

# NUMERICAL EVALUATION OF TERRAIN LANDSCAPE INFLUENCE ON HYDROGEN EXPLOSION CONSEQUENCES

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## ABSTRACT

The aim of this study is to assess numerically the influence of terrain landscape on the distribution of probable harmful consequences to personnel of hydrogen fueling station caused by an accidentally released and exploded hydrogen. In order to extract damaging factors of the hydrogen explosion wave (maximum overpressure and impulse of pressure phase), a three-dimensional mathematical model of gas mixture dynamics with chemical interaction is used. It allows controlling current pressure in every local point of actual space taking into account complex terrain. This information is used locally in every computational cell to evaluate the conditional probability of such consequences on human beings as ear-drum rupture and lethal ones on the basis of probit analysis. In order to use this technique automatically during the computational process, the tabular dependence "probit-function-impact probability" is replaced by a piecewise cubic spline. To evaluate the influence of the landscape profile on the non-stationary three-dimensional overpressure distribution above the earth surface near an epicenter of accidental hydrogen explosion a series of computational experiments with different variants of the terrain is carried out. Each variant differs in the level of mutual arrangement of the explosion epicenter and the places of possible location of personnel. Two control points with different distances from the explosion epicenter are considered. Diagrams of lethal and ear-drum rupture conditional probabilities are built to compare different variants of landscape profile. It is found that the increase or decrease in the level of the location of the control points relative to the level of the epicenter of the explosion significantly changes the scale of the consequences in the actual zone around the working places and should be taken into account by the risk managing experts at the stage of deciding on the level of safety at hydrogen fueling stations.

## INTRODUCTION

It is well-known that hydrogen is one of the most explosive gases [1]. Therefore, increasing the use of hydrogen in the industry creates high risks of accidents, which lead to severe social and economic consequences [2]. Even not significant violations of safety precautions or accidental equipment failures can cause hydrogen release into the atmosphere, mixing processes with air, and explosion which generates pressure waves propagated away from accident epicenter (Fig. 1) [3, 4].

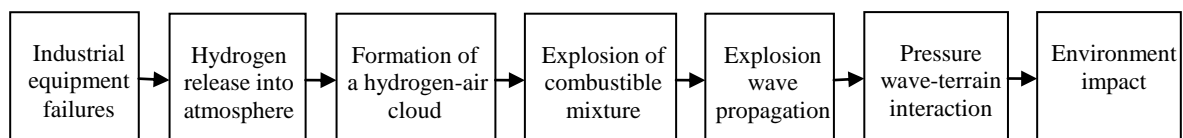


Figure 1. The development of technogenic accident

Explosion waves make a shock-impulse impact on the environment, threatening the life and health of industrial workers, destroying infrastructure, and damaging equipment placed at industrial sites. As a result of such accidents, social, material, and financial losses can be of catastrophic proportions.

In order to ensure the safety of working conditions on industrial sites, it is necessary to develop and apply protective equipment that can prevent or reduce to an acceptable level the possible harmful consequences caused by hydrogen-air explosions [3]. The effectiveness of protection methods can be tested experimentally [5]. However, a full-scale physical experiment with hydrogen explosion is difficult to implement, cumbersome, and too expensive. That is why a computational experiment based on computer information systems [6] implementing the considered accident scenarios (Fig. 2) is widely used in practice. Thus, an engineering problem of mathematical modeling of physical processes of the considered emergency scenario is relevant.

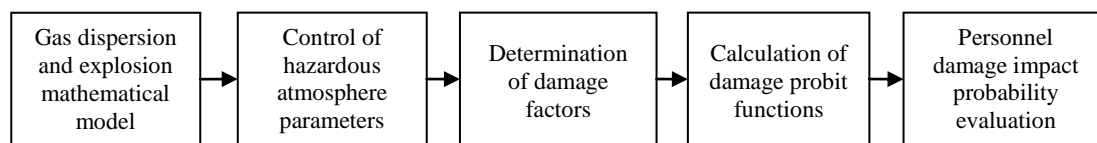


Figure 2. Accident consequences probabilistic evaluation scheme

A mathematical model of the explosion of a hydrogen-air mixture cloud at a hydrogen fueling station site is considered in this paper. An influence of the terrain shape near the accidental hydrogen explosion on the formation of a shock-impulse load in an open space and the resulting fields of the conditional probability of damage to working personnel are analyzed. A state of the gas-dynamic environment at the site before an accident can be described as a set of normal values of overpressure, temperature, velocity vector, the chemical composition of the atmosphere. During an accidental explosion, these parameters become locally temporarily disturbed, and excess values of hazardous parameters form damaging factors that have harmful effects on the human body. Some time after the accident, the environment returns to an unperturbed steady state again.

The purpose of this work is to use an effective mathematical model of the considered hydrogen explosion processes, for three-dimensional analysis and prediction of non-stationary fields of a damaging factor, a shock-impulse load, in order to determine the fields of the conditional probability of human damage based on probit analysis methodology.

An adequate description of the physical processes of dispersion of chemically reacting gases, mixing them with air, and further spreading the mixture into the open space [6], tunnel [7], or closed ventilated space [8] is possible only using the Navier-Stokes system of non-stationary equations for compressible gas [9]. Currently, numerical simulation of turbulent flows is carried out by solving the Reynolds-Favre-averaged Navier-Stokes equations, supplemented by a model of turbulence [10]. However, most turbulence models do not describe with an equal degree of adequacy the various types of flows that can appear [11]. This is especially true for currents with intense flow breaks and/or large pressure and temperature gradients.

