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NUMERICAL STUDY OF THE SUSUPLUME AIR POLLUTION MODEL

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In this paper, we propose a SUSUPLUME air pollution as a modern application of the classical Gaussian plume model. The presented model takes into account meteorological conditions and parameters of the pollution sources. The classical model is supplemented by the equations of motion of the center of mass of a single emission. A numerical study has shown that in stationary weather conditions the presented model qualitatively coincides with other known models. The results of calculating the concentrations of pollutants do not contradict the obtained values based on the official methodology for calculating the maximum concentrations of pollutants approved for usege in the territory of the Russian Federation. The SUSUPLUME model contains a number of identifiable parameters and it can be adapted to real conditions. The computational model consists of two blocks: a block for recording measurement information and a block for calculating the concentrations of pollutants. The measurement information registration unit has a low labor intensity (over a million registrations per second). The pollutant concentrations calculation block is laborious (400 points of calculations per second). Concentrations are calculated independently, it allows to use parallelization of the computational process in the future.

Keywords: air pollution model; Gaussian plume model; Romberg's method.

Introduction

At present, the problem of air pollution in large cities is extremely acute. For example, in Chelyabinsk, up to one third of days per year the maximum permissible concentrations of pollutants are exceeded [1]. In this situation the issue of identifying sources of air pollution becomes particularly relevant. The existing methods for monitoring the state of atmospheric air based on empirical methods for calculating the concentrations of pollutants [2] do not meet the current needs. The deployment of an extensive network of physicochemical air condition monitoring and the use of modern methods of mathematical modelling allow taking into account the variety of pollution sources in large cities, as well as the peculiarities of meteorological conditions formed under the influence of urban development and life.

Air pollution models can be divided into: empirical, computational fluid dynamics and semi-empirical models. Models are also distinguished by the scale of the computational grid: mesoscale models (grid spacing at least 10 km), as well as microscale models (grid spacing about 2 meters). Mesoscale models are used to calculate weather changes, e.g. WRF/LSM/Urban modelling system [3], NU-WRF model [4], WRF/Chem-NCSU scale

transport [5, 6] and WRF/hem-ROMS [6] and others. Microscale models are used to calculate air pollution of a city, street, enterprise, for example, the WACFD-RANS model which was applied in Madrid to two different areas of the city [7–10]. On the basis of empirical models, the Russian official methodology for calculating MRR-2017 [11] has been developed. Such models are well applicable for calculating quasi-stationary processes, for example, when the time of movement of pollutants is insignificant compared to the time of their release. The disadvantage of such models is their "rigid" structure and a large number of simplifications, which undoubtedly leads to inaccuracies in the calculation. Moreover, the introduction of additional correction factors does not increase their accuracy [12]. Compared to other models, computational fluid dynamics models allow to take into account complex flows in an urban environment, air flow around obstacles on a micro scale, and much more. For example, the WACFD-RANS model used in Spain [7–9] or the TAPM model developed and used in Australia [13, 14]. CFD models look very promising, but they have one significant drawback. The calculation of these models requires significant computational resources. Semi-empirical models have found wide practical application in calculating air pollution in an urban environment. The most widespread is the Pasquill–Gifford model [15], which is based on the hypothesis of the normal distribution of the pollutants concentration along spatial coordinates. This model was recommended in 1986 for the creation of national local models for IAEA member countries [16]. In Russia, national models DV-2010 [17] and NPO Typhoon [18, 19] were developed to calculate the propagation of radionuclides. Although the Pasquill–Gifford model was developed in the 50s of the last century, it has not lost its relevance up to the present time, in view of its simplicity and ability to adapt to local problems. In this paper, numerical modelling is presented within the framework of the SUSUPLUME model proposed by the authors, which is based on the classical Gauss model, supplemented by the equations of motion of the center of mass of a single emission. The motivation for the development of the model was the creation of a toolkit for an industrial enterprise, which allows calculating the concentration of pollutants within the boundaries of the sanitary zone to improve emission control. The main attention was paid to solving the key problem of constructing a tunable model for specific parameters of plant emissions, in contrast to the widely used AERMOD [20] and CALPUFF [21] models recommended by the US EPA.

