охраны труда и промышленной безопасности и выявлены проблемы, которые могут способствовать повышению уровня профессионального риска на предприятиях Украины. Предложены приоритетные пути правового и организационного характера по повышению уровня охраны труда и промышленной безопасности в Украине.

Научная новизна. Впервые разработана система автоматизированного учета и контроля изменений нормативно-правовых актов по охране труда и промышленной безопасности. Проанализированы взаимосвязи между уровнем охраны труда и реформами в законодательной и образовательной системах.

Практическая значимость. Результаты исследований могут быть использованы для создания и внедрения на государственном уровне системы автоматизированного учета и контроля изменений нормативно-правовых актов по охране труда и промышленной безопасности как в Украине, так и в странах ЕС.

Ключевые слова: *охрана труда, производственный травматизм, промышленная безопасность, профессиональный риск, нормативно-правовая база, высшее образование*

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MODIFICATION OF THE METHOD OF LARGE PARTICLES IN THE PROBLEM OF CALCULATION OF AN ACCIDENTAL EXPLOSION IN MINE ATMOSPHERE

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МОДИФІКАЦІЯ МЕТОДУ ВЕЛИКИХ ЧАСТОК У ЗАДАЧІ РОЗРАХУНКУ АВАРІЙНИХ ВИБУХІВ РУДНИЧНОЇ АТМОСФЕРИ

Purpose. Development of an effective scheme for numerical calculation of the joint solution of the problem of gas dynamics and the chemical kinetics of combustion of a gas-air medium on the basis of the large-particle method.

Methodology. Mathematical modeling, numerical experiment, analysis and generalization and results.

Findings. For joint solution of problems of gas dynamics and chemical kinetics of combustion gas environments it is proposed to introduce concentration function into the numerical scheme of the method of large particles, which allows taking into account the multicomponent composition of the gas medium. This function is defined at the stage of formation of the estimated area and it defines the mole fraction of each substance in each cell of the design scheme. The function is involved in the calculation of the mass flows across the boundaries of computational cells, determining the mass flow for each substance. The concentration function allows introducing equation of chemical kinetics into the numerical scheme in the form of the Arrhenius equation and differentiating chemical reaction components and combustion products. In the problem of calculation of detonation explosions there are strong gradients of pressures, which, at the exit of the shock front on the border of the "free exit" generate non-physical fluctuations of the parameter. To exclude their influence on the process analysis of different types of approximation of the parameters in the fictitious layer design scheme is conducted. From the analysis of physical processes effective form of the boundary conditions of "free exit" for the problem of shock wave propagation in the channel is found.

Originality. Due to the introduction of a concentration function, modification of the numerical method of large particles allows for the joint solution of problems of gas dynamics and chemical kinetics of combustion of an explosive gas-air environment. For correct operation of the boundary conditions of "free access" in terms of discontinuous currents approximation scheme of the parameter in a dummy layer based on shock adiabats of a specific gas has been developed.

Practical value. The conducted modification of the method of large particles allows carrying out numerical experiment on the calculation of safe distances in case of emergency of gas explosions in coal mines as well as determining the dynamic blast load on structures based on the calculation of distribution of air shock wave on the channel.

Keywords: *the gas-air mixture, accidental explosion, numerical calculation, method of large particles, concentration function, non-reflective border*

Introduction. The current level of design engineering and technology is impossible without the use of mathematical modeling of processes and, in particular, the use of numerical methods for solving differential equations. This contributes to a significant progress in increasing computing power of personal computers. This is especially true for fast emergency processes, the consequences of which have to be predicted with a sufficient degree of accuracy and taken into account in the measures to protect personnel and to reduce the negative consequences of emergency situations.

In the conditions of mine workings in coal mines, underground fires and explosions of mine atmosphere are the most dangerous and destructive types of accidents with insufficiently predictable consequences. Moreover, with underground fires there is danger of repeated explosions of the atmosphere enriched by the products of pyrolysis of the coal substance. To protect rescuers from air shock waves the protection distance and the construction of an explosion-proof construction are used. Forecasting of the parameters of air shock waves in these conditions is the main challenge for reliable determination of safe distances while conducting emergency work and determining the dynamic load to calculate the resistance of an explosion-proof construction.

Analysis of the recent research and publications. Calculation of parameters of air shock waves has interested researchers for a very long time. Initially, to assess the consequences of the explosions at industrial facilities and in the military empirical methods were used that summarized the data of the occurred explosions. Later they began to use experimental methods. Thus, while modeling explosive processes based on patterns of similarity theory, the "cube root" principle by Hopkins-Krantz was formulated which was the basis for predicting the effects of point explosions

$$K = R / \sqrt[3]{E},$$

where R is the distance from the center of the charge; E is the total energy of the explosion.

This principle is laid down in the formula by A. Sadovsky, which has hitherto been used in normative documents on calculation of explosive loads of engineering structures (nuclear power plants, shelter) from the action of air shock waves

$$\Delta P_e = 95\frac{\sqrt[3]{G}}{R} + 390\left(\frac{\sqrt[3]{G}}{R}\right)^2 + 1300\frac{G}{R^3},$$

where ΔP_e is the excess pressure in front air shock wave (AShW); G is the mass of the explosive in a trotyl equivalent, R is the distance from the point of explosion.

