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CONSTRUCTING A METHOD FOR ASSESSING THE EFFECTIVENESS OF USING PROTECTIVE BARRIERS NEAR HIGHWAYS TO DECREASE THE LEVEL OF AIR POLLUTION

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Highways are an intensive source of environmental pollution. Atmospheric air is exposed to the fastest anthropogenic influence. Therefore, a particularly important task is to minimize the level of air pollution near the highway. An effective method for solving this problem is the use of protective barriers of various shapes installed near highways. At the stage of designing these protective structures, an important task arises to assess their effectiveness.

Estimation of the effectiveness of protective barriers by the method of the physical experiment takes considerable time to set up and conduct an experiment, as well as analyze the results of physical modeling. This method is not always convenient during design work. An alternative method is the method of mathematical modeling. For the designer, it is very important to have mathematical models that make it possible to quickly obtain a predictive result and take into consideration a set of important factors on which the effectiveness of the protective barrier depends.

A method has been devised that makes it possible to assess the effectiveness of using protective barriers to reduce the level of air pollution near the highway. It was found that an increase in barrier height by 80 % leads to a 22 % decrease in the concentration of impurities behind the barrier. It was established that applying a barrier with a height of 1.5 m leads to a 26 % decrease in the concentration of impurities in buildings adjacent to the highway. A method has been devised to assess the effectiveness of using absorbent "TX Active" surfaces on the protective barrier located near the highway. This study's result revealed that the application of a barrier with one "TX Active" surface leads to a decrease in the concentration of NO behind the barrier by an average of 43 %. When using a barrier with two "TX Active" surfaces, a decrease in the NO concentration behind the barrier is 85 % on average

Keywords: air pollution, protective barrier, highway, numerical modeling, "TX Active" surface

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1. Introduction

The modern highway is a complex engineering structure, which is a powerful source of man-made impact on the environment due to the formation of intensive pollution zones near the highway. The emission of pollutants on the highway is a particular threat to humans [1]. Therefore, significant attention is paid to determining the patterns of formation of pollution zones near the highway [2], as well as the impact of this pollution on human health [3]. Over time, the requirements for the results from studying the patterns of formation of pollution zones near highways have increased. In such an analysis, it is necessary to take into consideration the chemical transformation of pollutants contained in emissions from cars [4]. Due to the significant negative impact of highways on environmental pollution and human beings, there is an important task to reduce this impact [5].

Therefore, when designing and building a highway, a set of tasks is resolved to reduce its negative impact on the environment. The solution to this problem is based on the implementation of special protective methods. The purpose of these methods is to limit the spread of pollution from the highway to person. The most common method of protecting air from pollution near highways in the world is the use of roadside protective barriers [6]. At the stage of designing a highway, it is very important to assess in advance the effectiveness of protective barriers that will be erected near the highway. To solve this problem, it is necessary to have specialized calculation methods. These methods should take into consideration the terrain of the area where the highway runs. Existing methods for assessing the effectiveness of protective barriers do not comprehensively take into consideration such significant factors as the body of the car, relief, protective barrier. Therefore, the assessment of the effectiveness of using protective barriers based on existing calculation methods is quite approximate. That renders relevance to the scientific research aimed at devising methods that make it possible to analyze the impact of protective barriers in order to reduce the level of air pollution near highways, taking into consideration the most significant factors.

2. Literature review and problem statement

The issue related to minimizing the level of air pollution near highways is typically based on the solution to two problems. The first task is to analyze the intensity of air pollution near the highway. The second task is the development of means aimed at reducing the level of air pollution near the highway. It should be noted that the most common means of air protection near highways is the use of protective barriers (obstacles) that change the direction of airflow near the highway and change the direction of distribution of impurities near the highway – up from the highway. That leads to a decrease in the concentration of impurities near the highway at the level of the human respiratory system. It is important to note that the construction of roadside protective barriers does not require significant investments and can be carried out through the use of typical construction equipment.

In [7], experimental studies were conducted to determine the intensity of air pollution near the highway. The value of the reported results is that the study was conducted in the form of a "field experiment". The data can be used only for the analysis of the formation of the pollution zone in the range of those parameters of meteorological conditions that took place during the experiment. Therefore, it is impossible to use them for other weather conditions or other terrains, which must be done during the design work.

Work [8] validated a set of mathematical models used to predict the level of air pollution near highways. But these models (AERMOD, CALINE, etc.) are based on the Gauss model. With this approach, it is impossible to determine the effect of protective barriers to reduce the intensity of air pollution. This is due to the fact that those models use a uniform field of wind speed, that is, a wind field that is formed in the absence of obstacles. Those models can be used to expressly assess the intensity and size of air pollution zones near highways.

Paper [9] reports the results of experiments on the analysis of the intensity of air pollution near highways in the presence or absence of obstacles. The measurement data make it possible to determine the intensity of reducing the level of air pollution under different weather conditions. But, during the experiments in [9], there were not enough sensors for measurements. Therefore, the results obtained are of a "pilot" nature and cannot be used in design work.

In work [10], experimental research was carried out under laboratory conditions to determine the effectiveness of suction systems to reduce the level of air pollution near a highway. The cited work also proposed a mathematical model that makes it possible to determine the effectiveness of the suction system. But the cited work does not take into consideration the impact of car bodies on the formation of pollution zones. From an aerodynamic point of view, the body of a car is an obstacle in the path of the wind flow, which radically changes the profile of the airspeed, and, therefore, the shape of the chemical contamination zone.

Study [11] considers the construction of a numerical model, which makes it possible to determine the effectiveness of using a vertical barrier near a highway, but the model does not make it possible to determine this effectiveness under conditions of complicated terrain.

In [12], a set of computational experiments on determining zones of chemical contamination from roads under conditions of obstacles was carried out. The authors used the Navier-Stokes equation to solve aerodynamic problems – calculating the field of airflow speed. But when using the Navier-Stokes equations, the computer time significantly increased when implementing the model, to several days to calculate one variant of the problem. Such a significant time is a very inconvenient factor in serial calculations at the stage of design work. The reason for the above is that during the working day it is necessary to determine the effectiveness of a large number of obstacle options for choosing the most effective.

