NUMERICAL MODELING OF HYDROGEN RELEASE, MIXTURE AND DISPERSION IN ATMOSPHERE

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ABSTRACT

The method of the numerical solution of a three-dimensional problem of atmospheric release, dispersion and explosion of gaseous admixtures is presented. It can be equally applied for gases of different densities, including hydrogen. The system of simplified Navier-Stocks equations received by truncation of viscous members (Euler equations with source members) is used to obtain a numerical solution. The algorithm is based on explicit finite-difference Godunov scheme of arbitrary parameters breakup disintegration. To verify the developed model and computer system comparisons of numerical calculations with the published experimental data on dispersion of methane and hydrocarbons explosions have been carried out. Computational experiments on evaporation and dispersion of spilled liquid hydrogen and released gaseous hydrogen at different wind speeds have been conducted. The largest mass concentrations of hydrogen between bottom and top limits of flame propagation and cloud borders have been determined. The problem of explosion of hydrogen-air cloud of the complex form generated by large-scale spillage of liquid hydrogen and instant release of gaseous hydrogen has been numerically solved at low wind speed. Shock-wave loadings affecting the buildings located on distance of 52 m from a hydrogen release place have been shown.

INTRODUCTION

Hydrogen is widely applied in the different industries. Particular danger of its application is conditioned by the large energy of combustion, fast transition from burning to detonation and, as a consequence, powerful explosion of the cloud in the atmosphere after release. Hydrogen differs essentially from other explosive compressed gases and liquids, firstly, by very small density, and, secondly, by very low liquid stage temperature. The quantity of hydrogen participating in explosion is defined by conditions of its evaporation (in case of release and spillage in liquefied form), dispersion and mixing with air. These processes will be influenced by specified above properties of liquefied and compressed hydrogen.

Atmospheric dispersion of gaseous admixtures is usually modeled under the assumption of Gaussian distribution of the admixture concentration and on the basis of corresponding analytical functional dependences. But for neutral, heavy and light gases only the partial solutions are obtained. In presented work an attempt to solve numerically a three-dimensional problem of the admixture dispersion in the atmosphere and explosion equally applied for different density gases (including hydrogen) have been made.

1.0. MATHEMATICAL MODEL

1.1. Basic equations

An adequate description of physical processes of nonreactive gas mixture with air and further admixture dissipation in the atmosphere (or enclosed ventilated premise) is possible only with the use of time-dependent Navier-Stocks equations for compressible gas. The limited resources of modern computers do not allow obtaining effectively the direct numerical solution of these equations. As a rule, numerical modeling of large space turbulent flows is carried out by solving of Reynolds-averaged Navier-Stocks equations added by turbulence model [1, 2]. However the majority of turbulence models do not describe with an identical degree of adequacy all various types of flows. It especially relates to flows with intensive stream separation and large-scale gradients of pressure and temperature.

As a result of the flow structural analysis and decomposition of the full gas-dynamic mathematical model it is assumed that the convective mass exchange mainly influences on the process considered. Thus, for the description of processes of two-component gas mixture and dissipation it is enough to use the simplified Navier-Stocks equations received by the truncation of viscous members (Euler's approach with source members).

The calculated space Ω is a parallelepiped located in the right-hand Cartesian system of coordinates (X, Y, Z) with the basis in plane XOZ (axis Y is directed opposite to the Earth's gravity). The calculated space is broken into spatial cells. The full system of the time-dependent equations describing three-dimensional two-component gas mixture flow looks like [3, 4]:

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

where $\bar{a},\bar{b},\bar{c},\bar{d},\bar{f}$ – vector-columns of a kind:

$$\vec{a}=\left[r,\, ru,\, rv,\, rw, E\right]^T, \qquad (2)$$

$$\vec{b}=\left[ru, P+ru^2,\, ruv,\, ruw,(E+P)u\right]^T, \qquad (3)$$

$$\vec{c}=\left[rv,\, ruv, P+rv^2,\, rvw,(E+P)v\right]^T, \qquad (4)$$

$$\vec{d}=\left[rw,\, ruw,\, rvw, P+rw^2,(E+P)w\right]^T, \qquad (5)$$

$$\vec{f}=\left[0,0,-g,0,-gv+e_S\,/\,r\right]^T; \qquad (6)$$

t – time; u,v,w – components of speed vector $\vec{q}$; P,r – pressure and density; E – full energy of volume unit of gas mixture:

$$E=r(e+\frac{1}{2}(u^2+v^2+w^2)); \qquad (7)$$

e – internal energy of gas mass unit; components of the vector $\vec{f}$ – projections of the distributed volumetric sources; g – gravitational acceleration; e_S – intensity of a thermal emission in gas volume unit as a result of chemical reaction.

