MATHEMATICAL MODELING OF TRANSFER OF HARMFUL EMISSIONS TO THE ENVIRONMENT

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The work is devoted to topical problems of studying the statistical characteristics of vortex structures. The intensities of turbulent velocity pulsations are considered in the mathematical description of turbulent pulsations. Statistical-phenomenological theories of turbulent transport are used. Using the probable-statistical model, various options for calculating the trajectories of gas impurity particles in a turbulent flow are performed. The concentration of harmful gas impurities is calculated. The dynamics of the changes occurring in the admixture is assessed. The intensities of turbulent pulsations in the corresponding directions are determined. Methodical calculations of the transport of gas impurities from point and linear sources are performed. The results of calculations of the transfer of harmful gas impurities from linear sources on a horizontal section are demonstrated.

Keywords:*turbulent motion, atmosphere, gas impurities, chaotic pulsations, turbulent diffusion, disordered process, flow core, equation of motion, hydraulic resistance, vortex flow.*

Introduction. The atmosphere, as the gaseous envelope of the planet, is a particularly complex turbulent and dynamic system in which various dynamic and physicochemical processes are constantly taking place. Mathematical modeling of the nonstationarity and constant variability of both the gaseous and aerosol composition of the atmosphere, as well as the assessment of the impact of atmospheric impurities on the environment, become problematic issues when describing the transport of harmful impurities in the atmosphere.

The turbulent motion of the atmosphere is characterized by characteristic random and chaotic pulsations of the velocity vector at all points of the flow and in all directions, which impart a stochastic character of changes for all ongoing processes. The formation of specific turbulent diffusion and random intensive mixing are a direct consequence of chaotic pulsating movements, which to a greater extent exceed the molecular turbulent viscosity of the gas and a more uniform flow, compared to laminar flow, the distribution of the average velocity occurs and even its sharp decrease in the region of the wall, and also a large increase in friction losses.

Purpose of work: For this purpose, it is required to develop models of the dynamic variability of the composition of the atmosphere. At the same time, the applied statistical theory will require preliminary data on the turbulent characteristics of the air flow. Proceeding from this, the most widespread in theory and practice began to receive statistical and phenomenological theories of turbulent transfer, which characterize themselves by scale and intensity, or otherwise, by the kinetic energy of pulsating motion and the rate of transition to energy of disordered processes. Along with the system of equations for the averaged turbulent flow, to describe the processes of turbulent transfer, the system of equations for the balance of pulsation energy is also involved, and additional hypotheses are accepted to ensure the closure of all equations of the system.

Main results. Most often it is assumed that stochastic motion can be determined only by the turbulence of the flow, and the mutual influence of their particles can be neglected. At the same time, to determine the diffusion behavior and the coefficient of turbulent diffusion of particles, due to the complex turbulent structure of the flow, depending on the parameters of this flow and the characteristics of its particles, significant simplifying assumptions are made. In addition, it is customary to use assumptions about the observed isotropic turbulence, which are confirmed with a satisfactory degree of accuracy by the data of experimental studies under normal conditions.

The main disadvantage for all diffusion models is the assumption of the homogeneity of the existing field of turbulent pulsations acting in all directions, moreover, the current character of the dispersed phase movement in the investigated turbulent flow is probable stochastic in nature, and all attempts to describe it by deterministic dependences will significantly reduce the quality capabilities of the analysis and the effectiveness of management decisions. As practice shows, in most cases, the use of deterministic methods makes it possible to determine only averaged or approximate values of the parameters and characteristics of the process, which quite often leads to the need to include empirical coefficients in the system of equations or to reduce the level of accuracy in calculations. The use of diffusion models leads, in addition, to the need to introduce indefinite coefficients of effective diffusion or longitudinal mixing that do not have a clear physical meaning.

