Worthy of note, that the computational time to solve the problem was about 10 *sec*. So the developed model can be used to predict very quickly the concentration field in the settler having comprehensive geometrical form. In future the 3-D CFD model is proposed to be developed.

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NUMERICAL SIMULATION OF AIR JET SUPPLY TO REDUCE CONTAMINATION NEAR THE BUILDING IN THE CASE OF CHEMICAL OUTDOOR RELEASE

Розроблено чисельну модель для моделювання захисту будівлі від потрапляння в нього хімічно небезпечних речовин шляхом застосування повітряної завіси. Розроблена модель базується на чисельному інтегруванні рівняння переносу домішки та моделі потенціальної течії. Для чисельного інтегрування використовуються неявні різницеві схеми. Наведено результати розрахунків на базі розробленої моделі.

Ключові слова: забруднення атмосфери, чисельне моделювання, захист будівель.

Разработана численная модель для моделирования защиты здания от попадания в него химически опасных веществ путем использования воздушной завесы. Разработанная модель основывается на численном интегрировании уравнения переноса примеси и модели потенциального течения. Для численного интегрирования используются неявные разностные схемы. Приведены результаты расчетов на базе разработанной модели.

Ключевые слова: загрязнение атмосферы, численное моделирование, защита зданий.

A numerical model was developed to simulate building protection from toxic chemical penetration using air jet. 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. Results of numerical experiment are presented.

Key words: the atmosphere pollution, numerical simulation, protection of building

Introduction. At present problem of people protection inside buildings in the case of chemical attack (outdoor release of chemicals) is of great interest**.** To protect people means to reduce the value of the hitting factor, the concentration inside the building. The toxic chemical penetration inside the building can be reduced if the special measures will take place near the building, for example, the air jet supply near the building. This air jet makes the obstacle on the way of toxic chemical dispersion and it results in decreasing of contamination near the building. It means that in case of the atmosphere air infiltration less contaminated air will infiltrate the building.

This work is dedicated to the problem of the numerical model development which can be used to compute the efficiency of the air jet supply to reduce the level of contamination near the building and thus protect building from intensive toxic chemical penetration.

Literature review. The analysis of the modern methods of the atmosphere pollution prediction after accidents with dangerous substances was carried out. Nowadays in Ukraine two models are widely used to predict the threat in the case with accidents with the toxic substance emissions. This the empirical model adopted by the Ukrainian authorities [7] and Gaussian plume model (in some case the analytical model of the instant ejection) [10; 11]. These 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 with the account of buildings or other obstacles influence on the process of pollutant dispersion [1; 4; 5]. Such models will be very useful for prediction of the atmosphere pollution in cities.

The purpose. The main purpose of this work is to give the engineers the tool, which can be used to estimate the efficiency of the air jet supply to protect building from chemical attack.

Governing equations. To simulate the process of toxic chemical dispersion in the atmosphere the convective – diffusive equation is used [6]:

$$\frac{\partial C}{\partial t}+\frac{\partial uC}{\partial x}+\frac{\partial (v-w)C}{\partial y}+\sigma C=div\left(\mu gradC\right) \qquad (1)$$

where u, v are the velocity components in x, y direction respectively; C is the concentration of toxic chemical; w – is the fallout speed; σ is the parameter taking into account the process of toxic chemical decay or washing by rain; μ_x, μ_y are the coefficients of turbulent diffusion in x, y direction respectively.

In the developed numerical model, the following profile of velocity component u and coefficient of diffusion μ_z is used [2,3]:

$$u=u_1\left(\frac{y}{y_1}\right)^n, \qquad \mu_y=k_1\left(\frac{y}{y_1}\right)^m,$$

where u_1 is the velocity at height y_1; k_1=0,2; n=0,16; $m\approx 1$.

The transport equation is used with the following boundary conditions [4, 5]:

– inlet boundary: $C\big|_{inlet} = C_E$, 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, ground and solid surfaces: $\frac{\partial C}{\partial n} = 0$.

To simulate the wind flow over buildings the model of potential flow is used. In this case, the governing equation is [5]:

$$\frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2} = 0, \tag{2}$$

where P is the potential of velocity.