The law of admixture component transfer, taking into account a diffusion speed, looks like [5]:

$$\frac{\partial(\,rQ\,)}{\partial t}+\frac{\partial(\,ruQ\,)}{\partial x}+\frac{\partial(\,rvQ\,)}{\partial y}+\frac{\partial(\,rwQ\,)}{\partial z}=r_{Qt}+r_{Qs}\,, \qquad (8)$$

where Q – relative mass density of an admixture (the ratio of gaseous admixture substance density to the mixture density); r_{Qt} – an admixture density change rate as a result of diffusion (according to Fick law, $r_{Qt}=div(\,r\,J_D gradQ\,)$, and the factor of diffusion J_D is defined according to Berljand [6]); r_{Qs} – an admixture density change rate as a result of chemical reaction.

The system of the equations (1, 8) is completed by the mixture component heat-transfer properties equations [7]. For ideal gas the value of e is related to the values of P and r of the mixture by the following dependence $e = \frac{P}{(k-1)r}$.

1.3. Boundary conditions

It is assumed that the air flow quantity component of velocity does not surpass sound speed. Entry boundary conditions are set on the finite-difference cells surfaces through which atmospheric air enters. The approaching flow is defined by values of total enthalpy

$$I_0 = \frac{k}{k-1}\frac{P}{r} + \frac{1}{2}(u^2 + v^2 + w^2), \tag{9}$$

entropy function

$$S_0 = \frac{P}{r^k}, \tag{10}$$

flow velocity vector (angles a_x, a_z), and relative admixture mass density Q ($Q \le 1$ if the gaseous admixture flows in). The entry flow parameters are defined by equations (3, 4) (if angles a_x, a_z are set) using "left" Riemannian invariant correlation [4, 7]. On impermeable computational cells' surfaces the "no passing" conditions are satisfied: q_n = 0 where $\bar{n}$ is a vector of normal to considered surface. Exit boundary conditions are set on the computational cells surfaces through which the mixture flows out (except for the atmospheric pressure P_A, the "right" Riemannian invariant correlation [4, 7] is used).

1.4. Initial conditions

At start time in all "gaseous" cells of the computational space the parameters of an ambient air are assigned. In cells, where the admixture cloud takes place, relative mass concentration of an admixture equals 1 (100%). In cells with hydrogen evaporation (or outflow) the law of admixture consumption variation is set.

1.5. Algorithm of the numerical solution

The vector equation (1) is a consequence of the mass, impulse and energy conservation laws which can be presented in the integrated form for each calculated cell

$$\frac{\partial}{\partial t}\iiint_V \bar{a}\,dV + \oint\!\!\oint_\sigma \hat{A}\,d\sigma = \iiint_V r\,\bar{f}\,dV, \tag{11}$$

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

The mixture component transfer law (8) can be presented also in the integrated form for each computational cell:

$$\frac{\partial}{\partial t}\iiint_V rQ\,dV + \oint\!\!\oint_\sigma rQ\bar{q}\,d\bar{\sigma} = \iiint_V (r_{Qt} + r_{Qs})\,dV. \tag{12}$$

The equations (11, 12) suppose occurrence and existence of parameters break surfaces of two types: shock waves and tangential breaks. The functions, satisfying to the equations (11, 12), can be considered as the gas dynamics equations generalized solutions. The use of integrated conservation laws as initial for construction of finite-difference equations provides the formation of breakup solutions without isolation of breaks.

The set of gas-dynamic parameters in all computational cells at the moment of time t^n represents the known solution. Gas-dynamic parameters at the moment of time $t^{n+1} = t^n + t$ are calculated by means of explicit finite-difference approximations for equations (5) according to Godunov method [7]. At first stage continuous distribution of parameters is replaced with piecewise constant integral-averaged values in each computational cell. At the same time the borders of a cell represent unstable surfaces of arbitrary breakup which disintegrate to steady wave elements: a shock wave, a contact surface and a wave of rarefaction. For each such breakup the streams of mass, impulse and energy through sides of gas cells are defined. The stability of the finite-difference scheme is provided due to a choice of time step size.

