Impact Factor:

ISRA (India)	= **6.317**	**SIS** (USA)	= **0.912**	**ICV** (Poland)	= **6.630**
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JIF	= **1.500**	**SJIF** (Morocco)	= **7.184**	**OAJI** (USA)	= **0.350**

SOI: 1.1/TAS DOI: 10.15863/TAS

International Scientific Journal

Theoretical & Applied Science

p-ISSN: 2308-4944 (print) **e-ISSN:** 2409-0085 (online)

Year: 2022 **Issue:** 06 **Volume:** 110

Published: 06.06.2022 **http://T-Science.org**

Issue **Article**

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MODEL AND NUMERICAL ALGORITHM OF THE PROCESS OF TRANSFER AND DIFFUSION OF ACTIVE FINE HARMFUL PARTICLES IN THE ATMOSPHERE

Abstract: *The article discusses the relevance of solving the problem of monitoring and forecasting the ecological state of industrial regions, where there is a violation of the balance of the sanitary norm of the environment due to a large number of emissions of harmful finely dispersed active aerosol particles and carbon dioxide into the atmosphere. A mathematical model of the process of distribution of pollutants released into the environment from production facilities is presented, which is described by a system of differential equations in partial derivatives with appropriate initial and boundary conditions. The main parameters that play a significant role in the process of transfer and diffusion of harmful substances in the atmosphere are indicated: wind speed and direction; terrain; absorption coefficient of harmful aerosol fine particles in the atmosphere, etc. In this work, a differential equation is obtained for calculating the settling rate of fine and aerosol particles propagating in the boundary layer of the atmosphere, when the main parameters affecting the particle settling rate are taken into account: the mass and radius of aerosol particles, the density of the atmosphere, and the air resistance force. For the numerical solution of the problem, an efficient numerical algorithm based on the "method of lines" is proposed. The algorithm makes it possible to reduce a multidimensional problem described by a partial differential equation to the integration of an ordinary differential equation.*

Key words: *mathematical model, transfer and diffusion of harmful substances, weather-climatic factor, hydromechanics, numerical algorithm.*

Language: *English*

Citation: Muradov, F. A., Kucharov, O. R., & Ravshanov, I. A. (2022). Model and numerical algorithm of the process of transfer and diffusion of active fine harmful particles in the atmosphere. *ISJ Theoretical & Applied Science, 06 (110),* 63-88.

Soi: http://s-o-i.org/1.1/TAS-06-110-11 ***Doi***: crossref https://dx.doi.org/10.15863/TAS.2022.06.110.11

Scopus ASCC: *2604.*

Introduction

Construction and launch of industrial facilities and the growth of their capacities, without taking into account the sanitary standards, the development and commissioning of new oil and gas fields, the extraction of ores from the bowels of the earth, the increase in transport systems in cities and metropolitan areas, etc. violate the ecological balance of the region and the adjacent territory. The imbalance arises as a result of an increase in the gas content of the atmosphere and the concentration of harmful fine particles in its surface layer. These "negative" effects adversely affect the living system - the flora and fauna of the region, and at the global level contribute to climate change on the globe.

As noted by the International Committee on Health, the number of cases of cancer, asthma, allergies, etc. has sharply increased in recent years. diseases due to the deterioration of the ecological state of the environment around the world.

In ITAR TASS reports for the month of December 2016 г. critical levels of air pollution have been declared in China, France, Mongolia, the Balkans and other regions. In particular, in Beijing, measures to eliminate the environmental threat included stopping the operation of industrial facilities for several days, classes in schools, children's institutions, and restrictions on the movement of vehicles within the metropolis.

Based on the foregoing, the issues of monitoring, forecasting and assessing the pollution of the atmosphere and the underlying ¬surface of the earth by passive and active aerosol emissions and fine impurities; placement of industrial ¬enterprises in compliance with sanitary standards ; determination of the amount of suspended particles over the region and their distribution into the environment are relevant in the tasks of environmental protection.

The problems of mathematical modeling of the processes of transfer, diffusion and transport of harmful substances (carbon dioxide, fine aerosol passive and active particles) are studied in scientific schools created under the direction of G.I. Marchuk, V.V. Penenko, A.E. Aloyan, L.T. Matveeva, V.P. Dymnikova I.E. Naatsa, E.A. Zakarina, I.A. Kibel, L.N. Gutman, F.B. Abutaliev, as well as foreign scientists WJ Layton, JH Ferziger, JW Deardorff, M. Germano, U. Piomelli, LC Berselli, GS Winckelmans, WC Reynolds, H. Zidisk, K.A. Welds, K.I. Nappo, J. Gothaas, M. Müllioland, S. Trap, M. Mathies, W. Edelman and others.

Developed under their leadership are widely used in monitoring, forecasting and assessing the impact of anthropogenic impacts on the environment.

When deriving mathematical models of the above objects of study, scientists took as a basis the basic laws of hydrothermodynamics, conservation of mass and momentum, energy and motion.

A significant contribution in this direction was made by A.A. Samarsky, A.A. Tikhonov, G.I. Marchuk, R. Temam, V.V. Penenko, A.E. Aloyan and others. They proposed new efficient numerical algorithms for carrying out computational experiments and solving problems on a computer.

In particular, in [1-3], mathematical models and numerical algorithms and their software were developed for predicting and monitoring the movement of a multicomponent air environment and the transport of pollutants in the atmosphere, as well as the problem of the movement of a multicomponent air environment in the atmosphere, taking into account vaporization and condensation .

The work [4] is devoted to the study of the process of transfer and diffusion of active aerosol particles in the atmosphere, taking into account chemical transformations in the air. The chemical reactions occurring with aerosol particles in the atmosphere are given.

In [5], the processes of transformation of substances during the process of transfer and diffusion of harmful substances in the air over long and medium distances were studied. The methods and results of measuring the concentration of aerosol particles in the atmosphere emitted from various sources and involved in long-range transport are presented. The paper also studies trajectory and evolutionary models of the propagation of aerosol particles in the atmosphere and compares the results of calculations with field measurements.

To describe the physical process of transport of suspended particles in the atmosphere, there are also a number of works that present various approaches. These include methods for studying the process using statistical models based on the Gaussian distribution function [6–8].

In [9], problems and principles of mathematical modeling, a numerical algorithm and a software tool for macroscale physical processes in the atmosphere are considered. The article describes the modeling of atmospheric pollution by biogas released during the decomposition of waste.

The work [10] considers the non-stationary process of transport of bioaerosol harmful substances, taking into account the particle size, as well as the physical processes of condensation and evaporation of gaseous substances.

The work [11] is devoted to the development of a mathematical model of the dynamics of a two-velocity granular medium, including the phase equilibrium of temperature and in the absence of phase equilibrium of pressure. The authors assess the ecological state of the atmospheric air of the oil and gas condensate field. The assessment is made according to the data of continuous monitoring of atmospheric air, obtained by means of an automatic post of environmental control. 14 parameters are measured in this field: concentrations of hydrocarbons, nitrogen oxides, carbon monoxide, ozone and meteorological parameters such as temperature, pressure, wind speed, exposure dose, and oxygen content in the atmospheric air.

In [12-19], a mathematical model was developed for calculating and predicting the transfer of pollutants in the Akhangaran industrial zone of Uzbekistan; local hydrodynamic model and design scheme for the distribution of pollutants in the atmosphere for an industrial region; a three-dimensional numerical model for assessing air pollution in the Akhangaran Valley by industrial emissions of sulfur dioxide (SO2) and arsenic compounds (As); a new approach that makes it possible to use experimental data on the wind regime in one of the Western Tien Shan valleys for other valleys with similar morphometric characteristics. The authors assessed the state of the air basin of the Akhangaran valley under various types of circulation in the warm and cold half-years ; the values of wind speed were established, providing favorable and unfavorable conditions for the purification of the atmosphere from emissions of harmful substances in the valley; connection of favorable and unfavorable conditions of air purification with the types of synoptic processes in Central Asia was revealed; a monitoring scheme is proposed, which includes a short-term forecast of the state of the air basin.

The study of the process of spreading harmful substances into the environment showed that the main factors that directly affect the course of the process are: the speed of movement of the air mass in the atmosphere; diffusion coefficient and vertical turbulent mixing coefficient; wind rose with time and depending on the orography of the area; taking into account the phase transition of the substance due to changes in the temperature regime in the layers of the atmosphere, as well as the rate of settling of fine and aerosol particles propagating in the boundary layer of the atmosphere.

Considering the above factors affecting the process of transfer and diffusion of harmful emissions in the atmosphere, it is necessary to develop an easily implemented effective tool - a model, a numerical algorithm, a software and instrumental complex for monitoring, forecasting and making management decisions to prevent negative consequences for the environment.

Statement of the problem

To study and predict the process of propagation, aerosol emissions into the atmosphere, taking into account the above factors, a mathematical model of the object has been developed, which is described by the equation of transfer and diffusion and based on the law of conservation of mass, momentum:

$$\frac{\partial\theta_1}{\partial t}+\left(w-w_g\right)\frac{\partial\theta_1}{\partial z}=\mu_1\left(\frac{\partial^2\theta_1}{\partial x^2}+\frac{\partial^2\theta_1}{\partial y^2}\right)+\frac{\partial}{\partial z}\left(k\frac{\partial\theta_1}{\partial z}\right)+\delta Q_1+F_1+\Phi_1\ ; \qquad (1)$$

$$\frac{\partial\theta_2}{\partial t}+\left(w-w_g\right)\frac{\partial\theta_2}{\partial z}=\mu_1\left(\frac{\partial^2\theta_2}{\partial x^2}+\frac{\partial^2\theta_2}{\partial y^2}\right)+\frac{\partial}{\partial z}\left(k\frac{\partial\theta_2}{\partial z}\right)+\delta Q_2+F_2+\Phi_2; \qquad (2)$$

$$\frac{dw_g}{dt}=\frac{mg-6\pi krw_g-0.5c\rho Sw_g^2}{m}; \qquad (3)$$

$$\theta_1\left(x,y,z,\dot{0}\right)=\theta_1^0\left(x,y,z\right);\quad \theta_2=\theta_2^0\left(x,y,z\right); w_g(0)=w_g^0\ \text{при}\ t=0; \qquad (3)$$

$$\left.\frac{\partial\theta_1}{\partial x}\right|_{x=0}=0;\quad \left.\frac{\partial\theta_1}{\partial x}\right|_{x=L_x}=0;\quad \left.\frac{\partial\theta_1}{\partial y}\right|_{y=0}=0;\quad \left.\frac{\partial\theta_1}{\partial y}\right|_{y=L_y}=0; \qquad (4)$$

$$\left.\frac{\partial\theta_1}{\partial z}\right|_{z=0}=\eta_1\theta_1;\quad \left.\frac{\partial\theta_1}{\partial z}\right|_{z=L_z}=0; \qquad (5)$$

$$\left.\frac{\partial\theta_2}{\partial x}\right|_{x=0}=0;\quad \left.\frac{\partial\theta_2}{\partial x}\right|_{x=L_x}=0;\quad \left.\frac{\partial\theta_2}{\partial y}\right|_{y=0}=0;\quad \left.\frac{\partial\theta_2}{\partial y}\right|_{y=hy}=0; \qquad (6)$$

$$\left.\frac{\partial\theta_2}{\partial z}\right|_{z=0}=\eta_2\theta_2;\quad \left.\frac{\partial\theta_2}{\partial z}\right|_{z=L_z}=0, \qquad (7)$$

where

$$F_1^{n+1}=\left(\alpha_2\theta_2-\beta_1\theta_1\right);\quad \Phi_1^n=u\frac{\partial\theta_1^n}{\partial x}+v\frac{\partial\theta_1^n}{\partial y};$$

$$F_2^{n+1}=\left(\alpha_1\theta_1-\beta_2\theta_2\right);\quad \Phi_2^n=u\frac{\partial\theta_2^n}{\partial x}+v\frac{\partial\theta_2^n}{\partial y}.$$

Here θ_1, θ_2, is the concentration of the first and second components of the harmful substance propagating in the atmosphere, *t* is the time, *x, y, z* are the coordinates, *u, v, w* are the components of the wind speed in directions *x, y, z*, respectively, w_g is the particle settling velocity, *k* is the turbulent mixing coefficient, is μ the *i-1* diffusion α_i, β_i coefficient *i, i+1*-th type (i =1,2), η_1, η_2 - coefficients of interaction with the underlying surface of the earth, $Q_i(x,y,z,t)$ - power of the sources of the first and second components, *m* - mass of aerosol particles, *r* - particle radius, *c* - dimensionless value equal to 0.5, ρ - atmosphere density.

Problem solving methods.

