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ЕКОЛОГІЯ НА ТРАНСПОРТІ

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CALCULATION OF «VULNERABILITY» ZONE IN CASE OF TERRORIST ATTACK WITH CHEMICAL AGENTS

Purpose. The work involves the development of a numerical model for calculating the «vulnerability» zone of a possible terrorist attack objective with the use of a chemical agent in a built-up environment. The «vulnerability» zone is a territory near the attack objective, where the emission of a chemical agent during the attack will lead to undesirable consequences. The emission of a chemical agent outside the «vulnerability» zone will not create a dangerous concentration near the attack objective. **Methodology.** To solve this problem, we use the equation for the velocity potential, on the basis of which we determine the wind stream velocity field, and the equation adjoint to the equation of mass transfer in the atmospheric air of the chemical agent emitted in the event of a terrorist attack. During simulation, we take into account the uneven wind stream velocity field, atmospheric diffusion and the rate of emission of a chemically hazardous substance. For the numerical integration of the velocity potential equation, we use the method of A. A. Samarsky. For numerical solution of the adjoint equation, we introduce new variables and use an implicit difference splitting scheme. The peculiarity of the developed numerical model is the possibility of operative estimation of the «vulnerability» zone near a possible attack objective. **Findings**. The developed numerical model and computer program can be used for scientifically grounded assessment of the «vulnerability» zone near significant facilities in the event of possible attacks with the use of chemical (biological) agents. The constructed numerical model can be implemented on computers of small and medium power, which allows it to be widely used to solve the problems of this class when developing the emergency response plan. The results of the computational experiment are presented, which allow us to evaluate the possibilities of the proposed numerical model. **Originality**. An effective numerical model is proposed for calculating the «vulnerability» zone near the facility, which may be the target of a terrorist attack with the use of a chemical agent. The model is based on the numerical integration of the velocity potential equation and the equation adjoint to the equation of mass transfer of a chemically dangerous substance in the atmosphere. **Practical value.** The developed model can be used to organize protective actions near the target facility of a possible chemical attack by terrorists.

Keywords: terrorist attack; chemical pollution; «vulnerability» zone; adjoint equation; numerical simulation; air contamination

Introduction

Recently, special attention has been drawn to the tasks related to the assessment of the consequences of possible terrorist acts with the use of chemical (biological) agents [1, 2, 4–14]. Within the framework of this problem, it is possible to single out an extremely important and specific

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task – determining the «vulnerability» zone for the terrorist chemical attack objectives. The «vulnerability» zone is a territory near the attack objective, where the emission of a chemical agent during a terrorist act will lead to undesirable consequences at the facility. The release of a chemically hazardous substance outside this zone will not create a «problem» at the attacked facility.

Mathematically, this provision can be expressed as follows: at the objective of the potential terrorist chemical attack, up to the time point τ, the concentration of the hazardous substance must not exceed a certain dangerous value φ:

$$C\left(r_i, \tau\right) < \varphi. \quad (1)$$

Here φ is the concentration which results in a certain severity affects for a person.

It should be noted that the solution to this problem becomes quite complicated if the emission of a chemical agent is considered in a built-up environment – which is, in fact, the most obvious situation in the case of a chemical attack. As a «zero» approximation, one can neglect the influence of specific buildings and other facilities on the formation of chemical contamination area and use, for example, Gaussian models to solve the problem, as was done in the «ALOHA» code. For a more detailed assessment of the the contaminated areas, it is necessary to make calculations taking into account the influence of facilities on the formation of concentration fields. Such detailing can be different and determined by a number of factors (for example, availability of a sufficient amount of input information for modeling, available software package for calculations, time for obtaining results, etc.). The models used in practice for assessing the consequences of a terrorist act are based on solving the «direct» problem of mass transfer – i.e. direct solution of the equation of convective-diffusion dispersion of impurities in the *atmosphere at a given place* of emission of a hazardous substance. However, the use of such models requires considerable time to determine the «vulnerability» zone, since the solution to the problem is found by going through different emission points of a chemical agent during a possible terrorist attack, i.e. the problem is solved by the trial-and-error method. Using this approach requires a lot of time to obtain the desired result. In this regard, the actual problem is the development of effective methods for solving the «vulnerability» zone determination problems for various facilities in the context of the growing terrorist threat.

