воздействия. Исследования являются базовыми для разработки мероприятий по достижению безопасного экологического состояния в бассейнах рек, отвечают обязательствам Украины в рамках действий „Окружающая среда для Европы“ и улучшению сотрудничества со странами-членами ЕС.

Ключевые слова: *экологическая безопасность, качество воды, биоиндикационные индексы, мониторинг, бассейновая экосистема*

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MATHEMATICAL SIMULATION OF GAS MIXTURE FORSED IGNITION FOR THE CALCULATION OF THE DAMAGING FACTORS OF EMERGENCY EXPLOSION

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МАТЕМАТИЧНЕ МОДЕЛЮВАННЯ ВИМУШЕНОГО ЗАПАЛЮВАННЯ ГАЗОПОВІТРЯНОЇ СУМІШІ ПРИ РОЗРАХУНКУ ВРАЖАЮЧИХ ФАКТОРІВ АВАРІЙНИХ ВИБУХІВ

Purpose. Selection and substantiation of the method of calculating the parameters of the ignition of gas mixtures with a heated body, the calculation of parameters and the evaluation of the reliability of performance of the established criteria for the initiation of the gas explosion.

Methodology. Mathematical simulation, numerical experiment, analysis and synthesis of the results.

Findings. The task of unsteady-state conduction problem of finding the temperature distribution in the thermal layer, near a source of ignition of air-gas mixture was set. Boundary conditions for a spherical source of ignition were defined. To solve the problem it was proposed to use the method of integral heat balance in which the thermal conductivity equation is replaced by the integral heat balance. Solutions of this equation are sought in the form of a polynomial of the second degree, i.e., the desired temperature profile in the thermal layer is represented as a quadratic parabola. As a result, an equation of the parabola as a dependence of temperature on the coordinates, time, heat capacity and heat generation from the ignition source is obtained. This solution allowed determining the effect of thermal oxidation of methane and, on that basis showing the convergence of the numerical method with the results of the analytical solution.

Originality. On the basis of the theory of thermal ignition and quasi-static approach, an analytical solution of the problem is found by methods of the integral balance, non-stationary temperature distribution in the thermal layer near a source of ignition of air-gas mixture. The thermal effect of oxidation of methane near a source of ignition is defined and the convergence of the numerical method of calculation of parameters of shock airwaves with the results of the analytical solution in terms of performance of the ignition criterion is shown.

Practical value. The resulting solution makes it possible to analyze the accuracy of the computing process methods of numerical simulation of gasdynamic parameters of shock waves in the air of the initiation of combustion and explosion of gas-air mixtures. The analysis of the accuracy of the computational process allows the use of numerical methods in practical calculations of finding a safe distance from the centers of the explosion in the liquidation or predicting the consequences of accidents.

Keywords: *gas-air mixture, ignition criteria, transient heat transfer, kinetics of combustion, thermal layer, temperature profile, mathematical model, thermal profile*

Introduction. Studies of forced ignition of the atmosphere of mining are highly relevant in terms of finding safety criteria. Within the processes of the coal industry, oil, gas, chemical and other industries there is a high probability of accidental formation of explosive concentrations and volumes of gas mixture. In the case of initiation of combustion and explosion of gas volumes, the value of damage effects of shock air waves is significantly affected by ignition process parameters [1]. This may be the effect of the power and source size on the result of the ignition in the form of laminar, deflagration or detonation combustion, as well as the influence of the place of initiation on the parameters of pressure waves [2].

Unsolved aspects of the problem. Currently, physical and mathematical models of the process of gas explosion and propagation of shock waves of air have been developed which require substantiation of a model of initiation of explosive processes and assessment of the adequacy calculation. In [3] the calculation of gas explosions parameters is performed using a combined gas-dynamic model and chemical kinetics of combustion of hydrocarbon gases. In this connection, it seems appropriate to carry out an analytical calculation of the ignition source parameters in the form of a heated body and assess the accuracy of the performance criteria established by the initiation of a gas explosion in the proposed model.

Analysis of the recent research. In this direction, mainly two of forced ignition theories are prevalent: thermal and ionic ones. In the vast majority of works the calculation of ignition processes is considered from the perspective of the theory of heat: the ignition by glowing particles and bodies, gas jets, shocks, friction, local fire and electric spark. The mechanism of the last two methods of ignition, as it is shown in the works of S. I. Taubkin relates closer to the ionic theory, because it is accompanied by enrichment of the gas phase with active species (ions with a large energy content and free radicals) and strong increase in the gas temperature (about 10 000 °C). Regarding a spark, this is due to the high concentration of energy in a small volume of a gas-discharge plasma channel. However, in the calculations of these sources the thermal theory is favored as being the most reasonable, ranging from the works of Van't Hoff to D. A. Frank-Kamenetskiy, E. A. Averson and Ya. Zeldovich. Thus, in [4], based on the theory of heat, equations for determining the parameters of the ignition of gas-air mixture in the model of the explosion of the gas mixture in a closed volume of a flameproof enclosure are set. In [5] the thermal mechanism is used in the physical and mathematical modeling of ignition of silane with shock waves.

