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A.V. Chernai[1], Dr. Sci. (Phys.-Math.), Prof.,
M.M. Nalysko[2], Cand. Sci. (Tech.), Assoc. Prof.,
H.S. Derevianko[1]

1 – State Higher Educational Institution "National Mining University", Dnipropetrovsk, Ukraine, e-mail: chernayanatoliy@rambler.ru; derevjnkoanna@rambler.ru
2 – State Higher Educational Institution "Prydniprovska State Academy of Civil Engineering and Architecture", Dnipropetrovsk, Ukraine, e-mail: n59568@yandex.ru

THE KINETICS OF THE METHANE ACIDIFICATION BY THE OXYGEN AND ITS ROLE IN THE BLAST AIR WAVE FORMATION IN MINE WORKINGS

А.В. Чернай[1], д-р фіз.-мат. наук, проф.,
М.М. Налисько[2], канд. техн. наук, доц.,
Г.С. Дерев'янко[1]

1 – Державний вищий навчальний заклад „Національний гірничий університет“, м. Дніпропетровськ, Україна, e-mail: chernayanatoliy@rambler.ru; derevjnkoanna@rambler.ru
2 – Державний вищий навчальний заклад „Придніпровська державна академія будівництва та архітектури“, м. Дніпропетровськ, Україна, e-mail: n59568@yandex.ru

КІНЕТИКА ОКИСЛЕННЯ МЕТАНУ КИСНЕМ ТА ЙОГО РОЛЬ У ФОРМУВАННІ ВИБУХОВОЇ ПОВІТРЯНОЇ ХВИЛІ У ШАХТНИХ ВИРОБКАХ

Purpose. The numerical calculation of the gas explosion parameters subject to the kinetics of the methane oxidation by oxygen in mine atmosphere, carrying out the model testing accounts of the methane-air mixtures explosion.

Methodology. The mathematical modeling of the gas-dynamic and physicochemical processes of the gas explosion. The numerical experiment of the methane ignition process, deflagration and detonation combustion, formation and propagation the explosive airwaves.

Findings. The choice of the chemical kinetics model of methane combustion mechanism in open reactor has been substantiated. The nonstationary processes of the methane-air environment explosion, formation and spreading of the explosion wave in mine workings has been modeled. The numerical experiment results have been analyzed.

Originality. The new approach in realization of the pattern of gas dynamic process numerical account – methane explosion – has been developed, in which the kinetics of methane oxidation chemical reaction and dynamics of explosion energy transmission by explosion wave and gas environment streams have been combined.

Practical value. The results of the numerical account scheme modification are applied during the technical solutions substantiation regarding the explosion security of mine workings emergency areas.

Keywords: *mine working, air-gas mixture, combustion kinetics, shock airwave, numerical account, gas dynamics*

Problem statement. Methane explosions in mines belong to the most dangerous emergencies in which accidents with fatal case account for about 90%. That is why the research studies are urgent which are aimed at determining the real parameters of shock airwave to estimate risks of anthropogenic disasters [1].

Unsolved aspects of the problem. The destructive effect of blast waves in mines generally is determined by pressure value at a wave front and duration of wave impact on barriers, including protecting ones. The latest accidents, for example, at the Zasyadko mine, showed that explosion protective bulkheads, constructed in hazardous zone of mine working and calculated according to the effective regulatory documents, failed to prevent tragic consequences of methane explosions.

In acting rules of the State Military Rescue Service (SMRS) in coal industry, the calculation of permissible distances is generally made according to A.M. Chehovskih's and V.M. Plotnikov's methods [2]. However, these methods were developed on the basis of simplified analytical solutions and are far from specific task statement of experimental data; as a rule, they provide results which do not correspond to coal mines conditions. The main initial calculation parameter is an overpressure at a shock air wave front. The methods do not consider the reflection of shock waves

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from firm surfaces, shock waves interaction and formation of rarefaction waves.

The prominent works by Y.B. Zeldovich, K.K. Stanyukovich, B.N. Kutuzov, P.M. Petrukhin, V.M. Plotnikov and others show that proper calculation of gas and dust explosion impact parameters is possible only with gas-dynamic calculation of shock airwave propagation along mine workings net. Unfortunately, such estimation is restrained because of the lack of appropriate effective methods of computation and physicochemical models adequate for mine environment.