1. Model of Air Pollution from a Point Source

Consider a point pollution source. Let it be located in the coordinates (x_i, y_i, h_i), $i = \overline{1, N}$, where x_i, y_i are coordinates in meters in the horizontal plane. The X axis is directed from West to East, and the Y axis goes from South to North, h_i is the height of the mouth of the pollution source above the earth's surface in meters, i is the number of the pollution source, N is the total number of point sources. At each moment of time let us know the wind in the horizontal plane. Let $u(t)$ be the projection of the wind speed on the X axis and $v(t)$ be the projection of the wind speed on the Y axis.

Consider a single emission of pollutants during rather small time period $\triangle t$. Let us describe the motion dynamics of the center of mass for the single emission. Let $x_i(t_0, t), y_i(t_0, t), z_i(t_0, t)$ be coordinates of the single emission from the i-th source at time t, that left the source mouth at time t_0. Then the movement of the center of mass of

the single emission in the horizontal plane is described by the relations

$$x_i(t_0,t) = x_i + \int_{t_0}^{t} u(t)\,dt,\ y_i(t_0,t) = y_i + \int_{t_0}^{t} v(t)\,dt.$$

On the vertical axis, the emission is influenced by the forces of gravity, Archimedes and viscous friction. Write down the corresponding second Newton's law

$$m_g \ddot{z}_i(t_0,t) = -m_g g + m_a g - \mu m_g \dot{z}_i(t_0,t), \tag{1}$$

where m_g is the mass of the single emission, m_a is the mass of displaced air, μ is the viscosity coefficient, which describes the dependence of the medium resistance to the movement of the single emission. Now write the ideal gas equation for the single emission and displaced air volume. Since the pressures of these gases coincide, then

$$\frac{m_g}{M_g} R T_g = \frac{m_a}{M_a} R T_a,$$

where T_a is the air temperature, T_g is the temperature of the single emission, m_a is the mass of displaced air, M_a is the molar mass of air, M_g is the molar mass of the single emission, $R = 8,314\ J \cdot K^{-1} \cdot mol^{-1}$ is the universal gas constant. Hence

$$m_a = m_g \frac{M_a T_g}{M_g T_a}. \tag{2}$$

Since the exhaust temperature T_g can be different from the ambient air temperature T_a, the exhaust cooling process takes place simultaneously. This can be described by the relation

$$\dot{T}_i(t_0,t) = \gamma\left(T_a - T_i(t_0,t)\right), \tag{3}$$

where $T_i(t_0,t)$ is the temperature of the single emission from the i-th source, γ is the coefficient characterizing the rate of emission cooling depending on external conditions. Taking into account (3), as well as the initial discharge temperature T_i at the moment of leaving the source, we can write

$$T_g = T_i(t_0,t) = T_a + (T_i - T_a)\, e^{-\gamma(t-t_0)}. \tag{4}$$

Substituting (2) and (4) into (1), we get

$$m_g \ddot{z}_i(t_0,t) = -m_g g + m_g \frac{M_a}{M_g T_a} g\left(T_a + (T_i - T_a)\, e^{-\gamma(t-t_0)}\right) - \mu m_g \dot{z}_i(t_0,t).$$

Therefore

$$\ddot{z}_i(t_0,t) = \left(\frac{M_a}{M_g} - 1\right) g + \frac{M_a (T_i - T_a)\, g}{M_g T_a} e^{-\gamma(t-t_0)} - \mu \dot{z}_i(t_0,t).$$

