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MODELING POLLUTANT TRANSPORT AND DIFFUSION IN THE ATMOSPHERIC BOUNDARY LAYER CONSIDERING TERRAIN OROGRAPHY AND METEOROLOGICAL FACTORS

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The problem of modeling the transport and diffusion of pollutants and fine aerosol particles in the atmospheric boundary layer is examined in this article. It takes into consideration the orographic features of the earth's surface, the velocity of air masses, air temperature, humidity and density, particle diameter, diffusion and absorption coefficients, the interaction of pollutants with the underlying earth's surface, and other external factors. Computational experiments were conducted using the proposed mathematical framework. These investigations showed that high wind speeds, when coupled with unstable atmospheric stratification and strong pollution transport, significantly raise the concentration of dangerous compounds in the surface layer of the atmosphere. It was established that horizontal flows play a primary role in the dispersion of harmful substances in the atmosphere. Test problems were solved for various particle sizes ($d_p = 10^{-7}$ m; $d_p = 10^{-8}$ m; $d_p = 10^{-9}$ m). It was found that, over time, as the particle size decreases, the area of their propagation significantly expands in the direction of air mass movement. Computational experiments have shown that at wind speeds of $u = 2$ m/s, $v = 0$ m/s, $w = 0.05$ m/s and air temperatures in the range $T = 20$–$30\,^{\circ}$C, pollutants spread predominantly in the horizontal direction. At low wind speeds, pollutants accumulate near the source. However, with an increase in wind speed to $u = 4$ m/s, $v = 4.5$ m/s, $w = 0.05$ m/s, pollutants are removed from the source at an accelerated rate. At a vertical wind speed of $w = 4.5$ m/s, particles rise into the upper atmosphere, which contributes to a decrease in their concentration near the earth's surface over time. Numerical experiments were conducted at various values of relative atmospheric humidity. It was found that at a relative air humidity of 80 %, the particle settling velocity increases by a factor of 1.442; at 90 %, by a factor of 1.765; and at 95 %, by a factor of 2.190.

Keywords: mathematical modeling, numerical methods, meteorological conditions, terrain orography, pollutants, air humidity and temperature, computational experiments

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1 Introduction

It is well known that the growth of production volumes and the expansion of transportation systems in industrial regions significantly impact the environment; this is particularly noticeable in developing countries, where new industrial facilities are being built at a rapid pace. Increased emissions of pollutants and aerosol particles in the ground

layer of the atmosphere inevitably lead to environmental imbalances in industrial regions and may be accompanied by climate change.

Taking into account the above, the issues of assessing the level of pollution of the atmosphere and the underlying surface by passive and active aerosol emissions, the placement of new industrial facilities in compliance with sanitary standards, determining the intensity and degree of pollution of air and water basins, as well as assessing the impact of harmful emissions on the state of flora and fauna are urgent tasks in the field of environmental protection.

Mathematical modeling (MM) is one of the useful methods for carrying out thorough research, tracking and predicting the ecological status of the environment, and making well-informed decisions.

Meteorological conditions and terrain significantly influence the dispersion of pollutants. Taking these factors into account in MM allows for a more detailed description of pollutant dispersion processes and an assessment of the overall environmental condition of the studied object. Based on the above, a new, constructive methodology for monitoring and forecasting the environmental condition of the region under consideration is discussed in [1], based on obtaining spatially distributed data on turbulence characteristics and air quality parameters.

The approach of employing a multi-layer model to simulate the dispersion of hazardous materials in the atmospheric boundary layer while accounting for the topography and characteristics of the subsurface layer is described in [2]. The process is described by a system of partial differential equations with the corresponding initial and boundary conditions. The model is developed based on the equation of motion of a multicomponent air medium and equations for calculating the pressure and heat flows in the gas and condensed phases. Heat transfer in a multicomponent medium is calculated using the heat transfer equation for a gas, and the Mendeleev–Clapeyron equation is used to determine the vapor pressure as a function of temperature.

The process of pollutant transport and diffusion in the atmospheric boundary layer is mathematically modeled in [3]. The model takes into account atmospheric air mass movement, particle settling velocity, photochemical transformations, decomposition, and washout under the influence of precipitation. Particle settling velocity is determined based on their diameter and density, gravity, and air viscosity. The model also accounts for the influence of orography and allows for the determination of the air flow velocity field near the terrain, which can be used to estimate the concentration of atmospheric pollutants under various meteorological and topographic conditions.

In [4], the relationship between $PM_{2.5}$ pollution and complex terrain and meteorological conditions was investigated. Using radiosonde data and the WRF model, 334 pollution events from 2013 to 2017 were analyzed. The study took into account wind direction, Froude number, atmospheric boundary layer fluxes, wind speed differences, and vortex formation behind terrain. The results showed that atmospheric flow and orography have a significant impact on pollutant accumulation areas.

The study [5] analyzed the influence of atmospheric boundary layer parameterization schemes on the modeling of meteorological conditions and aerosol pollution. It was shown that non-local schemes provide more intense turbulent mixing, while local closure schemes are characterized by relatively less intense turbulent mixing under stable stratification conditions.

Scientists have studied the development of the atmospheric boundary layer and changes in air flows under complex terrain conditions [6]. The results of observations and mod-

eling using WRF showed that the influx of daytime sea breezes into the basin enhances the air flow and affects O_3 transport. At night, a stable boundary layer was formed, accompanied by a strong night current in the lower layers of the atmosphere. The results obtained indicate the relationship between meteorological conditions, characteristics of the atmospheric boundary layer and complex terrain with pollutant transport processes. The study [7] used the WRF–CALPUFF modeling system, in which experiments were conducted to assess the sensitivity of the modeling results to orographic features of the terrain. According to the study results, taking into account orographic features led to an average increase in NO_2 concentration in urban areas by approximately 30 %.

