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MATHEMATICAL MODEL AND COMPUTING EXPERIMENT FOR MONITORING AND PREDICTING THE ENVIRONMENTAL STATE OF THE BORDER LAYER OF THE ATMOSPHERE

Abstract: *In this article the current problem of the monitoring and forecasting of the ecological state of the air basin of industrial regions related to the solution, where a violation of the valance of the sanitary norm of the environment due to a large number of emissions of harmful substances will be considered. In this work to solve the above problem a mathematical model and its software describing the process under consideration with the help of hydro mechanical equations with the corresponding initial and boundary conditions for carrying out a complex study of the process of transport and diffusion of pollutants released into the environment from production facilities and the results of numerical calculations on a computer. To derive the mathematical model of the object, the basic laws of mechanics and hydro thermodynamics (equations of mass conservation and balance of forces) were used, taking into account the main parameters that play an important role in the process of aerosol particles in the atmosphere: wind speed and direction; terrain relief; absorption coefficient of harmful aerosol fine particles in the atmosphere, physical and mechanical properties of particles, etc. The differential equation for calculating the deposition rate of fine-dispersed and aerosol particles propagating in the near-boundary layer of the atmosphere is obtained. This article is devoted to numerical modeling of the vibration of rods in the static formulation of the problem. The results are presented in tabular and graphical form. The problems considered are solved with different values of the grid pitch and these results are given in the table. Numerical analysis of the results obtained.*

Key words: *mathematical model, numerical algorithm, approximation, transfer and diffusion, atmosphere, harmful aerosols, rate of particles deposition.*

Language: *English*

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Introduction

Monitoring, forecasting and assessing the pollution of the atmosphere and the underlying surface of the earth with passive and active impurities, fine particles and carbon dioxide, as well as the design and placement of industrial facilities in compliance with the maximum permissible sanitary standards are relevant in the problem of environmental protection.

An analysis of data on the state of the environment in recent years shows that an intensive increase in the volume of emissions of harmful substances into the atmosphere inevitably causes an imbalance in the ecological state. This is especially noticeable in states with a high rate of industrial development, for example, China, India, Russia, the USA, France, Great Britain, Japan, Korea, Malaysia, etc. than negatively affect the living system - the flora and fauna of these regions, and at the global level contribute to climate change around the globe.

Potential sources of pollution of the atmospheric basin in industrial regions are divided into stationary and variable.

Information and a detailed analysis of the processes of air pollution in industrial cities and regions, as well as the difference between pollution produced by permanent and mobile variable sources, can be emphasized in the works of many foreign authors dealing with the problem of environmental protection. Here we note that a stationary (point) source of pollution is a source that is constantly located in a certain place. For example, chimneys of factories and plants, thermal power plants, technological installations, heating boilers, furnaces and dryers, exhaust shafts, ventilation pipes, hoods emitting fine harmful particles, etc. Statistical processing of the accumulated databases showed that in industrial regions, nitrogen oxides, sulfur dioxide, carbon monoxide, sulfuric acid, phenols and other aerosol substances are emitted into the environment in large quantities by constant sources, depending on the specifics of the industrial production of the city and the composition used in it. Fuel As is known, one of the main properties of stationary sources is that their emissions of harmful aerosol particles (unlike mobile sources) occur, as a rule, at high altitudes. Therefore, the process of diffusion and transfer of aerosol particles in the atmosphere emitted by production facilities spreads over a large area. As a result, due to the interaction between harmful particles, their concentration increases, and areas of stable pollution are formed, extending to a height of up to 180 200 мand more.

Recently, there has been growing research work aimed at developing problems of modeling the processes of transfer and diffusion of harmful substances in the atmosphere with the aim of systematic monitoring and forecasting the state of the atmosphere of industrial regions.

Simulations of the processes of distribution of harmful substances are carried out in advanced scientific centers and higher educational institutions of the world, which include California line Source Model , General Finite line Source Model (USA), Karlsruhe Institute of Technology Institute _ of Applied Geosciences (Germany), Center for Ecology and Hydrology _ _ for water Science (UK), Contaninants in the Air from a road , By the Finnish meteorological Institute (Finland), National Institute of Hydrology , Waterloo Hydro geologic (India), Institute of Atmospheric Physics. A.M. Obuzova , Institute of Computational Mathematics and Mathematical Geophysics (Russia), Research and Design and Technological Institute “Atmosphere”, National University of Uzbekistan (Uzbekistan).

In [1], an analytical model was developed for the process of transport of impurities in the atmosphere. As the authors of the article emphasize, the main advantages of the analytical model lie in its simple numerical implementation on a computer. Using an analytical solution, one can obtain a fragmented distribution of pollutants in any given area without solving a boundary value problem. But here it should be noted that the analytical model well describes the process of emission propagation in the atmosphere at constant transfer coefficients and can be used as a test to verify numerical calculations and to quickly obtain preliminary information on the propagation of pollutants. Such models can be used for the following purposes: control of pollution sources – rapid measurement of pollution emissions; measurement of pollution transport - monitoring at the surface layer and at altitude over large geographic areas.

In [2], a mathematical model was created, which consists in the use of systematic methodological methods of research, which made it possible to assess the quality of the surface layer of atmospheric air. A numerical algorithm has been proposed and new software has been created that satisfactorily describes the process of pollutant propagation in the atmospheric air of a limited area, which consists in using a flow correction algorithm, the results of which correlate with the data. The paper considers the two-dimensional distribution of aerosol matter in the lower layer of the atmosphere, where the chain of its transformation from one chemical state to another consists of three links. Whereas a free chemical is released into the air (substrate), an air mixture (complex) is first created in the course of a reversible reaction, which, in turn, irreversibly decomposes, re-forming the free chemical and product.

The authors showed not only the systematization of the known physicochemical properties and regularities of aerosols, but also the need for deeper further research.

In [3], a comprehensive assessment of atmospheric air pollution in a large industrial city is given in detail. The article summarizes the main problems of a hygienic and environmental nature that determine the state of the main environmental objects in a large industrial city. Such aspects of the ecological situation as air pollution in the metropolis are analyzed in detail. The features of the atmospheric air quality formation are studied based on the analysis of retrospective data on the dynamics of harmful substances entering the atmosphere with gross emissions from the leading industrial enterprises of the metropolis, the individual residential sector. An assessment of the contribution of motor transport to the level of air pollution is given. The main pollutants of the atmospheric air in Almaty are identified, which determine the greatest contribution to environmental damage and the risk to public health.

The work [4] presents a mathematical model of the process of movement of a multicomponent air environment in the surface layer for the coastal zone, taking into account the presence of green spaces. The transition to a two-dimensional model for the equations of motion of the air medium in the absence of a pressure gradient is briefly considered. This approach allows to significantly reduce the computational costs for the numerical solution of the grid equations of diffusion-convection (motion) and reduce the execution time of information exchange operations of interprocessor exchanges when simulating on multiprocessor systems.

Article [5] is devoted to the method of calculating the process of neutralization of toxic gas in the atmosphere. The method is based on the numerical integration of the two-dimensional equation of the convective-diffusion impurity transfer. An implicit difference scheme is used for the calculation.

The article [6] presents a numerical model and, on its basis, a method for calculating the process of propagation of a heavy toxic gas in the atmosphere is constructed. Three-dimensional equations of impurity transfer and potential air flow are used as a mathematical model. The calculation is carried out using implicit difference schemes. The results of a computational experiment on modeling air pollution in the event of an emergency leakage of a toxic substance are presented.

In [7], numerical models have been developed that allow calculating the 3D aerodynamics of the wind flow in urban areas and the process of mass transfer of emissions from the highway. Calculations were made to determine the pollution zone, which is formed near buildings located along the highway. The paper considers effective numerical models that can be applied in the development of environmental protection measures during the operation of road transport in the city. The developed models make it possible to estimate the size, shape and intensity of the pollution zone near the highway.