In work [12] it is indicated that modern engineering methods for predicting the consequences of accidents on chemically hazardous objects (such as [13], [14]) implement the Gauss model or the analytical solution of the mass transfer equation and do not take into account the blockage of the calculated space by impenetrable objects. The use of numerical kinematic models [15] to assess territorial risk is also limited to cases of impurity dispersion over a flat surface. Some papers take into account the complex terrain in the process of solving the mass transfer equation by the finite-difference method [12, 14], but either there is no consideration for the three-dimensional nature of the flow around obstacles [12] or the effect of compressibility of the flow is not taken into account, which does not allow to use these mathematical models to calculate effects of all damaging factors (explosion shock wave load, thermal radiation, toxic dose), which may be present simultaneously during accidents.

In addition, modern techniques for assessing the technogenic impact on the environment are mainly based on a deterministic approach [16], and during probabilistic consequences assessment based on probit analysis, the table-view dependence of probability on the probit function is used for expert analysis [17]. It is not possible to apply this approach automatically in a computer system to obtain non-stationary fields of damaging factors and probability of damage and it requires an improvement in computational methods and techniques.

Therefore, there is a need to build effective mathematical models and computational schemes for numerical modeling of three-dimensional flows of multicomponent gas mixtures, taking into account the complicated terrain shape in actual calculation space, compressibility, and chemical interaction effects, which allow determining the full set of hazardous flow parameters for various scenarios of man-made accidents, calculate the damaging factors (including the shock-impulse load) and build space-time fields of human damage conditional probability needed to assess individual risk.

## 1.0 METHOD OF ASSESSING THE IMPACT CAUSED BY AN EXPLOSION WAVE

It is necessary to determine the peculiarities of the influence of terrain shape near an explosion accident on the spatial and temporal distribution of the shock-impulse load and the probability of personnel harmful damage during an explosion of a hydrogen-air cloud at fueling station site with a two-level landscape based on a mathematical model of the considered physical processes [18].

An accidental release of hydrogen at an industrial site is usually accompanied by the formation of a hydrogen-air mixture, which can explode under the influence of external factors. The resulting explosion wave spreads through the site, causing a shock-impulse load on the fueling station workers and leading to harmful consequences for their healths and lives (Fig. 1).

The harmful damaging impact of the shock wave according to a probabilistic assessment approach is determined by the maximum overpressure  $\Delta P_+$  (relative to atmospheric pressure  $P_0$ ) of the wavefront and compression phase impulse  $I_+$  (Fig. 3).

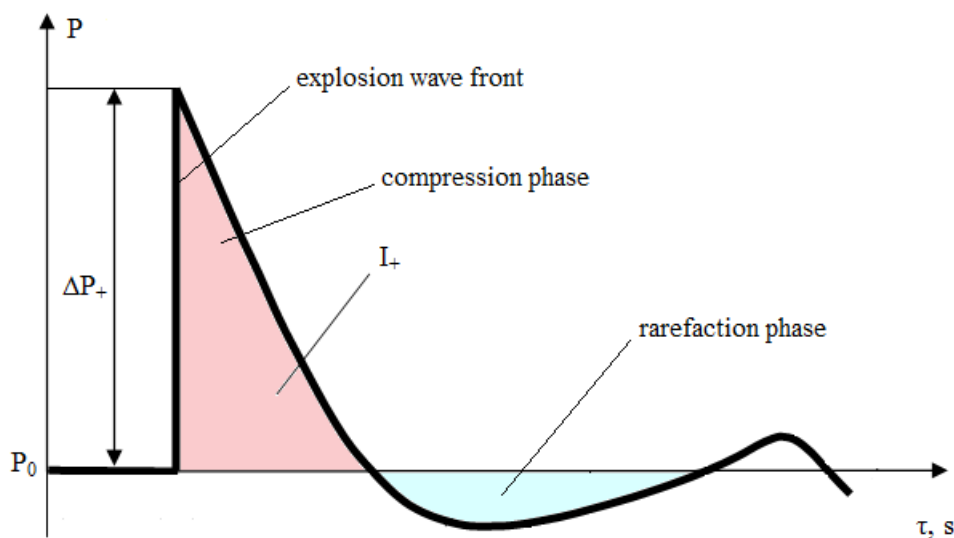


Figure 3. The typical profile of an explosion wave

The values of these indicators in each control point can be used to determine the individual risk of personnel's negative impact. The risk assessment of the harmful effects of damaging factors on the human body in the accident site is one of the main stages of the safety analysis process of an industrial object. It allows to draw conclusions about the acceptability of risk and evaluate the effectiveness of protective facilities. The probability of a specific scenario for the development of an accident  $P_s$  depends on the statistical probability of the occurrence of such an accident  $P_a$  and the conditional damage probability of an affected person  $P_c$ , which can be obtained using mathematical modeling.

The conditional probability  $P$  of harmful impact on a person that is under the influence of an explosion shock wave depends on the probit-function  $Pr$  – the upper limit of a definite integral of the normal distribution law with mathematical expectation 5 and variance 1

$$P = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{Pr} e^{-\frac{1}{2}(t-5)^2} dt, \quad (1)$$

where  $t$  is an integral degree of impact.

