ISSN 1995-0802, Lobachevskii Journal of Mathematics, 2024, Vol. 45, No. 3, pp. 1156–1169. © Pleiades Publishing, Ltd., 2024.

# Modeling the Process of Pollutant Spread in the Atmosphere with Account for the Capture of Particles by Vegetation Elements

**N. Ravshanov[1*], Sh. E. Nazarov[2**], and B. Boborakhimov[2***]**

(Submitted by T. K. Yuldashev)

[1]*Research Institute for the Development of Digital Technologies and Artificial Intelligence, Tashkent, 100125 Uzbekistan*

[2]*Bukhara State University, Bukhara, 200118 Uzbekistan*

Received June 17, 2023; revised October 28, 2023; accepted November 14, 2023

**Abstract**—The problems of forecasting the pollutant concentration in the atmosphere by means of mathematical modeling remain one of the most relevant scientific areas. Such a conclusion can be drawn from the analysis of scientific publications related to the problems of mathematical modeling of complex processes of mass transfer in the atmosphere. In this regard, the aim of this study is to develop a mathematical model for the transport and diffusion of emissions of polluting particles of technogenic and natural origin and an effective numerical algorithm for solving the problem with a high-order approximation in time and space variables. A feature of the proposed mathematical apparatus is that, in addition to the main factors, the model takes into account the phenomenon of the capture of aerosol particles by elements of vegetation in the land environment. The solution algorithm is based on the method for splitting the original problem into physical factors: advection, diffusion, and absorption of a substance in the air mass of the atmosphere. Computational experiments were conducted using real meteorological parameters and data on sources of atmospheric pollution. An analysis of the results of numerical calculations showed their good agreement with the data of field measurements and the results obtained by other authors. Thus, the adequacy of the developed mathematical model and the accuracy of the numerical algorithm were sufficiently substantiated. In the course of experiments, the influence of the main factors on the process of transfer and diffusion of particles of harmful substances in the atmosphere was established. Particular attention was paid to the study of how the green cover on the terrain affects the propagation of particle concentration fields; what portion of pollutants can be absorbed by vegetation elements compared to other types of the underlying surface. The practical outcome of the study is the possibility of developing recommendations to support decision-making on maintaining the ecological balance of the environment in industrial regions and protecting it from the possible negative impact of technogenic factors.

**DOI:** 10.1134/S1995080224600638

Keywords and phrases: *mathematical model, finite difference method, computational experiment, transport and diffusion of pollutants, weather and climatic factors*

## 1. INTRODUCTION

Initial-boundary value problems for first- and second-order differential equations have many applications in various fields of science and technology. There are many effective methods for solving differential equations with initial boundary conditions [1–25]. One of the applications of differential equations with initial boundary conditions is the study of environmental problems, which are becoming more relevant every day.

[*]E-mail: ravshanzade-09@mail.ru
[**]E-mail: nazarovshakhzod4313@gmail.com
[***]E-mail: Uzbekpy@gmail.com

The growth in the number of industrial facilities over the past decades has caused an increase in air pollution and, consequently, increased risks to public health. The World Health Organization (WHO) estimates that air pollution causes more than 7.5 million premature deaths each year and is therefore considered one of the world's most dangerous environmental risks. Air pollution is a change in the composition of pure natural air due to the ingress of impurities of various origins and states of aggregation: organic, inorganic, gaseous, aerosol, etc. The most common anthropogenic sources of pollutant emissions are transport, energy facilities, manufacturing enterprises, the construction sector, housing and communal services, livestock and agricultural enterprises. Industrial enterprises of various types act as the main sources of pollution of the atmosphere and plant complexes. The suppression of tree species is significant not only near the source of pollution but also at considerable distances from it. This is explained by the fact that a mixture of chemical components, the concentration of each of which is small, has a greater effect on vegetation than one component with a high concentration. Simultaneous soil acidification, air pollution, and climate change as a result of active anthropogenic impact on the environment cause a negative effect on the plant complexes [26–28].

Among the inorganic substances of anthropogenic origin, emissions of nitrogen and sulfur oxides, carbon monoxide and dioxide are especially harmful. As noted in [29], emissions of nitrogen and sulfur oxides cause significant damage to vegetation. Note that in problems where it is explicitly possible to single out physical processes, for example, the substance transfer in the wind direction and molecular diffusion, it would be quite reasonable to use the method for splitting into physical processes at each time layer. The idea of the splitting method is to reduce the original multidimensional problem to problems of a simpler structure, which are then sequentially or in parallel solved by already-known numerical methods [30]. This can be achieved in various ways, therefore, to date, a large number of different difference schemes have been created. Information and communication technology (ICT) and digital tools for air quality measurement have provided enormous data on environmental pollution, enabling decision-makers to provide early warnings to citizens in urban areas [31]. In the last few years, we have witnessed the development and emergence of affordable and powerful computational tools that support machine learning processes [32]. The study in [33] proposed a comprehensive method for forecasting the air quality index (AQI). The study focused on predicting hourly environmental concentrations of PM 2.5 and PM 10 using artificial neural networks. The calculation of the air quality index was performed according to six pollutant criteria. Since there was a problem with incorrect or empty values in the data sets, the authors used the missForest algorithm to fill in the missing data. Various aspects of the problems of modeling the spread of harmful substances in the surface layer of the atmosphere and calculating the concentration of emissions of impurities from sources of atmospheric pollution were considered in [34–36]. A new mathematical model of aerodynamic processes was proposed in [37]; it takes into account high air humidity, atmospheric pressure, temperature variability, and other parameters typical of coastal areas. Parallel algorithms for solving these models were developed and implemented in the form of programs for high-performance systems. The authors of article [38] proposed a method for determining the average annual concentrations of PM 2.5 and ozone particles to estimate the population morbidity. The determination of atmospheric air pollution at the global level was conducted based on the integration of remote sensing data from satellites with the results of instrumental measurements of the ground-based monitoring network and modeling pollutant dispersion processes in the atmosphere. Using this technique, the authors obtained extensive information on air pollution by PM2.5 and ozone particles over the vast territory. In [39–41], comprehensive studies of the process of propagation of aerosol particles in the atmosphere were conducted, taking into account the orography of the area and weather and climatic factors. For the numerical integration of the problem posed, the authors used high-order finite-difference schemes of approximation and the method for splitting into physical processes. The study in [42] is devoted to the construction of a mathematical model and a numerical algorithm for the dispersion of impurities of any type in the meso-meteorological boundary layer of the atmosphere. Particular attention was paid to the description of wind erosion since most of the emissions in the Aral Sea occur due to the removal of salt and dust particles from the soil surface. A series of computational experiments was performed using the developed mathematical apparatus. The results obtained, illustrate the influence of various factors on the process of atmospheric dispersion. The authors of [43–54] considered a mathematical model for research, forecasting, and making managerial decisions on the process of the spread of harmful aerosol substances in the atmosphere. When obtaining a mathematical model of the object, the main weather and climatic factors affecting the process of transport and diffusion of harmful substances and the relief of the region under consideration were taken into account. Changes in wind direction and speed were calculated using the Navier–Stokes equation for the function stream and vortex velocity variables. The proposed software was implemented as the Borland C++ Builder software tool for conducting computational experiments. Based on the above, the aim of this study is to build an efficient numerical algorithm based on the method for splitting into physical processes with the second order of accuracy, taking into account the wind speed in three directions, the deposition velocity of aerosol particles on the underlying surface, and the factor of particle capture by vegetation elements.

