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Numerical Study Process Distribution of Contaminated Substances in the Atmosphere Taking Into Account the Physical and Mechanical Properties of Particles

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ABSTRACT The article deals with the numerical modeling of the processes of transfer and diffusion of air pollutants in the boundary layer of the atmosphere. A mathematical model of the spread of industrial emissions in the atmosphere was developed, taking into account the motion velocity of finely dispersed substances and a number of other factors affecting the change in the concentration of harmful substances in the atmosphere. The model is described by multidimensional partial differential equations with corresponding initial and boundary conditions. For the numerical integration of the problem, the method of splitting into physical processes (of transfer, diffusion and absorption) and an implicit finite-difference scheme of the second order of approximation in spatial variables and in time were used. A software tool was developed to conduct a computational experiment on a computer and to perform a comprehensive study of the processes of transfer and diffusion of harmful substances in the atmosphere.

Key words : mathematical model, transfer and diffusion of harmful substances, numerical algorithm

1. INTRODUCTION

The modern economies of countries are increasingly depleting the power and wealth of nature to accelerate scientific and technological progress. Often these processes bring negative results. Plants and factories are being built at a fast pace, being the main factor of the environmental problem of anthropogenic origin. The anthropogenic sources cause irreparable damage to nature, and the polluted atmosphere presents a critical threat to it. Therefore, forecasting, monitoring, and assessing the ecological state of the atmosphere, design and placement of industrial facilities in compliance with sanitary standards is a priority in the problem of environmental protection.

The study of statistic data on ecology shows that the deterioration of the ecology in the atmosphere of industrial zones occurs due to an increase in the concentration of harmful substances and atmospheric gas pollution. It follows that the relevance of mathematical modeling of the propagation of harmful aerosol particles is obvious and it is one of the effective tools for a comprehensive study of the above problem.

In recent years, scientists have developed mathematical tools to research, predict and monitor the ecological state in industrial regions, based on a mathematical model, a numerical algorithm and software for conducting experiments on a computer; significant theoretical and applied results on the above problem were obtained.

In particular, a mathematical model and software for a system of assessing atmospheric air pollution emissions from motor vehicles were developed in [1]. The mathematical model developed takes into account the traffic intensity, which differs on the streets of the city at a given time of the day, at a given day of the week, at a given month, considering also the basic characteristics of vehicles, features of traffic lines and traffic modulation by traffic lights at street intersections.

A lot of scientific research was done to assess and predict the ecological state of the environment using mathematical models, computational algorithms, and software systems. For example, in [2], topical problems related to solving the problems of salt transfer in soil were considered. The article is devoted to the numerical modeling of the processes of salt transfer and diffusion in soils. To study and predict the spread of harmful substances, a mathematical model and a numerical algorithm for conducting a computer experiment were developed.

The Aral Sea problem is very critical for the population of Uzbekistan and the territories bordering it. In [3], [4], studies of this aspect were conducted to analyze the ecological situation in the Aral Sea region of Uzbekistan. The main share of emissions of harmful substances in the Aral Sea region is dust, salts, and toxic chemicals carried away from the dried-up bottom of the Aral Sea. Thus, in mathematical modeling of the process of atmospheric scattering, it is necessary to take into account physical and mechanical properties of particles and the principal forces acting on them.

In [5], a conjugate mathematical model of the optimal placement of industrial facilities was investigated. To develop an adequate mathematical model of the processes of transfer and diffusion of harmful substances in the atmosphere, the authors of the article studied the following factors: soil erosion, which, under unstable stratification of the air mass, substantially changes the concentration of harmful substances in the atmosphere; mass flow rate of atmospheric air in three directions in time; change in the diffusion coefficient and the vertical turbulent mixing coefficient at stable and unstable atmospheric stratification; changes in wind direction over time and due to the orography of the area; change in the interaction coefficient, which depends on the characteristics of the underlying surface.

The analysis of scientific publications related to the problem of mathematical modeling of the propagation and diffusion processes of aerosol particles in the atmosphere showed that in mathematical modeling and research of the above processes, changes in the velocities of particles in the atmosphere, which change with time and depending on physical and mechanical properties of the substance under consideration were not studied.