The recent researches analysis. The publications analysis shows that the approach, based on the gas-dynamic method of calculating parameters of shock air wave at explosions in coal mines developed in the RusSRIMRW and Tomsk State University, may become an alternative to known analytical ones [3, 4]. In Ukraine similar works are held by the "Respirator", Scientific Research Institute of Mine-rescue Work (Donetsk) [5].

The feature of the physical model which is used in works by Russian scientists [3, 4] and others, is an assumption that methane explosion occurs immediately with a pressure profile set beforehand along the whole gas-polluted zone. At the same time, a pressure jump value is not substantiated by any means. As a rule, the chosen pressure varies from 0.5 to 2.8 MPa; according to experimental estimations, these pressure ranges are realized during methane explosion in mine workings (Fig. 1).

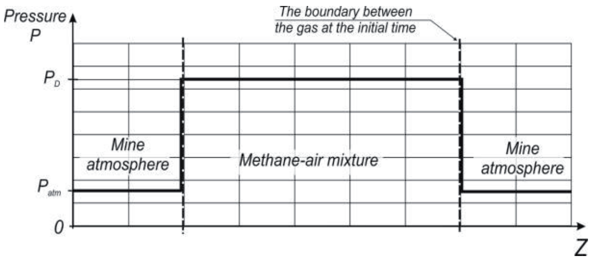


Fig. 1. The profile of the initial pressure jump along the excavation axis: P_p is explosion pressure of methane-air mixture; P_{atm} is atmospheric pressure; Z is a longitudinal axis of excavation

Work [5] suggests switching on a powerful momentary heat source within the whole gas-polluted zone rather than applying physical assumption on a momentary explosion. This source, according to the authors [6], corresponds to a chain reaction of methane and dust combustion. What kind of reaction it is and how its speed is chosen while operating, the work does not cover. But it follows from previous discussions that methane burns out completely, in other words development, attenuation and combustion process itself are not considered.

Emphasizing the part of the common problem unsolved earlier. Both models are beneath criticism, as in reality a pressure jump is determined by two processes: kinetics of chemical reaction and dynamics of methane-air environment motion.

Methods of numerical calculation of gas dynamics equations applied in the mentioned works should be regarded as their other drawbacks. Thus, the works [3, 4] apply an approach based on S.K. Godunov's method according to which the disintegration task of an optional disintegration is solved in every counting point of a computation area. This requires much computer time, even for one-dimensional problems. That is why such methods do not allow performing a huge value of calculations of the event development scenarios and choosing the most probable one.

The work [5] presents a difference scheme of calculation without grounding its stability and solution convergence. For flattering functions breaks, an artificial viscosity is used. However, artificial viscosity demands careful application to exclude overpressure of unphysical fluctuations, which do not correlate to experimental data. Besides, the work [5] notes that one cannot take the initial pressure allocation in the form of a jump at the area longer than 50 m, as this results in long-term attenuation of shock waves, which is not factually accurate.

Work purpose formulation. The purpose of the work is to state a task which considers the kinetics of methane acidification by oxygen in mine atmosphere as well as conducting model test computations of methane explosion in mine excavations.

Presentation of basic material. To computate the process of methane ignition, deflagration and detonation combustion as well as blast wave propagation in rectilinear areas of excavation, two-dimensional equations of gas dynamics recorded in a cylindrical coordinate system are used

$$\frac{\partial\rho}{\partial t}+div\left(\rho\vec{W}\right)=0;\quad continuity; \tag{1}$$

$$\left.\begin{aligned}&\frac{\partial\rho u}{\partial t}+div\left(\rho u\vec{W}\right)+\frac{\partial P}{\partial z}=\tau_{mp}\Pi\\&\frac{\partial\rho v}{\partial t}+div\left(\rho v\vec{W}\right)+\frac{\partial P}{\partial r}=0\end{aligned}\right\}\ motion; \tag{2}$$

$$\frac{\partial\rho E}{\partial t}+div\left(\rho E\vec{W}\right)+div\left(PW\right)=q\Pi\quad energy; \tag{3}$$

$$\begin{gathered}\tau_{mp}=\frac{1}{8}c_f\,\rho u^2;\quad c_f=0,0032+\frac{0,221}{R^{0,237}};\\R_e=\frac{\rho u D_{eqv}}{\mu};\quad D_{eqv}=\frac{4S}{\Pi};\end{gathered} \tag{4}$$