At mines experimental methods were also used. Existing normative methods of calculation of parameters of shock waves in mines, based on data from field measurements by M. A. Chekhovskykh and V. I. Gudkov in a mine tunnel "Karagaylinskaya" of "Kiselevskugol" Production Association in the late 60-ies of the last century.

In the last decade, numerical modeling of discontinuous gas dynamic flows is applied for calculating the parameters of air shock waves [1, 2]. So in works [3, 4] the finite difference method is used to solve systems of gas dynamic equations, which allows obtaining many values of distribution parameters of air shock waves on a network of mine workings. The paper [5] shows the application of this method in the FIRE® software package for the calculation of detonation parameters. As shown in the works of A. A. Samarskii, the complexity of the application of this method consists in the construction of homogeneous difference schemes for calculating discontinuous flows. The latter move in mass, and the flow parameters on both sides of the discontinuity are connected by the Hugoniot condition, which causes sharp fluctuations of the grid function behind the shock front (Fig. 1).

To address this question in a numerical scheme it is necessary to use the method of "smearing" of the front due to the introduction of the system of difference equations of the dissipative members (pseudoviscosity).

Unsolved aspects of the problem. The method of large particles is more stable in the calculations of discontinuous movements due to the presence of differential circuits in schematic viscosity. In [6] this method is used to calculate an accidental explosion in terms of camera gas boilers. However, the calculation does not take into account the kinetics of the process of explosive combustion of gaseous mixtures, which conditions the shock wave parameters. While calculating faults currents there generally occurs a problem of setting the correct conditions on the artificial boundaries of the computational domain. In the problem of calculation of detonation explosions there are strong gradients of pressures, which, at the exit of the shock front at the boundary of the free output generate non-physical fluctuations of the parameter. To exclude their influence on the process, it is necessary to set boundaries at considerable distances, which increases the amount of computation.

Objectives of the article. Development of an effective numerical scheme for the joint solution of problems of gas dynamics and chemical kinetics of combustion gas-air environment on the basis of the method of large particles.

Methods. Mathematical modeling by numerical approximation of partial differential equations of gas dynamics and chemical kinetics, numerical simulation, analysis and synthesis and results.

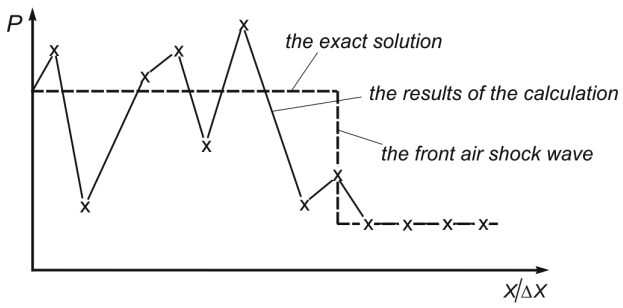

Fig. 1. Calculation of the motion of the shock wave

Presentation of the main research and explanation of scientific results. For the calculation of the process of gas mixture explosion and distribution of air shock waves in mines it is proposed to use the method of large particles (Davydov's method) [7]. The main provisions of this method in the following conditions are as follows.

Flow in a cylindrical coordinate system is described by the Euler equations (in divergence form) of the continuity, motion, energy

$$\frac{\partial \rho}{\partial t}+\operatorname{div}\left(\rho \bar{W}\right)=0;$$

$$\left.\begin{array}{l}\dfrac{\partial \rho u}{\partial t}+div\left(\rho u \bar{W}\right)+\dfrac{\partial P}{\partial z}=-\tau_{fr}\dfrac{\Pi}{S}\\ \dfrac{\partial \rho v}{\partial t}+div\left(\rho v \bar{W}\right)+\dfrac{\partial P}{\partial r}=0\end{array}\right\}; \qquad (1)$$

$$\frac{\partial \rho E}{\partial t}+\operatorname{div}\left(\rho E \bar{W}\right)+\operatorname{div}\left(\rho P \bar{W}\right)=q\Pi+q_x\rho\frac{\partial \alpha}{\partial t},$$

where ρ is density; P is pressure; $\bar{W}$ is the velocity vector; u, v are components of the velocity W in the z and r axis respectively; z, r are cylindrical coordinates; $E=J+\frac{1}{2}\left(u^2+v^2\right)$ is the total energy; J is the internal energy of the gas; τ_{fr} is the tension of surface friction forces of the gas flow on the wall; q is the density of the heat flux at the channel wall; S, Π is the cross section and perimeter generation; q_x is thermal effect of chemical reaction of combustion of hydrocarbons; α is the mole fraction of hydrogen in the mine atmosphere; t is time.

For closure of this system, the equation of ideal gas state is used

$$P=(\gamma-1)\rho\cdot J,$$

where γ is index of adiabatic.

The considered problem is solved in a cylindrical coordinate system in which the computational domain is presented in the form of a cylindrical channel. In fact, this scheme is a shock tube with a plot filled with gas mixture. Rapid combustion of the mixture (deflagration or detonation) causes the formation and spread of air shock waves in a cylindrical channel (Fig. 2).