The main reason for causing turbulent pulsation in the gas flow is its local emissions from the unstable zone of the near-wall region with a significant level of velocity gradient significance and periodicity. Such local ejections generate vortices that are directed into the flow core and thereby additionally stimulate the formation of new ejections. The comparability of the scale of primary vortices is similar to the scale of a gas flow, and its velocity is comparable to the flow velocity, but at the same time its frequency is comparatively low. The movement of large eddies, in a turbulent flow, has a very low stability and along the way can generate other smaller local eddies, and then even smaller ones, and so on down to the smallest ones. The flow inside the smallest vortices is laminar. It should be noted that the general direction of the gas flow does not affect the motion of small-scale vortices, i.e. the pulsations are practically isotropic and all directions are equally probable, and the pulsation frequency for these conditions is maximum and constant [1].

Substitution of expressions into the system of Navier-Stokes motion equations and by averaging over space and time leads to a system of Reynolds motion equations, which include additional tangential stresses that cause an increase in hydraulic resistance and viscosity. Empirical or statistical theories of turbulence are used to achieve the closure of a system of equations, and analogies between molecular and turbulent stresses are also applied, where experimental data on statistical relationships between pulsations in time and space are involved.

For any point of the gas flow, the instantaneous velocity of the atmosphere in each direction of propagation is represented as the sum of the average velocity and the velocity of pulsations:

$$u = \overline{u} + u^{'} \ , \quad v = \overline{v} + v^{'} \ , \quad w = \overline{w} + w' \ , \qquad (1)$$

The level of significance of the speed of turbulent pulsations determines the speed of friction (dynamic speed) - the average value of the transverse and longitudinal velocities that make up the total speed of the pulsations:

$$\omega^* = \sqrt{(\omega_z' \omega_y')} = \sqrt{\tau_0/\rho} \qquad (2)$$

The turbulence scaling parameter demonstrates less the average than the more probable dimension of turbulent eddies. In a deployed turbulent gas flow, the maximum fluctuation scaling parameter is comparable to the characteristic diameter (size) of the channel$l_{max} \sim D$, and the minimum is determined by the prevailing conditions for the viscous dissipation of a part of the kinetic energy of the pulsation $l_{min} \sim R/Re^{0,75}$. Experimental studies of the spectrum of transverse and longitudinal velocities of turbulent pulsations demonstrate that those turbulent pulsations are very likely for which the velocity is proportional to the gas flow velocity.

In the applied semi-empirical theory of turbulence, the concept of a mixing (mixing) path is involved, i.e. this is the distance at which the turbulent vortex begins to lose its integrity. When analyzing turbulent viscosity near the wall, the resulting mixing path length -l_m is most often proportional to the distance to the wall - ($l_m = k^* y$), where the coefficient of turbulence or turbulent structure k^* (proportionality coefficient) is taken $k^* \approx 0{,}4$or is found empirically. The number of changes in the amplitude values of the pulsation velocity per unit of time characterizes the frequency of turbulent pulsations. The generated statistical characteristics for medium-frequency turbulence do not depend on the viscosity and density of the medium; they depend on the rate of energy dissipation. The calculation of the lower limit of the frequency of large-scale turbulent pulsations of scale D:

$$\omega_0 \approx \omega_{cp}/D \quad (3)$$

For the general case, the speed of the pulsating motion of the gaseous medium is calculated using the Fourier integral formula [2,3]

$$\omega'(t) = \int_0^\infty (A\cos\omega t + B\sin\omega t)d\omega, \quad (4)$$

where ω is the value of the angular frequency of turbulent pulsations, c^{-1}; A and B - coefficients:

$$A = \frac{1}{\pi}\int_{-\infty}^{+\infty} \omega' \cos\omega t dt, \;\; B = \frac{1}{\pi}\int_{-\infty}^{+\infty} \omega' \sin\omega t dt, \quad (5)$$

However, in the formulaic representation of turbulent pulsations, the dynamics of changes in the velocity of the pulsating motion of a medium in all directions is usually represented by a monoharmonic function

$$\omega'(t) = W \cdot sin(\omega t) \quad (6)$$

where W is the amplitude of the pulsation velocity, m / s [3].