Article [8] is devoted to the construction of a two-dimensional mathematical model of the movement of the air medium, as well as writing a software package that implements the developed algorithms. For an adequate mathematical description of the processes occurring in the atmosphere, it is required to solve the problem of constructing its physical model, since it significantly affects the construction of the wind field and the description of the transport occurring in the air. The physical properties of atmospheric air (temperature, humidity, mobility, atmospheric pressure) are unstable and are associated with the climatic features of the geographical region. The paper presents an approximation of the problem with respect to the time variable, constructs a two-dimensional model of aerodynamics, and presents the results of numerical experiments.

The article [9] considers the main problems that arise when assessing the quality of the atmosphere in industrial cities. A model is proposed that allows taking into account the level of atmospheric pollution and predicting the occurrence of a particular environmental situation, taking into account a number of factors affecting the change in the concentration of pollutants in the atmosphere of industrial cities.

In [10], a mathematical numerical model was developed, and on its basis a package of applied programs was created, which allows to quickly carry out computational experiments to assess the level of atmospheric air pollution by vehicle emissions on city streets in the presence of several buildings located according to the “street canyon” scheme. As a result of the studies, regularities were established for changes in the concentration of carbon monoxide near the considered group of buildings at different pollutant emission rates. A numerical model has been developed that makes it possible to take into account the hydrodynamic effect of a group of buildings on the dispersion of pollutants when the wind speed and vertical diffusion coefficient change with height.

A detailed analysis of scientific works related to the problem of mathematical modeling of the process of transfer and diffusion of aerosol particles in the atmosphere, which, in mathematical modeling and research of the process of distribution of harmful substances in the atmosphere, firstly, does not consider changes in the deposition rate of aerosol particles, which changes with time and depending on the change speeds of the air flow, secondly, in all the above mathematical models of the process, the absorption coefficient of aerosol particles was taken constant, in the third, it was assumed that the spread of harmful substances emitted from sources does not reach the considered boundaries of the problem solution area and there is no inflow and outflow of harmful substances through them .

In this work, when studying the process of transfer and diffusion of harmful substances in the atmosphere, efforts were made to fill these gaps.

Based on the foregoing, the purpose of this work is to develop a mathematical model and a numerical algorithm for solving the problem of transport and diffusion of aerosol emissions in the atmospheric boundary layer.

Statement of the problem

To study the process of transfer and diffusion of aerosol particles in the atmosphere, taking into account an essential parameter - the deposition rate of fine particles w_g consider a mathematical model describing on the basis of the law of hydromechanics using a multidimensional differential equation in partial derivatives [11-13]

$$\frac{\partial\theta}{\partial t}+u\frac{\partial\theta}{\partial x}+v\frac{\partial\theta}{\partial x}+\left(w-w_g\right)\frac{\partial\theta}{\partial z}+$$
$$+\sigma\theta=\mu\left(\frac{\partial^2\theta}{\partial x^2}+\frac{\partial^2\theta}{\partial y^2}\right)+\frac{\partial}{\partial z}\left(k\frac{\partial\theta}{\partial z}\right)+\delta_{i,j}Q; \qquad (1)$$

$$\frac{\partial w_g}{\partial t}=\frac{m\cdot g-6\cdot\pi\cdot k\cdot r\cdot w_g-0,5\cdot c\cdot\rho\cdot s\cdot w_g^2}{m} \qquad (2)$$

and the corresponding initial and boundary conditions:

$$\theta(x,y,z,t)\big|_{t=0}=\theta^0(x,y,z);\quad \mathrm{w_g}(0)\big|_{t=0}=w_g^0\ ; \qquad (3)$$

$$\left.\frac{\partial\theta}{\partial x}\right|_{x=0}=\mu\left(\theta_t-\theta\right);\quad \left.\frac{\partial\theta}{\partial x}\right|_{x=Lx}=\mu\left(\theta_t-\theta\right); \qquad (4)$$

$$\left.\frac{\partial\theta}{\partial y}\right|_{y=0}=\mu\left(\theta_t-\theta\right);\quad \left.\frac{\partial\theta}{\partial y}\right|_{y=Ly}=\mu\left(\theta_t-\theta\right); \qquad (5)$$

$$\left.k\frac{\partial\theta}{\partial z}\right|_{z=0}=\beta\cdot\theta-f_0(x);\quad \left.\frac{\partial\theta}{\partial z}\right|_{z=H_z}= \qquad (6)$$
$$=k\left(\theta_t-\theta\right)0.$$

Here θ - the concentration of harmful substances in the atmosphere; θ_0 - primary concentration of harmful substances in the atmosphere; x, y, z - coordinate system; u, v, w - wind speed in three directions; w_g - particle settling rate; σ - coefficient of absorption of harmful substances in the atmosphere; μ , λ - coefficients of diffusion and turbulence; Q - source power; $\delta_{i,j}$ - Dirac function; f_0 - source of emission of harmful substances into the atmosphere; c - dimensionless value is equal to 0.5; ρ atmospheric density; r is the particle radius; S is the cross-sectional area of particles; g is the acceleration of gravity.

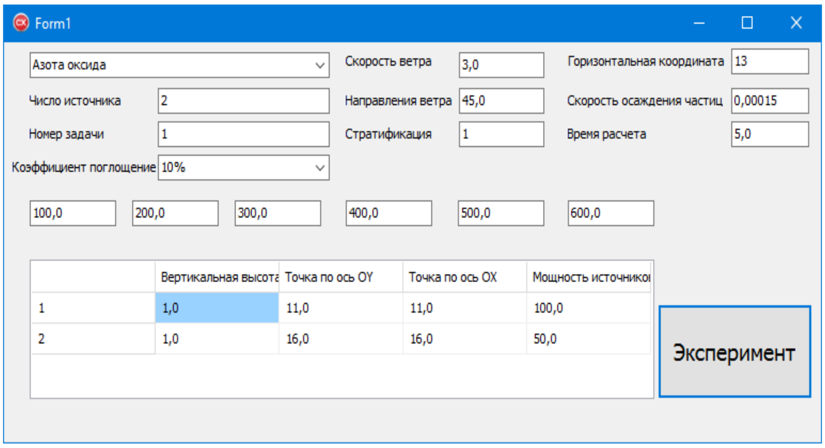
Methods for solving the problem

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.



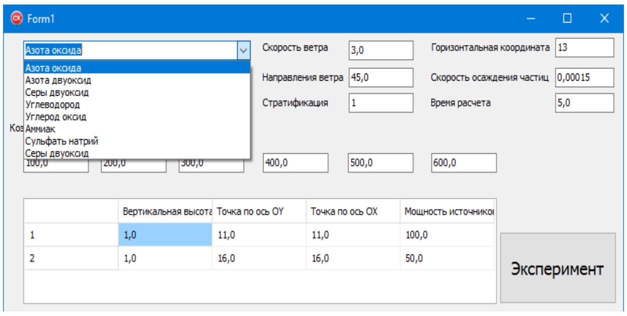
Азота оксида

Число источника: 2
Номер задачи: 1
Коэффициент поглощение: 10%
Скорость ветра: 3,0
Направления ветра: 45,0
Стратификация: 1
Горизонтальная координата: 13
Скорость осаждения частиц: 0,00015
Время расчета: 5,0

100,0 200,0 300,0 400,0 500,0 600,0

	Вертикальная высота	Точка по ось OY	Точка по ось OX	Мощность источникоі
1	1,0	11,0	11,0	100,0
2	1,0	16,0	16,0	50,0