The study [8] examined pollutant dispersion in the Akhangaran Valley using a hydrodynamic model. The model took into account the morphometric characteristics of the terrain, meteorological and synoptic conditions, as well as mountain-valley circulation and air flows. Calculations were performed using the finite difference method. The results showed that at wind speeds above 3 m/s, pollutants leave the valley more quickly, while at wind speeds below 2 m/s, pollution levels increase, especially near emission sources. Precipitation was also identified as an important factor contributing to atmospheric purification.

The issue of researching and forecasting the dispersion of dangerous compounds in the atmosphere is examined in [9]. The authors created a mathematical model that considers weather and climatic variables in addition to other process characteristics. Based on the suggested model, numerical experiments were carried out. The findings demonstrate that important variables like wind speed, soil moisture, and soil type have a big influence on how dangerous compounds spread throughout the atmosphere.

The identification of aerosols with different origins is another crucial challenge. The work of V. K. Danchenko and T. S. Ivlev [10] presents the primary methods for resolving this issue and the findings of the related investigations, while the article by R. F. Lavrinenko [11] focuses on the investigation of the formation of the chemical composition of precipitation. It gives quantitative features of the spatiotemporal changes in the chemical composition of precipitation and cloud water and summarizes the findings of measurements of their composition.

In [12], a mathematical model (MM) describing the dispersion of industrial emissions in the atmosphere is proposed. A method of splitting by physical processes, including migration, diffusion, and absorption, as well as a second-order finite-difference scheme in time, is used for the numerical solution of the problem. The influence of parameters such as wind speed and direction, absorption coefficient, and the physical and mechanical properties of particles on the dispersion of airborne contaminants is determined.

Scientists [13] proposed a model for predicting the environmental state of the atmospheric surface layer. This model takes into account the settling velocity of aerosol particles emitted from high pollution sources, turbulent dispersion in the horizontal direction, and vertical particle movement based on the Stokes equation. The effect of changes in wind direction on the particle settling area is also taken into account. The model was tested in the city of Barnaul to assess the dispersion of benzo(a)pyrene. The results showed good agreement between the calculated and experimental data.

Article [14] is devoted to mathematical modeling, analysis, and prediction of the dispersion of toxic substances in the atmospheric boundary layer. The model takes into account the velocity of particles in the air, as well as the horizontal and vertical diffusion coefficients, which depend on the ambient temperature, transport velocity, and particle

diameter. Computational experiments were conducted using the proposed mathematical model.

In the study [15], an MM was developed for monitoring and forecasting the processes of dispersion and propagation of aerosol particles in the lower layers of the atmosphere. A structural algorithm based on the method of integrating the model into computing systems was developed for its implementation.

The authors of [16] proposed a multicomponent air environment dynamics model describing the processes of pollutant and heat transport, as well as phase transitions during the dispersion of harmful compounds in the atmosphere. As part of the study, parallel algorithms for solving this model were developed and implemented in software for high-performance computing systems.

The study [17] presents a review of methods for modeling air pollution in urban canyons, focusing on the interaction of aerodynamic and chemical processes. For modeling airflow dynamics, computational fluid dynamics (CFD) is an effective numerical tool, primarily including RANS and LES models. Reynolds-averaged Navier–Stokes models are inherently steady-state methods, while large-eddy simulation models can account for the unsteadiness and discontinuity of canyon flows and reproduce transient turbulent structures in urban canyons.

An extended three-dimensional Eulerian model is proposed in [18] to model atmospheric pollution. The model takes into account the processes of pollutant advection and diffusion, particle deposition according to Stokes' law, temperature-dependent chemical decomposition, pollutant uptake by vegetation, washout by precipitation, and the influence of terrain. Turbulent diffusion is parameterized based on the Pasquill–Gifford stability classes. The Upwind/QUICK schemes and the CFL criterion are used in the calculations. The influence of terrain on pollutant dispersion for different wind directions and speeds is demonstrated.

Study [19] examines the Eulerian advection–diffusion model, designed to describe the wind dispersion of pollutants and their turbulent mixing. The book discusses the physical interpretation of the Monin–Obukhov length (L), its application to assessing the atmospheric stability class, and a method for calculating diffusion coefficients.

Thus, existing studies have considered factors such as terrain, meteorological conditions, atmospheric boundary layer conditions, turbulent diffusion, particle deposition, and chemical transformation—either individually or in combination—in MMs of atmospheric pollutant dispersion. However, in complex terrain, the challenge of comprehensively assessing the interaction of these factors within a single MM, taking into account local meteorological and orographic features, remains relevant.

It should be noted that, in the MM of pollutant propagation in the atmospheric boundary layer, many authors assume that the spread of pollutants emitted from sources does not reach the boundaries of the computational domain, and that there is no influx of pollutants across these boundaries. Studies of this process have shown that at high wind speeds, aerosol particles are carried beyond the computational domain.

This paper attempts to fill this gap and provide a more adequate description of the process under consideration by comprehensively considering key parameters, including atmospheric air velocity, air temperature, humidity and density, particle diameter, orographic features, diffusion and absorption coefficients, and particle interactions with the underlying earth's surface. These parameters depend on weather and climate conditions, time of day, and season.

In light of the aforementioned, the goal of this work is to create a mathematical model and a numerical technique for solving the problem of transport and diffusion of aerosol emissions in the atmospheric boundary layer while accounting for the aforementioned aspects.

