ISSN 2307–3489 (Print), ISSN 2307–6666 (Online)

Наука та прогрес транспорту, 2024, № 4 (108)

ЕКОЛОГІЯ ТА ПРОМИСЛОВА БЕЗПЕКА

UDC 331.42:[504.6:519.87]

M. M. BILIAIEV[1], V. V. BILIAIEVA[2], O. V. BERLOV[3*], V. A. KOZACHYNA[4],
P. B. MASHYKHINA[5]

[1]Dep. of «Hydraulics, Water Supply and Physics», Ukrainian State University of Science and Technologies, Lazaryana St., 2, Dnipro, Ukraine, 49010, tel. +38 (056) 373 15 09, e-mail biliaiev.m@gmail.com, ORCID 0000-0002-1531-7882
[2]Dep. of Energy Systems and Energy Management, Ukrainian State University of Science and Technologies, Nauky Ave., 4, Dnipro, Ukraine, 49010, tel. +38 (056) 374 82 89, e-mail water.supply.treatment@gmail.com, ORCID 0000-0003-2399-3124
[3*]Dep. of Labor Protection, Civil and Technogenic Safety, Ukrainian State University of Science and Technologies, St. Architect Oleg Petrov, 24-a, Dnipro, Ukraine, 49600, tel. +38 (056) 756 34 57, e-mail berlov.oleksandr@pdaba.edu.ua, ORCID 0000-0002-7442-0548
[4]Dep. «Hydraulics, Water Supply and Physics», Ukrainian State University of Science and Technologies, Lazaryana St., 2, Dnipro, Ukraine, 49010, tel. +38 (056) 373 15 09, e-mail v.kozachyna@gmail.com, ORCID 0000-0002-6894-5532
[5]Dep. of «Hydraulics and Water Supply», Ukrainian State University of Science and Technologies, Lazaryana St., 2, Dnipro, Ukraine, 49010, tel. +38 (056) 373 15 09, e-mail gidro_eko@ukr.net, ORCID ID 0000-0003-3057-9204

Quick computing CFD model to predict chemical pollution in room

Purpose. The problem of accidental contamination of workspaces attracts special attention, since in the event of such extreme situations, intense chemical contamination of the air in work areas occurs. This poses a threat of toxic exposure to workers. When assessing the consequences of such situations, it is necessary to take into account the time factor, in particular, to quickly determine the creation of concentrations of chemically hazardous substances. In this regard, an urgent task is to develop effective mathematical models for rapid assessment of the consequences of extreme situations in the working areas of chemically hazardous facilities. The paper considers a CFD model for analyzing the process of chemical air pollution in a workspace during an accidental release of a chemically hazardous substance. The solution of the problem is based on the numerical integration of the fundamental equations of continuum mechanics. **Methodology.** To calculate the air velocity field in the working room during the operation of supply and exhaust ventilation, a mathematical model of the motion of an inviscid fluid was used. The equation of convective diffusion motion was used to calculate the concentration of a chemically hazardous substance in the workspace. The integration of the modeling equations was carried out using finite difference schemes. **Findings.** A dynamic model has been created to calculate the spread of a chemically hazardous substance in a workspace. On the basis of the built CFD model, a computer program was created to conduct a computational experiment. **Originality.** A CFD model has been created to predict the level of air pollution in a workspace in the event of toxic gas emissions. The model is based on the fundamental equations of aerodynamic mechanics and mass transfer. The model makes it possible to determine the effect of the ventilation mode, the intensity of emission of a chemically hazardous substance, the location of equipment in the workspace, and the dynamics of the formation of concentration fields. **Practical value.** The developed CFD model can be used to quickly analyze the consequences of accidental emissions of a chemically hazardous substance in a workplace and assess the risk of toxic exposure of workers.

Key words: chemical air pollution; workplace; mathematical modeling

Introduction

The problem of air pollution in working premises is particularly relevant. The range of practical tasks of this class includes tasks related to the emission of toxic substances in extreme situations. In such situations, very rapid damage to personnel at workplaces is possible [1, 3–9]. This is due to the fact that in extreme situations, areas of intense chemical pollution appear very quickly in the

doi: https://doi.org/10.15802/stp2024/317406

premises (Fig. 1). Therefore, it is extremely important to reasonably determine the parameters of emergency ventilation, taking into account the fact that stagnant areas may form in working areas. Such forecasting can be performed on the basis of mathematical models [1, 2]. However, at present there is a shortage of such models, which makes the development of mathematical models for solving problems of this class urgent.

