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TWO-DIMENSIONAL NONLINEAR MATHEMATICAL MODEL OF THE PROCESS OF DISTRIBUTION OF HARMFUL SUBSTANCES IN THE BOUNDARY LAYER OF THE ATMOSPHERE

Abstract: The article discusses in fact, to develop a mathematical model of an object using natural laws, we build an information model that includes complete information about the process or object under study. The choice of the most significant information when creating an information model and its degree of complexity is determined by the purpose of mathematical modeling. It should be noted that the construction of an information model is the main point in the development of a mathematical model of the object of study. All input parameters of the object selected during the analysis are ranked, and based on the selection methods, the model is simplified in accordance with the purpose of modeling. At the same time, factors that are not informative in the mathematical modeling of the object of study are discarded.

Key words: rate of deposition of particles, the process of transfer and diffusion of aerosol particles in the atmosphere, numerical algorithm.

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Introduction

In addition to industrial and economic facilities, natural phenomena are also a significant source of harmful emissions, mainly, the removal of particles from the soil surface as a result of the turbulent movement of air masses in the surface layer of the

atmosphere. This example is very relevant for the Aral Sea region, due to the drying of the Aral Sea and the exposure of about 60 thousand km² of its bottom, composed mainly of solonchaks and saline soils containing a large amount of pesticides and other

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harmful chemicals brought into the sea by wastewater for many years [1].

The presence of a large amount of impurities in the atmosphere entails many negative effects on the living environment. In many respects, this affects the decrease in yield and quality of agricultural products as a result of damage to crops from "acid rain" [1].

The decrease in the quality of atmospheric air in places of residence causes significant harm to the health of the population. According to the International Committee on Health, the number of cases of cancer, asthma, allergies, etc. has increased dramatically in recent years. diseases due to the deterioration of the ecological state of the environment around the world [2].

Thus, in the tasks of environmental protection, the issues of monitoring and forecasting pollution of the atmosphere and the underlying surface of the earth by passive and active aerosol emissions, the location of new industrial facilities in compliance with sanitary standards and the determination of the amount of suspended particles in the air basins of the regions under consideration become extremely relevant [3].

Since the ecology of the atmosphere is one of the most important indicators of the state of the environment, it becomes necessary to carry out forecasts of the concentration of impurities in the surface layer of the atmosphere for various time frames. Of practical interest here are short-term forecasts related to the control of the maximum permissible concentration of harmful impurities in the design of structures of new enterprises[4, 5].

Pollution of the surface layer of the atmosphere and the underlying surface, including the transfer and diffusion of harmful substances, as well as their deposition and concentration, is a very complex process influenced by various factors that need to be taken into account in a detailed analysis of its state and in the performance of prognostic estimates, including geographical and weather and climatic conditions characteristic of a particular region under consideration, etc. Moreover, it is important to take into account the fact that meteorological conditions change during the day and seasons [6, 7].

Therefore, to date, one of the main approaches to the study of the process of distribution of harmful emissions in the atmosphere, the most acceptable in terms of economic and environmental criteria, is mathematical modeling, which can provide sufficient accuracy in describing and predicting changes [6].

The available means of mathematical modeling are able to provide comprehensive research, the purpose of which is to develop adequate models, efficient computational algorithms and software tools for automating the solution of problems of predicting the ecological state of industrial regions and making decisions on protecting the environment from harmful effects with a sufficiently high degree of certainty [6].

It should be noted that the current level of development of information technologies, computer hardware and software makes it possible to conduct computational experiments on problems of almost any complexity and dimension based on complex computer models that take into account a large number of various factors that affect the processes under study.

In response to the actualization of the problems of the ecological state of the atmosphere, the issues of mathematical modeling of the processes of transfer and diffusion of harmful substances in the boundary layer of the atmosphere are currently being actively studied by many scientists around the world. With the use of computer simulation tools for the process of transfer and diffusion of harmful substances in the boundary layer of the atmosphere, many studies of both applied and fundamental nature have already been carried out and are being carried out [1, 6].

As noted in the introduction, scientific research aimed at developing and improving mathematical models, computational algorithms and software systems for solving problems of monitoring and predicting the process of atmospheric pollution is carried out in many leading scientific centers and universities in the world.

Among the most significant scientific works on various aspects of the methodology of mathematical modeling in this area are the works of such prominent foreign and domestic scientists as E. Naslund, WJ Layton, WC Reynolds, G.I. Marchuk, M.E. Berlyand, V.V. Penenko, F.B. Abutaliev, K.S. Karimberdieva, M.L. Arushanov, N. Ravshanov and others.

The results obtained by the noted researchers in the field of mathematical modeling of the process of transfer and diffusion of aerosol particles and carbon dioxide in the atmosphere, in water and soils are of great theoretical and practical importance. Their efforts have created entire scientific schools that are effectively working today around the world.

Summarizing the experience of the published works of many authors, it can be argued that the key to successful comprehensive studies of the process of spreading emissions of harmful substances into the atmosphere, taking into account various internal and external disturbances acting on the process, is the development of an effective tool expressed by the triad - a mathematical model, a computational algorithm and a software tool for conducting computational experiments on a computer[6, 3].

Many works on the study of atmospheric dispersion models emphasize the need for a more thorough description of the features of aerosol particle deposition when calculating concentration fields in different layers of the atmosphere and directly on the underlying surface.

In particular, in the study [8] the authors, using the analytical solution of the advection-diffusion equation of the form

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$$u_n \frac{\partial c_n}{\partial x} = K_n \frac{\partial^2 c_n}{\partial z^2} + w_s \frac{\partial c_n}{\partial z} \quad z_n \leq z \leq z_{n+1}, \quad n = 1 : N,$$

showed that the sedimentation rate changes the concentration of particles along the entire length of the atmospheric boundary layer. Modeling has shown that gravitational settling can strongly influence the final distribution of the concentration of harmful particles in the air and the maximum concentration near the ground. The authors considered particles with a diameter of 10 to 100 μm at different heights of emission sources and under conditions of stable and unstable atmosphere. The particle settling rate was calculated according to the Stokes law, and the height of the atmospheric boundary layer was taken equal to 1000 m. The authors also showed the influence of particle diameters on the concentration distribution at ground level depending on the conditions of atmospheric stability. The results obtained by the authors show that under conditions of an unstable atmosphere for particles with a diameter of less than 10 μm , the gravitational component of the settling rate can be neglected. It should be noted that the authors applied a stepwise approximation to the problem posed by discretizing the height h into sublayers. The solution of the problem was obtained using the Laplace transform, but, due to the complexity of the integrand, the integration was performed numerically using the Talbot algorithm.

The authors of [9] developed a mathematical model for the transfer of aerosols emitted from a point ground source, taking into account the rate of deposition of particles. Two-dimensional stationary mass transfer equation

$$u(z) \frac{\partial c}{\partial x} - w_s \frac{\partial c}{\partial z} = \frac{\partial}{\partial z} \left(k_z \frac{\partial c}{\partial z} \right)$$

with the corresponding boundary conditions was solved by the authors by applying the method of the generalized integral Laplace transform. The solution area was limited to the surface layer of the atmosphere, and changes in wind speed and vertical eddy diffusion were taken into account. The results obtained by the authors demonstrate the influence of the gravitational regime and dry deposition of particles on the distribution of their concentration at ground level, and are generally consistent with the results of other researchers.

In [10] the authors carried out a capacious review of recent achievements in the field of mathematical modeling of the processes of transfer and diffusion of pollutants in the atmosphere. The paper discusses the advantages and disadvantages of the most popular approaches and modeling strategies, namely Gaussian, Lagrangian, Euler, and computational fluid dynamics (CFD) models. Particular attention is paid to the parametrization of turbulent mixing in the atmospheric boundary layer and particle settling, and the influence of these processes on the distribution of pollution concentrations is analyzed. The authors also

highlight the main methods for numerically solving problems based on finite-difference approximation of derivatives, including the method of splitting the original problem into physical processes. Due to the fact that the class of problems under consideration has a large computational capacity, the authors also pay attention to the trends in the use of parallel computing technologies using graphic modules or adaptive mesh refinement.

Menshov M.V. [11] proposes a modification of the model for the movement and settling of a polydisperse aerosol cloud resulting from the spraying of liquid fertilizers by agricultural aircraft. To describe the migration of an aerosol cloud, M.V. Menshov uses the equation of the semi-empirical theory of transport and turbulent diffusion with a set of corresponding initial-boundary conditions. The author carries out vertical averaging of the main equation under the assumption that the vertical distribution of concentration is close to the normal distribution. The method for solving the problem is based on the discretization of the original systems in the grid domain. Spatial approximation of differential operators is based on monotone schemes and schemes with increasing total variation, algebraic systems of finite-difference equations are solved iteratively using incomplete factorization methods, and implicit splitting methods are used for time integration. Comparison of calculation results with field data shows that the proposed model of aerosol formation migration and settling has a modeling error not exceeding 12-18%, which can be considered quite acceptable for field experiments due to the natural possibility of anomalous wind profiles.

In the article by Menshov M.V. [12] the results of mathematical modeling of the transfer of aerosol formation in conditions of rugged terrain using the model described in [11]. The above results show that the presence of even low gentle hills introduces significant changes in the nature of the distribution and deposition of aerosols [12].