## 2. STATEMENT OF THE PROBLEM

Let us consider a mathematical model for the propagation of aerosol particles in the atmosphere, described by the complete equation of hydromechanics, taking into account the capture of pollutant particles by vegetation elements

$$\frac{\partial\theta}{\partial t}+u\frac{\partial\theta}{\partial x}+v\frac{\partial\theta}{\partial y}+(w-w_g)\frac{\partial\theta}{\partial z}+\sigma\theta+\alpha\theta=\mu\frac{\partial^2\theta}{\partial x^2}+\mu\frac{\partial^2\theta}{\partial y^2}+\frac{\partial}{\partial z}(\kappa\frac{\partial\theta}{\partial z})+\delta_{i,j,k}\mathbb{Q} \tag{1}$$

with initial and boundary conditions

$$\theta|_{t=0}=\theta_0, \tag{2}$$

$$-\mu\frac{\partial\theta}{\partial x}|_{x=0}=\xi(\theta_E-\theta),\quad \mu\frac{\partial\theta}{\partial x}|_{x=L_x}=\xi(\theta_E-\theta), \tag{3}$$

$$-\mu\frac{\partial\theta}{\partial y}|_{y=0}=\xi(\theta_E-\theta),\quad \mu\frac{\partial\theta}{\partial y}|_{y=L_y}=\xi(\theta_E-\theta), \tag{4}$$

$$-\kappa\mu\frac{\partial\theta}{\partial z}|_{z=0}=(\beta\theta-f_0),\quad \kappa\frac{\partial\theta}{\partial z}|_{z=L_z}=\xi(\theta_E-\theta). \tag{5}$$

Here $\theta$ is the concentration of harmful substances in the atmosphere; $t$ is the time; $\theta_0$ is the primary concentration of harmful substances in the atmosphere; $\theta_E$ is the concentration entering through the boundaries of the domain under consideration; $(x,y,z)$ is the coordinate system; $(u,v,\omega)$ is the wind speed in three directions; $w_g$ the particle deposition velocity; $\sigma$ is the coefficient of absorption of harmful substances in the atmosphere; $\alpha(z)$ is the coefficient characterizing the capture of particles by vegetation elements; $\mu,\kappa$ are the diffusion and turbulence coefficients; $\mathbb{Q}$ is the source power; $\delta$ is the Dirac function; $\xi$ is the coefficient of mass transfer through the boundaries of the calculation domain; $\beta$ is the coefficient of particle interaction with the underlying surface; $f_0$ is the stationary source of emission of harmful substances from the underlying surface.

## 3. SOLUTION METHOD

Since problem (1)–(5) is described by a three-dimensional partial differential equation with the corresponding initial and boundary conditions, it is difficult to find its exact solution in an analytical form. At that, we note that in equation (1) two physical processes are clearly distinguished: the first process is the substance transfer in the direction of movement of the atmospheric air mass; the second process is the molecular diffusion of the substance in the atmosphere. Besides, the third process can also be distinguished – the absorption of the substance by the air mass of the atmosphere, mainly due to high humidity. Given this circumstance, it would be quite reasonable to use the method for splitting into physical processes at each time layer. Therefore, to effectively solve the problem, we split it into physical processes—the advection part and the diffusion part. For the numerical solution to problem (1)–(5) we assume that the sought-for solution is a smooth function over the entire space. Using the additivity of fundamentally different physical processes of transfer and diffusion of a substance in the atmosphere in a small time interval $t_n\leqslant t\leqslant t_{n+1}$,we consider them as separate problems. The process of substance transfer with its preservation along the trajectory is considered **problem A**:

$$\frac{\partial\theta_1}{\partial t}+u\frac{\partial\theta_1}{\partial x}+v\frac{\partial\theta_1}{\partial y}+(w-w_g)\frac{\partial\theta_1}{\partial z}=\frac{1}{3}\delta_{i,j,k}\mathbb{Q} \tag{6}$$

with initial and boundary conditions

$$\theta_1|_{t=0} = \theta_3^n, \tag{7}$$

$$-\mu\frac{\partial\theta_1}{\partial x}|_{x=0} = \xi(\theta_E - \theta_1), \quad \mu\frac{\partial\theta_1}{\partial x}|_{x=L_x} = \xi(\theta_E - \theta_1), \tag{8}$$

$$-\mu\frac{\partial\theta_1}{\partial y}|_{y=0} = \xi(\theta_E - \theta_1), \quad \mu\frac{\partial\theta_1}{\partial y}|_{y=L_y} = \xi(\theta_E - \theta_1), \tag{9}$$

$$-\kappa\frac{\partial\theta_1}{\partial z}|_{y=0} = (\beta\theta_1 - f_0), \quad \kappa\frac{\partial\theta_1}{\partial z}|_{z=L_z} = \xi(\theta_E - \theta_1). \tag{10}$$

The process of diffusion of a substance in the atmosphere without taking into account the absorption of particles in the air mass is considered **problem B**:

$$\frac{\partial\theta_2}{\partial t} = \mu\frac{\partial^2\theta_2}{\partial x^2} + \mu\frac{\partial^2\theta_2}{\partial y^2} + \frac{\partial}{\partial z}(\kappa\frac{\partial\theta_2}{\partial z}) + \frac{1}{3}\delta_{i,j,k}\mathbb{Q} \tag{11}$$

with initial and boundary conditions

$$\theta_2|_{t=0} = \theta_1^{n+1}, \tag{12}$$

$$-\mu\frac{\partial\theta_2}{\partial x}|_{x=0} = \xi(\theta_E - \theta_2), \quad \mu\frac{\partial\theta_2}{\partial x}|_{x=L_x} = \xi(\theta_E - \theta_2), \tag{13}$$

$$-\mu\frac{\partial\theta_2}{\partial y}|_{y=0} = \xi(\theta_E - \theta_2), \quad \mu\frac{\partial\theta_2}{\partial y}|_{y=L_y} = \xi(\theta_E - \theta_2), \tag{14}$$

$$-\kappa\frac{\partial\theta_2}{\partial z}|_{z=0} = (\beta\theta_2 - f_0), \quad \kappa\frac{\partial\theta_2}{\partial z}|_{y=z_z} = \xi(\theta_E - \theta_2). \tag{15}$$

Taking into account the absorption and capture of particles of harmful substances in the atmosphere, **problem C** has the following form

$$\frac{\partial\theta_3}{\partial t} + \sigma\theta_3 + \alpha\theta_3 = \frac{1}{3}\delta_{i,j,k}\mathbb{Q} \tag{16}$$

with initial and boundary conditions

$$\theta_3|_{t=0} = \theta_2^{n+1}, \tag{17}$$

$$-\mu\frac{\partial\theta_3}{\partial x}|_{x=0} = \xi(\theta_E - \theta_3), \quad \mu\frac{\partial\theta_3}{\partial x}|_{x=L_x} = \xi(\theta_E - \theta_3), \tag{18}$$

$$-\mu\frac{\partial\theta_3}{\partial y}|_{y=0} = \xi(\theta_E - \theta_3), \quad \mu\frac{\partial\theta_3}{\partial y}|_{y=L_y} = \xi(\theta_E - \theta_3), \tag{19}$$

$$-\kappa\frac{\partial\theta_3}{\partial z}|_{z=0} = (\beta\theta_3 - f_0), \quad \kappa\frac{\partial\theta_3}{\partial z}|_{y=z_z} = \xi(\theta_E - \theta_3). \tag{20}$$

