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METHODOLOGICAL APPROACHES TO MATHEMATICAL MODELING OF METHANE DISPERSION IN ATMOSPHERIC AIR

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Abstract. Nowadays, the amount of methane entering the environment from various sources remains a serious problem. Methane is released into the atmosphere during the production, processing, storage, transportation and distribution of natural gas and crude oil. Coal mining, household and business waste, domestic and industrial wastewater treatment and landfills are the main sources of methane emissions. The development of the economy, the increase in the consumption of various products leads to an increased number of natural and household waste storages. Currently, much attention is paid to the methane collection and utilization. However, there is no growing tendency to reduce the sources of methane emissions. In this regard, to estimate level of methane concentration coming from the sources of its release remains an urgent task. The task is quite complex as it requires taking into account physical and meteorological parameters, as well as different types of sources and their location. The authors propose a numerical model based on the three-dimensional equation of mass transfer. The solution of this equation is performed by finite-difference methods, which allows obtaining methane concentration field at any height from the earth's surface. The developed numerical model allows taking into account location of the methane source, a point or area source, the change in air flow speed with height, atmospheric turbulent diffusion coefficients. On the basis of the developed numerical model, a computer code was created for the operational forecast of methane concentration fields under the influence of a pollution source. Based on the developed program, the model task of forecasting atmospheric air pollution zones during methane emission from the future waste storage facility was solved, the predicted pollution zone was obtained in the form of isolines of methane concentration. The obtained results can be useful while conducting many numerical calculations when new methods of selection, disposal and protection are implemented.

Keywords: methane concentration, mathematical modeling, numerical calculation, pollution level, waste storage

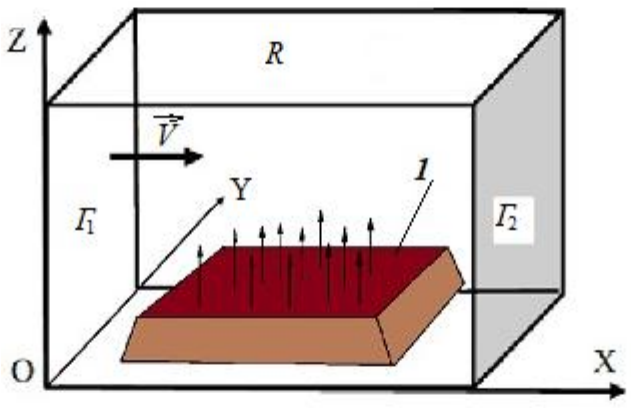
Introduction. Over the past two centuries, there has been a significant increase in the concentration of methane in the atmosphere. According to some sources, this increase is more than twice. Considering the fact that methane belongs to greenhouse gases, it can be argued that the increase in its concentration in the atmosphere is one of the factors contributing to the warming of the Earth's climate. In this regard, much attention is currently being paid to solving two problems: assessing the intensity of methane entering the atmosphere from various sources and its subsequent dispersion under the influence of wind and atmospheric diffusion, chemical transformations [1-2, 4]. To solve these important tasks, it is necessary to have scientifically based methods of forecasting the concentration of methane in the atmosphere.

The theoretical solution to the problem of methane dispersion in the atmosphere is a difficult task, since it is necessary to comprehensively take into account the influence of wind, atmospheric diffusion, chemical transformation of methane in atmospheric air on the formation of its concentration fields. There is no universal method of solving such a problem. Abroad, the Gaussian model [3-4] or numerical models implemented in the form of specialized codes WRF-Che, MOZART-4 and others [1] are used to estimate the concentration fields of impurities in atmospheric air. Such codes require the use of very powerful computers and a great amount of input information, which is not always available. There is also a problem to specifying correctly methane emission sources when using some codes. Therefore, there is an urgent problem of creating effective numerical models that can be used to estimate methane concentration fields in the atmosphere when it is emitted from various sources.

Methods. The purpose of this work is to create a fast numerical model for forecasting methane concentration fields in the atmosphere when it is emitted from various sources.

