

NUMERICAL MODELING OF HYDROGEN DEFLAGRATION DYNAMICS IN ENCLOSED SPACE

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ABSTRACT

A three-dimensional mathematical model of gaseous hydrogen deflagration in the enclosed space is developed. The process is described by the system of gas dynamics differential equations. Thermodynamic parameters of the mixture and its components are defined as functions of the local temperature and mixture composition. The concentration changes of the fuel and combustion products are determined using conservation laws taking into account rates of component disappearance and formation and turbulent diffusion. It is assumed, that the chemical reaction takes place only in the volume where the fuel concentration is within the limits of inflammability. The mathematical model is validated during an intercomparison test to predict deflagration of a large-scale hydrogen-air mixture in open atmosphere. An algorithm of numerical solution based on the Godunov method is developed. A computer system of engineering analysis of gas-dynamic processes of hydrogen-air mixture formation and combustion in enclosed space with natural ventilation is created. It allows predicting the history of the changes of overpressure, temperature, concentrations of hydrogen and combustion products and other thermogas-dynamic parameters of the mixture in space. This prognosis can be used to estimate dangerous zones of destruction and recommend some safety measures.

1. INTRODUCTION

An estimation of the fire safety level of the production area is a problem of extreme actuality and high practical importance [1, 2]. The thorough study of all aspects of the deflagration dynamics using mathematical and computer modeling (Computational Fluid Dynamics methods) is the most perspective way of scientific research in this area [3, 4].

A three-dimensional mathematical model of gaseous hydrogen-air deflagration in the enclosed space with natural ventilation is presented. It takes into account the process of combustion products formation. The results of some problem solutions obtained with the use of the developed computer complex Expert-2 are described. Firstly, the results of an intercomparison test to predict deflagration of a large-scale hydrogen-air mixture cloud in open atmosphere, formation of spherical blast wave and dynamics of temperature and concentration changes are considered. Then the scenario of the instant release of high compressed hydrogen, consequent formation and combustion of hydrogen-air mixture in the production area with natural ventilation is simulated. The calculations are carried out in order to estimate an influence of the combustible loading value on the deflagration factors (total heat generation rate, volume averaged overpressure and temperature) in the production area at different scenarios of deflagration origin and development. Some specific features of hydrogen dispersion and combustion in the air, conditioned by its low density, high diffusion constant, high rate of chemical reaction with an oxygen, wide range between concentration inflammability limits and high speed of the flame propagation are exposed.

2. MATHEMATICAL MODEL

The most adequate modeling of physical processes of mixing of reacting gases with an air, their combustion (taking into account chemical interaction of the mixture components) and further dispersion of the mixture in the open space or enclosed area with ventilation is possible only using of Navier-Stokes nonsteady equation system for the compressible gas. At present, the effective numerical modeling of turbulent flows is carried out by the solution of the Reynolds-averaged Navier-Stokes equations, complemented by the turbulence model [5, 6]. However the majority of turbulence models do not describe different types of flows with the identical degree of adequacy. Especially it relates to the flows with an intensive separation and/or large pressure and temperature gradients. Therefore there is the barest necessity to develop new mathematical models and computation schemes for the numerical modeling of such flows.

The main purposes of this work are the development of the simplified mathematical model adequately describing the nonsteady processes of mixing of the reacting gases with air, their combustion (taking into account chemical interaction of the mixture components) and further dispersion of mixture in the open space or enclosed area with the forced (or natural) ventilation, the creation of the effective algorithm of numerical solution and realization it into a computer system which can be an instrument to simulate these complex gas-dynamic processes.

As a result of structural analysis of the described flow and decomposition of the complete gas-dynamic mathematical model such an assumption is accepted that a convective exchange of mass, impulse and energy have the basic influence on the process. Thus, for modeling of mixing processes of three-component gas it is enough to use the truncated Navier-Stokes equations (Euler approach with the use of source members). But turbulence-combustion interaction is a powerful feedback mechanism that produces components' concentration exchange, and this phenomenon can be taken into account using sources terms in the mixture components' mass conservation laws.

The calculated space Ω is a parallelepiped located in the right-hand coordinate system (fig. 1) and it is partitioned to spatial cells the scale of which depends on characteristic sizes of the calculated space (roughness of streamlined surfaces, dimensions of streamlined objects).

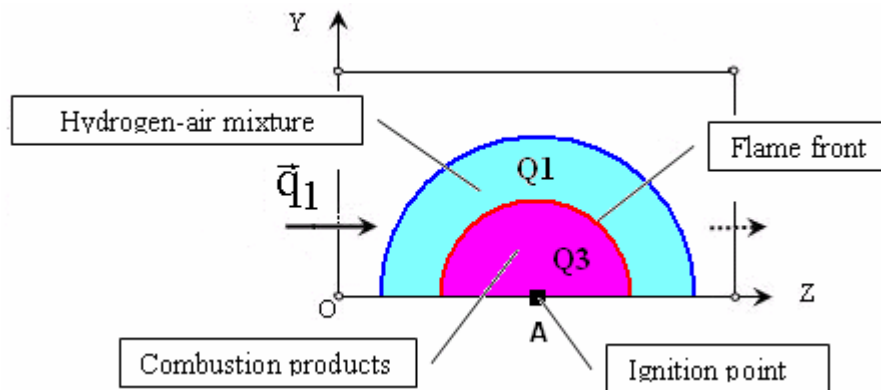


Figure 1. Analytical model of hydrogen-air mixture formation, its combustion and products dispersion

