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Probabilistic and Statistical Modelling of the Harmful Transport Impurities in the Atmosphere from Motor Vehicles

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1. Introduction

Realization of the concept of sustainable development depends, among others, on preservation of the caring capacity of global environment. Transport contributes significantly to deterioration of the environment in two ways: rise of CO_2 emissions and thus accelerated climate change (Olejnik & Sobiecka 2017, Drastichowa 2017, Cel et al. 2016, Żukowska et al. 2016) and rising local concentration of particulate matter, mostly PM 2.5 and nitrogen oxides causing acid rain (Cao et al. 2016). Therefore, mitigation of the negative impact of the transport is of great importance.

One of the central problems of describing the transport of harmful impurities in the atmosphere is the mathematical modelling of the gas and aerosol composition variability in the atmosphere, as well as the assessment of the effect of atmospheric contaminants on the environment.

The atmosphere is a complex dynamic and turbulent system in which various dynamic and physicochemical processes occur.

For the turbulent flow of the atmosphere, chaotic random velocity pulsations are characteristic in all directions at all points of the flow, giving almost all stochastic processes to all the processes taking place. The consequence of chaotic pulsation motions is disorderly intensive mixing and specific turbulent diffusion, considerably exceeding the molecular, turbulent viscosity of the gas, more uniform than in laminar flow, the distribution of the averaged velocity and its sharp drop in the wall region, a sharp increase in friction losses.

2. Modelling

The instantaneous velocity of the atmosphere at any point of the flow in each direction can be represented as the sum of the averaged velocity and the velocity of pulsations:

$$u = \overline{u} + u', \quad v = \overline{v} + v', \quad u = \overline{w} + w' \tag{1}$$

The statement of these expressions in the Navier-Stokes equations of motion and averaging over time and space leads to the Reynolds equations of motion, which include additional tangential stresses,

Causing increased viscosity and hydraulic resistance. Statistical or semiempirical theories of turbulence are used to close the system of equations, an analogy between turbulent and molecular stresses is used, experimental data on the statistical relationships between pulsations in space and in time (Antonia & Luxton 1971, Betchov 1977, Riahi 2000). However, the use of the statistical theory requires preliminary information about the turbulent flow characteristics, therefore the statistical-phenomenological theories of turbulent transport that are characterized by the intensity and scale or kinetic energy of the pulsation motion and the rate of its dissipation have become most widespread (Tennekes & Lumley 1972, Simpson et al. 1990, Trunev 1996, Holt & Raman 1988). To describe the processes of turbulent transport, along with the equations of the averaged turbulent flow, the balance equations of the pulsating energy are applied, additional hypotheses are adopted for closing the system of equations (Hurley 1997, Hogstrom 1996).

It is usually assumed that the mutual influence of particles can be neglected and their stochastic motion is determined only by the turbulence of the flow (Castillo 1997, Swinney & Gollub 1981). Due to the complicated turbulent structure of the flow, considerable simplifying assumptions are made in determining the diffusion behaviour and the turbulent diffusion coefficient of the particles, depending on the flow parameters and particle characteristics. In addition, it is often assumed that isotropic turbulence which is satisfactorily confirmed under normal conditions by experimental data.

The main drawback of all diffusion models is the assumption that the field of turbulent pulsations is homogeneous in all directions, in addition, as already noted, the nature of the motion of a dispersed phase in a turbulent flow is probably stochastic, and attempts to describe it by deterministic dependencies significantly reduce the possibilities for analyzing and making managerial decisions . The use of deterministic methods in most cases makes it possible to determine only the approximate or averaged values of the parameters and characteristics of the process, which often leads to errors, a decrease in the accuracy of calculations, or the need for introducing empirical coefficients. And the use of diffusion models leads, in addition, to the necessity of introducing very vague coefficients of longitudinal mixing or effective diffusion, which do not have a clear physical meaning (Edward 1993, Paladin & Vulpiani 1986).

In this paper, we consider the numerical implementation of the probably statistical model described in (Sugak 2003) for modelling the distribution of harmful impurities in the atmosphere from vehicles using the example of the city of Ust-Kamenogorsk.

In the atmosphere, a particle of an impurity can move together with air currents or under the influence of external forces, or through turbulent diffusion under the influence of turbulent pulsations of the atmosphere. Accordingly, the trajectory of motion of impurity particles can be considered as a total random path: any of its coordinates at any time can be represented as the sum of the deterministic and random components:

$$x(t) = \int_0^t u_x(t)dt + x'(t), \qquad (2)$$

where $x(t)$ is the projection of the deterministic velocity, m/s and $x'(t)$ is Random process.