Introduce the notation $a = -\mu$, $b = \left(\frac{M_a}{M_g} - 1\right) g$, $c = \frac{M_a (T_i - T_a) g}{M_g T_a}$. Taking into account that $z_i(t_0,t) \geq 0$, the solution to equation (1) can be written as

$$z_i(t_0,t) = \max\left[\hat{z}_i(t_0,t), 0\right],$$

where

$$\hat{z}_i(t_0,t) = h_i - \frac{c}{\gamma(a+\gamma)} + \left(w_i + \frac{b}{a} + \frac{c}{(a+\gamma)}\right)\left(\frac{e^{a(t-t_0)}-1}{a}\right) + \\ + \frac{ce^{-\gamma(t-t_0)}}{\gamma(a+\gamma)} - \frac{b(t-t_0)}{a},$$

h_i is the height of the i-th source mouth, and w_i is the initial vertical velocity of the single emission when leaving the i-th source mouth.

Concentration $c_i(x,y,z,t_0,t)$ at point (x,y,z) at time t, created by the single emission with a center of mass at point $(x_i(t_0,t), y_i(t_0,t), z_i(t_0,t))$ is described by a certain distribution characterizing the diffusion process of the single emission. In the ideal case, this process is described by the heat conduction equation or explicitly

$$\hat{c}_i(x,y,z,t_0,t) = \frac{m_g}{(2\pi)^{3/2}\sigma_x(t-t_0)\sigma_y(t-t_0)\sigma_z(t-t_0)} e^{-\left(\frac{(x_i(t_0,t)-x)^2}{2\sigma_x^2(t-t_0)} + \frac{(y_i(t_0,t)-y)^2}{2\sigma_y^2(t-t_0)} + \frac{(z_i(t_0,t)-z)^2}{2\sigma_z^2(t-t_0)}\right)},$$

where $\sigma_x(t-t_0), \sigma_y(t-t_0), \sigma_z(t-t_0)$ are functions that describe the expansion dynamics for the "cloud" of the single emission. To take into account the earth's surface, introduce a virtual source for each point source, which has coordinates $(x_i, y_i, -h_i)$. Then the concentration distribution from a point source will be described as

$$c_i(x,y,z,t_0,t) = \hat{c}_i(x,y,z,t_0,t) + \hat{c}_i(x,y,-z,t_0,t).$$

The concentration generated by the source can be calculated as

$$C_i(x,y,z,t) = \int_{-\infty}^{t} c_i(x,y,z,t_0,t)\,dt_0, \tag{5}$$

where $C_i(x,y,z,t)$ is the concentration created by the i-th source at the point (x,y,z) at time t. Then the pollutant concentration at a given point at time t is determined as follows

$$C(x,y,z,t) = \sum_{i=1}^{N} C_i(x,y,z,t).$$

2. Numerical Implementation of the SUSUPLUME Air Pollution Model

It is assumed that data on meteorological conditions are received discretely with step t_w. For the numerical integration algorithms to work, the values $u(t)$ and $v(t)$ are approximated by piecewise linear functions.

For dispersion functions $\sigma_x(t-t_0), \sigma_y(t-t_0), \sigma_z(t-t_0)$ we consider two sets of functions: the Pasquill–Briggs functions [23] and the MESOPUFF [24] functions, where the relation

$$\hat{x}(t,t_0) = \int_{t_0}^{t} \sqrt{u(s)^2 + v(s)^2}\,ds$$

is used to estimate $\hat{x}$.