Fig.1. Form for entering the main process parameters



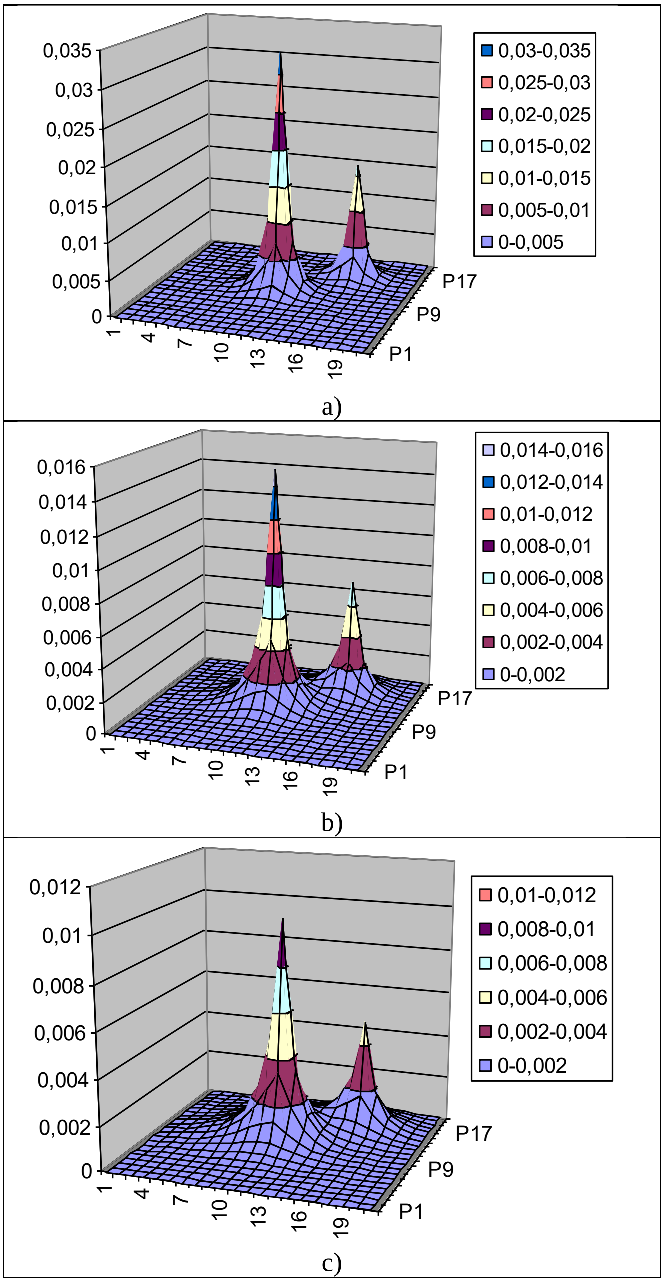
Скорость ветра 3,0
Напрвления ветра 45,0
Стратификация 1
Горизонтальная координата 13
Скорость осаждения частиц 0,00015
Время расчета 5,0

100,0 200,0 300,0 400,0 500,0 600,0

	Вертикальная высота	Точка по ось OY	Точка по ось OX	Мощность источнико
1	1,0	11,0	11,0	100,0
2	1,0	16,0	16,0	50,0

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.



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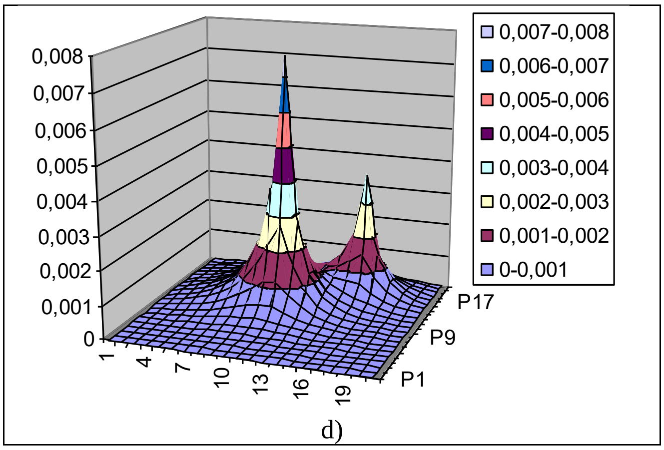
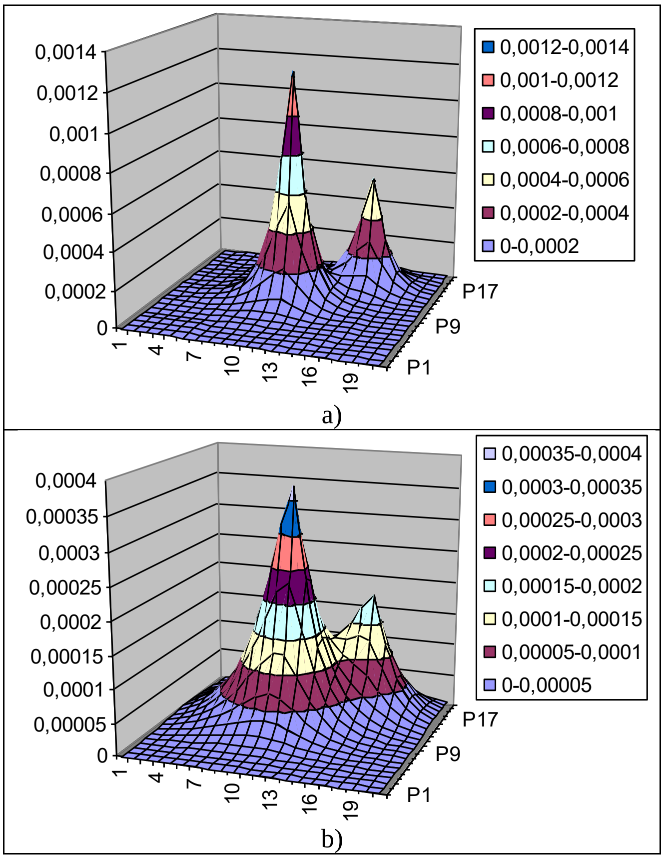


d)

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.***

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.