Since problem (1)-(7) is described by a multidimensional partial differential equation, it is difficult to obtain its solution in an analytical form. To solve the problem, we use a semi-implicit finite-difference scheme in time and obtain [20-23]:

$$\frac{\theta_1^{n+1}-\theta_1^n}{\Delta t}+\left(w-w_g^{n+1}\right)\frac{\partial\theta_1^{n+1}}{\partial z}=\mu_1\left(\frac{\partial^2\theta_1}{\partial x^2}+\frac{\partial^2\theta_1}{\partial y^2}\right)^{n+1}+\frac{\partial}{\partial z}\left(k\frac{\partial\theta_1}{\partial z}\right)^{n+1}+\delta Q_1^{n+1}+F_1^{n+1}+\Phi_1^n\ ;$$

$$\frac{\theta_2^{n+1}-\theta_2^n}{\Delta t}+\left(w-w_g^{n+1}\right)\frac{\partial\theta_2^{n+1}}{\partial z}=\mu_1\left(\frac{\partial^2\theta_2}{\partial x^2}+\frac{\partial^2\theta_2}{\partial y^2}\right)^{n+1}+\frac{\partial}{\partial z}\left(k\frac{\partial\theta_2}{\partial z}\right)^{n+1}+\delta Q_2^{n+1}+F_2^{n+1}+\Phi_2^n;$$

$$\frac{\theta_1^{n+1}-\theta_1^n}{\Delta t}+\left(w-w_g^{n+1}\right)\frac{\partial\theta_1^{n+1}}{\partial z}=\mu_1\left(\frac{\partial^2\theta_1}{\partial x^2}+\frac{\partial^2\theta_1}{\partial y^2}\right)^{n+1}+\frac{\partial}{\partial z}\left(k\frac{\partial\theta_1}{\partial z}\right)^{n+1}+\delta Q_1^{n+1}+F_1^{n+1}+\Phi_1^n\ ;$$

$$\frac{\theta_2^{n+1}-\theta_2^n}{\Delta t}+\left(w-w_g^{n+1}\right)\frac{\partial\theta_2^{n+1}}{\partial z}=\mu_1\left(\frac{\partial^2\theta_2}{\partial x^2}+\frac{\partial^2\theta_2}{\partial y^2}\right)^{n+1}+\frac{\partial}{\partial z}\left(k\frac{\partial\theta_2}{\partial z}\right)^{n+1}+\delta Q_2^{n+1}+F_2^{n+1}+\Phi_2^n.$$

Since equation (3) is nonlinear, we use the iterative method to solve it

$$\frac{w_g^{n+1}-w_g^n}{\Delta t}=\frac{mg-6\pi krw_g^n-0.5c\rho S(2\widetilde{w}_g w_g^n-\widetilde{w}_g^2)}{m},$$

and the convergence conditions of the iterative process have the following form:

$$\left|w_g^{(s+1)}-w_g^{(s)}\right|\le\varepsilon\ ,$$

where ε is the given value (10^{-6}), s is the number of iterations.

From the statement of problem (1) - (7) it can be seen that the coefficients of equation (1) - (2) do not depend on *x* and *y*, therefore, the method of lines can be used for integration [24].

To solve the problem in leading the grid over the variables *x* and *y*

$$\omega_x=\left(x_i=ih_x,\ \ i=0,1,3,\mathrm{N}_1+1;\ h_x=\frac{L_x}{(\mathrm{N}_1+1)}\right);$$

$$\omega_y=\left(y_j=jh_y,\ \ j=0,1,2,3,\mathrm{N}_2+1;\ h_y=\frac{L_y}{(\mathrm{N}_2+1)}\right).$$

Further, writing equations (1), (2) for , $x=x_i$ we obtain a system of linear equations

$$\frac{1}{\Delta t}\theta_{1,i}+\left(w-w_g^{n+1}\right)\frac{\partial\theta_{1,i}}{\partial z}=\mu_1\frac{\theta_{1,i-1}-2\theta_{1,i}+\theta_{1,i+1}}{h_x^{\ 2}}+$$
$$+\mu_1\frac{\partial^2\theta_{1,i}}{\partial y^2}+\frac{\partial}{\partial z}\left(k\frac{\partial\theta_{1,i}}{\partial z}\right)+\delta_i Q_{1,i}+F_{1,i}+\Phi_{1,i}+\frac{1}{\Delta\tau}\overline{\theta}_{1,i};\qquad(8)$$

$$\frac{1}{\Delta t}\theta_{2,i}+\left(w-w_g\right)\frac{\partial\theta_{2,i}}{\partial z}=\mu_1\frac{\theta_{2,i-1}-2\theta_{2,i}+\theta_{2,i+1}}{h_x^{\ 2}}+$$
$$+\mu_1\frac{\partial^2\theta_{2,i}}{\partial y^2}+\frac{\partial}{\partial z}\left(k\frac{\partial\theta_{2,i}}{\partial z}\right)+\delta_i Q_{2,i}+F_{2,i}+\Phi_{2,i}+\frac{1}{\Delta\tau}\overline{\theta}_{2,i},\qquad(9)$$

there

$$\Phi_{1,i}=\left[\frac{U+|U|}{2}\left(\overline{\theta}_{1,i}-\overline{\theta}_{1,i-1}\right)/h_x\right|+\left.\frac{V+|V|}{2}\frac{\partial\overline{\theta}_1}{\partial y}\right];$$

$$\Phi_{2,i}=\left[\frac{U+|U|}{2}\left(\overline{\theta}_{2,i}-\overline{\theta}_{2,i-1}\right)/h_x\right|+\left.\frac{V+|V|}{2}\frac{\partial\overline{\theta}_2}{\partial y}\right].$$

For convenience, equation (8)-(9) can be written in a compact form

$$\frac{1}{\Delta t}\theta_{1,i}+\left(w-w_g\right)\frac{\partial\theta_{1,i}}{\partial z}=\mu_1\frac{M_1}{h_x^{\,2}}\theta_{1,i}+\mu_1\frac{\partial^2\theta_{1,i}}{\partial y^2}+$$
$$+\frac{\partial}{\partial z}\left(k\frac{\partial\theta_{1,i}}{\partial z}\right)+\delta_i Q_{1,i}+F_{1,i}+\Phi_{1,i}+\frac{1}{\Delta t}\bar{\theta}_{1,i};\qquad(10)$$

$$\frac{1}{\Delta t}\theta_{2,i}+\left(w-w_g\right)\frac{\partial\theta_{2,i}}{\partial z}=\mu_1\frac{M_1}{h_x^{\,2}}\theta_{2,i}+\mu_1\frac{\partial^2\theta_{2,i}}{\partial y^2}+$$
$$+\frac{\partial}{\partial z}\left(k\frac{\partial\theta_{2,i}}{\partial z}\right)+\delta_i Q_{2,i}+F_{2,i}+\Phi_{2,i}+\frac{1}{\Delta t}\bar{\theta}_{2,i}.\qquad(11)$$

Here

$$M_1=\begin{pmatrix}-2 & 1 & 0 & \dots & \dots & 0\\ 1 & -2 & 1 & \dots & \dots & 0\\ 0 & 1 & -2 & 1 & \dots & \dots\\ \dots & \dots & \dots & \dots & \dots & \dots\\ \dots & \dots & \dots & \dots & 1 & -2\end{pmatrix}$$

Since the matrix M_1 is a matrix of simple structure, it can be represented as $M_1=B_1\lambda_{1,i}B_1^t$, $\lambda_{1,i}=B_1^tM_1B_1$, $B_1^{-1}=B_1^t$, λ a diagonal matrix whose elements are the eigenvalues of the matrix M_1, i.e.

$$\lambda_{1,i}=\begin{pmatrix}\lambda_1 & 0 & 0 & 0 & \\ 0 & \lambda_2 & 0 & 0 & \\ 0 & 0 & \lambda_3 & 0 & \\ 0 & 0 & \dots & \dots & \\ & & & & \\ 0 & 0 & 0 & \dots & \lambda_{N_1}\end{pmatrix},$$

$\lambda_{1,i}$ and matrix elements are B_1 calculated by the formulas:

$$\lambda_{1,i}=-2\left(1-\cos\frac{i\pi}{N_1+1}\right);\quad b_{1,i,j}=(-1)^{i+j}\sqrt{\frac{2}{N_1+1}}\sin\frac{ij\pi}{N_1+1};$$
$$\left(i,j=\overline{1}N_1\right).$$

The resulting equations (10) and (11), multiplying by the matrix on the left B_1^t and introducing the notation $B_1^t\theta_1=\theta_1^{(1)}$, $B_1^t\theta_2=\theta_2^{(1)}$ we get:

$$\frac{1}{\Delta t}\theta_{1,i}^{(1)}+\left(w-w_g\right)\frac{\partial\theta_{1,i}^{(1)}}{\partial z}=\alpha_i^2\theta_{1,i}^{(1)}+\mu_1\frac{\partial^2\theta_{1,i}^{(1)}}{\partial y^2}+$$
$$+\frac{\partial}{\partial z}\left(k\frac{\partial\theta_{1,i}^{(1)}}{\partial z}\right)+\delta_i Q_{1,i}^{(1)}+F_{1,i}^{(1)}+\Phi_{1,i}^{(1)}+\frac{1}{\Delta t}\bar{\theta}_{1,i}^{(1)};\qquad(12)$$

$$\frac{1}{\Delta t}\theta_{2,i}^{(1)}+\left(w-w_g\right)\frac{\partial\theta_{2,i}^{(1)}}{\partial z}=\alpha_{1,i}^2\theta_{2,i}^{(1)}+\mu_1\frac{\partial^2\theta_{2,i}^{(1)}}{\partial y^2}+$$
$$+\frac{\partial}{\partial z}\left(k\frac{\partial\theta_{2,i}^{(1)}}{\partial z}\right)+\delta_i Q_{2,i}^{(1)}+F_{2,i}^{(1)}+\Phi_{2,i}^{(1)}+\frac{1}{\Delta t}\bar{\theta}_{2,i}^{(1)}.\qquad(13)$$

Here $\alpha_{1,i}^2=\frac{\gamma_{1,i}\mu_1}{h_x^{\,2}}$.

Similarly, in equations (12) and (13) y, replacing the differential operators with respect to by finite-difference operators, we obtain:

$$\frac{1}{\Delta t}\theta_{1,i,j}^{(1)}+\left(w-w_g\right)\frac{\partial\theta_{1,i,j}^{(1)}}{\partial z}=\alpha_{1,i}^2\theta_{1,i,j}^{(1)}+\mu_1\frac{M_1}{hy^2}\theta_{1,i,j}^{(1)}+$$
$$+\frac{\partial}{\partial z}\left(k\frac{\partial\theta_{1,i,j}^{(1)}}{\partial z}\right)+\delta_{ij}Q_{1,i,j}^{(1)}+F_{1,i,j}^{(1)}+\Phi_{1,i,j}^{(1)}+\frac{1}{\Delta t}\bar{\theta}_{1,i,j}^{(1)};\qquad(14)$$

$$\frac{1}{\Delta t}\theta^{(1)}_{2,i,j}+\left(w-w_g\right)\frac{\partial\theta^{(1)}_{2,i,j}}{\partial z}=\alpha_i^2\theta^{(1)}_{2,i,j}+\mu_1\frac{M_2}{hy^2}\theta^{(1)}_{2,i,j}+$$
$$+\frac{\partial}{\partial z}\left(k\frac{\partial\theta^{(1)}_{2,i,j}}{\partial z}\right)+\delta_{ij}Q^{(1)}_{2,i,j}+F^{(1)}_{2,i,j}+\Phi^{(1)}_{2,i,j}+\frac{1}{\Delta t}\bar{\theta}^{(1)}_{2,i,j}. \qquad (15)$$

matrix M_2 in the form $M_2=B_2\lambda_2B_2^t$ and $B_2^t=B_2^{-1}$. Equations (14) and (15) also multiplying by the matrix on the left B_2^t and introducing the notation, $B_2^t\theta^{(1)}_{1,i,j}=\theta^{(2)}_{1,i,j}$; $B_2^t\theta^{(1)}_{2,i,j}=\theta^{(2)}_{2,i,j}$ we get:

$$\frac{1}{\Delta t}\theta^{(2)}_{1,i,j}+\left(w-w_g\right)\frac{\partial\theta^{(2)}_{1,i,j}}{\partial z}=\left(\alpha^2_{1,i}+\beta^2_{1,j}\right)\theta^{(2)}_{1,i,j}+$$
$$+\frac{\partial}{\partial z}\left(k\frac{\partial\theta^{(2)}_{1,i,j}}{\partial z}\right)+\delta_{ij}Q^{(2)}_{1,i,j}+F^{(2)}_{1,i,j}+\Phi^{(2)}_{1,i,j}+\frac{1}{\Delta t}\bar{\theta}^{(2)}_{1,i,j}; \qquad (16)$$

$$\frac{1}{\Delta t}\theta^{(2)}_{2,i,j}+\left(w-w_g\right)\frac{\partial\theta^{(2)}_{2,i,j}}{\partial z}=\left(\alpha^2_{2,i}+\beta^2_{2,j}\right)\theta^{(2)}_{2,i,j}+$$
$$+\frac{\partial}{\partial z}\left(k\frac{\partial\theta^{(2)}_{2,i,j}}{\partial z}\right)+\delta_{ij}Q^{(2)}_{2,i,j}+F^{(2)}_{2,i,j}+\Phi^{(2)}_{2,i,j}+\frac{1}{\Delta t}\bar{\theta}^{(2)}_{2,i,j}. \qquad (17)$$

