практичного застосування при рішенні завдань розробки перспективних методів і технічних засобів пожежогасіння.

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SIMULATION OF AIR POLLUTION IN WORKPLACES USING CODE «ACCAM-2»

Introduction. Along the Toliatti-Odessa ammonia pipeline there are several pumping stations which support the correct pressure in the pipeline. From the point view of industrial safety these pump stations are the chemically dangerous objects [5]. According to the Law of Ukraine for high-risk objects, a PLAS (Emergency Response Plan) document must be developed for such industrial object. Prediction of air pollution in workplaces after unplanned toxic chemical emission is the basis of this document. Therefore, the actual task is to estimate the level of contamination in working areas of the pump station in the case of unplanned ammonia release at the pump station territory.

Review of literature sources. To solve the problem of chemical contamination zones formation in the case of unplanned ammonia emissions analytical models or Gaussian plume are widely used [2, 3, 9, 10]. These models have significant lacks because they cannot be used when we model toxic chemical dispersion among buildings. For this purpose it is necessary to use numerical models [1, 4, 6-8] which are based on Fluid Dynamics equations. In Ukraine, there is a certain deficit of such models [1, 7, 8].

The purpose of this paper is to develop a code which is based on numerical model for computing the chemical contamination of air on the territory of the ammonia pump station for unplanned ammonia release.

Mathematical model. To simulate the ammonia dispersion 2D mass transport model is used [1, 3, 4, 7, 8]:

$$\frac{\partial C}{\partial t}+\frac{\partial uC}{\partial x}+\frac{\partial vC}{\partial y}+\sigma C=\frac{\partial}{\partial x}\left(\mu_x\frac{\partial C}{\partial x}\right)+ +\frac{\partial}{\partial y}\left(\mu_y\frac{\partial C}{\partial y}\right)+\sum Q_i(t)\delta(x-x_i)\delta(y-y_i), \qquad (1)$$

where C is mean concentration; u, v are the wind velocity components; σ is the parameter taking into account the process of pollutant chemical decay or washout; $\mu=(\mu_x , \mu_y)$ are the diffusion coefficients; Q is intensity of point source emission; $\delta(r-r_i)$ are Dirak delta function; $r_i = (x_i, y_i)$ are the coordinates of the point source.

To simulate the wind flow in the case of the buildings at the territory of Pump Station the 2D model of potential flow is used [6]:

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

where P is the potential of velocity.

The wind velocity components are calculated as follows:

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

Boundary conditions for modeling equations are discussed in [1, 4, 6].

Numerical model. To solve numerically Eq. (1) the implicit difference scheme [1, 6] is used. To solve Eq. (2) A.A. Samarskii's change-triangle difference scheme is used.

First of all equation (2) is transformed into the "evolution type"

$$\frac{\partial P}{\partial \eta} = \frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2}, \qquad (3),$$

where η is 'fictitious' time.

For $\eta \to \infty$ the solution of equation (3) tends to the solution of equation (2).

According to A.A. Samarskii's change-triangle difference scheme the solution of equation (3) is split into two steps:

-at the first step the difference equation is

$$\frac{P_{i,j}^{n+1/2} - P_{i,j}^{n}}{0{,}5\Delta\eta} = \frac{P_{i+1,j}^{n} - P_{i,j}^{n}}{\Delta x^2} + $$
$$+ \frac{-P_{i,j}^{n+1/2} + P_{i-1,j}^{n+1/2}}{\Delta x^2} + \frac{P_{i,j+1}^{n} - P_{i,j}^{n}}{\Delta y^2} +,$$
$$+ \frac{-P_{i,j}^{n+1/2} + P_{i,j-1}^{n+1/2}}{\Delta y^2}$$

- at the second step the difference equation is

$$\frac{P_{i,j}^{n+1} - P_{i,j}^{n+1/2}}{0{,}5\Delta\eta} = \frac{P_{i+1,j}^{n+1} - P_{i,j}^{n+1}}{\Delta x^2} + $$
$$+ \frac{-P_{i,j}^{n+1/2} + P_{i-1,j}^{n+1/2}}{\Delta x^2} + \frac{P_{i,j+1}^{n+1} - P_{i,j}^{n+1}}{\Delta y^2} + .$$
$$+ \frac{-P_{i,j}^{n+1/2} + P_{i,j-1}^{n+1/2}}{\Delta y^2}$$