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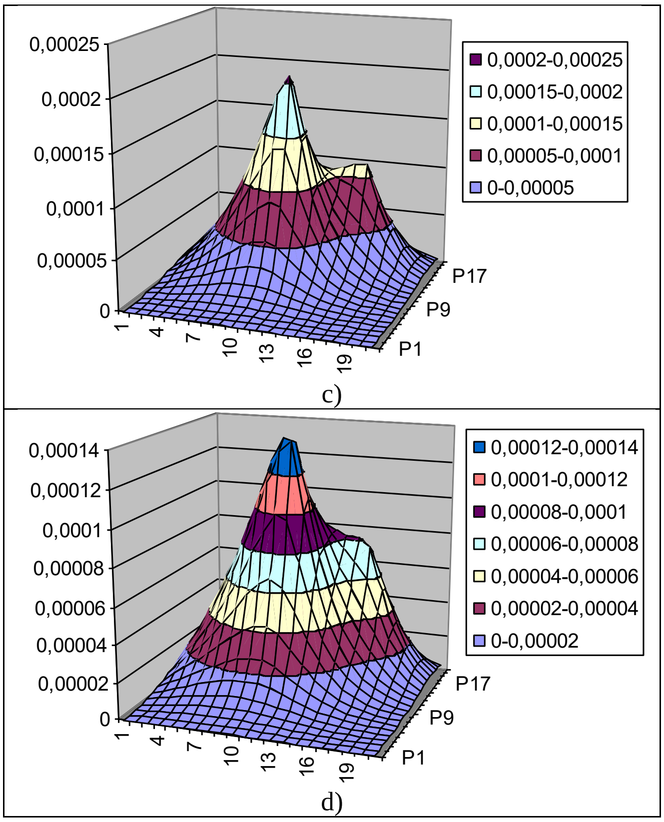
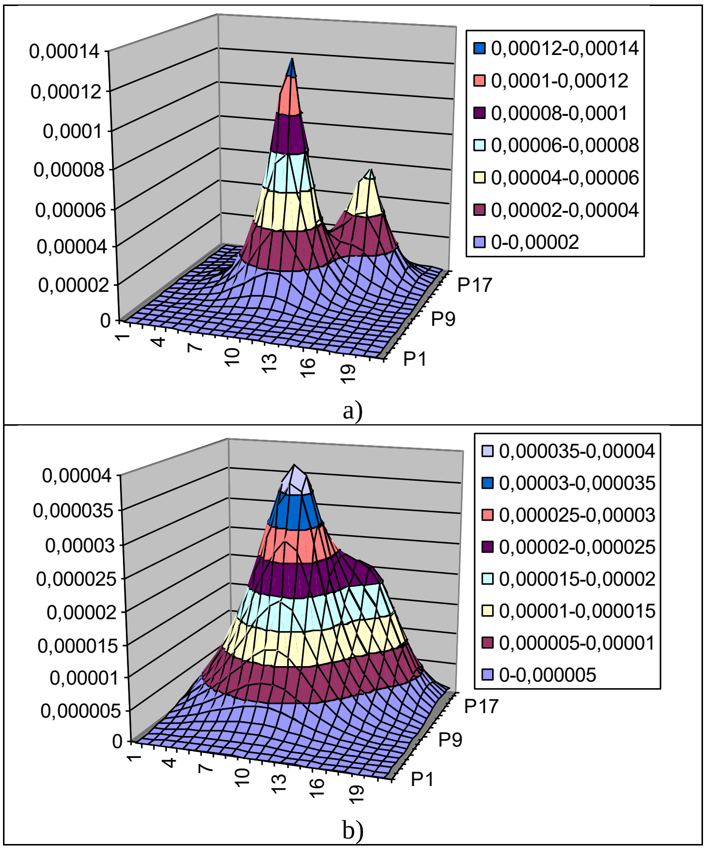
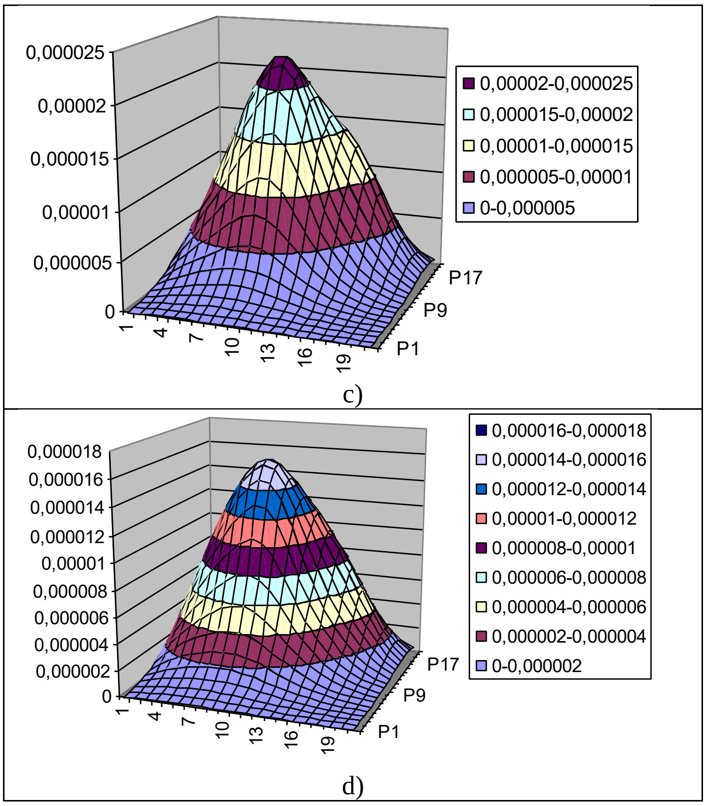


Fig.4. Change in the concentration of harmful substances in the first layer of the atmosphere (H = 200m) at wind speed: ***a) u = 1 m/s.; b) u = 3 m/s; c) u = 4 m/s; d) u = 5 m/s.***

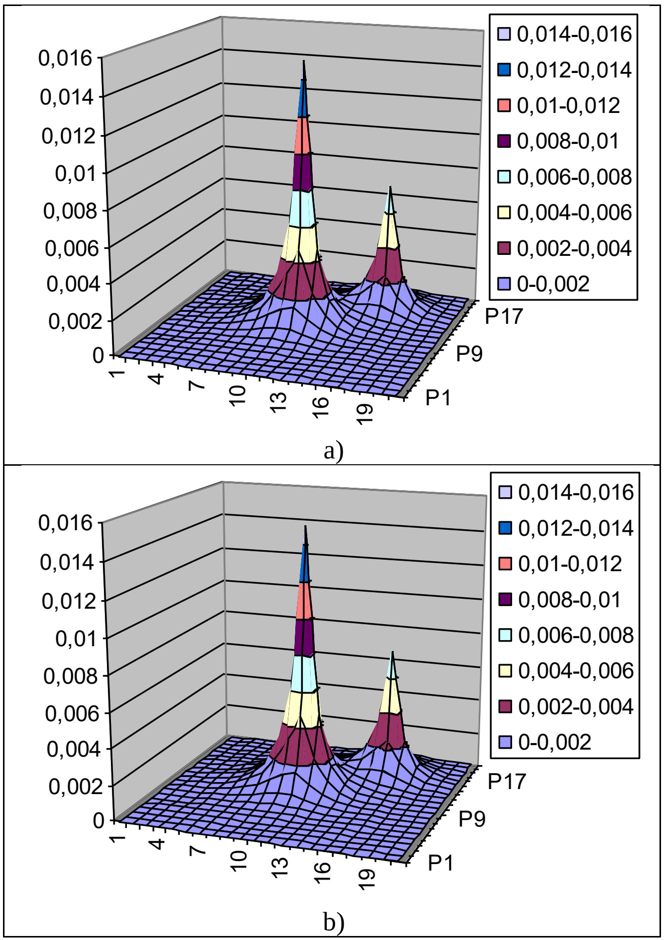




c)

d)

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.*



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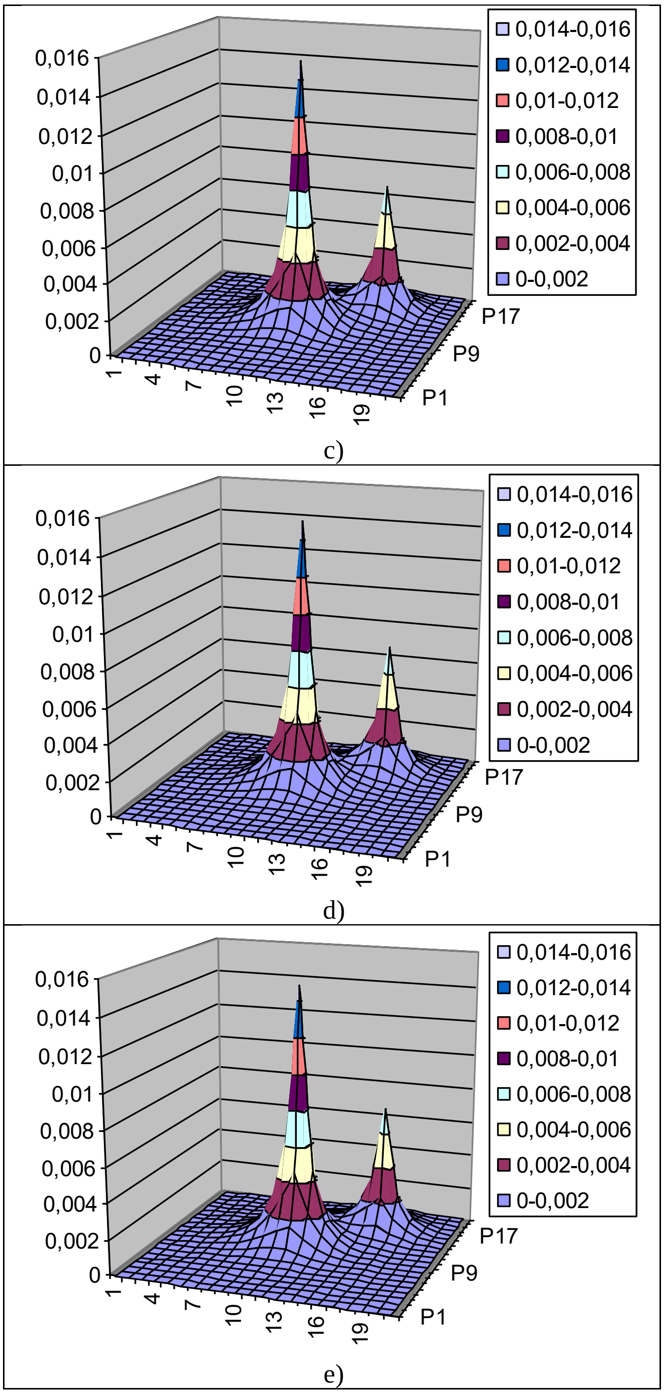

