_{N-1,j,k} \theta_{N,j,k}^{n+1/3} + \beta_{N-1,j,k} \right) + \beta_{N-2,j,k} = = \alpha_{N-2,j,k} \alpha_{N-1,j,k} \theta_{N,j,k}^{n+1/3} + \alpha_{N-2,j,k} \beta_{N-1,j,k} + \beta_{N-2,j,k}.$$
(13)

Substituting $\theta_{N-1,j,k}^{n+1/3}$ and $\theta_{N-2,j,k}^{n+1/3}$ from (12) and (13), instead $\theta_{N-1,j,k}^{n+1/3}$ and $\theta_{N-2,j,k}^{n+1/3}$ from (11) we find $\theta_{N,j,k}^{n+1/3}$: $\alpha_{N-2,j,k}\alpha_{N-1,j,k}\mu\theta_{N,j,k}^{n+1/3} + \alpha_{N-2,j,k}\beta_{N-1,j,k}\mu + \beta_{N-2,j,k}\mu - 4\alpha_{N-1,j,k}\mu\theta_{N,j,k}^{n+1/3} -$

$$\chi_{N-2,j,k}\alpha_{N-1,j,k}\mu\theta_{N,j,k} + \alpha_{N-2,j,k}\beta_{N-1,j,k}\mu + \beta_{N-2,j,k}\mu - 4\alpha_{N-1,j,k}\mu\theta_{N,j,k} - 4\beta_{N-1,j,k}\mu + 3\mu\theta_{N,j,k}^{n+1/3} = 2\Delta x\xi\theta_E - 2\Delta x\xi\theta_{N,j,k}^{n+1/3};$$

$$\theta_{N,j,k}^{n+1/3} = \frac{2\Delta x \xi \,\theta_E - \left(\beta_{N-2,j,k} + \alpha_{N-2,j,k} \beta_{N-1,j,k} - 4\beta_{N-1,j,k}\right) \mu}{2\Delta x \xi + \left(\alpha_{N-2,j,k} \alpha_{N-1,j,k} - 4\alpha_{N-1,j,k} + 3\right) \mu}.$$
(14)

In the reverse course of the sweep in successively decreasing order of the index i, the concentration values are determined $\theta_{N-1,j,k}^{n+1/3}$, $\theta_{N-2,j,k}^{n+1/3}$, ..., $\theta_{0,j,k}^{n+1/3}$:

$$\theta_{i,j,k}^{n+1/3} = \alpha_{i,j,k} \theta_{i+1,j,k}^{n+1/3} + \beta_{i,j,k}; \ i = \overline{N-1,0}, \ j = \overline{1,M-1}, \ k = \overline{1,L-1}.$$
(15)

Similarly, applying the above procedures for equation (1) in the direction of the axis Oy, we have the following tridiagonal system of linear algebraic equations:

$$\overline{a}_{i,j,k}\theta_{i,j-1,k}^{n+2/3} - \overline{b}_{i,j,k}\theta_{i,j,k}^{n+2/3} + \overline{c}_{i,j,k}\theta_{i,j+1,k}^{n+2/3} = -\overline{d}_{i,j,k}.$$
(16)

Using formulas (16), we find the values of the sweep coefficients $\overline{\alpha}_{i,0,k}$ and $\overline{\beta}_{i,0,k}$:

$$\overline{\alpha}_{i,0,k} = \frac{4\mu\overline{c}_{i,1,k} - \overline{b}_{i,1,k}\mu}{3\mu\overline{c}_{i,1,k} - \overline{a}_{i,1,k}\mu + 2\Delta y\xi}; \ \overline{\beta}_{i,0,k} = \frac{\mu\overline{d}_{i,1,k} + 2\Delta y\xi\overline{c}_{i,1,k}\theta_E}{3\mu\overline{c}_{i,1,k} - \overline{a}_{i,1,k}\mu + 2\Delta y\xi}.$$
(17)

Similarly, using the above actions in the boundary condition (4), with the direction of the axis $y = L_y$, we obtain:

$$\theta_{i,M,k}^{n+2/3} = \frac{2\Delta y \xi \theta_E - \mu \overline{\alpha}_{i,M-2,k} \overline{\beta}_{i,M-1,k} - \mu \overline{\beta}_{i,M-2,k} + 4\mu \overline{\beta}_{i,M-1,k}}{2\Delta y \xi + \overline{\alpha}_{i,M-2,k} \overline{\alpha}_{i,M-1,k} \mu - 4\mu \overline{\alpha}_{i,M-1,k} + 3\mu}.$$
(18)

