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MODELING OF THE ATMOSPHERE POLLUTION IN THE CITY AFTER ACCIDENT AT THE RAILWAY STATION

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Introduction. Different toxic chemicals are transported by railways. In the case of the accident the problem of the atmosphere pollution takes the first place. To predict the air pollution after accidents with toxic substances, the special standard model is used in Ukraine [3]. It is a common knowledge that this model doesn't take into account the influence of the wind velocity and buildings on the concentration dispersion. The analytical models, like Gaussian model, also do not take into account the buildings influence on the concentration dispersion [2,4, 5,6]. So it is very important to develop the numerical models to predict the atmosphere pollution with account of different obstacles.

The main purpose of this work is development of the numerical model for the prompt prediction of the atmosphere pollution in the case of the toxic chemicals release.

Governing equations. The process of the toxic chemical dispersion in the atmospher

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

e is simulated using the following equation [1,2,7,9,10,11]:

where *u, v, w* are the wind velocity components in *x, y* and *z* direction respectively;

C is the concentration of toxic chemical;

σ is the parameter which takes into account the process of toxic chemical decay in the atmosphere;

μx , μy , μz are the coefficients of turbulent diffusion in x, y and z direction respectively;

xi , yi , zi are the coordinates of point source of emission;

Qi(t) is the intensity of pollutant emission;

$\delta(x-x_i)\delta(y-y_i)\delta(z-z_i)$ is Dirac's delta-function.

In the numerical model, to simulate the profile of wind velocity and the coefficient of diffusion μ_z the following models are used [2,4]:

$$u=u_1\left(\frac{z}{z_1}\right)^n,\quad \mu_z=k_1\left(\frac{z}{z_1}\right)^m,$$

where u1 is the velocity at height *z1; k1=0,2; n=0,16; m 1*.

The advective - diffusive equation (1) is used with the following boundary conditions [1, 7, 9, 11]:

– inlet boundary: $C|_{inlet} = C_E$, where C_E is the known concentration (very often);

– outlet boundary: in numerical model the condition $C(i+1, j, k) = C(i, j, k)$ is used (this boundary condition means that we neglect the process of diffusion at this plane);

– top boundary and ground surface $\frac{\partial C}{\partial n} = 0$.

As we consider the problem of toxic chemical dispersion in the city it is necessary to simulate wind flow over buildings. To solve this problem the model of potential flow is used. In this case, the governing equation is [1,9,11]:

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

where P is the potential of velocity.

The boundary conditions for Eq. (2) are as following:

– at the «solid» boundaries we have: $\frac{\partial P}{\partial n} = 0$,

where n is a normal to the boundary;

– at the inlet boundary we have:

$$\frac{\partial P}{\partial n} = V_n ,$$

where *Vn* is the known meaning of the speed;

– at the outlet boundary we have: $P = P_0 + const$ (Dirichle condition).

The components of velocity are calculated as follows:

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

Numerical methods. To solve equation of the toxic chemical dispersion the change – triangle difference scheme of splitting is used [1,9,11].

To solve Eq. (2) A.A. Samarskii's difference scheme is used [8]. In this case, instead of equation (2) the «time-dependent» equation for the potential of velocity is used in the model:

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

where η is the «fictitious» time.

For $\eta \to \infty$ the solution of this equation tends to the solution of Laplas equation.

According to A.A. Samarskii's difference scheme the process of the numerical integration of equation (3) is split in two steps:

– at the first step the finite - difference equation is:

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

– at the second step the finite - difference equation is:

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

From these expressions, the unknown value P is calculated using the explicit formulae at each step (the «method of running calculation»). The calculation is completed if the condition:

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

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:

$$u_{i,j,k}=\frac{P_{i,j,k}-P_{i-1,j,k}}{\Delta x}$$

$$v_{i,j,k}=\frac{P_{i,j,k}-P_{i,j-1,k}}{\Delta y}$$

$$w_{i,j,k}=\frac{P_{i,j,k}-P_{i,j,k-1}}{\Delta z}$$

Results. The numerical model was used to calculate the atmosphere pollution in the case study of the NH3 emission at the railway station 'Dnipropetrovsk - Centralny'. It is a common knowledge that this toxic chemical is transported in a large volumes by railway. So it is very important to predict the area where the toxic hitting of people could take place. This case study was carried out using the following parameters: the length of the computational region is 540m, the width of the computational region is 420m (Fig.1), the height of the computational region is 80m; wind speed is u1=5m/c, emission of NH3 is 10kg/s. It was assumed that NH3 emission takes place near the main building of the railway station.

Fig. 1. Concentration contours of NH3, t= 35s

Fig. 2. Concentration contours of NH3, t= 86s

Fig. 3. Concentration contours of NH3, t= 97s

The results of the numerical simulation are shown in Fig. 1 - 3. These Figures present the concentration contours (section z=60m) for different time after accident. It is clear that in the case of the toxic chemical emission toxic plume very quickly will cover the residential districts. It is obvious that in the case of the accident the concentration of the toxic chemical will exceed the threshold level in urban districts. This is a real danger for the people living near the railway station.

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