The total system of the time-dependent equations describing the three-dimensional three-component gas mixture flow looks like [7, 8]:

$$\frac{\partial \vec{a}}{\partial t} + \frac{\partial \vec{b}}{\partial x} + \frac{\partial \vec{c}}{\partial y} + \frac{\partial \vec{d}}{\partial z} = \rho \vec{f}, \quad (1)$$

where $\vec{a}, \vec{b}, \vec{c}, \vec{d}, \vec{f}$ are the following vector-columns:

$$\vec{a} = [\rho, \rho u, \rho v, \rho w, E]^T, \quad (2)$$

$$\vec{b} = [\rho u, P + \rho u^2, \rho uv, \rho uw, (E + P)u]^T, \quad (3)$$

$$\vec{c} = [\rho v, \rho vu, P + \rho v^2, \rho vw, (E + P)v]^T, \quad (4)$$

$$\vec{d} = [\rho w, \rho wu, \rho wv, P + \rho w^2, (E + P)w]^T, \quad (5)$$

$$\vec{f} = [0, 0, -g, 0, -gv + e_s / \rho]^T, \quad (6)$$

where t – time; u, v, w – components of velocity vector \vec{q} ; P, ρ – pressure and density; E – total energy of the gas mixture volume unit:

$$E = \rho \left(e + \frac{1}{2} (u^2 + v^2 + w^2) \right); \quad (7)$$

e – internal energy of a gas mass unit; components of the vector \vec{f} – projections of the distributed volume sources; g – gravitational acceleration, e_s – thermo generation intensity of gas volume unit caused by the chemical reaction.

The conservation laws of admixture components (combustible gas, air and combustion materials) that take into account diffusion and chemical reaction rates look like [7, 8]:

$$\frac{\partial(\rho Q_i)}{\partial t} + \frac{\partial(\rho u Q_i)}{\partial x} + \frac{\partial(\rho v Q_i)}{\partial y} + \frac{\partial(\rho w Q_i)}{\partial z} = \rho_{Q_{it}} + \rho_{Q_{is}}, \quad (8)$$

where Q_i – relative mass density of the admixture (the ratio of the gaseous admixture substance density to the mixture density), $i = 1 \dots 3$: 1 – fuel, 2 – air, 3 – combustion products; $\rho_{Q_{it}}$ – an admixture density change rate as a result of turbulence diffusion (according to Fick law $\rho_{Q_{it}} = \text{div}(\rho \mathcal{G}_D \text{grad} Q_i)$ and a diffusion factor \mathcal{G}_D is defined according to Berljang [9]); $\rho_{Q_{is}}$ – change intensity of mixture component density caused by chemical reaction.

The set of equations (1-8) is incomplete. It is complemented with equations defining thermal and physical properties of mixture components.

$$\mu = \frac{1}{\sum_{i=1}^3 \frac{Q_i}{\mu_i}}; C_P = \sum_{i=1}^3 Q_i (C_P)_i; C_v = \sum_{i=1}^3 Q_i (C_v)_i; \sum_{i=1}^3 Q_i = 1, k = \frac{C_P}{C_v}. \quad (9)$$

For an ideal polytropic gas the value e is related to the values P and ρ of the mixture by the following dependence: $e = \frac{P}{(k-1)\rho}$.

The rate of fuel density change $\rho_{Q_{1s}}$ caused by chemical reaction is determined as a product of molecular mass of fuel μ_1 and its molar change rate w_1 . The chemical “brutto”-reaction is considered:



where ν_i – stoichiometrical coefficients, χ_i – chemical agents. The molar change rate w_1 is determined:

$$w_1 = -\nu_1 A_1 T^{\beta_1} \exp[-E_1 / (R_{yh} T)] \prod_{i=1}^2 [\chi_i]^{\nu'_i}, \quad (11)$$

where $A_1, \beta_1, E_1, \nu'_1, \nu'_2$ – the parameters obtained on the basis of experimental data generalization [10], $[\chi_i]$ – molar concentration of the mixture i -component: $[\chi_i] = \frac{\rho Q_i}{\mu_i \nu_i}$. The Arrhenius reaction constant

A_1 was adjusted in order to use large control volume sizes during solving of large-scale problems. The density change rate of the combustion products $\rho_{Q_{3s}}$ it is determined on the basis of law of locomotive the masses:

$$\frac{\rho_{Q_{1s}}}{\mu_1 \nu_1} = \frac{\rho_{Q_{2s}}}{\mu_2 \nu_2} = -\frac{\rho_{Q_{3s}}}{\mu_3 \nu_3}. \quad (12)$$

The heat-evolution intensity of the gas volume unit caused by chemical reaction e_s is determined:

$$e_s = -\xi H_{u1} \rho_{Q_{1s}}, \quad (13)$$

where ξ – completeness of combustion coefficient, H_{u1} – lower heat of fuel combustion.