2 Problem statement

Considering the orography of the region, the MM of the process of propagation of dangerous substances in the atmospheric boundary layer has the following form [20–22]:

$$\frac{\partial\theta}{\partial t}+\frac{\partial}{\partial x}(uH\theta)+\frac{\partial}{\partial y}(vH\theta)+\frac{\partial}{\partial z}\big((w-w_g)H\theta\big)+(\sigma+\alpha)H\theta= \\ =\frac{\partial}{\partial x}\left(D_xH\frac{\partial\theta}{\partial x}\right)+\frac{\partial}{\partial y}\left(D_yH\frac{\partial\theta}{\partial y}\right)+\frac{\partial}{\partial z}\left(D_zH\frac{\partial\theta}{\partial z}\right)+\delta_{i,j,k}Q; \quad (1)$$

$$\theta\big|_{t=0}=\theta_0; \quad (2)$$

$$D_x\frac{\partial\theta}{\partial x}\bigg|_{x=0}=(\theta-\theta_0); \quad (3)$$

$$D_x\frac{\partial\theta}{\partial x}\bigg|_{x=L_x}=(\theta-\theta_0); \quad (4)$$

$$D_y\frac{\partial\theta}{\partial y}\bigg|_{y=0}=(\theta-\theta_0); \quad (5)$$

$$D_y\frac{\partial\theta}{\partial y}\bigg|_{y=L_y}=(\theta-\theta_0); \quad (6)$$

$$D_zH\frac{\partial\theta}{\partial z}\bigg|_{z=0}=H\beta F_0; \quad (7)$$

$$D_z\frac{\partial\theta}{\partial z}\bigg|_{z=L_z}=(\theta-\theta_0). \quad (8)$$

Here x, y, z is the coordinate system; θ is the concentration of dangerous substances in the atmosphere; θ_0 is the primary concentration of dangerous substances in the atmosphere; the wind speed in three directions is denoted by u, v, and w; the particle deposition velocity is denoted by w_g; the coefficients of absorption and capture of dangerous chemicals in the atmosphere are denoted by σ and α, respectively; D_x, D_y, D_z are the diffusion and turbulence coefficients; $\delta_{i,j,k}$ is the Dirac function; Q and F_0 are the sources of hazardous material emissions from industrial facilities and the earth's underlying surface, respectively.

In the problem under consideration, the parameters H and β take into account the orography of the terrain as well as the mechanical and physical properties of the underlying earth's surface. The parameter H can have the following values: 0 indicates that the layer is underground, 1 indicates that it is in the atmosphere, and $(\eta-z_{k-0.5})/\Delta z$ indicates that it is beneath the orographic surface, where $\Delta z=z_{k+0.5}-z_{k-0.5}$ and η is the elevation above the plane parallel to sea level. The degree of airflow obstruction is determined by introducing a multiplier H $(0\leqslant H\leqslant 1)$ for each layer of the model (Fig. 1).

To integrate the given problem, the main parameters of the mathematical model of the process u, v, w will be defined in the form of power functions

$$u(x,t)=|v_1|\Big(\frac{z}{z_1}\Big)^n\cos\beta; \qquad v(z,t)=|v_1|\Big(\frac{z}{z_1}\Big)^n; \qquad w(z,t)=|v_1|\Big(\frac{z}{z_1}\Big)^n\sin\beta,$$

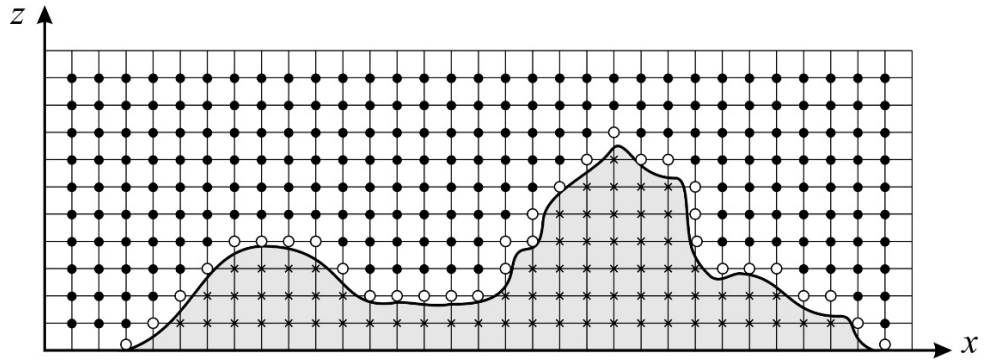


Figure 1 Terrain along the area of aerosol emission transfer: ∘ — $H = (\eta - z_{k-0.5})/\Delta z$, × — $H = 0$, • — $H = 1$.

where $|v_1|$ is the modulus of the wind speed at $z = 1$ m.

From the formulation of the problem it follows that, in order to take into account the interaction of aerosol particles with the underlying surface of the earth, the coefficient β must be calculated using the formula [9, 23]

$$\beta(x, y, z) = \begin{cases} 0, & z > z_k; \\ 0.264\, u(z)^{1.65} w_g s(z), & z < z_h. \end{cases}$$

Here z_h, z_k are the heights of vegetation and the critical layer, $s(z)$ is the specific surface area of vegetation, and w_g is the settling velocity of aerosol particles.

To calculate the capture coefficient of fine aerosol particles in the boundary layer, the following relation can be used [14, 23–25]:

$$\alpha(x, y, z, U) = \begin{cases} -\rho C_d L(x, y, z) U u_i, & \text{for } z > z_k; \\ 0, & \text{for } z > z_{r\,\max}, \end{cases}$$

where $L(x, y, z)$ is the vegetation's leaf area density profile (or the leaf surface area per unit volume); U is the air flow velocity; u_i is the flow velocity in the direction of interest; ρ is the air density (kg/m^3); C_d is the drag coefficient.

Leaf area density $L(x, y, z)$, which is defined as the total leaf area per unit volume or area of plant mass, is a metric used to characterize the structure of a plant canopy. Typically, it is expressed in square meters per cubic meter (m^2/m^3) [14, 23, 25], or as leaf area per unit volume or area:

$$L(x, y, z) = L_m \left(\frac{z_h - z_m}{z_h - z} \right)^{\gamma} \Big/ \exp\left[\gamma \left(1 - \frac{z_h - z_m}{z_h - z} \right) \right],$$

where

$$\gamma = \begin{cases} 6, & 0 \leqslant z < z_m; \\ 0.5, & z_m \leqslant z \leqslant h; \end{cases}$$

L_m is the coefficient of maximum leaf area density within the vegetation; z_m is the height at which L_m is reached ($z_m = 0.4h$).