On the basis of mathematical model the computer system of the engineering analysis of the gas-dynamic processes of release, mixture and dispersion was developed which is used in the research computer complex “Rizex”. It allows predicting an admixture concentration change in time and space in the calculated area and computing shock-wave parameters formed after detonation in the atmosphere during fuel-air mixture dispersion process with the use of personal computers for practically reasonable time.

2.0. VERIFICATION OF MATHEMATICAL MODEL

Since we did not possess hydrogen experimental data, we have used propane and methane experimental data to verify mathematical model and developed computer system.

2.1. Propane evaporation from a water surface

In order to verify the developed model for gaseous admixture dispersion in the atmosphere the comparison of the computation results with experimental data [8] was conducted (Fig. 1).

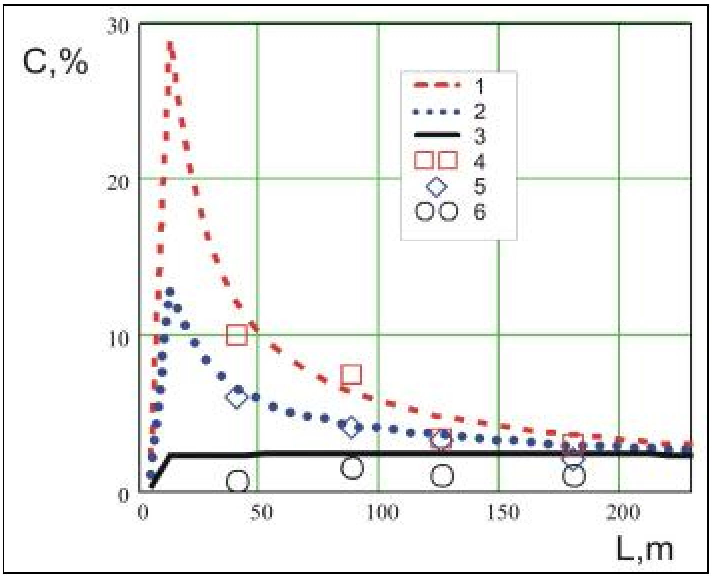

Figure 1. The maximal propane concentrations: 1, 2 and 3 – computations, 4, 5 and 6 – experimental data at heights 0.8, 1.4 and 2.3 m, accordingly

The evaporation process of liquid propane from a spillage pond occupying the area of 256 m^2 was modeled at ambient air parameters: pressure 101325 Pa, temperature 291 K, wind speed 8.1 m/s. The propane evaporated with the consumption of 27.6 kg/sec and had the temperature 230 K in a gaseous stage. The calculated propane concentration distributions at heights 0.8, 1.4 and 2.3 m at the moment of time 450 sec from the evaporation start time in comparison with experimental gauging [8] are well enough conformed to experimental data.

2.2. Gas cloud explosions in the atmosphere

For verification of calculation model of atmospheric gas cloud explosions a comparison with experimental data [9] was conducted (Fig. 2).