Thus, after splitting the original problem into physical processes, we got three sub-problems (6)–(10), (11)–(15), and (16)–(20), which can be solved independently of each other by the finite difference method. However, here it must be emphasized that the solution to sub-**problem A** is the initial condition for sub-**problem B**, the solution to sub-**problem B** serves as the initial condition for sub-**problem C** and the solution to sub-**problem C** serves as the initial condition for sub-**problem A** at the next time layer. From the formulation of the above sub-problems, it follows that the numerical solution to the main problem is greatly simplified when it is split into physical properties and parameters. It should be noted that the restriction of the integration step in terms of space variables and time is required when solving **problem A**; this is due to the presence of derivatives of the sought-for first-order variables in the equation for the transport of harmful substances in the atmosphere. Problems (6)–(10), (11)–(15), and (16)–(20) are solved using an implicit finite-difference scheme in time and with the second order of accuracy in coordinates (20), replacing the continuous domain of the sought-for variables by the grid domain with step $\Delta x$, $\Delta y$, and $\Delta z$:

$$\Omega_{xyzt} = (x_i = i\Delta x, \quad y_i = j\Delta y, \quad z_k = k\Delta z, \quad \tau_n = n\Delta t),$$

$$i = \overline{0, N}, \quad j = \overline{0, M}, \quad k = \overline{0, L}, \quad n = \overline{0, N_t}, \quad \Delta t = \frac{T}{N_t}.$$

To ensure a high-order approximation in time and space variables and the stability of the calculation process, we use an implicit finite-difference scheme for equation (6) in the $Ox$ direction

$$\frac{1}{2}\frac{\theta^{n+1/3}_{1,i,j,k} - \theta^n_{1,i,j,k}}{\Delta t/3} + \frac{1}{2}\frac{\theta^{n+1/3}_{1,i+1,j,k} - \theta^n_{1,i+1,j,k}}{\Delta t/3} + \left(\frac{u-|u|}{4}\right)\frac{\theta^{n+1/3}_{1,i+1,j,k} - \theta^{n+1/3}_{1,i,j,k}}{\Delta x}$$
$$+ \left(\frac{u-|u|}{4}\right)\frac{\theta^{n}_{1,i+1,j,k} - \theta^{n}_{1,i,j,k}}{\Delta x} + \left(\frac{u+|u|}{4}\right)\frac{\theta^{n+1/3}_{1,i,j,k} - \theta^{n+1/3}_{1,i-1,j,k}}{\Delta x} + \left(\frac{u+|u|}{4}\right)\frac{\theta^{n}_{1,i,j,k} - \theta^{n}_{1,i-1,j,k}}{\Delta x}$$
$$+ \left(\frac{v-|v|}{2}\right)\frac{\theta^{n}_{1,i,j+1,k} - \theta^{n}_{1,i,j,k}}{\Delta y} + \left(\frac{v+|v|}{2}\right)\frac{\theta^{n}_{1,i,j,k} - \theta^{n}_{1,i,j-1,k}}{\Delta y} + \left(\frac{w_a-|w_a|}{2}\right)\frac{\theta^{n}_{1,i,j,k+1} - \theta^{n}_{1,i,j,k}}{\Delta z}$$
$$+ \left(\frac{w_a+|w_a|}{2}\right)\frac{\theta^{n}_{1,i,j,k} - \theta^{n}_{1,i,j,k-1}}{\Delta z} = \frac{1}{9}\delta_{i,j,k}\mathbb{Q}. \tag{21}$$

Grouping similar terms in equation (21), we obtain a system of linear tridiagonal algebraic equations

$$a_{1,i,j,k}\theta^{n+1/3}_{1,i-1,j,k} - b_{1,i,j,k}\theta^{n+1/3}_{1,i,j,k} + c_{1,i,j,k}\theta^{n+1/3}_{1,i+1,j,k} = -c_{1,i,j,k}. \tag{22}$$

Here the coefficients of equation (22) are defined as follows

$$a_{1,i,j,k} = \frac{u+|u|}{4\Delta x}, \quad b_{1,i,j,k} = \frac{|u|}{2\Delta x} + \frac{3}{2\Delta t}, \quad c_{1,i,j,k} = -\frac{u-|u|}{4\Delta x} - \frac{3}{2\Delta t},$$

$$d_{1,i,j,k} = \left(\frac{3}{2\Delta t} - \frac{|u|}{2\Delta x} - \frac{|v|}{2\Delta y} - \frac{|w_a|}{2\Delta z}\right)\theta^n_{1,i,j,k} + (\frac{u+|u|}{4\Delta x})\theta^n_{1,i-1,j,k}$$
$$+ \left(\frac{3}{2\Delta t} - \frac{u-|u|}{4\Delta x}\right)\theta^n_{1,i+1,j,k} + \frac{v+|v|}{2\Delta y}\theta^n_{1,i,j-1,k} - \frac{v-|v|}{2\Delta y}\theta^n_{1,i,j+1,k}$$
$$+ \frac{w_a+|w_a|}{2\Delta z}\theta^n_{1,i,j,k-1} - \frac{w_a-|w_a|}{2\Delta z}\theta^n_{1,i,j,k+1} + \frac{1}{9}\delta_{i,j,k}\mathbb{Q}.$$

Next, we approximate boundary condition (8) for $x = 0$ with respect to Ox with the second order of accuracy and obtain

$$-\mu\frac{-3\theta^{n+1/3}_{1,0,j,k} + 4\theta^{n+1/3}_{1,1,j,k} - \theta^{n+1/3}_{1,2,j,k}}{2\Delta x} = \xi\theta_E - \xi\theta^{n+1/3}_{1,0,j,k}. \tag{23}$$

From relation (23), using the sweep method, we find the values of the sweep coefficients $\alpha_{1,0,j,k}$ and $\beta_{1,0,j,k}$:

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

Similarly, we approximate the boundary condition (8) in direction $Ox$ for $x = L_x$:

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

Hence, we find the concentration value at the boundary of the $Ox$-axis for $i = N$:

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

The values of the concentration sequence $\theta_{1,N-1,j,k}^{n+1/3}$, $\theta_{1,N-2,j,k}^{n+1/3}$, $\ldots$, $\theta_{1,0,j,k}^{n+1/3}$ are determined by the backward-sweep method by decreasing the $i$th sequence

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

Then, we perform similar actions in direction $Oy$ and instead of equation (6), we obtain

$$\bar{a}_{1,i,j,k}\theta_{1,N,j-1,k}^{n+2/3}-\bar{b}_{1,i,j,k}\theta_{1,N,j-1,k}^{n+2/3}+\bar{c}_{1,i,j,k}\theta_{1,N,j-1,k}^{n+2/3}=-\bar{d}_{1,i,j,k}, \tag{24}$$

where

$$\bar{a}_{1,i,j,k}=\frac{v+|v|}{4\Delta y},\quad \bar{b}_{1,i,j,k}=\frac{|v|}{2\Delta y}+\frac{3}{2\Delta t},\quad \bar{c}_{1,i,j,k}=-\frac{v-|v|}{4\Delta y}-\frac{3}{2\Delta t},$$

$$\begin{aligned}\bar{d}_{1,i,j,k}=&\left(\frac{3}{2\Delta t}-\frac{|u|}{\Delta x}-\frac{|v|}{2\Delta y}-\frac{|w_a|}{\Delta z}\right)\theta_{1,i,j,k}^{n+1/3}+\frac{u+|u|}{2\Delta x}\theta_{1,i-1,j,k}^{n+1/3}-\frac{u-|u|}{2\Delta x}\theta_{1,i+1,j,k}^{n+1/3}\\&+\frac{v+|v|}{4\Delta y}\theta_{1,i,j-1,k}^{n+1/3}+\left(\frac{3}{2\Delta t}-\frac{v-|v|}{4\Delta y}\right)\theta_{1,i,j+1,k}^{n+1/3}\\&+\frac{w_a+|w_a|}{2\Delta z}\theta_{1,i,j,k-1}^{n+1/3}-\frac{w_a-|w_a|}{2\Delta z}\theta_{1,i,j,k+1}^{n+1/3}+\frac{1}{9}\delta_{i,j,k}\mathbb{Q}.\end{aligned}$$