The scheme of the method of large particles and the issues of its stability and approximation order have been examined in detail in the literature (Belotserkovskyi O. M., Davydov Yu. M.). The difference scheme for solution of non-stationary system of differential equations (1) is based on the idea of splitting this system by physical processes. The problem is solved in three stages: the Euler, Lagrangian and final. At Eulerian stage, the intermediate values of the velocity $\tilde{u}$, $\tilde{v}$ and energy flow $\tilde{E}$ are determined from the condition of "freezing" density fields $\left(\frac{\partial \rho}{\partial t}=0\right)$, therefore, the numerical approximation of the equations of motion and energy (1), at time t^n, in cylindrical coordinates r, z will be represented by the following explicit finite-difference algebraic equations of the first order accuracy in time and second order in space

$$\tilde{u}^n_{i,j}=u^n_{i,j}-\frac{P^n_{i+0,5,j}-P^n_{i-0,5,j}}{\Delta z}\frac{\Delta t}{\rho^n_{i,j}};$$

$$\tilde{v}^n_{i,j}=v^n_{i,j}-\frac{P^n_{i,j+0,5}-P^n_{i,j-0,5}}{\Delta r}\frac{\Delta t}{\rho^n_{i,j}};$$

$$\tilde{E}^n_{i,j}=E^n_{i,j}-\left[\frac{jP^n_{i,j+0,5}v^n_{i,j-0,5}-(j-1)P^n_{i,j-0,5}v^n_{i,j-0,5}}{(j-0,5)\Delta r}+\right.$$

$$\left.+\frac{P^n_{i+0,5,j}u^n_{i+0,5,j}-P^n_{i-0,5,j}u^n_{i-0,5,j}}{\Delta z}\right]\frac{\Delta t}{\rho^n_{i,j}},$$

where i, j is the cell address of the rectangular computational grid.

At Lagrangian phase, the flows of matter in time Δt between the cells in the following algebraic equations obtained from the numerical approximation of the continuity equation (1) are calculated.

The flows of mass along the z-axis (depending on direction) are

$$\Delta M^n_{i\pm0,5,j}=\begin{cases}\text{if } \tilde{u}^n_{i,j}+\tilde{u}^n_{i+1,j}>0\\ (j-0,5)\Delta r^2\rho^n_{i,j}\dfrac{\tilde{u}^n_{i,j}+\tilde{u}^n_{i+1,j}}{2}\Delta t\\ \text{if } \tilde{u}^n_{i,j}+\tilde{u}^n_{i+1,j}<0\\ (j-0,5)\Delta r^2\rho^n_{i+1,j}\dfrac{\tilde{u}^n_{i,j}+\tilde{u}^n_{i+1,j}}{2}\Delta t\end{cases}. \qquad (2)$$

The flows of mass along the axis r (depending on direction) are

$$\Delta M^n_{i,j\pm0,5}=\begin{cases}\text{if } \tilde{v}^n_{i,j+1}+\tilde{v}^n_{i,j}>0\\ (j-0,5)\Delta r\Delta z\rho^n_{i,j}\dfrac{\tilde{v}^n_{i,j+1}+\tilde{v}^n_{i,j}}{2}\Delta t\\ \text{if } \tilde{v}^n_{i,j+1}+\tilde{v}^n_{i,j}<0\\ (j-0,5)\Delta r\Delta z\rho^n_{i,j+1}\dfrac{\tilde{v}^n_{i,j+1}+\tilde{v}^n_{i,j}}{2}\Delta t\end{cases}.$$

At the final stage the new values of all flow parameters taking into account the flow of the masses are calculated

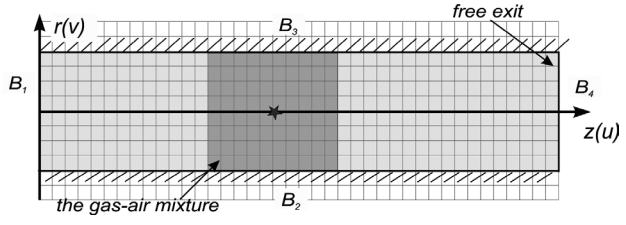

Fig. 2. The General structure of the computational grid in the flattened representation:
B1, B4 – type of "free exit" settlement boundaries; B2, B3, – type of "non-leakage" settlement boundaries; v, u – components of the velocity vector

$$X_{i,j}^{n+1}(j-0,5)\Delta r^2\Delta z\rho_{i,j}^{n+1} = \Big\{ D_{i,j}^n(1)\tilde{X}_{i-1,j}^n\Delta M_{i-0,5,j}^n + $$
$$+ D_{i,j}^n(2)\tilde{X}_{i,j}^n\Delta M_{i,j-0,5}^n + D_{i,j}^n(3)\tilde{X}_{i+1,j}^n\Delta M_{i+0,5,j}^n +$$
$$+ D_{i,j}^n(4)\tilde{X}_{i,j+1}^n\Delta M_{i,j+0,5}^n + \tilde{X}_{i,j}^n\{(j-0,5)\Delta r^2\Delta z\rho_{i,j}^n -$$
$$-[1-D_{i,j}^n(1)]\Delta M_{i-0,5,j}^n - [1-D_{i,j}^n(2)]\Delta M_{i,j-0,5}^n -$$
$$-[1-D_{i,j}^n(3)]\Delta M_{i+0,5,j}^n - [1-D_{i,j}^n(4)]\Delta M_{i,j+0,5}^n\}\Big\},$$

where $D_{i,j}^n$ is the function-sign of the direction of flow of mass through the boundary of computational cells; $X_{i,j}^{n+1}$, $\tilde{X}_{i,j}^n$ stand for the value of the parameter time on the new layer and its intermediate value.