A number of studies by Raputa V.F., Shlychkov V.A., Lezhenina A.A., Romanov A.N. and Yaroslavtseva T.V. is devoted to the problem of the transfer of heavy inhomogeneous impurities in the atmosphere [13, 14]. The authors proposed a model for reconstructing the fields of impurity particle fallout from a high-altitude source. The authors note that, in contrast to the situation with low-lying emission sources, when modeling the transport of aerosols in the atmosphere from high-altitude sources, there are significant difficulties associated with uncertainties in the height and power of the source, the initial distribution of aerosol particles in the cloud, and meteorological conditions. This explains the need to create reconstruction models. To describe the impurity propagation process, the authors use the semi-kinematic approximation, i.e. it is assumed that turbulent scattering occurs only in horizontal

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directions, while particles move vertically at a constant Stokes velocity. The authors considered the influence of the effects of wind turns in the boundary layer of the atmosphere on the formation of the field of long-term fallout of aerosol impurities. The developed model was tested in the numerical analysis of snow cover pollution with benzopyrene in the vicinity of one of the thermal power plants in Barnaul. An analysis of the simulation results showed quite satisfactory agreement between the measured and calculated values of pollutant concentrations at control measurement points.

2. Statement of the problem

An analysis of previous studies, including by other authors, showed that one of the significant

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

$$\frac{dw_g}{dt} = \frac{mg - 6\pi\gamma r w_g - 0,5c\rho s w_g^2}{m} \quad (2)$$

with the corresponding initial and boundary conditions:

$$\theta|_{t=0} = \theta^0; \quad w_g|_{t=0} = w_g^0; \quad (3)$$

$$-\mu \frac{\partial \theta}{\partial x} \Big|_{x=0} = \xi(\theta_E - \theta); \quad \mu \frac{\partial \theta}{\partial x} \Big|_{x=Lx} = \xi(\theta_E - \theta); \quad (4)$$

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

Here θ , is the concentration of harmful substances in the atmosphere; t is time; θ_0 – primary concentration of harmful substances in the atmosphere; θ_E - concentration entering through the boundaries of the area under consideration; x, z - coordinate system; u, w – wind speed in two directions; w_g is the particle settling rate; σ - coefficient of absorption of harmful substances in the atmosphere; μ, κ are the diffusion and turbulence coefficients; Q is the power of the source; δ is the Dirac function; ξ is the mass transfer coefficient across the calculation boundaries; β is the coefficient of particle interaction with the underlying surface; f_0 - a source of emission of harmful substances into the atmosphere from the underlying surface of the earth; c is a dimensionless quantity equal to 0.5; ρ is the particle density; r is the particle radius; s is the cross-sectional area of particles; g is the acceleration of gravity, m is the mass of the particles, γ is the specific gravity of the particles.

It should be noted that in this formulation, equations (1), (2) and the corresponding initial and boundary conditions (3)–(5) describe three physical processes: convective transport of aerosol particles in the atmosphere due to the action of the atmospheric

variables affecting the process of transfer and diffusion of fine particles in the atmosphere is the rate of particle deposition on the underlying surface of the earth. This factor directly affects changes in the concentration of harmful substances over time [15].

Therefore, to study the process of transfer and diffusion of aerosol particles in the atmosphere, taking into account this essential parameter, a mathematical model was developed, which is described on the basis of the law of hydromechanics using a two-dimensional differential equation in partial derivatives [15]:

air flow; diffusion propagation of aerosol particles in the atmosphere due to molecular and turbulent diffusion; absorption of aerosol particles in the atmosphere due to the moisture content of the air mass in the atmosphere.

Unlike the works of other authors [16, 17, 18, 19, 20, 21, 22, 23], here the particle settling rate w_g is variable and depends on the physical and mechanical properties of fine particles (density, radius, cross-sectional area of particles, gravity acceleration, mass) ejected from industrial sites and production facilities, and is described by equation (2) and the corresponding initial condition (3).

According to [23, 24, 25, 26, 27], to determine the initial particle settling velocity, it is necessary to take into account three main forces that act on particles when moving in the atmosphere: gravity M_t , buoyancy N_v force resistance force R_s , which are determined using the equalities

$$M_t = mg; \quad N_v = m_p g; \quad R_s = k_c S \frac{\rho w_g^2}{2},$$

where m_p is the mass of air in the volume; k_c - coefficient of air resistance.

Since, in general, aerosol particles emitted from production facilities are spherical with a diameter

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equal to d , these three forces are calculated using the following formulas:

$$M_t = \frac{\pi d^3}{6} \rho g; \quad N_v = \frac{\pi d^3}{6} \rho g; \quad R_s = k_c \frac{\pi d^2}{4} \rho \frac{w_g^2}{2}.$$

Using the equilibrium equation, one can find the initial particle settling velocity:

$$w_g(0) = \sqrt{\frac{4dg(\rho_a - \rho)}{3k_c \rho}},$$

where ρ_a is the particle density.

It should be noted that depending on the Reindols number [24, 28, 26] you can calculate the air resistance coefficient using the following formulas:

$$a) k_c = \frac{24}{Re}; \quad b) k_c = \frac{18,5}{Re} \quad c) k_c = 0.44.$$

We also emphasize that, unlike the works performed on the problem of mathematical modeling of the process of distribution of harmful substances in the atmosphere [22, 4, 5], here we consider a two-dimensional formulation of the problem of transfer and diffusion of harmful aerosol particles in the atmosphere, taking into account the inflow and outflow of substance through the boundaries of the considered solution area with stable, indifferent and unstable stratification of the atmospheric air mass.

We consider industrial production facilities as sources of emissions of harmful substances into the atmosphere, as well as, with unstable wind stratification, the surface of the earth, which is an additional generator of emissions of harmful substances due to wind erosion of the soil [10].

Summarizing, we note that as a result, a mathematical model (1) - (5) was developed to study, monitor and predict the concentration of harmful substances emitted from production facilities into the atmosphere, taking into account changes in the rate of deposition of aerosol particles on the underlying surface of the region under consideration, changes in the rates atmospheric air mass, as well as changes in the turbulence coefficient along the height of the atmospheric layer and other external disturbances acting on the object of study.

3. Problem solving methods.

It should be noted here that for the numerical solution of Eq. (2), it is necessary to set the initial condition and the initial iterative value for $w_g(0)$, w_g^s . According to [24, 27], the initial values and the initial iteration for these variables are given by the following relations:

a) with stable stratification

$$w_g(0) = \frac{d^2 g(\rho - \rho_z)}{18k}; \quad w_g^s = \frac{d^2 g(\rho - \rho_z)}{18k};$$

b) with indifferent stratification

$$w_g(0) = c_1 \frac{d^{1.14} (\rho - \rho_z)^{0.714}}{\rho_z^{0.286} k^{0.43}}; \quad w_g^s = c_1 \frac{d^{1.14} (\rho - \rho_z)^{0.714}}{\rho_z^{0.286} k^{0.43}};$$

c) with unstable stratification

$$w_g(0) = 5.46 \sqrt{\frac{d(\rho - \rho_z)}{\rho_z}}; \quad w_g^s = 5.46 \sqrt{\frac{d(\rho - \rho_z)}{\rho_z}}.$$

Here ρ_z is the particle density; $c_1 = 0.78$.

So, to solve the problem (1)-(5), a numerical algorithm has been developed, using which it is possible to carry out numerical experiments on a computer for monitoring, forecasting and making managerial decisions in order to protect the ecological state of industrial regions [15].

The numerical calculations carried out on the processes of transfer and diffusion of harmful substances in the atmosphere showed that one of the main factors influencing the change in the concentration of harmful aerosol particles is the absorption coefficient. It depends on external factors (humidity and temperature of the air mass of the atmosphere, density of the atmosphere, saturation of the mass, etc.).

To determine the absorption coefficient, consider the simplest equation for the transfer of a substance in the atmosphere:

$$\frac{\partial \theta}{\partial t} + \text{div} \vec{U} \theta + \sigma \theta = 0,$$

where σ is the absorption coefficient or the reciprocal of the time interval during which the concentration of harmful substances θ_0 decreases several times compared to the initial concentration.

