Библиографические ссылки

1. **Антошкина Л.И.** Оценка экологического риска при авариях с химически опасными веществами / Л.И. Антошкина, Н.Н. Беляев, Е.Ю. Гунько. – Днепропетровск, 2008. – 132с.
2. **Беляев Н.Н.,** Лисняк В.М. Защита атмосферы от загрязнения при миграции токсичных веществ / Н.Н. Беляев. – Днепропетровск, 2006. – 150 с.
3. **Берлянд М. Е.** Прогноз и регулирование загрязнения атмосферы / М. Е. Берлянд. – Л., 1985. – 273 с.
4. **Згуровский М. З.** Численное моделирование распространения загрязнения в окружающей среде / М. З. Згуровский, В. В. Скопецкий, В. К. Хрущ, Н. Н. Беляев. – Киев, 1997. – 368 с.
5. **Лойцянский Л. Г.** Механика жидкости и газа / Л.Г. Лойцянский. – М., 1978. – 735с.
6. **Марчук Г. И.** Математическое моделирование в проблеме окружающей среды / Г.И. Марчук. – М., 1982. – 320 с.
7. **Роуч П.** Вычислительная гидродинамика / П. Роуч. – М., 1980. – 616 с.

Надійшла до редколегії 18.10.2013.

UDC 519.6

E. Gunko

Academician V. Lasarjan Dnepropetrovsk National University of Railway Engineering

CFD MODELING OF THE ATMOSPHERE POLLUTION IN THE CASE OF ACCIDENTS FOR SOLVING MONITORING PROBLEMS

Розроблено CFD модель та код для моделювання тривимірного процесу переносу забруднювача в умовах забудови. Розроблена модель базується на чисельному інтегруванні тривимірного рівняння переносу домішки та моделі потенціальної течії. Для чисельного інтегрування використовуються неявні різницеві схеми.

Ключові слова: забруднення атмосфери, чисельне моделювання, розсіювання домішки.

Разработано CFD модель и код для моделирования трехмерного процесса переноса загрязнителя в условиях застройки. Разработанная модель основывается на численном интегрировании трехмерного уравнения переноса примеси и модели потенциального течения. Для численного интегрирования используются неявные разностные схемы.

Ключевые слова: загрязнение атмосферы, численное моделирование, рассеивание примеси.

CFD model and code were developed to simulate the pollutant dispersion among buildings. The model is based on the K-gradient model of pollutant dispersion and the model of the potential flow. The implicit schemes are used for the numerical integration.

Key words: atmosphere pollution, numerical simulation, pollutant dispersion**.**

Introduction. In the problem of the ecological monitoring, the prediction of the atmosphere pollution after accidents is the problem of the great interest because the solution of this problem provides the experts with the necessary information about the hitting areas and the level of the danger. To predict the air pollution after accidents with toxic substances, the special standard model is used in Ukraine [7]. This is the empirical model. This model has a lot of lacks and is widely criticized in scientific circles. This model can provide the information about the square of contaminated area. This model doesn't take into account the influence of the wind velocity or wind direction on the concen

tration dispersion. The main lack of this model is that it cannot predict the change of the concentration of the toxic gas in the atmosphere after emission. However, the concentration of the toxic gas in the atmosphere is the main parameter, which is necessary to know to estimate the danger level or organize protection of population. So this model can't be used for the purposes of monitoring. The analytical models can't take into account the influence of buildings on the process of pollutant dispersion [3; 10; 11]. Therefore, it is important to develop CFD models to simulate the process of the atmosphere pollution after toxic substances emissions [1; 4; 5]. The main purpose of this work is to give the engineers the tool, which is more effective than the standard model and can be used for monitoring problems in the case of accidents.

Governing equations. To simulate the process of pollutant (toxic chemical substances) transfer in the atmosphere the transport equation is used [6]:

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

where u, v, w are the velocity components in x, y and z direction respectively; C is the concentration of toxic substance; σ is the parameter taking into account the process of toxic gas decay; 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's delta-function.

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

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

where u_1 is the velocity at height z_1; k_1=0,2; n=0,16; $m\approx 1$.

The transport equation is used with the following boundary conditions [6, 9]:

– 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 simulate the 3-D wind flow over buildings the model of potential flow is used. In this case, the governing equation is [9]:

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

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 V_n is the known meaning of the speed;

– at the outlet boundary we have: $P = P_0 + const$ (Dirichlet 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 integration of the equations. To develop the numerical model the following splitting of Eq.1 is carried out [1]:

$$\frac{\partial c}{\partial t} + \frac{\partial u c}{\partial x} + \frac{\partial vc}{\partial x} + \frac{\partial wc}{\partial z} + \sigma c = 0,$$

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(\mu_x \frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu_y \frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(\mu_z \frac{\partial c}{\partial z}\right),$$

$$\frac{\partial c}{\partial t} = \sum Q_i(t)\delta(r - r_i).$$

To solve these equations the change – triangle difference scheme is used [9].