Table

Dispersion functions for different models

Atmospheric stability category	Pasquill–Briggs model	MESOPUFF model
A	$\sigma_x(\hat{x}) = \sigma_y(\hat{x}) = 0,32\hat{x}\left(1+\frac{\hat{x}}{2500}\right)^{-0,5}$, $\sigma_z(\hat{x}) = 0,24\hat{x}\sqrt{1+\frac{\hat{x}}{1000}}$	$\sigma_x(\hat{x}) = \sigma_y(\hat{x}) = 0,36\hat{x}^{0,9}$, $\sigma_z(\hat{x}) = 0,000236\hat{x}^{2,1}$
B	$\sigma_x(\hat{x}) = \sigma_y(\hat{x}) = 0,22\hat{x}\left(1+\frac{\hat{x}}{2500}\right)^{-0,5}$, $\sigma_z(\hat{x}) = 0,24\hat{x}\sqrt{1+\frac{\hat{x}}{1000}}$	$\sigma_x(\hat{x}) = \sigma_y(\hat{x}) = 0,25\hat{x}^{0,9}$, $\sigma_z(\hat{x}) = 0,058\hat{x}^{1,09}$
C	$\sigma_x(\hat{x}) = \sigma_y(\hat{x}) = 0,32\hat{x}\left(1+\frac{\hat{x}}{2500}\right)^{-0,5}$, $\sigma_z(\hat{x}) = 0,2\hat{x}$	$\sigma_x(\hat{x}) = \sigma_y(\hat{x}) = 0,19\hat{x}^{0,9}$, $\sigma_z(\hat{x}) = 0,11\hat{x}^{0,91}$
D	$\sigma_x(\hat{x}) = \sigma_y(\hat{x}) = 0,16\hat{x}\left(1+\frac{\hat{x}}{2500}\right)^{-0,5}$, $\sigma_z(\hat{x}) = 0,14\hat{x}\left(1+\frac{\hat{x}}{1000}\right)^{-0,5}$	$\sigma_x(\hat{x}) = \sigma_y(\hat{x}) = 0,13\hat{x}^{0,9}$, $\sigma_z(\hat{x}) = 0,57\hat{x}^{0,58}$
E	$\sigma_x(\hat{x}) = \sigma_y(\hat{x}) = 0,11\hat{x}\left(1+\frac{\hat{x}}{2500}\right)^{-0,5}$, $\sigma_z(\hat{x}) = 0,08\hat{x}\left(1+\frac{\hat{x}}{1000}\right)^{-0,5}$	$\sigma_x(\hat{x}) = \sigma_y(\hat{x}) = 0,096\hat{x}^{0,9}$, $\sigma_z(\hat{x}) = 0,85\hat{x}^{0,47}$
F	$\sigma_x(\hat{x}) = \sigma_y(\hat{x}) = 0,11\hat{x}\left(1+\frac{\hat{x}}{2500}\right)^{-0,5}$, $\sigma_z(\hat{x}) = 0,08\hat{x}\left(1+\frac{\hat{x}}{1000}\right)^{-0,5}$	$\sigma_x(\hat{x}) = \sigma_y(\hat{x}) = 0,063\hat{x}^{0,9}$, $\sigma_z(\hat{x}) = 0,77\hat{x}^{0,42}$

In (5), the lower limit of integration is $-\infty$, but in practice, we are interested in calculating the concentration in a limited area near pollution sources. We assume that if the center of mass of the single emission is located far enough from the area of interest, then its contribution can be neglected. Suppose that the minimum wind speed for which the developed model can be applied is u_{min}, and the size of the concentration calculation area is D, then in time $t_{max} = \frac{2D}{u_{min}}$ the single emission will leave the concentration calculation area. Accordingly, (5) can be written as

$$C_i(x,y,z,t) = \int\limits_{t-\frac{2D}{u_{min}}}^{t} c_i(x,y,z,t_0,t)\,dt_0. \tag{6}$$

To calculate (6) numerically, we use the modified Romberg's method [25]. The modification consists in the fact that the segment of integration $\left[t-\frac{2D}{u_{min}};t\right]$ is divided into several subsegments and the integral is calculated on each segment by the Romberg's method until the specified relative error ε is reached. Let the integral be calculated on the segment $[a;b]$. The integration algorithm is presented below.

