Probabilistic Statistical Modeling of Air Pollution from Vehicles

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

One of the central problems of describing the transport of harmful impurities in the atmosphere is the mathematical modeling of the gas and aerosol composition variability of 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.

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:

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

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 are used [1, 2, 3]. 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 [1]. 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 [4].

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 [3]. Due to the complicated turbulent structure of the flow, considerable

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simplifying assumptions are made in determining the diffusion behavior and the turbulent diffusion coefficient of the particles, depending on the flow parameters and particle characteristics. In addition, it is often assumed that there is 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 [5].

In this paper, we consider the numerical implementation of the probably statistical model described in [6] for modeling 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:

$$x(t) = \int_0^t u_x(t)dt + x'(t), \tag{2}$$

where $x(t)$ is the projection of the deterministic velocity, *m/s*; $x'(t)$ is a 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 $(p_{+x}(t) + p_{-x}(t) + p_{+z}(t) + p_{-z}(t) = 1)$.

Obviously, in the absence of wind and isotropic turbulence $p_{+x}(t) = p_{-x}(t) = p_{+z}(t) = p_{-z}(t) = \frac{1}{4}$, 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 $p_{+x} > p_{-x} = p_{+z} = p_{-z}$.

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 (Figure 1 and 2, respectively).

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 $P(i, j, t)$ (i, j is the number 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 neighboring nodes $((i-1), (i+1, j), (i, j-1)$ and $(i, j+1))$; the second is when flowing into neighboring nodes $((i-1, j), (i+1, j), (i, j-1)$ and $(i, j+1))$ (Figure 3). Presumably at each moment of time

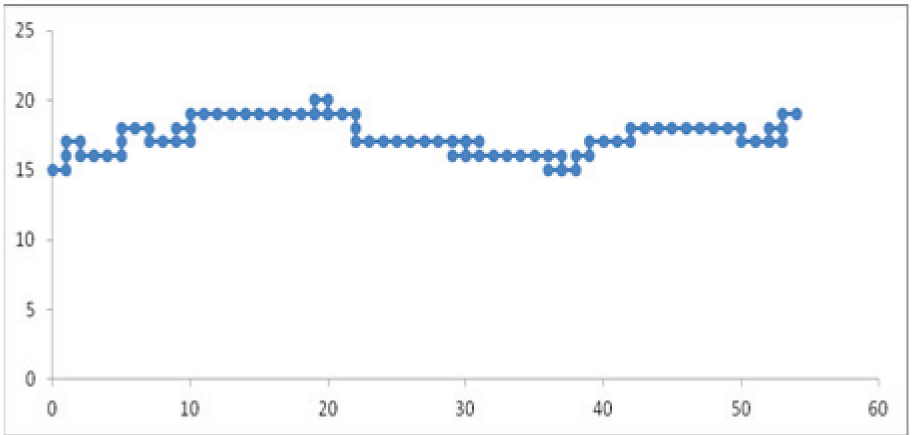

FIGURE 1. One particle, $p_{+x} = 0.7$, $p_{-x} = p_{+y} = p_{-y} = 0.1$ (100 steps)

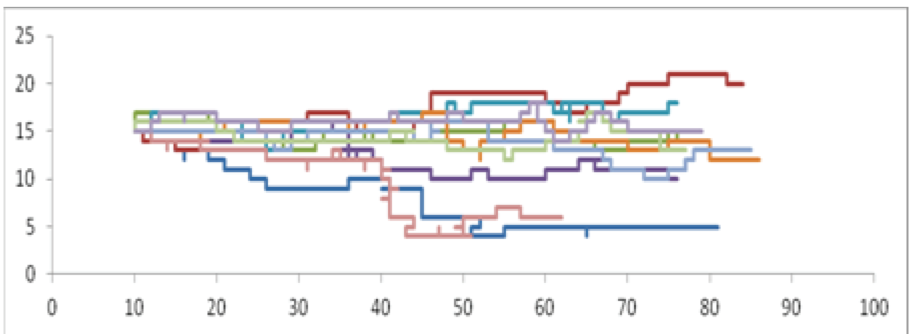

FIGURE 2. 10 particles, $p_{+x} = 0.7$, $p_{-x} = p_{+y} = p_{-y} = 0.1$ (10×100 steps)

$t + \Delta t$, the position (i, j) is determined by the probable direction of the particle's transition $p^{n+1}_{l,i,j}$ $(l = +x, -x, +z, -z)$, and accordingly what is flowing in is added, but what is flowing out 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:

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

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 $t + \Delta t$.