Purpose

The purpose of this work is to create a numerical model to determine the «vulnerability» zone of a facility in case of a chemical attack by terrorists in a built-up environment.

Methodology

We consider the solution method on the example of solving two problems that can be formulated when analyzing terrorist acts with the use of a chemical or biological agent.

Direct problem. If a chemical (biological) agent is used in a terrorist attack, contaminated area can be calculated on the basis of the following mass transfer equation (plan task) [2–5, 7, 8]:

$$\frac{\partial C}{\partial t} + \frac{\partial uC}{\partial x} + \frac{\partial vC}{\partial y} + \sigma C = \frac{\partial}{\partial x}\left(\mu_x \frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(\mu_y \frac{\partial C}{\partial y}\right) + Q\delta\left(x - x_0\right)\delta\left(y - y_0\right), \quad (2)$$

where C – average concentration of chemical (biological) agent in atmospheric air; σ – coefficient taking into account the agent decomposition in the atmosphere; u, v – components of the air velocity vector; $\mu = \left(\mu_x, \mu_y\right)$ – coefficients of atmospheric turbulent diffusion; Q – intensity of agent emission during the terrorist attack; $\delta\left(x - x_0\right)\left(y - y_0\right)$ – Dirac delta function; x_0, y_0 – coordinates of the agent emission source during the terrorist attack; t – time.

The boundary conditions for the equation (2) are written as [3]:

$$C = C_0 \quad \text{for } t = 0,$$

$C = 0$ at the boundaries of the calculated area, where C_0 is the known value.

When solving the «direct» problem, it is necessary to specify information about the chemical agent emission point (coordinates x_0, y_0), as well as the agent emission intensity Q).

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To apply the equation (1) in the case of dispersion of a chemical (biological) agent in a built-up environment, it is necessary to know the uneven velocity field of the wind flow, i.e. the value of the variables *u=f(x,y), v=f(x,y).* The definition of this field in the presence of buildings is a complex hydrodynamic problem. Abroad, to solve this problem, one traditionally uses the Navier-Stokes equations, supplemented by one or another turbulence model. This base allowed developing specialized software packages such as ANSYS Fluent, FAST, etc. These packages are a powerful tool for solving a wide class of problems. However, it is known that the use of the Navier-Stokes equations for calculating flows with large Reynolds numbers *(^{i}Re),* requires the use of a very small computational grid, which immediately leads to large expenditures of computer time in the practical implementation of the model. In addition, very powerful computers are needed. This becomes a significant obstacle when it is necessary to carry out serial calculations, for example, when developing the ERP (Emergency Response Plan). In MES or in other competent organizations it is necessary to have fast-reading models, which, in this case, would take into account the most significant physical factors of the simulated process. In this work, to determine the wind velocity field *u=f(x,y), v=f(x,y)* in the built-up environment, the potential flow model will be used [5]:

$$\frac{\partial^2 P}{\partial x^2}+\frac{\partial^2 P}{\partial y^2}=0, \qquad (3)$$

where *P* is the velocity potential.

The value of the components of the wind velocity vector are determined on the basis of the ratios:

$$u=\frac{\partial P}{\partial x},\ v=\frac{\partial P}{\partial y}. \qquad (4)$$

For equation (2) the following boundary conditions are set:

– On solid boundaries the impermeability condition is set:

$$\frac{\partial P}{\partial n}=0,$$

where *n* is the unit vector of the outer normal to the boundary;

– On the boundary of the «out-flow» from the computational domain, the Dirichle boundary condition of the form *P*=const is set;

– On the boundaries where the air «in-flow» occurs, the Neumann boundary condition is set: $\frac{\partial P}{\partial n}=V$, where *V* is the known velocity of the air flow.

The solution of problems for determining the size and intensity of contaminated area on the basis of equations (1), (2) is called the direct mass transfer problem solution.