Here

$$\beta_j^2=\frac{\alpha_{2,k}\mu_1}{h_y^{\ 2}};\quad \alpha_{2,k}=-2\left(1-\cos\frac{i\pi}{N_1+1}\right);$$

$$b_{2,i,j}=(-1)^{i+j}\sqrt{\frac{2}{N_2+1}}\sin\frac{ij\pi}{N_2+1},$$

$$\left(i,j=1,2,....,N_2\right).$$

After some transformation for the boundary conditions (5) and (7) we get:

$$k\frac{\partial\theta^{(2)}_{1,i,j}}{\partial z}=\eta_1\theta^{(2)}_{1,i,j}-\Phi^{(2)}_{1,i,j};$$

$$k\frac{\partial\theta^{(2)}_{2,i,j}}{\partial z}=\eta_2\theta^{(2)}_{2,i,j}-\Phi^{(2)}_{2,i,j}.$$

Here $\Phi^{(2)}_{1,i,j}$ and $\Phi^{(2)}_{2,i,j}$ are calculated using the formulas:

$$\Phi^{(2)}_{1,i,j}=\begin{cases}U\dfrac{\theta^{(2)}_{1,i,j}-\theta^{(2)}_{1,i-1,j}}{h_x} & npu\quad U\ge 0\\ U\dfrac{\theta^{(2)}_{1,i+1,j}-\theta^{(2)}_{1,i,j}}{h_x} & npu\quad U<0\end{cases}+$$
$$+\begin{cases}V\dfrac{\theta^{(2)}_{1,i,j}-\theta^{(2)}_{1,i,j-1}}{h_y} & npu\quad V\ge 0\\ V\dfrac{\theta^{(2)}_{1,i,j+1}-\theta^{(2)}_{1,i,j}}{h_y} & npu\quad V<0\end{cases};$$

$$\Phi^{(2)}_{2,i,j}=\begin{cases}U\dfrac{\theta^{(2)}_{2,i,j}-\theta^{(2)}_{2,i-1,j}}{h_x} & npu\quad U\ge 0\\ U\dfrac{\theta^{(2)}_{2,i+1,j}-\theta^{(2)}_{2,i,j}}{h_x} & npu\quad U<0\end{cases}+$$
$$+\begin{cases}V\dfrac{\theta^{(2)}_{2,i,j}-\theta^{(2)}_{2,i,j-1}}{h_y} & npu\quad V\ge 0\\ V\dfrac{\theta^{(2)}_{2,i,j+1}-\theta^{(2)}_{2,i,j}}{h_y} & npu\quad V<0\end{cases}.$$

Combining the obtained equations (16), (17) and the corresponding boundary conditions, we finally obtained ordinary differential equations that describe the process of transport and diffusion of harmful substances in the atmosphere in the vertical direction, with respect to the variable z.

For the final numerical integration of the problems, we introduce a grid with respect to the variable z

$$\omega_z=\left(z_k=z_{k-1}-h_z;\quad k=2,3,4,5,6\right),$$

replacing the differential operators of the differential equation with difference operators

$$\left(\frac{\partial\theta^{(2)}_{1,i,j}}{\partial z}\right)_\xi=\begin{cases}\dfrac{\theta^{(2)}_{1,i,j,\xi-1}-\theta^{(2)}_{1,i,j,\xi}}{hz}, npu\ \left(W-W_g\right)\ge 0\\ \dfrac{\theta^{(2)}_{1,i,j,\xi+1}-\theta^{(2)}_{1,i,j,\xi}}{hz}, npu\ \left(W-W_g\right)<0\end{cases}; \qquad (18)$$

$$\left(\frac{\partial \theta^{(2)}_{2,i,j}}{\partial z}\right)_{\xi} = \begin{cases} \dfrac{\theta^{(2)}_{2,i,j,\xi-1} - \theta^{(2)}_{2,i,j,\xi}}{hz}, \; npu \;\; (W - W_g) \geq 0 \\ \dfrac{\theta^{(2)}_{2,i,j,\xi+1} - \theta^{(2)}_{2,i,j,\xi}}{hz}, \; npu \;\; (W - W_g) < 0 \end{cases}; \tag{19}$$

$$\frac{\partial}{\partial z}\left(K\frac{\partial \theta^{(2)}_{1,i,j}}{\partial z}\right)_{\xi} = \left[K_{\xi+0.5}\theta^{(2)}_{1,i,j,\xi+1} - \left(K_{\xi+0.5} + K_{\xi-0.5}\right)\theta^{(2)}_{1,i,j,\xi} + K_{\xi-0.5}\theta^{(2)}_{1,i,j,\xi-1}\right] \Big/ h_z^2; \tag{20}$$

$$\frac{\partial}{\partial z}\left(K\frac{\partial \theta^{(2)}_{2,i,j}}{\partial z}\right)_{\xi} = \left[K_{\xi+0.5}\theta^{(2)}_{2,i,j,\xi+1} - \left(K_{\xi+0.5} + K_{\xi-0.5}\right)\theta^{(2)}_{2,i,j,\xi} + K_{\xi-0.5}\theta^{(2)}_{2,i,j,\xi-1}\right] \Big/ h_z^2, \tag{21}$$

releasing the indices i, j and grouping the same terms of the equation, we obtain

$$\frac{1}{h_z^2}k_{\xi+0.5} - \theta^{(2)}_{1,\xi+1} - \frac{1}{h_z^2}\left(k_{\xi+0.5} + k_{\xi-0.5}\right)\theta^{(2)}_{1,\xi} + \frac{1}{h_z^2}k_{\xi-0.5} - \theta^{(2)}_{1,\xi-1} + \\ + \begin{cases} \left(\dfrac{(w - w_g)}{h_z}\theta^{(2)}_{1,\xi-1} - \dfrac{(w - w_g)}{h_z}\theta^{(2)}_{1,\xi}\right) \; npu \;\; (w - w_g) \geq 0 \\ \left(\dfrac{(w - w_g)}{h_z}\theta^{(2)}_{1,\xi+1} - \dfrac{(w - w_g)}{h_z}\theta^{(2)}_{1,\xi}\right) \; npu \;\; (w - w_g) < 0 \end{cases} = \tag{22}$$

$$= q_1\theta^{(2)}_{1,\xi+1} - q_2\theta^{(2)}_{1,\xi} + q_3\theta^{(2)}_{1,\xi-1} + \begin{cases} \left(q_4\left(\theta^{(2)}_{1,\xi-1} - \theta^{(2)}_{1,\xi}\right)\right) \; npu \;\; (w - w_g) \geq 0 \\ \left(q_4\left(\theta^{(2)}_{1,\xi+1} - \theta^{(2)}_{1,\xi}\right)\right) \; npu \;\; (w - w_g) < 0 \end{cases};$$

$$\frac{1}{h_z^2}k_{\xi+0.5} - \theta^{(2)}_{2,\xi+1} - \frac{1}{h_z^2}\left(k_{\xi+0.5} + k_{\xi-0.5}\right)\theta^{(2)}_{2,\xi} + \frac{1}{h_z^2}k_{\xi-0.5} - \theta^{(2)}_{2,\xi-1} + \\ + \begin{cases} \left(\dfrac{(w - w_g)}{h_z}\theta^{(2)}_{2,\xi-1} - \dfrac{(w - w_g)}{h_z}\theta^{(2)}_{2,\xi}\right) \; npu \;\; (w - w_g) \geq 0 \\ \left(\dfrac{(w - w_g)}{h_z}\theta^{(2)}_{2,\xi+1} - \dfrac{(w - w_g)}{h_z}\theta^{(2)}_{2,\xi}\right) \; npu \;\; (w - w_g) < 0 \end{cases} = \tag{23}$$

$$= q_1\theta^{(2)}_{2,\xi+1} - q_2\theta^{(2)}_{2,\xi} + q_3\theta^{(2)}_{2,\xi-1} + \begin{cases} \left(q_4\left(\theta^{(2)}_{2,\xi-1} - \theta^{(2)}_{2,\xi}\right)\right) \; npu \;\; (w - w_g) \geq 0 \\ \left(q_4\left(\theta^{(2)}_{2,\xi+1} - \theta^{(2)}_{2,\xi}\right)\right) \; npu \;\; (w - w_g) < 0 \end{cases}.$$

Now using relations (22) and (23) instead of (16) and (17) we obtain

$$\frac{1}{\Delta t}\theta^{(2)}_{1,\xi} + q_1\theta^{(2)}_{1,\xi+1} - q_2\theta^{(2)}_{1,\xi} + q_3\theta^{(2)}_{1,\xi-1} + \begin{cases} \left(q_4\left(\theta^{(2)}_{1,\xi-1} - \theta^{(2)}_{1,\xi}\right)\right) \; npu \;\; (w - w_g) \geq 0 \\ \left(q_4\left(\theta^{(2)}_{1,\xi+1} - \theta^{(2)}_{1,\xi}\right)\right) \; npu \;\; (w - w_g) < 0 \end{cases} = \\ = \left(\alpha^2_{1,i} + \beta^2_{1,j}\right)\theta^{(2)}_{1,\xi} + \delta_{\xi}Q^{(2)}_{1,\xi} + F^{(2)}_{1,\xi} + \Phi^{(2)}_{1,\xi} + \frac{1}{\Delta t}\bar{\theta}^{(2)}_{1,\xi}; \tag{24}$$

$$\frac{1}{\Delta t}\theta^{(2)}_{2,\xi} + q_1\theta^{(2)}_{2,\xi+1} - q_2\theta^{(2)}_{2,\xi} + q_3\theta^{(2)}_{2,\xi-1} + \begin{cases} \left(q_4\left(\theta^{(2)}_{2,\xi-1} - \theta^{(2)}_{2,\xi}\right)\right) \; npu \;\; (w - w_g) \geq 0 \\ \left(q_4\left(\theta^{(2)}_{2,\xi+1} - \theta^{(2)}_{2,\xi}\right)\right) \; npu \;\; (w - w_g) < 0 \end{cases} = \\ = \left(\alpha^2_{2,i} + \beta^2_{2,j}\right)\theta^{(2)}_{2,\xi} + \delta_{\xi}Q^{(2)}_{2,\xi} + F^{(2)}_{2,\xi} + \Phi^{(2)}_{2,\xi} + \frac{1}{\Delta t}\bar{\theta}^{(2)}_{2,\xi}. \tag{25}$$

To determine the boundary conditions at $z = 0$ on the underlying surface of the earth, we integrate equations (16) and (17) from 0 to $h_{z/2}$ and obtain

$$\int_0^{h_z/2}\left[\frac{\partial}{\partial z}\left(k\frac{\partial\theta_{1,i,j}^{(2)}}{\partial z}\right)-\left(w-w_g\right)\frac{\partial\theta_{1,i,j}^{(2)}}{\partial z}+\left(\frac{1}{\Delta t}-\left(\alpha_{1,i}^2+\beta_{1,j}^2\right)\right)\theta_{1,i,j}^{(2)}\right]dz=\int_0^{h_z/2}\bar{G}_{1,i,j}^{(2)}dz, \tag{26}$$

$$\int_0^{h_z/2}\left[\frac{\partial}{\partial z}\left(k\frac{\partial\theta_{2,i,j}^{(2)}}{\partial z}\right)-\left(w-w_g\right)\frac{\partial\theta_{2,i,j}^{(2)}}{\partial z}+\left(\frac{1}{\Delta t}-\left(\alpha_{2,i}^2+\beta_{2,j}^2\right)\right)\theta_{2,i,j}^{(2)}\right]dz=\int_0^{h_z/2}\bar{G}_{2,i,j}^{(2)}dz, \tag{27}$$

where

$$\bar{G}_{1,i,j}^{(2)}=\delta_{i,j}Q_{1,i,j}^{(2)}+F_{1,i,j}^{(2)}+\Phi_{1,i,j}^{(2)}+\frac{1}{\Delta t}\bar{Q}_{1,i,j}^{(2)};$$

$$\bar{G}_{2,i,j}^{(2)}=\delta_{i,j}Q_{2,i,j}^{(2)}+F_{2,i,j}^{(2)}+\Phi_{2,i,j}^{(2)}+\frac{1}{\Delta t}\bar{Q}_{2,i,j}^{(2)}.$$