First of all, the development of mathematical models for the analysis of the spread of any impurity in atmospheric air is based on the determination of transfer scale. In practice, when considering industrial emissions, the most widely considered scale of transfer is "local" – transfer over a length of several hundreds of meters and "urban" – transfer over a length of 10-20 km. To determine the concentration of methane in atmospheric air within these scales, the three-dimensional equation of convective-diffusion transfer of impurities in air, which expresses the law of mass conservation for CH_4, will be used [5-9].

Mathematical model. The scheme of the calculation area for forecasting the level of methane concentration in the atmospheric air during its emission from the waste storage is shown in Figure 1.



1 – the waste storage; Γ_1, Γ_2, R – the left, right and upper faces of the calculation area, $\vec{V}$ – the velocity vector of the air flow at the entrance to the calculation area

Figure 1 – Scheme of the calculation area

A three-dimensional equation of impurity transfer is used for modelling CH_4 pollution (1) [5-9]:

$$\frac{\partial C}{\partial t}+\frac{\partial uC}{\partial x}+\frac{\partial vC}{\partial y}+\frac{\partial wC}{\partial z}+\sigma C= \\ =\frac{\partial}{\partial x}(\mu_x\frac{\partial C}{\partial x})+\frac{\partial}{\partial y}(\mu_y\frac{\partial C}{\partial y})+\frac{\partial}{\partial z}(\mu_z\frac{\partial C}{\partial z})+ \\ +\sum_{i=1}^{n}Q_i(t)\delta(x-x_i,y-y_i,z-z_i), \quad (1)$$

where C – the concentration of methane CH_4 in atmospheric air, [mg/ m^3]; $Q_i(t)$– the intensity of methane emission (it is assumed that this intensity depends on time, it is possible to simulate an increase or decrease of methane emission due to specific conditions), [mg/(s·m^3)]; *u(x,y,z), v(x,y,z), w(x,y,z)* – components of the air velocity vector, [m/s]; σ – a coefficient that takes into account the chemical transformations of methane in the air, as well as the "washing out" of the impurity by precipitation [1/s]; $\mu=(\mu_x,\mu_y,\mu_z)$ – the coefficients of atmospheric turbulent diffusion, [m^2/s]; x_i, y_i, z_i – the coordinates of the location of methane emission sources, [m]; $\delta(x-x_i, y-y_i, z-z_i)$ – the Dirac delta function, which simulates the location of the methane emission source; t – time, [s].

The following boundary conditions are applied in the transfer equation (1) [8-9]: on the lateral faces of the calculated three-dimensional area: on part of the face Γ_1, where the flow enters the calculation area, the concentration of pollution is known, the pollution introduced from outside is usually not taken into account, namely $C_{\Gamma_1}=0$, where $\vec{V}\cdot\vec{n}<0$; on part of the face Γ_2, where air masses flow out of the calculation area, diffusive transfer relative to convective transfer is neglected, i.e. $\left.\frac{\partial C}{\partial n}\right|_{\Gamma_2}=0$, where $\vec{V}\cdot\vec{n}\geq 0$.

The condition $\left.\frac{\partial C}{\partial z}\right|_{z=0}=\alpha C$, $\alpha>0$ is given for the plane $z=0$ (surface of the earth), where α is a coefficient that takes into account the nature of the interaction of the pollutant with the earth's surface.

At the upper face R of the possible spread of pollution, the vertical component of the velocity $w=0$, therefore, the condition of absence of diffusive transfer at the boundary $\left.\frac{\partial C}{\partial z}\right|_{z=Z}=0$ or the condition $C|_{z=Z}=0$ can be established.

If the condition that the amount of methane with concentration C_s flows from outside into the calculation area is met, then the boundary condition has the form $C_{\Gamma_1}=C_s$ on part of the border Γ_1, where $\vec{V}\cdot\vec{n}<0$.