To determine the «vulnerability» zone of a facility in case of a possible chemical attack, one can use the equations (1) and (2) and determine this zone by «brute force searching» for various coordinate values x_0, y_0, i.e. perform calculations for various points of chemical agent emission. It is quite obvious that such a solution of the problem for determining the «vulnerability» zone using the brute force method for parameters x_0, y_0 requires a lot of computational work, which is not always convenient.

Adjoint problem. Now we will consider a different approach to determining the facilty «vulnerability» zone in case of a chemical terrorist attack.

This approach is based on the application of the adjoint equation (3) [3]:

$$-\frac{\partial C^*}{\partial t}-\frac{\partial uC^*}{\partial x}-\frac{\partial vC^*}{\partial y}+\sigma C^*=$$
$$=\frac{\partial}{\partial x}\left(\mu_x\frac{\partial C^*}{\partial x}\right)+\frac{\partial}{\partial y}\left(\mu_y\frac{\partial C^*}{\partial y}\right)+p, \qquad (5)$$

where C^* is the function associated with the function C , *p* is a certain function [3].

The boundary conditions for the adjoint problem have the form [3]:

$C^*=C_T^*$ – concentration of the chemical agent in atmospheric air at *t=T*;

$C^*=0$ at the boundaries of the calculated area.

The peculiarity of applying the equation (3) is that the wind flow velocity field is uneven in a built-up environment and is determined by preliminary solving the equation (2) with the subsequent calculation of the velocity vector components by dependencies (3).

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The form of the function p can be extremely diverse [3], for example:

$$p(x,y,t)=\delta(x-x_i)\delta(y-y_i)\delta(t-\tau). \quad (6)$$

If the solution of the adjoint equation (5) is found, then, further, it is necessary to find the value of the following functional [3]

$$I=Q\int_0^T C^*(r_0,t)\,dt\,, \quad (7)$$

Having constructed the isolines of this functional, we find the solution of the problem posed out of the condition

$$I(r_0,\tau)<\varphi \quad (8)$$

We now consider the methodology for solving the adjoint equation. To solve the adjoint problem (4), we introduce new variables [3]:

$$u^{'}=-u\;,\; v^{'}=-v\,,\; t^{'}=T-t\,.$$

The solution of the adjoint problem begins with the time t = T.

When using new variables, the equation (5) takes the form of equation (2). Next, we will conduct an approximation of the derivatives, following [2, 5]. The approximation of the time derivative is as follows:

$$\frac{\partial C^*}{\partial t^{'}}\approx\frac{C_{ij}^{*\,n+1}-C_{ij}^{*\,n}}{\Delta t^{'}}.$$

Further, in the formulas, the symbols «*», «« will be omitted.

The first derivatives are approximated by the relations [5]

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

where

$$u^+=\frac{u+|u|}{2},u^-=\frac{u-|u|}{2},v^+=\frac{v+|v|}{2},v^-=\frac{v-|v|}{2}.$$

For approximation of the first derivatives, we use the formulas [2, 5]:

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

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

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

$$\frac{\partial v^-C}{\partial y}\approx\frac{v_{i,j+1}^-C_{i,j+1}^{n+1}-v_{ij}^-C_{ij}^{n+1}}{\Delta y}=L_y^-C^{n+1}.$$

Approximation of the second derivatives is carried out as follows [5]:

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

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

Taking into account the above designations of difference operators, we write the difference analogue of equation (2):

$$\frac{C_{ij}^{n+1}-C_{ij}^n}{\Delta t}+L_x^+C^{n+1}+L_x^-C^{n+1}+L_y^+C^{n+1}+$$
$$+L_y^-C^{n+1}+\sigma C_{ij}^{n+1}=$$
$$(M_{xx}^+C^{n+1}+L_{xx}^-C^{n+1}+L_{yy}^+C^{n+1}+L_{yy}^-C^{n+1})+$$
$$+Q_{ij}\delta_{ij}. \quad (9)$$

Now we carry out the splitting of the difference equation (9). The splitting equations at each step are written as:

At the first step ($k=n+\frac{1}{4}$):

$$\frac{C_{i,j}^{n+k}-C_{i,j}^n}{\Delta t}+\frac{1}{2}\left(L_x^+C^k+L_y^+C^k\right)+\frac{\sigma}{4}C_{i,j}^k=$$
$$=\frac{1}{4}\left(M_{xx}^+C^k+M_{xx}^-C^n+M_{yy}^+C^k+M_{yy}^-C^n\right), \quad (10)$$

At the second step ($k=n+\frac{1}{2};\,c=n+\frac{1}{4}$;):

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

$$= \frac{1}{4}\left(M_{xx}^- C^k + M_{xx}^+ C^c + M_{yy}^- C^k + M_{yy}^+ C^c\right), \quad (11)$$

At the third step ($k = n + \frac{3}{4}; c = n + \frac{1}{2}$;) the dependence (11) is applied.

At the fourth step ($k = n + 1; c = n + \frac{3}{4}$;) the dependence (10) is applied.

The desired value of the function C at each fractional step is determined by the «point-to-point computation» formula. At the last calculation step, we have the equation

$$\frac{\partial C^*}{\partial t'} = p.$$

To solve this equation, the Euler method is used.

For the numerical solution of the equation (2), the method by A.A. Samarskii is used. Preliminarily the equation (2) is reduced to evolutionary form.

$$\frac{\partial P}{\partial t} = \frac{\partial^2 P}{\partial x^2} + \frac{\partial^2 P}{\partial y^2}, \quad (12)$$

here t is fictitious time.

When $t \to \infty$, solution of the equation (12) tends to solution of the Laplace equation (3). To solve the equation (12), it is necessary to specify the potential field at t=0, for example, one can take P=0 in the entire computational domain.

The solution of equation (12) is split into two steps, at each step of splitting the difference equations have the form

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

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

The unknown value $P_{i,j}$, at each splitting step, is calculated using the explicit point-to-point computation formula.

For the software implementation of the constructed numerical model, FORTRAN was used.

Findings

Figures 1, 2 present the results of solving the «direct» task – the calculation of the chemical contamination zone during ammonia emission at a specific point of the area. The characteristic direction of the wind speed is shown by an arrow in the figure. As can be seen from the presented figures, the chemical contamination zone increases with time and covers the buildings located in the area of attack.

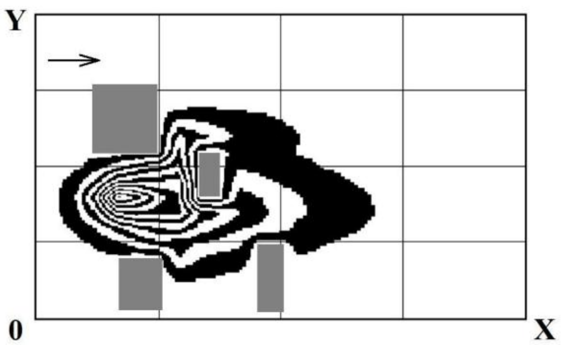

Fig. 1. Isolines of NH_3 concentration during a hypothetical terrorist attack $\tau = 9$ (nondimensional time, direct problem solution): *1* – point of agent emission

Fig. 2. Isolines of NH_3 concentration during a hypothetical terrorist attack $\tau = 14$ (nondimensional time, direct problem solution): *1* – point of agent emission n

The time to solve the direct problem is 3 seconds.

Fig. 3 shows the sketch of the computational domain in the second problem – «vulnerability»

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zone determination based on the adjoint equation. The situation of a possible chemical attack in the area of three buildings is simulated (Fig. 3). It was assumed that near the attack objective (building), the concentration of ammonia should not exceed the threshold value $\varphi = 9$ for time moment $\tau = 16$ (nondimensional concentration and time).