Taking into account the boundary conditions, equations (26) and (27) can be written as:

$$\int_0^{h_z/2}\frac{\partial}{\partial z}\left(k(z)\frac{\partial\theta_{1,i,j}^{(2)}}{\partial z}\right)dz=k\left(z_{1/2}\right)\frac{\partial\theta_{1,i,j}^{(2)}}{\partial z}\bigg|_{1/2}-k\left(z_{1/2}\right)\frac{\partial\theta_{1,i,j}^{(2)}}{\partial z}\bigg|_{0}=$$

$$=k\left(z_{1/2}\right)\frac{\theta_{1,i,j,2}^{(2)}-\theta_{1,i,j,1}^{(2)}}{h_z}-\eta_1\theta_{1,i,j,1}^{(2)},$$

$$\int_0^{h_z/2}\left(w-w_g\right)\frac{\partial\theta_{1,i,j}^{(2)}}{\partial z}dz=\left(w-w_g\right)_{1/4}\left(\theta_{1,i,j,1/2}^{(2)}-\theta_{1,i,j,0}^{(2)}\right)=$$

$$=\left(w-w_g\right)_{1/4}\frac{\theta_{1,i,j,1}^{(2)}-\theta_{1,i,j,0}^{(2)}}{2}-\theta_{1,i,j,0}^{(2)}=\left(w-w_g\right)_{1/4}\frac{1}{2}\left(\theta_{1,i,j,0}^{(2)}-\theta_{1,i,j,1}^{(2)}\right),$$

$$\int_0^{h_z/2}\bar{G}_{1,i,j}^{(2)}dz=\bar{G}_0^{(2)}\frac{h_z}{2},$$

$$k\left(z_{1/2}\right)\frac{\theta_{1,2}^{(2)}-\theta_{1,1}^{(2)}}{h_z}-\eta_1\theta_{1,1}^{(2)}-\left(w-w_g\right)_{1/4}\frac{1}{2}\left(\theta_{1,0}^{(2)}-\theta_{1,1}^{(2)}\right)-$$

$$-\left(\frac{1}{\Delta t}-\left(\alpha_{1,i}^2+\beta_{1,j}^2\right)\right)\theta_{1,1}^{(2)}=\bar{G}_{i,j,0}^2$$

or

$$2k\left(z_{1/2}\right)\left(\theta_{1,2}^{(2)}-\theta_{1,1}^{(2)}\right)-2h_z\eta_1\theta_{1,1}^{(2)}-\left(w-w_g\right)_{1/4}h_z\left(\theta_{1,0}^{(2)}-\theta_{1,1}^{(2)}\right)-$$

$$-2h_z\left(\frac{1}{\Delta t}-\left(\alpha_{1,i}^2+\beta_{1,j}^2\right)\right)\theta_{1,1}^{(2)}=2h_z\bar{G}_{i,j,0}^2.$$

Then we finally get

$$2k\left(z_{1/2}\right)\theta_{1,i,j,2}^{(2)}-\left[2K\left(z_{1/2}\right)+2h_z\eta_1+\left(w-w_g\right)h_z+\right.$$

$$\left.+2h_z\left(\frac{1}{\Delta t}-\left(\alpha_{1,i}^2+\beta_{1,j}^2\right)\right)\right]\theta_{1,i,j,1}^{(2)}-\left(w-w_g\right)h_z\theta_{1,i,j,0}^{(2)}=2h_z\bar{G}_{1,i,j,0}^{(2)},$$

and for $\theta_{2,i,j,\zeta}^{(2)}$

$$2k\left(z_{1/2}\right)\theta_{2,i,j,2}^{(2)}-\left[2k\left(z_{1/2}\right)+2h_z\eta_2+\left(w-w_g\right)h_z+\right.$$

$$\left.+2h_z\left(\frac{1}{\Delta t}-\left(\alpha_{2,i}^2+\beta_{2,j}^2\right)\right)\right]\theta_{2,i,j,1}^{(2)}-\left(w-w_g\right)h_z\theta_{1,i,j,0}^{(2)}=2h_z\bar{G}_{2,i,j,0}^{(2)}.$$

Also integrating equations (16) and (17) from $\left(N+\frac{1}{2}\right)h_z$ to $\left(N+1\right)h_z$ we obtain

$$\int_{G_H-\frac{1}{2}h_z}^{G_H} \frac{\partial}{\partial z}\left(k(z)\frac{\partial\theta_1^{(2)}}{\partial z}\right)dz = \left[k\left(z_{G_H}\right)\frac{\partial\theta_{1,i,j,N}^{(2)}}{\partial z} - k\left(z_{G_H-\frac{1}{2}h_z N}\right)\frac{\partial\theta^{(2)}_{1,i,j,H-\frac{1}{2}h_z N}}{\partial z}\right]=$$

$$= k\left(Z_{\frac{1}{2}}\right)\frac{\theta^{(2)}_{1,i,j,N+1}-\theta^{(2)}_{1,i,j,N}}{h_z} = k\left(Z_{G_H-\frac{1}{2}h_z}\right)\Big/h_z\,\theta^{(2)}_{1,i,j,N} + k\left(Z_{G_H-\frac{1}{2}h_z}\right)\Big/h_z\,\theta^{(2)}_{1,i,j,N+1};$$

$$\int_{G_H-\frac{1}{2}h_z}^{G_H}\left(w-w_g\right)\frac{\partial\theta_1^{(2)}}{\partial z}dz = \left(w-w_g\right)_{z_{G_H-\frac{1}{2}h_z}}\left(\theta^{(2)}_{1,i,j,N-1}-\theta^{(2)}_{1,i,j,N+0.5}\right).$$

And thus, when $z = G_H$ we have:

$$\frac{k\left(z_{G_H-\frac{1}{2}h_z}\right)}{h_z}\theta^{(2)}_{1,i,j,N} + \frac{k\left(z_{G_H-\frac{1}{4}h_z}\right)}{h_z}\theta^{(2)}_{1,i,j,N+1} + \left(\frac{1}{\Delta t}-\left(\alpha_{1,i}^2+\beta_{1,j}^2\right)\right)\theta^{(2)}_{1,i,j,N} -$$

$$-\left(w-w_g\right)_{z_{G_H-\frac{1}{4}h_z}}\left(\theta^{(2)}_{1,i,j,N-1}-\theta^{(2)}_{1,i,j,N+0.5}\right) = G^{(2)}_{1,i,j,N}$$

or

$$\gamma_1\theta^{(2)}_{1,i,j,N} + \gamma_2\theta^{(2)}_{1,i,j,N+1} + \gamma_3\theta^{(2)}_{1,i,j,N} - \gamma_4\theta^{(2)}_{1,i,j,N-1} -$$

$$-\gamma_4\frac{\theta^{(2)}_{1,i,j,N}+\theta^{(2)}_{1,i,j,N+1}}{2} = G^{(2)}_{1,i,j,N}$$

finally

$$\left(\gamma_2+\gamma_4/2\right)\theta^{(2)}_{1,i,j,N+1} + \left(\gamma_1+\gamma_3+\gamma_4/2\right)\theta^{(2)}_{1,i,j,N} + -\gamma_4\theta^{(2)}_{1,i,j,N-1} = G^{(2)}_{1,i,j,N}.$$

Here

$$\gamma_1 = \frac{k\left(z_{G_H-\frac{1}{2}h_z}\right)}{h_z};\quad \gamma_2 = \frac{k\left(z_{G_H-\frac{1}{4}h_z}\right)}{h_z};\quad \gamma_3 = \left(\frac{1}{\Delta t}-\left(\alpha_{1,i}^2+\beta_{1,j}^2\right)\right);\quad \gamma_4 = \left(w-w_g\right)_{z_{G_H-\frac{1}{4}h_z}}.$$

Similarly for $\theta^{(2)}_{2,i,j}$, we finally have the expression

$$\left(\gamma_2+\gamma_4/2\right)\theta^{(2)}_{2,i,j,N+1} + \left(\gamma_1+\gamma_3+\gamma_4/2\right)\theta^{(2)}_{2,i,j,N} - \gamma_4\theta^{(2)}_{2,i,j,N-1} = G^{(2)}_{2,i,j,N}.$$

So, as a result, to determine $\theta^{(2)}_{1,i,j,\xi}$ and $\theta^{(2)}_{2,i,j,\xi}$ we get a system of algebraic equations

$$\begin{cases} -b_{i,j,1}\theta^{(2)}_{m,i,j,1} + c_{i,j,1}\theta^{(2)}_{m,i,j,2} = -\bar{G}^{(2)}_{m,i,j,1}; \\ a_{i,j,2}\theta^{(2)}_{m,i,j,1} - b_{i,j,1}\theta^{(2)}_{m,i,j,2} + c_{i,j,1}\theta^{(2)}_{m,i,j,3} = -\bar{G}^{(2)}_{m,i,j,2}; \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ a_{i,j,N_1}\theta^{(2)}_{m,i,j,N_3-1} - b_{i,j,N_1}\theta^{(2)}_{m,i,j,N_3} + c_{i,j,N_1-1}\theta^{(2)}_{m,i,j,N_3+1} = -\bar{G}^{(2)}_{m,i,j,N_3}; \\ a_{i,j,N_3+1}\theta^{(2)}_{m,i,j,N_3} - b_{i,j,N_3+1}\theta^{(2)}_{m,i,j,N_3+1} = -\bar{G}^{(2)}_{m,i,j,N_3+1}. \end{cases}$$

where takes the value $m = 1, 2$.

Solving system (28), we find $\theta^{(2)}_{1,i,j,\xi}$, $\theta^{(2)}_{2,i,j,\xi}$ at $i = 0,1,2,...,N_1+1;$ $j = 0,1,2,...,N_2;$ $\xi = 0,1,2,...,N_3$. Then, using relations (16), (17) and from the desired values $\theta^{(2)}_{1,i,j,\xi}$, we $\theta^{(2)}_{2,i,j,\xi}$ pass to the desired values $\theta^{(1)}_{1,i,j,\xi}$, $\theta^{(1)}_{2,i,j,\xi}$. With the help of (12), (13) from $\theta^{(1)}_{1,i,j,\xi}$, $\theta^{(1)}_{2,i,j,\xi}$ we pass to the numerical solution of problems (8) and (9) at the moment of time $t = t_{n+1}$.

Methods for solving the problem

Since problem (1)-(5) is described by a multidimensional non-linear partial differential equation with appropriate initial and boundary conditions, it is difficult to obtain its solution in an analytical form. To solve the problem, we use an implicit finite-difference scheme in time with the second order of accuracy in time [14-15].

Computational experiment

To monitor and predict the ecological state of the industrial region, a web -oriented software tools using which computational experiments were carried out on a computer.

To enter the main parameters of the process of transfer and diffusion of aerosol particles and to carry out calculations on a computer, a graphical interface has been developed (Fig.1,2). With the help of the developed interface, the following is entered: types of harmful substances emitted from industrial facilities; number of potential sources of emission of harmful substances; problem number (1 - when the direct problem is solved, 2 - when the adjoint problem is solved); coefficient of absorption of harmful substances in the atmosphere; horizontal component of wind speed; Direction of the wind; atmospheric stratification; initial particle settling rate; calculation time; source power.

As can be seen from the numerical calculations performed on a computer (Fig. 3), with an increase in the horizontal component of the wind speed, aerosol particles ejected from industrial facilities are transported in the direction of the wind. The area of distribution of harmful substances in the surface layer of the atmosphere expands with an increase in the speed of the air mass of the atmosphere (Fig. 3-5). This can be especially observed at H=200- 300 м.

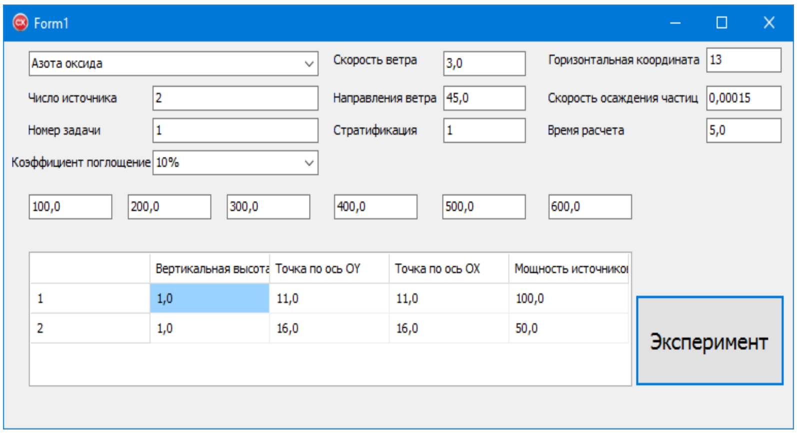


Fig.1. Form for entering the main process parameters

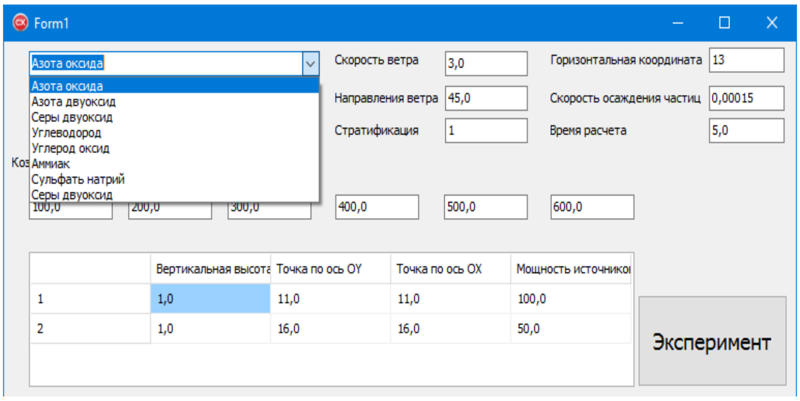


Fig.2. Form for entering the main process parameters

The results of the computational experiments carried out on a computer are shown in Figures 3-11.