As a result of these calculations we get the known values ρ^{n+1}, u^{n+1}, v^{n+1}, E^{n+1} on the new time layer.

Knowing these values, you can define the internal energy $J = \frac{E-W^2}{2}$, where $W^2 = u^2 + v^2$, consequently, to determine the value of the pressure according to the formulas and equations of state.

Initially, the numerical scheme of the method of large particles allows calculating the flow in one-component gas systems. In this case, it is necessary to consider the combustion of the gas mixture, and there may be several combustible components, i.e. in the computational cell there can be several substances, so to calculate pressure it is necessary to know the concentration of these substances. For this purpose, the function $C_{i,j}^n(k)$ of the concentration is introduced for which, for example, $k = 1$ corresponds to the hydrocarbon (methane), $k = 2$ is oxygen, $k = 3$ – nitrogen.

Before calculating mass flows through the surface of computational cells (3, 4), you need to know arrays $C_{i,j}^n(k)$, namely, to know the concentration of substances. This is defined as the initial conditions. When calculating mass fluxes across the boundaries of counting cells, after the introduction of $C_{i,j}^n(k)$, the fact that the total mass flow is equal to the sum of mass flows of individual components is taken into account.

To do this, first total mass flows are calculated, then the flows of the individual components (assuming single-speed model). This involves replacing $\rho_{i,j} \to \rho_{i,j}C_{i,j}$. Thus, $\rho_{i,j}^n(\alpha), \alpha = 1..3$ are determined.

After that we determine the concentration of

$$C_{i,j}^{n+1} = \frac{\rho_{i,j}^{n+1}(\alpha)}{\rho_{i,j}^{n+1}}.$$

Pressure needs to be estimated for the formula

$$P_{i,j}^{n+1} = \sum_{\alpha=1}^{4} P_{i,j}^{n+1}(\alpha)\cdot C_{i,j}^{n+1}(\alpha),$$

where $P_{i,j}^{n+1}(\alpha)$ is the partial pressure which is determined by the equations of state for each component of the gaseous medium.

The use of the concentration function allows solving the kinetic equation of a chemical reaction. The chemical reaction is represented in the form of one gross-out stage: "the initial substance → products" and the reaction rate is presented in the form of Arrhenius

$$-\frac{dc_i}{dt} = Z\cdot\exp\left(-\frac{E_a}{RT}\right)\Pi c_i^{v_i}, \qquad (3)$$

where Z, E_a, v_i stand for effective pre-exponential factor, activation energy and reaction order for the i^{th} component.

In our case, a bimolecular reaction proceeds, so the equation (3) for the component "methane" has the form

$$-\frac{dc_1}{dt} = Z\cdot\exp\left(-\frac{E_a}{RT}\right)c_1^{v_1}\cdot c_2^{v_2}. \qquad (4)$$

From macrokinetic equations of methane combustion it follows that the consumption rate of oxygen is 2 times higher than the rate of consumption of methane

$$-\frac{dc_1}{dt} = -\frac{1}{2}\cdot\frac{dc_2}{dt}. \qquad (5)$$

After numerical integration of equation (5), we obtain

$$c_2 = 2c_1 + A,$$

where A is constant of integration which can be determined from initial conditions

$$A = c_{2H} - 2c_{1H}.$$

The index "N" indicates the initial values of the concentrations.

As a result we obtain

$$c_2 = 2\left(c_1 - c_{1H}\right) + c_{2H} \Rightarrow c_2 = c_{2H} + 2\left(c_1 - c_{1H}\right). \qquad (6)$$

Thus, knowing the dependence of concentration on time $c_1(t)$, we define feature $c_2(t)$ by the formula (6).

Let $c_1 = c_{1H}$ at the initial moment of time, therefore, $c_2 = c_{2H}$. With the complete burnout of methane $c_1 = 0$, the oxygen concentration is equal to

$$c_2 = c_{2H} - 2c_{1H}.$$

With the stoichiometric composition $c_{2H} = 2c_{1H}$. Therefore, the methane and oxygen burn out completely at the same time $c_1 = 0$, $c_2 = 0$. If, $c_{2H} > c_{1H}$, then $c_2 > 0$, i.e. residue O_2 is observed. With $2c_{2H} < c_{1H}$ the oxygen burns out early, and the rest of the methane is equal to

$$c_1 = c_{1H} - \frac{c_{2H}}{2}.$$

To describe the combustion reaction of methane and oxygen it should be particularly noted that in equation (4) as the concentration "c" amount of substance (in moles) is used per unit volume in cm^3, i.e. dimensionality is $\left[c\right] = \frac{mol}{cm^3}$.

The equation of gas dynamics includes the density of the matter. The chemical reaction does not change this value because the source materials are just replaced

by the reaction products. Therefore, homogeneous density of the substances included in the composition of the atmosphere, are need only to specify initial conditions.