It is assumed that any component of air flow velocity is subsonic. The approaching flow is defined by the values of total enthalpy $I_0^* = \frac{k}{k-1} \frac{P}{\rho} + \frac{1}{2}(u^2 + v^2 + w^2)$, entropy function $S_0 = \frac{P}{\rho^k}$, flow velocity vector (angles $\alpha_x, \alpha_y, \alpha_z$), and relative admixture mass concentration Q_1 ($Q_1 \leq 1$ if the gas admixture

flows in). The entry flow parameters are defined using the "left" Riemann invariant correlation [11]. On the impermeable computational cells' surfaces the "no-flowing" condition is satisfied: $q_n = 0$ (where \vec{n} is a normal to the considered cell surface). Exit boundary conditions are set on the computational cells' surfaces where the mixture flows out from computational area using the "right" Riemann invariant correlation [11].

At start time in all "gaseous" cells of the computational space the ambient parameters are assigned. In the cells occupied by an admixture cloud, the relative mass concentration of the admixture equals $Q_1 \leq 1$. In cells with gas evaporation the law of change of mixture component flow discharge is set.

3. ALGORITHM OF NUMERICAL SOLUTION

The vector equation (1) can be presented in an integral form for every computational cell:

$$\frac{\partial}{\partial t} \iiint_V a dV + \iint_{\sigma} \hat{A} d\sigma = \iiint_V \rho f dV, \quad (14)$$

where V – a volume of the elementary computational cell; $\vec{\sigma}$ – a limiting surface of the cell which has an external normal \vec{n} ($\vec{\sigma} = \sigma \vec{n}$); \hat{A} – a tensor of flux density of the conservative variables \vec{a} the columns of which are the vectors $\vec{b}, \vec{c}, \vec{d}$.

The conservation law of each mixture component (8) can be also presented in an integral form for every computational cell:

$$\frac{\partial}{\partial t} \iiint_V \rho Q_i dV + \iint_{\sigma} \rho Q_i q d\sigma = \iiint_V (\rho_{Q_{it}} + \rho_{Q_{is}}) dV \quad (15)$$

The computational solution of the fundamental gas dynamics equations (14, 15) is obtained using Godunov method [11]. An explicit Godunov method is used to solve Euler equations complemented by the conservation law of the gas mixture concentration in the integrated form. The first order finite-differential scheme is used to approximate Euler equations. The second order central differences are used for the diffusion source member of the conservation law of the gas mixture concentration. The simple pressure interpolation in the vertical dimension is applied. Godunov method has a robust algorithm resistant to the large-scale disturbances of flow parameters and allows obtaining flow parameters when modeling large-scale gas mixture combustion. It is assumed that deflagration can occur in computational cells where the fuel concentration is within the limits of inflammability: $Q_{1\min} \leq Q_1 \leq Q_{1\max}$. The values $Q_{1\min}$ and $Q_{1\max}$ are assigned on the basis of experimental data generalization [12].

On the basis of the mathematical model a computer system of the engineering analysis of the gas mixture formation, its combustion and dispersion in the atmosphere has been developed. It is used in the research bundled software «Expert-2» at the Scientific Center of Risk Investigations «Rizikon» (Severodonetsk, Ukraine) and National Aerospace University "Kharkov Aviation Institute", Ukraine. The software allows simulating different dangerous scenarios in an acceptable time using stand-alone computers.

4. MATHEMATICAL MODEL VALIDATION

Instant release of high pressurized inflammable gas into the atmosphere and its combustion can cause the high temperature zones formation, pressure waves' propagation, personnel damage and destruction of the

vitaly important objects. The values of temperature and overpressure are usually used to evaluate pressure and thermal loadings on the building surfaces.

The accepted simplified combustion model is suitable for description of the examined processes both in the opened and confined spaces. A turbulent exchange is taken into account in mass conservation laws of mixture components (8, 15) in the form of source members. The validation of the mathematical model against experimental data is carried out. The deflagration of the hemispheric homogeneous stoichiometric hydrogen-air mixture cloud is modeled (experiments at Fraunhofer ICT [13]) under the following conditions: the total volume of the cloud is 2094 m³; the initial pressure is 98.9 kPa; the initial temperature is 283 K; the radius R of the hemispheric cloud is 10 m. The temperature, fuel and combustion products concentration and pressure development at the distances of 5 m (the control point B on the fig. 2), 8 m (the control point C) and 18 m (the control point D) from the epicenter of the deflagration (the point A) is examined during the computation.

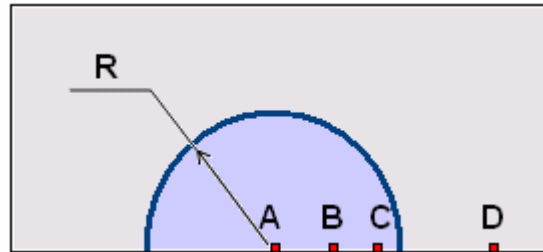


Figure 2. Computation area and control points' location

The computation space has the following dimensions: the length of 200 m; the width of 100 m, the height of 30 m. The computational grid has 200x100x30 sells. The computer has the following characteristics: 1 Intel® Celeron® CPU PCs (2.4 GHz), 0.75 Gb RAM, Windows XP. CPU time is 4 h.