The following relationship is used to determine the particle settling velocity [21–23]:

$$w_g(x,y,z,t) = \frac{(\rho_p - \rho_h)\, g\, d_n^2(x,y,z,t)}{18\mu};$$
$$d_n(x,y,z,t) = G\big(M(x,y,z,t)\big) d_q;$$
$$G\big(M(x,y,z,t)\big) = \left(1 + \varkappa \frac{M(x,y,z,t)}{100 - M(x,y,z,t)}\right)^{1/3},$$

where G is the hygroscopic parameter, M is the relative air humidity, d_q is the dry particle diameter, ρ_p is the particle density, ρ_h is the air density, μ is the air viscosity, g is the acceleration due to gravity, $\varkappa$ is the hygroscopic growth coefficient, and d_n is the diameter of the wet particle.

In this formulation, to determine the absorption coefficient of harmful substances in the atmosphere, a sinusoidal dependence was obtained on the basis of statistical processing of long-term data in the form of the following relationship:

$$\sigma(t) = \sigma_0 + \Delta\sigma \sin \omega t.$$

Here σ_0 is the average daily change in the absorption coefficient of aerosol emissions into the atmosphere; $\Delta\sigma$ is the amplitude of the change in the absorption coefficient per day; ω is the cyclic frequency of the daily change.

The Dirac delta function is additionally introduced into the advection–diffusion equation (1) in order to accurately describe the source of propagation in space and time:

$$Q = \begin{cases} \sum\limits_m q_m\, \delta\big((x_i - x_q)(y_j - y_q)(z_k - z_q)\big); \\ 0. \end{cases}$$
$$\forall (x_q, y_q, z_q) \in \Omega_q.$$

Here q_m is the power at each point of the source emitting a harmful substance, respectively outside and inside the region; δ is the Dirac function; $\delta(x_i - x_q, y_j - y_q, z_k - z_q)$ is the center; x_q, y_q, z_q is the source location point; x_i, y_j, z_k is the calculation point; Ω_q is the source location region.

As noted in [21–24], the coefficients of diffusion and transfer of harmful substances in the atmosphere D_x, D_y, D_z are calculated depending on the air flow velocity in the atmosphere, the particle diameter, the air temperature, the coefficient of molecular diffusion and the settling velocity of aerosol particles:

$$D_x = D_m \left(1 + a\frac{|u|}{d_p}\right); \qquad D_y = D_m \left(1 + a\frac{|v|}{d_p}\right); \qquad D_z = D_m \left(1 + a\frac{(w - w_g)}{d_p}\right); \tag{9}$$

$$D_m = \frac{k_B T}{6\pi\eta d_p}; \tag{10}$$

$$\eta(T) = \eta_0 \left(\frac{T}{T_0}\right)^{3/2} \left(\frac{T_0 + S}{T + S}\right); \tag{11}$$

$$
\begin{aligned}
D_x(T,|u|,d_p) &= \frac{k_B T}{6\pi\eta(T)d_p}\left(1+a\frac{|u|}{d_p}\right);\\
D_y(T,|v|,d_p) &= \frac{k_B T}{6\pi\eta(T)d_p}\left(1+a\frac{|v|}{d_p}\right);\\
D_z(T,|w-w_g|,d_p) &= \frac{k_B T}{6\pi\eta(T)d_p}\left(1+a\frac{|w-w_g|}{d_p}\right),
\end{aligned}
\tag{12}
$$

where D_m is the coefficient of molecular diffusion, k_B is the Boltzmann constant ($k_B = 1.38 \times 10^{-23}$ J/K), T is the absolute temperature, $T = t(^\circ\mathrm{C}) + 273.15$, η is the dynamic viscosity, T_0 is the initial temperature, $T_0 = 273$ K, S is the Sutherland temperature, $S = 110.4$ K, and η_0 is the initial viscosity, $\eta_0 = 1.716 \times 10^{-5}$ Pa·s.

As is well known, hills and mountain ranges located in open areas, as well as high-rise urban development, significantly influence changes in wind speed and direction. These orographic and anthropogenic factors significantly influence the formation of air currents and their direction and, consequently, the transport and diffusion of pollutants in the surface layer of the atmosphere.

According to the fundamental principles of hydrodynamics governing the movement of air masses in the atmosphere, wind speed rises as the atmospheric pressure differential increases, and the air flow velocity decreases to 20 m/s close to the ground as a result of friction against the rough surface.

3 Solution methods

From the formulation of problem (1)–(8), it is clear that it is difficult to obtain an analytical solution. As a result, a numerical technique based on substituting differential operators with finite-difference ones was created for the numerical integration of the problem.

It is also important to note that computational experiments using real data require a source of model parameter values relevant for a given area and at a given time. For this purpose, software interfaces for communicating with geoinformation and weather web services were developed. For example, the values of H for a given area are downloaded online using the Google Maps elevation data API. Weather data, in particular wind speed and direction (u, v, w), are retrieved from web services such as Weather Underground, World Weather Online, and WebserviceX.NET.

Auxiliary databases of elevation data based on the radar topographic survey (SRTM) and of average annual weather characteristics, including wind roses, were also created for a number of industrial regions of Uzbekistan, including Angren, Almalyk and Navoi.

To conduct a comprehensive study of the above process, based on the proposed mathematical apparatus, a software tool has been developed consisting of:

- a block for preparing, entering and formatting data;
- software modules that allow the creation of relief maps of varying levels of detail based on publicly available data from SRTM, the radar topographic survey of the Earth's surface project;
- a computing unit in which the main sought variables and parameters of the mathematical model of the object under study are calculated;
- a block for forming and filling a database with the results of numerical calculations performed on a computing cluster;
- a block for interpreting and analyzing data presented in graphical, animation and numerical formats;

– a block for making decisions and generating recommendations on the optimal placement of production facilities in order to preserve the environmental state of the region in question.