Unsolved aspects of the problem. The previously proposed method of numerical calculation of the gas-dynamic parameters of shock waves [3] allows you to set a safe distance for the construction of explosion protection facilities in mines with emergency response. However, for its effective application the issue of analysis of the accuracy of the computational process in the initiation of the combustion and explosion of gas-air mixture is to be solved. The same problem remains unsolved for similar numerical calculations using the method of large particles [6]. In this paper, the convergence of a numerical method with the results of the analytical solution of the problem is proposed to be used as the accuracy criteria [7].

Objectives of the article. Selection and substantiation of the method for calculating the parameters of the ignition of gas mixtures by a heated body, the calculation of parameters and the evaluation of the reliability performance of the established criteria for the initiation of the gas explosion.

Presentation of the main research. In the works of Averson E. A. it is noted that the division of the theory of ignition into the gas phase, heterogeneous and solid state regarding the physical sense is incorrect. They show that the pivotal role in the ignition does not belong to the stage of self-acceleration of a chemical reaction, but to the warm-up phase, during which conditions for the rapid development of the combustion reaction only occur while the reaction rate is still very low. Therefore, the main value in the calculations should be attached to the heat transfer processes for chemically inert substance. Features of the development of the chemical reaction become important while entering the combustion mode. Accordingly, in the gas-phase reaction a quasi-static period can be identified during which the heating of the initial reactive mixture occurs and it is possible to apply the methods of the theory of heat conduction implemented, for example, in [8, 9].

Most theoretical studies, the substance ignition is considered close to the unlimited hot surface. When studying the ignition of gas mixtures it has been established that laminar burning occurs in the initial source, while the source has a spherical shape. Obviously, in this case it is necessary to solve the problem for a spherical source.

As a criterion of the reactive gas mixture ignition, let us use the criterion of ignition by a heated body first substantiated by Ya. Zeldovich, according to which the ignition criterion includes not only the condition for the occurrence of the chemical reaction of combustion, but the conditions of the subsequent spread of flame and self-acceleration of a chemical reaction. The critical condition of the ignition by Zeldovich is

$$\left.\frac{dT}{dr}\right|_{r=r_0}=0;\quad \left.\frac{dT}{dr}\right|_{r>r_0}>0,$$

where dT is the temperature gradient at the boundary of the heated body; r_0 is spherical coordinate of the heated body boundaries.

With regard to this problem, the ignition occurs when the speed of the heat input from the ignition source Q_s and a chemical reaction Q_{ch} are compared

$$Q_s \le Q_{ch},$$

where

$$Q_{ch} = \frac{4}{3}\pi\int_{r_0}^{\infty} Q_g Z \exp\left(-\frac{E_a}{RT(x,t)}\right) r^3 dr;$$

$$Q_s = \frac{4}{3}\pi r_0^3 c_1\rho_1 T_s.$$

There $c_1\rho_1$ is volumetric heat capacity of the source of ignition, Q_g, Z, E_a stand for the thermal effect, preexponential factor, and the activation energy of the reaction.

Formulation of the problem. Implementation of the ignition criterion requires knowledge of transient thermal field in the computational domain. In the case where the heating time of the source is much smaller than the setting time of the temperature $r_0^2/æ_1$, the thermal conductivity of the source $æ_1$ can be considered endless. Therefore, the system of equations for thermal conductivity for particles and the medium can be replaced by one equation for a medium with boundary conditions on the surface of the source, which is the law of conservation of energy. Mathematical heat conduction equation for a spherical source is written as

$$\frac{\partial T}{\partial t} = \frac{æ}{r}\frac{\partial^2 (rT)}{\partial r^2}, \quad r \geq r_0, \qquad (1)$$

where T is medium temperature, K; t is time, s; æ is a coefficient of thermal conductivity, m^2/s; r is the current radius of the spherical coordinate system, m.

Let us define the boundary conditions: $T(r, 0) = T_s$, $T(\infty, 0) = T_s$, where T_s is the initial temperature of the gas environment, K.

According to Fourier's law, heat conduction equation for the consideration of (1) at the boundary of the spherical source (Fig. 1) will be written as

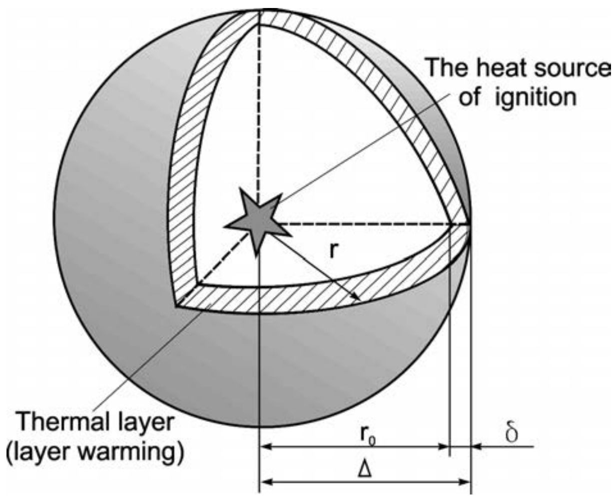

Fig. 1. The formulation of the reactive mixture ignition problem by spherical source: r_0 is radius of the spherical source of ignition; δ is thickness of the warming layer (thermal layer); Δ is the sum of the radius and thickness of the warming layer