The overpressure dynamics at the control milestone points B and D is presented on the fig. 3, 4 against the experimental data and computational results obtained using other codes [13]. Behavior of the curves in points B and C are similar. More sharp form of the calculated curve can be explained by particular features of the accepted combustion model. More intensive decrease of the overpressure as the blast-wave propagates from the point C to the point D can be referred to the first order scheme of the Godunov method.

The dynamics of the temperature in the control points B and D are represented on the fig. 5. The flame temperature of the stoichiometric hydrogen-air mixture (fig. 5a) somewhat higher than usually in experiment that could be explained by specific features of the model.

As a whole the computational results have quite a good agreement with experimental data. It allows using the developed mathematical model and code to simulate the large-scale deflagration of the hydrogen-air mixture in the atmosphere and to predict the pressure and thermal consequences generated by the hydrogen deflagration.

5. HYDROGEN DEFLAGRATION MODELING IN PRODUCTION AREA

The plan of the enclosed production area (where a hydrogen deflagration takes place) is represented on the fig. 6. Bearing constructions of building are the brick walls of 0.25 m width. Height of area is 3 m. The area consists of two production subspaces partially divided by internal wall of 0.25 m width. The thickness of the ceiling is 0.25 m. The area is equipped by two windows (1.5 m² each) and one doorway (2.5 m²). There are two gateways (4x2.5 m² each) for cars fuelled by hydrogen.

A balloon with high pressurized hydrogen is stored in the point A. The production area is situated in the three-dimensional space with ambient conditions.