Paper [5] reports the analysis of the impact of the height of the protective barrier on the formation of the air pollution zone near a highway. The cited work applied the Navier-Stokes equation (the FLUENT software package). But, during the computational experiments, the cited work did not take into consideration the impact of the body of a car on the formation of the pollution zone.

Work [13] considers the development of a CFD model to analyze the effectiveness of the use of a protective barrier to reduce the level of air pollution. The numerical model, proposed in the cited work, made it possible to determine the intensity and size of the pollution zone near a highway but that model did not take into consideration the complexity of the barrier shape and terrain.

Study [14] reports a numerical model for analyzing the use of protective barriers near highways located under conditions of complicated terrain. The model makes it possible to estimate the size and intensity of pollution zones for typical conditions: "embankment", "notch". But the disadvantage of the cited work is that a vehicle that emits pollutants is modeled as a point source of pollution.

Paper [15] describes the results of studies on reducing the concentration of pollutants near a highway in the case of the location of the plant protective barrier. The experimental data reported in the cited work make it possible to determine the effectiveness of this barrier in relation to a decrease in dust concentration at different heights. However, those data cannot be used to assess the effectiveness of these kinds of barriers, which are located differently relative to a highway and have a different height. That is, available scientific papers do not comprehensively take into consideration such significant factors as the barrier + relief + body of a car. All these factors are obstacles to the spread of impurities from the car and lead to the formation of an uneven field of airflow speed and, as a result, a complex zone of chemical contamination.

Study [16] reports the results of experimental studies on determining the effectiveness of the use of absorbent surfaces to reduce the level of chemical air pollution. It is shown in the cited work that such surfaces make it possible to locally reduce the concentration of NO_2 in the air. The cited study lacks mathematical models that could be used for a comprehensive analysis of this phenomenon.

In [17], the results of fundamental studies on reducing the level of air pollution near highways with absorbent coatings are given. Scientific data from the cited work confirm the effectiveness of the use of such coatings to minimize the negative impact of a highway on the environment.

In work [18], a numerical model was built to analyze the impact of the absorbent coating of a highway on the level of air pollution. The cited work also reports the results of experimental studies. The data in the cited work refer only to the configuration of the “canyon”, that is, for a highway with a coating, located between houses.

Based on papers in the scientific literature, it can be argued that issues related to the development of methods for evaluating the effectiveness of the use of protective barriers require further investigation.

3. The aim and objectives of the study

The purpose of this work is to build quick-computing CFD models to evaluate the effectiveness of the use of protective barriers near highways, taking into consideration various kinds of obstacles (terrain, barriers, buildings along the highway, car bodies, etc.). This would make it possible to reduce the time for research in this area.

To accomplish the aim, the following tasks have been set:

– to build a two-dimensional CFD model to calculate the effectiveness of the use of protective barriers installed near a highway under the conditions of difficult relief;

– to construct a three-dimensional CFD model to calculate the effectiveness of the use of a protective barrier with an absorbent coating;

– to conduct computational experiments based on the CFD models to be built.

4. The study materials and methods

Devising a method for evaluating the effectiveness of the use of protective barriers installed near highways is based on the construction of a numerical model (CFD model) that describes the physical process of impurity distribution in the atmospheric air.

To assess the effectiveness of the use of protective barriers, it is necessary to investigate how chemical air pollution zones are formed near a highway. This will take into consideration the complex terrain, the location near highways of protective barriers, the presence of an absorbent coating on the surface of protective barriers, an uneven wind speed field, atmospheric diffusion. These are the key factors influencing the formation of chemical contamination zones near highways.

Underlying the development of a method for evaluating the effectiveness of the use of protective barriers near a highway are multifactor numerical models. Below, the construction of such models is considered. To build a numerical model, finite-difference methods of integration of modeling equations [19] were used. Numerical integration of modeling equations is carried out on a rectangular difference grid.

5. Results of studying the construction of a method for evaluating the effectiveness of the use of protective barriers

5. 1. Devising a two-dimensional CFD model for calculating the effectiveness of the use of protective barriers under conditions of complex relief

To devise a method of express evaluation of the effectiveness of the use of vertical protective barriers under conditions of complex terrain, it makes sense to use two-dimensional mathematical models.

The construction of a method for calculating the effectiveness of the use of protective barriers near a highway is considered. This method is based on building a numerical model of the spread of impurities under conditions of complex relief. The scheme of the estimated area is shown in Fig. 1.

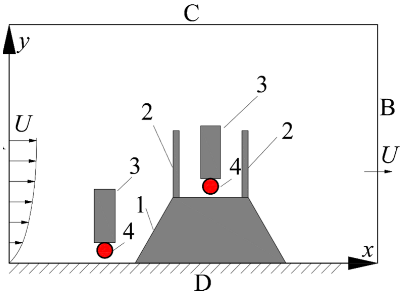

Fig. 1. Estimation scheme: 1 — embankment, 2 — protective barriers, 3 — car, 4 — emission source (exhaust pipe); A, B, C, D — boundaries of the estimated area

Emissions from ф car contain NO, NO_2. When constructing a mathematical model, we shall take into consideration the chemical transformations of these impurities as follows [4, 20]:

$$NO_2 + h_\nu \xrightarrow{J} NO + O, \tag{1}$$

$$O + O_2 \rightarrow O_3, \tag{2}$$

$$NO + O_3 \xrightarrow{k_1} NO_2 + O_2, \tag{3}$$

where J is the reaction rate parameter for the photolysis process depending on the amount of ultraviolet radiation, k_1 is the reaction speed parameter for NO, 1/s.