For instance, the probability of human lethal damage caused by overpressure can be estimated by the following ratio [19]

$$Pr_1 = 5 - 0,26 \ln \left[ (17500 / \Delta P_+)^{8,4} + (290 / I_+)^{9,3} \right]. \quad (2)$$

The probit-function for rupturing human eardrums depends on the level of overpressure only and can be found by the formula [20]

$$Pr_2 = -15,6 + 1,93 \ln \Delta P_+. \quad (3)$$

In order to automate the computational process of analysis and prediction, the table of discrete values of the “probit-function-probability”, that is usually in engineering practice, this dependence is replaced by a generalized piecewise cubic Hermitian spline [21]. The characteristics of such a spline allow you to avoid possible oscillations of the approximated function in the intervals.

## 2.0 EXPLOSION MATHEMATICAL MODEL AND CALCULATION ALGORITHM

For series of comparative computational experiments, in order to evaluate the influence of the two-level terrain shape on the distribution of the wave overpressure at the possible location of the working place, we use a mathematical model of an instantaneous explosion of hydrogen-air mixture [11-13]. It is assumed that the main factor influencing the physical processes under consideration is the convective transfer of mass, momentum, and energy. Therefore it is sufficient to use the simplified Navier-Stokes equations which are obtained by dropping the viscous terms in the mixture motion equations (Euler approach with source terms) [12].

The computational domain is a parallelepiped located in the right Cartesian coordinate system (Fig. 4). It is divided into spatial cells whose dimensions are determined by the scale of the characteristic features of the area (roughness of streamlined surface, dimensions of objects).

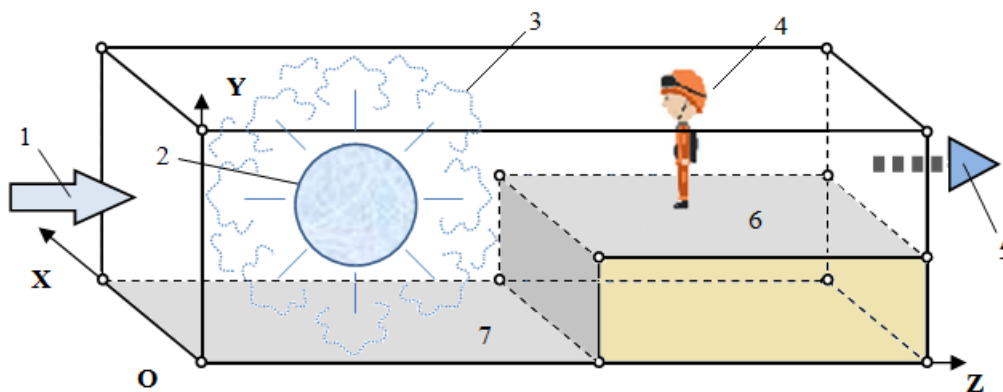


Figure 4. A computer model of the hydrogen-air cloud explosion:  
 1 – inlet air; 2 – hydrogen cloud; 3 – combustion products; 4 – personnel;  
 5 – output mixture; 6 – working place terrain level; 7 – explosion terrain level

According to the explosion model, it is assumed that the global instantaneous chemical reaction takes place in all elementary volumes of the computational grid where the hydrogen concentration is within the limits of ignition ( $Q_{\min} \leq Q \leq Q_{\max}$ ). This means that the parameters of the two-component mixture (air and fuel) in the control volume immediately get the new values of the parameters of the three-component mixture (air, combustion products, and residues of fuel). In other words, it is assumed that the flame front propagates with infinite velocity [16].

Computer solution of the fundamental equations of gas dynamics for a mixture supplemented by the mass conservation laws of admixtures in the integral form is obtained using the explicit Godunov's method [22]. To approximate the Euler equations the first-order finite-difference scheme is used. Central differences of second order are used for the diffusion source terms in the conservation equations of admixtures. Simple interpolation of the pressure is applied in the vertical direction. Godunov's method is characterized by a robust algorithm that is resistant to large disturbances of the flow parameters (e.g. pressure) which allows obtaining a solution for modeling large-scale explosions of gas mixtures.

A mathematical model was validated with respect to Fraunhofer ICT experimental data for hydrogen explosions and the explosion of propane [23].

To analyze the formation of hydrogen cloud, its explosion and dispersion of the combustion products in the atmosphere, as well as to forecast the pressure changes at the control points of the computational domain and to evaluate the differences between the various two-level terrain shape options of the actual calculated space a computer system «Explosion Safety»<sup>®</sup> [24] is used. The software allows calculating the density, velocity, pressure, temperature of the mixture, concentration of the mixture components (combustible gas, air, and combustion products), and the heat release rate within each control volume of the mixture at each discrete time step.

### 3.0 CALCULATION OF HYDROGEN CLOUD EXPLOSION

A computer simulation of the explosion of a cloud of the hydrogen-air mixture resulting from an accidental release from a destructed dispensing cylinder at the hydrogen fueling station is carried out. The calculated area is shown in Fig. 5. The computational experiment is carried out at an air velocity  $q = 0.0$  m/s, ambient temperature 293 K, pressure 101325 Pa at the entrance to the considered area. The dimensions of the computational domain and other specific sizes are the following: length  $L_z = 31.2$  m, height  $L_y = 14.0$  m, width  $L_x = 20.2$  m, a height of the first ground level  $Y_1 = 4.0$  m, a second-level part of the site begins from  $Z_2 = 13.2$  m and has changeable height  $H$ .