$$\begin{gathered}q=\alpha\left(T_S-T\right);\quad N_u=0,22\,R_e^{0,5}\,P_r^{0,47}\,B;\\P_r=\frac{\rho l}{\lambda_g};\quad N_u=\frac{\alpha D_{eqv}}{\lambda_B};\end{gathered} \tag{5}$$

$$B=\begin{cases}\exp\left[\dfrac{\left(\dfrac{l}{\delta}\right)_{ont}}{\left(\dfrac{l}{\delta}\right)}\right], & \left(\dfrac{l}{\delta}\right)\rangle\left(\dfrac{l}{\delta}\right)_{opt}\\ \exp\left[\dfrac{\left(\dfrac{l}{\delta}\right)}{\left(\dfrac{l}{\delta}\right)_{ont}}\right], & \left(\dfrac{l}{\delta}\right)\langle\left(\dfrac{l}{\delta}\right)_{opt}\end{cases}\quad \left(\frac{l}{\delta}\right)_{opt}=13\,. \tag{6}$$

Where ρ is density; P is pressure; $\vec{W}$ is velocity; u, v are components of velocity $\vec{W}$ on axes z and r correspondingly; z, r are cylindrical coordinates (z – along excavation, r – across it), t is time; Π is an excavation perimeter; τ_{mp} is channel wall friction force; c_f is a resistance coefficient; q is a heat flow in channel walls; α is a heat exchange coefficient; T_s is wall temperature; T is average gas temperature in an excavation cut set; R_e is the *Re*ynolds number; D_{eqv} is an equivalent diameter of excavation rectilinear area; S is a channel cut set; μ is a coefficient of gas dynamic tenacity; N_u is the Nusselt number, P_r is the Prandtl number; λ_g is a of gas heat conductivity coefficient, B is a correction coefficient, which considers influence of wall roughness on heat exchange process, l is a typical distance between roughness lugs; δ is a lug height.

Approximation formulas (4–6) are taken from works [3, 4].

Equations (1–3) are supplemented with an equation of state

$$P = (\gamma - 1)\, j\rho, \qquad (7)$$

which in form coincides with an ideal gas equation of state; however, in Equation (7) an adiabatic index γ and heat capacity c_p and c_v accordingly are assumed as temperature functions both for air and for methane-air mixture

$$c_v(T); \quad c_p(T); \quad \gamma = \gamma(T) = c_p(T) / c_v(T).$$

In contrast to the generally accepted statement of the problem of methane explosion in a mine, when a pressure profile of immediately exploded methane-air mixture is set in the gas-polluted area [2–4], the present work sets a concentration profile of methane, oxygen and other gases in mine atmosphere. A source of blast initiation is designed as a small volume area with high temperature whose heat exchange with surrounding gas leads to methane-air environment ignition and formation of a methane deflagration combustion wave or detonation wave (Fig. 2). To implement this problem statement, a chemical kinetics equation is added to equations (1–7); its specific form will be presented below. It is a fundamental difference between this work and preceding ones.

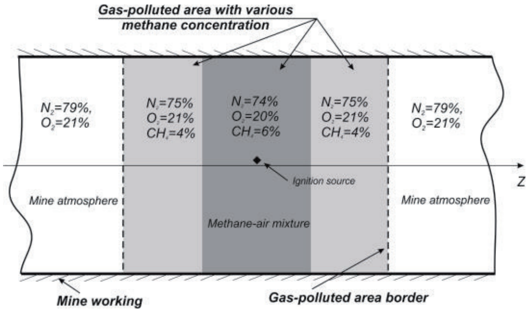


Fig. 2. The model of a gas-polluted area a mine working

Despite the fast development of computing means, appearance of improved detailed models of hydrocarbons combustion kinetics, their use in gas-dynamic flows calculation is currently impossible. That is why the usage of simple kinetic schemes which adequately describe combustion processes, is widely spread. The main advantage of such global models is their simplicity.

Detailed models may include hundreds of stages among dozens of reaction particles. Lack of kinetic data for many processes reduces the specification level of a kinetic process significantly. In this regard, various methods of presenting kinetics with simple models have been studied in recent years. They include simplified, generalized, schematic, quasi-global, compound and global ones.