The uptake of the substance in the environment will vary depending on weather conditions. Thus, in dry weather, substances are absorbed less and spread more in the atmosphere, while at high humidity or the presence of precipitation, the aerosol is absorbed more or, without spreading in the atmosphere, settles on the earth's surface. Consider how the coefficient behaves depending on the decrease θ on a simple transport equation when there is no pollution source $f(x, y, z, t)$ and $U=V=W=0$. In this case, the transport equation can be written in the form

$$\frac{\partial \theta}{\partial t} + \sigma \theta = 0.$$

We have found the following solution to this equation:

$$\theta = \theta_0 e^{-\sigma t}.$$

Suppose that at the initial moment of time a certain amount of harmful aerosol was released into the atmosphere. We also assume that 10, 20, 30, 40, 50, 60, 70, 80, and 90% of the aerosol substance is absorbed within an hour, depending on weather conditions. Let us calculate what the absorption coefficient should be under these conditions:

$$\theta = \theta_0 e^{-\sigma t},$$

$$\ln \theta = -\sigma t + \ln \theta_0,$$

$$-\sigma t = \ln \theta - \ln \theta_0.$$

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Let after an aerosol ejection for an hour ($t = 3600$ s) when interacting with the atmosphere

1. 10% of the substance was absorbed, then we have:

$$-\sigma t = \ln 9 - \ln 10 = 2,1972 - 2,3026 = -0,1054,$$

$$-\sigma = \frac{-0,1054}{3600} = -0,000029 \frac{1}{c},$$

$$\sigma = 0,000029 \frac{1}{c};$$

2. absorbed 20% of the substance:

$$-\sigma t = \ln 8 - \ln 10 = 2,0794 - 2,3026 = -0,2232, \quad \sigma = 0,000062 \frac{1}{c};$$

3. absorbed 30% of the substance:

$$-\sigma t = \ln 7 - \ln 10 = 1,9459 - 2,3026 = -0,3567, \quad \sigma = 0,000099 \frac{1}{c};$$

4. 40% of the substance was absorbed:

$$-\sigma t = \ln 6 - \ln 10 = 1,7918 - 2,3026 = -0,5108, \quad \sigma = 0,00014 \frac{1}{c};$$

5. Absorbed 50% of the substance:

$$-\sigma t = \ln 5 - \ln 10 = 1,6094 - 2,3026 = -0,6932, \quad \sigma = 0,00019 \frac{1}{c};$$

6. Absorbed 60% of the substance:

$$-\sigma t = \ln 4 - \ln 10 = 1,3863 - 2,3026 = -0,9163, \quad \sigma = 0,000254 \frac{1}{c};$$

7. 70% of the substance was absorbed:

$$-\sigma t = \ln 3 - \ln 10 = 1,0986 - 2,3026 = -1,204, \quad \sigma = 0,000334 \frac{1}{c};$$

8. 80% of the substance was absorbed:

$$-\sigma t = \ln 2 - \ln 10 = 0,6931 - 2,3026 = -1,6095, \quad \sigma = 0,00044 \frac{1}{c};$$

9. Absorbed 90% of the substance:

$$-\sigma t = \ln 1 - \ln 10 = 0 - 2,3026 = -2,3026, \quad \sigma = 0,000639 \frac{1}{c}.$$

In this example, we see that the relationship between σ and θ inversely proportional. It also shows that under different weather conditions, the absorption coefficients will be different. So, for example, in a dry climate, when up to 10% of the substance is absorbed, $\sigma = 0.000029$ 1/s, and in heavy rain or snow, up to 90% of the substance is absorbed and $\sigma = 0.000639$ 1/s.

According to [18], based on the analysis and statistical processing of long-term meteorological data, a sinusoidal dependence was obtained for calculating the absorption coefficient:

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

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

It follows from the studies carried out in the above works that the absorption coefficient depends significantly on the daily change in the state of the air

mass of the atmosphere and the season. In the spring and winter periods of the year, the amplitude of the absorption coefficient has the greatest value, as a result of which the maximum absorption of harmful substances in the atmosphere occurs at night. In summer, the values of the extinction coefficient between nighttime and daytime variations differ very little [60, 92].

Most authors believe that β is a constant value. This distorts the prediction of particle distribution on the underlying surface. To avoid such a problem, when developing a mathematical model of the process, it is necessary to take into account $\beta = \beta(x, y, z, r)$.

To take into account the absorption of aerosol particles in the vegetation cover, the coefficient of interaction with the underlying surface β must be calculated using the formula:

$$\beta(x, y, z) = \begin{cases} 0, & z > z_h, \\ 0,264u(z)^{1,65} w_g^{0,66} s(z), & z < z_h. \end{cases}$$

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Here z_h , is the height of the vegetation layer, and $s(z)$ is the specific surface area of vegetation.

Thus, in this section, a functional dependence is obtained for calculating the absorption coefficient of harmful aerosol particles in the atmosphere. This coefficient plays a significant role in changing the concentration of aerosol particles in the atmosphere. A dependence was also obtained for calculating the coefficient of interaction with the underlying surface, which depends on the specific vegetation cover of the earth's surface.

4. Methods for solving the problem

Since problem (1)-(5) is described by a multidimensional nonlinear differential equation in partial derivatives with the corresponding initial and boundary conditions, it is difficult to obtain its solution in an analytical form.

For simplicity of solving problem (1)-(5), we consider the area $D = (0 \leq x \leq L_x, 0 \leq z \leq H_z)$ as a rectangular one, and the source is assumed to be located in the surface layer.

As the experience accumulated in the world scientific community shows, for the numerical integration of problems similar to the stated problem (1)-(5), economical and universal finite-difference methods are used. This led to their comprehensive study in terms of analyzing and predicting the state of the considered process of propagation of harmful aerosol particles in the atmosphere over time and their impact through a combination of weather, climate, orographic and other external factors.

Based on the foregoing, for the numerical solution of problem (1) - (5), the area of change of the desired variables (concentration of harmful substances), taking into account the boundary conditions, will be covered with a square grid area with a step $\Delta x; \Delta z$:

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

To solve the problem and ensure the stability of the finite difference algorithm, as well as a high order of approximation in time and space variables, we use

an implicit difference scheme and obtain [15] with $(w - w_g) < 0$:

$$\begin{aligned} & \frac{1}{2} \frac{\theta_{i,j}^{n+\frac{1}{2}} - \theta_{i,j}^n}{\Delta t/2} + \frac{1}{2} \frac{\theta_{i+1,j}^{n+\frac{1}{2}} - \theta_{i+1,j}^n}{\Delta t/2} + \frac{1}{2} u \frac{\theta_{i,j}^{n+\frac{1}{2}} - \theta_{i-1,j}^{n+\frac{1}{2}}}{\Delta x} + \frac{1}{2} u \frac{\theta_{i,j}^n - \theta_{i-1,j}^n}{\Delta x} \\ & + (w - w_g) \frac{\theta_{i,j+1}^n - \theta_{i,j}^n}{\Delta z} + \sigma \theta_{i,j}^{n+\frac{1}{2}} = \frac{\mu}{\Delta x^2} \left(\theta_{i+1,j}^{n+\frac{1}{2}} - 2\theta_{i,j}^{n+\frac{1}{2}} + \theta_{i-1,j}^{n+\frac{1}{2}} \right) + \\ & + \frac{1}{\Delta z^2} \left(k_{i,j+0,5} \theta_{i,j+1}^n - (k_{i,j+0,5} + k_{i,j-0,5}) \theta_{i,j}^n + k_{i,j-0,5} \theta_{i,j-1}^n \right) + \frac{1}{2} Q_{i,j}^{n+\frac{1}{2}} \end{aligned}$$

or

$$\begin{aligned} & \frac{1}{\Delta t} \theta_{i,j}^{n+\frac{1}{2}} - \frac{1}{\Delta t} \theta_{i,j}^n + \frac{1}{\Delta t} \theta_{i+1,j}^{n+\frac{1}{2}} - \frac{1}{\Delta t} \theta_{i+1,j}^n + \frac{u}{2\Delta x} \theta_{i,j}^{n+\frac{1}{2}} - \frac{u}{2\Delta x} \theta_{i-1,j}^{n+\frac{1}{2}} + \\ & + \frac{u}{2\Delta x} \theta_{i,j}^n - \frac{u}{2\Delta x} \theta_{i-1,j}^n + \frac{w-w_g}{\Delta z} \theta_{i,j+1}^n - \frac{w-w_g}{\Delta z} \theta_{i,j}^n + \sigma \theta_{i,j}^{n+\frac{1}{2}} = \\ & = \frac{\mu}{\Delta x^2} \theta_{i+1,j}^{n+\frac{1}{2}} - \frac{2\mu}{\Delta x^2} \theta_{i,j}^{n+\frac{1}{2}} + \frac{\mu}{\Delta x^2} \theta_{i-1,j}^{n+\frac{1}{2}} + \frac{k_{i,j+0,5}}{\Delta z^2} \theta_{i,j+1}^n - \\ & - \frac{k_{i,j+0,5} + k_{i,j-0,5}}{\Delta z^2} \theta_{i,j}^n + \frac{k_{i,j-0,5}}{\Delta z^2} \theta_{i,j-1}^n + \frac{1}{2} Q_{i,j}^{n+\frac{1}{2}}. \end{aligned} \tag{6}$$

Grouping the terms of equation (6), we obtain

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$$\begin{aligned}
& -\left(\frac{u}{2\Delta x} + \frac{\mu}{\Delta x^2}\right)\theta_{i-1,j}^{n+\frac{1}{2}} + \left(\frac{1}{\Delta t} + \frac{u}{2\Delta x} + \sigma + \frac{2\mu}{\Delta x^2}\right)\theta_{i,j}^{n+\frac{1}{2}} - \left(\frac{\mu}{\Delta x^2} - \frac{1}{\Delta t}\right)\theta_{i+1,j}^{n+\frac{1}{2}} = \\
& = \frac{u}{2\Delta x}\theta_{i-1,j}^n + \left(\frac{1}{\Delta t} - \frac{u}{2\Delta x} + \frac{w-w_g}{\Delta z} - \frac{k_{i,j-0.5} + k_{i,j+0.5}}{\Delta z^2}\right)\theta_{i,j}^n - \\
& - \frac{1}{\Delta t}\theta_{i+1,j}^n + \frac{k_{i,j-0.5}}{\Delta z^2}\theta_{i,j-1}^n + \left(\frac{k_{i,j+0.5}}{\Delta z^2} - \frac{w-w_g}{\Delta z}\right)\theta_{i,j+1}^n + \frac{1}{2}Q_{i,j}^{n+\frac{1}{2}}.
\end{aligned} \tag{7}$$