Fig. 1. Emission in the workplace (http://surl.li/lrwqqj)

Purpose

Development of a numerical model for predicting emergency air pollution in the workplace.

Method

The calculation of the dynamics of chemical air pollution in a working room during an emergency release of chlorine is based on the numerical integration of aerodynamics and mass transfer equations. The modeling equation of aerodynamics is the following equation [1, 2]:

$$\frac{\partial P^2}{\partial x^2}+\frac{\partial P^2}{\partial y^2}=0. \qquad (1)$$

For the modeling equation (1), the following boundary conditions are set:

– at the boundary where the flow enters the calculation area (ventilation openings), the Neumann boundary condition is imposed on the velocity potential $\frac{\partial P}{\partial x}=U$, де U – known value of wind speed;

– at the boundary where the flow exits the computational domain (corresponding ventilation openings), a Dirichlet boundary condition is imposed on the velocity potential $P=P_0+const$, where P_0 – some numerical constant;

– on the upper boundary, a solid impermeable wall, the condition of impermeability is imposed $\frac{\partial P}{\partial y}=0$;

– on the lower boundary, a solid opaque wall, the condition of non-penetration is imposed $\frac{\partial P}{\partial y}=0$;

– the condition of non-penetration will be fulfilled on all solid walls (equipment).

If the velocity potential fields are known, then the following dependencies are used to determine the components of the air flow velocity vector [2]:

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

Numerical integration of the modeling equation (1), as well as for numerical integration of other differential equations of the ventilation and mass transfer model, a rectangular difference grid is used. For numerical integration of the equation for the velocity potential, its writing in evolutionary form is used [2]:

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

where t –fictitious time, when $t\to\infty$ the solution of equation (2) approaches the solution of Laplace's equation (1).

In this case, numerical integration was carried out in two stages. The differential dependencies at each stage have the form :

– at the first stage:

$$\frac{P_{i,j}^{n+\frac{1}{2}}-P_{i,j}^{n}}{\Delta t}=$$

$$=\left[\frac{-P_{i,j}^{n+\frac{1}{2}}+P_{i-1,j}^{n+\frac{1}{2}}}{\Delta x^2}\right]+\left[\frac{-P_{i,j}^{n+\frac{1}{2}}+P_{i,j-1}^{n+\frac{1}{2}}}{\Delta y^2}\right]; \qquad (3)$$

– at the second stage:

$$\frac{P_{i,j}^{n+1}-P_{i,j}^{n+\frac{1}{2}}}{\Delta t}=\left[\frac{P_{i+1,j}^{n+1}-P_{i,j}^{n+1}}{\Delta x^2}\right]+\left[\frac{P_{i,j+1}^{n+1}-P_{i,j}^{n+1}}{\Delta y^2}\right].(4)$$

doi: https://doi.org/10.15802/stp2024/317406

Next, the values of the air flow velocity components were determined based on the dependencies.

After calculating the air flow velocity, the solution of the energy equation begins. We also use a difference splitting scheme for the solution.

The calculation is carried out until the condition is met.

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

where ε – small number; n – iteration number.

The process of spreading a hazardous substance that enters the air of a workroom during an emergency emission is modeled based on the mass transfer equation [1, 2]:

$$\frac{\partial C}{\partial t} + \frac{\partial uC}{\partial x} + \frac{\partial \left(v - w_s \right) C}{\partial y} =$$
$$= \frac{\partial}{\partial x}\left(\mu_x \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y}\left(\mu_y \frac{\partial C}{\partial y} \right) +$$
$$+ \sum q_i \delta\left(x - x_i \right)\left(y - y_i \right), \quad (5)$$

where C – concentration of a chemically hazardous substance; u, v – components of the air flow velocity vector in the working space; w_s – rate of gravitational settling of matter; $\mu = \left(\mu_x, \mu_y \right)$ – turbulent diffusion coefficients; q_i – emission intensity of a chemically hazardous impurity; $\delta\left(x - x_i \right)\left(y - y_i \right)$ – Dirac delta function; $\left(x_i, y_i \right)$ – coordinates of the location of the emission source of a chemically hazardous impurity in the workplace; t – time.