1. Modeling the process of convective-diffusion distribution of pollutants in the air from the source of emission (car).

2. Chemical conversion of pollutants in the air.

For modeling the transfer of NO, NO_2, O_3 in the atmospheric air (the first stage), the following equations of mass transfer [21] are used:

$$\begin{aligned}&\frac{\partial C_{NO}}{\partial t}+\frac{\partial\left(uC_{NO}\right)}{\partial x}+\frac{\partial\left(vC_{NO}\right)}{\partial y}=\\&=\frac{\partial}{\partial x}\left(\mu_x\frac{\partial C_{NO}}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu_y\frac{\partial C_{NO}}{\partial y}\right)+\\&+\sum_{i=1}^{n}Q_{NOi}(t)\delta\left(x-x_{0i}\right)\delta\left(y-y_{0i}\right),\end{aligned}\tag{4}$$

$$\begin{aligned}&\frac{\partial C_{NO_2}}{\partial t}+\frac{\partial\left(uC_{NO_2}\right)}{\partial x}+\frac{\partial\left(vC_{NO_2}\right)}{\partial y}=\\&=\frac{\partial}{\partial x}\left(\mu_x\frac{\partial C_{NO_2}}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu_y\frac{\partial C_{NO_2}}{\partial y}\right)+\\&+\sum_{i=1}^{n}Q_{NO_2 i}(t)\delta\left(x-x_{0i}\right)\delta\left(y-y_{0i}\right),\end{aligned}\tag{5}$$

$$\begin{aligned}&\frac{\partial C_{O_3}}{\partial t}+\frac{\partial\left(uC_{O_3}\right)}{\partial x}+\frac{\partial\left(vC_{O_3}\right)}{\partial y}=\\&=\frac{\partial}{\partial x}\left(\mu_x\frac{\partial C_{O_3}}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu_y\frac{\partial C_{O_3}}{\partial y}\right),\end{aligned}\tag{6}$$

where $C_{NO}(x,y,t)$, $C_{NO_2}(x,y,t)$, $C_{O_3}(x,y,t)$ are the concentrations of NO, NO, NO_2, O_3, kg/m^3; $Q_{NO,i}$, $Q_{NO_2,i}$ are the emission intensities of NO, NO_2 from the i-th emission source (car), kg/(s·m^3); u, v are the components of wind speed vector, m/s; $\mu=\left(\mu_x,\mu_y\right)$ is the coefficient of turbulent diffusion, m^2/s; x_{0i}, y_{0i} are the coordinates of pollutant emission sources (a highway), m; $\delta\left(x-x_{0i}\right)\delta\left(y-y_{0i}\right)$ is the Dirac delta function, which simulates the presence of pollutant emission, m^{-2}.

The values of diffusion coefficients are calculated from formulas: $\mu_x=k_0\cdot U$, $k_0=(0.1\div 1)$ depending on the degree of atmospheric stability, U is the wind speed, m/s; $\mu_y=k_1\left(\frac{Y}{Y_1}\right)^m$, $k_1=(0.1\div 0.2)$ m^2/s within the height of the atmospheric near-Earth layer, Y_1=10 m, $m\approx 1$.

The boundary conditions for modeling equations are discussed in [19].

The delta function is zero everywhere except the sites where the i-th source of pollution is located. The emission of pollutants from vehicles is simulated by point sources of the predefined intensity Q_{NOi}, $Q_{NO_2 i}$, n is the number of sources of pollution. $\sum_{i=1}^{n}Q_{NO_2 i}(t)\delta\left(x-x_{0i}\right)\delta\left(y-y_{0i}\right)$ means that all sources of pollution with a specific pollutant intensity are taken into consideration, accounting for the principle of superposition.

At the second stage of solving the problem, the chemical transformation of substances in the atmospheric air is calculated using the following dependences:

$$\frac{\partial C_{NO}}{\partial t}=-k_1\cdot C_{NO}\cdot C_{O_3}+J\cdot C_{NO_2},\tag{7}$$

$$\frac{\partial C_{NO_2}}{\partial t}=k_1\cdot C_{NO}\cdot C_{O_3}-J\cdot C_{NO_2},\tag{8}$$

$$\frac{\partial C_{O_3}}{\partial t}=-k_1\cdot C_{NO}\cdot C_{O_3}+J\cdot C_{NO_2}.\tag{9}$$

During the calculations, we accepted: J=0.0045 s^{-1}, μ_y=0.00039 (ppm·s)$^{-1}$ [4].

In this model, it is accepted that the NO_2 emission is about 5 % of the NO_x emission, and the rest of the emission, about 95 %, is the NO emission.

This paper considers the dispersion of emissions from vehicles in the case when protective barriers are located near a highway, and the terrain has a complex relief, as shown in Fig. 1. In this case, an uneven field of airflow speed is formed in the examined region. This field must be known to solve modeling equations (4) to (6). To calculate the airflow under such conditions, a potential flow model is used. In this case, the modeling equation is the Laplace equation for the speed potential [19]:

$$\frac{\partial P^2}{\partial x^2}+\frac{\partial P^2}{\partial y^2}=0.\tag{10}$$

For equation (10), the following boundary conditions are set (Fig. 1):

– at boundary A – the flow enters the estimated region, the limit condition of Neiman is set for the speed potential

$$\frac{\partial P}{\partial x}=U,$$

where U is the known wind speed value

$$U=U_1\cdot\left(y/y_1\right)^{n_1},$$

where U_1 is the value of wind speed at some fixed height y_1=10 m $n_1\approx 0.15-0.69$, , since it depends on the roughness of the bedding surface and the class of stability of the atmosphere; the value n_1=0.15 was taken in this work;

– at boundary B – the flow leaves the estimated region, for the potential of the speed, the Dirichlet limit condition is set, $P=P_0$+const, where P_0 is a certain numeric constant equal to 100;

– at boundary C – the upper limit, a solid non-penetrable wall, the impenetrability condition is set, $\frac{\partial P}{\partial y}=0,$ since in the numerical calculations there can be no infinite boundary, it is chosen at a sufficient distance, where the curvature of the current lines is insignificant;

– at boundary D – the lower limit, solid opaque wall, the impenetrability condition is set $\frac{\partial P}{\partial y}=0;$

– on all rigid walls of the embankment, barriers, and car, depending on the direction of normal, the condition of impenetrability must be met.

Components of the airflow rate vector are calculated based on the following dependences [19]:

$$u=\frac{\partial P}{\partial x},\quad v=\frac{\partial P}{\partial y}.$$

Thus, the platform for predicting air quality near a highway with complex terrain and in the presence of barriers are modeling equations (4) to (10).

5. 2. Building a three-dimensional CFD model for calculating the effectiveness of the use of a protective barrier with an absorbing coating

The construction of a method for calculating the effectiveness of the use of absorbent surfaces on protective barriers located near a highway is considered. This method is based on building a numerical model of impurity propagation and its interaction with the absorbent surface.