Combined with data obtained from real-time weather web services, the developed approach enables monitoring and forecasting of the process in question in near-real time.

4 Results

Using the proposed mathematical tools, computational experiments were conducted on a computing cluster using a test example (Figs. 2–10). A material balance equation was used to control the accuracy of the calculations.

The obtained results differ in that the modeling takes into account weather and climate factors, as well as the features of the mountain-valley circulation of the atmosphere within the Central Asian region.

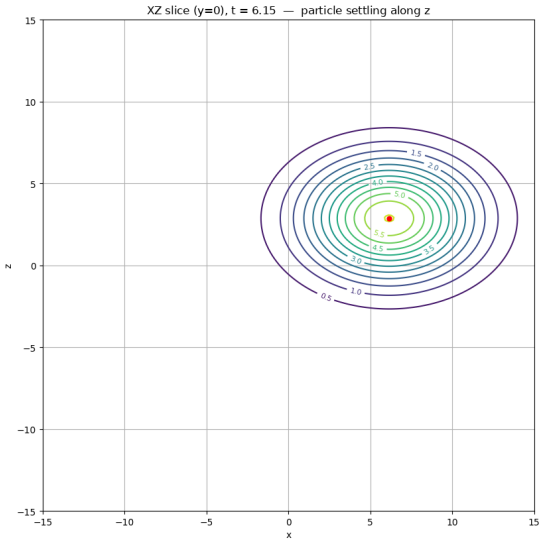


Figure 2 Concentrations of pollutants in the atmosphere at a height of $z = 100.0$ m at $t = 6.15$ h.

As can be seen from Figs. 2 and 3, the concentration of pollutants in the near-surface atmospheric layer under calm wind conditions varies significantly depending on the diffusion coefficient, which in turn depends on air temperature and humidity, as well as the diameter and density of the particles.

As can be seen from Figs. 6 and 7, the dynamics of changes in pollutant concentrations depend on the velocity of atmospheric air masses and the weather and climatic conditions of the region under consideration.

The computational experiments conducted revealed that the orographic features of the Earth's surface have a significant impact on the dispersion of pollutants in the atmosphere. Analysis of the simulation results showed that the accumulation of pollutants depends on the direction of airflow around obstacles and mountain ranges (Fig. 8).

Studies by many authors have noted that the highest levels of air pollution from low-lying sources are observed at light wind speeds of 0 to 1 m/s. For emissions from high-lying sources, maximum pollutant concentrations are typically recorded at so-called dangerous wind speeds, ranging from 3 to 6 m/s, depending on the velocity of gases exiting the exhaust stack.

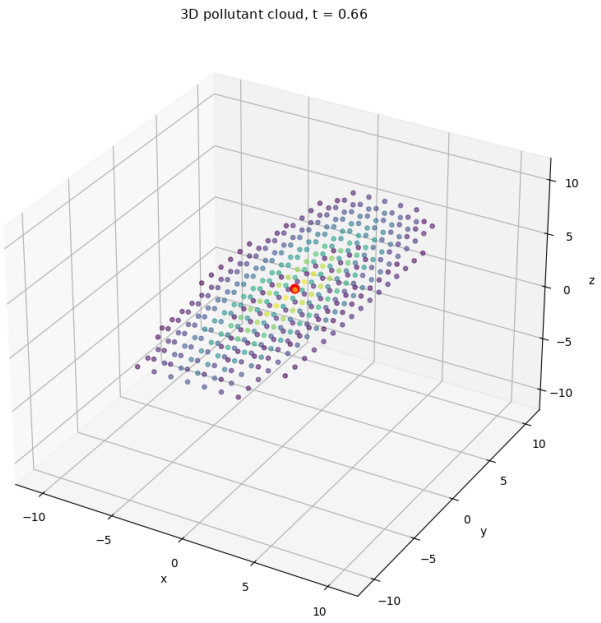


Figure 3 Concentrations of pollutants in the atmosphere at a height of $z = 50.0$ m at $t = 0.66$ h; $\sigma = 0.000254$; $\alpha = 5.0$.

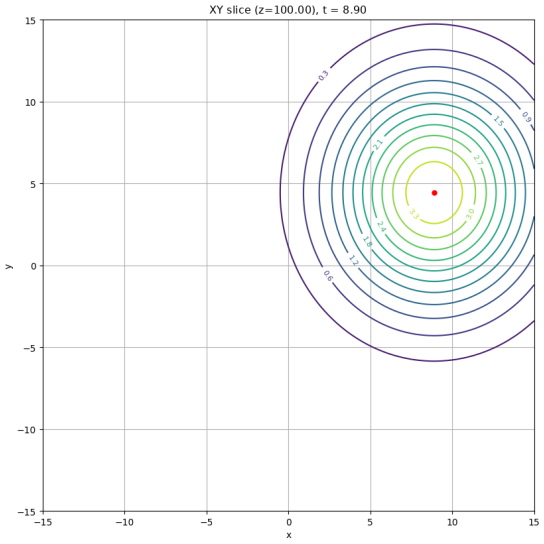


Figure 4 Concentrations of pollutants in the atmosphere at a height of $z = 100.0$ m at $t = = 8.90$ h; $\alpha = 5.0$.

One of the key factors significantly affecting the concentration of harmful substances in the atmosphere is the capture coefficient of fine aerosol particles (Figs. 9, 10). This coefficient varies depending on the vegetation density in the region under consideration and the leaf area density profile of the vegetation (i.e., the leaf surface area per unit volume). As the value of this coefficient increases, the concentration of harmful substances in the atmosphere decreases proportionally.

Dangerous wind speeds, combined with unstable atmospheric stratification and intense pollutant transport, lead to a maximum increase in the concentration of harmful substances in the ground layer of the atmosphere. Under these conditions, horizontal air currents play a primary role in the dispersion of harmful substances in the atmosphere.