c)

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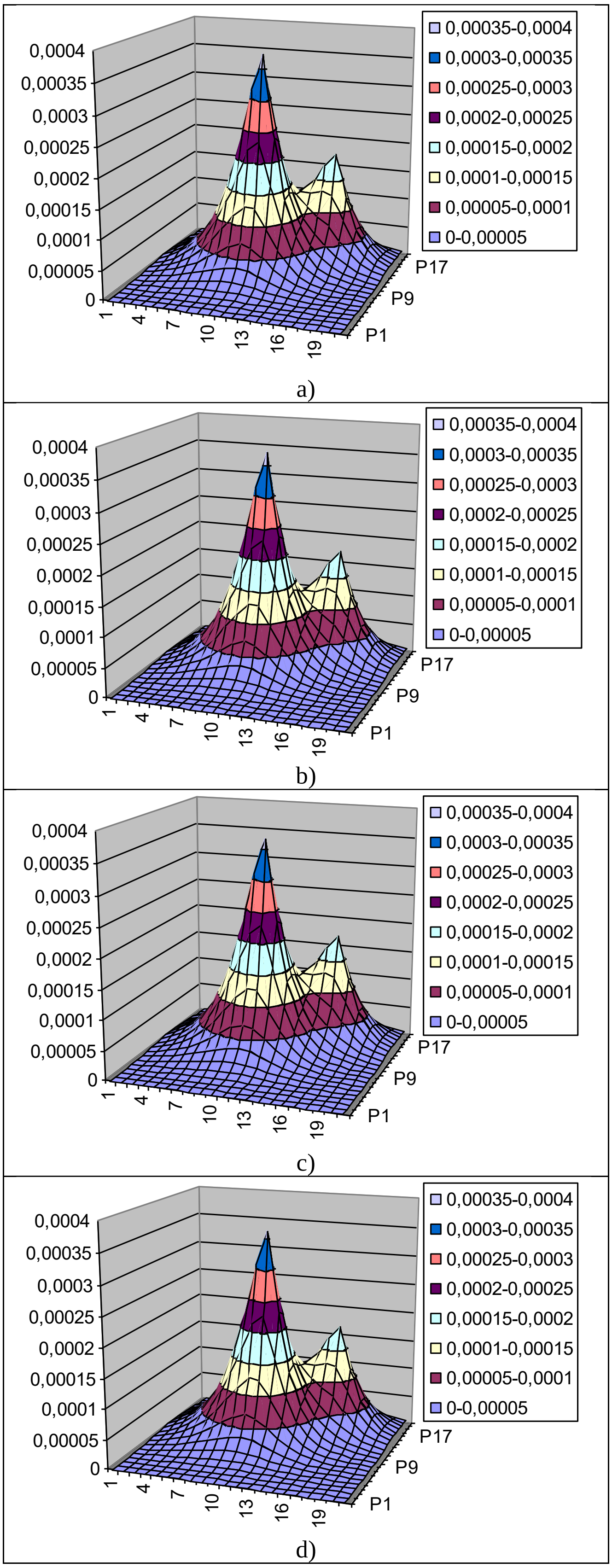
e)

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.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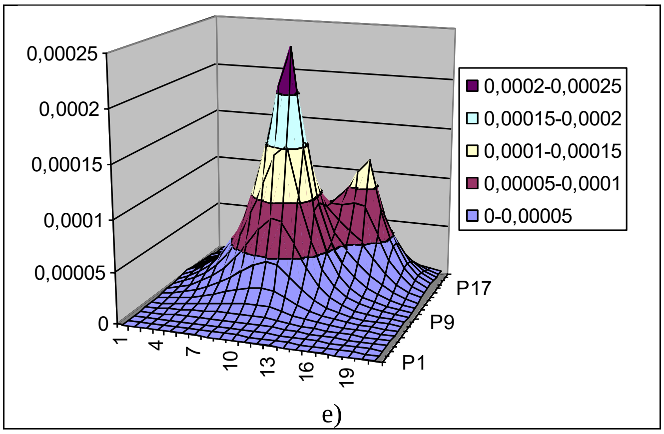
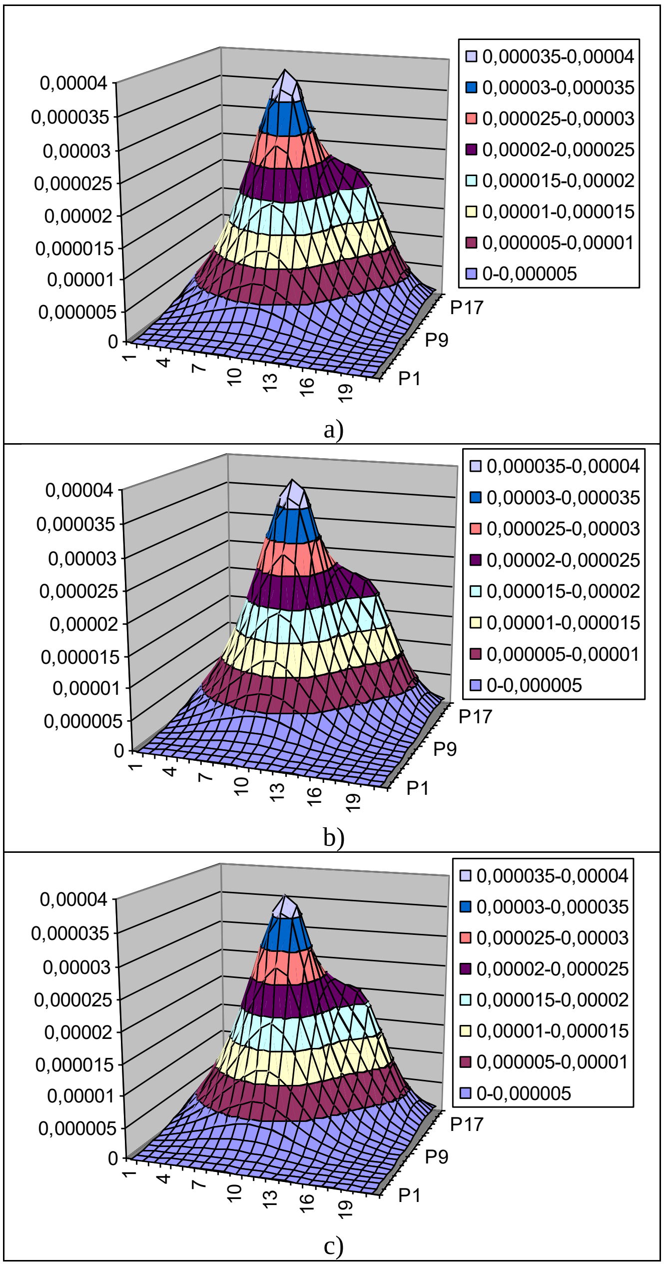


e)