The boundary conditions for equation (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: $P = P_0 + const$ (Dirichle condition).

The components of the wind velocity are calculated as follows:

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

After computing of the wind velocity components the convective – diffusion equation (1) is solved.

Numerical integration of the equations. To develop the numerical model on the basis of equation (1) the change – triangle difference scheme is used [1,7]. The following approximation is carried out

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

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

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

First order derivatives are approximated as follows

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

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

$$\frac{\partial v^{+}C}{\partial y} \approx \frac{v^{+}_{i,j+1}C^{n+1}_{ij} - v^{+}_{il}C^{n+1}_{i,j-1}}{\Delta y} = L^{+}_{y}C^{n+1},$$

$$\frac{\partial v^{-}C}{\partial y} \approx \frac{v^{-}_{i,j+1}C^{n+1}_{i,j+1} - v^{-}_{ij}C^{n+1}_{ij}}{\Delta y} = L^{-}_{y}C^{n+1}$$

Second order derivatives are approximated using such difference formulae:

$$\frac{\partial}{\partial x}(\mu_x \frac{\partial C}{\partial x}) \approx \mu_x \frac{C^{n+1}_{i+1,j} - C^{n+1}_{ij}}{\Delta x^2} - \mu_x \frac{C^{n+1}_{ij} - C^{n+1}_{i-1,j}}{\Delta x^2} = M^{-}_{xx}C^{n+1} + M^{+}_{xx}C^{n+1}$$

$$\frac{\partial}{\partial y}(\mu_y \frac{\partial C}{\partial y}) \approx \mu_y \frac{C^{n+1}_{i,j+1} - C^{n+1}_{ij}}{\Delta x^2} - \mu_y \frac{C^{n+1}_{ij} - C^{n+1}_{i,j-1}}{\Delta x^2} = M^{-}_{yy}C^{n+1} + M^{+}_{yy}C^{n+1}$$

The difference approximation of Eq.1 is now as follows

$$\frac{C^{n+1}_{ij} - C^{n}_{ij}}{\Delta t} + L^{+}_{x}C^{n+1} + L^{-}_{x}C^{n+1} + L^{+}_{y}C^{n+1} + L^{-}_{y}C^{n+1} + \sigma C^{n+1}_{ij} =$$
$$= (M^{+}_{xx}C^{n+1} + L^{-}_{xx}C^{n+1} + L^{+}_{yy}C^{n+1} + L^{-}_{yy}C^{n+1})$$

To solve this difference equation we split it:

Step 1: $k = \frac{1}{4}$:

$$\frac{C^{n+k}_{ij} - C^{n}_{ij}}{\Delta t} + \frac{1}{2}(L^{+}_{x}C^{k} + L^{+}_{y}C^{k}) + \frac{\sigma}{4}C^{k}_{ij} =$$
$$= \frac{1}{4}(M^{+}_{xx}C^{k} + M^{-}_{xx}C^{n} + M^{+}_{yy}C^{k} + M^{-}_{yy}C^{n})$$

Step 2: $k = n + \frac{1}{2}$; $c = n + \frac{1}{4}$:

$$\frac{C^{k}_{ij} - C^{c}_{ij}}{\Delta t} + \frac{1}{2}(L^{-}_{x}C^{k} + L^{-}_{y}C^{k}) + \frac{\sigma}{4}C^{k}_{ij} = \frac{1}{4}(M^{-}_{xx}C^{k} + M^{+}_{xx}C^{c} + M^{-}_{yy}C^{k} + M^{+}_{yy}C^{c})$$

Step 3: $k = n + \frac{3}{4}$; $c = n + \frac{1}{2}$:

$$\frac{C^{k}_{ij} - C^{c}_{ij}}{\Delta t} + \frac{1}{2}(L^{+}_{x}C^{k} + L^{-}_{y}C^{k}) + \frac{\sigma}{4}C^{k}_{ij} = \frac{1}{4}(M^{-}_{xx}C^{c} + M^{+}_{xx}C^{k} + M^{-}_{yy}C^{k} + M^{+}_{yy}C^{c})$$

Step 4: $k = n + 1$; $c = n + \frac{3}{4}$:

$$\frac{C^{k}_{ij} - C^{c}_{ij}}{\Delta t} + \frac{1}{2}(L^{-}_{x}C^{k} + L^{+}_{y}C^{k}) + \frac{\sigma}{4}C^{k}_{ij} = \frac{1}{4}(M^{-}_{xx}C^{k} + M^{+}_{xx}C^{c} + M^{-}_{yy}C^{c} + M^{+}_{yy}C^{k})$$

Unknown concentration C at each step can be easily computed using explicit formula of ‘*running calculation*’ [1, 5].