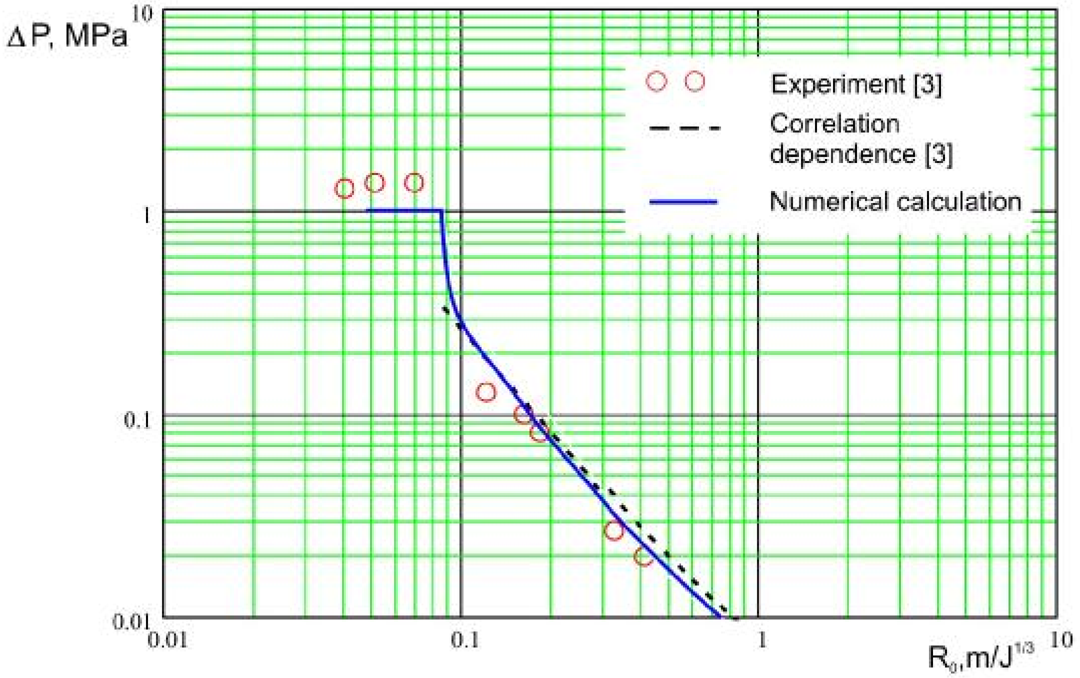

Figure 2. Explosion waves parameters in comparison with experimental data.

An explosion of a stoichiometrical propane-air mix cloud was calculated at conditions of experiment: volume of the gas mixture cloud - 1495 m^3; energy of explosion - 4940 MJ. On the basis of these data initial conditions for calculation, pressure and temperature of combustion products in the cloud, have been defined:

$$P=\frac{E(k-1)}{V}+P_A=\frac{4940*10^6(1.29-1)}{1495}+101325=1{,}06\,MPa\,, \tag{13}$$

$$T=\frac{Pm_{mix}}{r_{mix}R}=\frac{1{,}06\cdot 10^6\cdot 0.029}{1.29\cdot 8.31}=2868\,K\,, \tag{14}$$

where V - volume of the gas mixture cloud; E - energy of explosion; k - adiabatic coefficient; P_A - atmospheric pressure; m_{mix} - molar mass of the mixture; r_{mix} - mixture density; R - universal gas constant.

In work [9] on the basis of experiments of explosion of clouds of acetylene, propane and methane with air and propane and methane with oxygen the correlation dependence was received that allows to define the overpressure ΔP_f in the shock wave front from distance from an epicenter for the assigned energy of explosion:

$$\Delta P_f = \frac{0.6\cdot 10^{-1}}{R_0} + \frac{1.4\cdot 10^{-2}}{R_0^2} + \frac{2.5\cdot 10^{-3}}{R_0^3} \text{ if } R_0 \geq 0.3, \tag{15}$$

$$\Delta P_f = \frac{0.052}{R_0^{1.7}} \text{ if } 0.08 \leq R_0 < 0.3, \tag{16}$$

where $R_0 = \frac{R}{E^{1/3}}$ - dynamic radius; R - distance from an epicenter of explosion; E - energy of explosion.

In Fig. 2 the results of numerical calculations are presented which well enough coincide with experimental data and with correlation dependence [9].

3.0. NUMERICAL COMPUTATIONS OF HYDROGEN RELEASES

3.1. Release conditions

Processes of gaseous hydrogen release (spilled liquid hydrogen evaporation), hydrogen-air mixture formation, explosion and further dispersion of hydrogen-air cloud in the atmosphere (taking into account the movement of the air, gravity, presence of buildings, and thermodynamic gas properties) are considered.

Some possible scenarios at hydrogen dispensing station are modeled [10]. The station has the large cryogenic hydrogen tank (5.7 m^3) that feeds three 12-cylinder packages in total amount 799.2 m^3 in which gaseous hydrogen is stored at ambient temperature. The hydrogen under pressure is dispensed to vehicles' tanks. The station is separated from residential area by three zones:

- The region in the immediate vicinity of the equipment to protect the personnel from small leaks;

- An exclusion zone in the immediate area of the facility (23 m) to provide protection against unplanned minor releases of hydrogen;

- An additional margin, as large as 53 m is necessary to protect against large potentially catastrophic release of hydrogen.

The most dangerous scenarios from the potential catastrophe point of view have been numerically simulated using the created mathematical model and developed computer system:

1) spillage from the tank of all volume of liquid hydrogen, consecutive evaporation of cold liquid, mixture of gaseous hydrogen with moving air and the further dispersion of a mix towards residential area;

2) release of all volume of the gaseous hydrogen compressed under a high pressure from cylinders of distribution with formation of a cloud and its further dispersion in a stream of air;

3) explosion of a hydrogen-air cloud that is formed as a result of evaporation of spilled liquid hydrogen or instant gaseous hydrogen release.