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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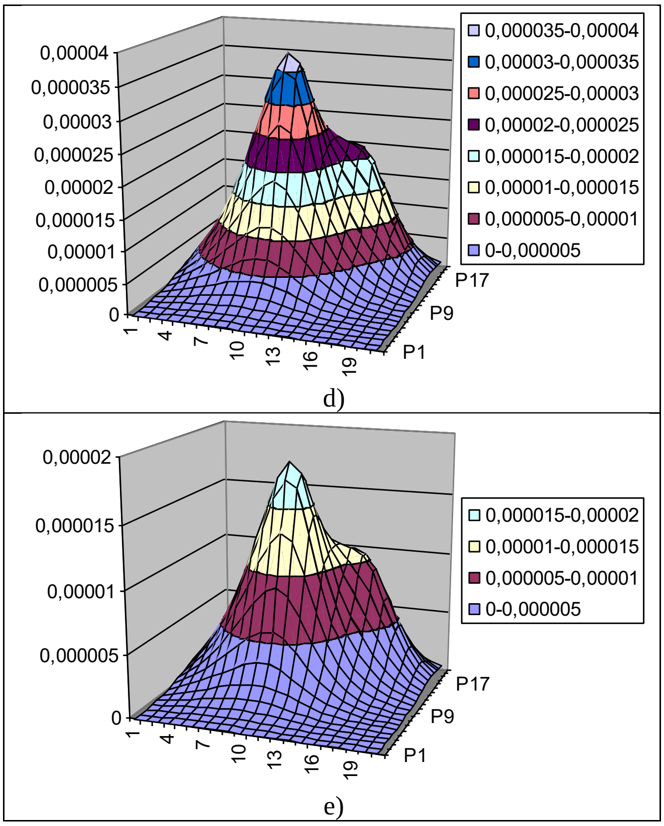

d)

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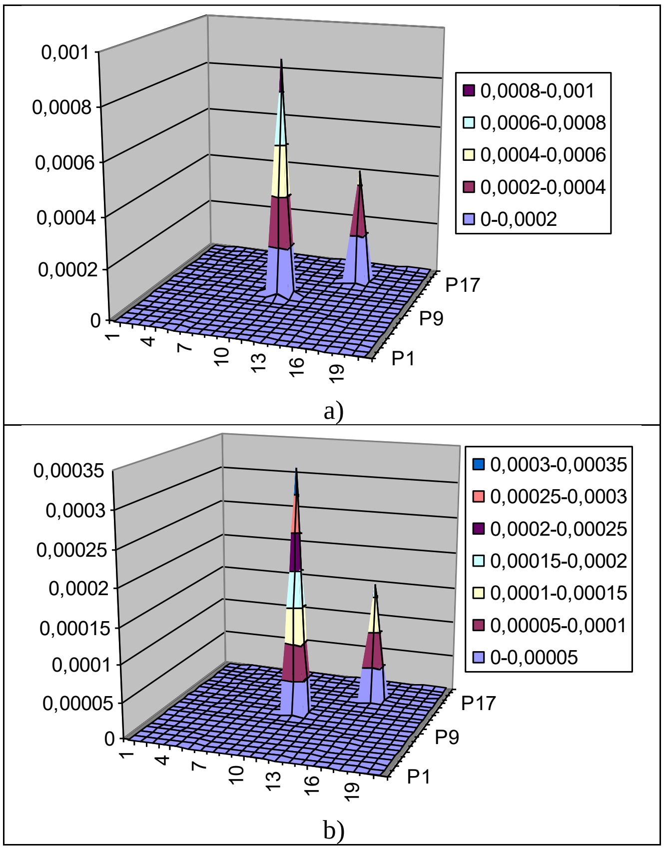
Fig.8. Change in the concentration of harmful substances in the third layer of the atmosphere (H=300m) at the initial particle settling velocity: ***a)*** $w_g = 0.00015$ ***m/s; b)*** $w_g = 0.0003$ ***m/s; c)*** w_g ***\u003d 0.0006 m / s .;***
d) $w_g = 0.0009$ ***m/s; e)*** $w_g = 0.009$ ***m/s.***



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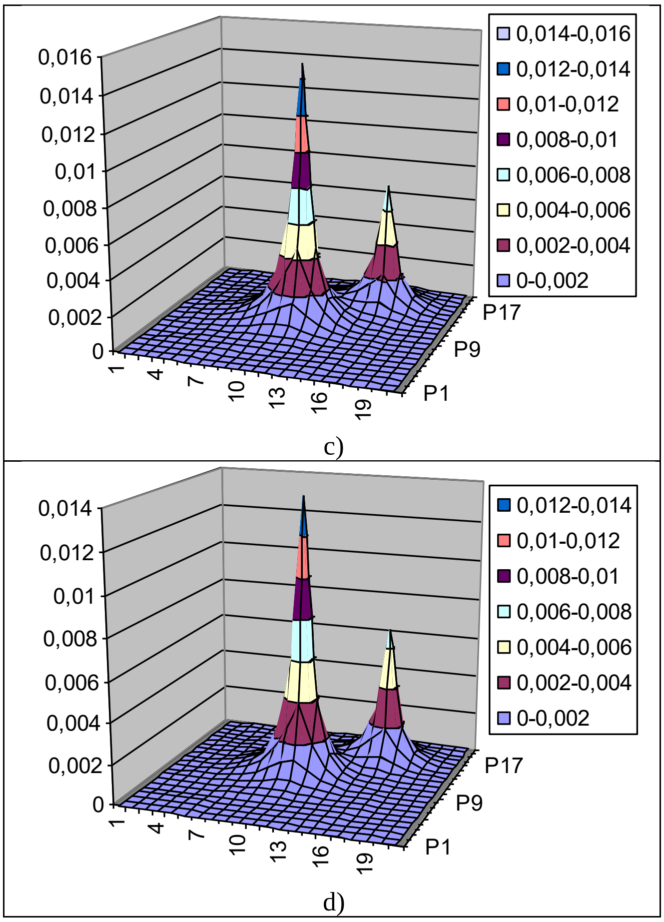
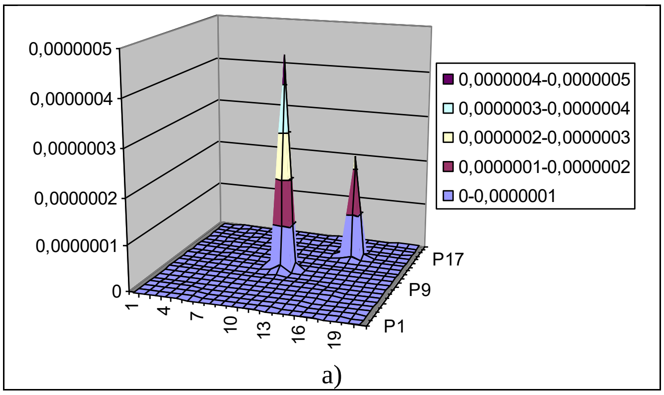


c)

d)

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%.

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].