When obtaining lower description levels, convolution of elementary stages and reaction particles in some generalized stages and parts is used. A global kinetic model is the simplest method of process kinetics description. The chemical reaction is presented in the form of one gross-stage "initial materials → products", while reaction rate is presented in the form of Arrhenius.

The global model is an approximate description of reaction behaviour kinetics. Reactions orders according to separate components may differ from stoichiometric ones, be fractional and even negative. To apply it, one should aim for correlated application of formulas on maximum number of parameters of experimental and theoretical characters, which belong to the task class considered.

The present work offers a new approach to solve the problem of methane explosion when the initial conditions include its concentration profile with further point chemical reaction initialization rather than the pressure profile of immediately exploded methane. Regarding its practical application, the approach is not entirely obvious.

That is why we should observe in detail a substantiation of the calculation method of chemical reaction kinetics in gas-dynamic computations of the problem class considered.

In practice, in technical literature and regulatory documents methane content in mine atmosphere is assigned by relative value of its volume concentration: $\alpha_1 = \frac{N_1}{N}$, where N_1 is the number of methane molecules, N is the total number of all gas molecules in certain volume V of mine atmosphere.

It follows therefrom that

$$\alpha_1 = \frac{(N_1 / V)}{(N / V)} = \frac{n_1}{n_1 + n_2 + n_3},$$

where n_1, n_2, n_3 are volumetric molecule concentration of methane, oxygen and all other molecules accordingly.

In terms of physics, this approach corresponds to assumption regarding the identity of peculiarities of interaction between molecules entering the air. In practical usage (not of an extreme character), this assumption justifies itself.

From what has been discussed above the next proposition follows.

$$\alpha_1 + \alpha_2 + \alpha_3 = 1.$$

To make calculations, we also need mass concentrations of molecules

$$n_i^m = \frac{N_i}{M}, \quad i = \overline{1, 3},$$

where $M = M_1 + M_2 + M_3$ is a mixture mass.

It is easy to determine the connection between the mass and volume concentrations

$$n_i^m = \frac{N_i}{M} = \frac{N_i / V}{M / V} = \frac{n_i}{\rho} \quad \text{or} \quad n_i = n_i^m \rho, \quad i = \overline{1, 3},$$

where ρ is mixture density.

We may assume that the mixture involved in gas-dynamic motion has density, which equals to the initial one.

It is also necessary to introduce the concept of molar concentration of molecules

$$n_i^{\mu} = n_i^m \cdot \mu, \quad i = \overline{1, 3}.$$

To calculate the mass concentration, it is essential to know the mixture density, which is introduced in the following way

$$\begin{aligned} \rho &= \frac{M}{V} = \frac{m_1 N_1 + m_2 N_2 + \overline{m_3} N_3}{V} = \\ &= \frac{m_1 \alpha_1 N + m_2 \alpha_2 N + \overline{m_3} N}{V} = \\ &= \alpha_1 \rho_1 + \alpha_2 \rho_2 + \alpha_3 \rho_3, \end{aligned} \tag{8}$$

where ρ_1, ρ_2, ρ_3 are initial densities of methane, oxygen and other air molecules correspondingly (for homogeneous substances, reference data are required); $\overline{m_3}$ is the average molecule mass without considering methane and oxygen.

The molar mass of gas mixture in mine atmosphere is defined according to Dalton's law

$$P = P_1 + P_2 + P_3,$$

where P is the pressure in the mixture, P_1, P_2, P_3 are partial pressures.

Using Mendeleev-Clapeyron equation $pv = \frac{m}{\mu} RT$, we obtain,

$$\frac{M}{\mu} \frac{RT}{V} = \frac{M_1}{\mu_1} \frac{RT}{V} + \frac{M_2}{\mu_2} \frac{RT}{V} + \frac{M_3}{\mu_3} \frac{RT}{V}.$$

From this equation it follows

$$\mu = \frac{M / V \cdot \mu_1 \mu_2 \mu_3}{M_1 / V \, \mu_2 \mu_3 + M_2 / V \, \mu_1 \mu_3 + M_3 / V \, \mu_1 \mu_3}.$$

Taking into account that

$$\frac{M_i}{V} = \frac{m_i N_i}{V} = \rho_i \alpha_{i,} \quad i = \overline{1, 3}.$$

Here ρ_1, ρ_2, ρ_3 are densities of homogeneous substances in normal conditions, for example, $\rho_1 = \frac{m_1 N}{V}$.