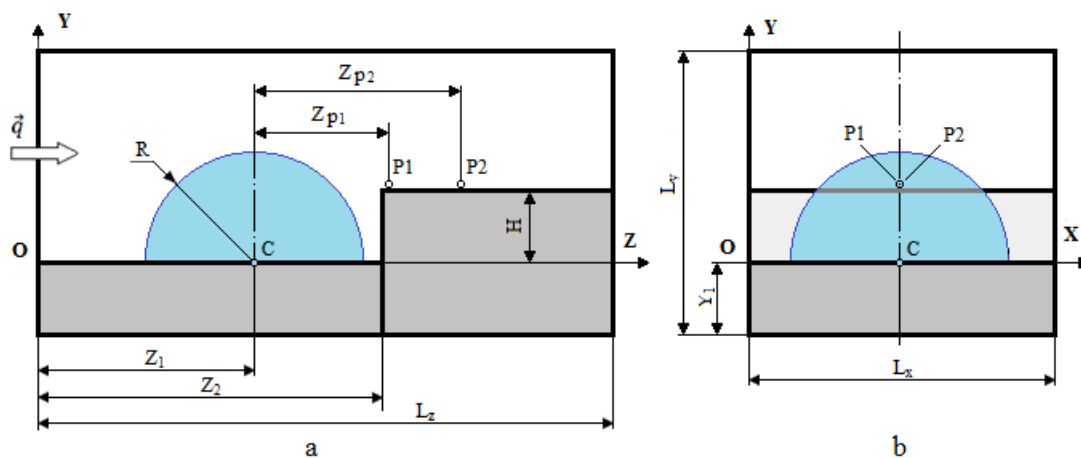


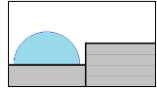
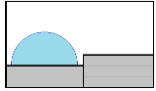
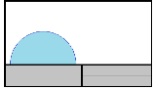
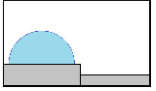
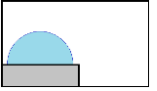
Figure 5. A scheme of the calculated area in YOZ and YOX planes

The cloud of the hydrogen is located at a distance of  $Z_1 = 10.1$  m from the origin of the computational domain, the radius of the cloud is  $R = 2.88$  m. Two control points P1 and P2 at the distances

$Z_{p1} = 3.2 \text{ m}$   $Z_{p2} = 7.1 \text{ m}$  from an explosion epicenter C are established in the characteristic places of the second-level part of the industrial site, where overpressure history is monitored.

In order to assess the influence of the complicated terrain shape at the site on the resulting fields of overpressure and the damage probability, five options of the design scheme V1-V5 are considered (table 1) which differ one from each other only by the height  $H_2$  of the terrain second part level.

Table 1. Types of calculation scheme.

Variants	V1	V2	V3	V4	V5
Scheme					
H, m	4.0	2.0	0.0	-2.0	-4.0

At the initial moment of time, as a result of the explosion of a hydrogen-air mixture, a cloud of combustion products with high pressure and temperature is formed. Further, the process of dispersion of combustion products takes place, accompanied by convective transfer and turbulent scattering of the gas mixture along with the domain, and propagation of the shock wave from an explosion epicenter. During the calculation process, it is possible to derive pressure fields at any moment of time in all three planes of the calculation domain (Fig. 6) in order to collect all the needed information to calculate conditional probability fields for personnel damage and gather overpressure collections.

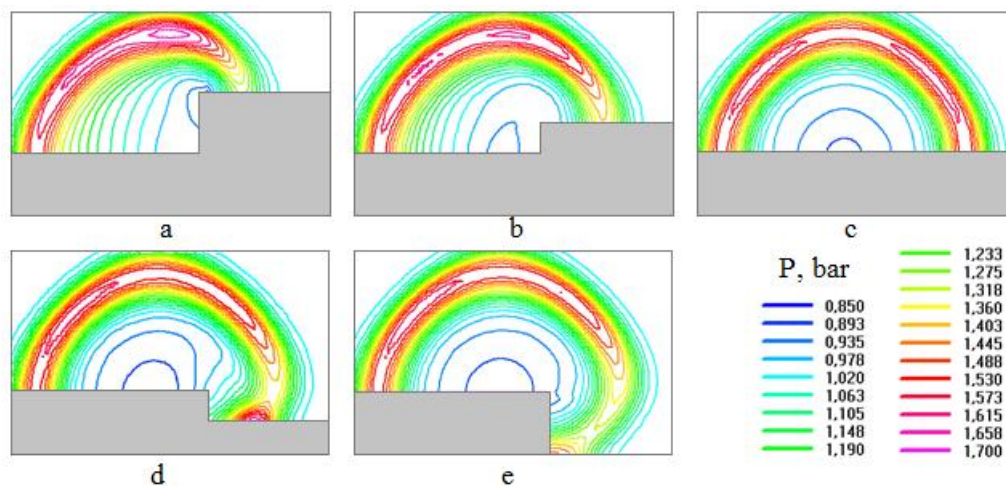


Figure 6. Pressure distribution in a plane YOZ at  $t = 0.01 \text{ s}$ : a-e – options V1-V6

The overpressure history at the control points P1 and P2 for different design scheme options V1-V5 are presented in Fig. 7. It is obvious, that the most dangerous variant of the landscape terrain corresponds to variant V3 where the terrain levels of both parts of the industrial site are of the same height  $H = 0 \text{ m}$ . Any other option of the calculation scheme leads to a decrease in both maximum overpressure and compression phase area that means less shock-impulse loads on people standing in control points P1 and P2. This trend can be noticed also from the comparison of pressure distribution in plane XOY at some moment of time (0.01 s) after the explosion (Fig. 6).