$$c_1\rho_1 \frac{4}{3}\pi r_0^3 \left.\frac{\partial T}{\partial t}\right|_{r=r_0} = q + 4\pi r_0^2 \lambda \left.\frac{\partial T}{\partial r}\right|_{r=r_0}, \qquad (2)$$

where you can write the boundary condition

$$\left.\frac{\partial T}{\partial t}\right|_{r=r_0} = \frac{3q}{4\pi r_0^3 c_1\rho_1} + \frac{4\pi r_0^2 3\lambda}{c\rho 4\pi r_0^3}\left.\frac{\partial T}{\partial r}\right|_{r=r_0},$$

where q is power of energy release at the source of ignition, J/s; $c_1\rho_1$, $c\rho$ are the volume heat capacity of the ignition source and the substance outside accordingly, J/m^3; λ is the thermal conductivity of the reactive gas environment, W/(m · K).

Let,

$$W = \frac{3q}{4\pi r_0^3 c_1\rho_1}; \quad K = \frac{3\lambda}{c_1\rho_1 r_0} = \frac{3æ}{r_0},$$

where $æ = \frac{\lambda}{c_1\rho_1}$.

Then the boundary conditions (1) with (2) takes the form

$$\left.\frac{\partial T}{\partial t}\right|_{r=r_0} = W + K\left.\frac{\partial T}{\partial r}\right|_{r=r_0}. \qquad (3)$$

As an approximation we take the dependence of thermal characteristics of the environment temperature.

To simplify the task, let us take $c_1\rho_1 = c\rho$ and introduce $T' = T - T_н$ value. Then the system (1) can be represented as follows (for simplicity, we omit the prime on the value of T)

$$\frac{\partial T}{\partial t} = \frac{æ}{r}\frac{\partial^2 (rT)}{\partial r^2}, \quad r \geq r_0. \qquad (4)$$

Border conditions are

$$T(r, 0) = 0; \quad T(\infty, 0) = 0; \quad T(r, 0) = 0; \qquad (5)$$

$$\left.\frac{\partial T}{\partial t}\right|_{r=r_0} = W + K\left.\frac{\partial T}{\partial r}\right|_{r=r_0}. \qquad (6)$$

For an approximate solution of the boundary transient heat conduction problem (4–6) we use the integral method of heat balance, which is presented, for example, in N. M. Beliaiev, A. A. Riadno. The integral method uses this model of the thermal conductivity process, where the value $\delta(t)$, called the thermal layer thickness (Fig. 1) is introduced for consideration and for all values of $r > \delta(t)$ it is believed that the heat does not extend beyond this layer $r = \delta(t)$ and the medium temperature with $r \geq \delta(t)$ is equal to the ambient temperature (Fig. 2).

According to the integral method, an integral heat balance replaces the heat equation. Let us multiply the left and right side of the equation (4) by r^2, in order to get rid of r in the denominator of the right side of the equation. In this case, the ratio (4–6) takes the form

$$\int_{r_0}^{\Delta} \frac{\partial}{\partial t}\left(r^2 T\right) dr = æ\int_{r_0}^{\Delta} r \frac{\partial^2}{\partial r^2}(rT) dr. \qquad (7)$$

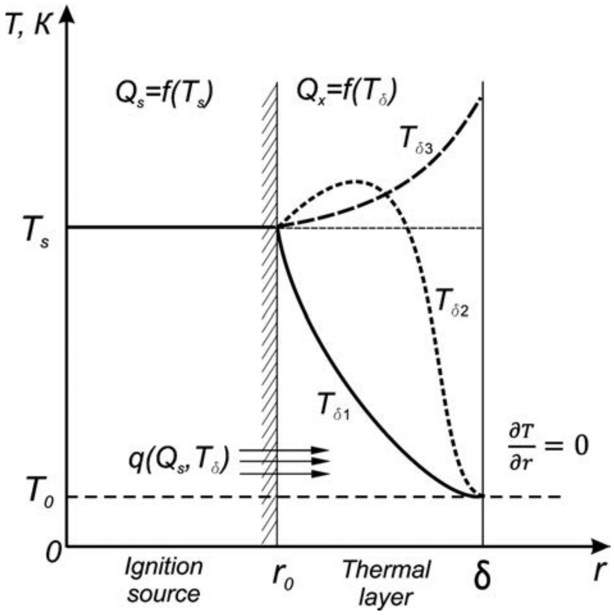

Fig. 2. The temperature distribution T (temperature profile) and the result of heating in the thermal layer due to conductive heat transfer: $T_{\delta 1}$ is heating result without initiating a chemical reaction; $T_{\delta 2}$ is ignition without flame propagation; $T_{\delta 3}$ is ignition and self-acceleration of the combustion reaction; r is the radius of the computational domain

The boundary condition is

$$T(\Delta,0)=\frac{\partial T}{\partial r}(\Delta,t)=0;\quad T(r,0)=0; \tag{8}$$

$$\left.\frac{\partial T}{\partial t}\right|_{r=r_0}=W+K\left.\frac{\partial T}{\partial r}\right|_{r=r_0}, \tag{9}$$

where $\Delta = r_0 + \delta$.