If we consider the motion of an impurity particle as a sequence of discontinuous displacements of length h in small intervals Δt in one of the six possible directions in an orthogonal coordinate system xyz, then the trajectory of motion will be a three-dimensional broken line, and the direction of motion at each instant of time will be determined by the corresponding probabilities: p_i: p_{+x}, p_{-x}, p_{+y}, p_{-y}, p_{+z}, p_{-z}.

It is obvious that at any time

$$p_{+x}(t)+p_{-x}(t)+p_{+y}(t)+p_{-y}(t)+p_{+z}(t)+p_{-z}(t)=1\,. \tag{3}$$

In the absence of convective motion and the influence of external forces, with isotropic turbulence, when a particle of an impurity performs only random movements, all directions of motion are equally probable and the probabilities are the same:

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

Let us consider the transfer of a single impurity particle from a point source (for example, from a tube of industrial enterprise). Let the wind direction coincide with the axis Ox. Then we can proceed to a two-dimensional coordinate system xOz, and at each instant of time consider the motion of impurity particles in one of four possible directions. And the probabilities of each direction will be p_{+x}, p_{-x}, p_{-z} and $p_{-z}\left(p_{+x}(t)+p_{-x}(t)+p_{+z}(t)+p_{-z}(t)=1\right)$.

Obviously, in the absence of wind and isotropic turbulence p_{+x} = p_{-x} = p_{+z}, = p_{-z} = 1/4. And in the presence of wind, with a direction coinciding with the axis, its influence can be expressed in terms of the ratio of the corresponding probabilities of the directions of motion: with ascending currents and isotropic turbulence in a fixed coordinate system $p_{+x}(t)\succ p_{-x}(t)=p_{+z}(t)=p_{-z}(t)$.

Using the above described model, for known values of probabilities p_i and a random number generator, variants of possible trajectories of one and ten impurity particles in a turbulent flow are calculated (Fig. 1 and Fig. 2, respectively).

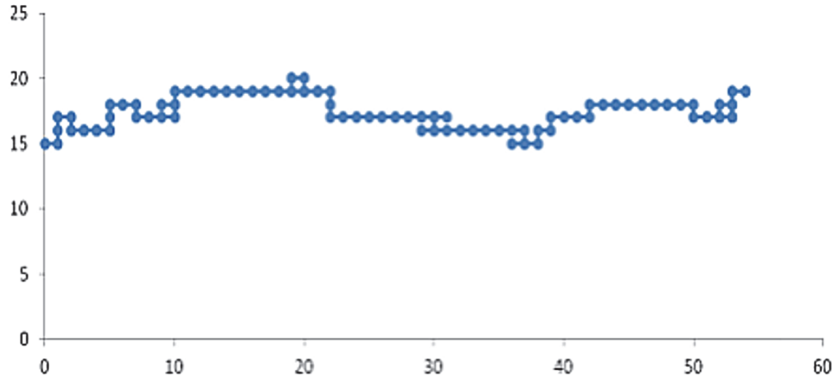

Fig. 1. One particle, $p_{+x} = 0.7$, $p_{-x} = p_{+y} = 0.1$ (100 steps)
Rys. 1. Jedna cząstka, $p_{+x} = 0{,}7$, $p_{-x} = p_{+y} = 0{,}1$ (100 kroków)

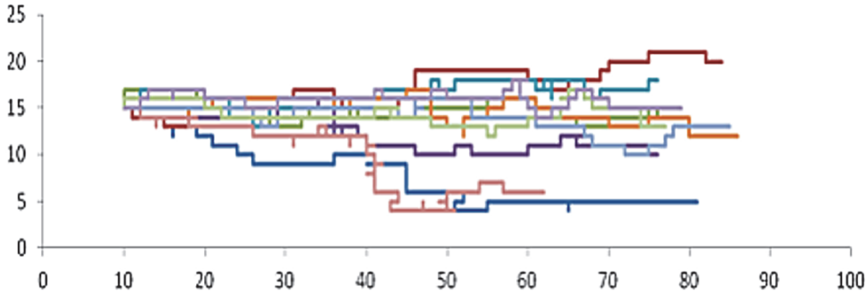

Fig. 2. 10 particles, $p_{+x} = 0.7$, $p_{-x} = p_{+y} = 0.1$ (10x100 steps)
Rys. 2. 10 cząstek, $p_{+x} = 0{,}7$, $p_{-x} = p_{+y} = 0{,}1$ (10 x 100 kroków)

But this approach makes it difficult to calculate when there are many sources and volumes of emissions of harmful substances. However, it can be noted that at any time, each particle can be in one of these grid nodes and each of these positions can be considered as a possible state of the particle at the time instant with a corresponding probability $P(i, j, t)$ where i, j are numbers of grid nodes).