Step 1. Put $i=0$. Calculate the scores $I_{0,0}, I_{1,0}$ using the formula

$$I_{i,0} = \frac{b-a}{2^i}\left[\frac{f(a)+f(b)}{2} + \sum_{k=1}^{2^i-1}\frac{f\left(a+k\frac{b-a}{2^i}\right)}{2}\right],\ i=0,1,\ldots. \tag{7}$$

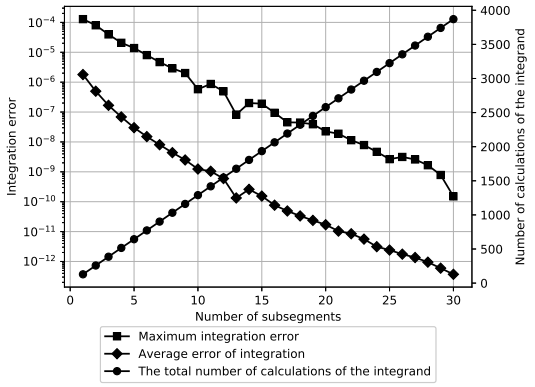

Fig. 1. Integration error depending on the number of subsegments

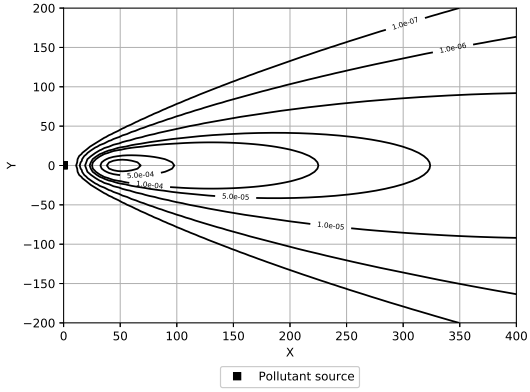

Fig. 2. Pollutant concentration for a point source

Step 2. Put $i = 1, j = 0$. Calculate the scores $I_{1,1}$ using the formula

$$I_{i,j+1} = I_{i,j} + \frac{I_{i,j} - I_{i-1,j}}{4^j - 1},\ i = 0, 1, \ldots,\ j = 0, .., \min(i, 5). \tag{8}$$

Step 3. If the condition

$$\left|I_{i,\min(i,5)} - I_{i-1,j-1}\right| \leq \varepsilon \left|I_{i,\min(i,5)}\right| \tag{9}$$

is satisfied, then the algorithm is completed. Otherwise, go to step 4.
Step 4. Put $i = i + 1$, calculate the estimates $I_{i,0}$ by formula (7).
Step 5. Calculate the estimates $I_{i,j}$ for all $j = 0, ..., \min(i, 5)$ by formula (8). Go to Step 3.

Typically, the maximum permissible concentration of the main pollutants is at least $10^{-3}\, mg \cdot m^{-3}$. To calculate the concentration of pollutants with an accuracy of 1%, the required accuracy for calculating the integral (6) is $\varepsilon = 10^{-8}$. Determine the number of segments into which it is necessary to split the segment of integration from the following computational experiment.

Let one source be $10\, m$ high, wind speed be $10\, m/s$ (Western), emission intensity be $1\, g/s$. Calculate the concentrations using formula (6) on a $5 * 5\, m$ grid for $x \in [0; 1000]$ (the emission does not spread upwind), $y \in [0; 100]$ (the concentration will be symmetrical). The height of the concentration calculation is $z = 2$ meters. To calculate the exact integral, we use the Romberg's method on the entire segment $\left[t - \frac{2D}{u_{min}}; t\right]$ with initial number of points equal to $100,000$ and accuracy of calculation $\varepsilon = 10^{-12}$.

The experimental results (Fig. 1) show that it is necessary to split the segment $\left[t - \frac{2D}{u_{min}}; t\right]$ into 23 subsegments, which is $49,19\, s$ per segment, to achieve the integration accuracy 10^{-8}. Romberg's method completed its work by calculating the objective function every $0,3\, s$.