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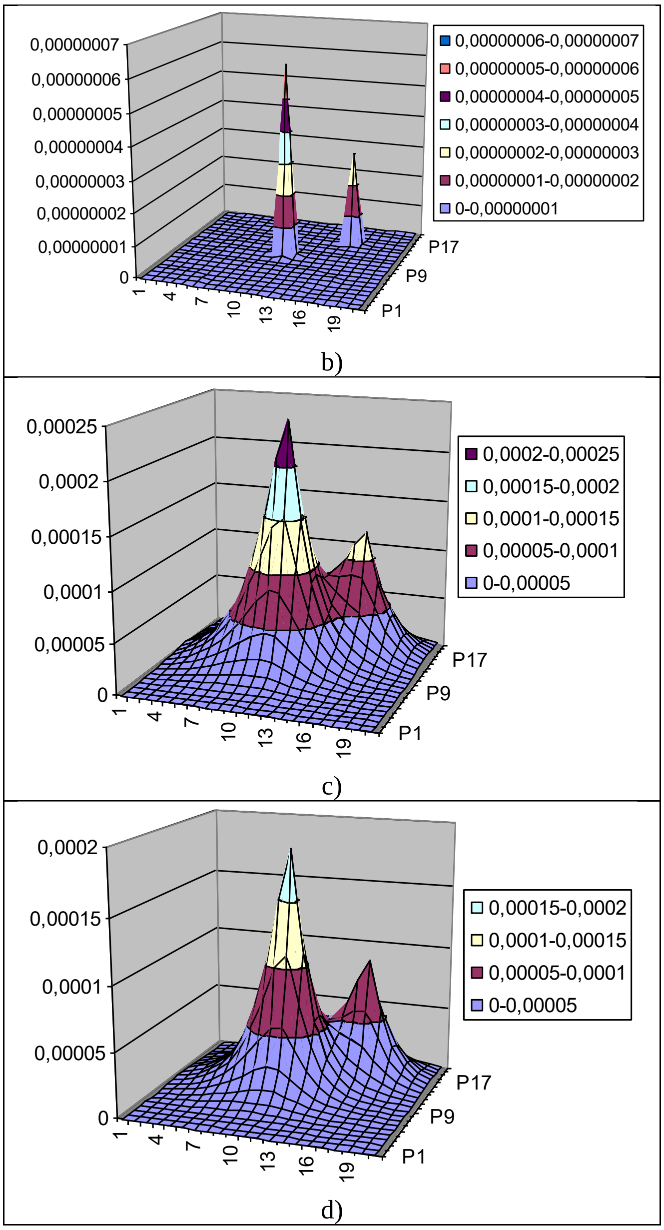
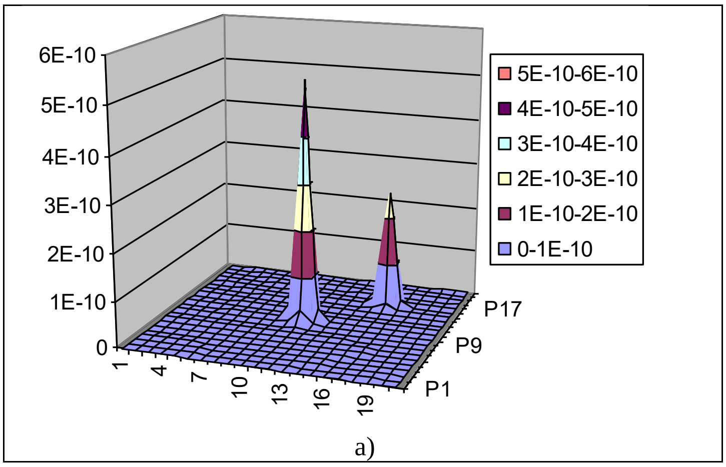


b)

c)

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%.*



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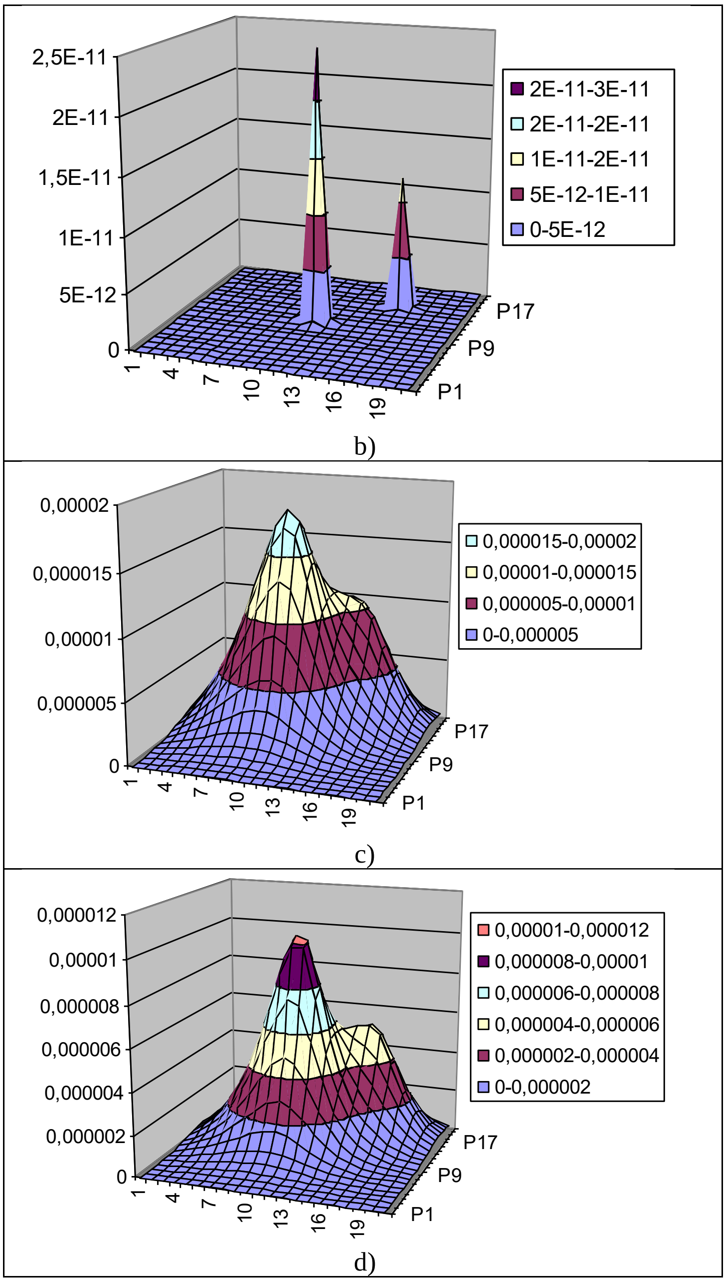

b)