Suppose that the probabilities of all positions of the particle are known at the time t, and we consider the change in the probability of finding the particle in position (i, j) through a small time interval Δt

At time $t + \Delta t$ the probability of a particle $P(i, j, t + \Delta t)$ can be determined by two cases: the first is when the position (i, j) flows in from neighbouring nodes $((i - 1), (i + 1, j), (i, j - 1)$ and $(i, j + 1))$; Second when flowing into neighbouring nodes $((i - 1, j), (i + 1, j), (i, j - 1)$ and

$(i, j + 1)$) (Figure 3). Presumably at each moment of time $t + \Delta t$, the position *(i, j)* is determined by the probable direction of the particle's transition $p^{n+1}_{l,i,j}, l = \{+z, -x, +z, -z\}$ and accordingly what is flowing in is added, but what is flowing is taken away. Thus, the equation for determining the probability of finding a particle at a position (i, j) at the time $t + \Delta t$ moment is as follows:

$$P^{n+1}_{i,j} = P^n_{i,j} + p^{n+1}_{+x,i,j} P^n_{i-1,j} + p^{n+1}_{-x,i,j} P^n_{i+1,j} + p^{n+1}_{+z,i,j} P^n_{i,j-1} + p^{n+1}_{-z,i,j} P^n_{i,j+1} + \\ + \left(p^{n+1}_{+x,i,j} + p^{n+1}_{-x,i,j} + p^{n+1}_{+z,i,j} + p^{n+1}_{+z,i,j} \right) P^n_{i,j} \tag{4}$$

where $P^{n+1}_{i,j}$ is the probability of finding a particle at the moment of time $t + \Delta t$ in position (i, j), $p^{n+1}_{+x,i,j}$ is the probability of transitions to (i, j), and from the position (i, j), at time $t + \Delta t$

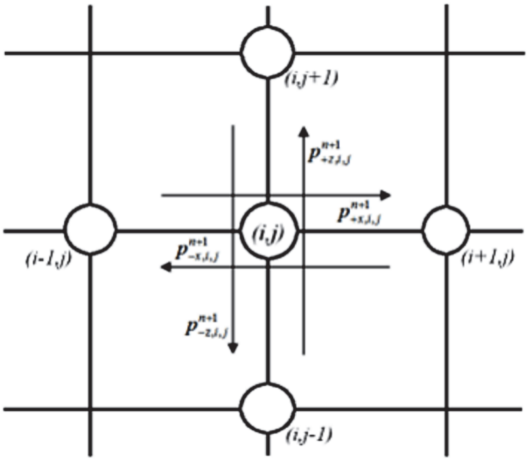

Fig. 3. Schemes of particle transitions
Rys. 3. Schematy przejścia cząstek

For a recurrent Poisson flow of events with $\mu_l(i, j)\Delta t << 1$:

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

where μ_l, $l = \{+z, -x, +z, -z\}$ is the intensity of the corresponding transitions, which in the turbulent flow are determined by the intensity of the turbulent pulsations c^{-1}.

Analogous approximations can also be written for all transitions denoting $\mu_{l,i,j}$. Then equation (4) takes the form

$$P_{i,j}^{n+1} = P_{i,j}^{n} + \mu_{+x,i,j}\Delta t P_{i-1,j}^{n} + \mu_{-x,i,j}\Delta t P_{i+1,j}^{n} + \mu_{+z,i,j}\Delta t P_{i,j-1}^{n} + \mu_{-z,i,j}\Delta t P_{i,j+1}^{n} - \\ -\left(\mu_{+x,i,j} + \mu_{-x,i,j} + \mu_{+z,i,j} + \mu_{-z,i,j}\right)P_{i,j}^{n}\Delta t \quad (5)$$

It is possible to obtain from expression (5)