From a computational point of view, the model consists of two blocks. The first block registers the measured values such as wind direction and strength, etc. Since the concentration calculation requires data for a limited $\frac{2D}{u_{min}}$ length, a circular buffer is used to

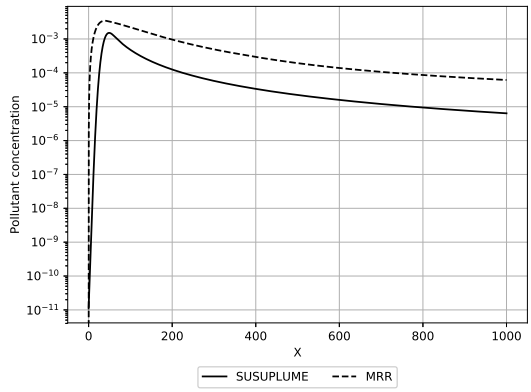

Fig. 3. Pollutant concentration along the X axis ($y = 0$)

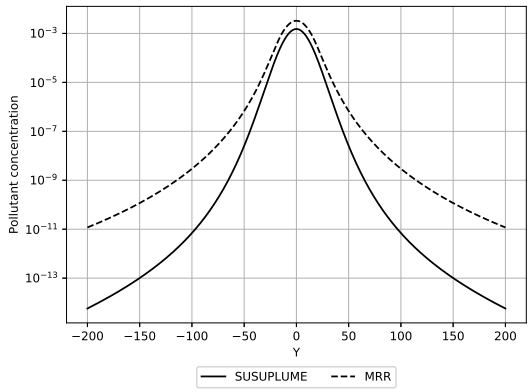

Fig. 4. Pollutant concentration along the Y axis ($x = 41,1$)

accumulate information. This allows information accumulation operations to be performed in $O(1)$ time. The second block calculates the pollutants concentration at the given points. Calculations of the pollutants concentrations at different points are independent and can be performed in parallel on different computers. The average time for calculating the concentration at one point from one source is about $10^{-4}\,s$ on an Intel Core 2 Duo T8300, 2,4 GHz processor for one subsegment.

3. Investigation of the SUSUPLUME Model

Let's consider a model situation. One point pollution source $10\,m$ high is located at point $(0;0)$. The source emits nitrogen dioxide ($M_g = 46$) with intensity equal to $1\,g/s$, temperature equal to $300°C$ and velocity equal to $3\,m/s$. The wind is considered to be constant with speed equal to $3\,m/s$, West. Consider atmospheric class – "D", air temperature $27°C$. Let us choose the Pasquill–Briggs functions as the dispersion functions (Table). Parameter values are $\gamma = 0,1$, $\mu = 1,0$. Let's calculate the concentration (Fig. 2) at a height of 2 m for the area $[0;400] \times [-200;200]$. The maximum concentration is reached at the point $(49,1;0)$ and is equal to $1,5 \cdot 10^{-3} g \cdot m^{-3}$.

Let us compare the obtained concentration values with the maximum calculated values calculated in accordance with [2]. Construct sections through the point $(49,1;0)$ along the X-axis (Fig. 3) and Y-axis (Fig. 4).

Now compare the concentration distribution calculated using the SUSUPLUME model and results of the official MRR-2017 method used in the Russian Federation. The maximum concentration according to the MRR-2017 technique (Fig. 5) is achieved at the point $(41,1;0)$. Qualitatively, the SUSUPLUME model repeats the concentration dynamics, however, quantitatively it may differ from MRR-2017.

The calculated values of concentrations according to the model do not exceed the values specified in the normative document. In this case, the MRR-2017 model does not take into account the type of substance that is emitted. Let us consider how the concentration of pollutants for sulfur dioxide will change ($M_g = 64$).

