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ATMOSPHERE POLLUTION MODELING IN THE CASE OF THE ACCIDENT AT THE ROCKET PROPELLANT STORAGE

Розроблено чисельну модель та код для моделювання тривимірного процесу переносу забруднювача при аварійному викиді небезпечної речовини. Розроблена модель базується на чисельному інтегруванні тривимірного рівняння переносу домішки. Для чисельного інтегрування використовується неявна різницеві схема.

Разработана численная модель и код для моделирования трехмерного процесса переноса загрязнителя при аварийном выбросе опасного вещества. Разработанная модель основывается на численном интегрировании трехмерного уравнения переноса примеси. Для численного интегрирования используется неявная разностная схема.

A numerical model and code were developed to simulate the pollutant dispersion in the case of the accident release of the toxic chemical. The model is based on the K-gradient model of pollutant dispersion. The implicit schemes is used for the numerical integration.

Introduction. The storage of the rocket propellant (this is the solid propellant of RS-22 rocket) which is situated at Pavlograd Chemical Plant is a very dangerous source of the atmosphere chemical pollution in the case of the possible accident (Fig.1, 2).

Fig. 1. Territory near the storage of rocket propellant: 1 – storage with rocket propellant; 2 – receptor (building at the territory of the plant)

Fig. 2. Solid propellant of the RS-22 system (Pavlograd Chemical Plant)

That is why the prediction of the atmosphere pollution in the case of the accident at the storage is of great interest. Nowadays to predict the dimensions of the hitting area in the case of outdoor toxic chemical release the special standard model is used in Ukraine [2]. This model is formed on the basis of some empirical models and it has a lot of lacks and is , without doubt, unrealistic . The model doesn't take into account the influence of the wind velocity and the atmosphere diffusion on the concentration dispersion in the atmosphere. The main lack of this model is that the standard model cannot calculate the change of toxic chemical concentration in the atmosphere after the accident. The main purpose of this work is the development of the numerical model to predict the atmosphere pollution which is more effective than the standard model and application of this model to predict the atmosphere pollution at the territory of the Pavlograd Chemical Plant.

Governing equation. To simulate the process of toxic chemical dispersion in the atmosphere the transport equation is used [1,4,5]:

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

where *u, v, w* are the velocity components in *x, y* and *z* direction respectively; *C* is the concentration of toxic chemical; σ is the parameter taking into account the process of toxic gas decay or rain wash out; μ_x, μ_y, μ_z are the coefficients of turbulent diffusion in *x, y* and *z* direction respectively; x_i , y_i , z_i 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 delta-function.

In the developed numerical model, the following profile of velocity component *u* and coefficient of diffusion μ_z is used [2]:

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

where u_1 is the velocity at height z_1; k_1=0,2; n=0,16; $m \approx 1$. The following models to calculate the other diffusive coefficients are used

$$\mu_y = \mu_x, \ \mu_y = \kappa_0 u,$$

where κ_0 is the empirical parameter..

The transport equation is used with the following boundary conditions [1,5]:

– inlet boundary: $C|_{inlet} = C_E$, where C_E is the known concentration (very often $C_E = 0$);

– 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 $\frac{\partial C}{\partial n} = 0$.

To develop the numerical model the implicit difference scheme was used [1].

Results. The developed numerical model was used to predict HCL (this is the product of the propellant firing) concentration in the case of the accident at the rocket propellant storage. The place of toxic chemical emission is shown on Fig.1. It is situated apart from the working buildings of Pavlograd Chemical Plant. The main interest was to compute the level of the atmosphere pollution at the territory of this plant to find out the risk of hitting at this place. The duration of HCL emission was supposed to be 15min. The emission rate was 4000 g/s, the wind speed was u_1=4.5m/s. The length of the region was 3500m, the width of the region was 2500m, the height of the computational region was 500m.

The height of the plume which is formed during the propellant firing was calculated using the following empirical model [6]

$$h = 4,71 \cdot \frac{Q^{0,444}}{u^{0,694}}$$

where u is wind speed, Q is the intensity of the heat emission (Q=4*10^3 kJ/kg).