Hence, $\bar{\alpha}_{1,i,0,k}$ and $\bar{\beta}_{1,i,0,k}$ are found by boundary conditions (9) for $y=0$ as follows

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

Similarly, approximating boundary condition (9) with respect to $Oy$ for $y=L_y$, we find the concentration values at the boundary for $j=M$:

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

In equation (6), replacing differential operators by finite-difference operators in the direction of the $Oz$-axis, we obtain

$$\bar{\bar{a}}_{1,i,j,k}\theta_{1,N,j,k-1}^{n+1}-\bar{\bar{b}}_{1,i,j,k}\theta_{1,N,j,k}^{n+1}+\bar{\bar{c}}_{1,i,j,k}\theta_{1,N,j,k+1}^{n+1}=-\bar{\bar{d}}_{1,i,j,k},$$

where

$$\bar{\bar{a}}_{1,i,j,k}=\frac{w_a+|w_a|}{4\Delta z},\quad \bar{\bar{b}}_{1,i,j,k}=\frac{|w_a|}{2\Delta z}+\frac{3}{2\Delta t},\quad \bar{\bar{c}}_{1,i,j,k}=-\frac{w_a-|w_a|}{4\Delta z}-\frac{3}{2\Delta t},$$

$$\begin{aligned}\bar{\bar{d}}_{1,i,j,k}=&\left(\frac{3}{2\Delta t}-\frac{|u|}{\Delta x}-\frac{|v|}{\Delta y}-\frac{|w_a|}{2\Delta z}\right)\theta_{1,i,j,k}^{n+2/3}+\frac{u+|u|}{2\Delta x}\theta_{1,i-1,j,k}^{n+2/3}-\frac{u-|u|}{2\Delta x}\theta_{1,i+1,j,k}^{n+2/3}\\&+\frac{v+|v|}{2\Delta y}\theta_{1,i,j-1,k}^{n+2/3}-\frac{v-|v|}{2\Delta y}\theta_{1,i,j+1,k}+\frac{w_a+|w_a|}{4\Delta z}\theta_{1,i,j,k-1}^{n+2/3}\\&+\left(\frac{3}{2\Delta t}-\frac{w_a-|w_a|}{4\Delta z}\right)\theta_{1,i,j-1,k}^{n+2/3}+\frac{1}{9}\delta_{i,j,k}\mathbb{Q}.\end{aligned}$$

Hence, $\bar{\alpha}_{1,i,j,0}$ and $\bar{\beta}_{1,i,j,0}$ are determined by boundary conditions (10) for $z=0$ as follows

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

Boundary condition (10) is approximated by $Oz$ for $z=L_z$ and the concentration values at the boundary for $k=L$ are determined

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

To solve problem $B$, the process of diffusion of a substance in the atmosphere, taking into account the absorption of particles in the air mass, we use an implicit finite-difference scheme of a high order of approximation in time and space (21), and in direction $Ox$ we obtain

$$a_{2,i,j,k}\theta^{n+1/3}_{2,i-1,j,k} - b_{2,i,j,k}\theta^{n+1/3}_{2,i,j,k} + c_{2,i,j,k}\theta^{n+1/3}_{2,i+1,j,k} = -d_{2,i,j,k}. \tag{25}$$

Here the coefficients of equation (25) are defined as

$$a_{2,i,j,k} = \frac{\mu}{\Delta x^2}, \quad b_{2,i,j,k} = \frac{2\mu}{2\Delta x^2} + \frac{3}{2\Delta t}, \quad c_{2,i,j,k} = -\frac{\mu}{2\Delta x^2} - \frac{3}{2\Delta t},$$

$$d_{2,i,j,k} = \left(\frac{3}{2\Delta t} - \frac{\mu}{\Delta y^2} - \frac{2\kappa_k}{\Delta z^2}\right)\theta^n_{2,i,j,k} - \frac{3}{2\Delta t}\theta^n_{2,i+1,j,k} + \frac{\mu}{\Delta y^2}\theta^n_{2,i,j-1,k}$$
$$- \frac{\mu}{\Delta y^2}\theta^n_{2,i,j+1,k} + \frac{\kappa_{k-1}}{\Delta z^2}\theta^n_{2,i,j,k-1} - \frac{\kappa_{k+1}}{\Delta z^2}\theta^n_{2,i,j,k+1} + \frac{1}{9}\delta_{i,j,k}\mathbb{Q},$$

$\alpha_{2,0,j,k}$ and $\beta_{2,0,j,k}$ are found by the boundary conditions (13) for $x = 0$ as follows

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

Similarly, we approximate the boundary condition (13) along the $Ox$ direction for $У = L_x$, and find the concentration value at the boundary of the $Ox$-axis for $i = N$:

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

Then, we perform similar actions in direction$Oy$ and instead of equation (11), we obtain

$$\bar{a}_{2,i,j,k}\theta^{n+2/3}_{2,i,j-1,k} - \bar{b}_{2,i,j,k}\theta^{n+2/3}_{2,i,j,k} + \bar{c}_{2,i,j,k}\theta^{n+2/3}_{2,i,j+1,k} = -\bar{d}_{2,i,j,k}, \tag{26}$$

where

$$\bar{a}_{2,i,j,k} = \frac{\mu}{\Delta y^2}, \quad \bar{b}_{2,i,j,k} = \frac{2\mu}{2\Delta y^2} + \frac{3}{2\Delta t}, \quad \bar{c}_{2,i,j,k} = -\frac{\mu}{\Delta y^2} - \frac{3}{2\Delta t},$$

$$\bar{d}_{2,i,j,k} = \left(\frac{3}{2\Delta t} - \frac{\mu}{\Delta x^2} - \frac{2\kappa_k}{\Delta z^2}\right)\theta^{n+1/3}_{2,i,j,k} + \frac{\mu}{\Delta x^2}\theta^{n+1/3}_{2,i-1,j,k} + \frac{\mu}{\Delta x^2}\theta^{n+1/3}_{2,i+1,j,k} + \frac{3}{2\Delta t}\theta^{n+1/3}_{2,i,j+1,k}$$
$$+ \frac{\kappa_{k-1}}{\Delta z^2}\theta^{n+1/3}_{2,i,j,k-1} + \frac{\kappa_{k+1}}{\Delta z^2}\theta^{n+1/3}_{2,i,j,k+1} + \frac{1}{9}\delta_{i,j,k}\mathbb{Q}.$$

Hence, $\bar{\alpha}_{2,i,0,k}$ and $\bar{\alpha}_{2,i,0,k}$ are found with boundary conditions (14) for $y = 0$ as follows

$$\bar{\alpha}_{2,i,0,k} = \frac{(4\bar{c}_{2,i,1,k} - \bar{b}_{2,i,1,k})\mu}{(3\bar{c}_{2,i,1,k} - \bar{a}_{2,i,1,k})\mu + 2\Delta y\alpha_3}, \quad \bar{\beta}_{2,i,0,k} = \frac{\bar{d}_{2,1,j,k}\mu + 2\Delta y\xi\bar{c}_{2,i,1,k}\theta_E}{(3\bar{c}_{2,i,1,k} - \bar{a}_{2,i,1,k})\mu + 2\Delta y\xi}.$$