For numerical integration of equation (5), the following transformations are made [2]:

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

$$u^+ = \left(u + |u| \right)/2, u^- = \left(u - |u| \right)/2,$$
$$v^+ = \left(v + |v| \right)/2, v^- = \left(v - |v| \right)/2,$$

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

$$\frac{\partial u^- C}{\partial x} \approx \frac{u^-_{i+1,j} C^{n+1}_{i+1,j} - u^-_{i,j} C^{n+1}_{i,j}}{\Delta x} = L^-_x C^{n+1},$$

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

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

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

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

$$\frac{\partial}{\partial y}\left(\mu_y \frac{\partial C}{\partial y} \right) \approx \tilde{\mu}_y \frac{C^{n+1}_{i,j+1} - C^{n+1}_{i,j}}{\Delta y^2} - \tilde{\mu}_y \frac{C^{n+1}_{i,j} - C^{n+1}_{i,j-1}}{\Delta y^2} =$$
$$= M^-_{yy} C^{n+1} + M^+_{yy} C^{n+1}.$$

Then, we can write an analogue of equation (1) in difference form:

$$\frac{C^{n+1}_{ij} - C^{n}_{ij}}{\Delta t} + L^+_x C^{n+1} + L^-_x C^{n+1} +$$
$$+ L^+_y C^{n+1} + L^-_y C^{n+1} + \sigma C^{n+1}_{ij} =$$
$$= (M^+_{xx} C^{n+1} + M^-_{xx} C^{n+1} +$$
$$+ M^+_{yy} C^{n+1} + M^-_{yy} C^{n+1}) + q_{ij} \delta_{ij} . (6)$$

The parameter δ_{ij} is 1 if there is a source of contamination in the differential cell, and 0 if there is no source of contamination in the cell.

Note that this entry uses the following dependency:

$$q_{i,j} = q_i / \Delta x / \Delta y ,$$

where q_i – intensity of the pollutant emission source.

Next, equation (6) is decomposed as follows [2]:

doi: https://doi.org/10.15802/stp2024/317406

– step 1 (k=1/4):

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

$$=\frac{1}{4}(M_{xx}^{+}C^{k}+M_{xx}^{-}C^{k}+$$

$$+M_{yy}^{+}C^{n}+M_{yy}^{-}C^{n})+\sum_{l=1}^{N}\frac{Q}{4}\delta_l\,. \quad (7)$$

– step 2 (k=n+1/2; c=n+1/4):

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

$$=\frac{1}{4}(M_{xx}^{-}C^{k}+M_{xx}^{+}C^{c}+$$

$$+M_{yy}^{-}C^{k}+M_{yy}^{+}C^{c})+\sum_{l=1}^{N}\frac{Q}{4}\delta_l\,. \quad (8)$$

– step 3 (k=n+3/4; c=n+1/2):

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

$$=\frac{1}{4}(M_{xx}^{-}C^{c}+M_{xx}^{+}C^{k}+$$

$$+M_{yy}^{-}C^{k}+M_{yy}^{+}C^{c})+\sum_{l=1}^{N}\frac{Q}{4}\delta_l\,. \quad (9)$$

– step 4 (k=n+1; c=n+3/4):

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

$$=\frac{1}{4}(M_{xx}^{-}C^{k}+M_{xx}^{+}C^{c}+$$

$$+M_{yy}^{-}C^{k}+M_{yy}^{+}C^{c})+\sum_{l=1}^{N}\frac{Q}{4}\delta_l\,. \quad (10)$$

A feature of the considered splitting scheme is that at each calculation step, the concentration of a chemically hazardous substance is determined by an explicit formula.

At the next stage, the software implementation of the constructed numerical models of aerodynamics and mass transfer was carried out.

Results

A computational experiment was conducted on the basis of the developed numerical models of aerodynamics and mass transfer. The scheme of the computational domain is shown in Fig. 2. In the working room, an emergency ammonia emission was considered. The emergency emission was carried out during 20s, and then the emission stopped. In the working room, air enters through an opening located at the middle of the left wall, and the outlet opening was situated at the right wall of the room. The both openings are shown by the «arrows» in Fig. 2.