Let us carry out a numerical implementation of a probable-statistical modeling on the spread of harmful gas impurities from vehicles in the atmosphere of an urban conglomerate.
An impurity particle can move in the atmosphere together with the gas flows of air under the influence of external forces, and due to turbulent diffusion under the influence of turbulent pulsations of the atmospheric flow. Consequently, the resulting trajectory of the impurity particles can be considered as a general total random path. Then, at any moment in time, any of its coordinates can be calculated as the sum of the random and deterministic components [4,5]:

$$x(t) = \int_0^t u_x(t)dt + x'(t) \quad (7)$$

where is the time projection of the deterministic velocity, m / s; $x'(t)$ is a random process.

When considering the movement of a gas impurity particle as repeated jump-like movements with length at small time intervals in one of the degrees of freedom of movement in an orthogonal coordinate system, then the resulting trajectory of particle motion will be a three-dimensional broken curve, and the vector of the direction of movement at each moment of time will be probabilistic characteristics $p_i : p_{+x}, p_{-x}, p_{+y}, p_{-y}, p_{+z}, p_{-z}$. Then it will become obvious that at any time:

$$p_{+x}(t) + p_{-x}(t) + p_{+y}(t) + p_{-y}(t) + p_{+z}(t) + p_{-z}(t) = 1 \quad (8)$$

Under the influence of external forces in isotropic turbulence and in the absence of convective motion, when a gas impurity particle makes only random movements, all probabilities are the same and the vector directions of displacement are equally probable:

$$p_{+x}(t)=p_{-x}(t)=p_{+y}(t)=p_{-y}(t)=p_{+z}(t)=p_{-z}(t)=\frac{1}{6}$$

Let us consider the process of transfer of one particle of a gas impurity from a point source. Let's assume that the wind direction coincides with the Ox axis. In this case, you can go to a two-dimensional xOz coordinate system and at each moment of time consider the motion of particles of a gas impurity in only one of four possible directions. Then, the probabilities of each direction will be p_{+x}, p_{-x}, p_{+z} and $p_{-z}(p_{+x}(t)+p_{-x}(t)+p_{+z}(t)+p_{-z}(t)=1)$.

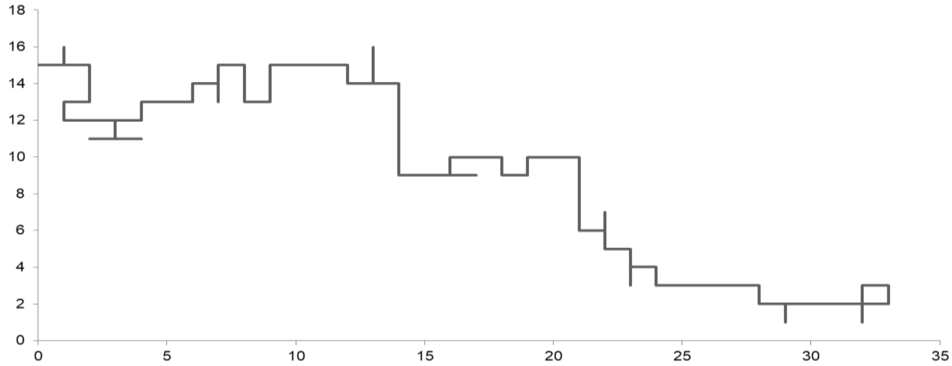

Figure 1 - Variants of calculating the trajectory of one particle of gas impurity in a turbulent flow

($p_{+x}=0.7,\ p_{-x}=p_{+y}=p_{-y}=0.1$ (100 steps))

Obviously, with isotropic turbulence and in the absence of wind $p_{+x}=p_{-x}=p_{+z}=p_{-z}=1/4$. In the case of the presence of a wind effect coinciding with the direction of the axis, this influence can be expressed by the ratio of the corresponding probabilities of the directions of movement, i.e. with isotropic turbulence in a stationary coordinate system and an upward flow $p_{+x}\succ p_{-x}=p_{+z}=p_{-z}$.

With the known values of the random number generator and probabilities p_i, using the above-described probable-statistical model, Figures 1 and 2, respectively, reflect the variants of the results of calculating the possible trajectories of one and ten particles of a gas impurity in a turbulent flow.