Then

$$\mu = \frac{(\alpha_1 \rho_1 + \alpha_2 \rho_2 + \alpha_3 \rho_3) \cdot \mu_1, \mu_2, \mu_3}{\alpha_1 \rho_1 \mu_2 \mu_3 + \alpha_2 \rho_2 \mu_1 \mu_3 + \alpha_3 \rho_3 \mu_1 \mu_2}. \tag{9}$$

Equations (8, 9) can be easily generalized for any quantity of gas in mine atmosphere, which are considered in calculations.

Calculation of the thermal capacity of mixtures. Kinetic equations of chemical reaction depend on the temperature, which is included in an exponent index. That is why one needs the most exact temperature value, which is determined by thermal capacity since gas dynamics equations, allow determining only specific internal energy of thermodynamic system.

In practice, mass, volume, and molar specific thermal capacities are used

$$C^m = \frac{1}{m} \frac{dQ}{dT}, \quad C^v, C^{\mu},$$

which depend on process type (constant volume or pressure).

To solve the problem of methane-air mixture ignition, thermal capacities with constant volume C_v^m, C_v^{μ} are appropriate. Further, we will omit the lower index "v".

Inflammation area is a small volume of mine atmosphere gas-polluted with methane in which temperature increases "immediately", and mixture ignition T_{ign} occurs. Reasons for this phenomenon can be various: discharge of static electricity, electrical covering disruption in working electromechanical equipment, materials friction, crystals cleavage, match burning, etc.

If we know specific volumetric thermal capacity, then specific mass and molar thermal capacities correspondingly equal to

$$C^m = \frac{C_V}{\rho}; \quad C^{\mu} = \frac{\mu \cdot C_V}{\rho} = \mu \cdot C^m,$$

where ρ, μ are density and molar mixture mass.

It is worth noting that temperatures depend on thermal capacity. All these correspondences can be found in reference literature. While making gas-dynamic calculations one needs constant adiabatic value

$$\gamma(T) = \frac{C_P(T)}{C_V(T)}.$$

Such functions are also known for some gas mixtures.

Kinetic equation of chemical reaction of methane-air mixture combustion. As a result of explosion of methane-polluted mine atmosphere, there proceeds a reaction of oxidation of methane by oxygen which is present in the air. The chemical reaction is presented as one gross-scheme

$$CH_4 + 2O_2 = CO_2 + 2H_2O. \tag{10}$$

The reaction speed by i component i=1, 2 is set in the Arrhenius form

$$-\frac{dc_i}{dt} = Z \cdot \exp\left(-\frac{E_a}{RT}\right) \Pi c_i^{v_i}, \tag{11}$$

where Z, E_a, v_i are effective pre-exponential multiplier, activation energy and reaction order by i component.

In this very case of the reaction (10), the equation (11) by a methane component looks like

$$-\frac{dc_1}{dt} = Z \cdot \exp\left(-\frac{E_a}{RT}\right) c_1^{v_1} \cdot c_2^{v_2}. \tag{12}$$

According to the equation (10) it follows that the speed of oxygen consumption is twice as high as the speed of methane consumption

$$-\frac{dc_1}{dt} = -\frac{1}{2}\cdot\frac{dc_2}{dt}\ . \qquad (13)$$

After integrating the equation (13) over the time, we will get $c_2 = 2c_1 + A$, where A is an integration constant, which can be obtained from the initial conditions

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

Index "*H*" shows the initial concentration value.

As a result, we get

$$c_2 = 2(c_1 - c_{1H}) + c_{2H} \Rightarrow c_2 = c_{2H} + 2(c_1 - c_{1H}). \qquad (14)$$

Thus, knowing the dependence of concentration change on time, we can find function $c_2(t)$ using the formula (14).

Let us assume that $c_1 = c_{1H}$ at the initial moment of time; that is why $c_2 = c_{2H}$. With the total methane burning $c_1=0$, oxygen concentration will equal

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

With stoichiometric composition $c_{2H} = 2c_{1H}$. That is why methane and oxygen totally burn out simultaneously $c_1=0$, $c_2=0$. If $c_{2H} > c_{1H}$, than $c_2 > 0$ i.e. we observe residuum of O_2. Regarding $2c_{2H} < c_{1H}$ oxygen burns out earlier, while the methane residuum is equal to $c_1 = c_{1H} - \dfrac{c_{2H}}{2}$.