Further, grouping like terms of Eq. (7), we finally have

$$a_{i,j}\theta_{i-1,j}^{n+\frac{1}{2}} - b_{i,j}\theta_{i,j}^{n+\frac{1}{2}} + c_{i,j}\theta_{i+1,j}^{n+\frac{1}{2}} = -d_{i,j}.$$

Here

$$\begin{aligned}
a_{i,j} &= \frac{u}{2\Delta x} + \frac{\mu}{\Delta x^2}; \quad b_{i,j} = \frac{1}{\Delta t} + \frac{u}{2\Delta x} + \sigma + \frac{2\mu}{\Delta x^2}; \quad c_{i,j} = \frac{\mu}{\Delta x^2} - \frac{1}{\Delta t}; \\
d_{i,j} &= \frac{u}{2\Delta x}\theta_{i-1,j}^n + \left(\frac{1}{\Delta t} - \frac{u}{2\Delta x} + \frac{w-w_g}{\Delta z} - \frac{k_{i,j-0.5} + k_{i,j+0.5}}{\Delta z^2}\right)\theta_{i,j}^n - \\
& - \frac{1}{\Delta t}\theta_{i+1,j}^n + \frac{k_{i,j-0.5}}{\Delta z^2}\theta_{i,j-1}^n + \left(\frac{k_{i,j+0.5}}{\Delta z^2} - \frac{w-w_g}{\Delta z}\right)\theta_{i,j+1}^n + \frac{1}{2}Q_{i,j}^{n+\frac{1}{2}}.
\end{aligned}$$

Similarly, when $(w-w_g) > 0$ we approximate differential operators by finite-difference operators and obtain

$$\begin{aligned}
& \frac{1}{2}\frac{\theta_{i,j}^{n+\frac{1}{2}} - \theta_{i,j}^n}{\Delta t/2} + \frac{1}{2}\frac{\theta_{i+1,j}^{n+\frac{1}{2}} - \theta_{i+1,j}^n}{\Delta t/2} + \frac{1}{2}u\frac{\theta_{i,j}^{n+\frac{1}{2}} - \theta_{i-1,j}^{n+\frac{1}{2}}}{\Delta x} + \frac{1}{2}u\frac{\theta_{i,j}^n - \theta_{i-1,j}^n}{\Delta x} + \\
& + (w-w_g)\frac{\theta_{i,j}^n - \theta_{i,j-1}^n}{\Delta z} + \sigma\theta_{i,j}^{n+\frac{1}{2}} = \frac{\mu}{\Delta x^2}\left(\theta_{i+1,j}^{n+\frac{1}{2}} - 2\theta_{i,j}^{n+\frac{1}{2}} + \theta_{i-1,j}^{n+\frac{1}{2}}\right) + \\
& + \frac{1}{\Delta z^2}\left(k_{i,j+0.5}\theta_{i,j+1}^n - (k_{i,j+0.5} + k_{i,j-0.5})\theta_{i,j}^n + k_{i,j-0.5}\theta_{i,j-1}^n\right) + \frac{1}{2}Q_{i,j}^{n+\frac{1}{2}}.
\end{aligned}$$

To calculate the value of the desired function (concentration of suspended particles in the atmosphere) for an integer time step, similarly, for $(w-w_g) < 0$ we get

$$\begin{aligned}
& \frac{1}{2}\frac{\theta_{i,j}^{n+1} - \theta_{i,j}^{n+\frac{1}{2}}}{\Delta t/2} + \frac{1}{2}\frac{\theta_{i,j+1}^{n+1} - \theta_{i,j+1}^{n+\frac{1}{2}}}{\Delta t/2} + u\frac{\theta_{i,j}^{n+\frac{1}{2}} - \theta_{i-1,j}^{n+\frac{1}{2}}}{\Delta x} + \frac{w-w_g}{2}\frac{\theta_{i,j+1}^{n+1} - \theta_{i,j}^{n+1}}{\Delta z} + \\
& + \frac{w-w_g}{2}\frac{\theta_{i,j+1}^{n+\frac{1}{2}} - \theta_{i,j}^{n+\frac{1}{2}}}{\Delta z} + \sigma\theta_{i,j}^{n+1} = \frac{\mu}{\Delta x^2}\left(\theta_{i+1,j}^{n+\frac{1}{2}} - 2\theta_{i,j}^{n+\frac{1}{2}} + \theta_{i-1,j}^{n+\frac{1}{2}}\right) + \\
& + \frac{1}{\Delta z^2}\left(k_{i,j+0.5}\theta_{i,j+1}^{n+1} - (k_{i,j+0.5} + k_{i,j-0.5})\theta_{i,j}^{n+1} + k_{i,j-0.5}\theta_{i,j-1}^{n+1}\right) + \frac{1}{2}Q_{i,j}^{n+1}
\end{aligned} \tag{8}$$

and, grouping like terms of equation (8), we finally have

$$\bar{a}_{i,j}\theta_{i,j-1}^{n+1} - \bar{b}_{i,j}\theta_{i,j}^{n+1} + \bar{c}_{i,j}\theta_{i,j+1}^{n+1} = -\bar{d}_{i,j}, \tag{9}$$

where

$$\bar{a}_{i,j} = \frac{k_{i,j-0.5}}{\Delta z^2}; \quad \bar{b}_{i,j} = \frac{1}{\Delta t} - \frac{w-w_g}{2\Delta z} + \sigma + \frac{k_{i,j-0.5} + k_{i,j+0.5}}{\Delta z^2}; \quad \bar{c}_{i,j} = \frac{k_{i,j+0.5}}{\Delta z^2} - \frac{1}{\Delta t} - \frac{w-w_g}{2\Delta z};$$

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$$\begin{aligned} \bar{d}_{i,j} = & \left(\frac{u}{\Delta x} + \frac{\mu}{\Delta x^2} \right) \theta_{i-1,j}^{n+\frac{1}{2}} + \left(\frac{1}{\Delta t} - \frac{u}{\Delta x} + \frac{w-w_g}{2\Delta z} - \frac{2\mu}{\Delta x^2} \right) \theta_{i,j}^{n+\frac{1}{2}} + \\ & + \frac{1}{\Delta t} \theta_{i+1,j}^{n+\frac{1}{2}} + \left(\frac{1}{\Delta t} - \frac{w-w_g}{2\Delta z} \right) \theta_{i,j+1}^{n+\frac{1}{2}} + \frac{1}{2} Q_{i,j}^{n+1}. \end{aligned}$$

equation (9) with $(w-w_g) > 0$ the coefficients of the transition matrix are determined using

$$\begin{aligned} \bar{a}_{i,j} = \frac{w-w_g}{2\Delta z} - \frac{k_{i,j-0,5}}{\Delta z^2}; \quad \bar{b}_{i,j} = \frac{1}{\Delta t} + \frac{w-w_g}{2\Delta z} + \sigma + \frac{k_{i,j-0,5} + k_{i,j+0,5}}{\Delta z^2}; \quad \bar{c}_{i,j} = \frac{k_{i,j+0,5}}{\Delta z^2} - \frac{1}{\Delta t}; \\ \bar{d}_{i,j} = \left(\frac{u}{\Delta x} + \frac{\mu}{\Delta x^2} \right) \theta_{i-1,j}^{n+\frac{1}{2}} + \left(\frac{1}{\Delta t} - \frac{u}{\Delta x} - \frac{w-w_g}{2\Delta z} - \frac{2\mu}{\Delta x^2} \right) \theta_{i,j}^{n+\frac{1}{2}} + \\ + \frac{\mu}{\Delta x^2} \theta_{i+1,j}^{n+\frac{1}{2}} + \frac{1}{\Delta t} \theta_{i,j+1}^{n+\frac{1}{2}} + \frac{w-w_g}{2\Delta z} \theta_{i,j-1}^{n+\frac{1}{2}} + \frac{1}{2} Q_{i,j}^{n+1}. \end{aligned}$$

To solve the problem numerically, we replace condition with the second order of accuracy and the boundary condition (4) with a finite-difference obtain

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

Grouping like terms in the equation, we end up with

$$\theta_{0,j}^{n+1/2} = \alpha_{0,j} \theta_{1,j}^{n+1/2} + \beta_{0,j},$$

where the sweep coefficients are calculated as follows:

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

Also, replacing the boundary condition (3) with a difference condition, we obtain

$$\theta_{1,N-2,j,k}^{n+\frac{1}{2}}$$

which allows you to calculate $\theta_{N,j}^{n+1/2}$ as follows:

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

We apply the above procedure for the boundary conditions (5) and finally obtain

$$\begin{aligned} \bar{\alpha}_{i,0} = \frac{4\kappa_1\bar{c}_{i,1} - \bar{b}_{i,1}\kappa_1}{3\kappa_1\bar{c}_{i,1} - \bar{a}_{i,1}\kappa_1 - 2\Delta z\beta\bar{c}_{i,1}}; \quad \bar{\beta}_{i,0} = \frac{\bar{d}_{i,1}\kappa_1 + 2\Delta z\bar{c}_{i,1}f}{3\kappa_1\bar{c}_{i,1} - \bar{a}_{i,1}\kappa_1 - 2\Delta z\beta\bar{c}_{i,1}}; \\ \theta_{i,L}^{n+1} = \frac{2\Delta z\xi\theta_E - (\bar{\beta}_{i,L-2} + \bar{\alpha}_{i,L-2}\bar{\beta}_{i,L-1} - 4\bar{\beta}_{i,L-1})\kappa_L}{2\Delta z\xi + (\bar{\alpha}_{i,L-2}\bar{\alpha}_{i,L-1} - 4\bar{\alpha}_{i,L-1} + 3)\kappa_L}. \end{aligned}$$

To solve the stated problem (1)-(5), linearizing schemes, we obtain an equation for calculating the equation (2) and replacing it with finite-difference intermediate result according to $w_g^{n+\frac{1}{2}}$ [15]:

$$\begin{aligned} \frac{w_g^{n+\frac{1}{2}} - w_g^n}{\Delta t / 2} = \frac{mg - 6\pi\gamma r w_g^{n+\frac{1}{2}} - 0,5c\rho s \left(2\tilde{w}_g w_g^{n+\frac{1}{2}} - \tilde{w}_g^2 \right)}{m}; \\ w_g^{n+\frac{1}{2}} = \frac{2m}{2m + 6\pi\gamma r \Delta t + c\rho s \Delta t \tilde{w}_g} w_g^n + \frac{mg\Delta t + 0,5c\rho s \Delta t \tilde{w}_g^2}{2m + 6\pi\gamma r \Delta t + c\rho s \Delta t \tilde{w}_g}. \end{aligned}$$

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To calculate, w_g^{n+1} we obtain the following relation:

$$\frac{w_g^{n+1} - w_g^{n+\frac{1}{2}}}{\Delta t / 2} = \frac{mg - 6\pi\gamma r w_g^{n+1} - 0,5c\rho s(2\tilde{w}_g w_g^{n+1} - \tilde{w}_g^2)}{m};$$

$$w_g^{n+1} = \frac{2m}{2m + 6\pi\gamma r\Delta t + c\rho s\Delta t\tilde{w}_g} w_g^{n+\frac{1}{2}} + \frac{mg\Delta t + 0,5c\rho s\Delta t\tilde{w}_g^2}{2m + 6\pi\gamma r\Delta t + c\rho s\Delta t\tilde{w}_g}.$$

The resulting nonlinear equations for w_g are solved by simple iteration. The convergence of the iteration process is checked using the condition $|w_g^{S+1} - w_g^S| < \varepsilon$, where ε is the accuracy of the iteration process, S is the number of iterations [15].

5. Computational experiment

To carry out the SE on a computer, a software tool in the C++ language was created. The following input parameters were taken into account in the calculations: the size of the area for solving the problem is 21x21 km, while the emission source is located in the center of the area; height of the mouth of the discharge pipe - 100 m above the ground; source power - 100 mg / m³ per second; the initial value of the particle settling velocity is 0.00015 m/s; absorption coefficient - 0.00048 1/s; wind speed - 5 m/s; wind direction - 130°.

The effectiveness of the developed algorithm for solving the problem based on the physical splitting method was evaluated by comparing the calculation results with field measurement data and calculations based on other numerical methods for solving the above problem. On fig. 1-4, the concentration distribution of fine particles in each case is given for time $t = 5$ h at a height of 200 m above the earth's surface. Colors indicate concentration values in kg/m³ per second.

The sizes and shapes of the loops in fig. 1-4 visually have minimal differences. Nevertheless, the analysis of the numerical results shows a quite tangible advantage of the developed computational algorithm based on the method of splitting by physical processes.

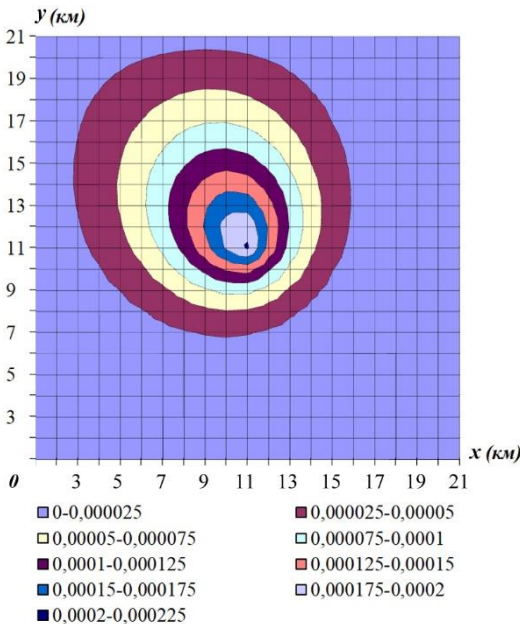


Fig. 1. Field measurement data

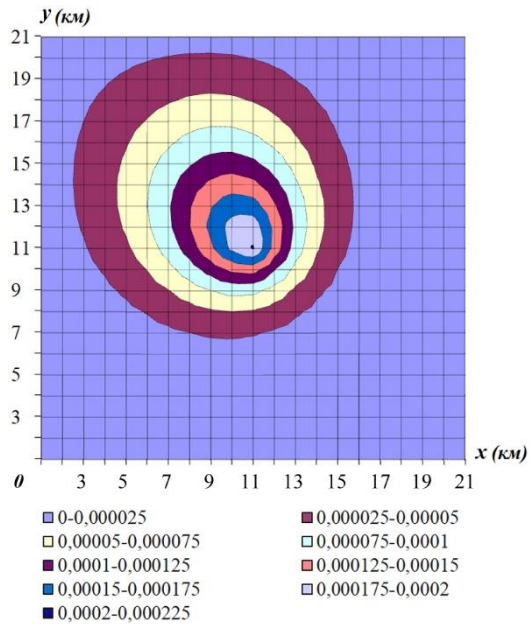


Fig. 2. Method of physical splitting

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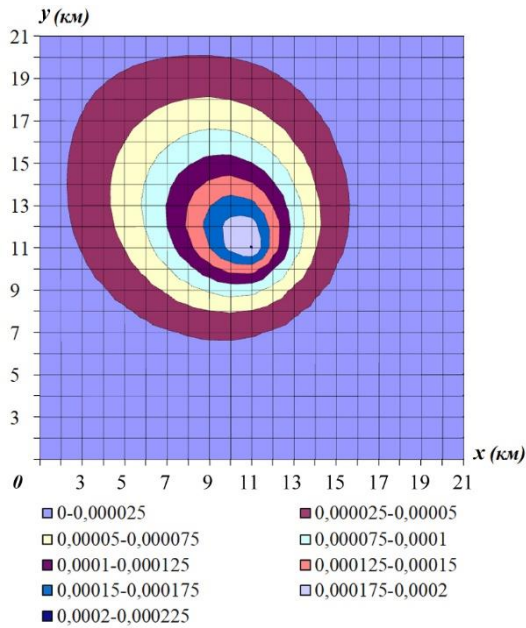


Fig. 3. Finite-difference scheme of the 2nd order of approximation

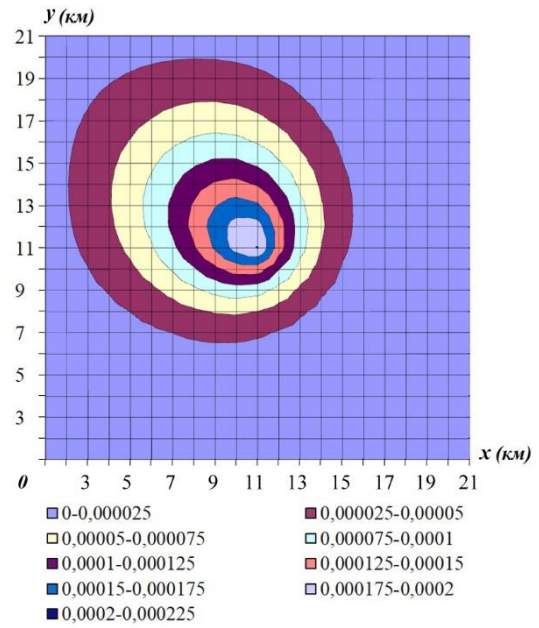


Fig. 4. Solution based on the change of variables method

On fig. Figure 5 shows a graph of the values of the concentration of harmful particles along the middle line of the problem solution area for x , θ ($\mu\text{g}/\text{m}^3$)

obtained by various methods, and the table shows the performance indicators of the algorithms developed on the basis of the considered numerical methods.