Similarly, approximating the boundary condition (14) with respect to $Oy$ for $y = L_y$, we find the concentration values at the boundary along the $Oy$-axis for $j = M$:

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

Similarly, replacing the differential operators in equation (11) by finite-difference operators in the direction of the $Oz$-axis, we obtain

$$\bar{\bar{a}}_{2,i,j,k}\theta^{n+1}_{2,i,j,k-1} - \bar{\bar{b}}_{2,i,j,k}\theta^{n+1}_{2,i,j,k} + \bar{\bar{c}}_{2,i,j,k}\theta^{n+1}_{2,i,j,k+1} = -\bar{\bar{d}}_{2,i,j,k},$$

where

$$\bar{\bar{a}}_{2,i,j,k} = \frac{\kappa_{k-1}}{\Delta z^2}, \quad \bar{\bar{b}}_{2,i,j,k} = \frac{2\kappa_k}{\Delta z^2} + \frac{3}{2\Delta t}, \quad \bar{\bar{c}}_{2,i,j,k} = \frac{\kappa_{k+1}}{\Delta z^2} - \frac{3}{2\Delta t},$$

$$\bar{\bar{d}}_{2,i,j,k} = \left(\frac{3}{2\Delta t} - \frac{2\mu}{\Delta x^2} - \frac{2\mu}{\Delta y^2}\right)\theta^{n+2/3}_{2,i,j,k} + \frac{\mu}{\Delta x^2}\theta^{n+2/3}_{2,i-1,j,k} + \frac{\mu}{\Delta x^2}\theta^{n+1/3}_{2,i+1,j,k}$$

$$+\frac{\mu}{\Delta y^2}\theta_{2,i,j-1,k}^{n+2/3}+\frac{\mu}{\Delta y^2}\theta_{2,i,j+1,k}^{n+2/3}+\frac{3}{2\Delta t}\theta_{2,i,j+1,k}^{n+2/3}+\frac{1}{9}\delta_{i,j,k}\mathbb{Q}.$$

Next, we approximate the boundary condition (15) with respect to Oz for $z=0$ and obtain the following

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

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

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

Using the sweep method, we find the values of the sweep coefficients $\bar{\bar{\alpha}}_{2,i,j,0}$ and $\bar{\bar{\beta}}_{2,i,j,0}$ :

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

We approximate the boundary condition (15) with respect to $Oz$ for $z=L_z$ and find the concentration values at the boundary of the $Oz$-axis for $k=L$:

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

We proceed similarly when solving problem $C$:

$$\frac{1}{2}\frac{\theta_{3,i,j,k}^{n+1/3}-\theta_{3,i,j,k}^{n}}{\Delta t/3}+\frac{1}{2}\frac{\theta_{3,i+1,j,k}^{n+1/3}-\theta_{3,i+1,j,k}^{n}}{\Delta t/3}+\sigma\theta_{3,i,j,k}^{n+1/3}+\alpha\theta_{3,i,j,k}^{n+1/3}=\frac{1}{9}\delta_{i,j,k}\mathbb{Q}. \tag{27}$$

Grouping similar terms into equation (27), we obtain a system of linear tridiagonal algebraic equations

$$a_{3,i,j,k}\theta_{3,i-1,j,k}^{n+1/3}-b_{3,i,j,k}\theta_{3,i,j,k}^{n+1/3}+c_{3,i,j,k}\theta_{3,i+1,j,k}^{n+1/3}=-d_{3,i,j,k}. \tag{28}$$

The coefficients of equation (28) are defined as follows

$$a_{3,i,j,k}=0,\ b_{3,i,j,k}=\frac{3}{2\Delta t}+\sigma+\alpha,\ c_{3,i,j,k}=-\frac{3}{2\Delta t},$$
$$d_{3,i,j,k}=\frac{3}{2\Delta t}\theta_{3,i,j,k}^{n}+\frac{3}{2\Delta t}\theta_{3,i+1,j,k}^{n}+\frac{1}{9}\delta_{i,j,k}\mathbb{Q}.$$

Then, with boundary conditions (18) at $x=0$, $\alpha_{3,0,j,k}$ and $\beta_{3,0,j,k}$ are found as follows

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

Similarly, we approximate the boundary condition (18) in direction Ox for $x=L_x$ and determine the concentration value at the boundary of the $Ox$-axis for $i=N$:

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

Then, we perform similar actions in direction $Oy$ and instead of equation (16), we get

$$\bar{a}_{3,i,j,k}\theta_{3,i,j-1,k}^{n+2/3}-\bar{b}_{3,i,j,k}\theta_{3,i,j,k}^{n+2/3}+\bar{c}_{3,i,j,k}\theta_{3,i+1,j,k}^{n+2/3}=-\bar{d}_{3,i,j,k}, \tag{29}$$

where

$$\bar{a}_{3,i,j,k}=0,\quad \bar{b}_{3,i,j,k}=\frac{3}{2\Delta t}+\sigma+\alpha,\quad \bar{c}_{3,i,j,k}=-\frac{3}{2\Delta t},$$
$$\bar{d}_{3,i,j,k}=\frac{3}{2\Delta t}\theta_{3,i,j,k}^{n+1/3}+\frac{3}{2\Delta t}\theta_{3,i,j+1,k}^{n+1/3}+\frac{1}{9}\delta_{i,j,k}\mathbb{Q}.$$

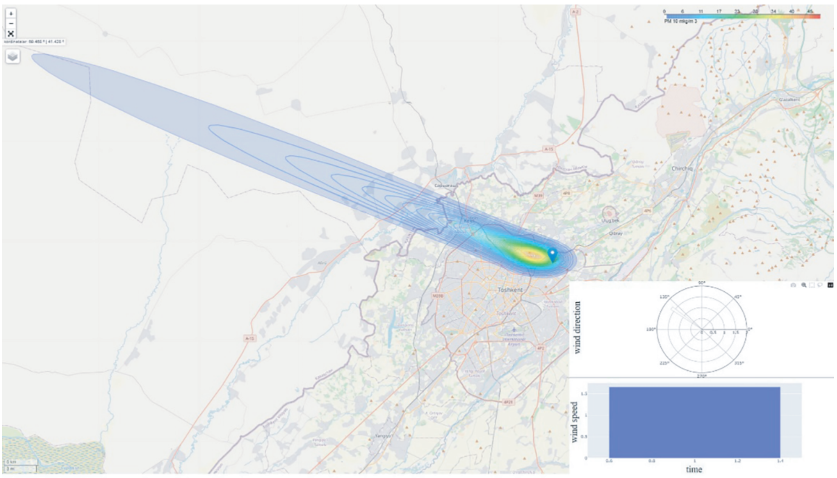


**Fig. 1.** Dynamics of transfer and diffusion of aerosol particles in the atmosphere at $Q = 1000$ mg/m$^3$; $H = 50$ m; $t = 1$ h.