To describe the reaction (10), it is necessary to note that in the equation (12) the substance quantity (in moles) is used as concentration "*c*", per a volume unit in cm^3, i.e. dimension $[c] = \dfrac{moles}{cm^3}$.

The gas dynamics equation includes material density. The chemical reaction does not change this value, as long as the initial materials are simply substituted by reaction products. That is why, homogeneous material densities, included in the atmosphere content, are only necessary to set the initial conditions.

Computer realization of the initial conditions of the problem.

The chemical kinetics equation was solved by the numerical method in combination with gas dynamics equations and state equations. The difference analogue of the equation (11) was represented as follows

$$-\frac{[c_1]^{n+1}_{i,j} - [c_1]^{n}_{i,j}}{\Delta t} = k\cdot\left([c_1]^{n}_{i,j}\right)^{\nu_1}\cdot\left([c_2]^{n}_{i,j}\right)^{\nu_2},$$

where $k = Z\cdot\exp(-E_a/RT)$ is a speed constant of the combustion reaction; *i, j* are integer-valued coordinates of a calculation cell (coarse part); *n* is the number of a temporary layer.

From the equations (11,13) it follows

$$[c_1]^{n+1}_{i,j} = [c_1]^{n}_{i,j} - \Delta t\cdot k\cdot\left([c_1]^{n}_{i,j}\right)^{\nu_1}\cdot\left([c_1]^{n}_{i,j}\right)^{\nu_2};$$

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

When calculating an equation of energy conservation, one adds the following item to the right part

$$\Delta t\cdot Q\cdot Z\cdot\exp(-E_a/RT)\cdot\left([c_1]^{n}_{i,j}\right)^{\nu_1}\cdot\left([c_2]^{n}_{i,j}\right)^{\nu_2},$$

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

Gas dynamics equation system and numerical approach to their solution with the help of modification method of coarse parts is presented in the work [7] and will be described in detail in our further publications.

The approbation of the kinetic approach for the computation task solution of methane-air mixture explosion parameters in mine atmosphere will be demonstrated by solving an axis-symmetric task by the example of mine working gas-polluted area ignition with П-type distribution of methane molecule concentration at methane-oxygen stoichiometric composition (Fig. 3). The task does not consider the influence of gas flow heat exchange on an excavation wall and its drag on account of channel wall friction.

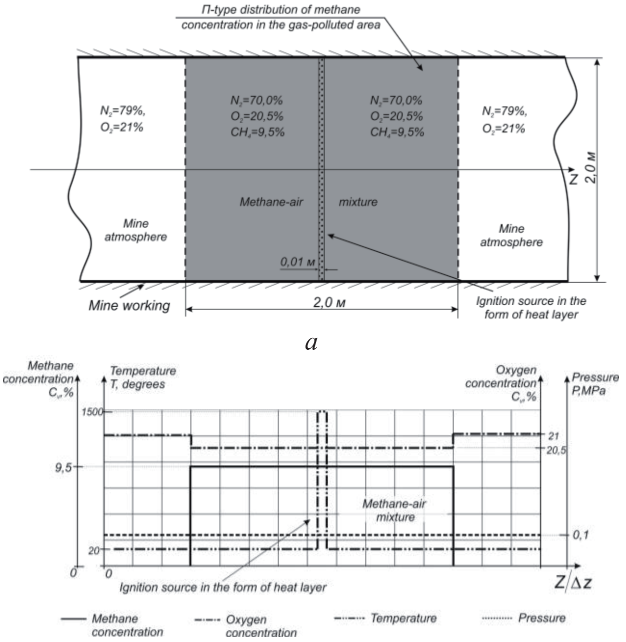


Fig. 3. The example of ignition and combustion calculation of methane-air mixture in the cylindrical channel: a) a gas-pollution scheme; b) a distribution diagram of CH_4, O_2, concentrations, temperature and pressure at the initial moment of time t=0 c

The following initial parameters were selected for the kinetic part of the task (Fig. 3, table). The air in the task is presented in the form of gas mixture of nitrogen 79% and oxygen 21%.

Current values of the thermal capacity C_p, adiabatic values γ and molar mass μ of the mixture are calculated according to its content.

Table

Parameters at the initial moment of time with n.c.