3.2. Spillage of liquid hydrogen

According to the scenario 1, numerical computations of an instant spillage of all volume of liquid hydrogen from the cryogenic tank of dispensing station with formation of a spillage pond with total area of 65.7 m^2 were conducted. Liquid hydrogen evaporation productivity was evaluated of 11.56 kg/sec [10]. The wind blew with speeds of 1, 3 and 10 m/sec, and its direction was towards residential area.

Hydrogen mass concentration distributions near the surface of the ground are presented on Fig. 3. With an increase in wind speed the rate of dispersion increased too (Fig. 4). According to comparison of hydrogen time-space concentration distributions at different wind conditions in the case of spilled liquid hydrogen its buoyancy is insignificant because of low vapor temperature and, as a consequence, small difference between densities of hydrogen and air.

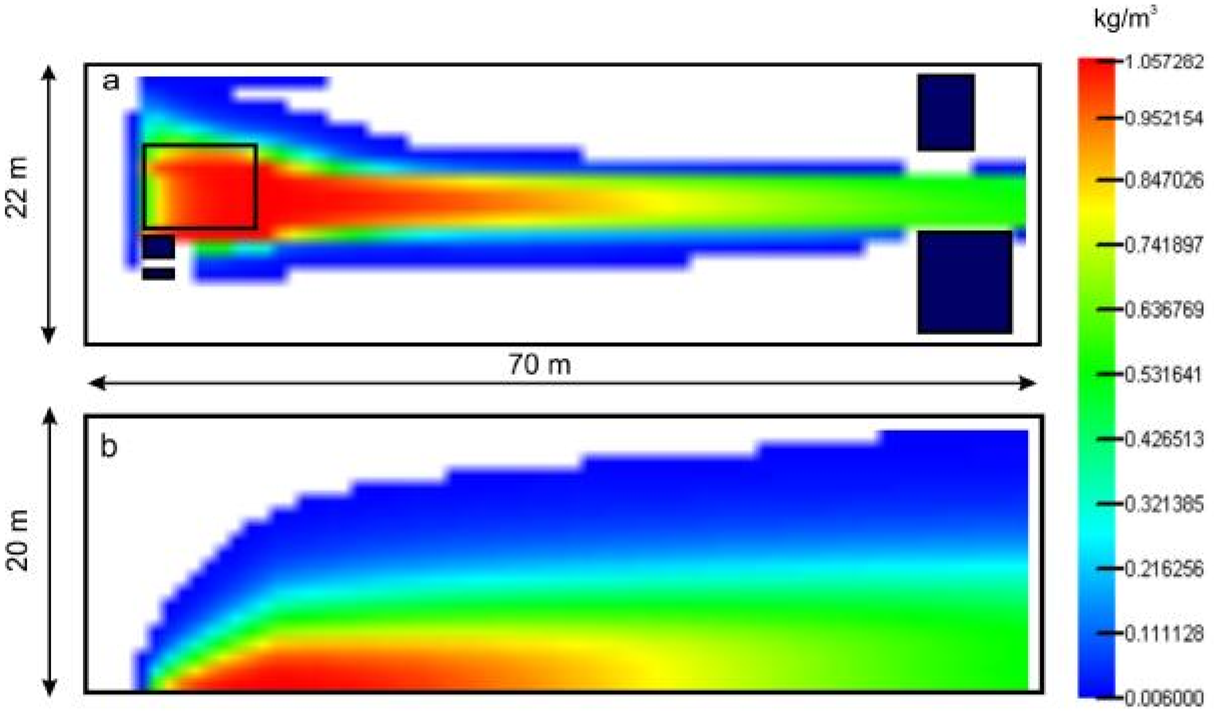

Figure 3. Numerical computations of spilled liquid hydrogen dispersion.
Wind speed equals 1 m/sec: a – top view; b – side view