To solve equation (2) Richardson scheme and Libman method were used. Special code ‘*InFLOW-2D*’ was created on the basis of the developed numerical model.

Results. The developed numerical model was used to estimate the efficiency of the jet supply to reduce the concentration near the building and thus protect building from toxic chemical penetration. The numerical experiment was carried out using the following data: the length of the computational domain is 100m, the height of the computational domain is 63m; wind speed is 5m/s; air jet speed is 10m/s; the dimensionless concentration in cloud is 1(at t=0). The sketch of the calculation domain is shown in Fig. 1. At t=0 the form of the toxic chemical (NH3) cloud is set.

The results of the computational experiment are shown in Fig.2,3. If we compare the concentration field near the second building for two cases (with air jet and without air jet) we can see that the air jet influence the intensity of the air contamination near that building. The concentration near the windward wall of the second building is less than in the case when the air jet is not used.

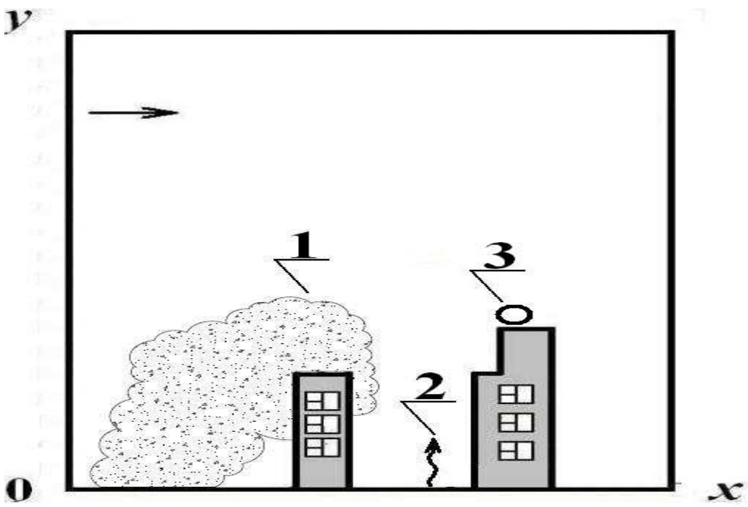

Fig. 1. Sketch of the computational domain: 1 – toxic cloud; 2 – position of air jet; 3 – position of receptor (intake of the ventilation system)