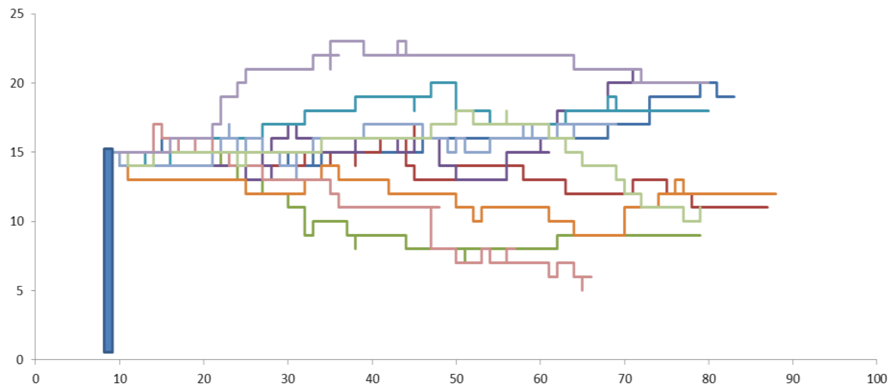

Figure 2 - Variants of calculating the possible trajectories of ten gas particles take in a turbulent flow ($p_{+x}=0.7,\ p_{-x}=p_{+y}=p_{-y}=0.1$ (10x100 steps))

It should be noted that when there are many emissions and many sources of pollutants, this approach will make the calculation difficult. Therefore, in every time interval, any particle can stay in one of such grid nodes and any of these positions should be perceived as a probabilistic state of a particle at a time with a corresponding probability $P(i, j, t)$ (i, j - numbers of grid nodes) [7].

Let us imagine that we have obtained the probabilities of all possible positions of the particle at a certain moment of time t, and analyze the dynamics of the change in the probability of the particle being in a certain position (i, j) after a short time period Δt.

The probability of a particle $P(i, j, t+\Delta t)$ at an instant of time $t+\Delta t$ is determined in two cases: the first is when they flow from the position (i, j) into neighboring nodes (,, and); the second, when they flow in from neighboring nodes ($(i-1, j)$, $(i+1, j)$, $(i, j-1)$ and $(i, j+1)$) (Figure 3). It can be assumed that in any time period $t+\Delta t$, in the position (i, j), the probable direction of the particle transition $p^{n+1}_{l,i,j}$ ($l=+x,-x,+z,-z$) is determined, and, accordingly, what follows is subtracted, and what flows in is added [8].

Therefore, the final equation for determining the probability of finding a particle in a position (i, j) at a certain point in time $t+\Delta t$ looks like this:

$$P^{n+1}_{i,j} = P^n_{i,j} + p^{n+1}_{+x,i,j}P^n_{i-1,j} + p^{n+1}_{-x,i,j}P^n_{i+1,j} + p^{n+1}_{+z,i,j}P^n_{i,j-1} + p^{n+1}_{-z,i,j}P^n_{i,j+1} - \left(p^{n+1}_{+x,i,j} + p^{n+1}_{-x,i,j} + p^{n+1}_{+z,i,j} + p^{n+1}_{-z,i,j}\right)P^n_{i,j} \quad (9)$$

Where $P^{n+1}_{i,j}$ is the probability of finding a particle at a certain moment in time $t+\Delta t$ in a position (i, j), $p^{n+1}_{+x,i,j}$ is the probability of transitions to the corresponding position (i, j) at a moment in time $t+\Delta t$ from position (i, j) [4].

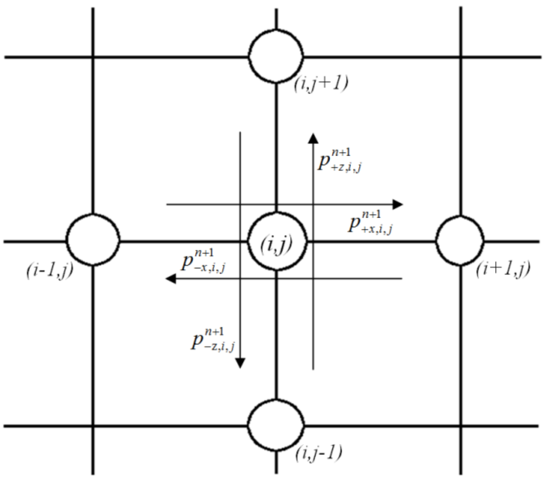

Figure 3 - Diagrams of the directions of particle transitions

$$p^{n+1}_{l,i,j} = 1 - \exp[-\mu_l(i, j)\Delta t] \approx 1 - [1 - \mu_l(i, j)\Delta t] = \mu_l(i, j)\Delta t \quad (10)$$