Collected data allow us to extract all the information needed to evaluate the damaging factors of the explosion shock wave (maximum overpressure (Fig. 8) and compression phase impulse (Fig. 9)) and calculate the values of the conditional probability of lethal consequences (Fig. 10) according to the formula (2) and eardrum rupture (Fig. 11) according to the formula (3) at control points P1 and P2 for different terrain options V1-V5.

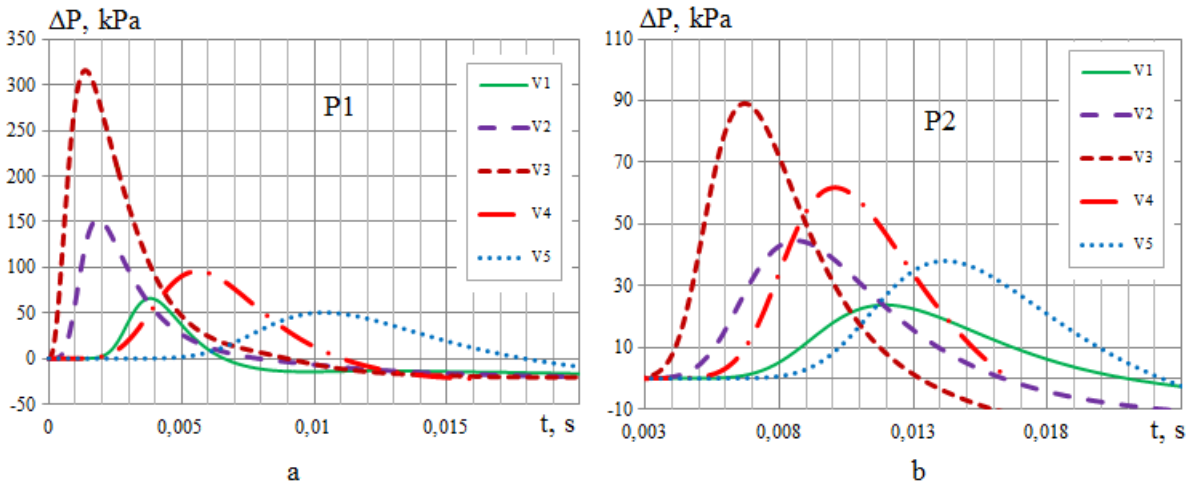


Figure 7. Overpressure history at the control points P1 (a) and P2 (b)

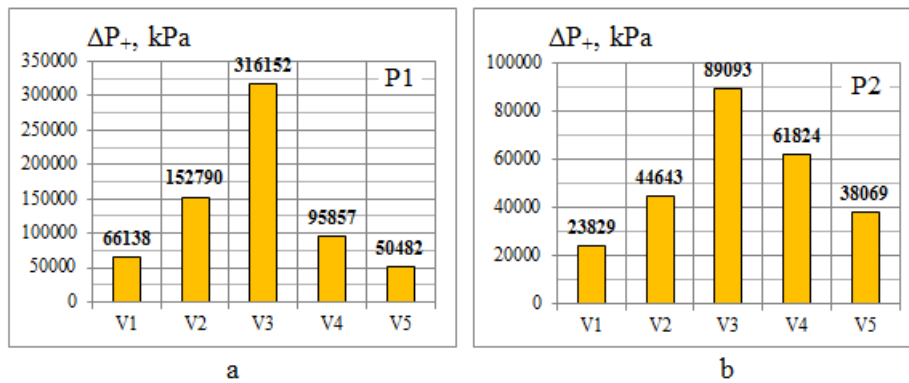


Figure 8. Maximum overpressure at control points: a – point P1; b – point P2

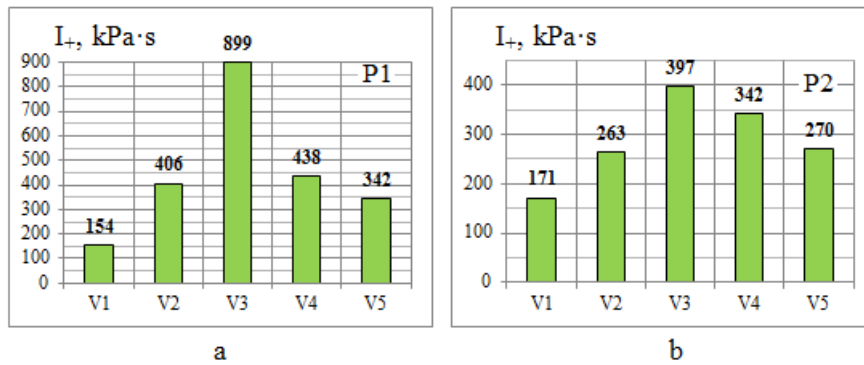


Figure 9. Compression phase impulse  $I_+$  at control points: a – point P1; b – point P2