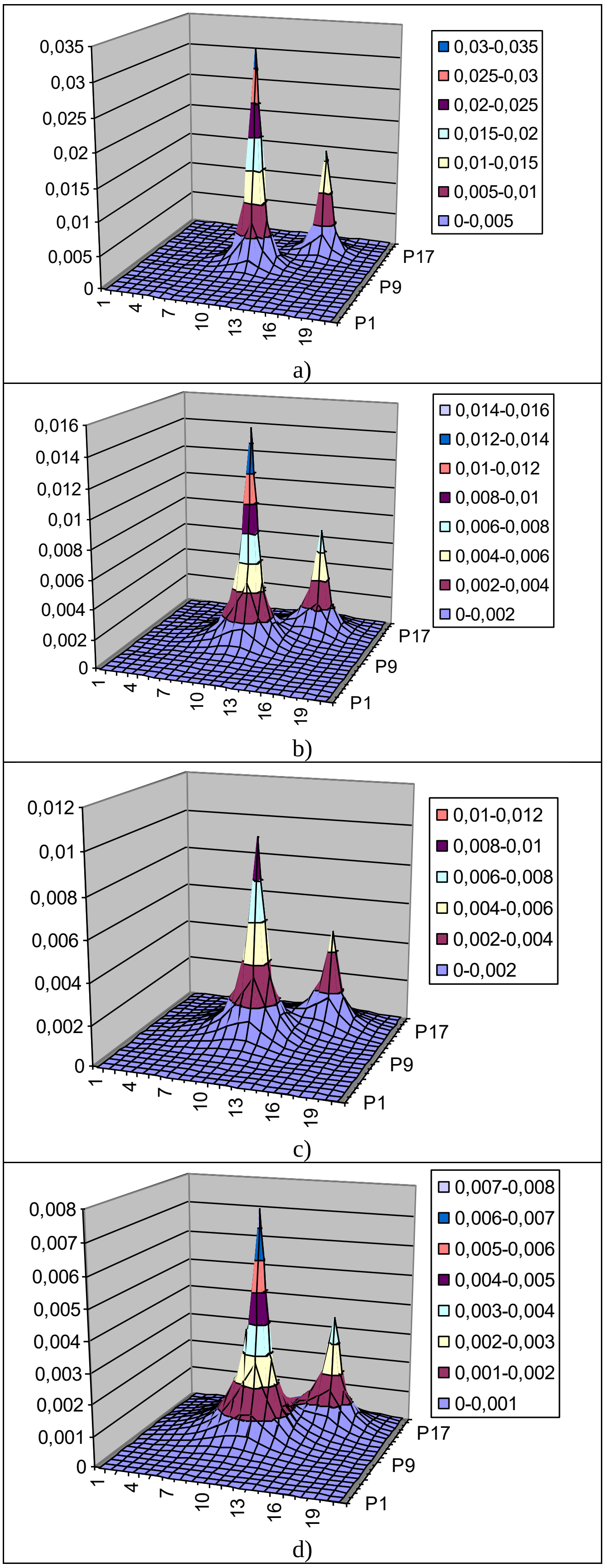


Fig.3. Change in the concentration of harmful substances in the first layer of the atmosphere (H = 100m) at wind speed: ***a) u = 1 m/s.; b) u = 3 m/s; c) u = 4 m/s; d) u = 5 m/s.***

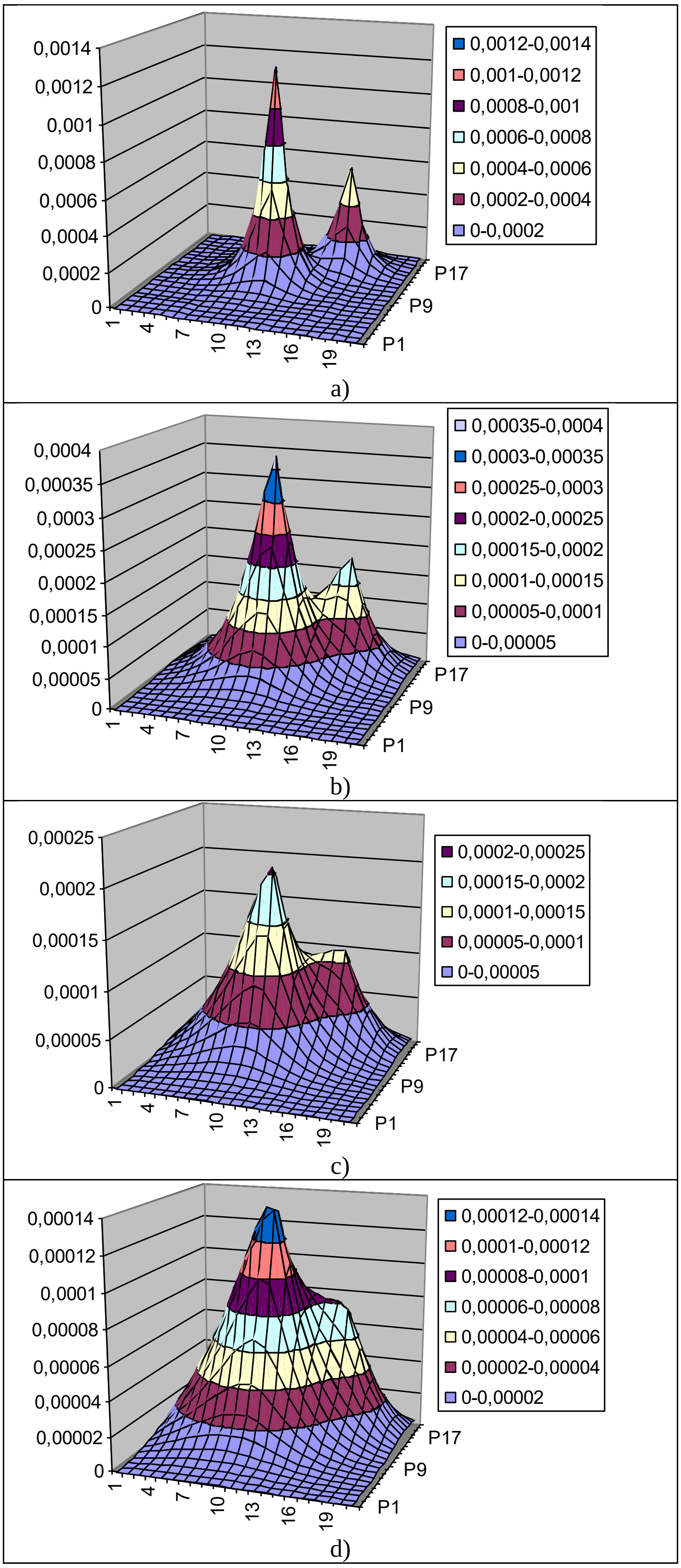


Fig.4. Change in the concentration of harmful substances in the first layer of the atmosphere (H = 200m) at wind speed: ***a) u = 1 m/s.; b) u = 3 m/s; c) u = 4 m/s; d) u = 5 m/s.***

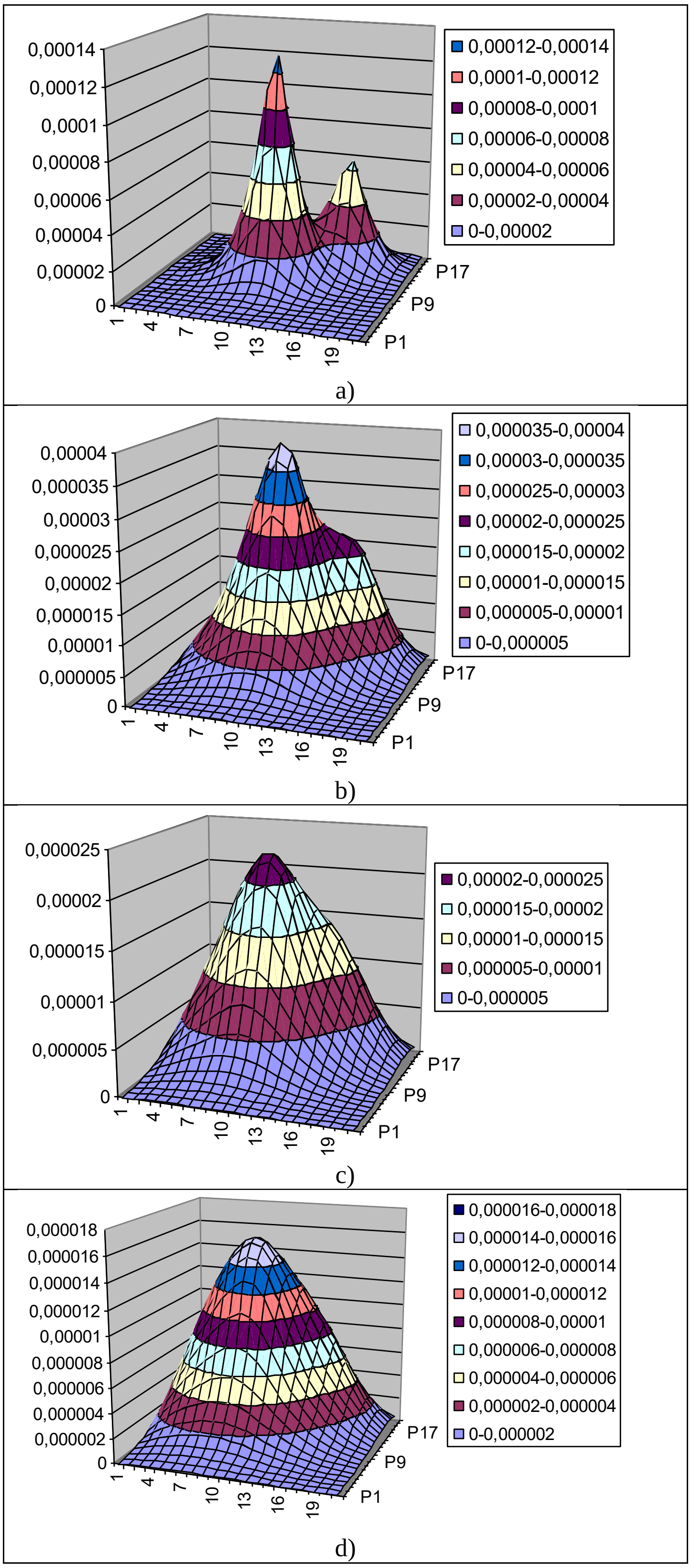
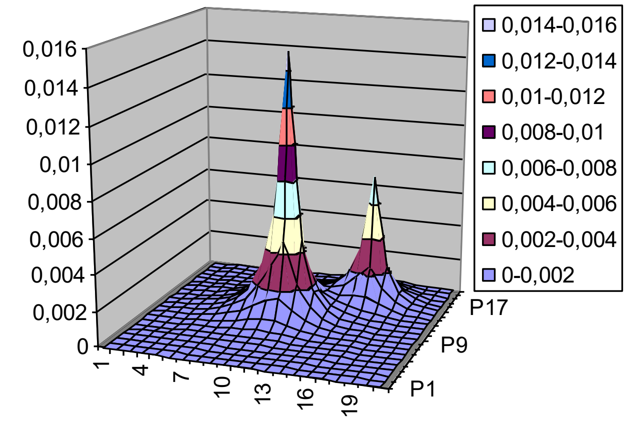


Fig.5. Change in the concentration of harmful substances in the third layer of the atmosphere (H = 300m) at wind speed: ***a) u = 1 m/s.; b) u = 3 m/s; c) u = 4 m/s; d) u = 5 m/s.***



0,014-0,016
0,012-0,014
0,01-0,012
0,008-0,01
0,006-0,008
0,004-0,006
0,002-0,004
0-0,002
0,016
0,014
0,012
0,01
0,008
0,006
0,004
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0
1
4
7
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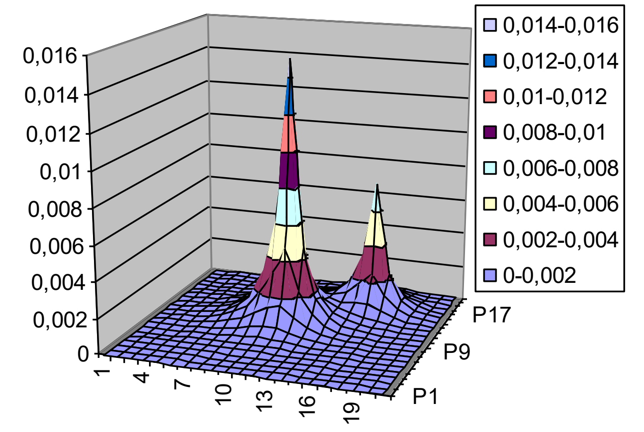
13
16
19
P1
P9
P17

a)