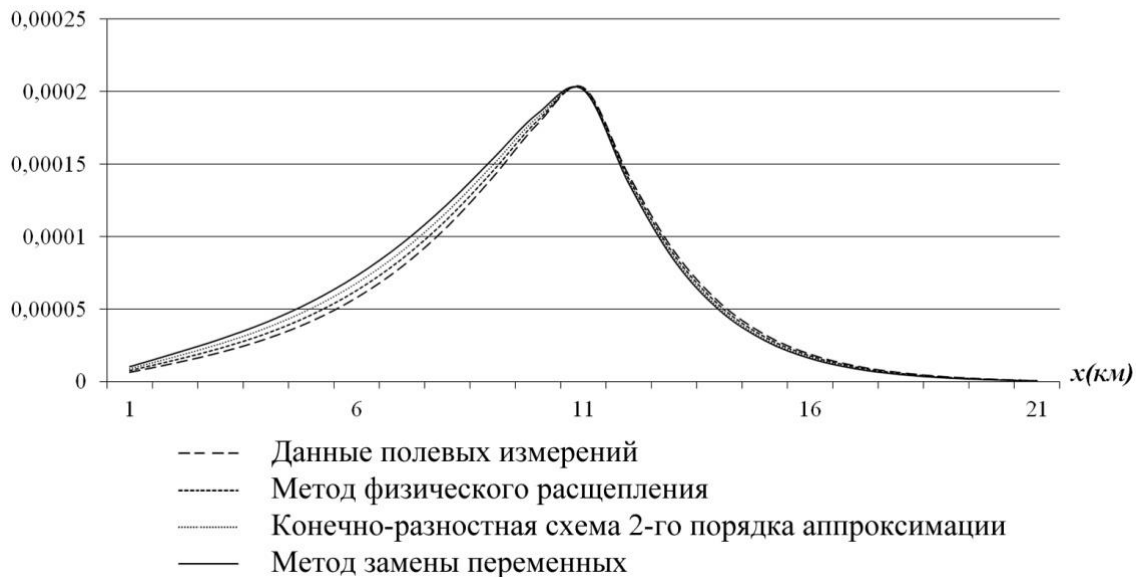


Fig. 5. Consistency of various numerical methods for solving the problem with real measurement data

According to the graphs shown in the figures, the results of the numerical solution of the problem of the distribution of harmful emissions in the atmosphere by the physical splitting method have a minimum

discrepancy with the measurement data. The accuracy is higher by 5-10%, while the calculation time is the smallest.

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Table 1. Performance indicators of computational algorithms

Indicators	Physical splitting method	Finite-difference scheme of the 2nd order of approximation	Variable substitution method
Accuracy (%)	95.07	90.25	85.53
Time (ms)	1.2	1.5	1.9

The SE found that with a decrease in the time integration step, the solution of individual problems tends to solve the main problem. Although the method of splitting into physical processes gives good results, inaccuracies in the solution of split problems can arise due to changes in parameters $u, v, w, w_g, \mu, \kappa(z)$ both in time and in space variables.

Comparison of the results of the conducted SE with the data of field measurements, as well as the regularities identified in the works of other authors, showed their fairly satisfactory agreement.

Based on the foregoing, we conclude that the developed model adequately describes the process of atmospheric dispersion of pollutants and their precipitation. The computational algorithm for solving the problem based on the method of splitting by physical processes is quite efficient and gives good results. The purpose of creating the considered model and algorithm, which was to provide the possibility of analyzing, monitoring and predicting the process of distribution of harmful industrial emissions in the surface layer of the atmosphere, was achieved to a sufficient extent.

As an example, consider **Farkhad village, Samarkand region**. For the experiment, an assessment was made of the spread of aerosol emissions from one of the industrial enterprises near the village of Farhad, Samarkand region. The area under consideration is a flat area at the foot of the Zerafshan Range. The soil cover here is represented mainly by sands and meadow-serozem soils. The climate is inland with hot dry summers and cold winters. The average annual temperature is $+16.5^{\circ}$, the average annual rainfall is 310-330 mm. In the area

under consideration, weak winds up to 4-5 m/s prevail, blowing mainly from the north-west direction.

The following input parameters were taken in the calculations: the initial value of the particle settling velocity - 45.762×10^{-5} m/s; the size of the area for solving the problem is 21x21 km, while the emission source is located in the center of the area; height of the mouth of the discharge pipe - 100 m above the ground; absorption coefficient - 30%, i.e. 0.00048 1/s; source power - $10 \text{ mg} / \text{m}^3 \text{ in s}$.

Numerical calculations have established that the change in the concentration of aerosols in the atmosphere depends significantly on the absorption coefficient of particles in the atmosphere. This parameter varies depending on the degree of humidity of the air mass of the atmosphere, time of year and day. At the same time, the maximum absorption of harmful aerosol particles in the atmosphere is typical for the morning and evening hours of the day. In general, the region under consideration is characterized by absorption from 10 to 18% of aerosol particles.

Of the numerical experiments performed, the most significant parameters affecting the distribution and accumulation of harmful aerosol particles in the atmosphere of the region under consideration are the horizontal and vertical components of the wind speed and their direction, as well as the particle settling rate. As might be expected, under moderate wind (when the wind speed components approach zero), the concentration of harmful substances accumulates around the emission sources and the change in the concentration of aerosol particles in the atmosphere mainly occurs due to an increase in the particle settling rate w_g (Fig. 6).

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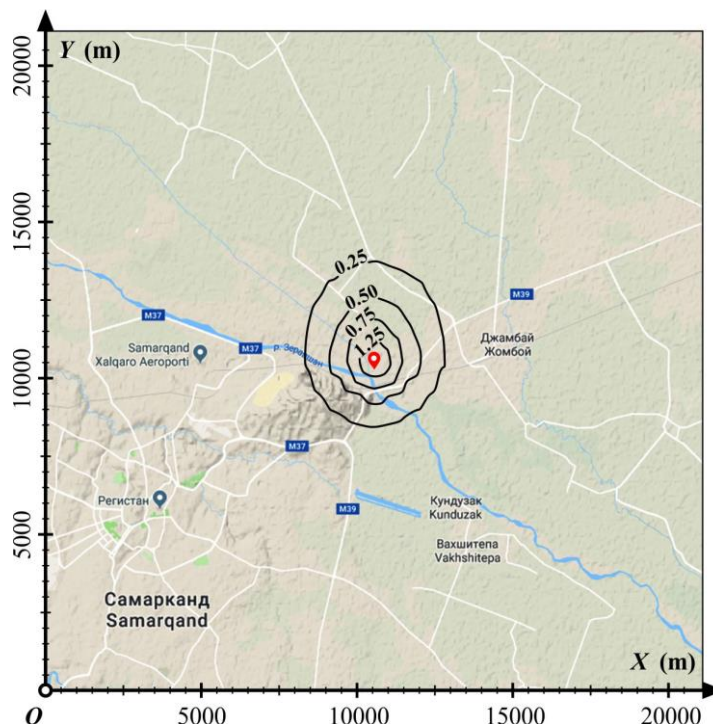


Fig. 6 . The concentration of fine particles of cement dust (mg/m^3) at a height of 200 m with a southerly wind of 1 m/s and calculation time $t = 4$ h

The SE were carried out under the condition that aerosol particles with different diameters are emitted into the atmosphere, which also plays a significant role in the process of transfer and the rate of particle deposition. Thus, it follows from the calculations that the transportation of aerosol particles along the vertical largely depends on both the vertical component of the wind speed and the physicochemical properties of the particles (radius, mass and cross-sectional area, density), as well as the acceleration of gravity.

With an increase in wind speed due to the horizontal transfer of aerosol particles, the concentration of harmful substances around the source decreases proportionally, and the area of their transportation expands over time. The maximum accumulation of aerosol particles in the atmosphere is observed at a level of 200-350 m. The concentration of pollution decreases exponentially with distance from the source. The maximum concentration of harmful particles is observed in the axial part of the atmospheric transport plume at a distance of up to 10 km from the source (Fig. 7, 8).