Surfaces that absorb NO ("photocatalytic" surfaces, "TX Active" surfaces) are used not only to cover the road surface but also to cover protective barriers. To solve the problem of determining the impact of barriers with the "photocatalytic" surface on the formation of air medium quality near a highway, a mathematical model was built. The modeling equations of this model are as follows [19, 20]:

$$\frac{\partial C}{\partial t}+\frac{\partial uC}{\partial x}+\frac{\partial vC}{\partial y}+\frac{\partial (w-w_s)C}{\partial z}+\sigma C=$$
$$=\frac{\partial}{\partial x}\left(\mu_x\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu_y\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial z}\left(\mu_z\frac{\partial V}{\partial z}\right)+$$
$$+\sum_{i=1}^{n}Q_i(t)\delta(x-x_i)\delta(y-y_i)\delta(z-z_i), \qquad (11)$$

$$\frac{\partial^2 P}{\partial x^2}+\frac{\partial^2 P}{\partial y^2}+\frac{\partial^2 P}{\partial z^2}=0, \qquad (12)$$

$$u=\frac{\partial P}{\partial x},\quad v=\frac{\partial P}{\partial y},\quad w=\frac{\partial P}{\partial z}, \qquad (13)$$

where P is the speed potential;

C is the concentration of the pollutant (NO);

$Q_i(t)$ is the intensity of pollutant emission;

u, v, w are the projections of the airflow rate vector on axes in the Cartesian coordinate system, m/s;

t – time, s;

w_s is the rate of settling of the pollutant, m/s;

σ is a parameter that takes into consideration the washing out of the pollutant, s^{-1};

$\mu=(\mu_x,\mu_y,\mu_z)$are the coefficients of turbulent diffusion, m^2/s,

x_i, y_i, z_i are the coordinates of the emission source, m;

$\delta(x-x_i)\delta(y-y_i)$ $\delta(z-z_i)$ is the Dirac delta function, m^{-3}.

The boundary conditions for modeling equations (11) to (13) are as follows:

1. $\frac{\partial P}{\partial n}=0$ at impenetrable boundaries.

2. $\frac{\partial P}{\partial n}=0$ at the upper surface.

3. $\frac{\partial P}{\partial n}=V_n$ at the boundary where the flow flows in (V_n is the airflow speed).

4. P=const – at the boundary of the flow outlet.

5. At the boundary of the flow inlet: C=0.

6. At the boundary of the flow outlet: $\left.\frac{\partial C}{\partial n}\right|_{\Gamma_2}=0$.

7. At the boundary z=0, $z=L_z$ (L_z is the region's upper boundary):

$$\frac{\partial C}{\partial n}=0,$$

where n is the unit vector of the outer normal to the surface.

For the time t=0, the starting condition is written as C=0.

To simulate the absorption process of "TX Active" by the surface, the following boundary condition is used on this surface (for NO concentration):

$$C=0. \qquad (14)$$

To determine the amount of pollutant absorbed by the "TX Active" surface during dt, the boundary condition (14) and Fick's law are used. Fick's law for a given process is written as follows:

$$J=-\mu S\frac{\partial C}{\partial n}dt,$$

where J is the flow of the mass of the pollutant to the surface that falls on the surface; μ is the diffusion coefficient; S is the surface area through which the diffusion flow passes.

The concentration gradient is as follows:

$$\frac{\partial C}{\partial n}=\frac{C_{i,j}-C_{surf}}{s_x},$$

where $s_x=0.5\cdot h_x$; h_x is the step of the difference grid in the direction of the Ox axis;

C_{surf} is the concentration of a pollutant on a photocatalytic surface; $C_{i,j}$ is the concentration of the pollutant in the difference cell adjacent to the photocatalytic surface.

It should be noted that the concentration of the pollutant is calculated in the center of the difference cell.

Thus, the mass of the pollutant that "escaped" from the difference cell during the time dt on the "TX Active" surface is calculated. The following is the concentration of the pollutant in the difference cell adjacent to the photocatalytic surface. In the numerical model built, the absorbent surface is set with the help of markers.

Fundamental models in the mechanics of a continuous environment allow only a numerical solution within the framework of the considered boundary-value problems. Therefore, it is necessary to construct numerical models based on modeling equations (4) to (13).

Numerical integration of modeling equations is carried out on a rectangular difference grid. For the numerical integration of mass transfer equations (4) to (6), the physical splitting of modeling equations is carried out. An example of such splitting is given only for equation (4):

$$\frac{\partial C_{\mathrm{NO}}}{\partial t}+\frac{\partial uC_{\mathrm{NO}}}{\partial x}=\frac{\partial}{\partial x}\left(\mu_x\frac{\partial C_{\mathrm{NO}}}{\partial x}\right), \qquad (15)$$

$$\frac{\partial C_{\mathrm{NO}}}{\partial t}+\frac{\partial vC_{\mathrm{NO}}}{\partial y}=\frac{\partial}{\partial y}\left(\mu_y\frac{\partial C_{\mathrm{NO}}}{\partial y}\right), \qquad (16)$$

$$\frac{\partial C_{\mathrm{NO}}}{\partial t}=\sum_{i=1}^{n}Q_{\mathrm{NO}\,i}(t)\delta(x-x_{0i})\delta(y-y_{0i}). \qquad (17)$$

In order to solve equations (15), (16) numerically, a two-step splitting scheme [19] is used. For equation (15), this scheme is:

– the first step is to use the following dependence:

$$C^{n+\frac{1}{2}}_{\mathrm{NO}i,j}=C^{n}_{\mathrm{NO}i,j}-\Delta t\frac{u^{+}_{i+1,j}C^{n+\frac{1}{2}}_{\mathrm{NO}i,j}-u^{+}_{i,j}C^{n+\frac{1}{2}}_{\mathrm{NO}i-1,j}}{\Delta x}+$$
$$+\Delta t\,\mu_x\frac{-C^{n+\frac{1}{2}}_{\mathrm{NO}i,j}+C^{n+\frac{1}{2}}_{\mathrm{NO}i-1,j}}{2\Delta x^2}+\Delta t\,\mu_x\frac{-C^{n}_{\mathrm{NO}i,j}+C^{n}_{\mathrm{NO}i+1,j}}{2\Delta x^2};$$

– the second step uses the following dependence:

$$C_{NOi,j}^{n+1} = C_{NOi,j}^{n+\frac{1}{2}} - \Delta t \frac{u_{i+1,j}^{-} C_{NOi+1,j}^{n+1} - u_{i,j}^{-} C_{NOi,j}^{n+1}}{\Delta x} + \Delta t \mu_x \frac{-C_{NOi,j}^{n+\frac{1}{2}} + C_{NOi-1,j}^{n+\frac{1}{2}}}{2\Delta x^2} + \Delta t \mu_x \frac{-C_{NOi,j}^{n+1} + C_{NOi+1,j}^{n+1}}{2\Delta x^2},$$

where

$$u^{+} = \frac{u+|u|}{2}, \quad u^{-} = \frac{u-|u|}{2}.$$

A similar scheme is written for equation (16). In order to solve equation (17) numerically, the Euler method is used [22]. For numerical integration of equation (10), an implicit difference scheme [22] is applied.