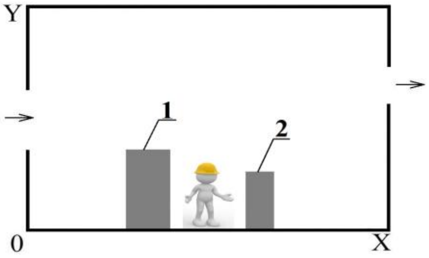

Fig. 2. Calculation scheme:
1 – ammonia emission site; *2* – equipment

The intensity of ammonia emission was 3 g/s, the dimensions of the calculation area were 10m*5m. When performing calculations, the following dependencies were used to determine the value of the diffusion coefficients:

$$\mu_x=0{,}1\cdot \mathrm{u}\,;\ \mu_y=0{,}1\cdot v\,.$$

The results of the numerical experiment are shown in two forms: a matrix of the distribution of ammonia concentration in the working room (Fig. 3–6) and in the form of ammonia concentration isolines (Fig. 7–10). The matrices make it possible to obtain quickly a «quantitative» assessment of the level of chemical air pollution in the working room, or in a certain area of the room, and change of this level during time. The modeling results, shown in the form of isolines (Fig. 3–6), make it possible to determine quickly the shape of the chemical pollution zone and the influence of the equipment on the «deformation» of the pollution zone.

The matrix figures show the ammonia concentration field in dimensionless form. Each number in the figure shows the concentration value as a percentage of $C_{\max}$ (maximum concentration).

doi: https://doi.org/10.15802/stp2024/317406

The maximum ammonia concentration changes over time in the working room.

Figure 7–10 shows how the shape of the contamination zone in the workroom changes at different times after the accident. Figure 3–6 shows the ammonia concentration field in dimensionless form. Each number in the figure shows the concentration value as a percentage of its maximum value at a given time.