To solve Eq. (2) A.A. Samarskii's change-triangle 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:

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

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 change-triangle difference scheme the solution of equation (3) is split in two steps:

– at the first step the 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 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 developed CFD model was used to predict Cl_2 concentrations in the case of the accident at the Nizhnedneprovsk Filtration Station. There is the storage of liquid Cl_2 at this station. This storage is situated near Nizovaya Street where there are many civil buildings (Fig. 1).The numerical modeling was carried out using the following initial parameters: the length of the region is 300 m, the width of the region is 250 m, the height of the computational region is 70 m. The wind speed is u_1=3 m/c, the emission of the toxic substance is 180 kg and this amount of Cl_2 is ejected during 2 seconds.

Fig. 1. Urban territory near the storange of toxic substance:
1 – storage with Cl_2; 2 – civil buildings

Fig. 2. Concentration of Cl_2, t=20 s (level z=12 m):
1 – C=9 mg/m^3; 2 – C=20 mg/m^3; 3 – C=28 mg/m^3

Fig. 3. Concentration of Cl_2, t=23 s (level z=12 m):
1 – C=7 mg/m^3; 2 – C=17 mg/m^3; 3 – C=25 mg/m^3

The results of the CFD modeling are shown in Fig. 2 and Fig. 3. These Figures illustrate the concentration field for different time after accident. It is clear that in the case of the accident the toxic gas cloud very quickly will cover the urban area. In Table 1 the concentration of Cl_2 at the different distance from the point of emission is shown.

Table 1

Cl_2 concentration at the different distance from the point of emission (for time t=22 s)

X, m	60	72	98
C, mg/m^3	27	19	8,1

Conclusions. It is obvious that in the case of the accident the concentration of the toxic substance will exceed the level of the hitting concentration. This is a real danger for the people living near this Filtration Station.

References

1. **Антошкина Л. И.** Оценка экологического риска при авариях с химически опасными веществами / Л. И. Антошкина, Н. Н. Беляев, Е. Ю. Гунько. – Днепропетровск, 2008. – 136 с.

2. **Берлянд М. Е.** Современные проблемы атмосферной диффузии и загрязнения атмосферы / М. Е. Берлянд. – Л., 1975. – 448 с.

7. Методика прогнозування наслідків виливу (викиду) небезпечних хімічних речовин при аваріях на промислових об'єктах і транспорті – Київ, 2001. – 33 с.

3. **Бруяцкий Е. В.** Теория атмосферной диффузии радиоактивных выбросов / Е. В. Бруяцкий. – Киев, 2000. – 443 с.

10. **Hanna S.** Hybrid Plume Dispersion Model (HPDM) Improvements and Testing / S. Hanna, J. Chang // College on Atmospheric Boundary Layer and Air Pollution Modelling: 16 May–3 June 1994. № SMR/760–4. – P. 1491–1508.

11. **Tirabashi T.** Analytical Air Pollution Advection and Diffusion Models / T. Tirabashi // College on Atmospheric Boundary Layer and Air Pollution Modeling. – 16 May–3 June 1994. – № SMR / 760–9.

6. **Марчук Г. И.** Математическое моделирование в проблеме окружающей среды / Г. И. Марчук. – М., 1982. – 320 с.

8. **Самарский А. А.** Теория разностных схем / А. А. Самарский. – М., 1983. – 616 с.

4. **Гунько Е. Ю.** Моделирование загрязнения атмосферы при испарении жидкости из грунта / Е. Ю. Гунько // Вісник Дніпропетр. національного ун-ту залізничного транспорту ім. академіка В. Лазаряна. – 2007. – Вип. 19. – С. 35–39.

5. **Гунько Е. Ю.** Оценка риска токсичного поражения людей при аварийном выбросе химически опасного вещества / Е. Ю. Гунько // Вісник Дніпропетр. національного ун-ту залізничного транспорту ім. академіка В. Лазаряна. – 2008. – Вип. 20. – С. 87–90.

9. **Згуровский М. З.**Численное моделирование распространения загрязнения в окружающей среде / М. З. Згуровский, В. В. Скопецкий, В. К. Хрущ, Н. Н. Беляев. – Киев, 1997. – 368 с.

Надійшла до редколегії 18.10.2013.

УДК 519.6

Н. Н. Беляев, Д. О. Затынайченко

Днепропетровский национальный университет
железнодорожного транспорта им. академика В. Лазаряна

ЧИСЛЕННОЕ МОДЕЛИРОВАНИЕ АЭРОИОННОГО РЕЖИМА В РАБОЧЕМ ПОМЕЩЕНИИ

Розроблена двомірна модель для прогнозу аероіонного режиму у приміщеннях. Модель базується на використанні рівнянь переносу аероіонів та моделі нев'язкої нестислої рідини. Розв'язання задачі знаходиться за допомогою різницевих схем.

Ключові слова: аероіонний режим, приміщення, чисельне моделювання.

Разработана двухмерная модель для прогноза аэроионного режима в помещениях. Модель базируется на использовании уравнений переноса аэроионов и модели невязкой несжимаемой жидкости. Решение задачи находится с помощью разностных схем.