2. PROBLEM STATEMENT

Considering the above, to study the process of transfer and diffusion of aerosol particles in the atmosphere, taking into account essential parameters u_p, v_p, w_p that are the components of the particle velocity in x, y, z directions, respectively, we address a mathematical model described on the basis of the law of hydromechanics using a multidimensional partial differential equation [6], [7]:

$$\frac{\partial\theta}{\partial t}+u_p\frac{\partial\theta}{\partial x}+v_p\frac{\partial\theta}{\partial y}+w_p\frac{\partial\theta}{\partial z}+\sigma\theta= =\mu\left(\frac{\partial^2\theta}{\partial x^2}+\frac{\partial^2\theta}{\partial y^2}\right)+\frac{\partial}{\partial z}\left(\kappa\frac{\partial\theta}{\partial z}\right)+\delta Q; \quad (1)$$

$$m\frac{du_p}{dt}=c_f\pi r^2\rho_a(u_p-U)^2; \quad (2)$$

$$m\frac{dv_p}{dt}=c_f\pi r^2\rho_a(v_p-U)^2; \quad (3)$$

$$m\frac{dw_p}{dt}=-\frac{4}{3}\pi r^3(\rho_p-\rho_a)g-k_f\mu_a\pi r w_p+F_n \quad (4)$$

with corresponding initial conditions

$$\left.\begin{array}{l}\theta(x,y,z,0)=\theta^0(x,y,z),\ \tilde{u}=u(0),\\ \tilde{v}=v(0),\ \ \tilde{w}=w(0),\ \ \text{at t}=0\end{array}\right\} \quad (5)$$

and boundary conditions

$$-\mu\frac{\partial\theta}{\partial x}\bigg|_{x=0}=\xi\left(\theta_e-\theta\right); \qquad \mu\frac{\partial\theta}{\partial x}\bigg|_{x=L_x}=\xi\left(\theta_e-\theta\right); \quad (6)$$

$$-\mu\frac{\partial\theta}{\partial y}\bigg|_{y=0}=\xi\left(\theta_e-\theta\right); \qquad \mu\frac{\partial\theta}{\partial y}\bigg|_{y=L_y}=\xi\left(\theta_e-\theta\right); \quad (7)$$

$$-\kappa\frac{\partial\theta}{\partial z}\bigg|_{z=0}=\left(\beta\theta-F_0\right); \qquad \kappa\frac{\partial\theta}{\partial z}\bigg|_{z=H}=\xi\left(\theta_e-\theta\right); \quad (8)$$

where $U=\sqrt{\tilde{u}^2+\tilde{v}^2+\tilde{w}^2}$.

Here t is time; x, y, z are the coordinates; θ is the concentration of the spreading substance; σ is the coefficient of absorption of harmful substances in the atmosphere; µ is the diffusion coefficient; κ is the turbulence coefficient; δ is the Dirac function; Q is the power of sources; θ^0 is the primary concentration of harmful substances in the atmosphere; *m* is the mass of the particle; c_f is the coefficient of drag of particles; *r* is the radius of the particle; ρ_a is the air density; ρ_p is the particle density; *g* is the acceleration of free fall; k_f is the body shape coefficient for the drag force; μ_a is the air viscosity; F_n is the lifting force of the air flow; β is the coefficient of interaction with the underlying surface; F_0 is the number of aerosol particles detached from the ground roughness; ξ is the coefficient to reduce the boundary condition to the dimensional form; θ_e is the concentration of suspended solids in neighboring areas of the problem being solved.

3. SOLUTION METHOD

Since the problem formulated in (1) - (8) is described by a multidimensional nonlinear partial differential equation with corresponding initial and boundary conditions, it is difficult to find its exact solution in an analytical form.

From the statement of the problem and equation (1), it is clear that they describe three physical processes - the transfer of a substance in the motion direction of the atmospheric air mass, molecular diffusion of a substance in the atmosphere, and absorption of harmful substances in the atmosphere.

Considering the above, the method of splitting into physical processes at each time level was used in solving the problem. Therefore, in order to effectively solve the problem posed, we split it by physical processes - into the convection part, the diffusion part and the part of the substance absorption in the atmosphere.

The method of splitting into physical processes is based on a high-order approximation [8], on the substantiation of the additivity of processes for sufficiently small time steps [9], and on the proof of original equation by total approximation due to splitting. The general theory of splitting is given in detail in [10], and the singularities of splitting for the convection problem in rectangular regions and in parallelepipeds are given in [11] - [13].

For the numerical solution of the problem posed (1) - (9), we assume that the sought solution is a smooth function in the entire space. Using the additivity of fundamentally different physical processes of mass transfer and diffusion in the atmosphere in a short time interval $t_n \le t \le t_{n+1}$, we will consider them as separate problems.