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

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

where μ_l $(l = +x, -x, +z, -z)$ 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

$$P^{n+1}_{i,j} = P^n_{i,j} + \mu_{+x,i,j}\Delta t P^n_{i-1,j} + \mu_{-x,i,j}\Delta t P^n_{i+1,j} + \mu_{+z,i,j}\Delta t P^n_{i,j-1} + \mu_{-z,i,j}\Delta t P^n_{i,j+1} - \\ -(\mu_{+x,i,j} + \mu_{-x,i,j} + \mu_{+z,i,j} + \mu_{-z,i,j})P^n_{i,j}\Delta t. \tag{5}$$

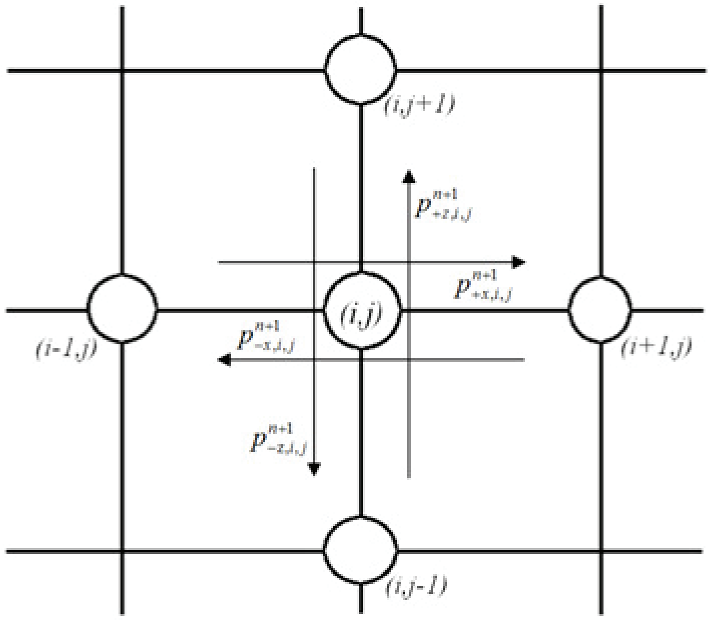

FIGURE 3. Schemes of particle transitions

It is possible to obtain from expression (5)

$$\frac{P^{n+1}_{i,j} - P^n_{i,j}}{\Delta t} = \mu_{+x,i,j} P^n_{i-1,j} + \mu_{-x,i,j} P^n_{i+1,j} + \mu_{+z,i,j} P^n_{i,j-1} + \mu_{-z,i,j} P^n_{i,j+1} -$$
$$-(\mu_{+x,i,j} + \mu_{-x,i,j} + \mu_{+z,i,j} + \mu_{-z,i,j}) P^n_{i,j}.$$

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

$$\frac{\partial P}{\partial t} = \mu_{+x,i,j} P^n_{i-1,j} + \mu_{-x,i,j} P^n_{i+1,j} + \mu_{+z,i,j} P^n_{i,j-1} + \mu_{-z,i,j} P^n_{i,j+1} -$$
$$-(\mu_{+x,i,j} + \mu_{-x,i,j} + \mu_{+z,i,j} + \mu_{-z,i,j}) P^n_{i,j}. \quad (6)$$

The probability of finding a single particle in any position $P^n_{i,j}$ 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,

$$P^n_{i,j} = \frac{N(i, j, t)}{N} = \varphi^n_{i,j} \frac{V(i, j)}{N}, \quad (7)$$

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

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

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

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

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

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 $x = X$:

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

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 $z = 0$:

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

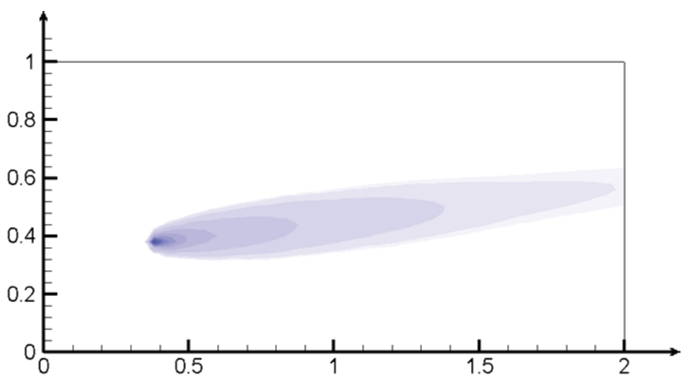

FIGURE 4. Wind speed 3 m / s, point source

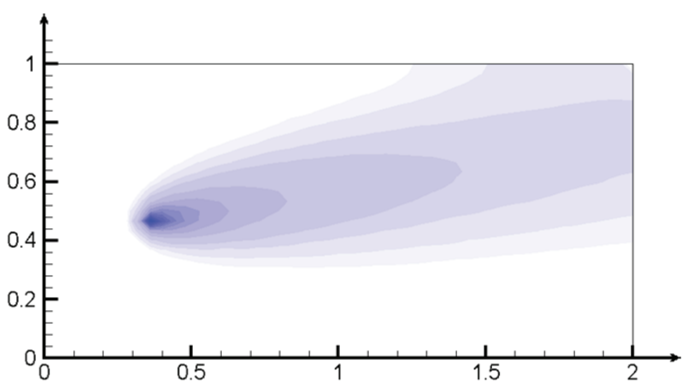

FIGURE 5. Wind speed 1 m / s, point source

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

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

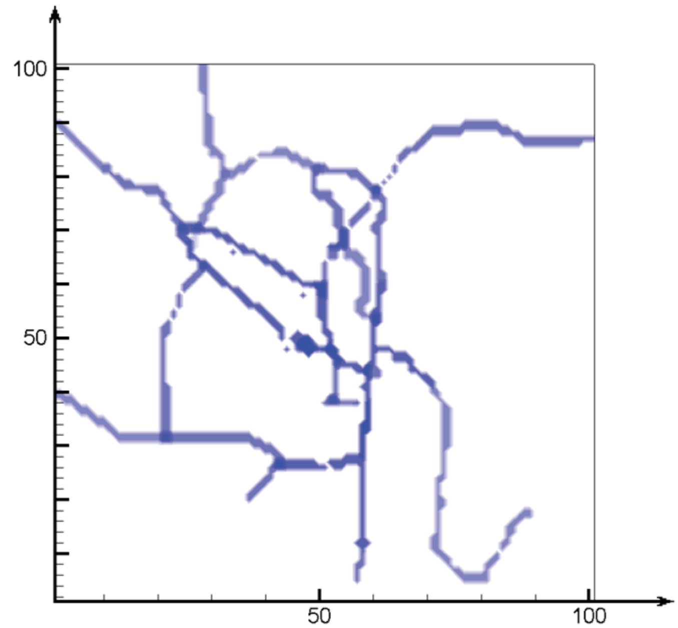

FIGURE 6. Input from a linear source

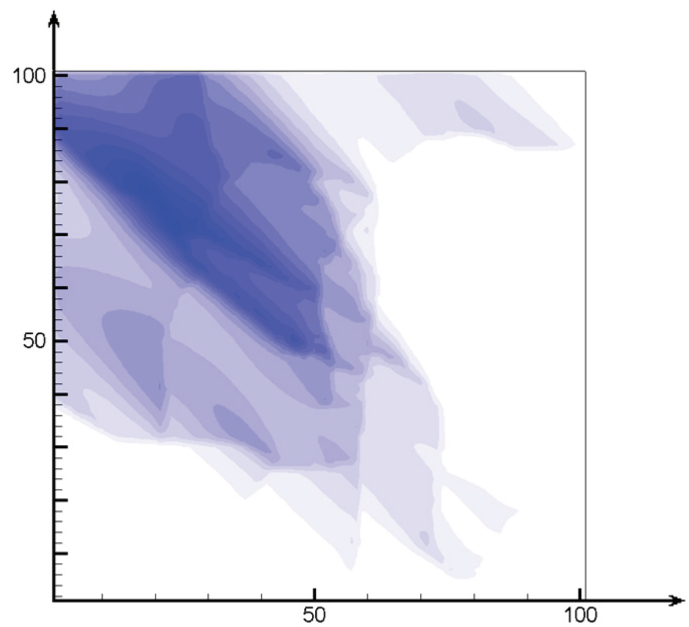

FIGURE 7. Propagation from a linear source, wind speed 5 m / s, North-west direction

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

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

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:

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

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. 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.

In Figure 6 and 7, the results of calculations of the transport of harmful impurities from linear sources on the horizontal section are presented. In Figure 6, there are shown the initial values of emissions on the main roads of the city used in [7, 8, 9], and in Figure 7, there are given the results of numerical calculations of the problem (9) - (11), which coincide with the results of [7, 8, 9, 10].

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

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