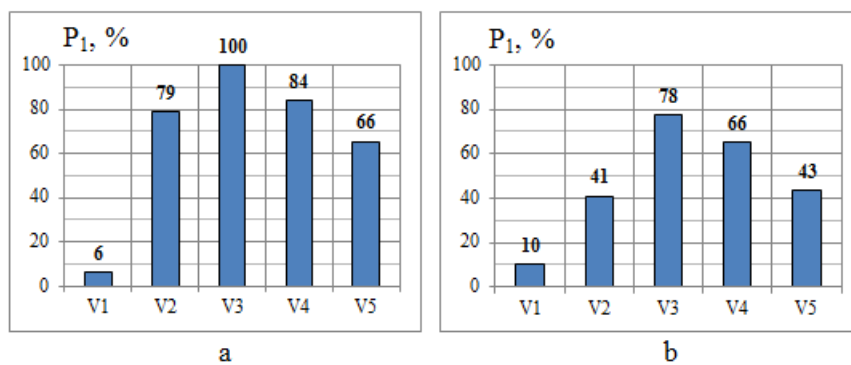


Figure 10. Lethal probability in control points: a – point P1; b – point P2

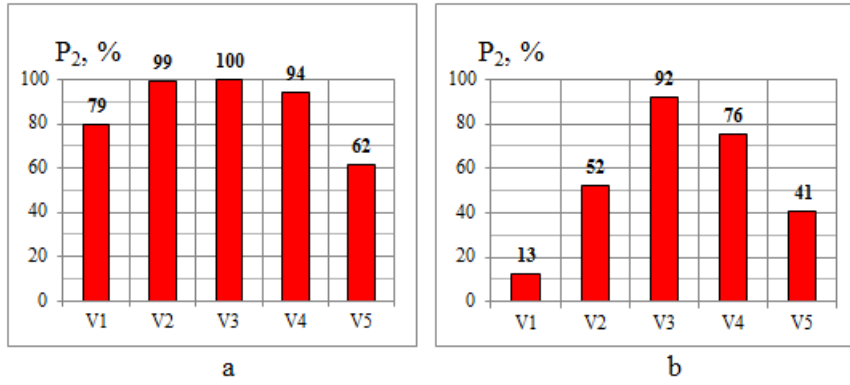


Figure 11. Eardrum rupture probability in control points: a – point P1; b – point P2

The lethal consequence conditional probability in the most exposed to overpressure vertically centered plane YOZ and on the surface of the second part of the industrial site (possible working places location) in the plane XOZ are displayed (Fig. 12-16).

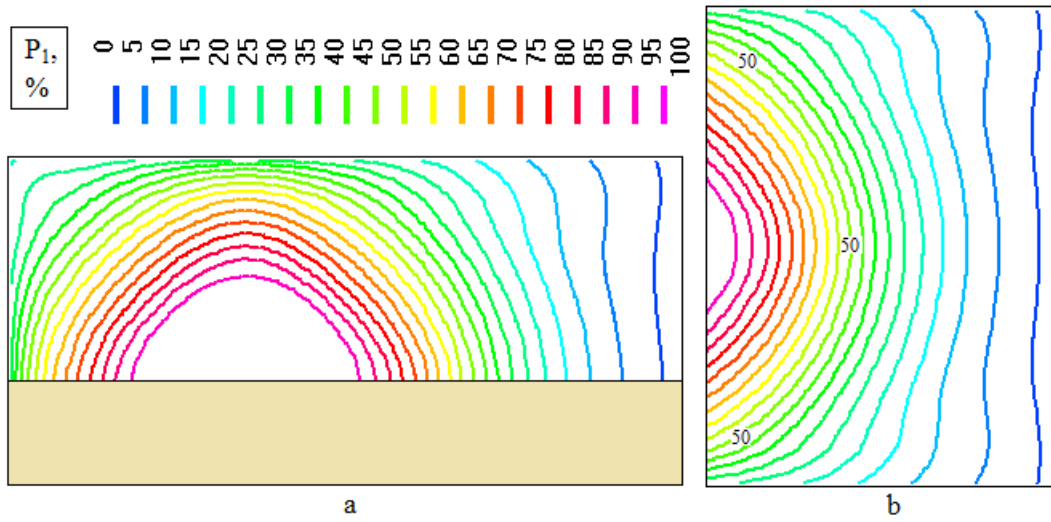


Figure 12. Lethal probability fields for option V3: a – plane YOZ; b – plane XOZ (a working place)