In the left side of the equation (7) we take $\frac{\partial}{\partial t}$ out of the integral sign, since the integration is according to r

$$\int_{r_0}^{\Delta}\frac{\partial}{\partial t}\left(r^2T\right)dr=\frac{\partial}{\partial t}\int_{r_0}^{\Delta}r^2Tdr.$$

Having integrated the equation (7) according to the ratio $\frac{\partial T}{\partial r}(\Delta,t)=0,$ we get

$$\frac{d\Theta}{dt}=-æ r_0^2\left.\frac{\partial T}{\partial r}\right|_{r=r_0}, \tag{10}$$

where $\Theta=\int_{r_0}^{\Delta}r^2Tdr.$

Considering (9), equation (10) can be simplified to the form

$$\frac{d\Theta}{dt}=-\frac{æ r_0^2}{K}\left[\left.\frac{\partial T}{\partial t}\right|_{r=r_0}-W\right]. \tag{11}$$

Having integrated the equation (11), we find that

$$\Theta=-b\left[T\big|_{r=r_0}-Wt\right]+A,$$

where $b=\frac{æ r_0^2}{K}$, since $K=\frac{3æ}{r_0}$, then $b=\frac{r_0^3}{3}$.

A is an integrating constant.

Taking into account that $t = 0$, $\Theta = T = 0$, we find

$$\Theta=b\left[Wt-T\big|_{r=r_0}\right]. \tag{12}$$

The solution of equation (12) with the boundary conditions (8, 9), according to the integral method, is found in the form of a polynomial of the second degree, i.e. the desired temperature profile in the thermal layer can be represented as a quadratic parabola

$$T=\left[a_0+a_1\left(r-r_0\right)+a_2\left(r-r_0\right)^2\right]\frac{1}{r}. \tag{13}$$

Let us define the temperature and temperature gradient in the medium at the boundary thermal layer ($T = 0$) from equation (13). From the boundary conditions (8) $r - r_0 = \delta$, then

$$T=\left[a_0+a_1\delta+a_2\delta^2\right]\frac{1}{r}. \tag{14}$$

To determine three coefficients of a parabola let us differentiate (14) for δ, and require that the temperature T and temperature change $\left.\frac{\partial T}{\partial r}\right|_{r=r_0}$ meet the boundary condition, namely, be equal to zer; we obtain the system of equations

$$\begin{cases}a_0+a_1\delta+a_2\delta^2=0\\ a_1+2a_2\delta=0\end{cases}. \tag{15}$$

From the second equation (15) we express a_1 и a_2

$$a_1=-2a_2\delta;\quad a_2=-\frac{a_1}{2\delta}.$$

Let us substitute the expressions a_1 and a_2 in the first equation of (15) and determine the a_1 and a_2 coefficients as a function of a_0

$$a_1=-\frac{2a_0}{\partial};\quad a_2=\frac{a_0}{\partial^2}. \tag{16}$$

Let us substitute the value of T (13) with (16) in equation (9) and differentiate the right side $\frac{\partial T}{\partial r}$.

$$\left.\frac{\partial T}{\partial r}\right|_{r=r_0}=\frac{\partial}{\partial r}\left[a_0-\frac{2a_0}{\partial}\left(r-r_0\right)+\frac{a_0}{\partial^2}\left(r-r_0\right)^2\right]\frac{1}{r}.$$

From the condition on the border of an ignition source (9), we obtain the equation

$$\left.\frac{\partial T}{\partial r}\right|_{r=r_0}=\frac{1}{r_0}\frac{da_0}{dt}=W-K\frac{a_0\left(2r_0+\delta\right)}{r_0^2\delta}. \tag{17}$$

Substituting solution (13) with (16) into the expression $\Theta = \int_{r_0}^{\Delta} r^2 T dr,$ we find that

$$\Theta = \int_{r_0}^{\Delta} r^2 \left[a_0 - \frac{2a_0}{\delta}(r-r_0) + \frac{a_0}{\delta^2}(r-r_0)^2 \right] \frac{1}{r} dr =$$

$$= \frac{a_0}{\delta^2} \int_{r_0}^{\Delta} r\left(\delta - (r-r_0)\right)^2 dr;$$

$$\Theta = \frac{a_0}{\partial^2} \int_{r_0}^{\Delta} r(\Delta - r)^2 dr.$$

Let us integrate the last equation in parts. We replace

$$\left\{ \begin{array}{l} u = r \\ du = dr \\ dv = (\Delta - r)^2 \end{array} \right\}.$$

Let us integrate $(\Delta - r)^2$ by r

$$\int (\Delta - r)^2 dr = \left\{ \begin{array}{l} \Delta - r = x \\ dx = -dr \\ dr = -dx \end{array} \right\} = \int x^2(-dx) =$$

$$= -\int x^2 dx = -\frac{1}{3}x^3 = -\frac{1}{3}(\Delta - r)^3.$$

Thus, according to the formula of integration in parts

$$\left\{ \begin{array}{l} u = r \\ du = dr \end{array} \right\} \ldots \left\{ \begin{array}{l} dv = (\Delta - r)^2 \\ v = -\frac{1}{3}(\Delta - r)^3 dr \end{array} \right\}.$$