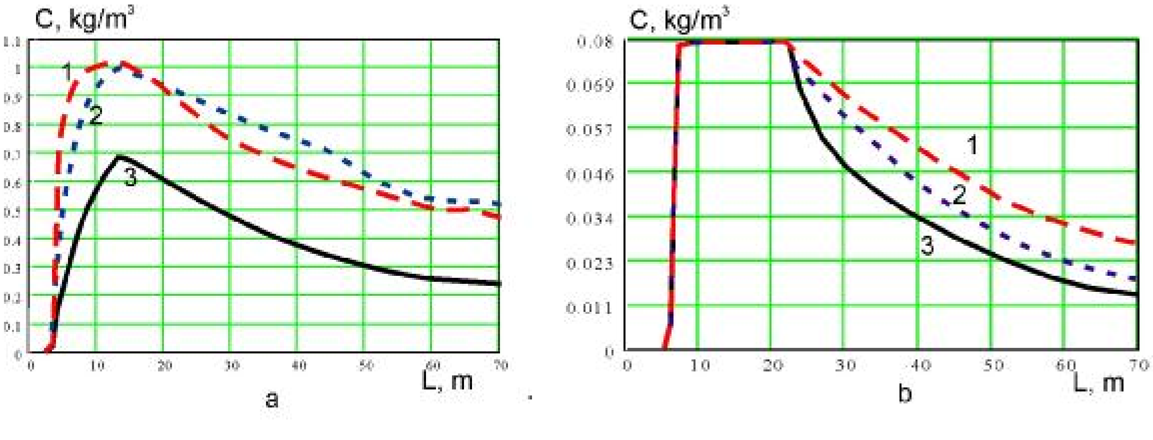

Figure 4. The maximal concentration of hydrogen in the mixture depending on distance from a spillage place: a – spillage; b – instant release. Speed of a wind: 1 - 1 m/sec; 2 - 3 m/sec; 3 - 10 m/sec

3.3. Dispersion of gaseous hydrogen cloud

An instant release of all gaseous hydrogen from a package of dispensing cylinders with the formation of a cloud in volume 799.2 m^3 have been numerically simulated according to the scenario 2. According to results of numerical experiments, buoyancy of hydrogen is essential only at low wind speeds (Fig. 5). With an increase of speed the wind prevents an emersion of the cloud pressing it to the ground.

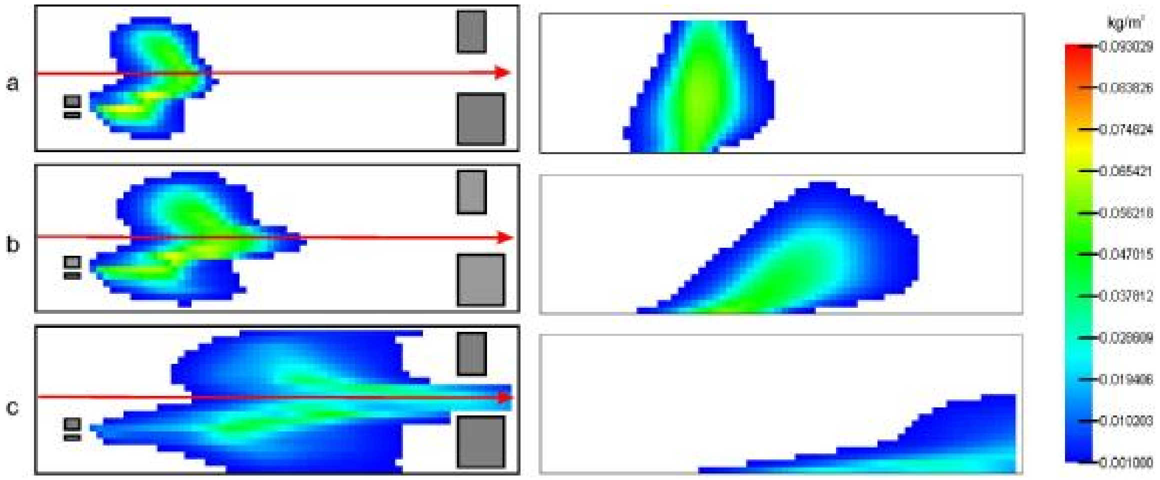

Figure 5. Hydrogen concentration distribution in the cloud in 5 seconds after release.
Wind speed: a - 1 m/sec; b - 3 m/sec; c - 10 m/sec

Obviously, if wind speed is greater then hydrogen’s buoyancy, hydrogen behaves as a neutral gas. Both in the case of spilled hydrogen dispersion and dispersion of instantly released gaseous hydrogen, the presence of construction facilities and residential buildings essentially affect flow symmetry decreasing transfer and mixing processes in the space before the buildings and accelerating these processes between constructions.

3.4. Explosion of hydrogen-air cloud

In computations on dispersion the dependence of hydrogen mass in the cloud between top and bottom limits of flame propagation was determined (Fig. 6). The largest mass of hydrogen and, consequently, maximal explosion energy will be under low wind speed conditions. But, as evident from Fig. 5, an explosive cloud with less hydrogen mass and larger energy of explosion can be located closer to residential constructions.