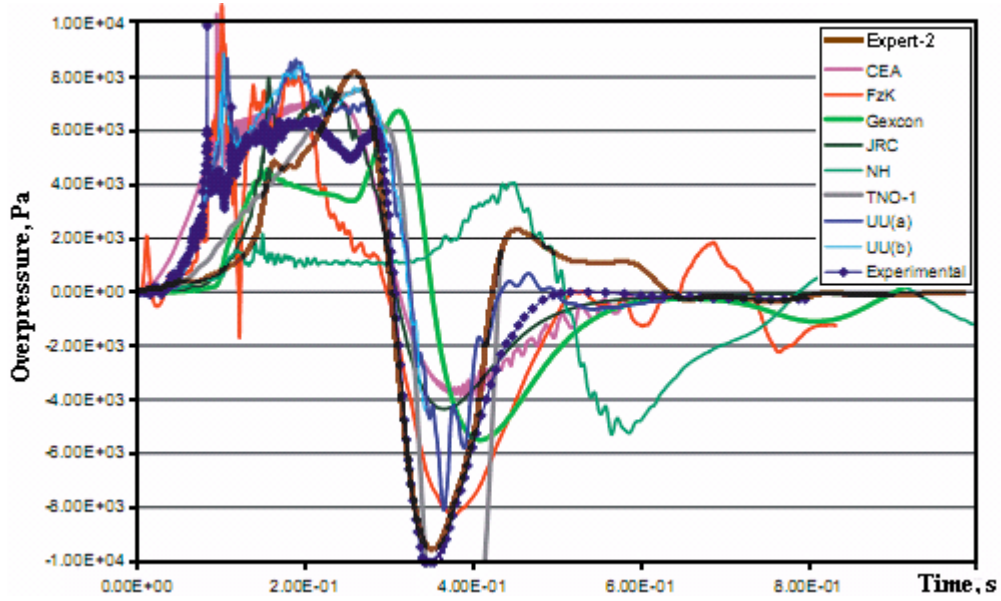


Figure 3. Pressure history in the control point B

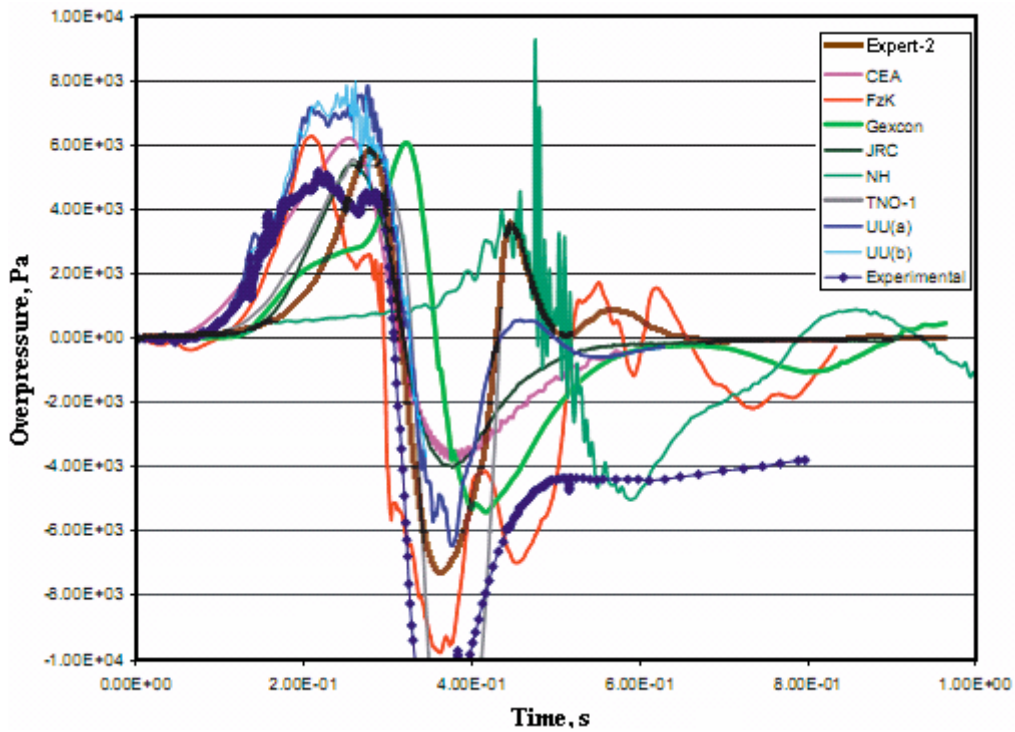


Figure 4. Pressure history in the control point D

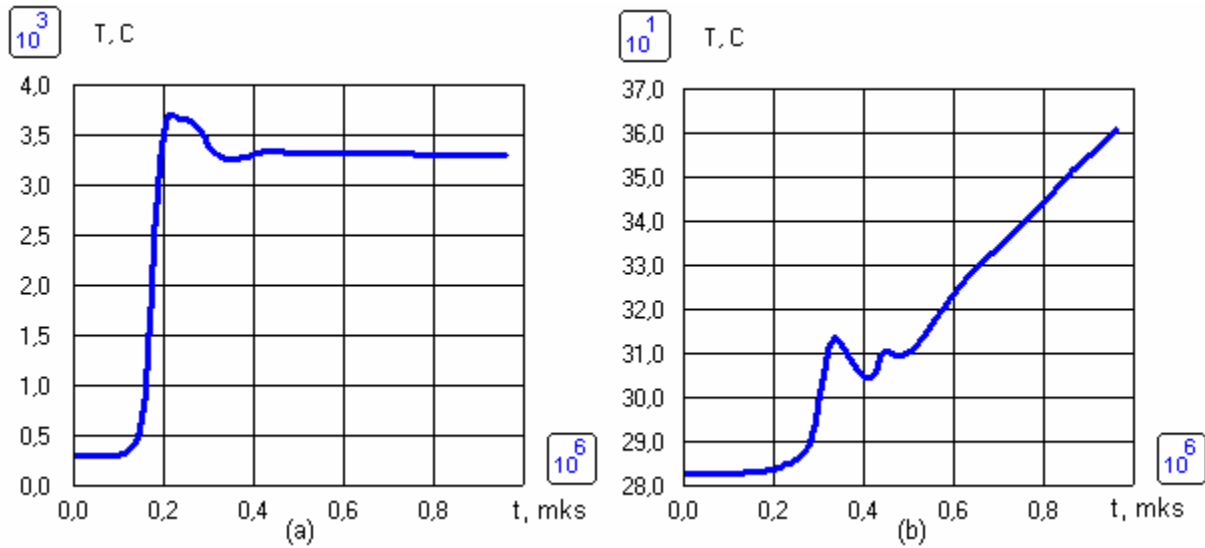


Figure 5. Temperature history in the control points B (a) and D (b)

6. SCENARIOS OF DEFLAGRATION DEVELOPMENT

Such factors as a place of deflagration origin, location and state (opened or closed) of the windows and doorways, capacity and character of hydrogen release can substantially influence deflagration dynamics in the production area. Two possible assumed scenarios with different parameters of released hydrogen cloud (in particular, hydrogen mass concentration) are simulated in order to determine the influence of them on deflagration dynamics in the production area (fig. 6).

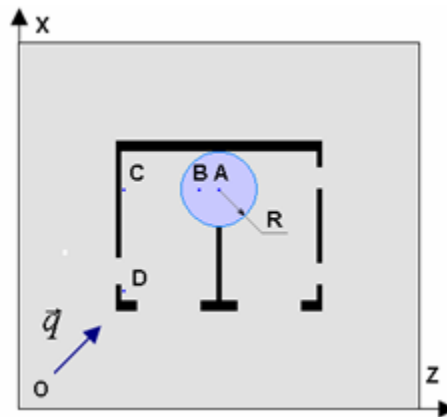


Figure 6. Computation area and control points' location

It is assumed that the hydrogen is released due to the destruction of (or leakage from) the fueling balloon stored in the production space. The doors, windows and gateways of the production building during the deflagration are open. In first case, the leakage from the balloon causes the formation of the stoichiometrical hydrogen-air cloud (2 m radius) with ambient atmospheric parameters (scenario 1). In second case, the instant destruction of the 12-balloon fueling set (volume of each 0.51 m^3) generates hydrogen-air cloud (2 m radius) with the ambient temperature, pressure 134 213 Pa, and mass concentration of hydrogen $Q_1 = 0.111$ (scenario 2). It is assumed, that for both scenarios the center of the cloud (and the point of flame ignition) is located in the point A (fig. 6). The sizes of the building are $10.5 \times 3.25 \times 12.75 \text{ m}$. The dimensions of the computational cells are $0.25 \times 0.25 \times 0.25 \text{ m}$. The sizes of the

computational domain are 22.5x4.25x15.75 m. The height of the all control points B, C, D and deflagration ignition point A (center of the cloud) is 1.125 m.