Then

$$\Theta = \frac{a_0}{\delta^2}\left(-\frac{1}{3} r (\Delta - r)^3 \Big|_{r_0}^{\Delta} + \frac{1}{3}\int_{r_0}^{\Delta} (\Delta - r)^3 dr \right).$$

Let us integrate the right term

$$\Theta = \frac{a_0}{\delta^2}\left(-\frac{1}{3} r (\Delta - r)^3 \Big|_{r_0}^{\Delta} - \frac{1}{12}(\Delta - r)^4 \Big|_{r_0}^{\Delta} \right).$$

Let us substitute limits of integration

$$\Theta = \frac{a_0}{\delta^2}\left(-\frac{1}{3}\Delta(\Delta-\Delta)^3 + \frac{1}{3}r_0(\Delta - r_0)^3 - \frac{1}{12}(\Delta-\Delta)^4 + \right.$$

$$\left. + \frac{1}{12}(\Delta - r_0)^4 \right) = \left(\frac{1}{4}r_0 + \frac{1}{12}\Delta \right);$$

$$\Theta = \frac{a_0}{\delta^2}(\Delta - r_0)^3 \left(\frac{1}{4}r_0 + \frac{1}{12}\Delta \right).$$

Let us substitute according to conditions of the problem, $\Delta = r_0 + \delta$

$$\Theta = \frac{a_0}{\delta^2}(r_0 + \delta - r_0)^3 \left(\frac{1}{4}r_0 + \frac{1}{12}(r_0 + \delta) \right);$$

$$\Theta = \frac{a_0 \delta}{12}(4r_0 + \delta). \quad (18)$$

Substituting (18) into (12), we find that

$$a_0 = \frac{12 r_0 b W t}{\delta^2 r_0 + 4r_0^2 \delta + 12b} = \frac{4r_0^3 W t}{(\delta + 2r_0)^2}. \quad (19)$$

Substituting (19) into (17), we find that

$$\frac{\mu}{\nu} - \frac{\mu t \nu}{\nu^2} = W r_0 - \frac{3æ}{r_0^2}\frac{1}{\delta}\frac{\mu t}{\sqrt{\nu}},$$

where $\mu = 4r_0^3 W$; $\nu = (2r_0 + \delta)^2$.

Let us transform this equation to the following form

$$\nu - t\frac{d\nu}{dt} = \frac{1}{4r_0^2}\left[1 - \frac{12æt}{\delta\sqrt{\nu}} \right]\nu^2. \quad (20)$$

Let us find the solution of this equation for the two extreme cases, $r_0 \ll \delta$ and $\delta \ll r_0$. In the first case the equation (16) takes the form

$$\delta^2 = 12æt. \quad (21)$$

When $\delta \ll r_0$ equation (20) can be transformed to $\left(\nu \to 4r_0^2, \;\; \frac{d\nu}{dt} \to 4r_0 \frac{d\nu}{dt} \right)$

$$16r_0^4\delta - 16r_0^3 \delta t \frac{d\delta}{dt} = \left[\delta - \frac{12æt}{2r_0} \right] 16 r_0^4,$$

from which we obtain

$$\delta \frac{d\delta}{dt} = 6æt.$$

Integrating this equation provided $\delta(0) = 0$, we obtain the solution

$$\delta = \sqrt{12æt}. \quad (22)$$

As it can be seen from (21), (22), the solutions of equation (20) for large and small ignition sources are of the same size. On this basis, we will assume approximately that the thickness of the thermal layer is defined by $\delta = \sqrt{12æt}$, regardless of the ignition source size.

Thus, an approximate solution of problem (1) is written as

$$T = \frac{a_0}{r\delta^2}(\Delta - r)^2 = \frac{4r_0^3 W t}{(\delta + 2r_0)^2};$$

$$r_0 \le r \le \Delta, \quad \Delta = \delta + r_0, \quad (23)$$

where $\delta = \sqrt{12æt}$.

Substituting the expression W in (23), we get

$$T(r,\tau) = \frac{3qt}{\pi c_1 \rho_1 \delta^2 (\delta + 2r_0)^2}\frac{(\Delta - r)^2}{r},$$

where $\delta = \sqrt{12æt}$; $r_0 \le r \le \Delta$.

The results of calculating the temperature profile in the thermal layer. As a source of ignition, we consider a heated metal body of a spherical shape, which is placed immediately in the medium of methane. We used the following characteristics of the source (iron) and the environment: $r_0 = 0.01$ m; $c_1 = 0.444$ kJ/(kg · K); $\rho_1 = 7000$ kg/m^3; $c = 1.005$ kJ/(kg · K); $\rho = 1.22$ kg/m^3; the volume fraction of methane – 0.09; $æ_{15°} = 1.9 \cdot 10^{-5}$ m^2/s; $æ_{1500°} = 3.5 \cdot 10^{-4}$ m^2/s. As for gases, the coefficient of temperature conductivity is strongly dependent on its temperature (for example, when gas is heated from 0 to 1200 °C, its value increases almost 17-fold). This must be considered when calculating δ.