Parameter Name	*Unit of Measurement*	*Value*
CH_4 density, (homogeneous gas), ρ_1	kg/m^3	0,716
O_2 density, (homogeneous gas), ρ_2	kg/m^3	1,429
N_2 density, (homogeneous gas), ρ_3	kg/m^3	1,25
Isochoric thermal capacity of CH_4, C_{1v}^{m},	J/(kg·K)	$1{,}644\cdot 10^3$
Isochoric thermal capacity of O_2, C_{2v}^{m},	J/(kg·K)	$0{,}653\cdot 10^3$
Isochoric thermal capacity of N_2, C_{3v}^{m},	J/(kg·K)	$0{,}776\cdot 10^3$
Heating capacity of the mixture, Q_m	J/(kg·K)	$50\cdot 10^6$

The following equation was taken as a specific form of the Arrhenius equation for deflagration methane combustion conditions in mine workings [8]

$$-\frac{dc_1}{dt} = 8{,}3\cdot 10^5 \exp\left(-\frac{30}{RT}\right) c_1^{-0{,}3} c_2^{1{,}3} .$$

The boundary conditions of the task include conditions of leakproofness $v_{imax,j} = -v_{imax+1,j}$ on the walls of the cylindrical channel, and conditions of a "transparent" wall in the boundary region of the calculation area on an Z axis.

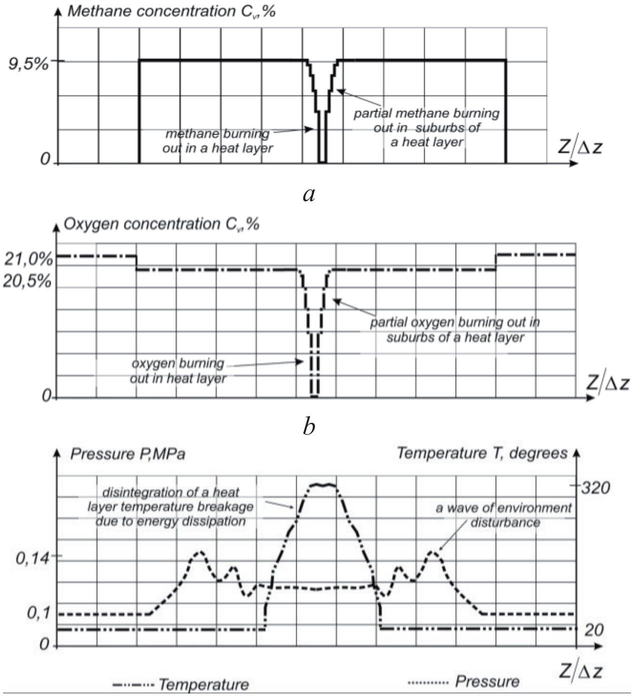
The numerical account was made with the time step $\Delta t=1$ mcs.

To carry out test calculations, the initial temperature of initialization (T_i) in the heat layer was increased smoothly from 500°C. Within the interval to 1850°C the ignition did not occur, further there appeared methane ignition with its partial burning out in the heat layer and its surroundings.

From T_i=2650°C upwards there occurs ignition and total burning out of methane in the heat layer as well as its partial burning out in surrounding layers. However, due to the small volume of the ignition source the processes of energy dissipation prevail over the activation process of the combustion reaction, which leads to a combustion chain break and correspondingly stopping of flame spread. Fig. 4, *a–b* shows the system state at the moment of time $t=500$ mcs after combustion cessation, which is proved by a pressure drop in the reaction area, sharp temperature drop and disintegration of a heat layer temperature breakage (Fig. 4, *c*).

As the numerical calculation showed, stable combustion was obtained beginning from T_i>3900°C. The character of the obtained combustion features deflagration, which is proved by low propagation speed of the reaction zone and formation of a shock wave, which comes from combustion front (Fig. 5).

Conclusions and prospects for the direction development. The results obtained show that the devised scheme of a numerical calculation, which considers the methane combustion kinetics, is the base for solving gas-dynamic problems of ignition processes and methane-air mixture combustion. The method will be developed in the direction of total account of physical phenomena in a concerned gas-dynamic process; for example, while computing temperature and gas pressure it is necessary to consider energy losses for friction and heat exchange with excavation walls, for inter-facial transition and dissociation of molecules in combustion products.