Numerical solution of the equations of chemical kinetics in conjunction with the gas dynamics equations and equations of state is as follows. The difference analogue of equation (4) is presented in the form

$$-\frac{\left[c_1\right]_{i,j}^{n+1}-\left[c_1\right]_{i,j}^{n}}{\Delta t}=k\cdot\left(\left[c_1\right]_{i,j}^{n}\right)^{v_1}\cdot\left(\left[c_2\right]_{i,j}^{n}\right)^{v_2},$$

where $k=Z\cdot\exp\left(-E_a/RT\right)$ is the rate constant for the chemical reaction of combustion; *i, j* are the integer coordinates of the calculated cell (large particles); *n* is the number of the temporary layer.

From equations (3, 5) it follows that

$$\left[c_1\right]_{i,j}^{n+1}=\left[c_1\right]_{i,j}^{n}-\Delta t\cdot k\cdot\left(\left[c_1\right]_{i,j}^{n}\right)^{v_1}\cdot\left(\left[c_1\right]_{i,j}^{n}\right)^{v_2};$$

$$\left[c_2\right]_{i,j}^{n+1}=\left[c_2\right]_{i,j}^{n}+2\left(\left[c_1\right]_{i,j}^{n+1}-\left[c_1\right]_{i,j}^{n}\right).$$

When calculating the equation of conservation of energy the addend is added to the right part

$$\Delta t\cdot Q\cdot Z\cdot\exp\left(-E_a/RT\right)\cdot\left(\left[c_1\right]_{i,j}^{n}\right)^{v_1}\cdot\left(\left[c_2\right]_{i,j}^{n}\right)^{v_2},$$

where Q is the calorific value of methane burning in air at stoichiometric composition, the methane-oxygen, J/m^3.

At the boundaries of the computational domain $j = jm$, $i = im$ it is necessary to specify conditions which do not affect the parameters in the estimated region. To do this, a dummy computational cell in which parameter values are determined by extrapolation are introduced (Fig. 3, *a*).

According to the algorithm of the method of large particles on non-reflecting boundaries extrapolation of the zero, first and second order can be used. For boundaries B_2, B_3, the condition of non-flow is used: zero dummy cell is introduced, in which $v_{i,0} = v_{i,1}$, so

$$v_{i,0,5}=\frac{v_{i,0}+v_{i,1}}{2}=0.$$

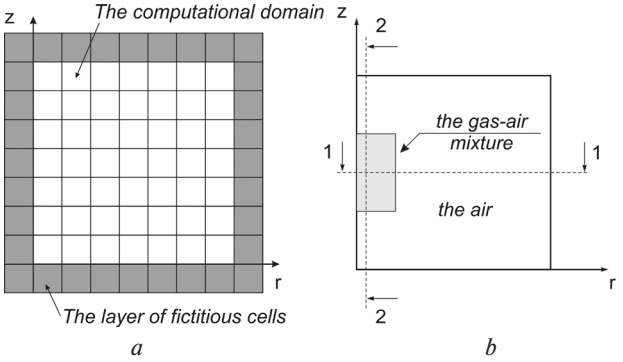

Fig. 3. The structure of the computational grid (dummy cell shaded) – a, scheme of test problem of choosing the order of extrapolation – b

The choice of procedure of extrapolation for non-reflecting boundary B_1, B_4 is made on the basis of the study of a test problem – the explosion of the gas cloud in an unlimited space (Fig. 3, *b*).

The zero extrapolation $y_{im+1,j} = y_{im,j}$, $y_{i,jm+1} = y_{i,jm}$ gives the "cut" parameter values (Fig. 4).

Linear extrapolation parameters can be obtained from the following considerations (Fig. 5)

$$y_{im+1}=y_{im}+\left(\frac{\partial y}{\partial x}\right)_{im}\cdot\Delta x=$$

$$=y_{im}+\frac{y_{im}-y_{im-1}}{\Delta x}=2y_{im}-y_{im-1};$$

$$y_0=y_1-\left(\frac{\partial y}{\partial x}\right)_{1}\cdot\Delta x=$$

$$=y_1+\frac{y_2-y_1}{\Delta x}=2y_1-y_2.$$

Right (or left) derivatives of a linear extrapolation give higher values of the parameters in the dummy cell. The most acceptable values are obtained with the use of the central derivative, which largely takes into account the gradient of the graph in the vicinity of the boundaries of the computational domain (Fig. 5)

$$y_{im+1}=y_{im}+\left(\frac{\partial y}{\partial x}\right)_{im}\cdot\Delta x=y_{im}+\frac{y_{im}-y_{im-2}}{2\Delta x}=$$