Fig. 3. Area of contamination in the workplace $t = 2$s, $C_{max} = 1,34$ g/m^3

Fig. 4. Area of contamination in the workplace $t = 4$s, $C_{max} = 1,56$ g/m^3

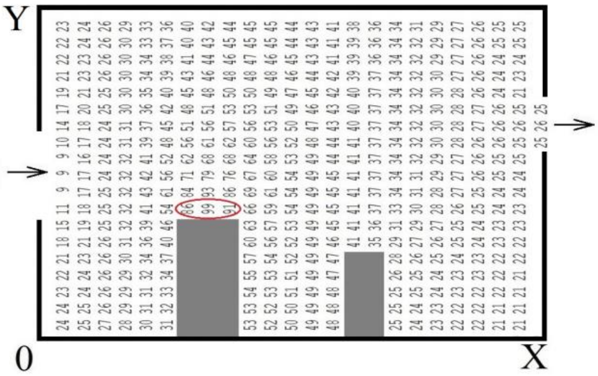

Fig. 5. Area of contamination in the workplace $t = 10$s, $C_{max} = 1,95$ g/m^3

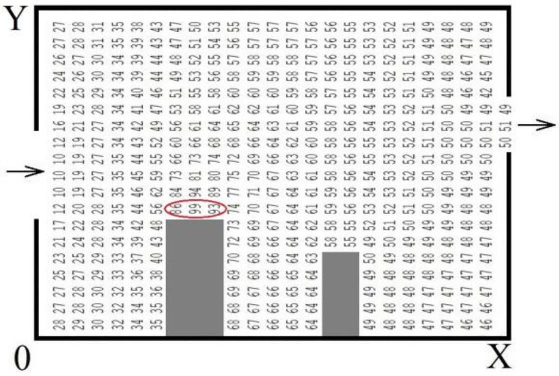

Fig. 6. Area of contamination in the workplace $t = 20$s, $C_{max} = 2,25$ g/m^3

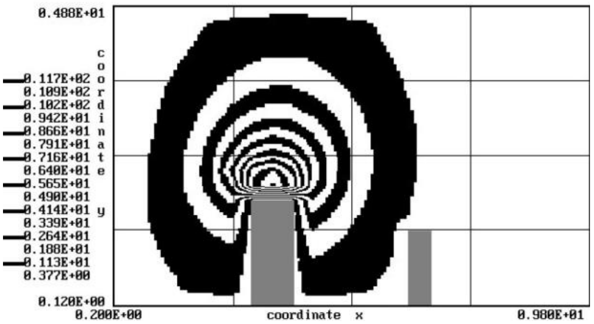

Fig. 7. Isolines of impurity concentration in the working room $t = 1$s

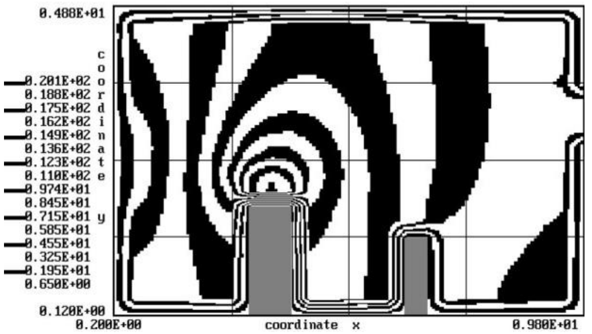

Fig. 8. Isolines of impurity concentration in the working room $t = 10$s

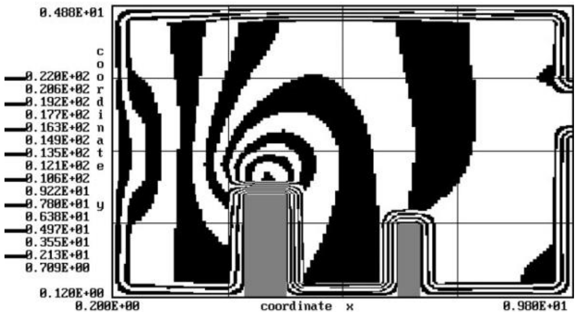

Fig. 9. Isolines of impurity concentration in the working room $t = 15$s

doi: https://doi.org/10.15802/stp2024/317406

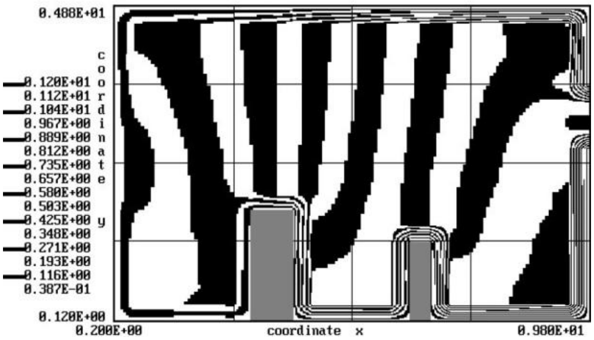

Fig. 10. Isolines of impurity concentration
in the working room t = 70s

As can be seen from the figures, the contamination zone increased in size very quickly. By the time t = 4s, this zone «occupied» all the working room. That means that the room was filled with toxic gas. The concentration of toxic gas will significantly exceed the maximum permissible concentration. And this can be seen clearly in Fig. 11. Fig. 11 shows the change in the maximum ammonia concentration in the room at different times.

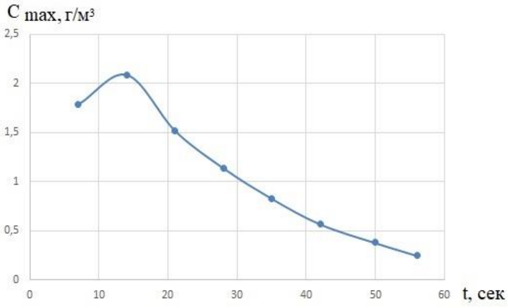

Fig. 11. Changing the maximum indoor ammonia concentration in room

As can be seen from Fig. 11, over time there is a decrease of ammonia concentration in room, which is associated with the leak of a chemically hazardous substance. An intensive decrease of the ammonia concentration is explained by the work of emergency ventilation system and emission source stop. The calculation time is 3 seconds.

Scientific novelty and practical significance

A numerical model has been created to predict the level of air pollution in a work environment due to toxic gas emissions.

The model is based on the numerical integration of fundamental equations of the mechanics of a solid medium. A feature of the numerical model is the consideration of the main physical factors that affect the spread of toxic gas in the room (the presence of equipment in the room, the position of ventilation openings, the location of the emission of the toxic substance, etc.) and the speed of calculation.

Conclusions

1. A dynamic multifactorial numerical model has been developed to analyze and predict the process of chemical contamination of the work space.
2. A feature of the numerical model is the ability to take into account the main physical factors that influence the formation of pollution areas in work areas.
3. The developed numerical model can be used to scientifically substantiate emergency ventilation parameters to quickly reduce the concentration of a toxic (or explosive) substance in a workroom.