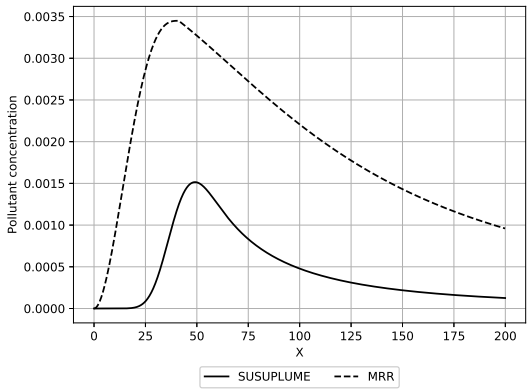

Fig. 5. Comparison of the maximum concentration of pollutants in different models

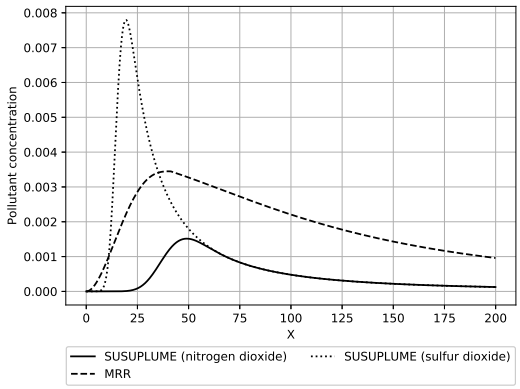

Fig. 6. Pollutant concentration for nitrogen dioxide and sulfur dioxide

In this case, the maximum concentration value exceeds the value calculated by the MRR-2017 (Fig. 6). Let us consider the possibility of ensuring a decrease in the calculated concentration due to the correct selection of the γ, μ parameters. Let's assume that $\gamma, \mu \in [0; 4,6]$. With $\gamma = \mu = 4,6$, the single blowout will decrease vertical speed by 99% in 1 second and decrease temperature by 99% in 1 second in relation to the environment. Consider such pairs $(\gamma; \mu)$ for which the inequality $\max\limits_{x \in [0;200]} (c(x,0,2) - c_{mrr}(x,0,2)) \leq 0$. The allowed range of parameters is shown in Fig. 7.

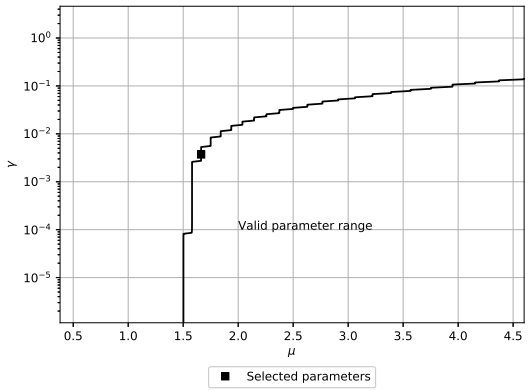

Fig. 7. Values $(\mu; \gamma)$ at which the concentration value does not exceed the MRR-2017 model data

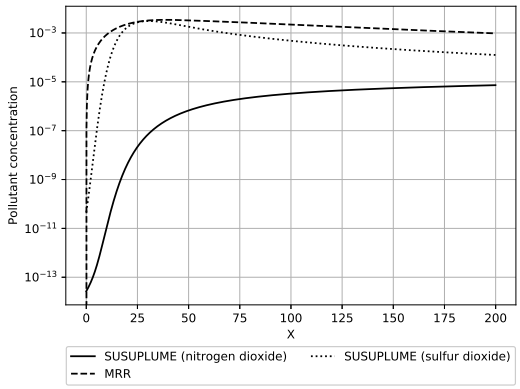

Fig. 8. Pollutant concentration for identified parameters

Let $\gamma = 0,003714$ and $\mu = 1,66310$, then the calculated concentrations are shown in Fig. 8. The maximum concentration of sulfur dioxide fits into the calculation according to MPR-2017, however, with the given parameters, the concentration of nitrogen dioxide has dropped sharply.

Let us calculate the concentration of pollutants for the dispersion functions MESOPUFF (Table) for the initial conditions (Fig. 9, 10).