The software implementation of the devised numerical model was carried out; the code "Barrier-2" was developed in the programming language FORTRAN.

A similar approach was used for the numerical integration of three-dimensional equations (11), (12). The software implementation of the constructed three-dimensional numerical model was carried out; the code "Barrier-TX" was developed in the programming language FORTRAN.

5. 3. Conducting computational experiments based on the built CFD models

Below are the results from solving two problems based on the built CFD models. The first problem is to simulate air pollution near a highway (Fig. 1) based on the "Barrier-2" code. Two scenarios were considered: there are no barriers on the embankment and there are protective barriers to the embankment. Calculations were carried out with the following data: airflow rate, 5 m/s; the average intensity of nitrogen oxide emission, Q_{NOx}=4.8 g/s. It was assumed that the share of NO_2 is 5 % of NO_x emissions, and NO – 95 %. The geometric dimensions of the region are 28 m along the Ox axis and 14 m along the Oy axis, which is directed vertically upwards. The coordinates of the emission source of NO and NO_2 are the coordinates of the location of the exhaust pipe hole of a car.

Fig. 2, 3 show the NO concentration field for both scenarios. For the convenience of analyzing the pollution zone, the concentration of impurities is shown as a percentage of the maximum value of NO concentration in the estimated region.

After analyzing the data given in Fig. 2, 3, it can be seen that subzones with a significant gradient of impurity concentration are formed near cars. The use of protective barriers can reduce the level of pollution behind the barrier on the leeward side of the embankment (zone "*B*" in Fig. 2, 3). However, the use of protective barriers leads to an increase in the zone of pollution for height.

Fig. 4 shows how the concentration of NO on the leeward side of the embankment changes for the different heights of barriers (zone "*B*" in Fig. 3).

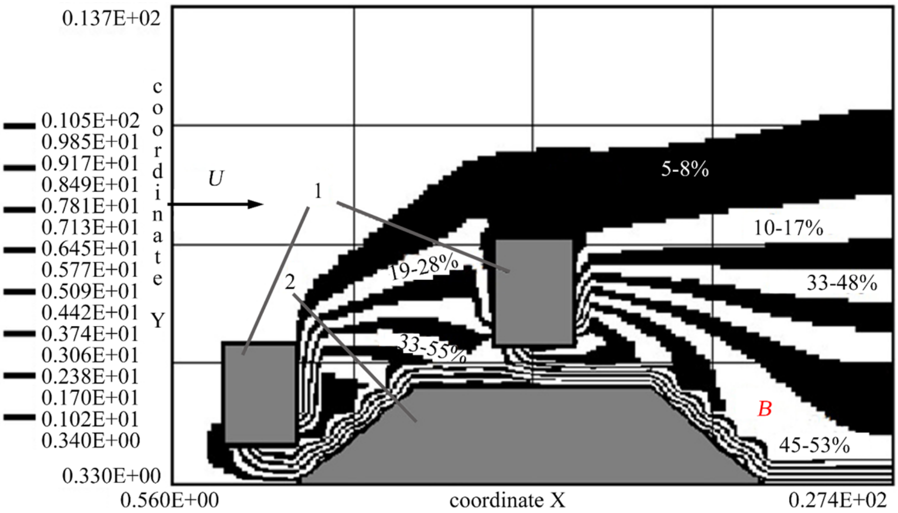

Fig. 2. Concentration field of NO (no protective barriers): 1 — car, 2 — embankment

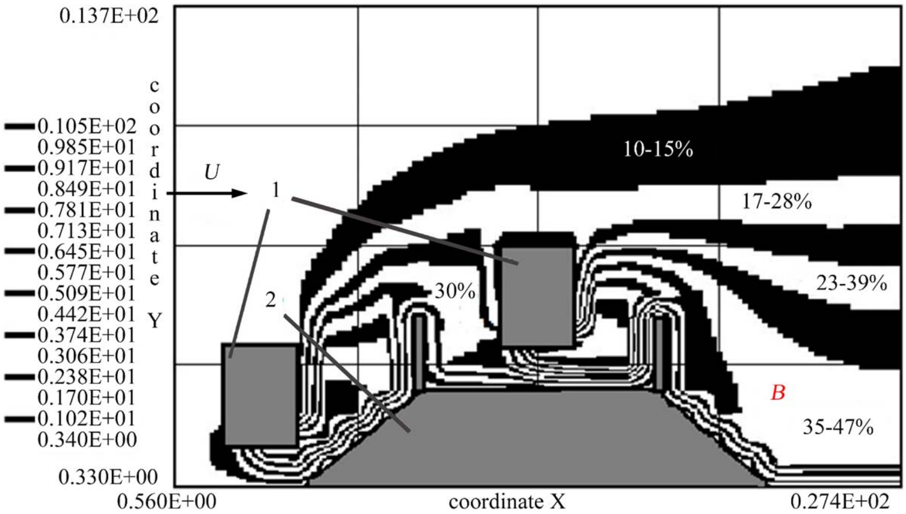

Fig. 3. Concentration field of NO (height of protective barriers, *H*=2.5 m): 1 — car, 2 — embankment

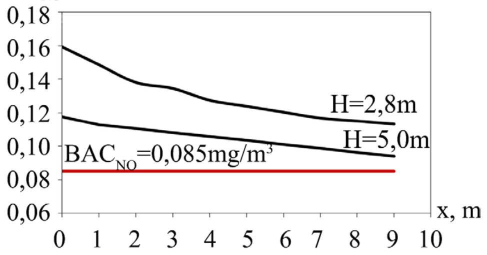

Fig. 4. Change in the NO concentration at a height of 1.7 m along the Ox axis in region *B* (behind the second barrier)

Analysis of the data given in Fig. 4 reveals that when using a barrier with a height of 2.8 m, the concentration of impurities behind the barrier is in the range of 0.16–0.115 mg/m^3. When using a barrier with a height of 5 m, the concentration of impurities behind the barrier is in the range of 0.12–0.09 mg/m^3. Thus, an increase in the barrier height by 80 % leads to a decrease in concentration by 22 %.