The initial condition for equation (1) is $C|_{t=0}=0$ or $C|_{t=0}=C_0$ (where C_0 – the known background concentration).

The speed of the air flow is modeled by the dependence (2) [5; 7]:

$$V=V_1\frac{lgz/z_0}{lgz_1/z_0}, \tag{2}$$

where V_1 – wind speed at altitude z_1; z_0 – surface roughness.

When calculating methane concentration, atmospheric turbulent diffusion coefficients are calculated as follows [5; 7]:

– for height $z>h$, where h is the height of the surface layer, in the numerical calculation, $\mu_x\approx\mu_y\approx\mu_z$ are accepted, the vertical diffusion coefficient

$\mu_z = \gamma + k_1 \frac{h}{z_1}$, where γ – molecular diffusion coefficient, k_1 – turbulent diffusion coefficient at altitude $z = 1$ m;

– for height $z < h$, $\mu_x \approx \mu_y$, the horizontal turbulent diffusion coefficient is calculated $\mu_y = k_0 \cdot V$, where $k_0 = 0,1 \div 1$ m depending on the stability of the atmosphere, the vertical diffusion coefficient $\mu_z = \gamma + k_1 \frac{h}{z_1}$, where $k_1 = 0,1 \div 0,2$ m^2/ s, the height of the surface layer $h = 50 \div 100$ m or $\mu_z = k_1 \left(\frac{z}{z_1} \right)^m$, $m \approx 1$ – dimensionless parameter.

The dependencies are used to determine other coefficients of atmospheric turbulent diffusion [5; 7]: $\mu_y = k_0 \cdot V$, $\mu_x = \mu_y$, where k_0 – empirical constant (for example, k_0=0,1 [5; 8]).

The input data for modeling the process of methane transfer within the considered model (1) are the following data: wind direction for this region and parameters characterizing the meteorological regime in the region; quantitative characteristics of methane emission intensity and its change over time; the location of the emission source.

The sources of methane emissions are very diverse. Thus, in the paper [1] we are talking about 11 sources of emission: swamps, mines, storage of household waste and others. Therefore, for the practical use of the modeling equation (1), the methane emission sources should be typified. This allows us to adequately describe, from a mathematical point of view, the "action" of the source of methane emissions. When using model (1), the following typification of methane emission sources is proposed:

1. Methane emission from the mine ventilation system (Fig. 2).

Figure 2 – Methane emission from the pipe

For a given type of methane emission, the emission source is modeled as a "point" with known coordinates x_i, y_i, z_i.

2. Release of methane to the surface of the earth through cracks (Fig. 3).

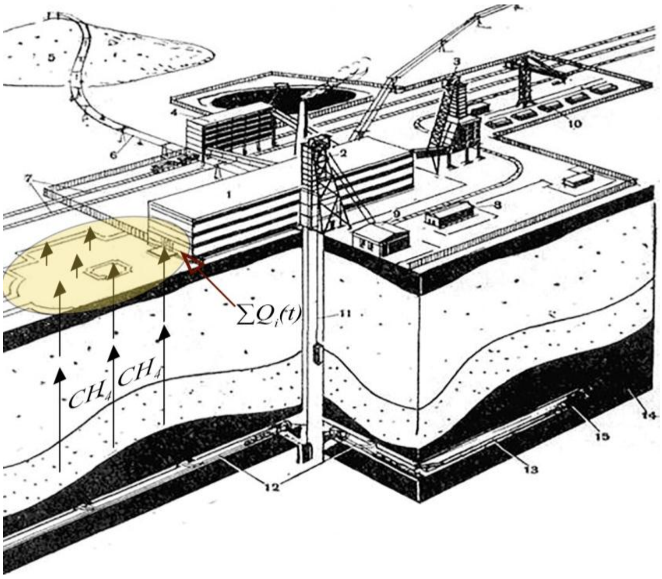


Figure 3 – Scheme of methane release through cracks

3. Emission of methane from waste storage facilities (Fig. 4).

Figure 4 – Scheme of methane emissions from waste storage facilities

For the second and third types of methane emission, the emission source is modeled by a set of points $\sum_{i=1}^{n} Q_i(t)\delta(x - x_i, y - y_i, z - z_i)$ with known coordinates x_i, y_i, z_i, which means that an area emission source is specified.