0,014-0,016
0,012-0,014
0,01-0,012
0,008-0,01
0,006-0,008
0,004-0,006
0,002-0,004
0-0,002
0,016
0,014
0,012
0,01
0,008
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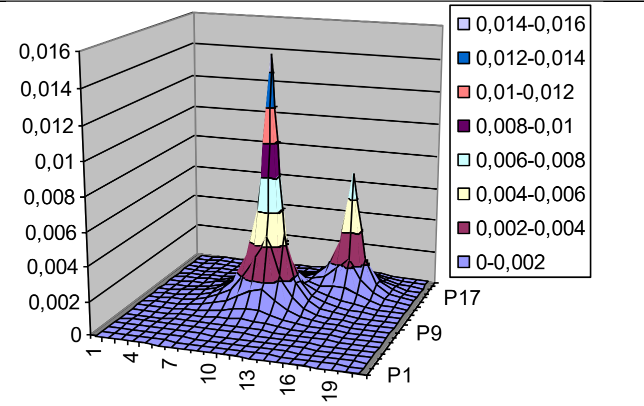
P1
P9
P17

b)



0,014-0,016
0,012-0,014
0,01-0,012
0,008-0,01
0,006-0,008
0,004-0,006
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0,016
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P1
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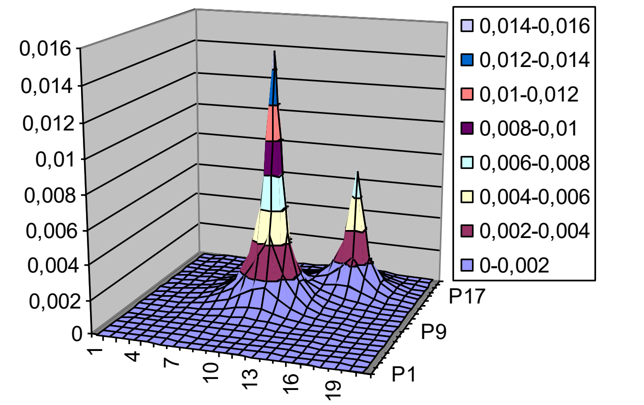
P17

c)



0,014-0,016
0,012-0,014
0,01-0,012
0,008-0,01
0,006-0,008
0,004-0,006
0,002-0,004
0-0,002
0,016
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0,012
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P1
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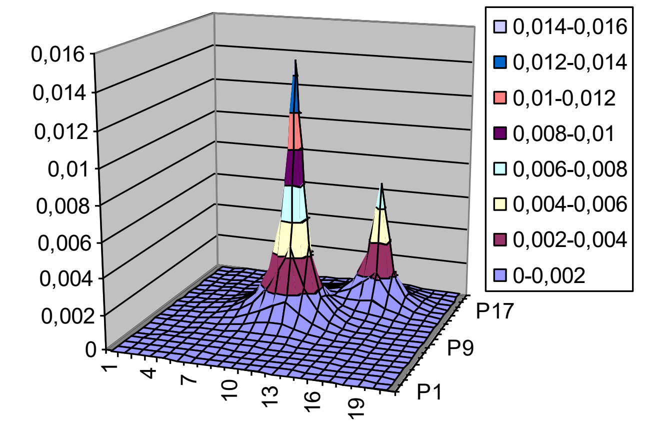
P17

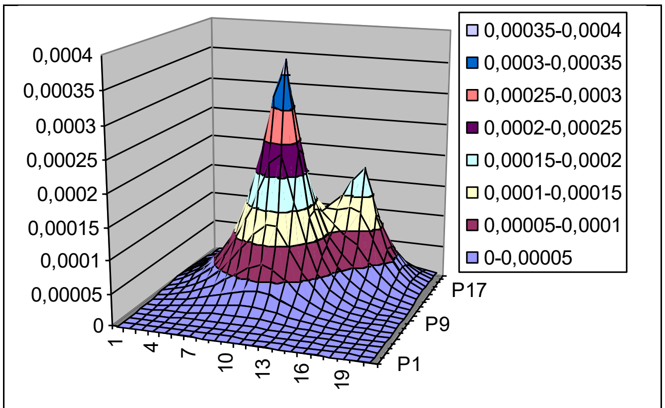
d)



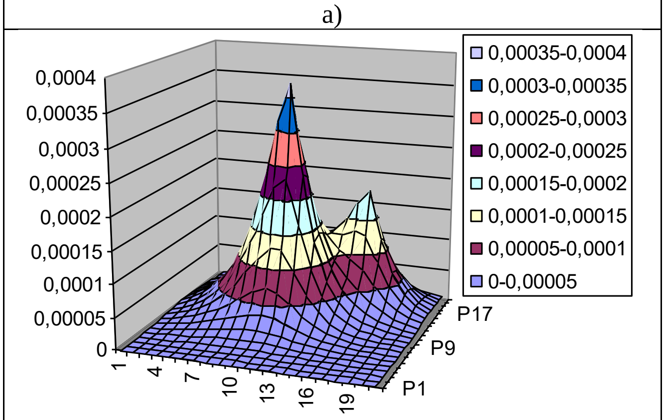
e)

Fig.6. Change in the concentration of harmful substances in the first layer of the atmosphere (H=100m) at the initial particle settling velocity: ***a)*** w_g ***= 0.00015 m/s; b)*** w_g ***= 0.0003 m/s; c)*** w_g ***\u003d 0.0006 m / s .; d)*** w_g ***= 0.0009 m/s; e)*** w_g ***= 0.009 m/s.***

Another parameter that significantly affects the change in the concentration of harmful substances in the atmosphere, on the earth's surface is the rate of deposition of harmful particles (Fig. 6-8). As it was established by the computational experiments carried out on a computer, the vertical transfer of harmful substances into the atmosphere depends: firstly, on the initial rate of particle settling; secondly, on the vertical speed of the air mass of the atmosphere; in thirds of the physico-mechanical properties of particles (radius of particles; cross-sectional area of particles) and properties of the atmosphere (ρ atmospheric density); fourthly from the acceleration of gravity.



a)



b)

Impact Factor:

ISRA (India) = **6.317**	**SIS** (USA) = **0.912**	**ICV** (Poland) = **6.630**
ISI (Dubai, UAE) = **1.582**	**РИНЦ** (Russia) = **3.939**	**PIF** (India) = **1.940**
GIF (Australia) = **0.564**	**ESJI** (KZ) = **8.771**	**IBI** (India) = **4.260**
JIF = **1.500**	**SJIF** (Morocco) = **7.184**	**OAJI** (USA) = **0.350**

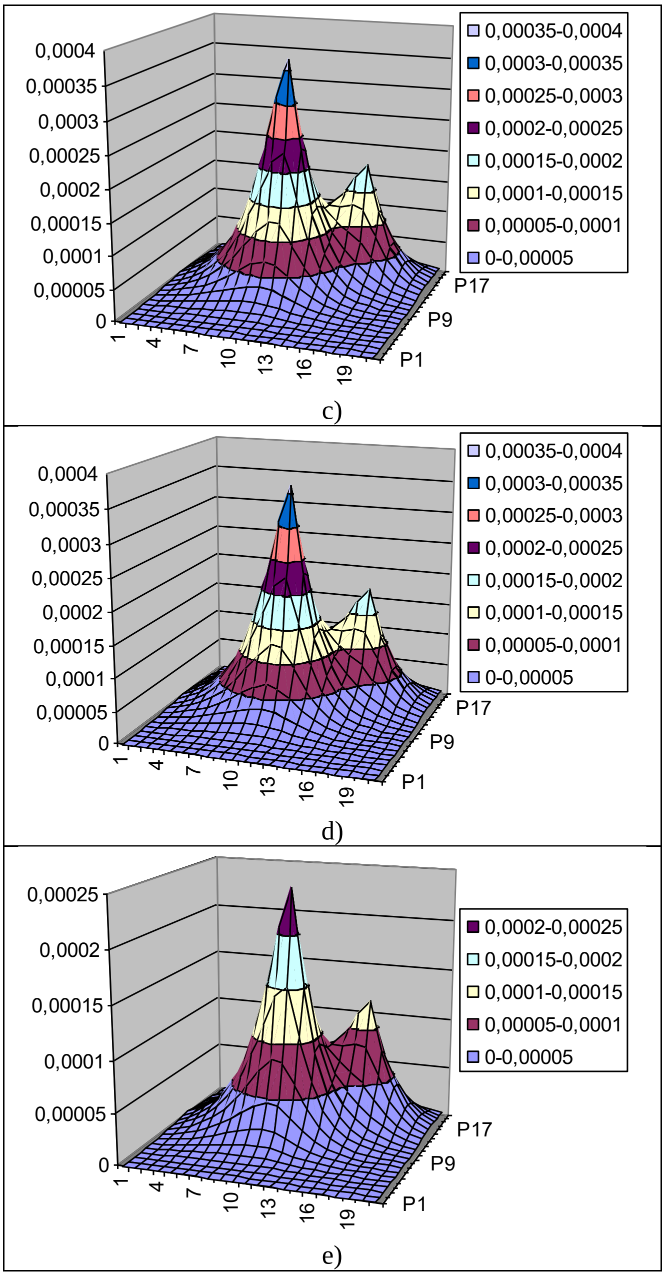
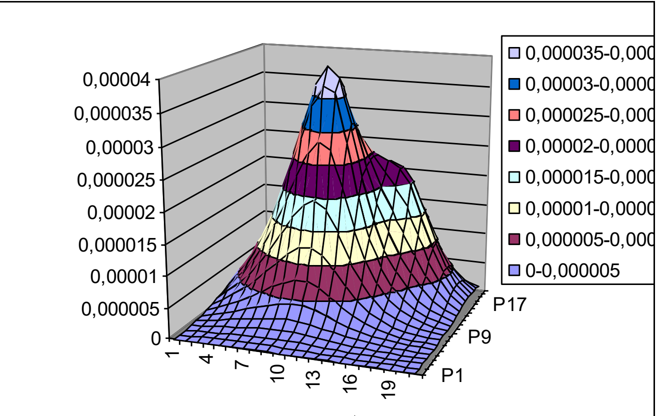


Fig.7. Change in the concentration of harmful substances in the second layer of the atmosphere (H=200m) at the initial particle settling velocity: ***a)*** $w_g = 0.00015$ *m/s;* ***b)*** $w_g = 0.0003$ *m/s;* ***c)*** w_g *\u003d 0.0006 m / s .;* ***d)*** $w_g = 0.0009$ *m/s;* ***e)*** $w_g = 0.009$ *m/s.*



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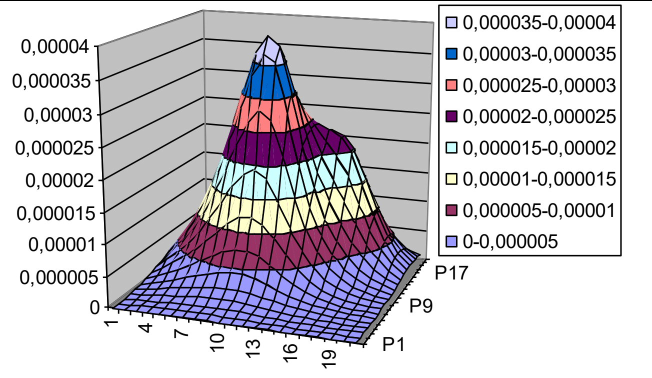
a)



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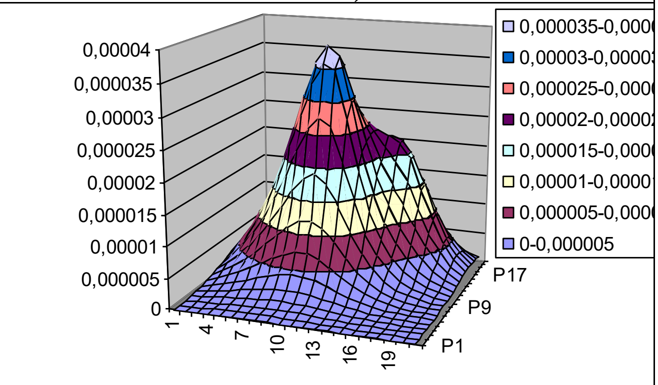
b)