Fig. 3 shows the dependence of the ambient temperature on the coordinate in the thermal layer for different initial temperatures under specified conditions. It is evident that due to the low thermal conductivity gas graph is exponential.

With the thermal conductivity if the environment increasing, the temperature profile smoothes out, the thermal layer width increases (Fig. 4).

The resulting temperature profile allows us to take the next step – to solve the problem of chemical kinetics for the calculation of the thermal effect of methane oxidation in the thermal layer and, thus, determine Q_{ch}. In view of the spherical shape of the thermal layer and the content of the fuel component of the gas mixture, the thermal effect is determined by the Arrhenius equation

$$Q_{ch} = \frac{4}{3}\pi(\Delta^3 - r_0^3)\int_{r_0}^{\Delta} Q_g Z \exp\left(-\frac{E_a}{RT}\right) dr \cdot c_1^n c_2^m, \quad (24)$$

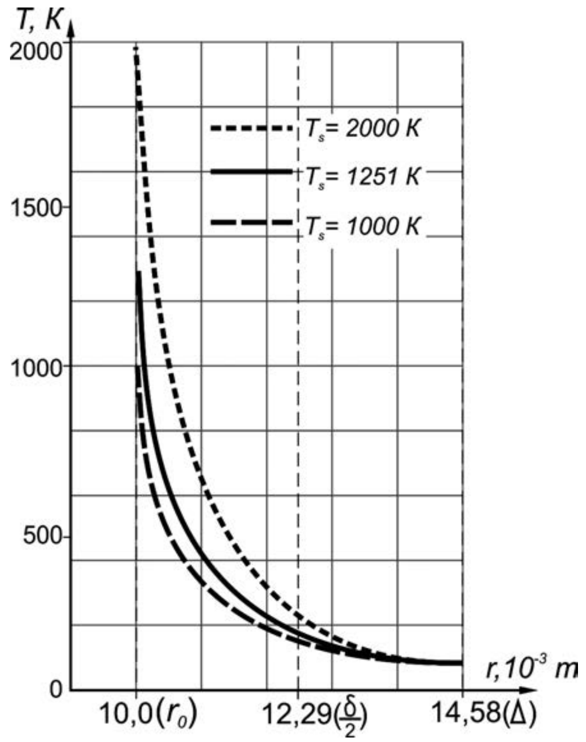

Fig. 3. The temperature profile T in the thermal layer under different initial temperatures of the ignition source, the period of time of 5 ms

where c_1, c_2 are concentration of methane and oxygen in the gas medium; n, m stand for the order of the reaction.

The integral equation (24) does not have an analytical solution, so to determine Q_{ch} we use the numerical solution. To do this, the resulting temperature profile in the interval $[r_0; \Delta]$ is divided into 20 sections and the heat q_{chi} is determined in each section with its average temperature (Fig. 5). According to the results of calculation of heat in the thermal layer, the rate of a chemical combustion reaction was established.

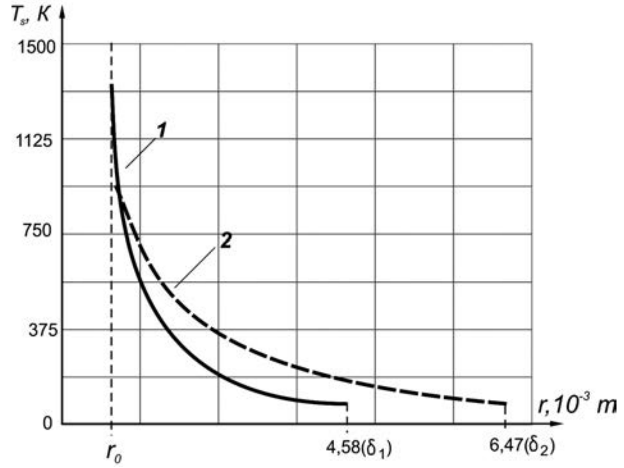

Fig. 4. The temperature profile in the thermal layer for different values of thermal conductivity of the gaseous medium:
1 – $æ = 3.5 \cdot 10^{-4}$ m^2/s; 2 – $æ = 3.7 \cdot 10^{4}$ m^2/s