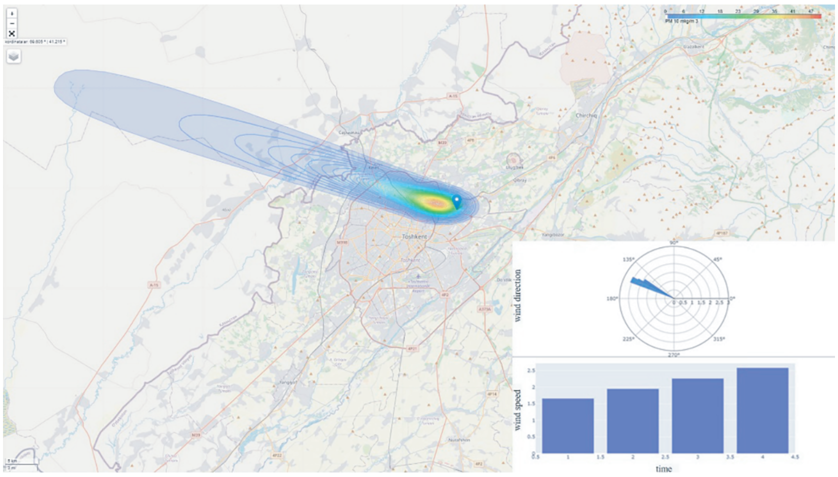


**Fig. 2.** Dynamics of transport and diffusion of aerosol particles in the atmosphere at $Q = 1000$ mg/m$^3$; $H = 50$ m; $t = 4$ h.

Hence, $\bar{\alpha}_{3,i,0,k}$ and $\bar{\beta}_{3,i,0,k}$ are found by the boundary conditions (19) for $y = 0$ in the following way

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

Similarly, approximating the boundary condition (19) with respect to $Oy$ for $y = L_y$, we find the concentration values at the boundary along the $Oy$-axis for $j = M$:

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

In equation (16), replacing the differential operators by finite-difference operators in the direction of the $Oz$-axis, we obtain

$$\bar{\bar{a}}_{3,i,j,k}\theta^{n+1}_{3,i,j,k-1} - \bar{\bar{b}}_{3,i,j,k}\theta^{n+1}_{3,i,j,k} + \bar{\bar{c}}_{3,i,j,k}\theta^{n+1}_{3,i,j,k+1} = -\bar{\bar{d}}_{3,i,j,k},$$

where

$$\bar{\bar{a}}_{3,i,j,k} = 0, \quad \bar{\bar{b}}_{3,i,j,k} = \frac{3}{2\Delta t} + \sigma + \alpha, \quad \bar{\bar{c}}_{3,i,j,k} = -\frac{3}{2\Delta t},$$
$$\bar{\bar{d}}_{3,i,j,k} = \frac{3}{2\Delta t}\theta^{n+2/3}_{3,i,j,k} + \frac{3}{2\Delta t}\theta^{n+2/3}_{3,i,j+1,k} + \frac{1}{9}\delta_{i,j,k}\mathbb{Q}.$$

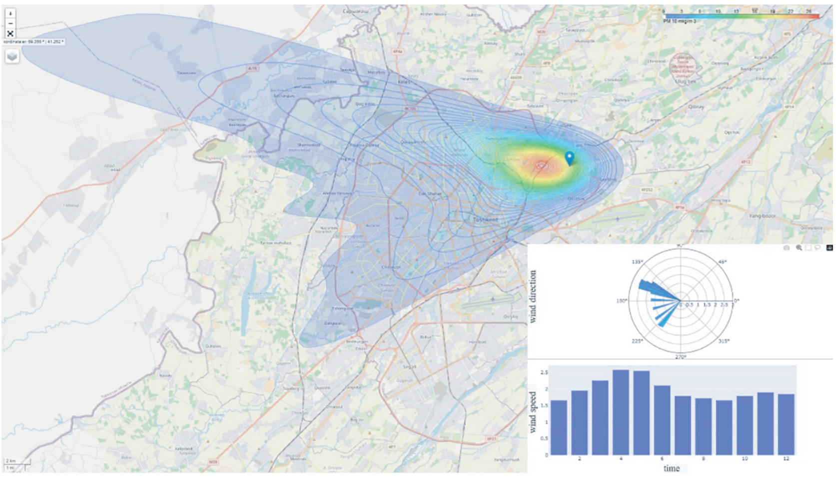


**Fig. 3.** Dynamics of transport and diffusion of aerosol particles in the atmosphere at $Q = 1000$ mg/m$^3$; $H = 50$ m; $t = 12$ hours.

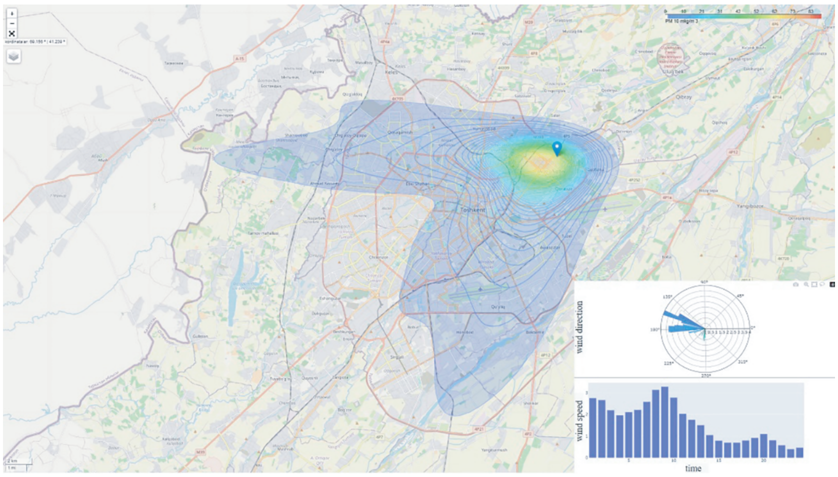


**Fig. 4.** Dynamics of transport and diffusion of aerosol particles in the atmosphere at $Q = 1000$ mg/m$^3$; $H = 50$ m; $t = 24$ h.

Further, $\bar{\alpha}_{3,i,j,0}$ and $\bar{\beta}_{3,i,j,0}$ are found by the boundary conditions (20) for $z = 0$ as follows

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

Boundary condition (20) is approximated by $Oz$ for $z = L_z$ and we find the concentration values at the boundary of the $Oz$-axis for $k = L$

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

So, a numerical algorithm was developed for solving the problem of transport and diffusion of aerosol particles in the boundary layer of the atmosphere; it can be used to study and predict the concentration of pollutants in industrial regions based on computational experiments.

## 4. RESULTS

Within the framework of this study, an object-oriented software and tool complex were developed, which include 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

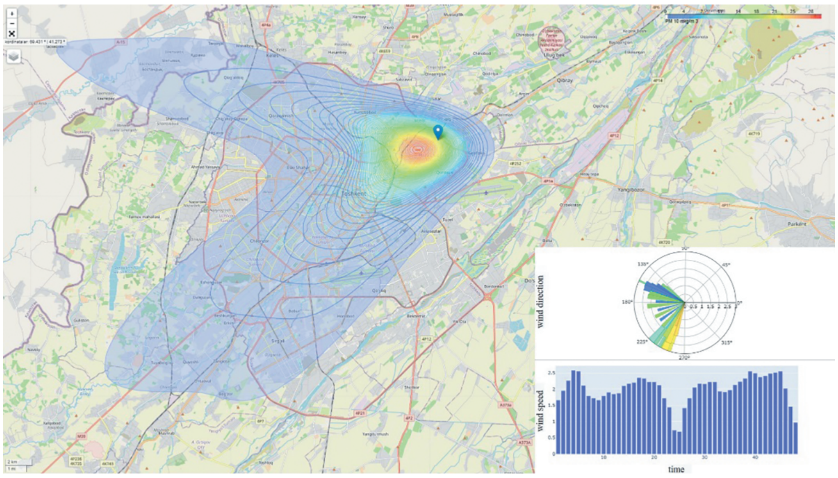

**Fig. 5.** Dynamics of transport and diffusion of aerosol particles in the atmosphere at $Q = 1000$ mg/m$^3$; $H = 50$ m; $t = 48$ h.

visualization libraries OSM, OWM, Googlemaps, numpy, pandas, scipy, matplotlib, requests, folium, bs4, etc. Computational experiments were conducted to study the process of transfer and diffusion of harmful substances in the atmosphere, taking into account the non-homogeneity and roughness of the earth's surface: vegetation cover, forest belts, and high-rise residential and industrial facilities.