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М. М. БІЛЯЄВ[1], В. В. БІЛЯЄВА[2], О. В. БЕРЛОВ[3*], В. А. КОЗАЧИНА[4],
П. Б. МАШИХІНА[5]

[1]Каф. «Гідравліка, водопостачання та фізика», Український державний університет науки і технологій, вул. Лазаряна, 2, Дніпро, Україна, 49010, тел. +38 (056) 373 15 09, ел. пошта biliaiev.m@gmail.com, ORCID 0000-0002-1531-7882
[2]Каф. Енергетичних систем та енергоменеджменту, Український державний університет науки і технологій, пр. Науки, 4, Дніпро, Україна, 49010, тел. +38 (056) 374 82 89, ел. пошта water.supply.treatment@gmail.com, ORCID 0000-0003-2399-3124
[3*]Каф. Охорони праці, цивільної та техногенної безпеки, Український державний університет науки і технологій, вул. Архітектора Олега Петрова, 24-а, Дніпро, Україна, 49600, тел. +38 (056) 247 16 01, ел. пошта berlov.oleksandr@pdaba.edu.ua, ORCID 0000-0002-7442-0548
[4]Каф. «Гідравліка, водопостачання та фізика», Український державний університет науки і технологій, вул. Лазаряна, 2, Дніпро, Україна, 49010, тел. +38 (056) 373 15 09, ел. пошта v.kozachyna@gmail.com, ORCID 0000-0002-6894-5532
[5]Каф. «Гідравліка, водопостачання та фізика», Український державний університет науки і технологій, вул. Лазаряна, 2, Дніпро, Україна, 49010, тел. +38 (056) 373 15 09, ел. пошта gidro_eko@ukr.net, ORCID 0000-0003-3057-9204

Швидка обчислювальна CFD-модель для прогнозування хімічного забруднення приміщення

Мета. Проблема аварійного забруднення робочих приміщень привертає до себе особливу увагу, оскільки в разі виникнення таких екстремальних ситуацій відбувається інтенсивне хімічне забруднення повітря в робочих зонах. Це створює загрозу токсичного ураження працівників. Під час оцінювання наслідків таких ситуацій потрібно враховувати часовий фактор, зокрема швидко визначити створення концентрацій хімічно небезпечних речовин. У зв’язку з цим актуальною задачею є розробка ефективних математичних моделей для оперативного оцінювання наслідків екстремальних ситуацій у робочих приміщеннях хімічно небезпечних об’єктів. Розглянуто побудовану CFD-модель для аналізу процесу хімічного забруднення повітря в робочому приміщенні під час аварійної емісії хімічно небезпечної речовини. Рішення задачі базується на чисельному інтегруванні фундаментальних рівнянь механіки суцільного середовища. **Методика.** Для розрахунку поля швидкості повітря в робочому приміщення під час роботи припливно-витяжної вентиляції використано математичну модель руху нев’язкої рідини. Для розрахунку концентрації хімічно небезпечної речовини в робочому приміщенні використано рівняння конвективно-дифузійного руху. Інтегрування моделювальних рівнянь здійснено за допомогою скінченнорізницевих схем. **Результати.** Створено динамічну модель для розрахунку поширення хімічно небезпечної речовини в робочому приміщенні. На базі побудованої CFD-моделі створено комп’ютерну програму для проведення обчислювального експерименту. **Наукова новизна.** Створено CFD-модель для прогнозування рівня забруднення повітря в робочому приміщенні в разі емісії токсичного газу. Основою моделі є фундаментальні рівняння механіки аеродинаміки та масопереносу. Модель дає можливість визначати вплив режиму вентиляції, інтенсивності емісії хімічно небезпечної речовини, розташування обладнання в робочому приміщенні та динаміку формування концентраційних полів. **Практична значимість.** Розроблена CFD-модель може бути використана для оперативного аналізу наслідків аварійної емісії хімічно небезпечної речовини в робочому приміщенні та оцінювання ризику токсичного ураження працівників.

Ключові слова: хімічне забруднення повітря; робоче приміщення; математичне моделювання

doi: https://doi.org/10.15802/stp2024/317406

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Надійшла до редколегії: 12.08.2024
Прийнята до друку: 10.12.2024

doi: https://doi.org/10.15802/stp2024/317406