From these expressions the unknown value $P_{i,j}$ is determined using the explicit formulae at each step of splitting ("method of running calculation"). The calculation is completed if the condition

$$\left| P_{i,j}^{n+1} - P_{i,j}^{n} \right| \le \varepsilon$$

is fulfilled (where ε is a small number, n is the number of iteration). The components of velocity vector are calculated on the sides of computational cell as follows

$$u_{i,j} = \frac{P_{i,j} - P_{i-1,j}}{\Delta x},$$
$$v_{i,j} = \frac{P_{i,j} - P_{i,j-1}}{\Delta y}.$$

To solve equation (1) we use change –triangle difference scheme [1, 7]. The time dependent derivative in Eq. (1) is approximated as follows:

$$\frac{\partial C}{\partial t} \approx \frac{C_{ij}^{n+1} - C_{ij}^{n}}{\Delta t}.$$

At the first step convective derivatives are represented in the following way:

$$\frac{\partial uC}{\partial x} = \frac{\partial u^{+}C}{\partial x} + \frac{\partial u^{-}C}{\partial x};$$
$$\frac{\partial vC}{\partial y} = \frac{\partial v^{+}C}{\partial y} + \frac{\partial v^{-}C}{\partial y},$$

where $u^{+} = \frac{u + |u|}{2}$; $u^{-} = \frac{u - |u|}{2}$; $v^{+} = \frac{v + |v|}{2}$; $v^{-} = \frac{v - |v|}{2}$.

At the second step the convective derivatives are approximated as follows:

$$\frac{\partial u^{+}C}{\partial x} \approx \frac{u_{i+1,j}^{+} C_{ij}^{n+1} - u_{ij}^{+} C_{i-1,j}^{n+1}}{\Delta x} = L_x^{+} C^{n+1},$$
$$\frac{\partial u^{-}C}{\partial x} \approx \frac{u_{i+1,j}^{-} C_{i+1,j}^{n+1} - u_{ij}^{-} C_{ij}^{n+1}}{\Delta x} = L_x^{-} C^{n+1},$$
$$\frac{\partial v^{+}C}{\partial y} \approx \frac{v_{i,j+1}^{+} C_{ij}^{n+1} - v_{il}^{+} C_{i,j-1}^{n+1}}{\Delta y} = L_y^{+} C^{n+1},$$
$$\frac{\partial v^{-}C}{\partial y} \approx \frac{v_{i,j+1}^{-} C_{i,j+1}^{n+1} - v_{ij}^{-} C_{ij}^{n+1}}{\Delta y} = L_y^{-} C^{n+1}.$$

The second order derivatives are approximated as follows:

$$\frac{\partial}{\partial x}\left(\mu_x \frac{\partial C}{\partial x}\right) \approx \tilde{\mu}_x \frac{C_{i+1,j}^{n+1} - C_{ij}^{n+1}}{\Delta x^2} - $$
$$- \tilde{\mu}_x \frac{C_{ij}^{n+1} - C_{i-1,j}^{n+1}}{\Delta x^2} = M_{xx}^{-} C^{n+1} + M_{xx}^{+} C^{n+1},$$

$$\frac{\partial}{\partial y}(\mu_y \frac{\partial C}{\partial y}) \approx \tilde{\mu}_y \frac{C_{i,j+1}^{n+1} - C_{ij}^{n+1}}{\Delta x^2} -$$

$$- \tilde{\mu}_y \frac{C_{ij}^{n+1} - C_{i,j-1}^{n+1}}{\Delta x^2} = M_{yy}^{-} C^{n+1} + M_{yy}^{+} C^{n+1} .$$

In these expressions $L_x^+, L_x^-, L_y^+, L_y^-, M_{xx}^+, M_{xx}^-, M_{yy}^+, M_{yy}^-$ are the difference operators. Using these expressions the difference scheme for the transport equation can be written as follows:

$$\frac{C_{ij}^{n+1} - C_{ij}^{n}}{\Delta t} + L_x^+ C^{n+1} + L_x^- C^{n+1} +$$

$$+ L_y^+ C^{n+1} + L_y^- C^{n+1} + \sigma C_{ij}^{n+1} =$$

$$= M_{xx}^+ C^{n+1} + M_{xx}^- C^{n+1} + M_{yy}^+ C^{n+1} + M_{yy}^- C^{n+1}.$$

Solution of the transport equation in finite - difference form is split in four steps on the time step of integration *dt*:

- at the first step ($k = \frac{1}{4}$) the difference equation is

$$\frac{C_{ij}^{n+k} - C_{ij}^{n}}{\Delta t} + \frac{1}{2}\left(L_x^+ C^k + L_y^+ C^k\right) + \frac{\sigma}{4} C_{ij}^k =$$

$$= \frac{1}{4}\left(M_{xx}^+ C^k + M_{xx}^- C^n + M_{yy}^+ C^k + M_{yy}^- C^n\right) ,(4)$$