Where μ_l ($l=+x,-x,+z,-z$) - the intensity of transitions in a turbulent flow, which are determined by the level of intensity of turbulent pulsations, c^{-1}.

Analogs of these approximations can be written for all other transitions, performing the appropriate designations $\mu_{l,i,j}$. In this case, equation (9) will take the form:

$$\begin{aligned} P^{n+1}_{i,j} &= P^n_{i,j} + \mu_{+x,i,j}\Delta t P^n_{i-1,j} + \mu_{-x,i,j}\Delta t P^n_{i+1,j} + \mu_{+z,i,j}\Delta t P^n_{i,j-1} + \\ &+ \mu_{-z,i,j}\Delta t P^n_{i,j+1} - \left(\mu_{+x,i,j} + \mu_{-x,i,j} + \mu_{+z,i,j} + \mu_{-z,i,j}\right)P^n_{i,j}\Delta t \end{aligned} \quad (11)$$

From expression (11) we obtain:

$$\frac{P_{i,j}^{n+1}-P_{i,j}^{n}}{\Delta t}=\mu_{+x,i,j}P_{i-1,j}^{n}+\mu_{-x,i,j}P_{i+1,j}^{n}+\mu_{+z,i,j}P_{i,j-1}^{n}+$$
$$+\mu_{-z,i,j}P_{i,j+1}^{n}-\left(\mu_{+x,i,j}+\mu_{-x,i,j}+\mu_{+z,i,j}+\mu_{-z,i,j}\right)P_{i,j}^{n} \quad (12)$$

Making the transition to the limit at $\Delta t \to 0$, we obtain a differential equation for the probability of finding a particle at a certain moment in time t at a point (i, j):

$$\frac{\partial P}{\partial t}=\mu_{+x,i,j}P_{i-1,j}^{n}+\mu_{-x,i,j}P_{i+1,j}^{n}+\mu_{+z,i,j}P_{i,j-1}^{n}+$$
$$+\mu_{-z,i,j}P_{i,j+1}^{n}-\left(\mu_{+x,i,j}+\mu_{-x,i,j}+\mu_{+z,i,j}+\mu_{-z,i,j}\right)P_{i,j}^{n} \quad (13)$$

In any position $P_{i,j}^{n}$, the probability of finding a single particle in accordance with the law of large numbers will simultaneously mean the fraction of particles $N(i, j,t)/N$ from their total number in the system, which are at the moment in time t in an elementary volume $V(i, j)$ of the cross section $h_x \times h_z$, i.e.:

$$P_{i,j}^{n}=\frac{N(i,j,t)}{N}=\varphi_{i,j}^{n}\frac{V(i,j)}{N} \quad (14)$$

Where $\varphi_{i,j}^{n}$ is the local numerical concentration of gas impurities, $м^{-3}$.
Substituting the equations, we get the following expression:

$$\frac{V(i,j)}{N}\frac{\partial\varphi}{\partial t}=\mu_{+x,i,j}\frac{V(i,j)}{N}\left(\varphi_{i-1,j}^{n}-\varphi_{i,j}^{n}\right)+\mu_{-x,i,j}\frac{V(i,j)}{N}\left(\varphi_{i+1,j}^{n}-\varphi_{i,j}^{n}\right)+$$
$$+\mu_{+z,i,j}\frac{V(i,j)}{N}\left(\varphi_{i,j-1}^{n}-\varphi_{i,j}^{n}\right)+\mu_{-z,i,j}\frac{V(i,j)}{N}\left(\varphi_{i,j+1}^{n}-\varphi_{i,j}^{n}\right) \quad (15)$$