In this way, the equation (1) allows to model the flow of methane from various sources on the basis of a single approach.

An important issue is also determining the power of methane emission Q_i, which can change over time. To determine this parameter, it is possible to use, for example, known empirical dependencies [4] or measurement data. Of course, it is impossible to obtain reliable data for this parameter without experimental research. In the absence of reliable data on the power of methane emission Q_i and if it is necessary to make an estimate of the level of atmospheric air pollution, this value can be set as a constant. Then we have to calculate on the basis of the modeling equation (1) and determine the field of methane concentration as a percentage of the emission source power. This makes it possible to obtain quite important information, which has not only a qualitative value for assessing the shape of pollution zones, but also a quantitative value that shows the "gradient of decrease" in the impurity concentration at different distances from the emission source. This approach can be called a pilot calculation or a trial one.

Numerical model. The finite-difference method is used for the numerical solution of the modeling equation (1). First, the equation (1) is split into five equations of system (3) at the differential level [6; 9]:

$$\begin{aligned}
&\frac{\partial \overset{1}{C}}{\partial t}+\frac{1}{2}div(\vec{V}^{+}\overset{1}{C})+\frac{1}{4}\sigma\overset{1}{C}=\frac{1}{4}\left(\frac{\partial}{\partial x}(\bar{\mu}_{1x}\frac{\partial \overset{1}{C}}{\partial x})+\frac{\partial}{\partial y}(\bar{\mu}_{1y}\frac{\partial \overset{1}{C}}{\partial y})+\frac{\partial}{\partial z}(\bar{\mu}_{1z}\frac{\partial \overset{1}{C}}{\partial z})\right);\\
&\frac{\partial \overset{2}{C}}{\partial t}+\frac{1}{2}div(\vec{V}^{-}\overset{2}{C})+\frac{1}{4}\sigma\overset{2}{C}=\frac{1}{4}\left(\frac{\partial}{\partial x}(\bar{\mu}_{2x}\frac{\partial \overset{2}{C}}{\partial x})+\frac{\partial}{\partial y}(\bar{\mu}_{2y}\frac{\partial \overset{2}{C}}{\partial y})+\frac{\partial}{\partial z}(\bar{\mu}_{2z}\frac{\partial \overset{2}{C}}{\partial z})\right);\\
&\frac{\partial \overset{3}{C}}{\partial t}+\frac{1}{2}div(\vec{V}^{-}\overset{3}{C})+\frac{1}{4}\sigma\overset{3}{C}=\frac{1}{4}\left(\frac{\partial}{\partial x}(\bar{\mu}_{2x}\frac{\partial \overset{3}{C}}{\partial x})+\frac{\partial}{\partial y}(\bar{\mu}_{2y}\frac{\partial \overset{3}{C}}{\partial y})+\frac{\partial}{\partial z}(\bar{\mu}_{2z}\frac{\partial \overset{3}{C}}{\partial z})\right);\quad (3)\\
&\frac{\partial \overset{4}{C}}{\partial t}+\frac{1}{2}div(\vec{V}^{+}\overset{4}{C})+\frac{1}{4}\sigma\overset{4}{C}=\frac{1}{4}\left(\frac{\partial}{\partial x}(\bar{\mu}_{1x}\frac{\partial \overset{4}{C}}{\partial x})+\frac{\partial}{\partial y}(\bar{\mu}_{1y}\frac{\partial \overset{4}{C}}{\partial y})+\frac{\partial}{\partial z}(\bar{\mu}_{1z}\frac{\partial \overset{4}{C}}{\partial z})\right);\\
&\frac{\partial \overset{5}{C}}{\partial t}=\sum_{i=1}^{n}Q_i(t)\delta(x-x_i,y-y_i,z-z_i).
\end{aligned}$$