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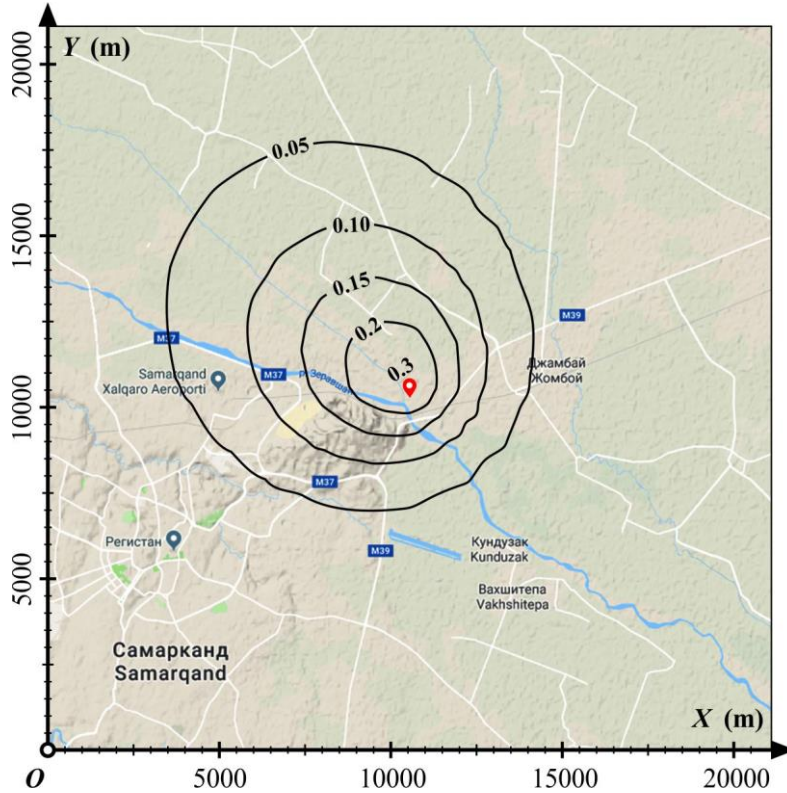


Fig. 7 . The concentration of fine particles of cement dust (mg/m^3) at a height of 200 m with a southeast wind of 3 m/s and calculation time $t = 4$ h

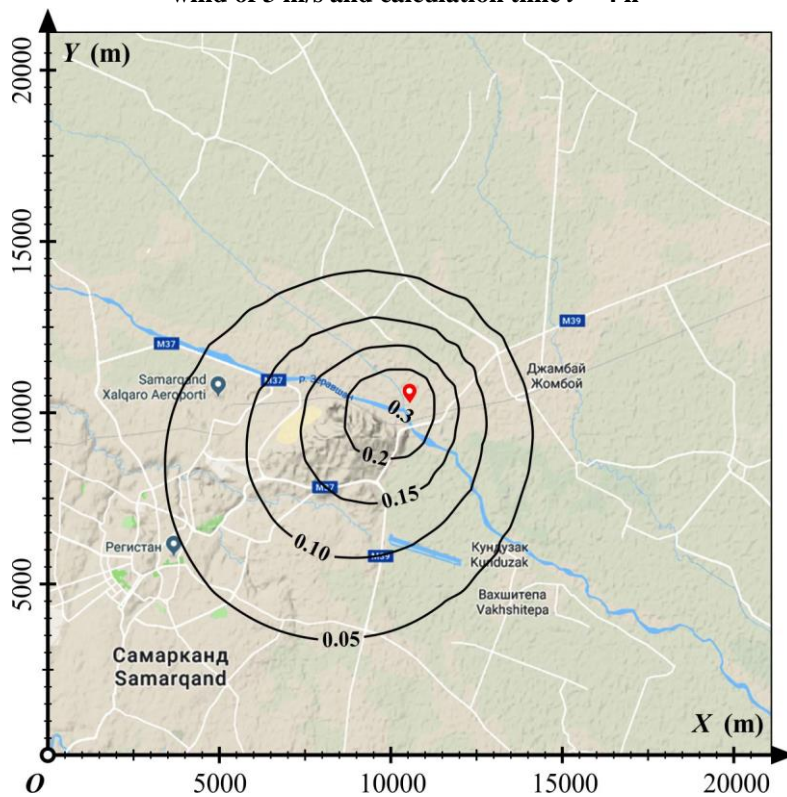


Fig. 8 . The concentration of fine particles of cement dust (mg / m^3) at a height of 200 m with a northeast wind - 4 m / s and calculation time $t = 4$ h

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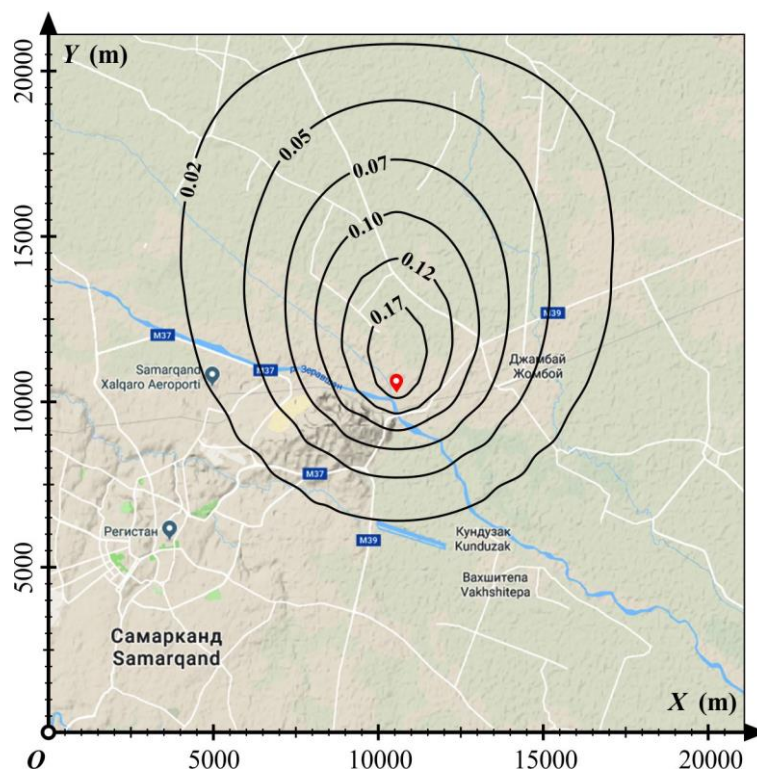


Fig. 9 . The concentration of fine particles of cement dust (mg / m^3) at a height of 200 m with a southerly wind of 6 m / s and calculation time $t = 4$ h

When emitted from a high source (>100 m), the maximum concentrations of pollution are recorded at dangerous wind speeds (in the range from 3 to 6 m/s, depending on the speed of the outflow of gases from the mouth of the exhaust pipes). Dangerous wind speed combined with unstable stratification leads to the maximum increase in the concentration of harmful substances in the surface layer of the atmosphere. In such cases, the main role in the dispersion of pollutants is played by horizontal flows (Fig. 9).

On the example of Nurabad district of Samarkand region. In this case, it was assumed that it was required to locate a new cement plant in the Nurabad district of the Samarkand region of Uzbekistan. The coordinates of the object are $39^{\circ}7'37''$ north latitude, $66^{\circ}3'8''$ east longitude south of the settlements of Charvadar, Kurusai, Maylidzhar.

The area under consideration, as in the previous case, is a flat area at the foot of the Zerafshan Range with similar geographical and weather-climatic characteristics.

In the calculations, the following input parameters were taken: source power $50 \text{ mg}/\text{m}^3$ per

second, height of the mouth of the exhaust pipe - 100 m above the earth's surface.

The results of calculations of the concentration fields of cement dust particles in Figs. 10, fig. 11, 12 are given at a height of 200 m above the earth's surface with a calculation time of 2 hours for various wind speeds and directions. Note that the MPC value for cement dust is $0.3 \text{ mg}/\text{m}^3$ - the maximum single concentration and $0.1 \text{ mg}/\text{m}^3$ - the average daily concentration.

From the numerical calculations carried out on a computer, it follows that with moderate wind and calm, the concentration of harmful substances accumulates around the source of emission of fine particles in the atmosphere at a level of $z = 200$ m (Fig. 10).

According to fig. 11, 12, with an increase in the horizontal wind speed component, the process of horizontal transfer of cement dust occurs. The concentration of harmful substances around the source decreases proportionally, and the area of their transportation expands over time.

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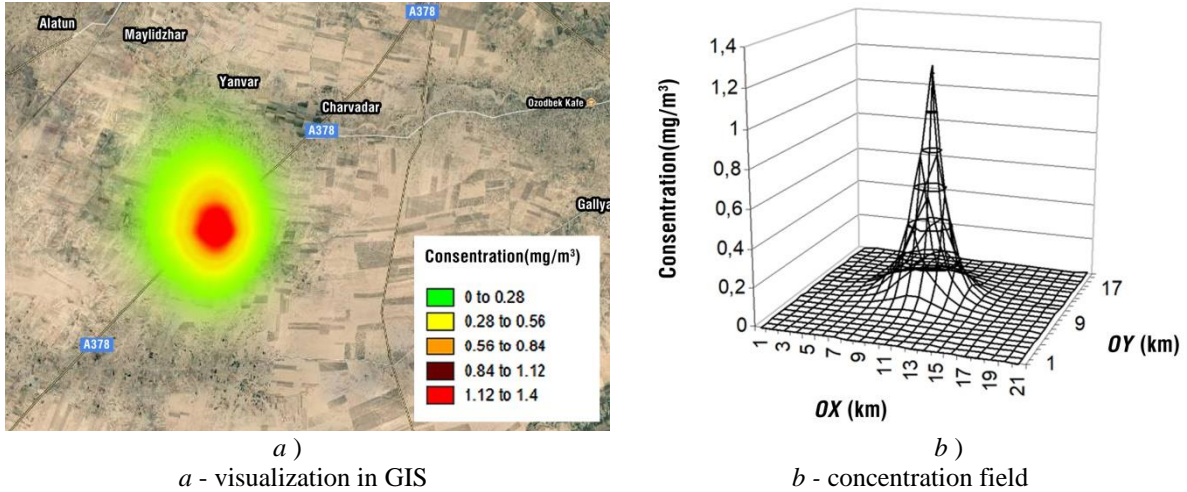