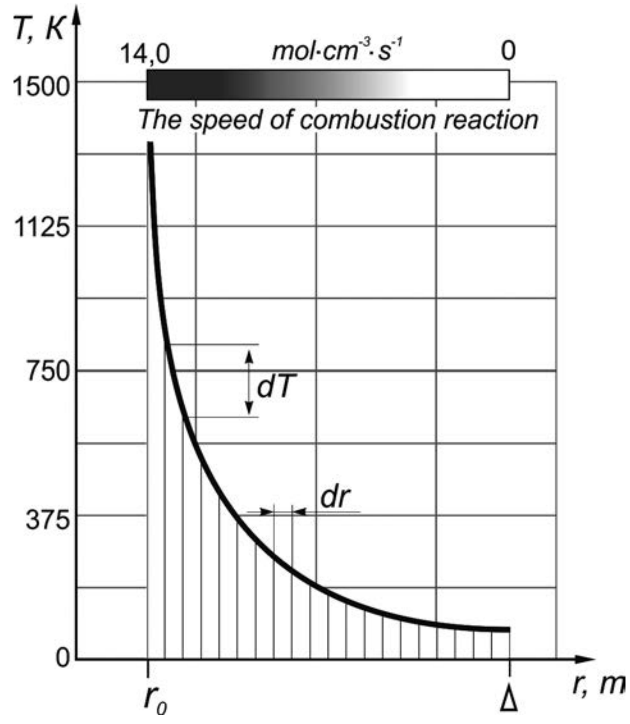

Fig. 5. Diagram of the numerical solution of the integral equation of thermal effect of methane oxidation: T is the gas temperature; r is the radius of the computational domain

Fig. 6 shows the thermal profile q_{ch}, the result of a chemical reaction, which is determined by the temperature profile T.

As it can be seen from the graph (Fig. 6), in spite of the warming of the whole thermal layer, the reaction rate is important only in a thin boundary layer that is in accord with the known data [2].

As a result, showing a heat input related the source of ignition Q_s and chemical reaction Q_{ch} we can determine the ignition temperature under specific conditions (Fig. 7). For the examined terms, the temperatures of methane-air mixture ignition were obtained 978, 1013, 1059 °C, respectively, for 9, 7 и 5 % volume content of methane.

To assess the reproducibility of numerical calculation by the method of large particles of the process of gas mixture ignition, a numerical experiment of ignition of mixture of methane and air was conducted with the parameters adopted for analytical calculation. The ignition source was defined in a form of a cylinder with dimensions of height and diameter having close values while the volume of a cylinder $V_c \approx V_{ball}$. The density and heat capacity of the environment in the area of the ignition source were assumed as equal to the characteristics of iron. The numerical experiment showed a stable ignition of a 9 % methane-air mixture at a source temperature of 930 °C. For 7 and 5 % methane-air mixtures, ignition test was carried out at temperatures of 983 and 996 °C. Thus, discrepancies between the numerical calculation and the analytical solution do not exceed 7 %, which can be explained by a simplification of the adopted model of the physical process in the analytical decision as opposed to the numerical solution, namely, the lack of consideration of mass transfer (in the formula (24) concentrations of c_1, c_2 are taken as permanent, though they actually manage to change to nearly zero during the accepted amount of time).

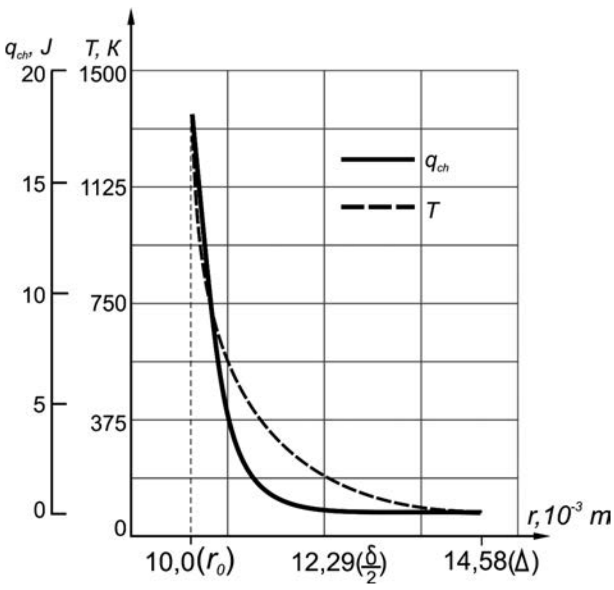

Fig. 6. Heat q_{ch} and temperature T profile in the thermal layer

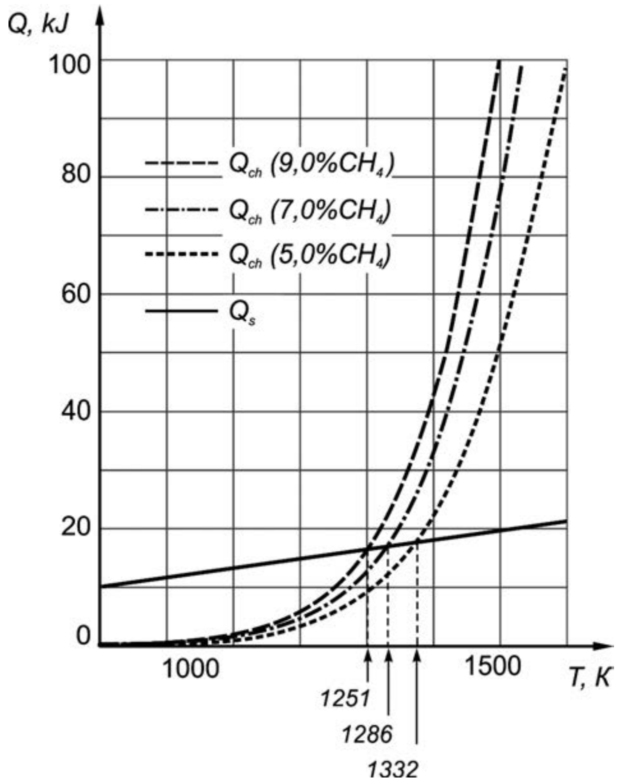

Fig. 7. Determination of the ignition temperature regarding the dependence of heat input of the ignition source Q_s and chemical reaction Q_{ch} on the initial temperature T