In the reverse course of the sweep in a successively decreasing index j, the concentration values are determined $\theta_{i,M-1,k}^{n+2/3}$, $\theta_{i,M-2,k}^{n+2/3}$, ..., $\theta_{i,0,k}^{n+2/3}$ are in the following form:

$$\boldsymbol{\theta}_{i,j,k}^{n+2/3} = \overline{\boldsymbol{\alpha}}_{i,j,k} \boldsymbol{\theta}_{i,j,k}^{n+2/3} + \overline{\boldsymbol{\beta}}_{i,j,k}; \ i = \overline{1,N-1}, \ j = \overline{M-1,0}, \ k = \overline{1,L-1}.$$
(19)

Applying the above procedures for equation (1) along the direction of the Oz axis and we have the following tridiagonal system of linear algebraic equations:

$$\overline{\overline{a}}_{i,j,k}\boldsymbol{\theta}_{i,j,k-1}^{n+1} - \overline{\overline{b}}_{i,j,k}\boldsymbol{\theta}_{i,j,k}^{n+1} + \overline{\overline{c}}_{i,j,k}\boldsymbol{\theta}_{i,j,k+1}^{n+1} = -\overline{\overline{\overline{d}}}_{i,j,k}.$$
(20)

For the boundary condition (3) we use the approximation of the second order of accuracy, and for z=0 we have

$$-\kappa \frac{-3\theta_{i,j,0}^{n+1} + 4\theta_{i,j,1}^{n+1} - \theta_{i,j,2}^{n+1}}{2\Delta z} = f_0 - \beta \theta_{i,j,0}^{n+1}$$

or

$$3\kappa\theta_{i,j,0}^{n+1} - 4\kappa\theta_{i,j,1}^{n+1} + \kappa\theta_{i,j,2}^{n+1} = 2\Delta z f_0 - 2\Delta z \beta \theta_{i,j,0}^{n+1}.$$
(21)

From the resulting tridiagonal system of linear algebraic equations for y=1 we have

$$\overline{\overline{a}}_{i,j,1}\boldsymbol{\theta}_{i,j,0}^{n+1} - \overline{\overline{b}}_{i,j,1}\boldsymbol{\theta}_{i,j,1}^{n+1} + \overline{\overline{c}}_{i,j,1}\boldsymbol{\theta}_{i,j,2}^{n+1} = -\overline{\overline{d}}_{i,j,1};$$

where is calculated $\theta_{i,j,2}^{n+1}$ in the following way:

$$\boldsymbol{\theta}_{i,j,2}^{n+1} = -\frac{\overline{\overline{a}}_{i,j,1}}{\overline{\overline{c}}_{i,j,1}} \boldsymbol{\theta}_{i,j,0}^{n+1} + \frac{\overline{b}_{i,j,1}}{\overline{\overline{c}}_{i,j,1}} \boldsymbol{\theta}_{i,j,1}^{n+1} - \frac{\overline{d}_{i,j,1}}{\overline{\overline{c}}_{i,j,1}}.$$
(22)

Equation 28 is substituted for $\theta_{i,j,2}^{n+1}$ in (21)

$$3\kappa\theta_{i,j,0}^{n+1} - 4\kappa\theta_{i,j,1}^{n+1} + \kappa \overline{\overline{\overline{c}}_{i,j,1}}^{\overline{a}_{i,j,1}} \theta_{i,j,0}^{n+1} + \kappa \overline{\overline{\overline{c}}_{i,j,1}}^{\overline{b}_{i,j,1}} \theta_{i,j,1}^{n+1} - \kappa \overline{\overline{\overline{c}}_{i,j,1}}^{\overline{a}_{i,j,1}} = 2\Delta z f_0 - 2\Delta z \beta \theta_{i,j,0}^{n+1};$$

and find $\theta_{i,j,0}^{n+1}$ in the following way:

$$\theta_{i,j,0}^{n+1} = \frac{4\kappa\overline{\bar{c}}_{i,j,1} - \kappa\overline{\bar{b}}_{i,j,1}}{3\kappa\overline{\bar{c}}_{i,j,1} + 2\Delta z\beta\overline{\bar{c}}_{i,j,1} - \kappa\overline{\bar{a}}_{i,j,1}} \theta_{i,j,1}^{n+1} + \frac{\kappa\overline{\bar{d}}_{i,j,1} + 2\Delta z\overline{\bar{c}}_{i,j,1}f_0}{3\kappa\overline{\bar{c}}_{i,j,1} + 2\Delta z\beta\overline{\bar{c}}_{i,j,1} - \kappa\overline{\bar{a}}_{i,j,1}}.$$
(23)