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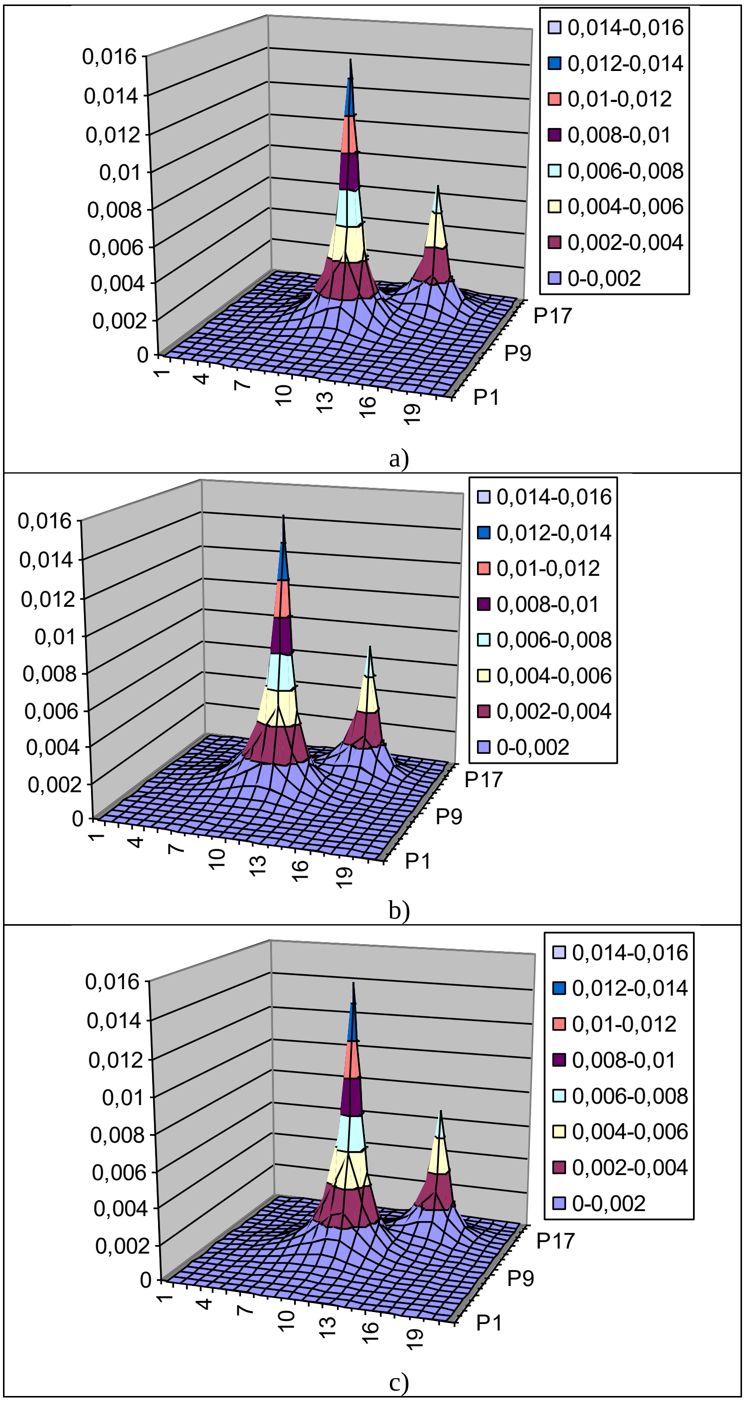
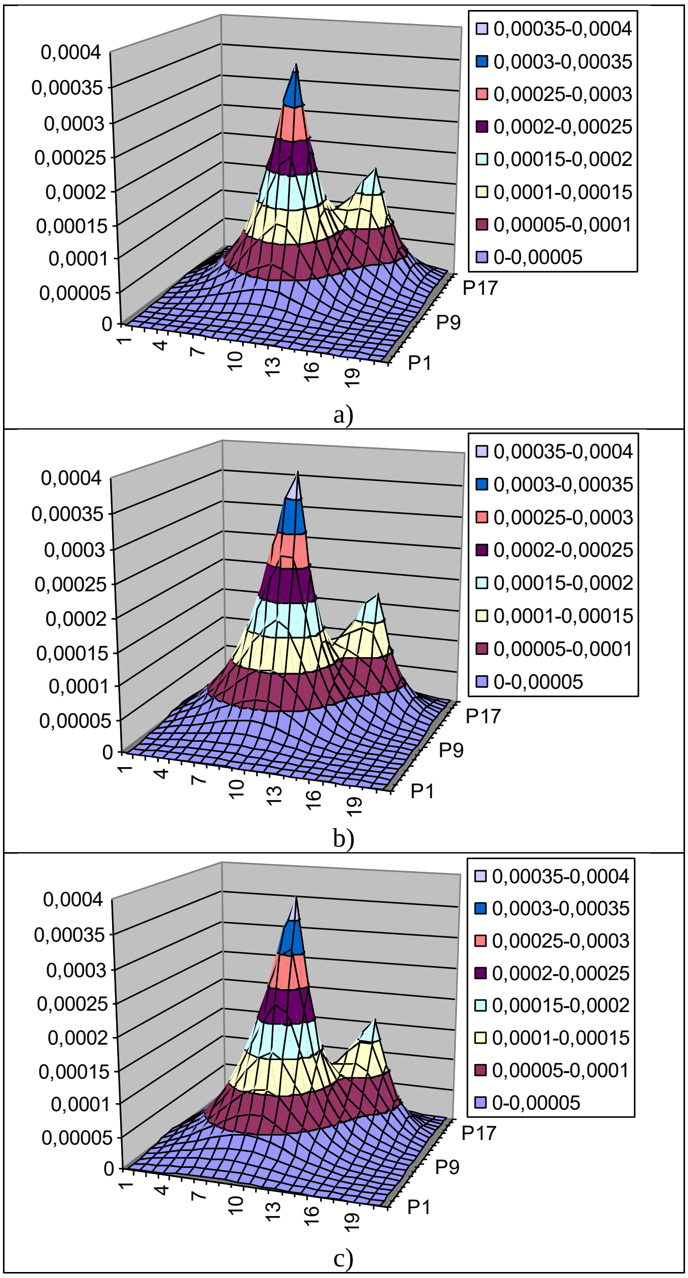
Fig.11. Change in the concentration of harmful substances in the third layer of the atmosphere (H=300m) for different values of the absorption coefficient
a) σ = 10%; b) σ = 20%; c) σ = 30%; d) σ = 40%.



a)
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).



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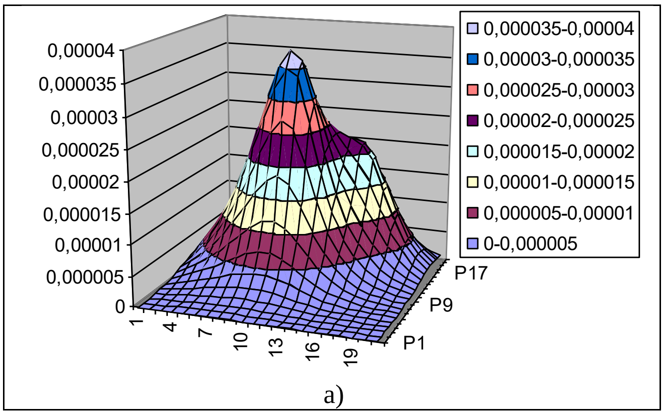
b)

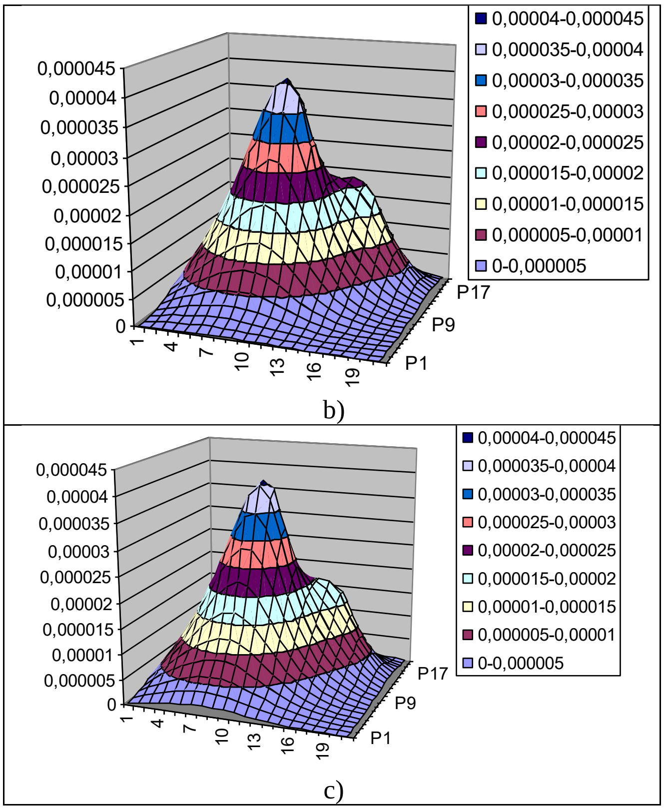
c)

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.

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