To conduct a comprehensive study of the process of pollutant spread in the atmosphere, computational experiments were performed with real weather and climatic factors obtained online. As follows from the results of the numerical calculations, the dynamics of changes in the concentration of harmful substances in the atmosphere significantly depends on the wind speed in the surface layer of the atmosphere (Fig. 1). At critical values of wind speeds, changes in the concentration of harmful substances in the atmosphere mainly occur due to the transfer of atmospheric air mass in the surface layer, while the height of the source of harmful substances indirectly affects the transfer distance. The area covered by the concentration of harmful substances in the atmosphere significantly depends on the velocity direction of the air mass of the atmosphere (Fig. 2).

From the dynamics of the transfer of pollutants in the atmosphere, it is seen (Figs. 3–5) that, depending on the change in the direction and speed of the wind, the concentration of pollutants in the atmosphere and the area of their transfer change over time. The numerical calculations performed showed that another significant factor affecting the change in the concentration of pollutants in the surface layer of the atmosphere is the vegetation cover and the coefficient of absorption of harmful substances in the atmosphere, which depend on the time of year and time of day.

## 5. CONCLUSIONS

A mathematical model (1)–(5) and an efficient numerical algorithm were developed based on the method for splitting into physical processes with the second order of accuracy in space variables (6)–(29). It 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 plays a significant role in the dynamics of the process.To check the adequacy of the developed mathematical tool, computational experiments were conducted, the results of which were compared with field data. A comprehensive analysis of the processes of atmospheric pollution of a real production facility located in the Tashkent region of Uzbekistan was performed. It can be seen from the Figs. 2–5, that the change in the concentration of aerosols in the atmosphere depends significantly on the actual change in wind speed by day, the coefficient characterizing the capture of particles by vegetation elements, the horizontal diffusion coefficient, and the vertical turbulence coefficient. The concentration of pollutants in the surface layer of the atmosphere changes over time depending on the actual wind speed. With an increase in wind speed, the concentration of pollutants around the source does not accumulate, and the area of distribution of pollutants increases with time Fig. 1. The results obtained in the form of software can be successfully used to monitor the spread of harmful substances in the atmosphere. As numerical calculations have shown, at the moderate wind and calm, the concentration of harmful substances around the source accumulates at a distance of 280 to 350 m. At the same time, the concentration of harmful substances in the atmosphere will increase with increasing source power. With an increase in the intensity of aerosol sources and horizontal components of the wind speed, the area of pollutant transfer in the atmosphere increases.

## FUNDING

The authors of this work have no funding.

## CONFLICTS OF INTEREST

The authors of this work declare that they have no conflicts of interest.

## REFERENCES

1. R. D. Aloev and M. U. Khudoyberganov, "Implicit upwind difference scheme for a symmetric t-hyperbolic system with variable coefficients and lowest terms," Lobachevskii J. Math. **44**, 510–522 (2023). https://doi.org/10.1134/S1995080223020075
2. D. Baigereyev, D. Omariyeva, N. Temirbekov, Y. Yergaliyev, and K. Boranbek, "Numerical method for a filtration model involving a nonlinear partial integro-differential equation," Mathematics **10**, 1319 (2022). https://doi.org/10.3390/math10081319
3. A. Berdyshev, R. Aloev, Zh. Abdiramanov, and M. Ovlayeva, "An explicit-implicit upwind difference splitting scheme in directions for a mixed boundary control problem for a two-dimensional symmetric t-hyperbolic system," Symmetry **15**, 1863 (2023). https://doi.org/10.3390/sym15101863
4. A. Berdyshev and Zh. Abdiramanov, "Initial-boundary value problems solution for a hyperbolic equation with memory," Vestn. KazNPU Abaya, Ser. Fiz. Mat. Nauk **63** (3), 50–53 (2018). https://bulletin-phmath.kaznpu.kz/index.php/ped/issue/view/12/10
5. D. Bliyeva, D. Baigereyev, and Kh. Imomnazarov, "Computer simulation of the seismic wave propagation in poroelastic medium," Symmetry **14**, 1516 (2022). https://doi.org/10.3390/sym14081516
6. V. Ya. Glizer and M. G. Dmitriev, "Asymptotics of the solution of some discrete optimal control problems with a small step," Differ. Uravn. **15**, 1681–1691 (1979).
7. J. A. Ferreira and L. Pinto, "An integro-differential model for non-Fickian tracer transport in porous media: Validation and numerical simulation," Math. Meth. Appl. Sci. **39**, 4736–4749 (2016). https://doi.org/10.1002/mma.3446
8. M. Hasan, L. N. Jahan, T.-U. Zaman, S. Imtiaz, and M. E. Hossain, "Modeling of fluid flow through porous media using memory approach: A review," Math. Comput. Simul. **177**, 643–673 (2020). https://doi.org/10.1016/j.matcom.2020.05.026
9. Kh. Kh. Imomnazarov, A. S. Berdyshev, and Zh. A. Abdiramanov, "Classical solution of the first mixed problem for the equation of porous media with memory in a curvilinear half-strip," Vestn. Univ. Yassawi **8** (1), 7–19 (2019).
10. D. A. Koc, "A numerical scheme for time-fractional fourth-order reaction-diffusion model," J. Appl. Math. Comput. Mech. **22** (2), 15–25 (2023). https://doi.org/10.17512/jamcm.2023.2.02
11. V. I. Korzyuk and I. I. Smolyarchuk, "Mixed problems for the Klein–Gordon–Fock equation," in *Proceedings of the 9th International Workshop AMADE* (2018), pp. 1–2. https://elib.bsu.by/bitstream/123456789/207514/1/
12. F. Mirzaev, "Solving a class of nonlinear Volterra integral equations by using two-dimensional triangular orthogonal functions," J. Math. Model. **1**, 28–40 (2013).
13. N. N. Moiseev, *Asymptotic Methods of Nonlinear Mechanics* (Nauka, Moscow, 1981) [in Russian].
14. A. I. Propoi, *Elements of the Theory of Optimal Discrete Processes* (Nauka, Moscow, 1973) [in Russian].
15. A. A. Samarskii, *The Theory of Difference Schemes* (CRC, Boca Raton, FL, 2001). https://doi.org/10.1201/9780203908518
16. A. I. Sing, *Elements of the Theory of Optimal Discrete Systems* (Nauka, Moscow, 1973) [in Russian].
17. W. A. Strauss, *Partial Differential Equations: An Introduction* (Wiley, New York, 2007). https://www.wiley.com/en-au/
18. E. Wegrzyn-Skrzypczak and T. Skrzypczak, "Numerical modeling of the solidification process with consideration of shrinkage cavities formation and the influence of solid phase content on the feeding of the casting," J. Appl. Math. Comput. Mech. **22**, 75–86 (2023).