The process of a substance transfer with its preservation along the trajectory is considered as problem A:

$$\frac{\partial\theta_1}{\partial t} + u_p\frac{\partial\theta_1}{\partial x} + v_p\frac{\partial\theta_1}{\partial y} + w_p\frac{\partial\theta_1}{\partial z} = \frac{1}{3}\delta Q; \qquad (9)$$

$$m\frac{du_p}{dt} = c_f\pi r^2\rho_a(u_p - U)^2; \qquad (10)$$

$$m\frac{dv_p}{dt} = c_f\pi r^2\rho_a(v_p - U)^2; \qquad (11)$$

$$m\frac{dw_p}{dt} = -\frac{4}{3}\pi r^3(\rho_p - \rho_a)g - k_f\mu_в\pi r w_p + F_n \qquad (12)$$

with initial condition

$$\left.\begin{array}{l}\theta_1^0 = \theta_3^n; \quad \tilde{u} = u_ч(t_n), \quad \tilde{v} = v_ч(t_n), \\ \tilde{w} = w_ч(t_n), \text{ at } t = t_n;\end{array}\right\} \qquad (13)$$

and boundary conditions

$$-\mu\left.\frac{\partial\theta_1}{\partial x}\right|_{x=0} = \xi\left(\theta_e - \theta_1\right); \qquad \mu\left.\frac{\partial\theta_1}{\partial x}\right|_{x=L_x} = \xi\left(\theta_e - \theta_1\right); \qquad (14)$$

$$-\mu\left.\frac{\partial\theta_1}{\partial y}\right|_{y=0} = \xi\left(\theta_e - \theta_1\right); \qquad \mu\left.\frac{\partial\theta_1}{\partial y}\right|_{y=L_y} = \xi\left(\theta_e - \theta_1\right); \qquad (15)$$

$$-\kappa\left.\frac{\partial\theta_1}{\partial z}\right|_{z=0} = \left(\beta\theta_1 - F_0\right); \qquad \kappa\left.\frac{\partial\theta_1}{\partial z}\right|_{z=H} = \xi\left(\theta_e - \theta_1\right). \qquad (16)$$

Let us consider the process of diffusion of a substance in the atmosphere as problem B:

$$\frac{\partial\theta_2}{\partial t} = \mu\left(\frac{\partial^2\theta_2}{\partial x^2} + \frac{\partial^2\theta_2}{\partial y^2}\right) + \frac{\partial}{\partial z}\left(\kappa\frac{\partial\theta_2}{\partial z}\right) + \frac{1}{3}\delta Q; \qquad (17)$$

with initial conditions

$$\theta_2^0 = \theta_1^{n+1}; \qquad (18)$$

and boundary conditions

$$-\mu\left.\frac{\partial\theta_2}{\partial x}\right|_{x=0} = \xi\left(\theta_в - \theta_2\right); \qquad \mu\left.\frac{\partial\theta_2}{\partial x}\right|_{x=L_x} = \xi\left(\theta_в - \theta_2\right); \qquad (19)$$

$$-\mu\left.\frac{\partial\theta_2}{\partial y}\right|_{y=0} = \xi\left(\theta_e - \theta_2\right); \qquad \mu\left.\frac{\partial\theta_2}{\partial y}\right|_{y=L_y} = \xi\left(\theta_e - \theta_2\right); \qquad (20)$$

$$-\kappa\left.\frac{\partial\theta_2}{\partial z}\right|_{z=0} = \beta\theta_2 - F_0; \qquad \kappa\left.\frac{\partial\theta_2}{\partial z}\right|_{z=H} = \xi\left(\theta_в - \theta_2\right). \qquad (21)$$