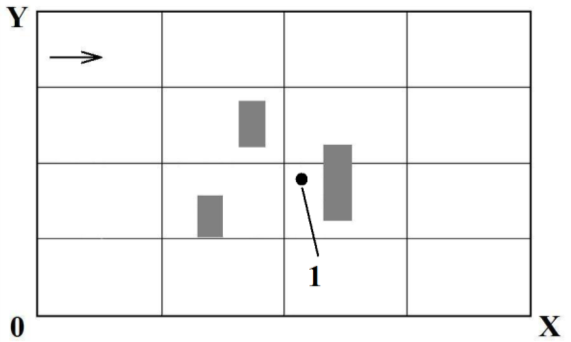

Fig. 3. Sketch of computational domain (the second task – «vulnerability» zone determination for the facility):
1 – target of terrorist attack

Figure 4 shows the lines of the functional (7) defined after solving the adjoint equation (5). The arrow in Fig. 3 and 4 indicates the wind direction.

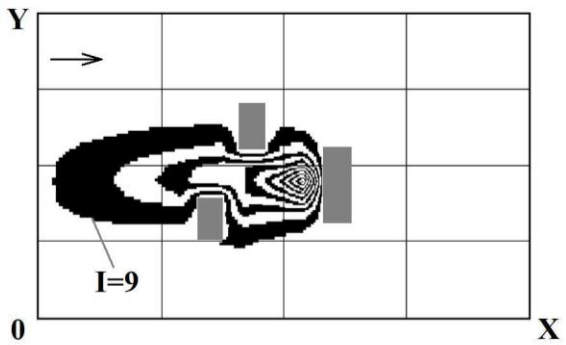

Fig. 4. Isolines of functional (7) for time moment $\tau = 16$ (nondimensional time)

The isolines in Fig. 4 show that if the chemical agent emission source is along one of the lines *I=const*, then the chemical effect on the objective of attack will be the same. Thus, isoline *I=9* shows that if the chemical agent emission is at one of the points on this isoline, then at the time moment $\tau = 16$ the concentration of the chemical agent near the objective of attack will correspond to a given value $\varphi = 9$ (here the concentration is nondimensional value).

The chemical agent emission inside the zone constrained by this isoline will lead to an even greater degree of atmospheric air contamination near the objective of attack.

It should be noted that the calculation time of the «vulnerability» zone is about 3 seconds.

Originality and practical value

The numerical model has been developed that allows determining the «vulnerability» zone near the objective of a possible terrorist attack with the use of a chemical (biological) agent.

The peculiarity of the developed model is the use of the adjoint equation to solve the problem together with the potential flow equation for calculating the wind velocity field in build-up environment. The computer time consumed for the implementation of the model is a few seconds.

Conclusions

The numerical model has been developed for determining the «vulnerability» zone of a facility during a possible chemical attack by a terrorist in build-up environment. The calculation basis is the solution of the adjoint mass transfer equation. The constructed model can be used to develop a strategy to minimize the consequences of terrorist attacks with the use of chemical (biological) agents. Further improvement in this direction should be carried out for developing a three-dimensional numerical model that allows determining the dimensions of the facility «vulnerability» zone during a possible terrorist attack.

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РОЗРАХУНОК ЗОНИ «УРАЗЛИВОСТІ» ОБ’ЄКТА ЗА МОЖЛИВОГО ТЕРАКТУ ІЗ ЗАСТОСУВАННЯМ ХІМІЧНОГО АГЕНТА

Мета. Робота передбачає розробку чисельної моделі для розрахунку зони «уразливості» можливого об’єкта атаки терориста із застосуванням хімічного агента в умовах забудови. Зона «уразливості» являє собою територію біля об’єкта атаки, де емісія хімічного агента під час теракту призведе до небажаних наслідків. Емісія хімічного агента поза зоною «уразливості» не створить небезпечну концентрацію біля об’єкта атаки. **Методика**. Для вирішення поставленого завдання використано рівняння для потенціалу швидкості, на базі якого визначено поле швидкості вітрового потоку, і рівняння, спряжене з рівнянням масопереносу в атмосферному повітрі хімічного агента, викинутого в разі теракту. Під час моделювання