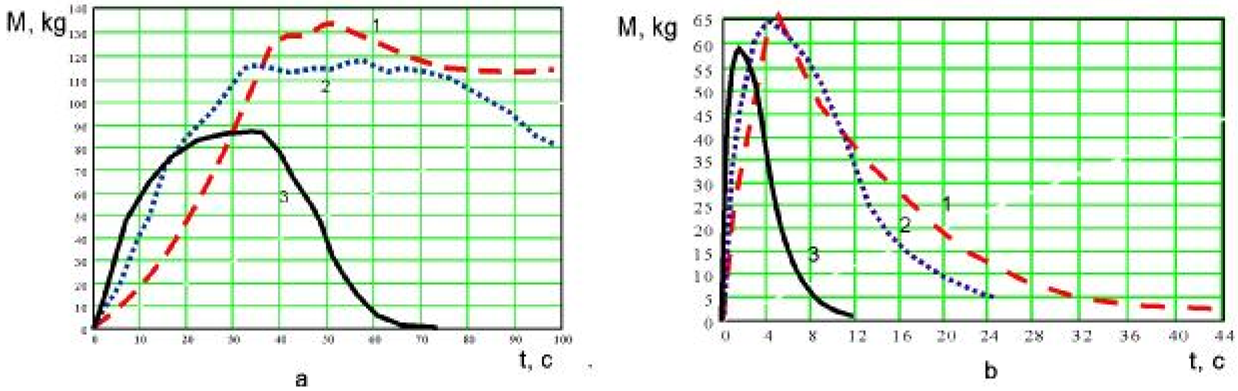

Figure 6. Hydrogen mass history in explosive cloud between bottom and top limits of flame propagation: a – after spillage; b – after instant release of gas. Wind conditions: 1 – 1 m/sec; 2 – 3 m/sec; 3 – 10 m/sec

In case of instant release of compressed gaseous hydrogen, the cloud is compact enough (Fig. 5) and it can be considered as spherical cloud. But, in case of presence of constant source of assigned productivity (hydrogen spillage evaporation), an explosive mixture occupies the space of complex form (Fig. 7).

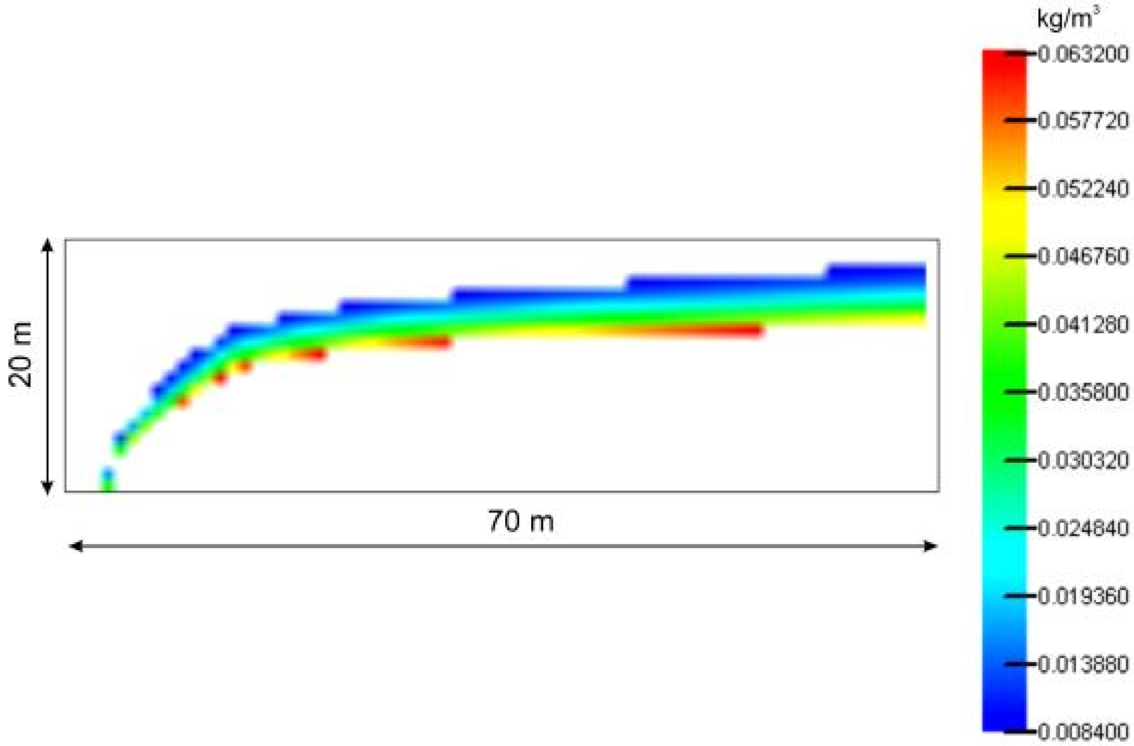

Figure 7. Concentration distribution in the explosive cloud with maximal hydrogen mass formed after spillage. Wind speed – 1 m/sec.