Let us consider the process of absorption of particles in the air mass as problem C:

$$\frac{\partial\theta_3}{\partial t} + \sigma\theta_3 = \frac{1}{3}\delta Q; \qquad (22)$$

with initial conditions

$$\theta_3^0 = \theta_2^{n+1}; \qquad (23)$$

and boundary conditions

$$-\mu\left.\frac{\partial\theta_3}{\partial x}\right|_{x=0} = \xi\left(\theta_e - \theta_3\right); \qquad \mu\left.\frac{\partial\theta_3}{\partial x}\right|_{x=L_x} = \xi\left(\theta_e - \theta_3\right); \qquad (24)$$

$$-\mu\left.\frac{\partial\theta_3}{\partial y}\right|_{y=0} = \xi\left(\theta_e - \theta_3\right); \qquad \mu\left.\frac{\partial\theta_3}{\partial y}\right|_{y=L_y} = \xi\left(\theta_e - \theta_3\right); \qquad (25)$$

$$-\kappa\left.\frac{\partial\theta_3}{\partial z}\right|_{z=0} = \left(\beta\theta_3 - F_0\right); \qquad \kappa\left.\frac{\partial\theta_3}{\partial z}\right|_{z=H} = \xi\left(\theta_e - \theta_3\right). \qquad (26)$$

Thus, after splitting the original problem into physical processes, we obtained three sub problems (9) - (16), (17) - (21) and (22) - (26), which can be solved independently of each other by the finite-difference method. The complete solution to this problem is given in the authors' article [14].

To conduct computational experiments on a PC based on the developed mathematical model and computational algorithm, a software-instrumental complex is needed. It is possible to simulate the process under study, using this software package, under different conditions: unfavorable weather conditions, different values of the absorption coefficient of harmful substances, with different physical and mechanical properties of particles, etc.

The software developed serves to solve applied problems related to monitoring and predicting the ecological state of the environment of the region in question and makes it possible to assess the impact of harmful substances on the environment of the territories adjacent to the object, taking into account the norms of the maximum permissible concentration for each type of pollutant.

Within the framework of this research, an object-oriented software-tool complex has been developed; it includes a number of related software tools obtained using modern, most widespread technologies, such as Microsoft Visual Studio (C# language), Microsoft Frameworks, NET Framework 4.6.2, sets of visualization libraries ILNumerics, etc.

This software allows monitoring and predicting the process of transfer and diffusion of harmful substances emitted into the atmosphere from industrial facilities, taking into account physical and mechanical properties of particles: mass, density, radius, drag coefficient, environmental factors: ambient temperature, density, air viscosity and other factors influencing the object as a whole. A schematic diagram of software operation is shown in Fig. 1.

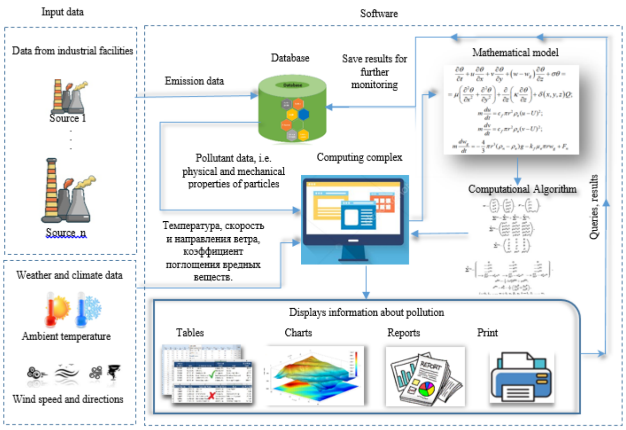


Figure 1. Schematic diagram of software operation

There are two ways to conduct a computational experiment (CE) on a computer, the first is to manually enter all the parameters for conducting CE, the second is to select data from the software interface; from the database management system (DBMS). When the parameters are input manually, the following values should be displayed: wind velocity and direction, initial velocities of a harmful substance, source power, absorption coefficient of harmful substances, initial concentration of harmful substances, diffusion coefficient, dimensions along the x, y, z coordinates, density and mass of the considered harmful substance, drag coefficient, air density and viscosity and calculation time. In the second method, the appropriate parameters for conducting CE on a computer can be selected from the DBMS.

After conducting the CE, the values of the concentration of harmful substances are displayed in the table. Having chosen the desired height, the information can be presented graphically or be sent to a Microsoft Excel file for further use.

4. RESULTS

In the calculations, the following input parameters were taken: wind velocity 4 m/s, initial values of particle velocities: $u_ч(0) = 3$ m/s, $v_ч(0) = 1{,}5$ m/s, $w_ч(0) = 0{,}5$ m/s, wind angle 90^0; calculation time t =10 hours, dimensions of the problem solution region 21x21 km; the emission source is located in the center of the region; the height of the outlet of the exhaust pipe - 100 m above the ground; source power - 10 mg/m^3.