The initial condition for each splitting equation has the following form:

$$\overset{1}{C}\big|_{t=t^n}=C(x,y,z,t^n),\quad \overset{k}{C}\big|_{t=t^n}=\overset{k-1}{C}\big|_{t=t^{n+1}},\quad C(x,y,z,t^{n+1})=\overset{5}{C}\big|_{t=t^{n+1}}. \qquad (4)$$

In the system of equations (3), the notations are used:

$$\vec{V}^{+}=\{u^{+},v^{+},w^{+}\},\quad \vec{V}^{-}=\{u^{-},v^{-},w^{-}\},$$
$$u^{+}=\frac{u+|u|}{2},\ u^{-}=\frac{u-|u|}{2},\ v^{+}=\frac{v+|v|}{2},\ v^{-}=\frac{v-|v|}{2},\ w^{+}=\frac{w+|w|}{2},\ w^{-}=\frac{w-|w|}{2}.$$

The difference analog of system (2) is written in the form of ratios (5) – (6) [6; 9].

– The first step of splitting:

$$\frac{\overset{1}{C}{}_{ijk}^{n+1}-\overset{1}{C}{}_{ijk}^{n}}{\Delta t}+(L_x^{+}+L_y^{+}+L_z^{+})(\overset{1}{C}{}_{ijk}^{n+1}\xi+\overset{1}{C}{}_{ijk}^{n}(1-\xi))+\frac{\sigma}{4}\overset{1}{C}{}_{ijk}^{n+1/2}=$$
$$=\frac{1}{4}\left[(M_{xx}^{+}+M_{yy}^{+}+M_{zz}^{+})\overset{1}{C}{}_{ijk}^{n+1}+(M_{xx}^{-}+M_{yy}^{-}+M_{zz}^{-})\overset{1}{C}{}_{ijk}^{n}\right], \qquad (5)$$

where $\xi\in[0,1]$ – parameter. $\overset{1}{C}{}_{ijk}^{n+1/2}=\dfrac{\overset{1}{C}{}_{ijk}^{n+1}+\overset{1}{C}{}_{ijk}^{n}}{2}$.

– The second step of splitting:

$$\frac{\overset{2}{C}{}_{ijk}^{n+1}-\overset{2}{C}{}_{ijk}^{n}}{\Delta t}+(L_x^{-}+L_y^{-}+L_z^{-})(\overset{2}{C}{}_{ijk}^{n+1}\xi+\overset{2}{C}{}_{ijk}^{n}(1-\xi))+\frac{\sigma}{4}\overset{2}{C}{}_{ijk}^{n+1/2}=$$
$$=\frac{1}{4}\left[\left(M_{xx}^{-}+M_{yy}^{-}+M_{zz}^{-}\right)\overset{2}{C}{}_{ijk}^{n+1}+\left(M_{xx}^{+}+M_{yy}^{+}+M_{zz}^{+}\right)\overset{2}{C}{}_{ijk}^{n}\right]. \qquad (6)$$

– The third step of splitting – a difference equation is used (6), the fourth step of splitting – differential equation (5) is applied, the fifth step is performed according to relation (7) [10]:

$$\frac{\overset{5}{C}{}_{ijk}^{n+1}-\overset{5}{C}{}_{ijk}^{n}}{\Delta t}=\sum_{i=1}^{n}\frac{Q_i(t^{n+1/2})(x-x_i,y-y_i,z-z_i)}{\Delta x\Delta y\Delta z}. \qquad (7)$$

In the discrete form, the Dirac delta function is "smeared" over the volume of the difference cell while preserving the total amount of pollution, the delta function is equal to zero everywhere, except for the cells where the i-th source of pollution is located.