19. E. Wegrzyn-Skrzypczak, “Investigation of the influence of liquid phase motion on the solidification process in the three-dimensional region,” J. Appl. Math. Comput. Mech. **20**, 103–111 (2021).
20. T. K. Yuldashev, “Mixed problem for pseudoparabolic integro-differential equation with degenerate kernel,” Differ. Equat. **53**, 99–108 (2017).
21. T. K. Yuldashev, “Nonlocal mixed-value problem for a Boussinesq-type integrodifferential equation with degenerate kernel,” Ukr. Math. J. **68**, 1278–1296 (2017).
22. T. K. Yuldashev, “Solvability of a boundary value problem for a differential equation of the Boussinesq type,” Differ. Equat. **54**, 1384–1393 (2018).
23. T. K. Yuldashev, “Inverse problem for a nonlinear Benney–Luke type integro-differential equations with degenerate kernel,” Russ. Math. **60** (8), 53–60 (2016).
24. T. K. Yuldashev, “Nonlinear optimal control of thermal processes in a nonlinear inverse problem,” Lobachevskii J. Math. **41**, 124–136 (2020).
25. T. K. Yuldashev and B. Y. Ashirbaev, “Optimal feedback control problem for a singularly perturbed discrete system,” Lobachevskii J. Math. **44**, 661–668 (2023).
26. C. S. Chen and S. C. Lu, “The removal of sulphur dioxide in a long-lived line echo system: A numerical study,” Atmos. Environ., Part A: Gen. Top. **24**, 1561–1571 (1990).
27. R. Baldauf, “Roadside vegetation design characteristics that can improve local, near-road air quality,” Transp. Res., Part D: Transp. Environ. **52**, 354–361 (2017).
28. D. Leone and S. Turns, “Active chlorine and nitric oxide formation from chemical rocket plume after burning,” in *Proceedings of the AIAA 32nd Aerospace Sciences Meeting and Exhibit, 1994* (1994), pp. 1–14.
29. X. Huang, He Li, He Zhengwei, Nan Xi, Lyu Pengyi, and Ye Haiyan, “An improved Carnegie-Ames-Stanford approach model for estimating ecological carbon sequestration in mountain vegetation,” Front. Ecol. Evolut. **10** (2022). https://doi.org/10.3389/fevo.2022.1048607
30. A. Havasi, J. Bartholy, and I. Farago, “Musicales influences on wind fields,” Idojaras **105**, 39–58 (2001).
31. A. Bekkar, B. Hssina, S. Douzi, and Kh. Douzi, “Air-pollution prediction in smart city, deep learning approach,” J. Big Data **8** (1), 1–21 (2021).
32. L. Zhang, D. Li, and Q. Guo, “Deep learning from spatio-temporal data using orthogonal regularizaion residual CNN for air prediction,” IEEE Access **8**, 66037–66047 (2020).
33. H. Alkabbani, A. Ramadan, Q. Zhu, and A. Elkamel, “An improved air quality index machine learning-based forecasting with multivariate data imputation approach,” Atmosphere (Basel) **13** (7) (2022).
34. M. Z. Liang, Chao Ye, Tu Yu, and Xu Te, “Vehicle pollutant dispersion in the urban atmospheric environment: A review of mechanism, modeling and application,” Atmosphere (Basel) **14** (2) (2023).
35. H. Zhou, W. Song, and K. Xiao, “Flow and hazardous gas dispersion by using WRF-CFD coupled model under different atmospheric stability conditions,” Atmosphere (Basel) **13** (7) (2022).
36. T. Ekkachai and W. Suttida, “Modeling and numerical experiments of air pollution on a complex modeling and numerical experiments of air pollution on a complex terrain,” J. Phys.: Conf. Ser. **1850**, 1–12 (2021).
37. A. Sukhinov, D. Khachuns, and A. Chistyakov, “Mathematical model of impurity propagation in the surface layer of the atmosphere and its software implementation on a multiprocessor computer system,” Vestn. UGATU **19**, 185–195 (2015).
38. M. Brauer, M. Amann, R. T. Burnett, A. Cohen, F. Dentener, M. Ezzati, S. Henderson, M. Kryzanowski, R. Martin, R. Dingenen, A. Donkelaar, and G. Thurston, “Exposure assessment for estimation of the global burden of disease attributable to outdoor air pollution,” Environ. Sci. Technol. **46**, 652–660 (2012).
39. N. Ravshanov, Z. Ravshanov, and V. Bolnokin, “Modeling the salt-dust aerosols distribution in the atmosphere, taking into account the soil erosion,” IOP Conf. Ser.: Mater. Sci. Eng. **862**, 62004 (2020).
40. N. Ravshanov and T. Shafiev “Nonlinear mathematical model for monitoring and predicting the process of transfer and diffusion of fine-dispersed aerosol particles in the atmosphere,” J. Phys.: Conf. Ser. **1260**, 1–7 (2019).
41. N. Ravshanov, M. Shertaev, and N. Toshtemirova, “A mathematical model for the study and forecast of the concentration of harmful substances in the atmosphere,” Am. J. Model. Optim. **3** (2), 35–39 (2015).
42. Z. Ravshanov, Z. Abdullaev, and O. Khafizov, “Atmospheric dispersion modelling of dust emissions from the dried bottom of the Aral Sea,” IOP Conf. Ser.: Mater. Sci. Eng. **896**, 12045 (2020).
43. D. Sharipov, Z. Abdullaev, and O. Khafizov, “The process of distribution computer modeling of hazardous substances in the atmosphere taking into account the terrain relief,” E3S Web Conf. **264**, 1–7 (2021).
44. N. Ravshanov, Z. Abdullaev, and T. Shafiyev, “Mathematical model and numerical algortm to study the process of aerosol particles distribution in the atmosphere,” in *Proceedings of the International Conference on Information Science and Communications Technologies* (Uzb. Acad. Sci., Tashkent, 2019), pp. 1–7.
45. N. Ravshanov, F. Muradov, and D. Akhmedov, “Operator splitting method for numerical solving the atmospheric pollutant dispersion problem,” J. Phys.: Conf. Ser. **1441**, 012164 (2020).

46. F. Muradov and D. Akhmedov, "Numerical modeling of atmospheric pollutants dispersion taking into account particles settling velocity," in *Proceedings of the International Conference on Information Science and Communications Technologies* (Uzb. Acad. Sci., Tashkent, 2019), pp. 1–5. https://doi.org/10.1109/ICISCT47635.2019.9011915
47. P. Haertel, "A Lagrangian ocean model for climate studies," Climate **7** (41), 1–24 (2019).
48. F. Hosoi and K. Omasa, "Factors contributing to accuracy in the estimation of the woody canopy leaf-area-density profile using 3D portable lidar imaging," J. Exp. Botany **58**, 3464–3473 (2007).
49. M. Kawka, J. Struzewska, and J. W. Kaminski, "Downscaling of regional air quality model using Gaussian plume model and random forest regression," Atmosphere **14**, 1171 (2023).
50. B. Y. Kim, R. L. Wayson, and G. G. Fleming, "Development of traffic air quality simulation model," Transp. Res. Record **1987**, 73–81 (2006).
51. J. C. Lopes da Costa, F. A. Castro, and C. S. Santos, "Large-eddy simulation of thermally stratified forest canopy flow for wind energy studies purposes," Energy Proc. **136**, 501–506 (2017).
52. N. Ravshanov, D. D. Akhmedov, and G. Roziyeva, "GIS based estimation of the vertical wind profile effect on air pollutants disperse in the atmosphere," AIP Conf. Proc. **2781**, 020078-1–6 (2023).
53. R. H. Shaw and U. Schumann, "Large-eddy simulation of turbulent flow above and within a forest," Boundary-Layer Meteorol. **61**, 47–64 (1992).
54. N. Zaman, K. D. Kanniah, D. G. Kaskaoutis, and M. T. Latif, "Evaluation of machine learning models for estimating PM 2.5 concentrations across Malaysia," Appl. Sci. **11**, 7326-1–24 (2021).