$$=y_{im}+\frac{y_{im}-y_{im-2}}{2}=\frac{3}{2}y_{im}+\frac{1}{2}y_{im-2}.$$

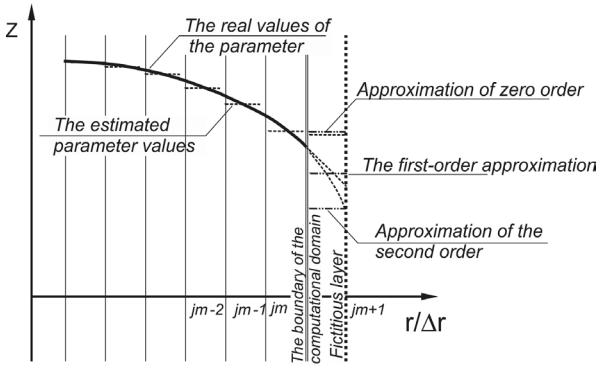

Fig. 4. The approximation parameter in the fictitious layer

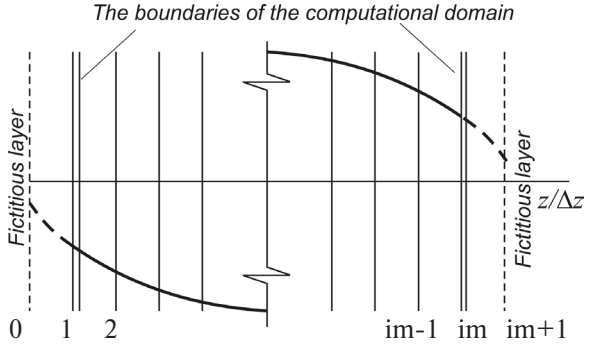

Fig. 5. The output of the shock wave on the boundary of the computational domain with linear extrapolation

The equation of the extrapolation of the parameters of shock waves in the dummy cell 2 in order is

$$y_{im+1} = y_{im} + \frac{1}{1!}\left(\frac{\partial y}{\partial x}\right)\Delta x + \frac{1}{2!}\left(\frac{\partial^2 y}{\partial x^2}\right)\Delta x^2,$$

where

$$\left(\frac{\partial y}{\partial x}\right) = \frac{y_i - y_{i-1}}{\Delta x}, \quad \left(\frac{\partial^2 y}{\partial x^2}\right) = \frac{\left(\frac{\partial y}{\partial x}\right)_{im} - \left(\frac{\partial y}{\partial x}\right)_{im-1}}{\Delta x}.$$

After substitution we get

$$y_{im+1} = 2y_{im} - y_{im-1} + \frac{1}{2}(y_{im} - 2y_{im-1} + y_{im-2}).$$

Analysis of the results of calculation of parameter values defined by (4), showed that they are highly inflated (Fig. 4). Thus, the most acceptable is the use of the linear extrapolation of parameters.

However, this type of extrapolation is possible at small gradients of the function. With discontinuous characteristics, i.e. in front of the shock wave, the linear approximation leads to the opposite signs of the parameter values, which contradicts the physical sense of the problem (Fig. 6).

In the calculation, it manifests itself by appearance of generating fluctuations pressure after passing the peak of the shock wave through the border (Fig. 7). A similar effect is observed in the zero approximation: at the time of the shock wave on the boundary of the computational domain, in the fictitious layer, there appears pressure equal to the amplitude in the shock wave. A braking effect on the flow at the border "free exit" is formed.

Problems of the correct operation of the nonreflecting boundary conditions (NBC) exist in almost all numerical schemes in the calculation of the break-governmental movements [8]. To enable the NBC to open borders, a variety of techniques is used: the buffer volumes with the calculated cells are attached, the heuristic dependencies of pressure on the time of the relaxation process are applied or one-dimensional characteristic NBC is used [9]. Such techniques focus on solving specific

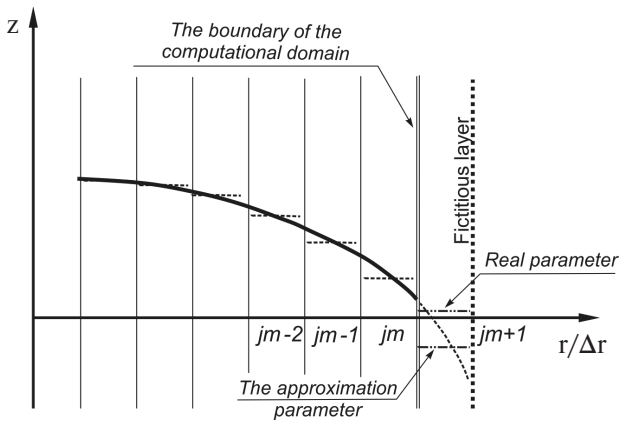

Fig. 6. The parameter approximation is negative

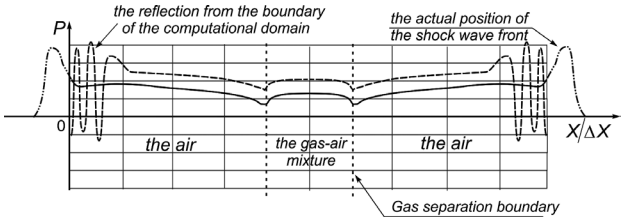

Fig. 7. The generation of pressure surges in the approximation parameter in the negative region on the nonreflective border

tasks [10, 11]. The general approach to the formulation of the NBC, to date, is absent. An example of the error of the NBC can be demonstrated in the FlowVision system. In the model of a completely compressible medium, the boundary conditions of the type of the Riemann invariant, intended for the calculation of trans- and supersonic flows, a pressure drop in the undisturbed flow is given (Fig. 8).

The task of finding the correct solution is performed by conducting a joint study of boundary conditions and physical processes. So in [8] the zero-order extrapolation for the velocity of flow is determined by the ratio derived from shows that Hugoniot conditions on the shock seals

$$v = \frac{1}{a_\infty}\sqrt{\frac{(p - p_\infty)(\rho - \rho_\infty)}{\rho\rho_\infty}},$$

where a_∞, ρ_∞, p_∞ are the speed of sound, density, and pressure in the undisturbed gas stream.