The equations (5) – (6) use the following designations of difference operators [6; 9-10]:

$$L_x^{+}=\frac{u_{i+1,j,k}^{+}C_{ijk}-u_{i,j,k}^{+}C_{i-1,j,k}}{2\Delta x},\ L_x^{-}=\frac{u_{i+1,j,k}^{-}C_{i+1,j,k}-u_{i,j,k}^{-}C_{i,j,k}}{2\Delta x},$$
$$L_y^{+}=\frac{v_{i,j+1,k}^{+}C_{ijk}-v_{i,j,k}^{+}C_{i,j-1,k}}{2\Delta y},\ L_y^{-}=\frac{v_{i,j+1,k}^{-}C_{i,j+1,k}-v_{i,j,k}^{-}C_{i,j,k}}{2\Delta y},$$
$$L_z^{+}=\frac{w_{i,j,k+1}^{+}C_{ijk}-w_{i,j,k}^{+}C_{i,j,k-1}}{2\Delta x},\ L_z^{-}=\frac{w_{i,j,k+1}^{-}C_{i,j,k+1}-w_{i,j,k}^{-}C_{i,j,k}}{2\Delta z}.$$

The notation of other operators coincides with the corresponding notation.

Results and discussion. A computer code was created on the basis of the developed numerical model. FORTRAN was the programming language. This code contains subroutines of type SUBROUTINE:

– *CH14* – The numerical calculation of methane concentration in the first and fourth steps of splitting according to the calculated dependence (5).

– *CH23* – The numerical calculation of methane concentration in the second and third steps of splitting according to the calculated dependence (6).

– *CH5* – The numerical calculation of the concentration of methane under the influence of the source of pollution according to the calculated dependence (7).

– *CHPR* – Subroutine for printing the results of a computational experiment.

The main program MAIN.PRG is based on the work of all the subroutines listed above.

Based on the modeling equation (1), the model problem was solved. The task of forecasting a zone of atmospheric air pollution during methane emission from the future waste storage facility is considered (Fig. 5).

Figure 5 – Layout of the waste storage: *1* – storage

The calculation was performed with the following parameters:

1) wind speed at a height of 10 m is 6 m/s;

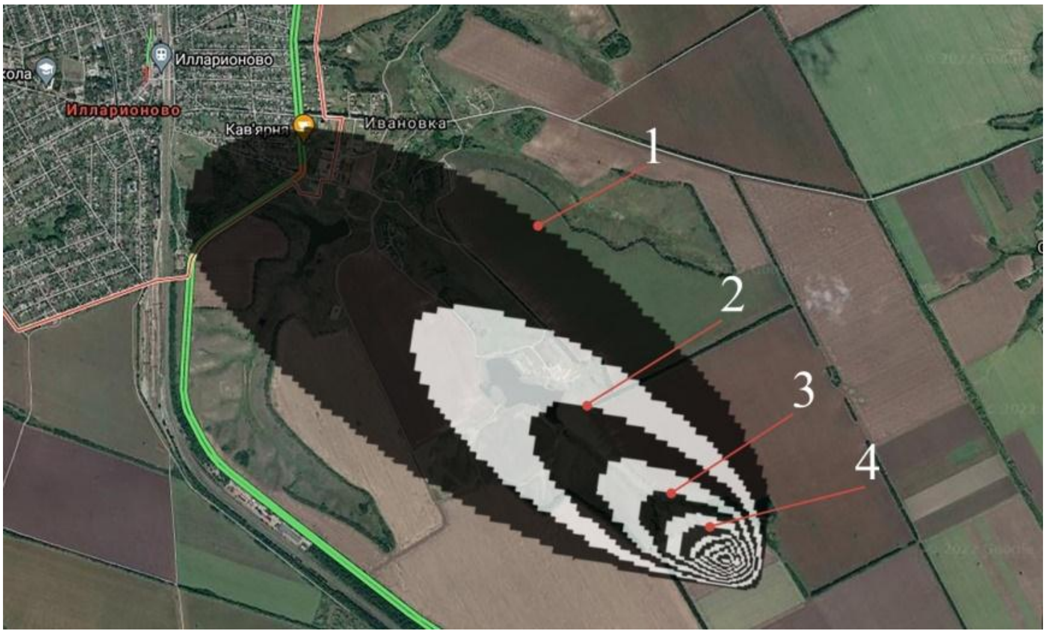
2) methane emission intensity is 1 kg/s;

3) atmospheric diffusion coefficients are calculated according to the dependencies given above;

4) the direction of the wind is southeast;

5) the dimensions of the calculation area are 6 km×3.7 km.