- at the second step ($k = n + \frac{1}{2}$, $c = n + \frac{1}{4}$):the difference equation is

$$\frac{C_{ij}^{k} - C_{ij}^{c}}{\Delta t} + \frac{1}{2}\left(L_x^- C^k + L_y^- C^k\right) + \frac{\sigma}{4} C_{ij}^k =$$

$$= \frac{1}{4}\left(M_{xx}^- C^k + M_{xx}^+ C^c + M_{yy}^- C^k + M_{yy}^+ C^c\right) , \quad (5)$$

- at the third step ($k = n + \frac{3}{4}$, $c = n + \frac{1}{2}$) the expression (5) is used;
- at the fourth step ($k = n + 1$, $c = n + \frac{3}{4}$) the expression (4) is used.

At the fifth step (at this step the influence of the source of pollutant emission is taken into account) the following approximation is used:

$$\frac{\overset{5}{C}{}_{i,j}^{\,n+1} - \overset{5}{C}{}_{i,j}^{\,n}}{\Delta t} = \sum_{l=1}^{N} \frac{q_l\left(t^n\right)}{\Delta x \Delta y} \delta_l .$$

Function δ_l is equal to zero in all cells accept the cells where source of emission is situated.

Practical implementation of the model. Calculation of velocity components on the sides of computational cell allows to develop the conservative numerical scheme for pollutant dispersion.

For coding of difference formulae FORTRAN language was used.

Description of code «ACCAM-2». This code includes:

1. Subroutine «TRIANG» for numerical integration of mass transport equation.
2. Subroutine «SAMTRI» for numerical integration of Laplas equation for potential flow.
3. Subroutine «UVCAL» for calculation of wind flow components.
4. Subroutine «RISK2» for concentration presentation in the region (fig. 1).

The developed code can solve such problems: prediction of air pollution in workplaces in the case of unplanned emissions; prediction of air pollution in workplaces in the case of continuous source of emission; short time ejections of toxic chemicals.

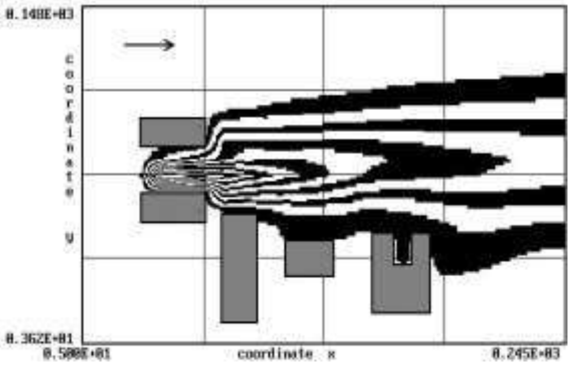

Fig. 1. Computed ammonia concentration at pump station, t=170 s

Conclusions. Code «ACCAM-2» for assessing the level of air pollution in workplaces during the unplanned ammonia emissions is proposed. Developed code allows to predict the level of air pollution in workplaces among buildings. In this code the solution of the aerodynamic problem is based on the numerical integration of the equation for the velocity potential. To predict the air pollution the equation of mass transfer is numerically integrated. The mass transfer equation takes into account the convective and diffusive transport of pollutants in atmosphere, taking into account buildings situated near the source of emission. In this code ammonia emission is simulated by a point source, which is modeled using the Dirac's delta function.

Further improvement of the model should be carried out in the direction of creating a 3D numerical model to predict air pollution in workplaces in the case of unplanned ammonia emission.

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УМЕНЬШЕНИЕ ИНТЕНСИВНОСТИ ПЫЛЕВОГО ЗАГРЯЗНЕНИЯ РАБОЧИХ ЗОН ВОЗЛЕ УГОЛЬНОГО ШТАБЕЛЯ

Вступление. Складирование угля в виде штабелей приводит к интенсивному загрязнению рабочих зон угольной пылью [6, 8, 9]. Причиной такого загрязнения является унос угольной пыли от поверх-ности штабеля. На интенсивность уноса влияет комплекс факторов, однако важнейшим из которых является аэродинамический режим возле штабеля. Угольная пыль попадает как на производственный персонал, работающий на промышленной площадке. Поэтому важной задачей является минимизация такого загрязнения рабочих зон возле штабелей угля путем использования эффективных и не дорогих методов защиты [1, 2].

Анализ литературы. Оценка уровня загрязнения рабочих зон возле штабелей