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

Passing to the limit for $\Delta t \to 0$, we obtain a differential equation with respect to the probability of finding the particle at the time t instant at the point (i, j):

$$\frac{\partial P}{\partial t} = \mu_{+x,i,j}P_{i-1,j}^{n} + \mu_{-x,i,j}P_{i+1,j}^{n} + \mu_{+z,i,j}P_{i,j-1}^{n} + \mu_{-z,i,j}P_{i,j+1}^{n} - \\ -\left(\mu_{+x,i,j} + \mu_{-x,i,j} + \mu_{+z,i,j} + \mu_{-z,i,j}\right)P_{i,j}^{n} \quad (6)$$

The probability of finding a single particle in any position $P_{i,j}^{n}$ in accordance with the law of large numbers simultaneously means the fraction of particles $N(i, j, t)/N$ from their total number in the system that are in an elementary volume $V(i, j)$ by the cross $h_x \times h_z$ section at time t, that is,

$$P_{i,j}^{n} = \frac{N(i, j, t)}{N} = \varphi_{i,j}^{n}\frac{V(i, j)}{N} \quad (7)$$

where $\varphi_{i,j}^{n}$ is the local numerical impurity concentration, m^{-3}.

Substituting expressions (7) into equations (6), we can obtain the following expression

$$\frac{V(i,j)}{N}\frac{\partial \varphi}{\partial t} = \mu_{+x,i,j}\frac{V(i,j)}{N}\left(\varphi_{i-1,j}^{n} - \varphi_{i,j}^{n}\right) + \mu_{-x,i,j}\frac{V(i,j)}{N}\left(\varphi_{i+1,j}^{n} - \varphi_{i,j}^{n}\right) + \\ + \mu_{+z,i,j}\frac{V(i,j)}{N}\left(\varphi_{i,j-1}^{n} - \varphi_{i,j}^{n}\right) + \mu_{-z,i,j}\frac{V(i,j)}{N}\left(\varphi_{i,j+1}^{n} - \varphi_{i,j}^{n}\right) \quad (8)$$

Taking into account that the total number of divisions and the elementary volume is constant and adding a function describing the sources of harmful emissions into equations (8), we obtain

$$\frac{\partial\varphi}{\partial t} = \mu_{+x,i,j}\left(\varphi^n_{i-1,j} - \varphi^n_{i,j}\right) + \mu_{-x,i,j}\left(\varphi^n_{i+1,j} - \varphi^n_{i,j}\right) + \\ + \mu_{+z,i,j}\left(\varphi^n_{i,j-1} - \varphi^n_{i,j}\right) + \mu_{-z,i,j}\left(\varphi^n_{i,j+1} - \varphi^n_{i,j}\right) + f \tag{9}$$

where f is the function describing the source of emission of harmful substances.

The system of differential equations (9) for given initial and boundary conditions makes it possible to determine the concentration of harmful impurities and its variation. We will consider two types of boundary conditions: a free boundary and a solid wall. In a free boundary, we exclude those terms that go beyond the boundary. For example, on the border $x = X$:

$$\left.\frac{\partial\varphi}{\partial t}\right|_{x=X} = \mu_{+x,n_1,j}\left(\varphi^n_{n_1-1,j} - \varphi^n_{n_1,j}\right) + \mu_{-x,n_1,j}\left(-\varphi^n_{n_1,j}\right) + \\ + \mu_{+z,i,j}\left(\varphi^n_{n_1,j-1} - \varphi^n_{n_1,j}\right) + \mu_{-z,i,j}\left(\varphi^n_{n_1,j+1} - \varphi^n_{n_1,j}\right) + f \tag{10}$$

This means that the admixture from the calculated region flows unhindered, but does not flow in. Thus, if necessary, it is possible to determine the volume of impurities derived from the calculated region, to determine the self-cleaning of the atmosphere by wind regimes.

If the boundary is a solid wall, for example, on the boundary $z = 0$:

$$\left.\frac{\partial\varphi}{\partial t}\right|_{z=0} = \mu_{+x,i,1}\left(\varphi^n_{i-1,1} - \varphi^n_{i,1}\right) + \mu_{-x,i,1}\left(\varphi^n_{i+1,1} - \varphi^n_{i,1}\right) + \\ + \mu_{+z,i,1}\left(-\varphi^n_{i,1}\right) + \mu_{-z,i,1}\left(\varphi^n_{n_1,2}\right) + f \; . \tag{11}$$

In this case, the impurity does not flow in and out. Similarly, one can obtain boundary conditions for all boundaries of the region under consideration.