Taking into account that the elementary volume and the total number of divisions are constant, we add a function that describes the sources of emissions of harmful substances into the resulting equation:

$$\frac{\partial\varphi}{\partial t}=\mu_{+x,i,j}\left(\varphi_{i-1,j}^{n}-\varphi_{i,j}^{n}\right)+\mu_{-x,i,j}\left(\varphi_{i+1,j}^{n}-\varphi_{i,j}^{n}\right)+\mu_{+z,i,j}\left(\varphi_{i,j-1}^{n}-\varphi_{i,j}^{n}\right)+\mu_{-z,i,j}\left(\varphi_{i,j+1}^{n}-\varphi_{i,j}^{n}\right)+f \quad (16)$$

where f is a function that describes the source of the emission of harmful substances.
For given initial and boundary conditions, the system of differential equations (16) makes it possible to calculate the concentration of harmful gas impurities and evaluate the dynamics of its change. Consider two types of boundary conditions: 1. free boundary; 2. solid wall. For a free boundary, we take those terms that go beyond the boundary. For example, at the border $x = X$:

$$\left.\frac{\partial\varphi}{\partial t}\right|_{x=X}=\mu_{+x,n_1,j}\left(\varphi_{n_1-1,j}^{n}-\varphi_{n_1,j}^{n}\right)+\mu_{-x,n_1,j}\left(-\varphi_{n_1,j}^{n}\right)+\mu_{+z,n_1,j}\left(\varphi_{n_1,j-1}^{n}-\varphi_{n_1,j}^{n}\right)+\mu_{-z,n_1,j}\left(\varphi_{n_1,j+1}^{n}-\varphi_{n_1,j}^{n}\right)+f$$
(17)

This will mean that the impurity flows out of the computational domain without hindrance, but does not flow in.

Then, if necessary, it is possible to calculate the volumes of impurities removed from the computational domain to determine the self-cleaning of the atmosphere by wind regimes.
If the boundary is a solid wall, for example, at the boundary $z = 0$:

$$\left.\frac{\partial \varphi}{\partial t}\right|_{z=0} = \mu_{+x,i,1}\left(\varphi_{i-1,1}^{n} - \varphi_{i,1}^{n}\right) + \mu_{-x,i,1}\left(\varphi_{i+1,1}^{n} - \varphi_{i,1}^{n}\right) + \mu_{+z,i,j}\left(-\varphi_{i,1}^{n}\right) + \mu_{-z,i,1}\left(\varphi_{i,2}^{n}\right) + f \qquad (18)$$

Then, the impurity does not flow out or flow in. Similarly, it is possible to obtain boundary conditions for all other boundaries of the considered area.
The calculated values of the intensity of transitions $\mu_{+x,i,j}, \mu_{-x,i,j}, \mu_{+z,i,j}$ and $\mu_{-z,i,j}$ are determined by the intensities of turbulent pulsations and deterministic velocities in the corresponding directions. The velocity of particles of gaseous impurities for any directions is calculated in the sum of the deterministic and random components:

$$u = \bar{u} + u' \qquad (19)$$

In this case, the total intensity of transitions along any of the axes is determined by the sum of the averaged deterministic velocity and turbulent pulsations.

$$\mu_{+x} = \bar{u}_x + \mu_{+x}, \ \mu_{-x} = \mu_{+z} = \mu_{-z}$$

In the computational realization of equations (16) from the intensity of transitions $\mu_{+x,i,j}, \mu_{-x,i,j}, \mu_{+z,i,j}$ and $\mu_{-z,i,j}$ only one of them takes the value 1, and the rest of 0. This approach will ensure the fulfillment of conditions (8). And the one that takes the value 1 is determined on the basis of the random number generator.
Using the probabilistic-stochastic model, let us carry out methodical calculations of the transfer of gas impurities from point and linear sources [9, 10].
Figures 4 and 5 reflect the effect of the high-speed wind regime on a point source. For example, at a wind speed of 3 m / s, the gas impurity displaces faster, not even having time to be involved in diffusion processes (Figure 4). At a wind speed of 1 m / s, the process of transport of gas impurities proceeds more slowly (Figure 5).