It should be noted that the computation time of each problem was 5 s.

Next, a model problem is considered in this work when a trade or service pavilion is located near the road. In the absence of a barrier, polluted air penetrates the pavilion, thereby harming the respiratory system of employees and visitors to the pavilion. Fig. 5 clearly shows the distribution of zones of pollution of harmful impurities *NO* near a highway, inside and outside the pavilion.

Fig. 6 shows the distribution of zones of pollution of harmful impurities NO both within the highway and in the adjacent territory, but in the presence of a barrier. This barrier is an obstacle that inhibits and redistributes the flow. As a result, the concentration behind the barrier decreases, namely inside the pavilion.

The comparative analysis of the estimated values of *NO* concentration and maximum permissible concentration for *NO* are shown in Fig. 7. It is clearly visible that in the presence of a barrier, the concentration value inside the pavilion decreases by 26 % and does not exceed $\mathrm{MPC}_{NO}=0.085$ mg/m^3.

Below are the results of solving the problem of determining the effectiveness of the use of the protective barrier with the “TX Active” surface. Modeling was carried out with the following initial data: dimensions of the estimated area, 25×25×12 m; emission intensity $Q_{NO_x}=1$ (in dimensionless form), of which NO_2 is 5 % of NO_x emission, and NO – 95 %; air speed, 5.2 m/s. In the cross-section, x=11 m, y=11 m, there is a car; the height of the barrier is 3 m (Fig. 8).

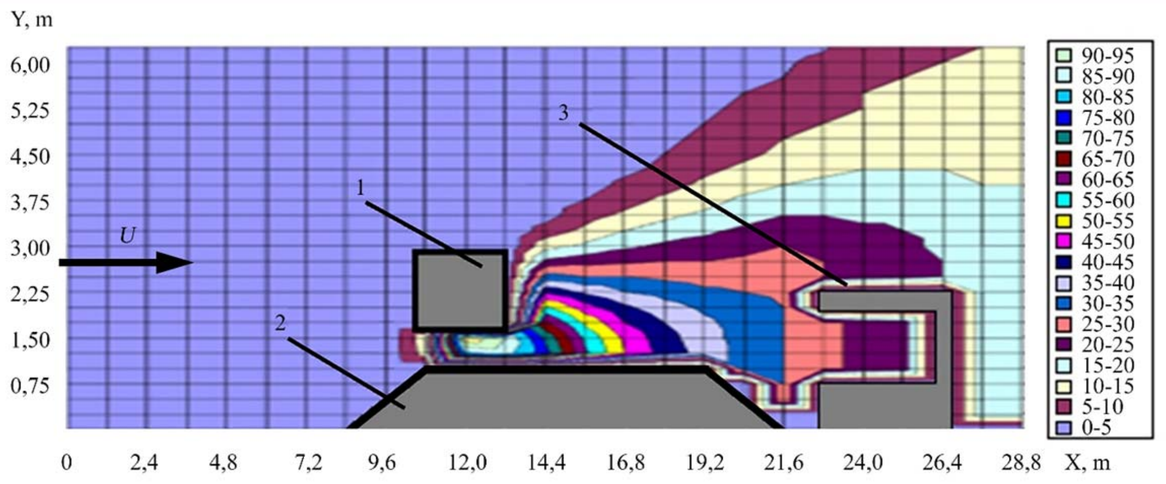

Fig. 5. Distribution of NO concentration field in the absence of a barrier (H=1.5 m): 1 – emission source (cars); 2 – embankment; 3 – pavilion, (C_{NO} as a percentage of $(C_{NO})_{max}$=0.4128 mg/m^3)

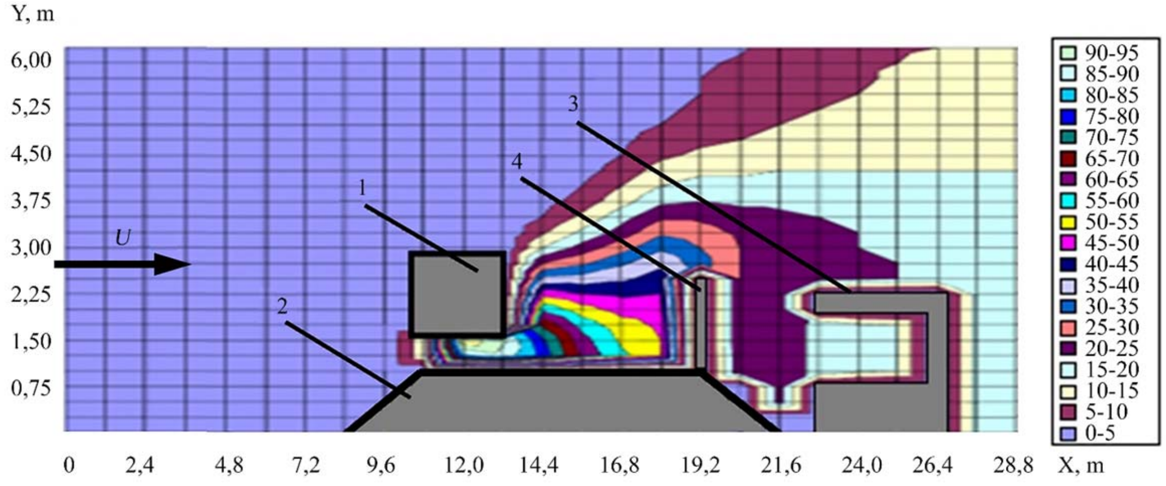

Fig. 6. Distribution of NO concentration field in the presence of a barrier (H=1.5 m): 1 – emission source (cars); 2 – embankment; 3 – pavilion; 4 – barrier (C_{NO} as a percentage of $(C_{NO})_{max}$ =0.4194 mg/m^3)