Zone of chemical pollution is shown in figure 6, namely the isolines of CH_4 concentration at a height of 5 m.



1 – C=0,01 g/m^3; 2 – C=0,05 g/m^3; 3 – C=0,07 g/m^3; 4 – C=0,11 g/m^3

Figure 6 – Predicted pollution zone

As it can be seen from figure 6, zone of chemical pollution reaches the border of the village located near the waste storage facility. A pond and agricultural land are also affected by the source of pollution. The calculation time of one scenario is 2 seconds.

Conclusions. As a result of the conducted research, the following results were obtained:

1. The numerical model is proposed for operational forecasting of methane concentration fields.
2. The modeling of methane emission sources in the form of a delta function in the developed model allows making a mathematical description of various sources of methane emission from a unified standpoint.
3. The numerical model takes into account the main physical factors affecting the formation of pollution zones in atmospheric air during methane emission.
4. The feature of developed numerical model is the high speed of calculation, which is an important factor for organizations and institutions when conducting comprehensive research in the field of environmental protection.

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МЕТОДОЛОГІЧНІ ПІДХОДИ ДО МАТЕМАТИЧНОГО МОДЕЛЮВАННЯ РОЗСІЮВАННЯ МЕТАНУ В АТМОСФЕРНОМУ ПОВІТРІ

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Анотація. Сьогодні залишається великою проблемою кількість метану, що надходить у довкілля від різноманітних джерел. Метан викидається в атмосферу при виробництві, переробці, зберіганні, транспортуванні та розподілі природного газу та сирої нафти. Видобуток вугілля, відходи будинків і підприємств, очищення побутових і промислових стічних вод, звалища – це основні джерела викиду метану. Розвиток економіки, зростання споживання різноманітної продукції, призводить до збільшення сховищ відходів, як природного походження так і побутового. В даний час велика увага приділяється збору та утилізації метану. Проте немає тенденції скорочення джерел викидів метану. У зв'язку з цим залишається актуальним завданням оцінка рівня концентрації метану, що надходить від джерел викиду. Завдання є досить складним, оскільки вимагає врахування фізичних та метеорологічних параметрів, а також різного типу джерел та їх розташування. У роботі запропоновано чисельну модель, яка ґрунтується на тривимірному рівнянні масопереносу. Розв'язання цього рівняння виконується різницевими методами, що дозволяє отримати поле концентрації метану на будь-якій висоті від поверхні землі. Розроблена чисельна модель дозволяє враховувати місце розташування джерела метану, точкове або майданне джерело, зміну швидкості повітряного потоку з висотою, коефіцієнти атмосферної турбулентної дифузії. На базі розробленої чисельної моделі створено комп'ютерний код для оперативного прогнозу концентраційних полів метану під дією джерела забруднення. На основі розробленої програми вирішено модельну задачу прогнозу зон забруднення атмосферного повітря при емісії метану від майбутнього сховища відходів, прогнозовану зону забруднення отримано у вигляді ізоліній концентрації метану. Одержані результати можуть бути корисними під час проведення великої кількості чисельних розрахунків, коли впроваджуються нові способи відбору, утилізації та захисту, тобто при вирішенні актуальних питань відносно технологій охорони та захисту навколишнього середовища.

Ключові слова: концентрація метану, математичне моделювання, чисельний розрахунок, рівень забруднення, сховище відходів.

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