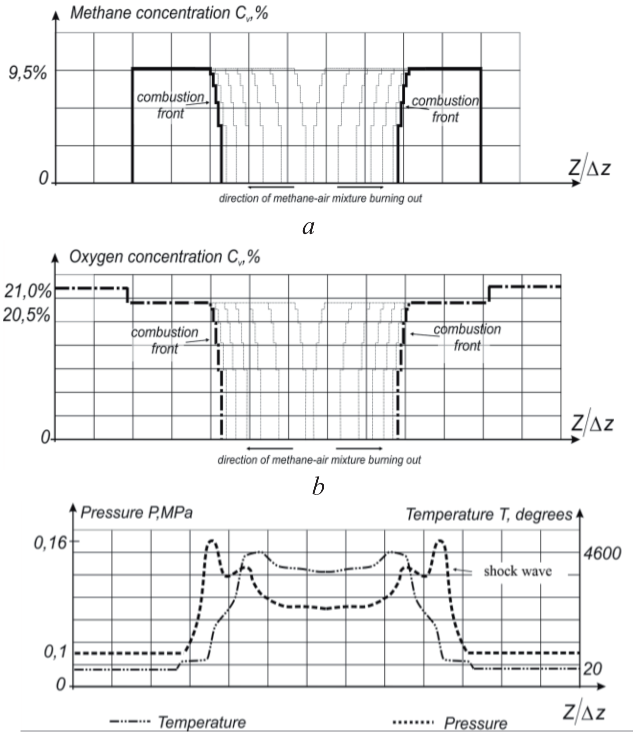


a

b

c

Fig. 4. The work of the ignition kinetic mechanism and partial burning out of methane-air mixture at the moment of time t=500 mcs after combustion stoppage



a

b

c

Fig. 5. The system state during the deflagration combustion (at the moment t=500 mcs)

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Мета. Чисельний розрахунок параметрів газових вибухів з урахуванням кінетики окислення метану киснем у шахтній атмосфері, проведення модельних тестових розрахунків вибуху метаноповітряної суміші.

Методика. Математичне моделювання газодинамічних і фізико-хімічних процесів газових вибухів. Чисельний експеримент процесу запалювання метану, дефлаграційного та детонаційного горіння, формування та розповсюдження вибухових повітряних хвиль.

Результати. Обгрунтовано вибір моделі хімічної кінетики механізму горіння метану у відкритому реакторі. Змодельовані нестаціонарні процеси вибуху метаноповітряного середовища, формування та розповсюдження вибухової хвилі в гірничих виробках. Аналіз результатів чисельного експерименту.

Наукова новизна. Розроблено новий підхід у реалізації схеми чисельного розрахунку газодинамічного процесу – вибуху метану, в якому об'єднані кінетика хімічної реакції окислення метану та динаміка перенесення енергії вибуху ударною хвилею й потоками газового середовища

Практична значимість. Результати модифікації схеми чисельного рахунку використовуються при обґрунтуванні технічних рішень з вибухозахисту аварійних ділянок гірничих виробок.

Ключові слова: *гірнича виробка, метаноповітряна суміш, кінетика горіння, вибухова повітряна хвиля, чисельний розрахунок, газова динаміка*

Цель. Численный расчет параметров газовых взрывов с учетом кинетики окисления метана кислородом в шахтной атмосфере, проведение модельных тестовых расчетов взрыва метановоздушных смесей.

Методика. Математическое моделирование газодинамических и физико-химических процессов газовых взрывов. Численный эксперимент процесса зажигания метана, дефлаграционного и детонационного горения, формирования и распространения взрывных воздушных волн.

Результаты. Обоснован выбор модели химической кинетики механизма горения метана в открытом реакторе. Смоделированы нестационарные процессы взрыва метановоздушной среды, формирования и распространения взрывной волны в горных выработках. Анализ результатов численного эксперимента.

Научная новизна. Разработан новый подход в реализации схемы численного счета газодинамического процесса – взрыва метана, в котором объединены кинетика химической реакции окисления метана и динамика переноса энергии взрыва ударной волной и потоками газовой среды.

Практическая значимость. Результаты модификации схемы численного счета используются при обосновании технических решений по взрывозащите аварийных участков горных выработок.

Ключевые слова: *горная выработка, метановоздушная смесь, кинетика горения, ударная воздушная волна, численный расчет, газовая динамика*

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