Numerical calculations have established that the change in the concentration of aerosols in the atmosphere depends substantially on the ambient temperature. This parameter varies with the time of year and day. When the ambient temperature changes, the humidity, viscosity and density of the air change as well. Therefore, the maximum absorption of harmful aerosol particles in the atmosphere is typical for the morning and evening hours of the day.

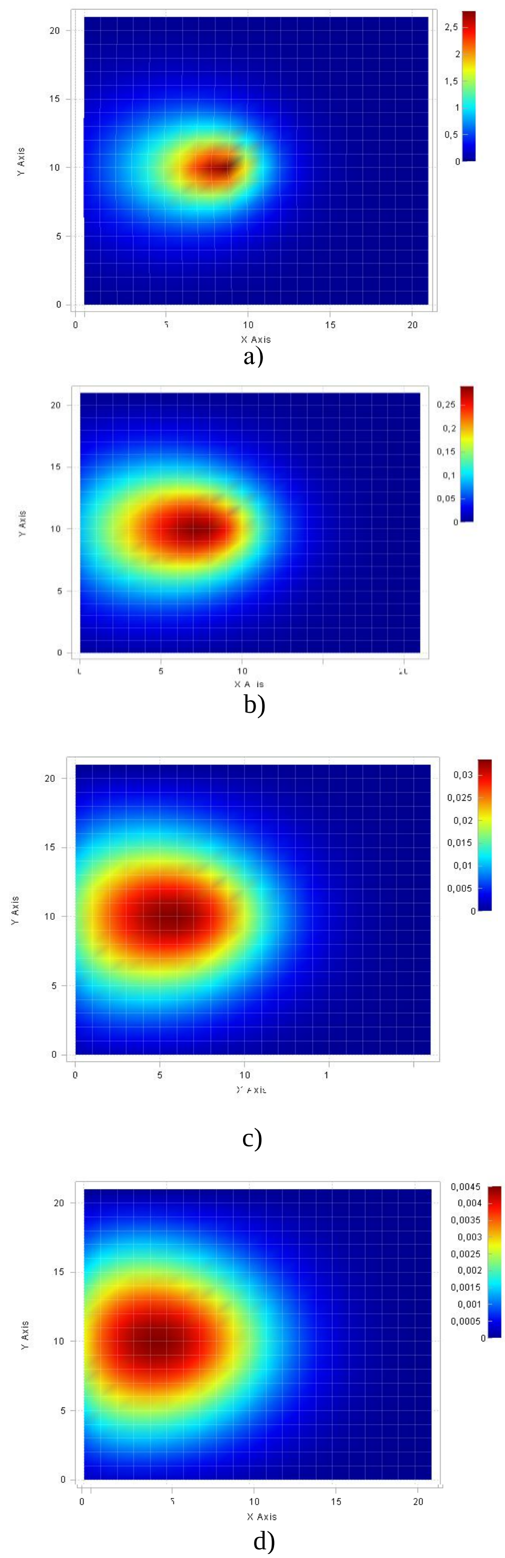


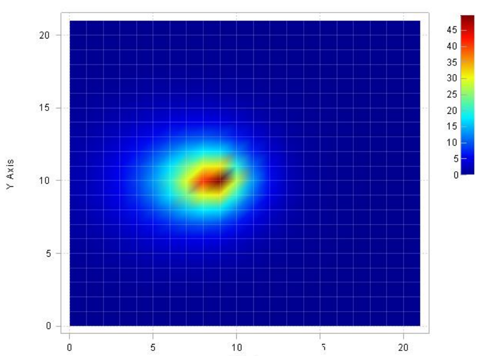
Figure 2. Visualization of the processes of transfer and diffusion of harmful substance - nitric oxide - in the atmosphere:*a) z = 200 m; b) z = 300 m; c) z = 400 m; d) z = 500 m.*

As seen from the numerical experiments conducted, the most significant parameters affecting the spread and accumulation of harmful aerosol particles in the atmosphere in the region under consideration are the horizontal and vertical components of the velocity of particles, and their direction, as well as the air flow rate. As might be expected, in moderate winds (when the components of the wind velocity approach zero), the concentration of harmful substances accumulates around the emission sources, and the change in the concentration of aerosol particles in the atmosphere is mainly due to an increase in the deposition rate of particles. The analysis of the performed numerical calculations showed that, in moderate winds, the aerosol emission in the atmosphere occurs due to their diffusive mixing in the atmosphere.