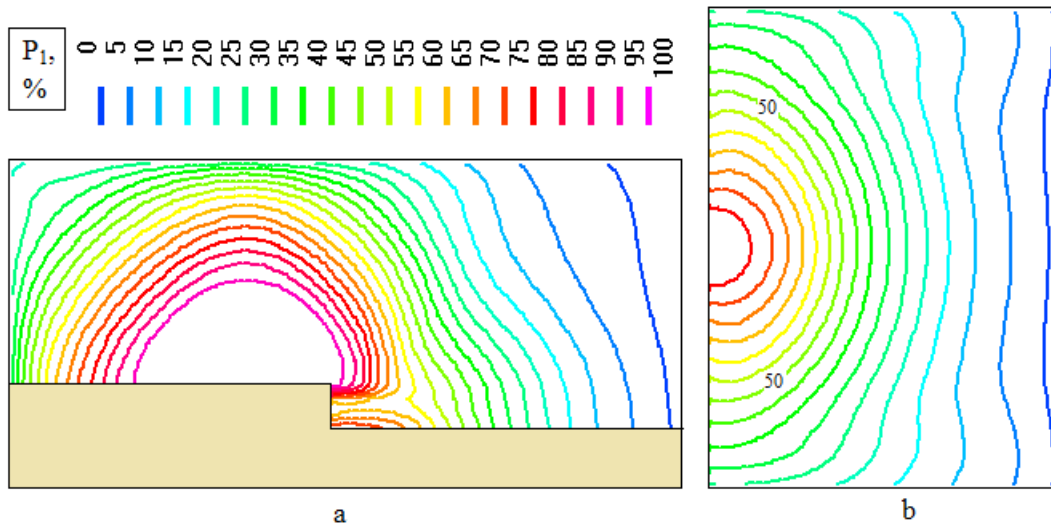


Figure 13. Lethal probability fields for option V4: a – plane YOZ; b – plane XOZ (a working place)



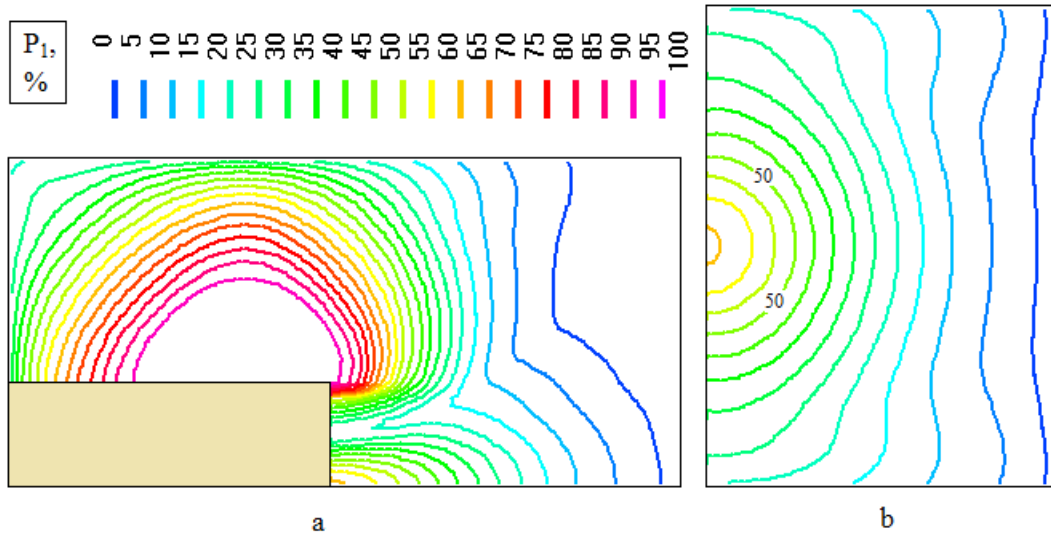


Figure 14. Lethal probability fields (option V5): a – plane YOZ; b – plane XOZ (level two)

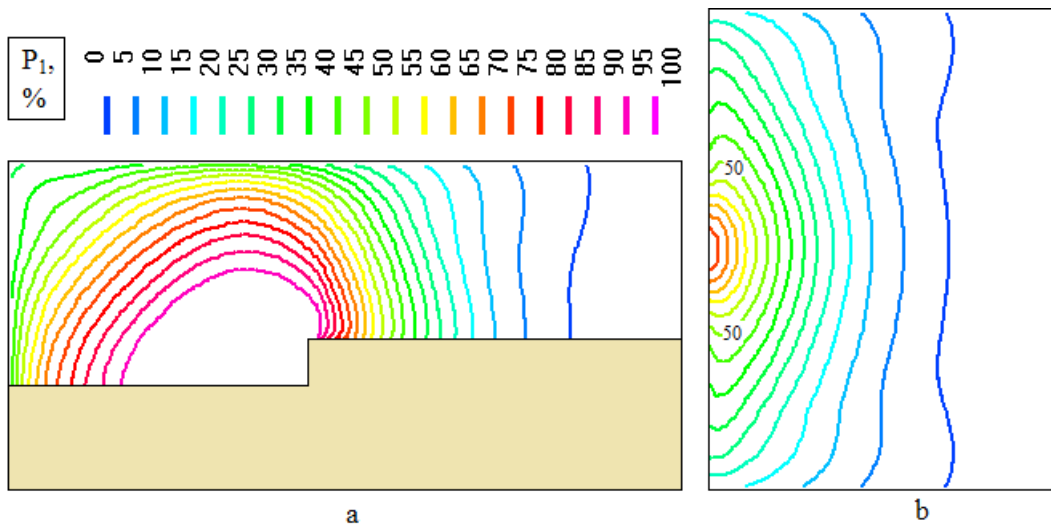


Figure 15. Lethal probability fields (option V2): a – plane YOZ; b – plane XOZ (level two)