Fig. 10 . Accumulation of concentration of harmful substances at $U=1 \text{ m/s}$, $\alpha = 45^\circ$, $\sigma = 0.0014 / c$ and calculation time $t=2 \text{ h}$

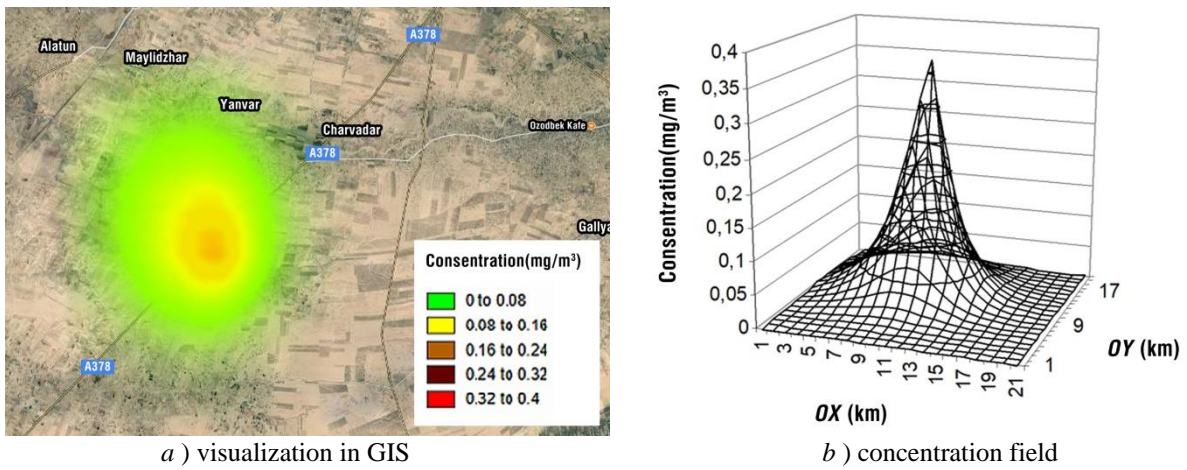


Fig. 11 . At $U = 3 \text{ m/s}$, $\alpha = 45^\circ$, $\sigma = 0.0014 / c$ and calculation time $t = 2 \text{ h}$

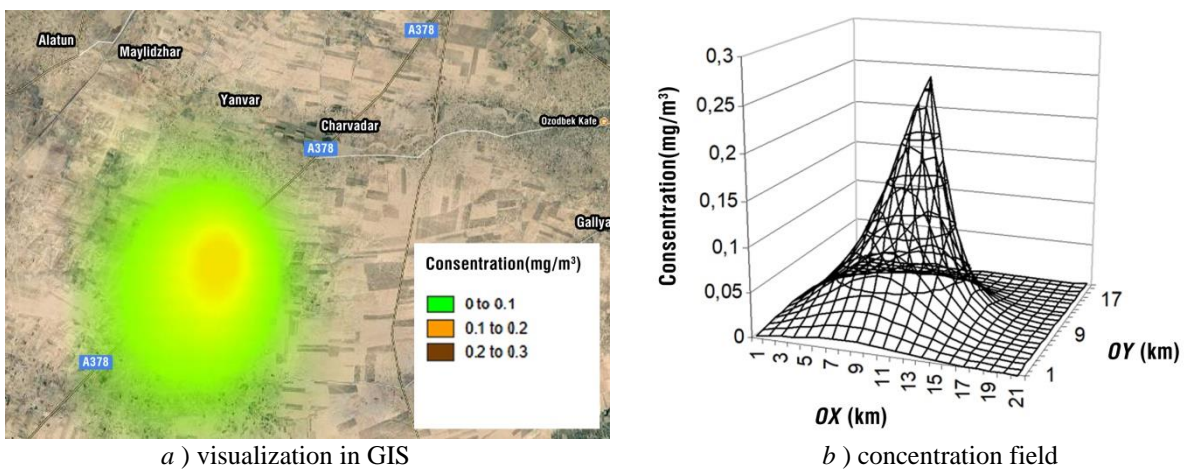


Fig. 12 . At $U = 4 \text{ m/s}$, $\alpha = 135^\circ$, $\sigma = 0.0014 / c$ and calculation time $t = 2 \text{ h}$

An analysis of the numerical calculations performed showed that the maximum values of the concentration of aerosol particles in the atmosphere are observed near the earth's surface when z changes

in the range from 200 to 350 m. The concentration of cement dust particles exponentially decreases with distance from the emission source (Fig. 11, 12) . Numerical calculations have shown that the particle

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concentration maximum is located in the axial part of the atmospheric transport plume. At the same time, the maximum concentration corresponds to a level of 400-425 m in calm and moderate wind.

The SE found that the process of transfer of fine particles is significantly affected by the components of the horizontal wind speed and their direction on the surface in the surface layer of the atmosphere. With the growth of this indicator, the area of distribution of harmful particles in the direction of the wind increases proportionally.

According to the results of numerical calculations on a computer, with an increase in the horizontal velocity of the air mass of the atmosphere, the concentration of harmful substances in the surface layer increases. This is especially noticeable at wind speed $u \geq 2.5$ m/s and is clearly observed at $h = 200-300$ m. It was also found that with an increase in the intensity of aerosol generators, the area where the concentration exceeds the permissible sanitary standards increases. With unstable stratification, the concentration distribution has a peak-like character, i.e. maximizes in a short period of time. In such cases, the main role in the dispersion of harmful substances in the atmosphere is played by horizontal flows.

In the vertical transport of aerosol particles, the role of the turbulence coefficient is extremely important. It has been established that the value of the turbulence coefficient increases significantly in the surface layer of the atmosphere in the range of height from 10 to 250 m. In addition, this coefficient directly affects the rate of deposition of aerosol particles.

An analysis of the experimental results shows that an increase in the absorption coefficient reduces the value of the concentration of pollutants in the atmosphere, and the parameter itself depends on the humidity of the air mass. The maximum concentration values correspond to the summer season, when the absorption coefficient tends to zero.

The SE found that the atmospheric basin of the industrial regions of Uzbekistan, on average, is characterized by absorption from 10 to 18% of aerosol particles. Absorption occurs at air humidity from 70 to 80%.

The obtained results of SE were compared with the results and revealed regularities given in the works of other authors, as well as with the real data of instrumental measurements, and their fairly satisfactory agreement was established.

It should also be noted that in the implementation of the developed software and tool complex, GIS technologies and web-based architecture were actively used with the use of online services that ensure the supply of geographic and meteorological operational data. Using the API of existing online information services, coupled with their constant development, active support and comprehensive documentation, has greatly simplified the development of software tools.

5. Conclusion

In the era of rapidly developing information technologies, the solution of transport and diffusion problems cannot be imagined without the development of an effective mathematical apparatus implemented on a computer in the form of mathematical models, analytical, approximate and approximate-analytical algorithms and their software. With the help of the developed software, it is possible to study the process under various natural and artificial conditions.

Among the universal methods for solving complex multidimensional problems of fluid and gas mechanics and solid mechanics, heat and mass transfer is the finite-difference method based on replacing the continuous domain of solving problems with a grid one.

Recently, the automation of solving boundary value problems has been widely developed on the basis of universal numerical methods created by the scientific schools of A.A. Dorodnitsin, A.N. Tikhonov, A.A. Samarsky, N.N. F.B. Abutaliev, C. Atkinson, S. Banerjee, G. Barenblatt, T. W. Patzek, D. Silin, F. Boyer, C. Lapuerta, S. Minjeaud, F. Golfier, R. Pongraz, M. K. Panga. These methods are sufficiently substantiated and are well suited for numerical simulation of mass transfer processes in the atmospheric boundary layer.

It should be noted that the universal difference schemes used for the numerical integration of problems must satisfy the requirements of convergence and stability of the method on any sequence of grids and for any input data and their small perturbations from the norm. When developing numerical algorithms, all available methods should be involved: exact approximate, approximate-analytical and numerical methods based on the replacement of differential operators by difference ones, as well as asymptotic estimates of the solution, dimensional analysis and experimental data.

When solving problems described using partial differential equations with lumped parameters and corresponding initial and boundary conditions, it is necessary to pay special attention to the conservatism of finite-difference analogs based on the laws of conservation of mass, energy, momentum, and process kinetics.

When solving the tasks set numerically, it is necessary to:

- a) choose the steps of integrating the problem set over the spatial and temporal layers, which ensure the conservatism of the finite difference model;
- b) replace the area of continuous change of prognostic variables with a discrete one;
- c) replace the differential operators of the mathematical model of the object with finite-difference operators, and also write out a difference analogue for the boundary conditions and initial input data.

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To study, predict and monitor the state of the atmosphere in industrial regions, two- and three-dimensional nonlinear mathematical models have been developed for the process of the spread of harmful substances in the boundary layer of the atmosphere, taking into account their absorption and the variable rate of particle settling.

To carry out computational experiments on a computer and solve the problem of transport and

diffusion of aerosol particles in the atmosphere, a numerical algorithm based on an implicit finite-difference approximation scheme with the second order of accuracy has been developed.

A functional dependence is obtained for calculating the absorption coefficient of aerosol particles in the atmosphere.

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