In the problem in question, the shock wave spreads through the gas mixture and the value of the amplitude in the next moment of time depends on the thermodynamic properties of this compound. The pressure in the gas is of thermal origin, it is related to the momentum transfer by the particles participating in the thermal motion and always determines the shock adiabats, and it is proportional to the volume and the temperature while in the air shock wave it is proportional to the flow velocity [12]. Therefore, to determine the excess pressure in the fictitious cell, we can obtain the equation of the shock adiabatic in the system *P-U*. According to the works of Y. B. Zeldovich, Y. P. Raiser the dependence between the velocity of the shock front and the velocity of the matter behind the wave front, in a wide range of amplitudes is linear

$$D = A + Bu, \qquad (7)$$

where A, B are the coefficients.

The velocity of the front shock air wave is also known

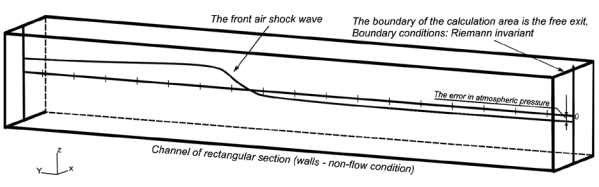

Fig. 8. The error in the operation of the boundary conditions is a free yield by the type of the Riemann invariant

$$D = \sqrt{\Delta P\left(\frac{1}{\rho_a} - \frac{1}{\rho}\right)}, \qquad (8)$$

where ρ_a, ρ are the density of the gas, and the atmospheric shock wave.

Solving equation (5, 6) we get the condition of "soft" walls

$$\Delta P_{jm+1} = \frac{\left(A + Bu_{jm+1}\right)^2}{V_a - V},$$

where u_{jm+1} is the speed of the substance in the dummy cell; V_a, V is specific gravity of gas.

In (5) value A is close to the speed of sound in the substance and is specified by the table. The value B of the coefficient is determined according to the boundary cell, by solving equations (7, 8) with respect to B

$$B = \frac{\sqrt{\Delta P\left(V_a - V\right)} - A}{u_{jm}}. \qquad (9)$$

The use according to (9) also has its own peculiarity. It is logical to define the value of the velocity of the matter in it for the boundary cells as full speed

$$\overline{U}_{jm} = \sqrt{u_{jm}^2 + v_{jm}^2}\ .$$

However, it does not give correct results of calculations of the pressure in the fictitious cell for two reasons. First: while calculating $\overline{U}_{jm}$ for the lower boundary there is a loss of the mark in the direction of the velocity, because speed has a negative value with the movement of a substance down (Fig. 9).

Second, the calculation flow of the substance according to the method of large particles is defined through the border of the cell, that is, vertically or horizontally. The actual speed of the substance in the cells at the periphery from the axis of symmetry is directed at an angle to it (maximum of 45°). Therefore, the pressure in the fictitious extreme cells will be defined incorrectly. To exclude such phenomena in the expression (7), the corresponding component of the flow velocity is to be used as the speed. In the calculation this is done by establishing separate conditions for left, right, upper and lower bounds of the computational region.

The method of large particles involves the execution of three calculation steps. Accordingly, the boundary conditions are met at the end of each stage. For the stability of the calculation the use of "soft" borders in the final part of the Lagrangian phase to calculate the pressure is of the necessary and sufficient condition while the boundary conditions in the Eulerian phase must be determined at zero approximation, because of the intermediate character of the results. As a result, a design scheme allows performing the transition of the shock front through the boundary of the computational domain correctly (Fig. 10).

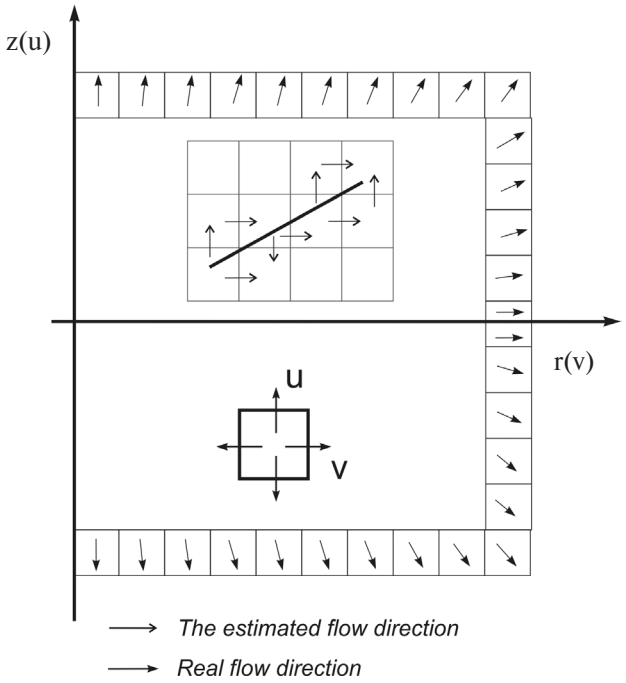

Fig. 9. The direction of movement of the substance in the dummy cells and the estimated flow direction