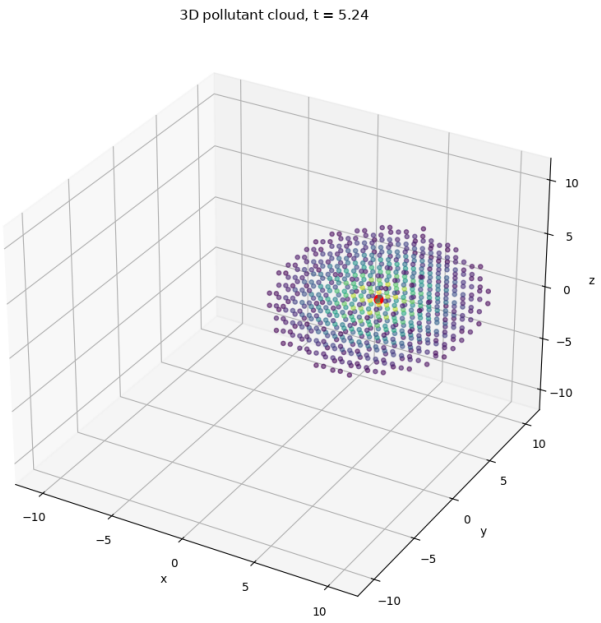


Figure 5 Variation in the concentration of pollutants in the atmosphere at a height of $z = 10.0$ m at $t = 5.24$ h; $\sigma = 0.000334$; $\alpha = 5.0$.

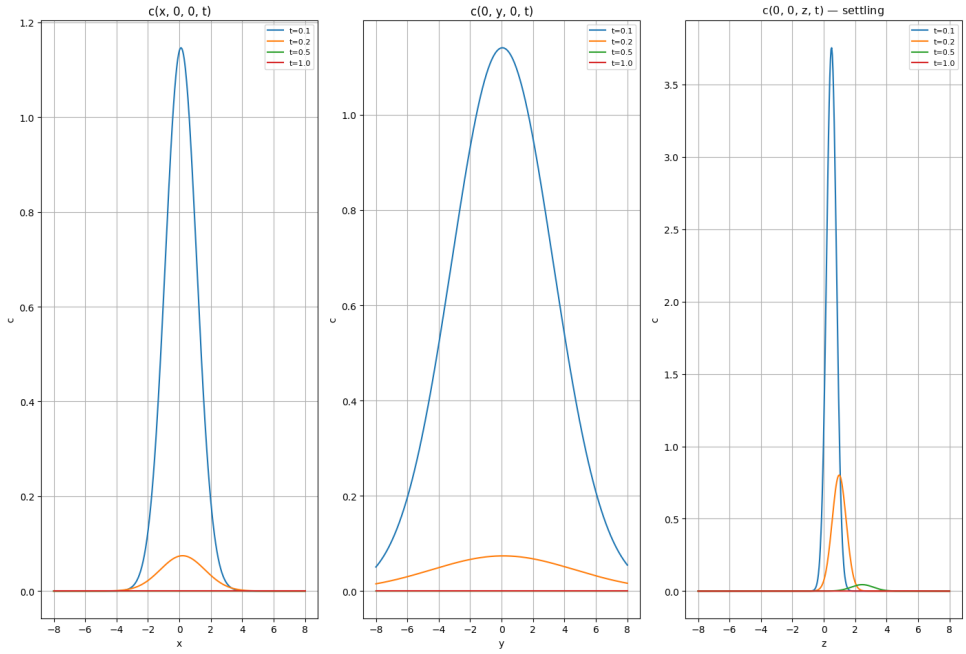


Figure 6 Concentrations of pollutants in the atmosphere at $t = 4.29$ h.

Test calculations were carried out for different particle sizes ($d_p = 10^{-7}$ m; $d_p = 10^{-8}$ m; $d_p = 10^{-9}$ m). Analysis of the obtained results showed that, over time, as the particle size decreases, the area of their distribution significantly expands in the direction of air mass movement (Figs. 7, 8).

As can be seen from the calculations, at wind speeds of $u = 2$ m/s, $v = 0$ m/s, and $w = 0.05$ m/s, and at air temperatures in the range $T = 20$–$30\,^{\circ}$C, the movement and dispersion of aerosol particles in the surface layer of the atmosphere occur predominantly in the horizontal direction under the influence of the wind flow (Figs. 9, 10). Consequently, at low wind speeds, pollutants accumulate near the source, whereas with increasing dis-

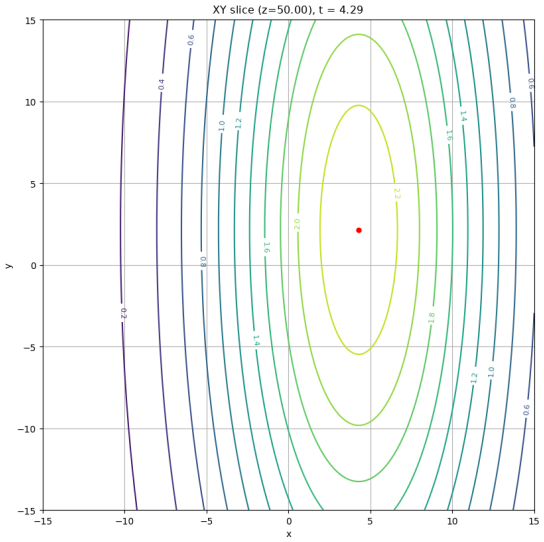


Figure 7 Variation in the concentration of pollutants in the atmosphere at a height of $z = 50.0$ m at $t = 4.29$ h.