The numerical results of blast wave parameters at detonation of the cloud generated after an instant gaseous hydrogen release are presented in Fig. 8. The mass of hydrogen in the cloud equals 63 kg.

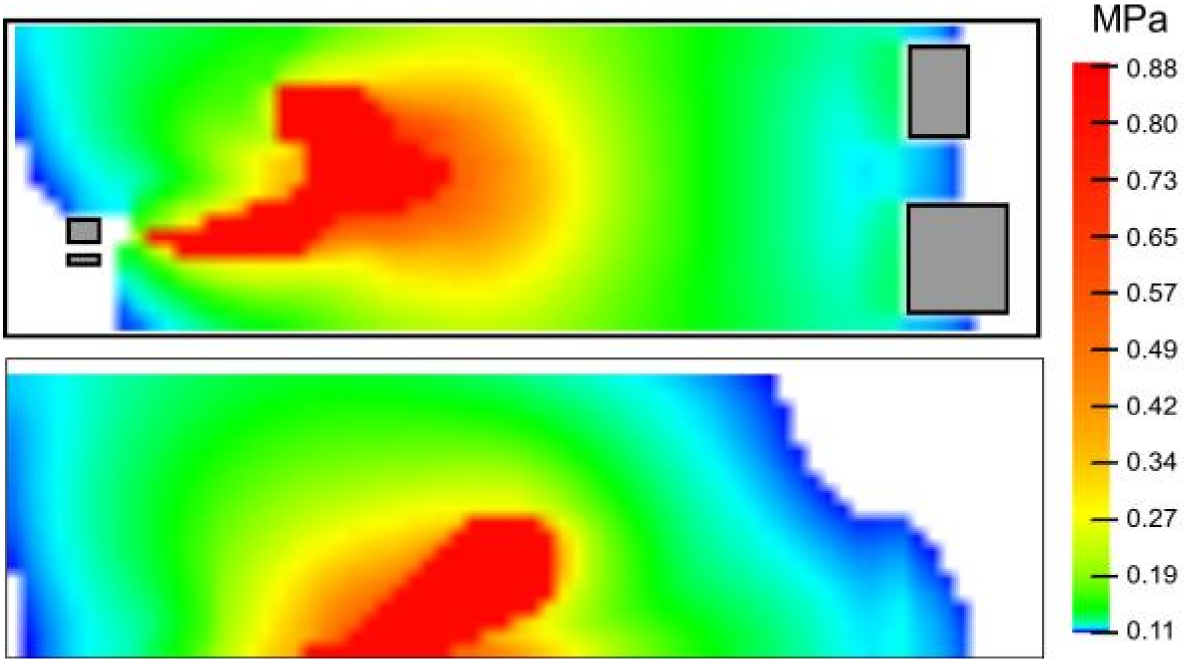

Figure 8. Pressure distributions at conditions of hydrogen explosion in the cloud with maximal hydrogen mass formed after spillage of 63 kg of hydrogen. Wind speed – 3 m/sec

An increase of pressure takes place between residential constructions, as it would be expected. Overpressure affecting the walls of buildings (on the right side of the Fig. 8) is about 28 kPa that allows suggesting the possibility of serious destructions of residential constructions and industrial facilities threatening personnel and inhabitants.

CONCLUSIONS

The three-dimensional model of the release and explosion of gaseous admixtures in the atmosphere has been developed. The verification of the numerical results shows acceptable accuracy in comparison with known experimental data.

Numerical computations for dispersion of spilled liquid and instantly released gaseous hydrogen and for explosion of the hydrogen-air cloud generated during dispersion have been carried out.

Obtained results can be usually predicted at qualitative level but presented numerical computations have allowed making quantitative forecasting with noncontradictory physical picture.

Numerical modeling of the harmful admixture dispersion in the atmosphere generated as a result of air-fuel mixture distribution in three-dimensional space with the use of the program complex “Rizex” is applicable to engineering calculations for different technological systems, including ones which work on liquefied and gaseous hydrogen.

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