The intensities of the transitions $\mu_{+x,i,j}$, $\mu_{-x,i,j}$, $\mu_{+z,i,j}$ and $\mu_{-z,i,j}$ are determined by the determined velocities and intensities of the turbulent pulsations in the corresponding directions. The velocity of a particle of impurities in any direction is determined by the sum of the deterministic and random components

$$u = \overline{u} + u' \tag{12}$$

Then the total intensity of the transitions along any of the axes is determined by the sum of the averaged deterministic velocity and the turbulent pulsations.

$$\mu_{+x} = u + \mu_{+x}, \mu_{-x} = |-u| + \mu_{-x}, \mu_{+z} = w + \mu_{+z}, \mu_{-z} = |-w| + \mu_{-z}$$

where *u, w* are the components of wind speed. In the atmosphere in the absence of wind, the intensity of turbulent pulsations in all directions can be considered identical, i.e. $\mu_{+x} = \mu_{-x} = \mu_{+z} = \mu_{-z}$.

If we assume that the wind direction coincides with the direction of the axis *Ox*, then the intensity of the transitions will be determined as follows:

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

When the equations (9) are numerically realized from the intensity of the transitions $\mu_{+x,i,j}$, $\mu_{-x,i,j}$, $\mu_{+z,i,j}$ and $\mu_{-z,i,j}$ only one takes the value 1, and the remaining ones 0. This approach ensures that conditions (3) are satisfied. And which of them takes the value 1, is determined with the help of a random number generator.

Using the above-described probabilistic-stochastic model, methodical calculations of impurity transfer from point and linear sources have been carried out.

Figures 4 and 5 clearly show the effect of the wind speed regime. At a wind speed of 3 m/s, the impurity is carried away faster, without having time to succumb to diffusion processes. And with a wind speed of 1 m/s, the transfer process is slower.

And in Figures 6 and 7 the results of calculations of the transport of harmful impurities from linear sources on the horizontal section are presented. In Figure 5, the initial values of emissions on the main roads of the city used in (Danaev et al. 2014), and in Figure 6, the results of numerical calculations of the problem (9)-(11), which coincides with the results of (Danaev et al. 2014).

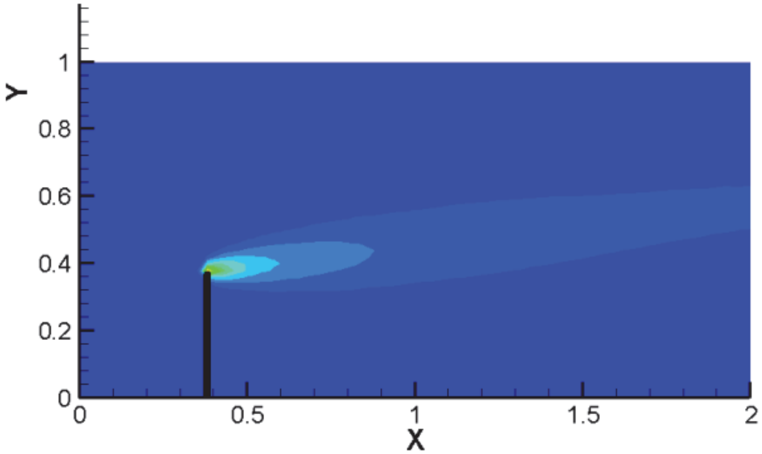

Fig. 4. Wind speed 3 m/s, point source
Rys. 4. Prędkość wiatru 3 m/s, źródło punktowe

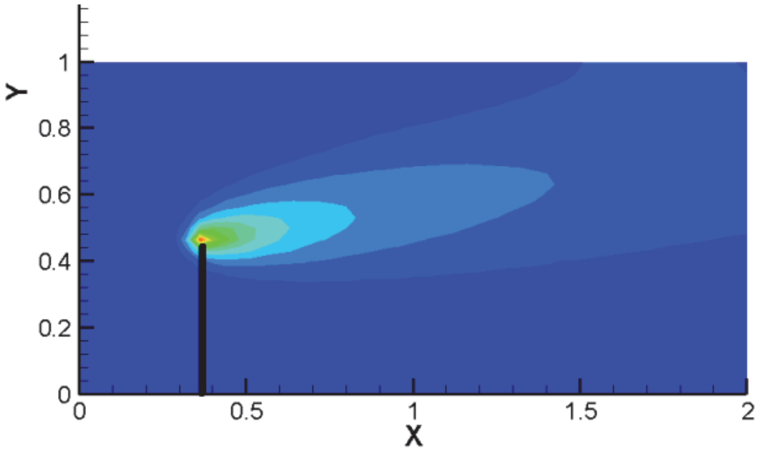

Fig. 5. Wind speed 1 m/s, point source
Rys. 5. Prędkość wiatru 1 m/s, źródło punktowe