Using the above relation (23), we find the values of the sweep coefficients $\overline{\overline{\alpha}}_{i,j,0}$ and $\overline{\overline{\beta}}_{i,j,0}$:

$$\overline{\overline{\alpha}}_{i,j,0} = \frac{4\kappa\overline{\overline{c}}_{i,j,1} - \kappa\overline{\overline{b}}_{i,j,1}}{3\kappa\overline{\overline{c}}_{i,j,1} + 2\Delta z\beta\overline{\overline{c}}_{i,j,1} - \kappa\overline{\overline{a}}_{i,j,1}}; \ \overline{\overline{\beta}}_{i,j,0} = \frac{\kappa\overline{d}_{i,j,1} + 2\Delta z\overline{\overline{c}}_{i,j,1}f_0}{3\kappa\overline{\overline{c}}_{i,j,1} + 2\Delta z\beta\overline{\overline{c}}_{i,j,1} - \kappa\overline{\overline{a}}_{i,j,1}}.$$
(24)

Similarly for boundary condition (4), at $z = H_z$ we find:

$$\theta_{i,j,L}^{n+1} = \frac{2\Delta z \xi \theta_E - \kappa \overline{\overline{\alpha}}_{i,j,L-2} \overline{\beta}_{i,j,L-1} - \kappa \overline{\beta}_{i,j,L-2} + 4\kappa \overline{\beta}_{i,j,L-1}}{2\Delta z \xi + \overline{\overline{\alpha}}_{i,j,L-2} \overline{\overline{\alpha}}_{i,j,L-1} \kappa - 4\kappa \overline{\overline{\alpha}}_{i,j,L-1} + 3\kappa}.$$
(25)

In the reverse course of the sweep in a successively decreasing index k, the concentration values are determined $\theta_{i,j,L-1}^{n+1}$, $\theta_{i,j,L-2}^{n+1}$, ..., $\theta_{i,j,0}^{n+1}$ are calculated in the following form:

$$\boldsymbol{\theta}_{i,j,k}^{n+1} = \overline{\overline{\alpha}}_{i,j,k} \boldsymbol{\theta}_{i,j,k+1}^{n+1} + \overline{\overline{\beta}}_{i,j,k}; \quad i = \overline{1, N-1}, \quad j = \overline{1, M-1}, \quad k = \overline{L-1, 0}.$$
(26)

And as a result, a mathematical model and a numerical algorithm were obtained for research, forecasting and management decision-making on the protection of the environment and air basins of industrial regions, which take into account the wind speed in three directions and the rate of deposition of aerosol particles on the underlying surface of the earth, as well as the capture of particles by elements vegetation, which plays a significant role in the dynamics of the considered process.

RESULTS

Within the framework of this study, an object-oriented software and tool complex has been developed, which includes a number of related software tools developed using modern, most widely used technologies, such as the python programming language, Django frameworks, Django-rest-framework, sets of visualization libraries OSM, OWM, Googlemaps, numpy, pandas, scipy, matplotlib, requests, folium, bs4, etc.

Computational experiments were carried out to study the process of transfer and diffusion of harmful substances in the atmosphere, taking into account the heterogeneity and roughness of the earth's surface: vegetation cover, forest belt, high-rise residential and industrial facilities. A computational experiment has established that the change in the concentration of aerosols in the atmosphere depends significantly on the actual change in wind speed in a day, the coefficient characterizing the capture of particles by vegetation elements and the horizontal diffusion coefficient, as well as the vertical turbulence coefficient. The concentration of pollutants in the surface layer of the atmosphere change over time depending on the actual wind speeds. With an increase in wind speed, there is no accumulation of concentrations of pollutants around the source, and their distribution area increases with time.



FIGURE 1. Dynamics of transfer and diffusion of aerosol particles in the atmosphere at $Q = 1000 \text{ mg/m}^3$; H = 40 m; S = 12 m; t = 1 hours; u = 10.32 m/s; wind direction 120°



FIGURE 2. Dynamics of transfer and diffusion of aerosol particles in the atmosphere at $Q = 1000 \text{ mg/m}^3$; H = 40 m; S = 12 m; t = 4 hours.



FIGURE 3. Dynamics of transfer and diffusion of aerosol particles in the atmosphere at $Q = 1000 \text{ mg/m}^3$; H = 40 m; S = 12 m; t = 24 hours.

CONCLUSION

To monitor and predict the concentration of pollutants in the atmosphere of the region under consideration, a mathematical model has been developed, which takes into consideration the wind speed in three directions and the rate of deposition of aerosol particles on the underlying surface, as well as the capture of particles by vegetation elements, which plays a significant role in the process dynamics.

Since the problem (1)-(5) is described by the field equations of hydromechanics, for its integration a numerical

algorithm was developed with the second order of approximation in time and space variables, numerical calculations were carried out on a computer based on the developed mathematical and software. As an object, a source was considered at the site of «Kuylyuk Asphalt Concrete Plant LLC», located in the Tashkent region, Yashnabad district (Fig. 1-3).

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