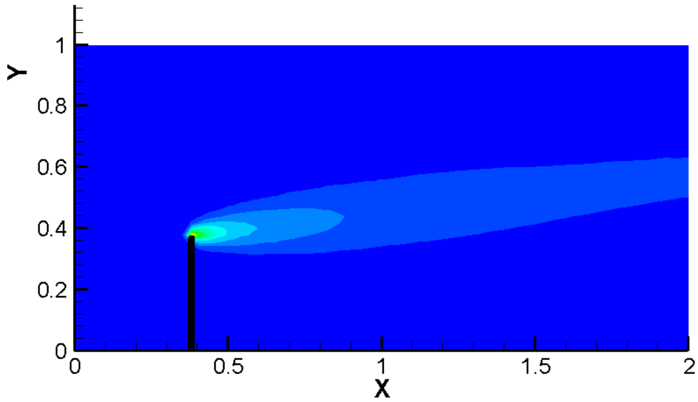

Figure 4 - Impact of high-speed wind conditions at speed wind 3m / s, point source

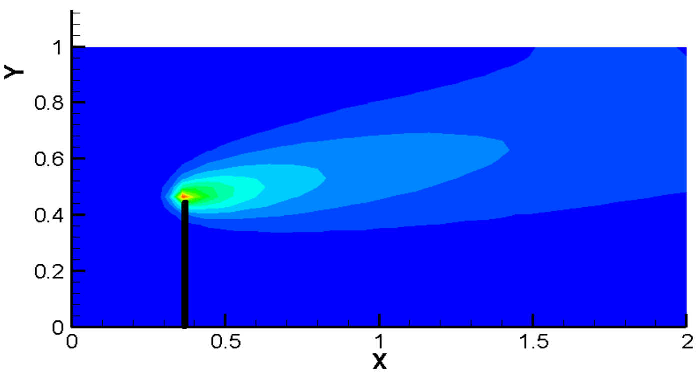

Figure 5 - Impact of high-speed wind conditions at speed
wind 1m / s, point source

Conclusion. Figures 6 and 7 show the results of calculations of the transfer of harmful gas impurities from linear sources on a horizontal section.

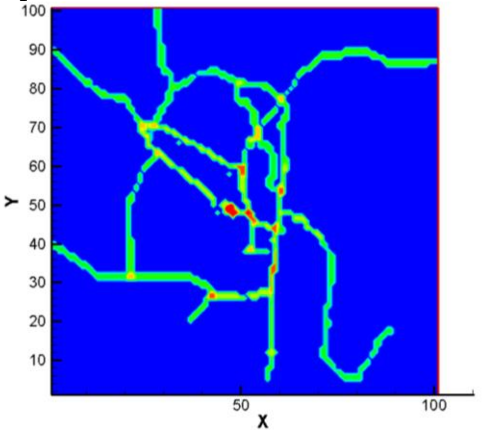

Figure 6 - Input data on the transport of harmful gas impurities
from line source

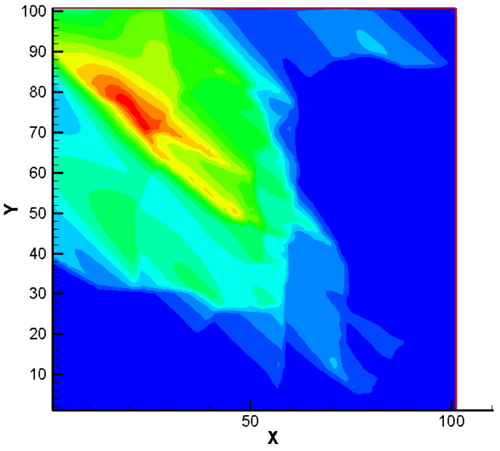

Figure 7 - The spread of harmful gas impurities from the linear
source at a wind speed of 5 m / s in the northwest direction

Thus, it can be stated that the use of even a simplified method of probabilistic-stochastic modeling provides good opportunities to build effective numerical algorithms for calculation, thereby significantly reducing the amount of calculations without losing their accuracy.

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