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були враховані нерівномірне поле швидкості вітрового потоку, атмосферна дифузія, інтенсивність викиду хімічно небезпечної речовини. Під час чисельного інтегрування рівняння для потенціалу швидкості використаний метод Самарського А. А. Для чисельного розв'язання спряженого рівняння введені нові змінні та застосована неявна різницева схема розщеплення. Особливістю розробленої чисельної моделі є можливість оперативної оцінки зони «уразливості» біля можливого об'єкта атаки. **Результати**. Розроблена чисельна модель і комп'ютерна програма можуть бути використані для науково обґрунтованої оцінки стану зони «уразливості» біля важливих об'єктів у разі можливих терактів із застосуванням хімічних (біологічних) агентів. Побудована чисельна модель може бути реалізована на комп'ютерах малої і середньої потужності, що дозволяє широко використовувати її для вирішення завдань зазначеного класу під час розробки плану ліквідації в аварійній ситуації. Наведені результати обчислювального експерименту, що дозволяють оцінити можливості цієї чисельної моделі. **Наукова новизна.** Запропоновано ефективну чисельну модель для розрахунку зони «уразливості» біля об'єкта, який може бути ціллю терористичної атаки із застосуванням хімічного агента. Модель заснована на чисельному інтегруванні рівняння для потенціалу швидкості й рівняння, що є спряженим до рівняння масопереносу хімічно небезпечної речовини в атмосфері. **Практична значимість.** Розроблена модель може бути використана для організації захисних заходів біля об'єктів можливої хімічної атаки терориста.

Ключові слова: теракт; хімічне забруднення; зона «уразливості»; спряжене рівняння; чисельне моделювання; забруднення атмосфери

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РАСЧЕТ ЗОНЫ «УЯЗВИМОСТИ» ОБЪЕКТА ПРИ ВОЗМОЖНОМ ТЕРАКТЕ С ПРИМЕНЕНИЕМ ХИМИЧЕСКОГО АГЕНТА

Цель. Работа предполагает разработку численной модели для расчета зоны «уязвимости» возможного объекта атаки террориста с применением химического агента в условиях застройки. Зона «уязвимости» представляет собой территорию возле объекта атаки, где эмиссия химического агента при теракте приведет к нежелательным последствиям. Эмиссия химического агента вне зоны «уязвимости» не создаст опасной концентрации возле объекта атаки. **Методика.** Для решения поставленной задачи использовано уравнение для потенциала скорости, на базе которого определено поле скорости ветрового потока, и уравнение, сопряженное с уравнением массопереноса в атмосферном воздухе химического агента, выброшенного в случае теракта. При моделировании были учтены неравномерное поле скорости ветрового потока, атмосферная диффузия, интенсивность выброса химически опасного вещества. При численном интегрировании уравнения для потенциала скорости использован метод Самарского А. А. Для численного решения сопряженного уравнения введены новые переменные и применена неявная разностная схема расщепления. Особенностью разработанной численной модели является возможность оперативной оценки зоны «уязвимости» возле возможного объекта атаки. **Результаты.** Разработанная численная модель и компьютерная программа могут быть использованы для научно обоснованной оценки положения зоны «уязвимости» возле значимых объектов в случае возможных терактов с применением химических (биологических) агентов. Построенная численная модель может быть реализована на компьютерах малой и средней мощности, что позволяет широко использовать ее для решения задач рассматриваемого класса при разработке плана ликвидации в аварийной ситуации. Представлены результаты вычислительного эксперимента, позволяющие оценить возможности этой численной модели. **Научная новизна.** Предложена эффективная численная модель для расчета зоны

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«уязвимости» возле объекта, который может быть целью террористической атаки с применением химического агента. Модель основана на численном интегрировании уравнения для потенциала скорости и уравнения, являющегося сопряженным к уравнению массопереноса химически опасного вещества в атмосфере. **Практическая значимость.** Разработанная модель может быть использована для организации защитных мероприятий возле объектов возможной химической атаки террориста.

Ключевые слова: теракт; химическое загрязнение; зона «уязвимости»; сопряженное уравнение; численное моделирование; загрязнение атмосферы

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