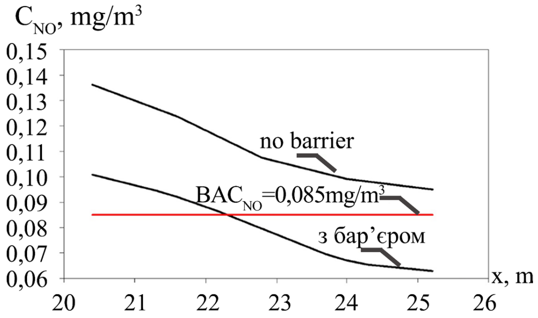

Fig. 7. Distribution of *NO* concentration in the pavilion at the human respiratory level (*H*=1.7 m) compared to MPC$_{NO}$=0.085 mg/m^3 with and without a barrier

Below is an estimated diagram (cross-section, *y*=12 m) for each scenario of examining the effectiveness of using a vertical barrier that has a "TX Active" surface:

1. Scenario #1 – the vertical barrier has a "TX Active" surface only on the windward side (Fig. 9).
2. Scenario #2 – the vertical barrier has a "TX Active" surface on the windward side and on the leeward side (Fig. 10).

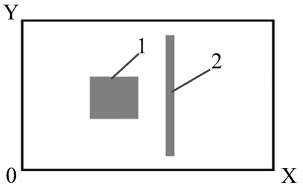

Fig. 8. Scheme of the estimated region (cross-section, *z*=0.7 m): 1 — car; 2 — barrier with a "TX Active" surface

Fig. 11, 12 show pollution zones for each problem scenario. The area of contamination (the distribution of NO concentration, dimensionless value·10^2) is shown in these figures for the cross-section *y*=12 m.

Fig. 13 shows the dimensionless value of *NO* concentration in the working area behind the barrier at a height of 1.5 m and at different lengths.

As can be seen from Fig. 13, the use of the "TX Active" surface makes it possible to significantly reduce the concentration of the pollutant in the working area.

It should be noted that solving each problem requires 6 s of computer time.

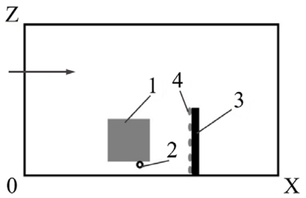

Fig. 9. Diagram of the estimated area (scenario #1): 1 — the body of a car; 2 — a place of the pollutant emission; 3 — barrier; 4 — "TX Active" surface

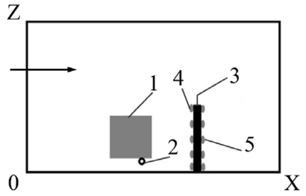

Fig. 10. Diagram of the estimated region (scenario #2): 1 — car body; 2 — place of the pollutant emission; 3 — barrier; 4 — "TX Active" surface; 5 — "TX Active" surface

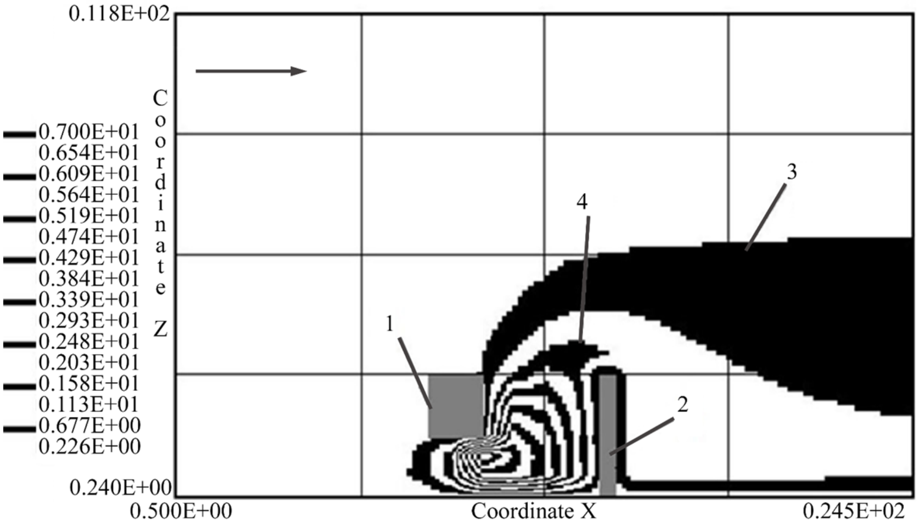

Fig. 11. Pollution zone (scenario #1): 1 — car body; 2 — barrier; 3 — *C*=0.67; 4 – *C*=1.50

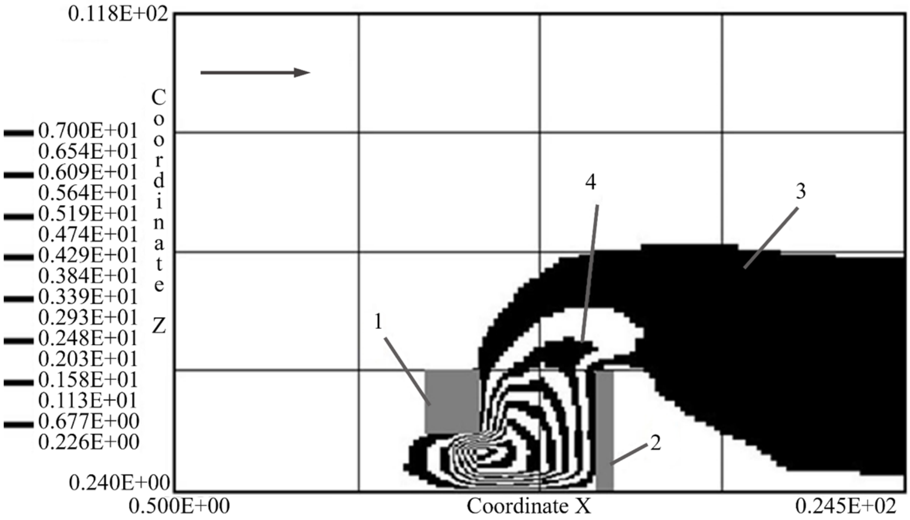

Fig. 12. Pollution zone (scenario #2): 1 — car body; 2 — barrier; 3 — *C*=0.67; 4 – *C*=1.50