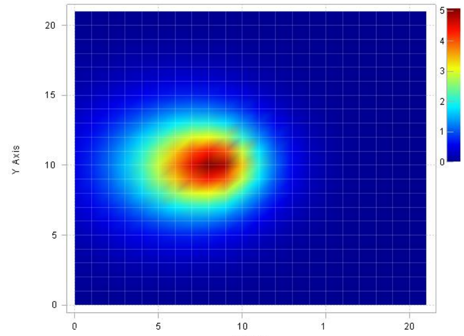
Analyzing the results given in Figs. 2-3, we can say that the mass of the harmful substances substantially affects the processes of transfer and diffusion in the atmosphere.

Computational experiments were conducted under the condition that aerosol particles of different radii are emitted into the atmosphere, which also plays an essential role in the processes of transfer and diffusion of particles. Therefore, it follows from the calculations that the transportation of aerosol particles along the vertical depends largely on the vertical component of the wind velocity and on physico-mechanical properties of particles (radius, mass, density, etc.).

According to the analysis of the calculations performed and their comparison with the real data of field measurements and with the results obtained by other authors, the developed mathematical software is fully appropriate for solving the problems of monitoring and predicting atmospheric pollution in industrial zones, in areas of unfavorable ecological situation, and for determination of the concentration of toxic substances in the air and on the underlying surface.



a)



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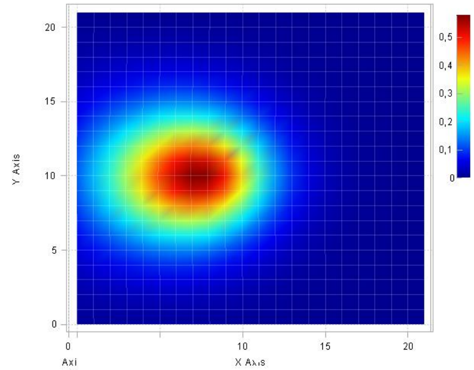
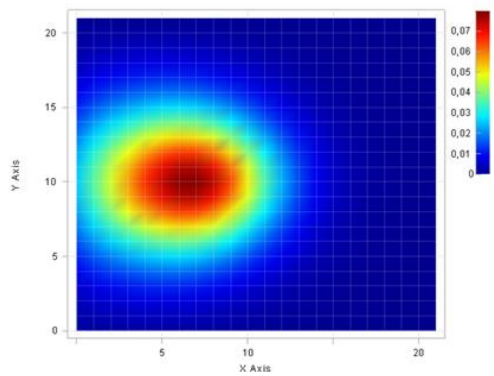


c)



d)

Figure 3. Visualization of the process of transfer and diffusion of harmful substance - sulfur oxide (IV) - in the atmosphere:
a) z = 200 m; b) z = 300 m; c) z = 400 m; d) z = 500 m

5. CONCLUSION

To solve the problem of predicting changes in the concentration of harmful substances in the atmosphere, an effective numerical algorithm based on the method of an implicit finite-difference scheme is implemented.
Analysis of numerical calculations performed to monitor and predict the process of movement and diffusion of harmful substances showed that the area of dispersion of harmful substances in the region under consideration depends

substantially on the physical and mechanical properties of particles, i.e. their density, mass, radius, shape and other properties.

For a comprehensive study of the processes of transfer and diffusion of harmful substances in the atmosphere, a numerical experiment was conducted to assess the effect of ambient temperature on the propagation of aerosols in the atmospheric air.

It was found by the calculated experiments that when the temperature changes, the dynamic viscosity and density of the air change as well, thereby these parameters significantly affect the absorption of harmful substances in the atmosphere. The developed mathematical support and software make it possible to analyze, monitor and predict the processes of transfer and diffusion of harmful aerosol emissions, taking into account the changing velocity of particle motion and their physical and mechanical properties.

The results obtained in the form of mathematical software can be successfully used for optimal placement of newly built facilities in industrial regions; to assess the scale of industrial emissions into the environment; to assess the concentration of harmful substances in the atmosphere and on the underlying surface with subsequent decision-making to minimize the risks of environmental disturbance.

The results obtained show that the proposed numerical approach was effective for solving the problems of salt transfer in soils. Suggested computational algorithms, i.e. the method based on the use of quadrature formulas in combination with the differential sweep method, as well as the corresponding computer software made it possible to successfully carry out calculations to determine the solution content in "through" and "dead-end" pores of soil. The above approach to solving the problem can be extended to the problems of heat- and water-transfer in soils on ameliorated lands.

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