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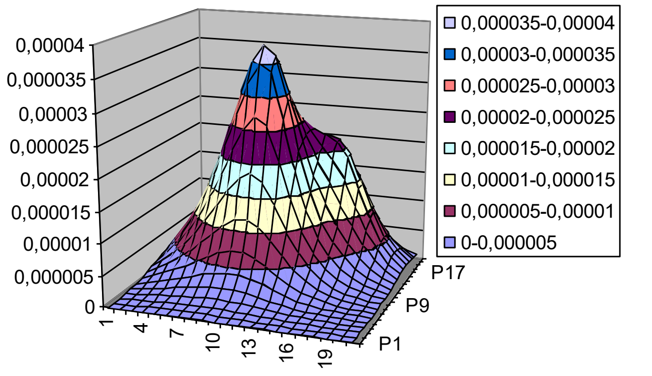
c)



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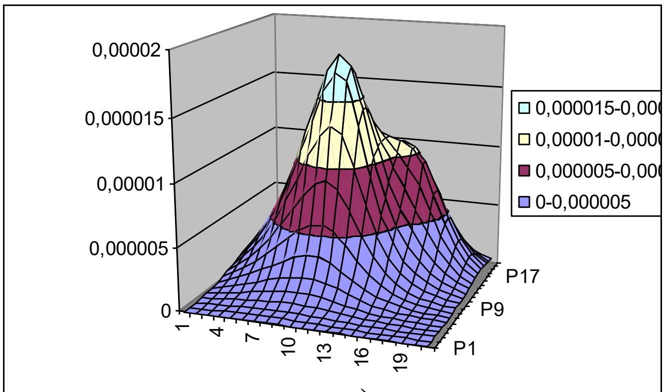
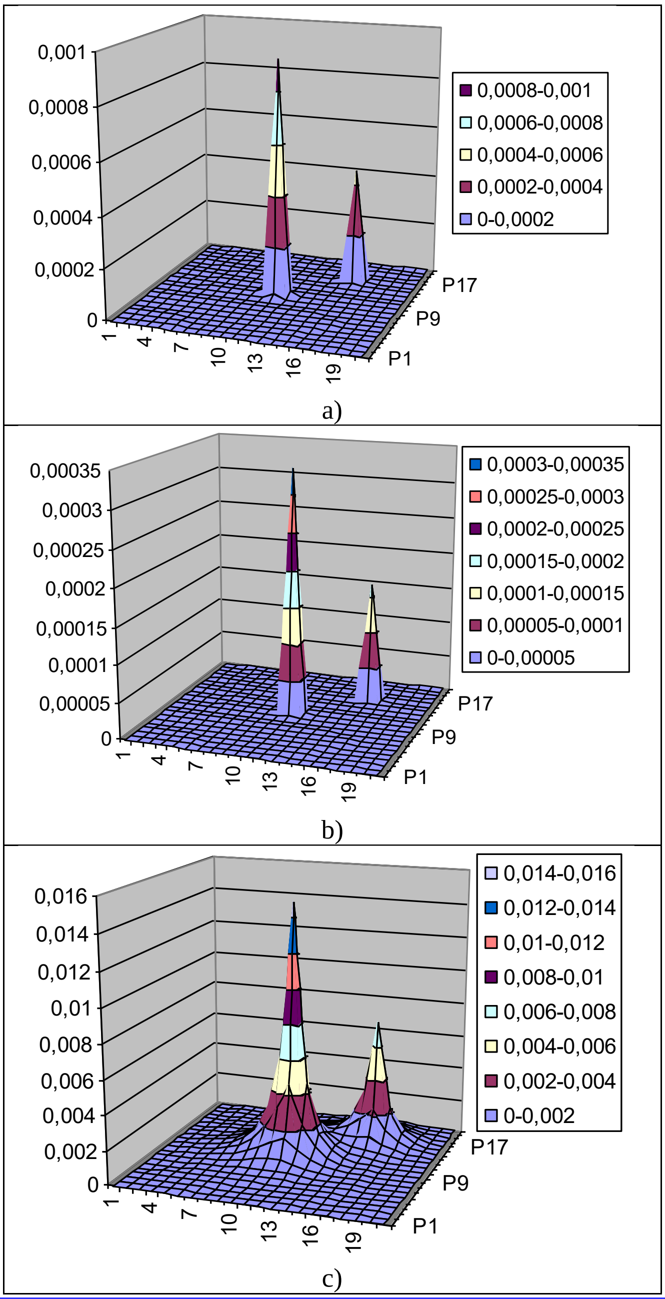
d)



e)

Fig.8. Change in the concentration of harmful substances in the third layer of the atmosphere (H=300m) at the initial particle settling velocity: *a) w_g = 0.00015 m/s; b) w_g = 0.0003 m/s; c) w_g \u003d 0.0006 m / s .; d) w_g = 0.0009 m/s; e) w_g = 0.009 m/s.*



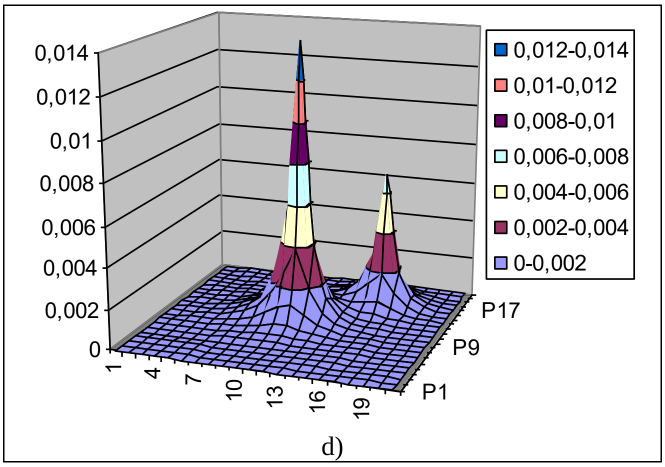
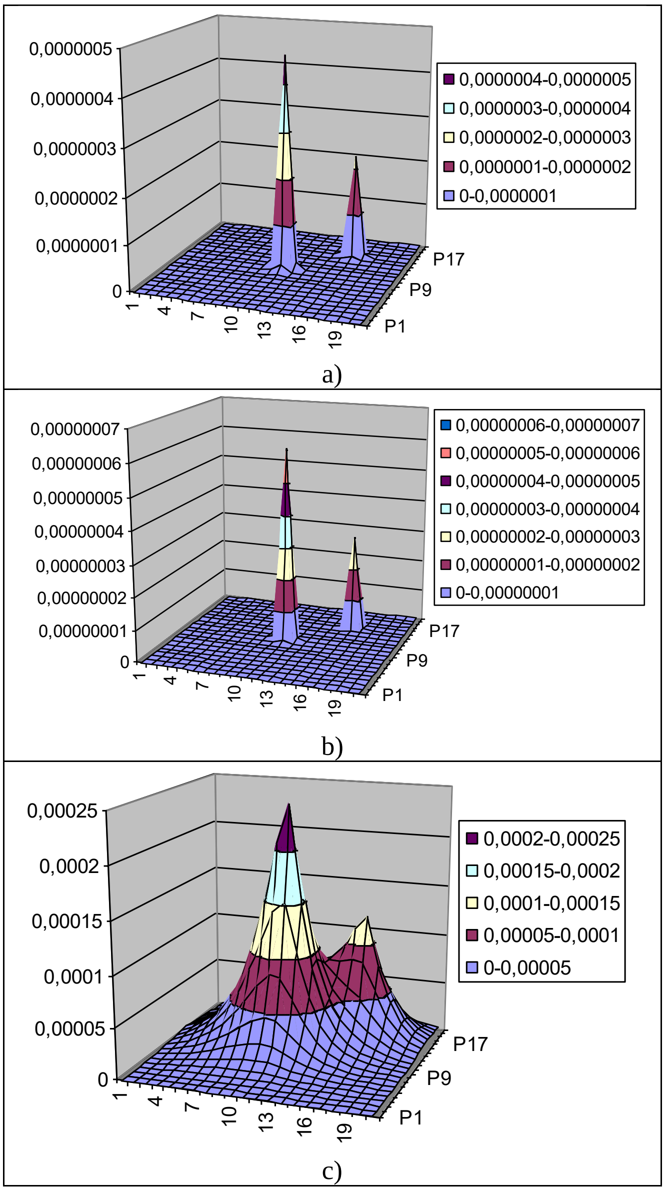
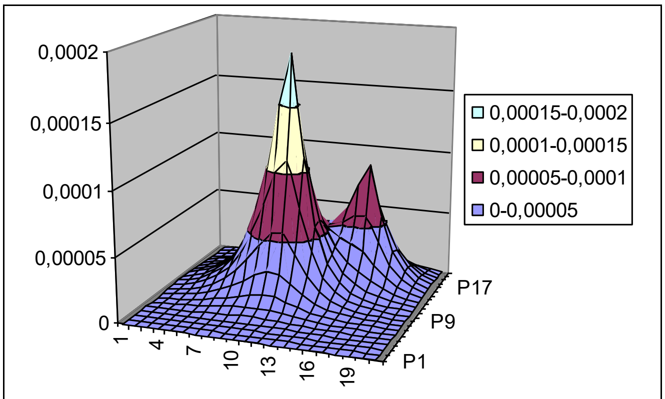


Fig.9. Change in the concentration of harmful substances in the first layer of the atmosphere (H=100m) for different absorption coefficient values
a) σ = 10%; b) σ = 20%; c) σ = 30%; d) σ = 40%.

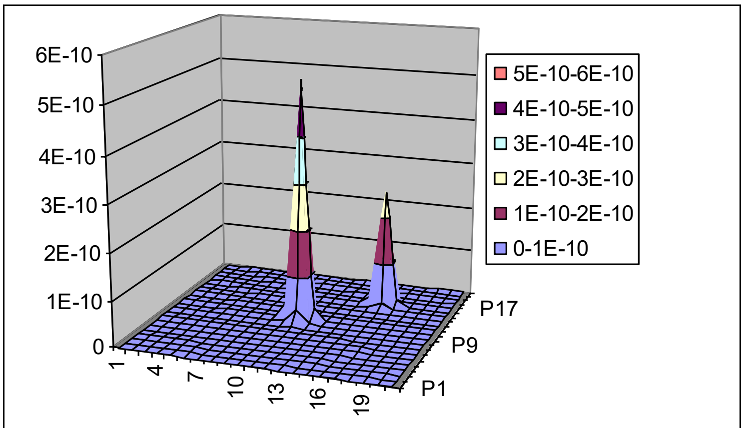




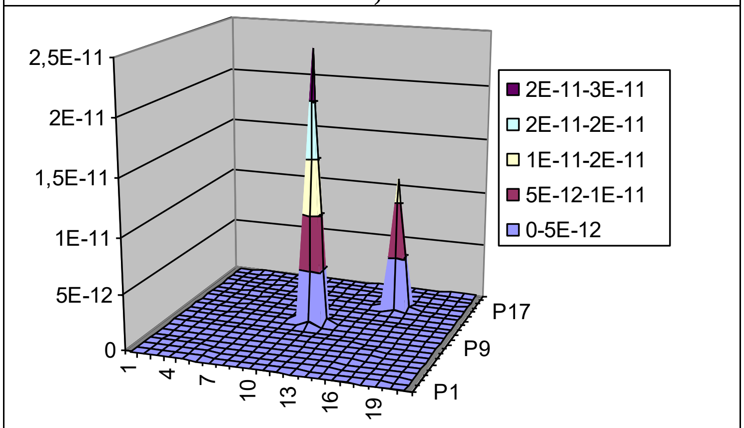
d)

Fig.10. Changes in the concentration of harmful substances in the second layer of the atmosphere (H=200m) for different values of the absorption coefficient *a) σ = 10%; b) σ = 20%; c) σ = 30%; d) σ = 40%.*

Numerical calculations on a computer were carried out at different values of the particle absorption coefficient (Fig. 9-11). Computational experiment established that 10 to 18 percent of aerosol particles are absorbed in the atmosphere. The growth of the absorption of harmful substances in the atmosphere depends on the humid state of the air mass of the atmosphere. The change in the absorption coefficient of direct images depends on the temperature and humidity of the atmosphere [16].



a)



b)