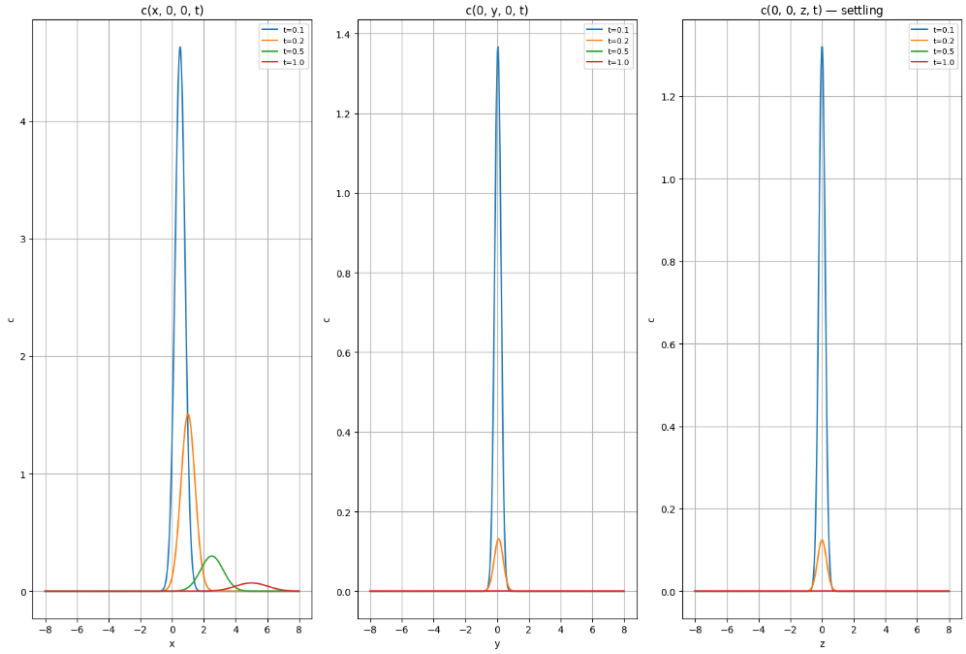


Figure 8 Variation in the concentration of pollutants in the atmosphere at a height of $z = = 150.0$ m at $V_{\text{medium}} = 5.0$ m/s; $\sigma = 0.000334$; $\alpha = 0.5$.

tance their concentration gradually decreases due to turbulent diffusion and atmospheric mixing.

Computational experiments have shown that at wind speeds of $u = 4$ m/s, $v = = 4.5$ m/s, and $w = 0.05$ m/s, $PM_{2.5}$ particles are rapidly carried away from their source and intensively mixed in the atmospheric boundary layer. As the vertical wind speed increases to $w = 4.5$ m/s, the particles rise into the upper atmosphere, which contributes to a decrease in their concentration near the earth's surface over time.

Calculations were also conducted at various relative atmospheric humidity levels. At 80 % relative humidity, the particle settling velocity increases by a factor of 1.442 and the sedimentation process accelerates by a factor of 2.080. At 90 % relative humidity, these

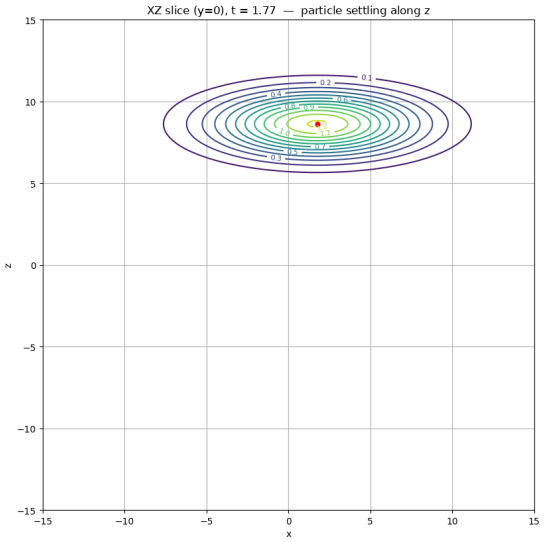


Figure 9 Concentrations of pollutants in the atmosphere at a height of $z = 50.0$ m at $V_{\text{medium}} =$ $= 5.0$ m/s; $t = 1.77$; $\sigma = 0.000334$; $\alpha = 5.0$.

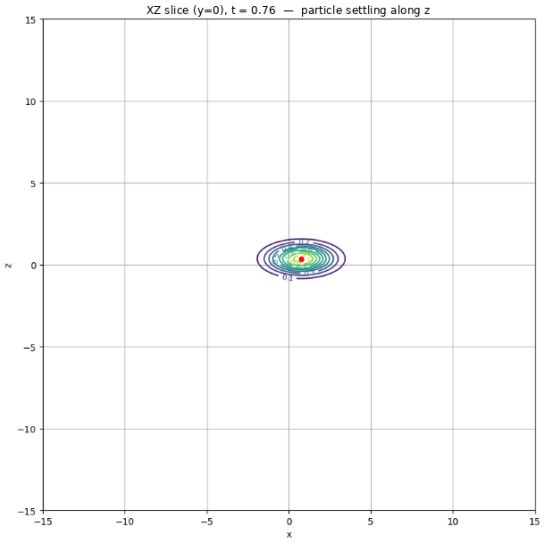


Figure 10 Concentrations of pollutants in the atmosphere at $V_{\text{medium}} = 3.5$ m/s; $t = 0.76$ h; $\sigma = 0.000334$; $\alpha = 0.55$.

figures are 1.765 and 3.116, respectively, and at 95 % relative humidity, they are 2.190 and 4.795.