7. RESULTS OF DEFLAGRATION SIMULATION

The following computational output data in the control points B, C, D (fig. 6) are considered to analyze hydrogen deflagration dynamics in both scenarios: hydrogen mass concentration time history; combustion products mass concentration time history; overpressure and temperature time history.

The distribution of hydrogen and combustion products mass concentration in the production area during hydrogen deflagration (0.15, 0.25 and 0.35 s from the inflammation moment) for the scenario 1 is represented on the fig. 7. The pocket of unburned hydrogen (fig. 7b, 7c) could be explained by wall influence. The time history of overpressure and temperature in the control point B for the scenario 1 is represented on the fig. 8. The overpressure in the point C behaves similar and the temperature changes are insignificant. Once again, the flame temperature of the hydrogen-air mixture (fig. 8b) somewhat higher than usually in experiment that could be explained by specific features of the model. The dynamics of distribution of hydrogen and combustion products mass concentration in the production area during hydrogen deflagration (0.10, 0.15 and 0.20 s from the deflagration initiation) for the scenario 2 is represented on the fig. 9. The time changes of overpressure and temperature in the control point B for the scenario 2 are represented on the fig. 10 (the overpressure in the points C and D behaves similar to point B and the temperature changes insignificantly as in scenario 1).

An inter-comparison analysis of the calculation results of both scenarios of hydrogen deflagration in the enclosed area shows that the control flow parameters differ substantially. In particular, combustion products concentration maximum in the scenario 2 (fig. 9) is more than one in the scenario 1 (fig. 7). Overpressure and temperature maximums in the scenario 2 are much bigger, than ones in the scenario 1. These differences are caused by greater hydrogen fuel mass, participating in combustion, and more intensive mixture dispersion in the case of scenario 2.

These exposed features of hydrogen dispersion and combustion in the air during deflagration development are conditioned by hydrogen's low density, high diffusion constant, high rate of chemical reaction with an oxygen, wide range between concentration inflammability limits and high speed of the flame propagation.

In order to prevent or minimize pressure and thermal consequences caused by the hydrogen deflagration in the enclosed production space it is recommended some measures (in the case when the high hydrogen concentration is registered by sensors): water dispersion (reduces the mixture temperature and, as a result, the speed of chemical reaction); blowing of the neutral gas (carbon dioxide) or chemically active admixtures (increases the minimum concentration inflammability limit and, as a result, reduces the mixture temperature).

8. CONCLUSIONS

A three-dimensional mathematical model of gaseous hydrogen deflagration in the enclosed space is developed. An algorithm of numerical solution of the basic gas dynamic differential equations system based on the Godunov method is developed. A computer system of engineering analysis of gas-dynamic processes of hydrogen-air mixture formation and combustion in enclosed space with natural ventilation is created. It allows predicting the history of the changes of overpressure, temperature, concentrations of hydrogen and combustion products and other thermo gas-dynamic parameters of the mixture in space. This prognosis can be used to estimate dangerous zones of destruction and recommend some safety measures.