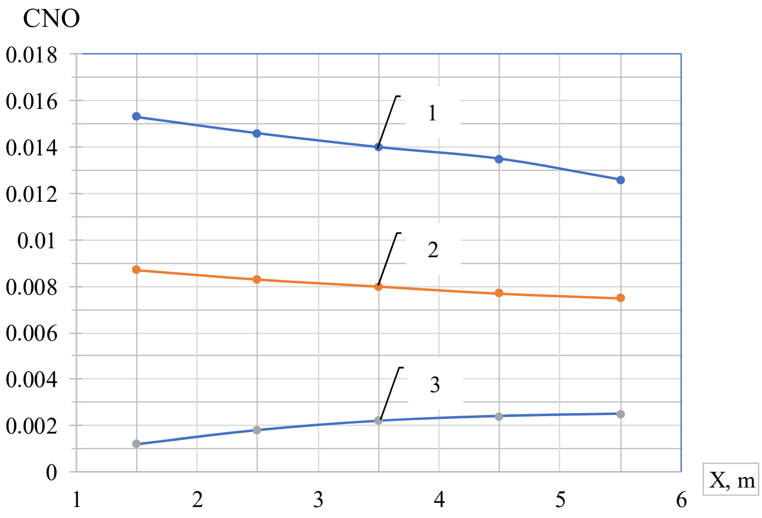

Fig. 13. Dimensionless value of *NO* concentration behind a barrier:
1 – base (barrier without "TX Active" surface);
2 – scenario #1 ("TX Active" surface only on one side of the barrier);
3 – scenario #2 ("TX Active" surface on both sides of the barrier)

6. Discussion of results of studying the construction of a method for evaluating the effectiveness of the use of protective barriers near highways

The built two-dimensional CFD model, based on equations (4) to (10), makes it possible to determine the field of air pollution near a highway (Fig. 2, 3, 5, 6) taking into consideration the chemical transformation of NO, NO_2 contained in emissions from a car (equations (7) to (9)). That is, it becomes possible to simulate the process of air pollution with a greater approximation to reality. Based on the devised CFD model, a study was carried out to determine the effectiveness of the use of protective barriers of different heights located under conditions of difficult terrain. Our studies have shown a significant impact of barrier height on reducing the concentration of impurities near a highway. With an increase in the height of the barrier, there is a more intense reversal of airflow from the barrier upwards, as a result of which the concentration of impurities in the territory adjacent to the highway decreases. It was found that an increase in barrier height by 80 % leads to a 22 % decrease in the concentration of impurities behind the barrier. It was established that the use of a barrier with a height of 1.5 m leads to a decrease in the concentration of impurities by 26 % in the facilities adjacent to the highway. The method devised could be used to scientifically substantiate the size of protective barriers and their location near highways to ensure the required level of air quality in areas of interest.

The built three-dimensional CFD model, based on equations (11) and (12), makes it possible to get predictive information about the effectiveness of the use of barriers with the "TX Active" surface (Fig. 13). This takes into consideration the location of this surface on the barrier. Our studies have shown that the use of a barrier with one "TX Active" surface leads to a decrease in the concentration of *NO* behind the barrier by an average of 43 %. When using a barrier with two "TX Active" surfaces, the decrease in the *NO* concentration behind the barrier is an average of 85 %. Therefore, it is recommended to use protective barriers with a two-sided "TX Active" surface

The computational experiments confirmed the possibility of using the built CFD models to analyze pollution zones near a highway in order to quickly obtain predictive information that is necessary to assess the effectiveness of the use of protective barriers near highways (Fig. 2, 3, 5, 6, 11, 12).

A special feature of the proposed method for assessing the effectiveness of barriers, based on the CFD models constructed, is the speed of calculation on a computer (computation time is a few seconds). High calculation speed becomes possible due to the fact that the wind speed field in the constructed CFD models is determined on the basis of simple equations (10), (12) – the dynamics equation of the "ideal" liquid. Known calculation methods, for example [12–14], involve a more complex model of aerodynamics – the viscous flow equation with an additional turbulence model where the calculation time is several days. When using a viscous flow model, a very fine grid is required so that when calculating, the circuit viscosity does not exceed the value of turbulent viscosity of the flow.

The disadvantages of the CFD models built include the fact that the model of airflow aerodynamics does not take into consideration turbulent viscosity. In addition, when using models, several empirical constants are employed, the values of which need to be clarified in some cases. The limitation of the proposed method of evaluating the effectiveness of protective barriers is also that it cannot be used when the barrier material is porous or air-penetrating (for example, a straw barrier).

The current study is to be advanced by building a numerical model that could additionally determine the effectiveness of barriers to reduce noise pollution of the environment.

7. Conclusions

1. A two-dimensional CFD model for the analysis of pollution zones formed near a highway, which is located under conditions of complex relief, has been built. The model makes it possible, during calculations, to take into consideration the influence of protective barriers, car bodies, the location of various kinds of structures, and other physical parameters on the formation of chemical pollution zones near a highway. It was found that an increase in barrier height by 80 % leads to a 22 % decrease in the concentration of impurities behind the barrier. It was established that the use of a barrier with a height of 1.5 m leads to a decrease in the concentration of impurities by 26 % in the facilities adjacent to the highway.

2. A three-dimensional CFD model has been constructed to analyze the pollution zones formed near a highway, which has protective barriers with the "TX Active" surface. The model makes it possible to take into consideration the set of important physical factors affecting the formation of pollution zones near highways when determining the effectiveness of these barriers.

3. The results of computational experiments obtained on the basis of the constructed CFD models show that the

models built have a wide working range, and make it possible to quickly get predictive data. These data could be useful in assessing the effectiveness of the use of protective barriers near highways. Our studies have shown that the use of a barrier with one "TX Active" surface leads to a decrease in the concentration of NO behind the barrier by an average of 43 %. When using a barrier with two "TX Active" surfaces, the decrease in the NO concentration behind the barrier is an average of 85 %. Thus, it is recommended to use protective barriers that have a two-sided "TX Active" surface.

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