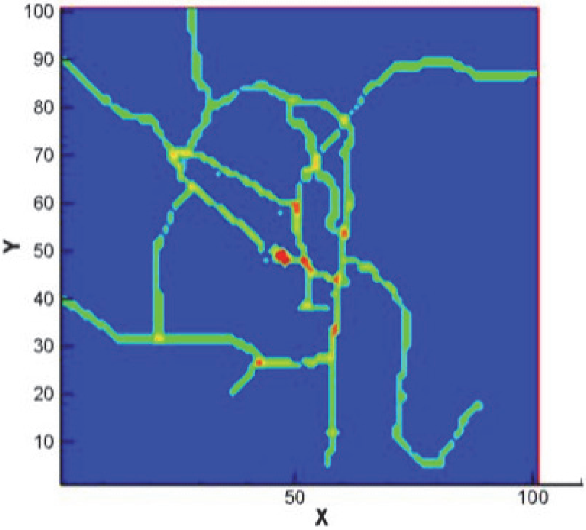

Fig. 6. Input from a linear source
Rys. 6. Napływ ze źródła liniowego

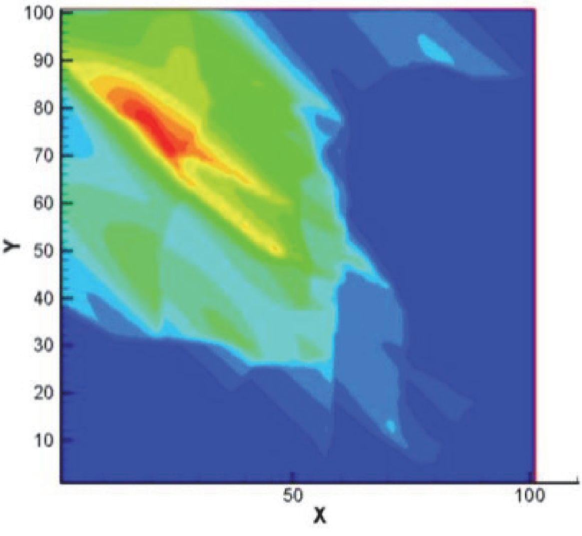

Fig. 6. Propagation from a linear source, wind speed 5 m/s, North-west direction
Rys. 6. Propagacja ze źródła liniowego, prędkość wiatru 5 m/s, kierunek północny-zachód

3. Conclusions

Using a simplified methodology of stochastic modelling, it is possible to construct effective numerical computational algorithms that significantly reduce the amount of computation without losing their accuracy.

From technical standpoint it is of great importance to control emissions from transport (Niewczas et al. 2002, Kordas et al. 2008, Droździel 2007).

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Probabilistyczne i statystyczne modelowanie rozprzestrzeniania się w atmosferze szkodliwych zanieczyszczeń z pojazdów silnikowych

Streszczenie

Celem pracy jest stworzenie matematycznego modelu rozprzestrzeniania się zanieczyszczeń z pojazdów. W tym artykule zaproponowano zastosowanie podejścia probabilistycznego i statystycznego do modelowania rozprzestrzeniania się szkodliwych zanieczyszczeń w atmosferze z pojazdów na przykładzie miasta Ust-Kamenogorsk. Stosując uproszczoną metodologię modelowania stochastycznego, można konstruować skuteczne numeryczne algorytmy obliczeniowe, które znacznie redukują ilość obliczeń bez utraty dokładności.

Abstract

The aim of the work is to create a mathematical model for the distribution of emissions from vehicles. In this article, it was proposed to use the probabilistic and statistical approach for modelling the distribution of harmful impurities in the atmosphere from vehicles using the example of the Ust-Kamenogorsk city. Using a simplified methodology of stochastic modelling, it is possible to construct effective numerical computational algorithms that significantly reduce the amount of computation without losing their accuracy.

Słowa kluczowe:
pulsacje turbulentne, model statystyczny, pojazdy mechaniczne,
rozwiązanie numeryczne, źródło,
rozprzestrzenianie się szkodliwych zanieczyszczeń

Keywords:
turbulent pulsations, statistical model, motor vehicles, numerical solution,
source, distribution of harmful impurities.