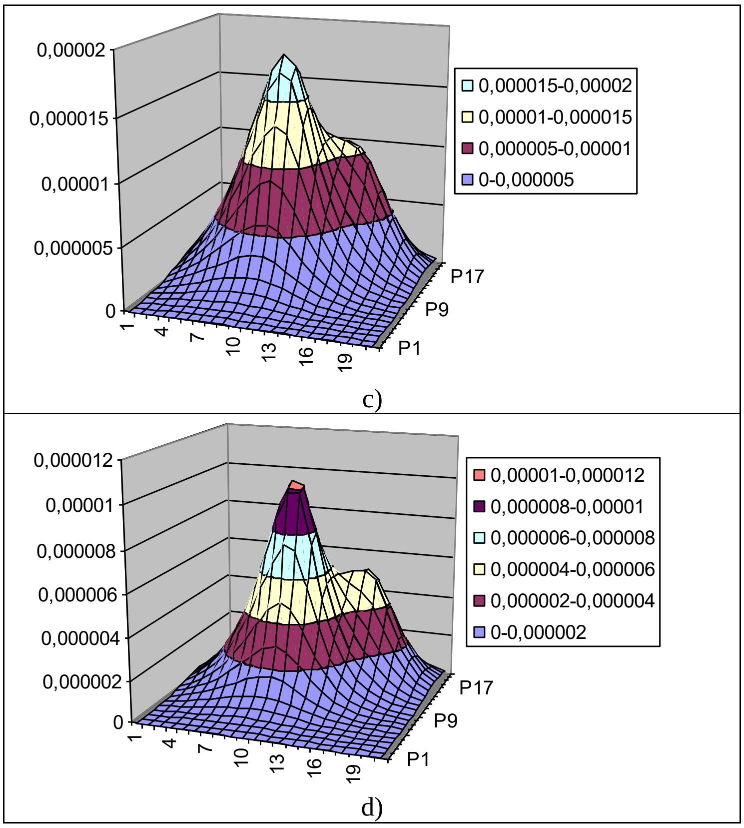
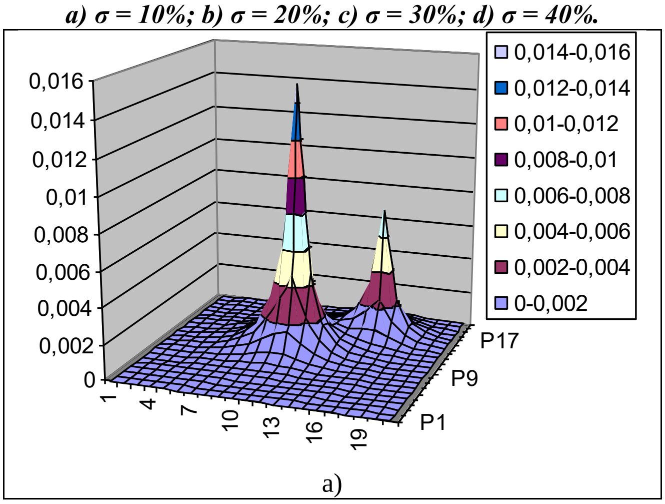
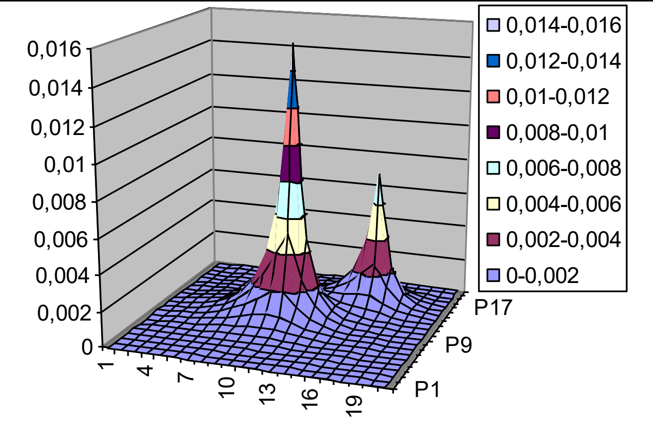


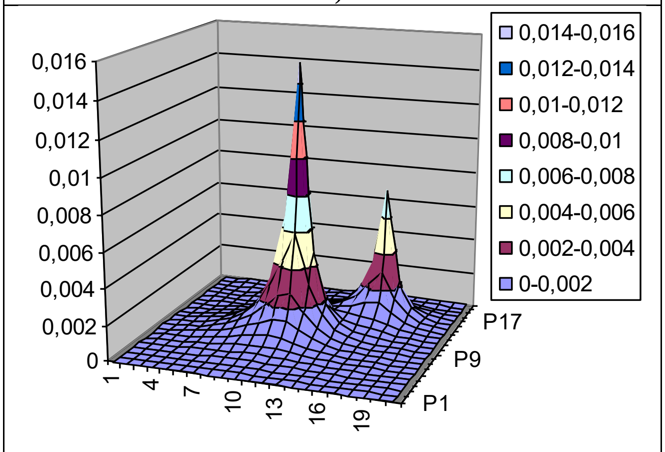
Fig.11. Change in the concentration of harmful substances in the third layer of the atmosphere (H=300m) for different values of the absorption coefficient

a) σ = 10%; b) σ = 20%; c) σ = 30%; d) σ = 40%.





b)

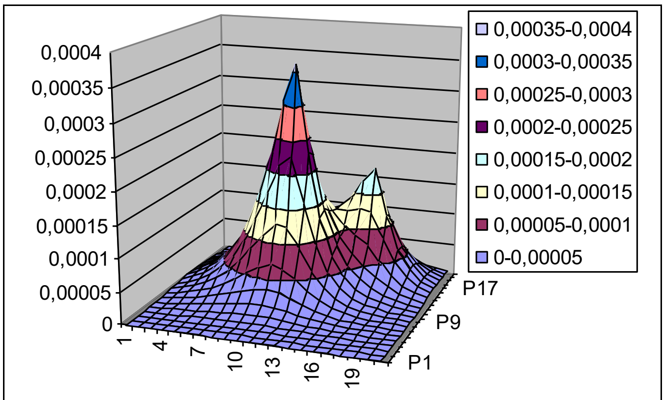


c)

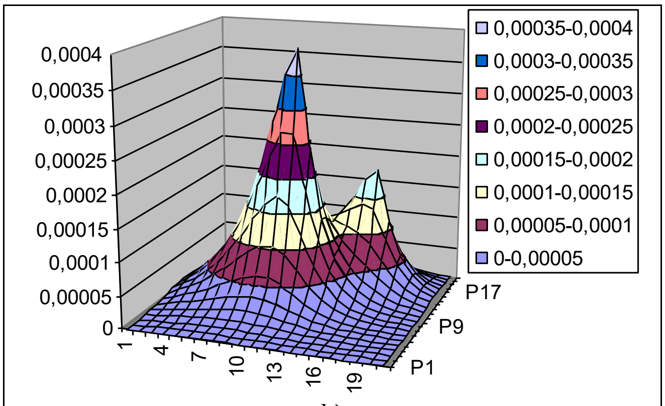
Fig.12. Change in the concentration of harmful substances in the first layer of the atmosphere (H=100m) for different values of the wind speed direction

a) α\u003d 45 ^{0}; b) α= 85 ^{0}; c)) α= 120 ^{0}

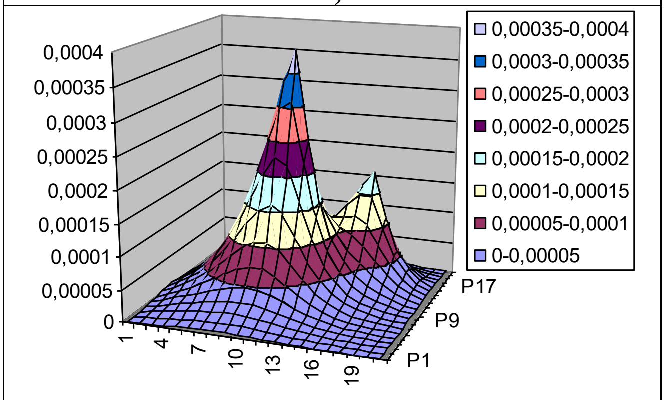
Another parameter that significantly affects the horizontal transfer and diffusion of harmful substances in the atmosphere is the direction of the horizontal wind speed (Fig. 12-14). As can be seen from the calculations carried out on a computer, the direction of the wind strongly affects the process of transport of harmful substances in the atmosphere when H changes from 300 to 300 м. (Fig. 14).



a)



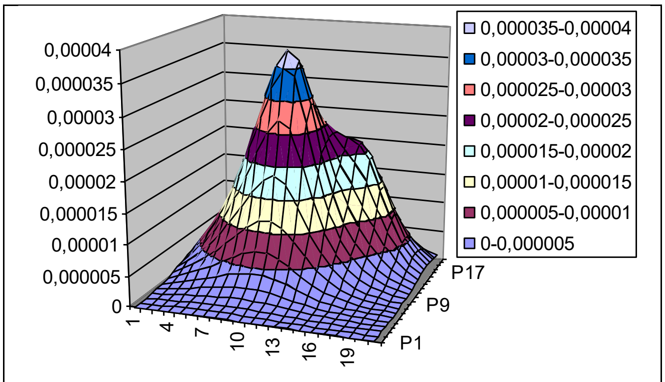
b)



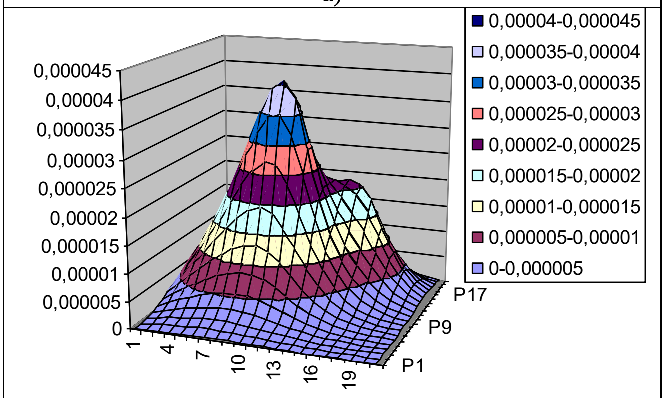
c)

Fig.13. Change in the concentration of harmful substances in the second layer of the atmosphere (H=200m) for different values of the wind speed direction

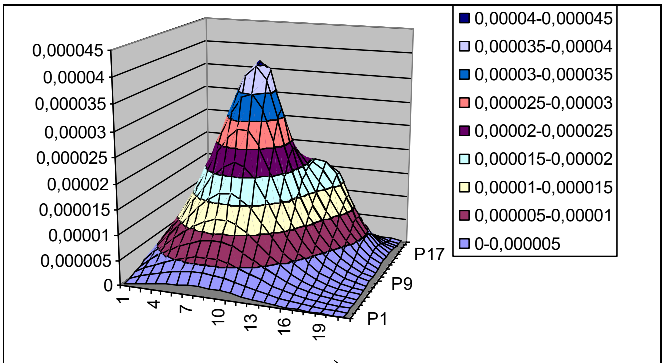
a) α\u003d 45 ^{0}; b) α= 85 ^{0}; c) α= 120 ^{0}



a)



b)



c)

Fig.14. Change in the concentration of harmful substances in the third layer of the atmosphere (H=300m) for different values of the wind speed direction

a) α \u003d 45 ^{0}; b) α = 85 ^{0}; c) α = 120 ^{0}

Conclusion

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.

Computational experiment established that 10 to 18 percent of aerosol particles are absorbed in the atmosphere. The growth of the absorption of harmful substances in the atmosphere depends on the humid state of the air mass of the atmosphere.

The numerical calculations carried out on a computer showed that the distribution of aerosol particles in the atmosphere along the vertical depends: firstly, on the initial rate of particle settling; secondly, on the vertical speed of the air mass of the atmosphere; in thirds of the physico-mechanical properties of particles (radius of particles; cross-sectional area of particles) and properties of the atmosphere (ρ atmospheric density); fourthly from the acceleration of gravity.

An analysis of numerical calculations showed that the area of distribution of harmful substances in the surface layer of the atmosphere expands with an increase in the speed of the air mass of the atmosphere. This can be especially observed at H=200- 300 м.

The numerical experiments carried out for different wind directions and speeds have shown that these parameters directly affect the change in the concentration of aerosol emissions in the atmosphere. It was also established that with an increase in the power of aerosol generators, the area of \u200b\u200bthe area where the concentration exceeds the permissible sanitary norm increases. With unstable wind stratification, the area of distribution of harmful substances has a sawtooth character, it maximizes over time and over a short period of time.

The calculated data showed that elevations - hills or mountain ranges located on an open landscape - play a significant role in changing the speed and direction of winds. Above the hills, the wind speed is higher compared to the surrounding flat area. Since the high pressure area actually expands some distance to the hill, the wind changes its direction before reaching it. If the air mass meets a steep hill with an uneven surface, then the wind speed increases sharply, which leads to an increase in the turbulence coefficient. The wind speed increases with an increase in the atmospheric pressure drop, and the air flow speed decreases near the ground due to friction due to the roughness of the underlying surface;

Computational experiments have established that when harmful fine particles propagate in the atmosphere, taking into account the coefficient of interaction with the underlying surface plays a special role.

When specifying different heights of the source of pollution, it was found that with emissions from high sources, 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 and intensive transport of impurities, leads to a 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 harmful substances in the atmosphere is played by horizontal flows.

To conduct a comprehensive study of the process of spreading harmful substances into the environment, taking into account the mutual transformation of aerosol particles in the atmosphere due to changes in weather and climate factors, a mathematical model was developed that more adequately describes the object of study.

A differential equation is obtained for calculating the settling rate of fine and aerosol particles propagating in the boundary layer of the atmosphere, where the mass and radius of aerosol particles, atmospheric density, and air resistance force are taken into account.

For the numerical solution of the problem, an efficient algorithm based on the "method of lines" has been developed, which allows reducing the multidimensional problem described by a partial differential equation to the integration of an ordinary equation.

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