Computational experiments were conducted at various air flow temperatures. When the temperature is −3 °C, the diffusion coefficient is at its lowest. Consequently, molecular diffusion is relatively weak, the pollutant remains concentrated around the emission source, and the cloud has a relatively small dispersion zone and a narrow spatial distribution. At −2 °C, a slight increase in temperature leads to an increase in the diffusion coefficient. Compared to −3 °C, the pollutant plume becomes slightly wider and extends further downwind. The concentration near the source decreases slightly due to increased diffusion. At 0 °C, the diffusion process becomes more pronounced. The pollutant is transported further from the source, and the concentration distribution becomes spatially more uniform. Thus, an increase in temperature leads to a noticeable expansion of the dispersion region. At 10 °C, the diffusion coefficient increases significantly compared to

subzero temperatures. As a result, the pollutant plume becomes wider and extends further. The pollutant concentration is distributed more uniformly across the computational domain, which leads to a decrease in peak concentrations near the source. At 20 °C, enhanced molecular diffusion leads to a significant expansion of the concentration region. The pollutant is transported over a greater distance in the direction of the prevailing wind. At the same time, the maximum concentration decreases due to stronger spatial dispersion. At 30 °C, the diffusion coefficient reaches its highest value among all the cases considered. Thus, the pollutant plume exhibits the greatest spatial expansion and the widest dispersion range in the downwind direction. The concentration is distributed over a significantly larger area, and the maximum concentration near the source is comparatively lower. Numerical results demonstrate a clear relationship between air temperature and pollutant dispersion. As the temperature increases from −3 °C to 30 °C, the diffusion coefficient increases, leading to an expansion of the pollutant concentration field in both the longitudinal and transverse directions. Conversely, at lower temperatures, diffusion is weaker, and pollutant concentrations remain higher near the source. Therefore, temperature should be considered as an important parameter when calculating the diffusion coefficient and predicting pollutant dispersion in the atmosphere.

5 Conclusion

The developed mathematical framework for the mechanisms by which dangerous compounds are transported and diffused in the atmosphere can be used for optimal siting of newly constructed industrial facilities, assessing the scale and spatial distribution of environmental emissions, determining the concentration of dangerous materials on the surface and in the atmosphere, and subsequently making informed decisions aimed at minimizing environmental risks.

Computational experiments have shown that wind speeds are higher over elevated areas than in the surrounding flatlands, resulting in more intense pollutant transport in this region. Since the high-pressure zone extends a certain distance ahead of the elevation, the airflow changes direction before reaching its slope. It should be noted that when an air mass interacts with a steep hill with an uneven surface, the wind speed can rise dramatically, increasing turbulence and the turbulent diffusion coefficient.

Computational tests have demonstrated that the combination of dangerous wind speeds, unstable atmospheric stratification, and intense pollutant transport leads to a significant increase in pollutant concentrations in the surface layer of the atmosphere. Furthermore, horizontal air currents are crucial in pollutant dispersion.

In the course of solving test problems for different values of particle diameter ($d_p = = 10^{-7}$ m; $d_p = 10^{-8}$ m; $d_p = 10^{-9}$ m), it was established that over time, as the particle size decreases, the area of their distribution significantly expands in the direction of movement of the air mass.

At wind speeds of $u = 2$ m/s, $v = 0$ m/s, and $w = 0.05$ m/s, and at air temperatures in the range $T = 20$–30 °C, the transport and diffusion of aerosol particles occur predominantly in the horizontal direction. At low wind speeds, pollutants accumulate near the source, whereas with an increase in wind speed to $u = 4$ m/s, $v = 4.5$ m/s, and $w = 0.05$ m/s, pollutants are rapidly carried away from the source. With an increase in vertical wind speed to $w = 4.5$ m/s, particles rise into the upper layers of the atmosphere, which contributes to a decrease in their concentration near the earth's surface over time.

Software interfaces have been developed for interaction with geoinformation and weather web services, allowing computational experiments to be conducted using real weather and climate data for a given territory.

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МОДЕЛИРОВАНИЕ ПЕРЕНОСА И ДИФФУЗИИ ЗАГРЯЗНЯЮЩИХ ВЕЩЕСТВ В ПОГРАНИЧНОМ СЛОЕ АТМОСФЕРЫ С УЧЁТОМ ОРОГРАФИИ МЕСТНОСТИ И МЕТЕОРОЛОГИЧЕСКИХ ФАКТОРОВ

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В статье рассматривается задача моделирования процесса переноса и диффузии загрязняющих веществ и аэрозольных мелкодисперсных частиц в пограничном слое атмосферы с учётом орографических особенностей земной поверхности, скорости движения воздушных масс, температуры, влажности и плотности воздуха, диаметра частиц, коэффициентов диффузии и поглощения, а также взаимодействия загрязняющих веществ с подстилающей земной поверхностью и других внешних факторов. На основе предложенного математического аппарата проведены вычислительные эксперименты, в ходе которых выявлено, что высокая скорость ветра в сочетании с неустойчивой стратификацией атмосферы и интенсивным переносом примесей приводит к значительному увеличению концентрации вредных веществ в приземном слое атмосферы. Установлено, что при рассеивании вредных веществ в атмосфере основную роль играют горизонтальные потоки. Решены тестовые задачи при различных значениях размера частиц ($d_p = 10^{-7}$, 10^{-8} и 10^{-9} м). Установлено, что с течением времени при уменьшении размера частиц область их распространения существенно расширяется в направлении движения воздушной массы. Вычислительными экспериментами установлено, что при скоростях ветра $u = 2$ м/с, $v = 0$ м/с, $w = 0{,}05$ м/с и температуре воздуха в диапазоне $T = 20$–$30\,^{\circ}$C распространение загрязняющих веществ происходит преимущественно в горизонтальном направлении. При низкой скорости ветра наблюдается накопление загрязняющих веществ вблизи источника, тогда как при увеличении скорости ветра до $u = 4$ м/с, $v = 4{,}5$ м/с, $w = 0{,}05$ м/с происходит ускоренное удаление загрязняющих веществ от источника. При вертикальной скорости ветра $w = 4{,}5$ м/с происходит подъём частиц в верхние слои атмосферы, что способствует снижению их концентрации у поверхности земли с течением времени. Установлено, что при относительной влажности воздуха 80 % скорость осаждения частиц увеличивается в 1,442 раза; при влажности 90 % — в 1,765 раза; а при влажности 95 % — в 2,190 раза.

Ключевые слова: математическое моделирование, численные методы, метеорологические условия, орография местности, загрязняющие вещества, влажность и температура воздуха, вычислительные эксперименты

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