Conclusions and recommendations for further research. The resulting analytical solution of temperature distribution in the thermal layer allowed determining the thermal effect of methane oxidation near the source of ignition, and on this basis showing the convergence of the numerical method with the results of the analytical solution in terms of implementation of the ignition criterion. The analysis of the accuracy of the computational process allows the use of numerical methods in practical calculations of finding a safe distance from the centers of the explosion while eliminating and forecasting consequences of accidents.

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Мета. Вибір і обґрунтування методу розрахунку параметрів запалювання газових сумішей нагрітим тілом, розрахунки параметрів і оцінка вірогідності виконання встановлених критеріїв ініціювання для газового вибуху.

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

Результати. Виконана постановка задачі нестаціонарної теплопровідності щодо знаходження температурного розподілу в тепловому шарі, поблизу джерела запалювання газоповітряної суміші. Визначені граничні умови для сферичного джерела запалювання. Для розв'язку задачі запропоновано використовувати метод інтегрального теплового балансу, в якому рівняння теплопровідності замінялося інтегралом теплового балансу. Рішення такого рівняння шукається у вигляді багаточлена другого ступеня, тобто шуканий профіль температури в тепловому шарі представляється у вигляді квадратичної параболи. У результаті отримане рівняння параболи у вигляді залежності температури від координати, часу, теплоємності й теплоприходу від джерела запалювання. Цей розв'язок дозволив визначити тепловий ефект реакції окиснення метану та на цій основі показати збіжність чисельного методу з результатами аналітичного розв'язку.

Наукова новизна. На основі теплової теорії запалювання й квазістатичного підходу отримано аналітичний розв'язок задачі методом інтегрального балансу, нестаціонарного розподілу температури в тепловому шарі поблизу джерела запалювання газоповітряної суміші. Визначено тепловий ефект реакції окиснення метану поблизу джерела запалювання та показана збіжність чисельного методу розрахунку параметрів поширення ударних повітряних хвиль із результатами аналітичного розв'язку в частині виконання критерію запалювання.

Практична значимість. Отриманий розв'язок дозволяє виконати аналіз точності обчислювального процесу методики чисельного розрахунку газодинамічних параметрів поширення ударних повітряних хвиль у частині ініціювання горіння та вибуху газоповітряних сумішей. Виконаний аналіз точності обчислювального процесу дозволяє застосовувати чисельний метод у практичних розрахунках знаходження безпечних відстаней від осередку вибуху при ліквідації або прогнозуванні наслідків аварійних ситуацій.

Ключові слова: *газоповітряна суміш, критерії запалювання, нестаціонарна теплопровідність, кінетика горіння, тепловий шар, температурний профіль, математична модель, тепловий профіль*

Цель. Выбор и обоснование метода расчета параметров зажигания газовых смесей нагретым телом, расчет параметров и оценка достоверности выполнения установленных критериев инициирования для газового взрыва.

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

Результаты. Выполнена постановка задачи нестационарной теплопроводности о нахождении температурного распределения в тепловом слое, вблизи источника зажигания газовоздушной смеси. Определены граничные условия для сферического источника зажигания. Для решения задачи предложено использовать метод интегрального теплового баланса, в котором уравнение теплопроводности заменялось интегралом теплового баланса. Решение такого уравнения ищется в виде многочлена второй степени, т.е. искомый профиль температуры в тепловом слое представляется в виде квадратичной параболы. В результате получено уравнение параболы в виде зависимости температуры от координаты, времени, теплоемкости и теплоприхода от источника зажигания. Это решение позволило определить тепловой эффект реакции окисления метана и на этой основе показать сходимость численного метода с результатами аналитического решения.

Научная новизна. На основе тепловой теории зажигания и квазистатического подхода получено аналитическое решение задачи методом интегрального баланса, нестационарного распределения температуры в тепловом слое вблизи источника зажигания газовоздушной смеси. Определен тепловой эффект реакции окисления метана вблизи источника зажигания и показана сходимость численного метода расчета параметров

распространения ударных воздушных волн с результатами аналитического решения в части выполнения критерия зажигания.

Практическая значимость. Полученное решение позволяет выполнить анализ точности вычислительного процесса методики численного расчета газодинамических параметров распространения ударных воздушных волн в части инициирования горения и взрыва газовоздушных смесей. Выполненный анализ точности вычислительного процесса позволяет применять численный метод в практических расчетах нахождения безопасных расстояний от очагов взрыва при ликвидации или прогнозировании последствий аварийных ситуаций.

Ключевые слова: *газовоздушная смесь, критерии зажигания, нестационарная теплопроводность, кинетика горения, тепловой слой, температурный профиль, математическая модель, тепловой профиль*

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