This vertical plume is simulated as the set of vertical point sources using Delta function.

The result of the numerical modeling is shown in Fig. 3. This Figure illustrates the HCL plume which covers the territory of the plant. In Table 1 the concentration of HCl near the industrial building (see Fig.1, position 2) at the plant territory is shown. Also one can see in this Table the ratio of the toxic chemical concentration to the threshold concentration which is equal to 0.02 mg/m^3.

Table 1

HCL concentration near the building at the territory of Pavlograd Chemical Plant

Time after accident	Concentration	Level of Contamination (concentration / threshold concentration)
450 sec	2.85 mg/m^3	14,2
510 sec	3.24 mg/m^3	16,2
550 sec	3.40 mg/m^3	17,0

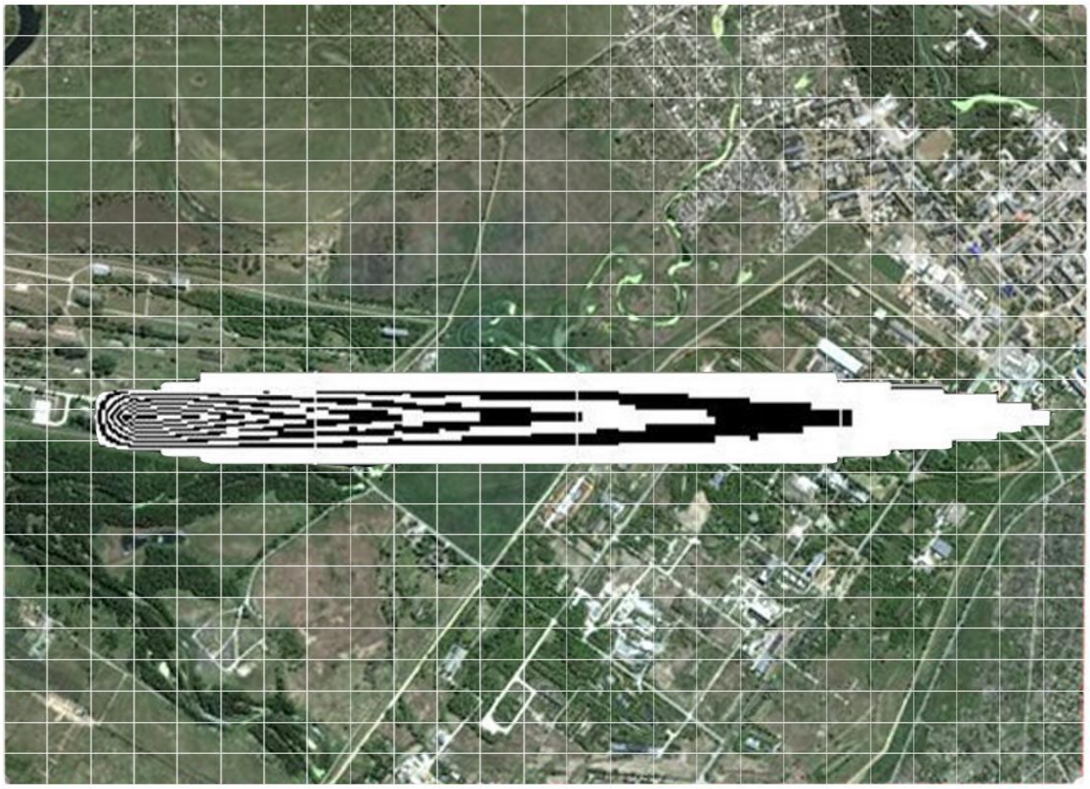

Fig. 3. Contours of HCL concentration, t=550 sec (level z=10 m):

It is clear that in the case of the accident at the storage the concentration of the toxic chemical concentration will quickly exceed the threshold level at the territory of Pavlograd Chemical Plant. This is a real danger for the people working at the plant. That is why the protection measures should be developed for the working people.

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