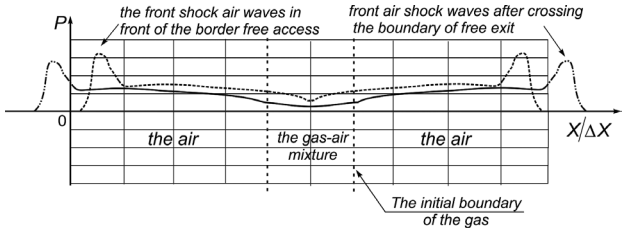

Fig. 10. The transition of the shock wave front across the border of free access to "soft" wall

Conclusions. A modification of the method of large particles allows extending the scope of its application to the solution of problems of gas dynamics and chemical kinetics of combustion of gas-air mixtures. The condition of the soft wall allows us to avoid distorting the settings of cutoff currents at the boundary of computational region and thus, enables to reduce the amount of calculations by reducing the size of computational domain.

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Мета. Розробка ефективної схеми чисельного розрахунку спільного розв'язку задачі газової динаміки й хімічної кінетики горіння газоповітряного середовища на основі методу великих часток.

Методика. Математичне моделювання, чисельний експеримент, аналіз і узагальнення результатів.

Результати. Для спільного рішення задачі газової динаміки й хімічної кінетики горіння газоповітряної суміші пропонується ввести до чисельної схеми методу великих часток концентраційну функцію, що дозволяє враховувати багатокомпонентний склад газового середовища. Ця функція визначається на стадії формування розрахункової області, і в кожній комірці розрахункової схеми вона визначає мольну частку кожної речовини. Функція бере участь у розрахунку перетоків мас через границі розрахункових комірок, визначаючи масу перетікання по кожній речовині. Концентраційна функція дає можливість вводити до чисельної схеми рівняння хімічної кінетики у вигляді рівняння Арреніуса й розрізняти компоненти хімічної реакції та продукти горіння. У задачі розрахунку детонаційних вибухів виникають сильні градієнти тисків, що, при виході фронту ударної хвилі на границю „вільний вихід“ генерують нефізичні флуктуації параметра. Для виключення їх впливу на процес проводиться аналіз різних видів апроксимації параметрів у фіктивний шар розрахункової схеми. З аналізу фізичних процесів знайдено ефективний вид граничних умов „вільний вихід“ для задачі поширення ударної хвилі в каналі.

Наукова новизна. Модифікація чисельного методу великих часток за рахунок уведення концентраційної функції дозволяє проводити спільне рішення задачі газової динаміки й хімічної кінетики вибухового горіння газоповітряної суміші. Для коректної роботи граничних умов „вільний вихід“ в умовах розривних течій розроблена схема апроксимації параметра у фіктивний шар на основі ударної адіабати конкретного газу.

Практична значимість. Виконана модифікація методу великих часток дозволяє проводити чисельний експеримент із розрахунку безпечних відстаней при аварійних газових вибухах в умовах вугільних шахт, а також на основі розрахунку поширення ударної повітряної хвилі по каналу визначати динамічні навантаження на вибухозахисні споруди.

Ключові слова: *газоповітряна суміш, аварійний вибух, чисельний розрахунок, метод великих часток, концентраційна функція, невідбиваюча межа*

Цель. Разработка эффективной схемы численного счета совместного решения задачи газовой динамики и химической кинетики горения газовоздушной среды на основе метода крупных частиц.

Методика. Математическое моделирование, численный эксперимент, анализ и обобщение результатов.

Результаты. Для совместного решения задачи газовой динамики и химической кинетики горения газовоздушной среды предлагается ввести в численную схему метода крупных частиц концентрационную функцию, которая позволяет учитывать многокомпонентный состав газовой среды. Данная функция определяется на стадии формирования расчетной области, и в каждой ячейке расчетной схемы она определяет мольную долю каждого вещества. Функция участвует в расчете перетоков масс через границы расчетных ячеек, определяя массу перетока по каждому веществу. Концентрационная функция дает возможность вводить в численную

схему уравнения химической кинетики в виде уравнения Аррениуса и различать компоненты химической реакции и продукты горения. В задаче расчета детонационных взрывов возникают сильные градиенты давлений, которые, при выходе фронта ударной волны на границу „свободный выход“ генерируют нефизические флуктуации параметра. Для исключения их влияния на рассматриваемый процесс проводится анализ различных видов аппроксимации параметров в фиктивный слой расчетной схемы. Из анализа физических процессов найден эффективный вид граничных условий „свободный выход“ для задачи распространения ударной волны в канале.

Научная новизна. Модификация численного метода крупных частиц за счет введения концентрационной функции позволяет проводить совместное решение задачи газовой динамики и химической кинетики взрывного горения газовоздушной среды. Для корректной работы граничных условий „свободный выход“ в условия разрывных течений разработана схема аппроксимации параметра в фиктивный слой на основе ударной адиабаты конкретного газа.

Практическая значимость. Проведенная модификация метода крупных частиц позволяет проводить численный эксперимент по расчету безопасных расстояний при аварийных газовых взрывах в условиях угольных шахт, а также на основе расчета распространения ударной воздушной волны по каналу определять динамические нагрузки на взрывозащитные сооружения.

Ключевые слова: *газовоздушная смесь, аварийный взрыв, численный расчет, метод крупных частиц, концентрационная функция, неотражающая граница*

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