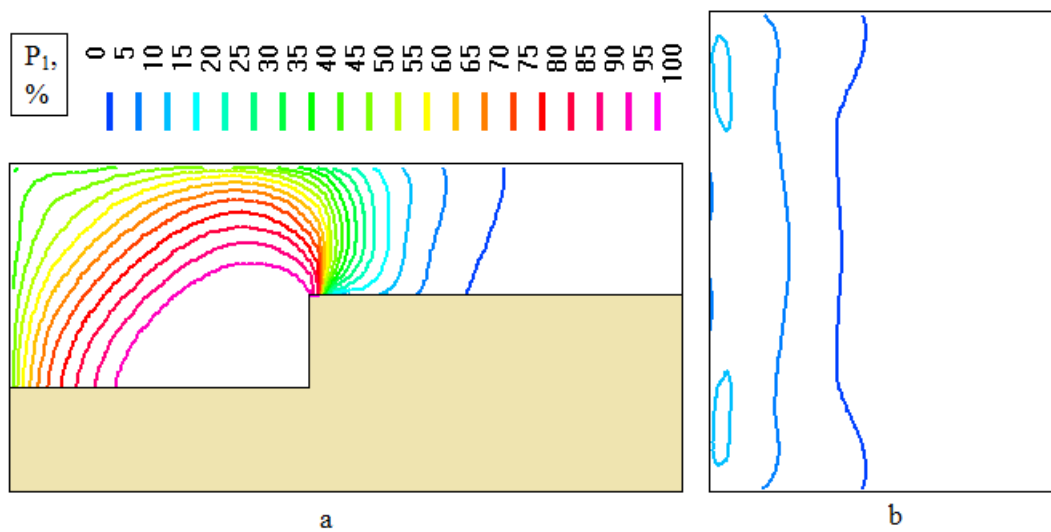


Figure 16. Lethal probability fields for option V1:  
a – plane YOZ; b – plane XOZ (a working place)

In order to compare different design schemes of the terrain landscape the area  $S_{50}$  on the surface of the second part of the industrial site where the lethal consequences conditional probability is greater than 50%, which is considered a dangerous zone in engineering practice, is calculated (Fig. 17).

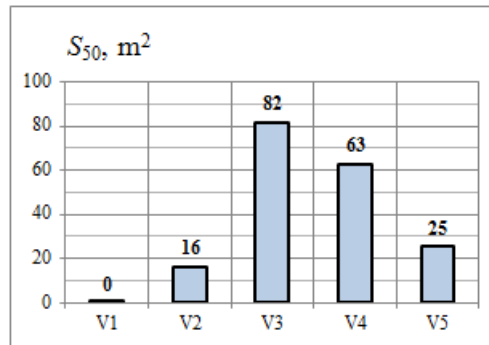


Figure 17. A dangerous area  $S_{50}$  at the working place level

#### 4.0 CALCULATION RESULTS DISCUSSION

From an analysis of the overpressure behavior (Figs. 7, 8), it can be seen that the biggest shock loads correspond to option V3 with equal terrain levels of two parts of the industrial site. It leads to the highest values of the ear-drum rupture conditional probabilities (Fig. 11) for both control points. Some decrease in shock loads in control point P2 (comparing to point P1 at the edge of level-two part) can be explained by the more distant location of this point from the explosion epicenter.

Any other design scheme of the level-two part gives a decrease in shock loads that especially noticeable for control point P2 (Figs. 7b, 8b, 11b). It has to be underlined that options V4 and V5, which correspond to deeper levels of the part two terrain, give less protection effect for point P2 than the corresponding options V2 and V1 with higher levels of the part two terrain. It can be explained that in options V2 and V1 part of the explosion wave meets an obstacle and is reflected backward. For control point P1 (Figs. 7a, 8a, 11a) the deepening makes a bigger effect in options V4 and V5 comparable to options V2 and V1 maybe because of the less intensive expansion process around the convex corners of the terrain.

Very similar behavior can be seen in compression phase impulse distribution (Figs. 7, 9). Higher levels of the terrain (options V2 and V1) create bigger protection in control points from impulse loads than deeper levels (options V4 and V5).

The total effect from maximum overpressure and impulse loads can be clearly seen in Fig. 10 for lethal probabilities in control points and in Figs. 12-16 for the fields of this consequence parameter. Higher levels of options V2 and V1, do better protect humans than deeper variants of terrain, especially in point P2 (Figs. 10b, 12b-16b). This conclusion can be confirmed by such safety characteristics as an area  $S_{50}$  of dangerously high values ( $> 50\%$ ) of the conditional lethal probability (Fig. 17) on the surface of the level-two part of the industrial site (working place). It is clearly seen that higher-level variants V2 and V1 protect the working place much more effectively than deeper level variants V4 and V5 of landscape terrain in relation to variant V3 with evenly leveled terrain.

#### CONCLUSIONS

The paper presents a useful methodology for probabilistic assessment of the influence of different variants of the landscape terrain on the probable damage consequences for the personnel of the hydrogen fueling station where an accidental hydrogen release and explosion takes place. The methodology is based on a three-dimensional mathematical model of the hydrogen dispersion and explosion taking into account complicated terrain shape.

The model allows obtaining fields of maximum overpressure and compression phase impulse of the explosion wave and, using the probit-analysis procedure, numerically estimate the conditional probability of damage to personnel who is exposed to explosion wave shock-impulse loads as a comparable indicator of the industrial object safety. It is obtained that higher terrain levels of the working place in relation to possible explosion epicenter terrain level can give better protection than deeper terrain levels of the working place. The obtained results can be used by safety experts to develop measures to reduce the risk of considered accidents at the industrial sites and to analyze their effectiveness. Further improvement of this methodology is possible in the direction of enhancing the accuracy of the gas-dynamics mathematical model and considering a combination of accidental scenarios with various damaging factors.

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