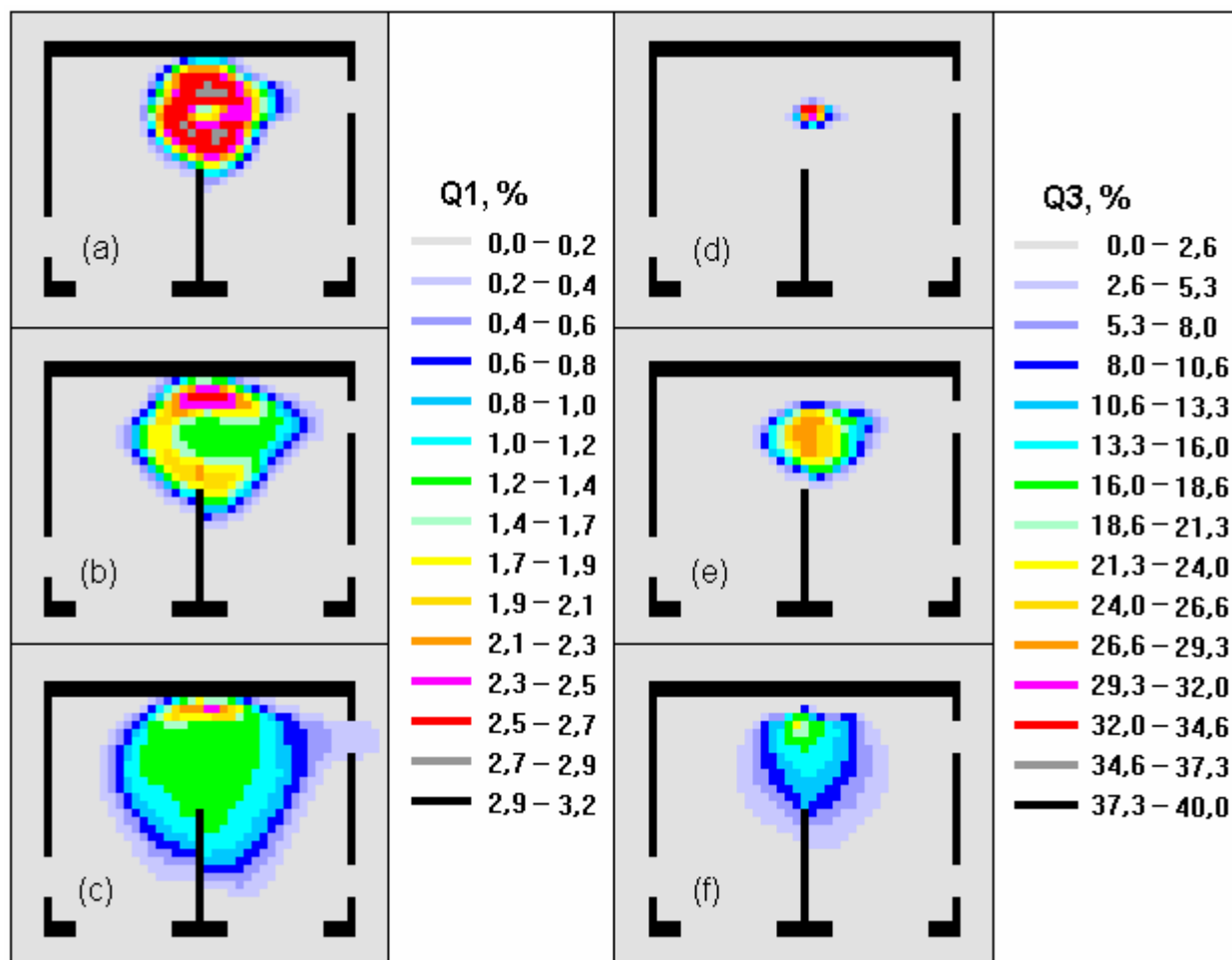


Figure 7. Mass concentration of hydrogen (a-c) and combustion products (d-f) distribution in 0.15, 0.25, 0.35 s from the moment of inflammation (scenario 1)

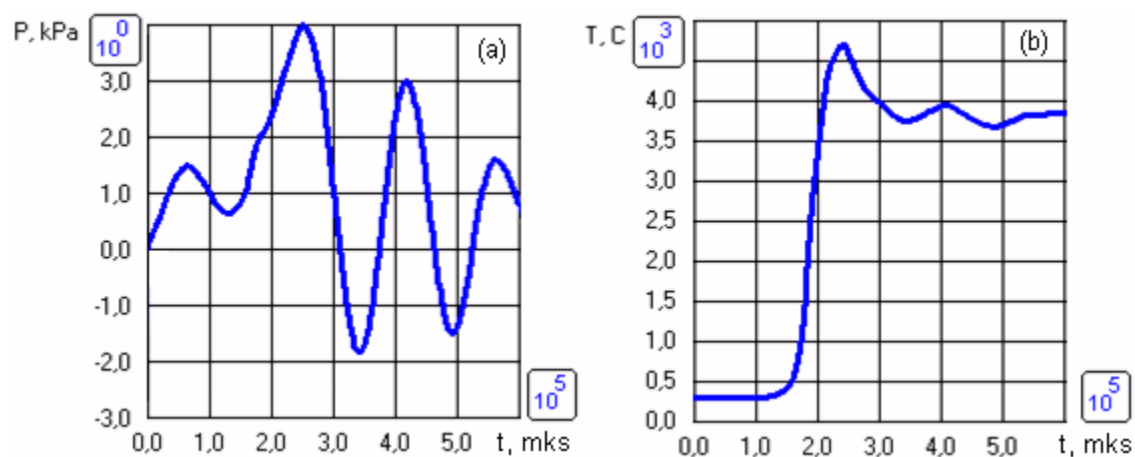


Figure 8. Overpressure (a) and temperature (b) history (point B, scenario 1)