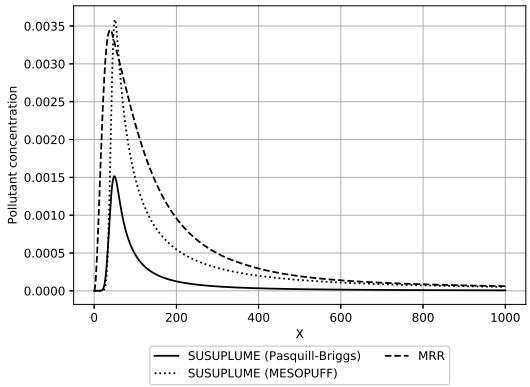

Fig. 9. Concentration of pollutants for different dispersion functions (along the X axis)

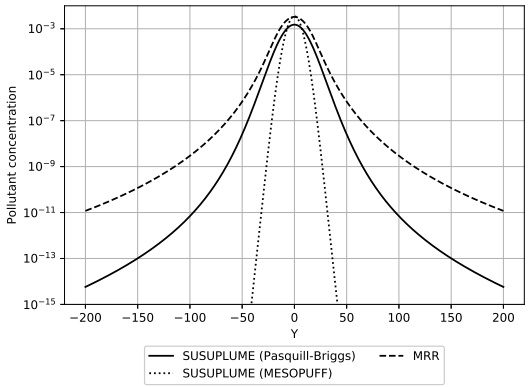

Fig. 10. Concentration of pollutants for different dispersion functions (along the Y axis)

Using the MESOPUFF functions simulates a distribution that is much "squeezed" on the Y axis and more "smeared" on the X axis. The identification of the dispersion function $\sigma_x, \sigma_y, \sigma_z$, in the presence of a large number of measurements, will improve the quality of modelling the air pollution.

When identifying model parameters on real data, it is necessary to identify the parameters γ, μ, and also take into account that the dynamics of the center of mass of the single emission is determined by the parameters of the gas-air mixture M_g, w, which are also subject to identification.

4. Advantages and Disadvantages of the Proposed Model

The constructed model makes it possible to simulate the dispersion of pollutants taking into account the real measurement of the wind over time. In addition, the model is able to take into account the type of emitted substance, the current season (through the ambient temperature), the possibility of parallelization when calculating the concentration. The disadvantage of the constructed model is the considerable time for calculating the concentration and the lack of taking into account the local movement of air masses.

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ЧИСЛЕННОЕ ИССЛЕДОВАНИЕ МОДЕЛИ SUSUPLUME РАСПРОСТРАНЕНИЯ ЗАГРЯЗНЯЮЩИХ ВЕЩЕСТВ В АТМОСФЕРЕ

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В настоящей работе предложена модель рассеивания загрязняющих веществ в атмосферном воздухе SUSUPLUME, представляющая собой модификацию классической

модели гауссового шлейфа (Gaussian plume model). Представленная модель описывает динамику рассеяния с учетом различных факторов: метеорологической обстановки, параметров источника загрязнения. Уравнения классической модели дополнены уравнениями движения центра масс единичного выброса. Численное исследование показало, что в стационарных метеоусловиях представленная модель качественно совпадет с другими известными моделями. Результаты расчета концентраций загрязняющих веществ не противоречат полученным значениям на основе методики ММР 2017, утвержденной к применению на территории Российской Федерации. Модель также содержит ряд идентифицируемых параметров, с помощью которых она может быть адаптирована к реальным условиям. Вычислительно модель состоит из двух блоков: блока регистрации измерительной информации и блока расчета концентраций загрязняющих веществ. Блок регистрации измерительной информации имеет низкую трудоемкость (свыше миллиона регистраций в секунду). Блок расчета концентраций загрязняющих веществ имеет высокую трудоемкость (около 400 точек вычислений концентрации в секунду), но поскольку все концентрации в представленной модели рассчитываются независимо, то это позволяет в перспективе использовать распараллеливание вычислительного процесса.

Ключевые слова: модель распространения загрязняющих веществ; гауссова модель; метод Ромберга.

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