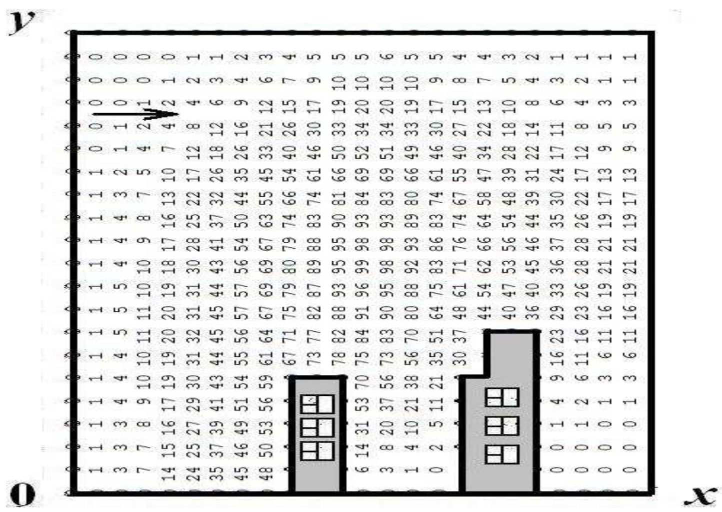

Fig. **2. Concentration of toxic gas, t=6 sec (no air jet)**

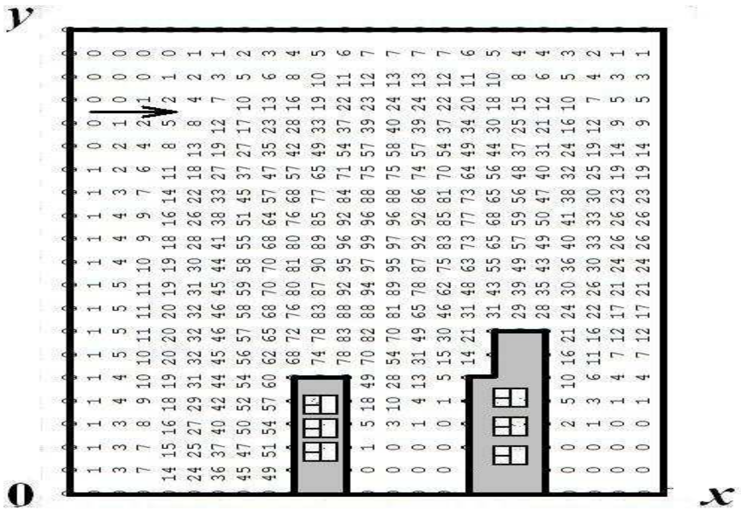

Fig. 3. Concentration of toxic gas, t=6 sec (with air jet)

The efficiency of this method of protection can be estimated if we compare the concentration of the chemical for both cases, for example, on the roof where the intake of the ventilation system is situated. This position on the roof is shown by '*circle*' in Fig.1. These results are shown in Tabl.1.

Table 1

Dimensionless concentration on the roof

t, sec	No jet	With jet
6	0,281	0,19
9	0,424	0,26
12	0,331	0,18

As we see from Tabl.1 the jet implementation can reduce the level of contamination even at the roof level.

The computational time to solve the problem was about 8 sec. It means that the developed model can be attractive from a designer's point of view.

The future work in this field should be directed to the development of the 3-D numerical model of this process.

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PROMPT CFD SIMULATION OF AIR IONS DISPERSION IN THE ROOMS

Представлена CFD модель для моделювання розсіювання аероіонів в приміщеннях. Модель заснована на використанні рівняння переносу домішки і моделі потенційного течії. Представлені результати обчислювального експерименту, проведеного на базі розробленої моделі.

Ключові слова: аероіони, CFD моделювання, мікроклімат приміщень.

Представлена CFD модель для моделирования рассеивания аэроионов в помещениях. Модель основана на использовании уравнения переноса примеси и модели потенциального течения. Представлены результаты вычислительного эксперимента, проведенного на базе разработанной модели.

Ключевые слова: аэроионы, CFD моделирование, микроклимат помещений.

A CFD model to simulate the air ions concentration in rooms was developed. This model is based on the equations of the admixture dispersion and the model of potential flow. The implicit schemes are used for the numerical simulation. The results of the numerical experiment are presented.

Key words: air ions, CFD simulation, rooms microclimate

Introduction. The prediction of the air ions concentration in industrial rooms, office rooms is now the problem of great interest. It is well known that the concentration of negative and positive air ions influence on the health of people. To provide the normal air ions conditions in industrial rooms it is necessary to predict the air ions concentration at the work places when the special equipment of air ions emission are proposed to be used. To solve this problem the researches need special mathematical models.

Literature review. Now in Ukraine to predict the air ions regimes in rooms only the analytical models are used [2 - 5]. These models allow to calculate rapidly the air ions concentration but the models can’t take into account the influence of the furniture deposition in rooms or the air flow induced by ventilation system on the air ions dispersion. CFD models developed abroad are based on Navier – Stokes equations [1] and need a lot of computational time. It is not very convenient at practical use especially when many variants of have to be solved. So it is necessary to have CFD models to provide researches with the more power tools of air ions prediction in industrial rooms.

The objective. The main objective of this paper is the development of the effective CFD model to predict the air ions concentration in rooms.