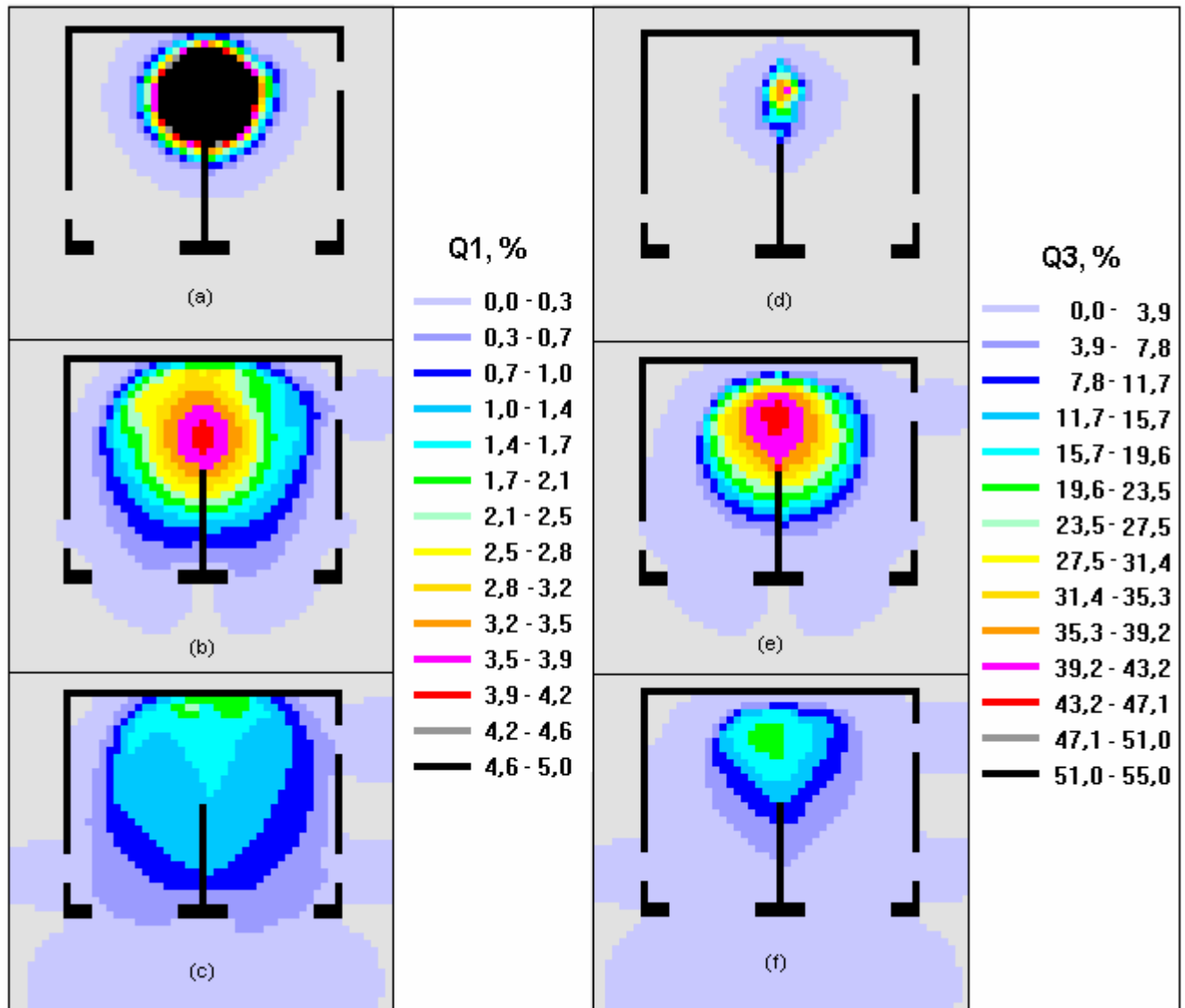


Figure 9. Mass concentration of hydrogen (a-c) and combustion products (d-f) distribution in 0.10, 0.15, 0.20 s from the moment of inflammation (scenario 2)

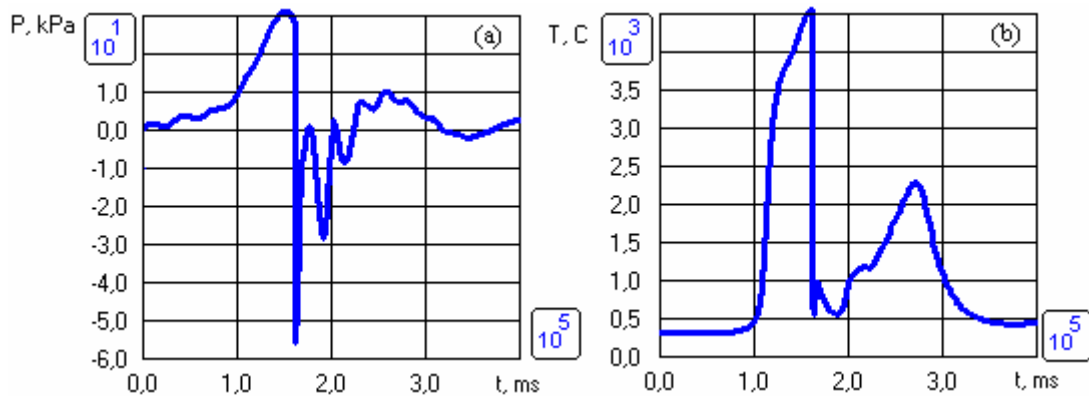


Figure 10. Overpressure (a) and temperature (b) history (point B, scenario 2)

The results of hydrogen deflagration simulation with different initial parameters of the released hydrogen-air cloud in the enclosed production area are considered. Specific features of hydrogen dispersion and combustion in the air during deflagration development are exposed. They are conditioned by hydrogen's low density, high diffusion constant, high rate of chemical reaction with an oxygen, wide range between concentration inflammability limits and high speed of the flame propagation. The computation results expose that the scale of the deflagration depends on the hydrogen concentration of the released mixture. Therefore, all the suggested safety measures that result in minimizing of the hydrogen concentration could prevent or reduce pressure and thermal consequences caused by the hydrogen deflagration in the confined space.

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