

## Numerical Modelling of Gas Explosion Overpressure Mitigation Effects

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**Abstract.** The main aims of this study are to assess numerically the mitigation effects caused by the solid wall installed at the fueling station in order to protect personnel from the consequences of the emergent gas explosion, evaluate the optimal location of the wall and choose the appropriate material the wall have to be made of in order not to be destructed. A three-dimensional mathematical model of an explosion of hydrogen-air cloud is used. A computer technology how to define the personnel damage probability fields on the basis of probit analysis of the explosion wave is developed. The mathematical model takes into account the complex terrain and three-dimensional non-stationary nature of the shock wave propagation process. The model allows obtaining time-spatial distribution of damaging factors (overpressure in the shock wave front and the compression phase impulse) required to determine the three-dimensional non-stationary damage probability fields based on probit analysis. The developed computer technology allows to carry out an automated analysis of the safety situation at the fueling station and to conduct a comparative analysis of the effectiveness of different types of material the protective facilities made of.

### Introduction

The level of safety at the industrial enterprises which use hydrogen (such as fueling stations) depends on reliable operation of the equipment and efficient safety measures protecting the staff and surrounding buildings from the negative effects of such emergencies as large-scale releases of compressed gaseous hydrogen from destroyed high-pressure vessels [1]. The most dangerous scenario of an emergency situation is an explosion of the hydrogen-air cloud generating a shock wave that spreads rapidly from the epicenter and has a negative impact on the environment. The major damaging factor in this case is the maximal overpressure in the shock wave front and impulse.

The effectiveness of protective measures is usually checked by field tests [2]. However, the unpredictable nature of the hydrogen requires replacement of expensive physical experiments by computer simulations based on adequate mathematical models of the physical processes of the release, dispersion and explosion of hydrogen in the atmosphere [3-5]. Modern computer systems allow carrying out a three-dimensional analysis of gas-dynamic flow parameters in the computational domain, including the protective measures, and to forecast changes in pressure at typical control points in space and draw conclusions about the effectiveness of protective device.

### Methods of Assessing the Impact Caused by an Explosion Wave

**Deterministic approach.** Technogenic accidents are usually accompanied by a sudden release or leakage of the hydrogen into the atmosphere, the formation of explosive hydrogen-air mixtures followed by their explosion and fire. As a result of such accidents the compression wave in the

atmosphere is formed and propagated, the impact-pulse effect of explosion may cause dangerous consequences to the personnel health and surrounding structures (Fig. 1).

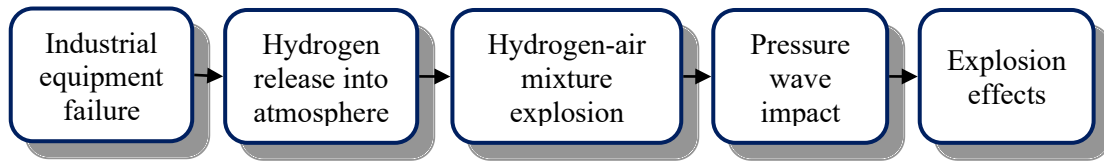


Fig. 1. Development scheme of technogenic accident

In general, a shock wave has a characteristic profile and its negative impact is determined by the maximal overpressure  $\Delta P_+$  and  $I_+$  – the compression phase impulse.

According to the deterministic method the damaging effect of the shock wave is determined by the overpressure  $\Delta P_+$  in the front of the shock wave. Comparison of overpressure with threshold values allows to determine the extent of human impact (Table 1) or destruction degree of the exposed constructions (Table 2) [6].

Table 1. The degree of the impact on human health at different overpressure range.

$\Delta P_+$ [kPa]	Less than 10 [kPa]	10...40 [kPa]	40...60 [kPa]	60...100 [kPa]	More than 100 [kPa]
Degree of impact	Safe overpressure	Light (bruises, hearing loss)	Average (bleeding)	Heavy (concussion)	Lethal effect

Table 2. The degree of the impact on the wall at different overpressure range.

Type number	Wall material	Wall destruction grade depending on overpressure [kPa] range			
		weak	medium	severe	total
1	Antiseismic concrete	25...35	80...120	150...200	200
2	Sectional ferroconcrete	10...20	20...30	–	30...60
3	Brick	8...15	15...25	25...35	35...45
4	Wood	6...8	8...12	12...20	20...30

**Probabilistic method.** 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  $t$  – integral degree of impact.

For example, the probability of human lethal injury can be estimated by the formula [7, 8]

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

The probit-function for eardrums rupture can be found by the formula [9]

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

Then using the method of probit-analysis it is possible to define the damage probability for every type of impact [4].

### Explosion Mathematical Model and Calculation Algorithm

In order to evaluate the effectiveness of overpressure protective wall it is used a mathematical model of an instantaneous explosion of hydrogen-air mixture [5]. 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 without viscous terms in the mixture motion equations (Euler approach with source terms).

### Calculation of Hydrogen Cloud Explosion

Assume that some of the high-pressure dispensing cylinders at the refueling station are instantly destroyed, resulting in the release of compressed hydrogen into the atmosphere near the ground, its expansion to atmospheric pressure, and formation of the hemispherical stoichiometric hydrogen-air cloud with radius of 1.5 [m] and ambient temperature 293 [K] (Fig. 2). Consider an instantaneous explosion of this hydrogen cloud that causes the formation of combustion products with the following parameters: temperature 3450 [K], pressure 901 [kPa], molar mass 0.02441 [kg/mol] and adiabatic coefficient 1.24.

The computation space has the following dimensions (Fig. 5): the length  $L_z = 31$  [m], the width  $L_x = 20$  [m], and the height  $L_y = 14$  [m]. All sides of the computational cells have the same size 0.2 [m], so the computational grid has 155 x 100 x 70 cells respectively. The time step is calculated in order to keep the stability of explicit finite-difference Godunov method.

The protective wall has the following dimensions: the length  $X_w = 10.0$  [m]; the width  $Z_w = 0.2$  [m], the height  $Y_w = 2.2$  [m] (Fig. 5). For each option of experiments the wall is installed at some distance  $L_w$  from an explosion epicenter (Table 1). To analyze the effectiveness of the protective measure the overpressure is controlled in several points  $P_i$  (P0-P4) near the ground at the distance  $Z_p$  (4 [m], 5 [m], 6 [m], 7 [m], and 8 [m] respectively). Except point P0 one of the rest control points in some option is located before the wall in order to evaluate overpressure loading to the wall surface. For example, for the option V2 of the wall location (see Table 1) control points P0, P1 and P2 are between the explosion epicenter and the wall, point P2 is near the wall and control points P3 and P4 are behind the wall and protected from the main overpressure exposure.

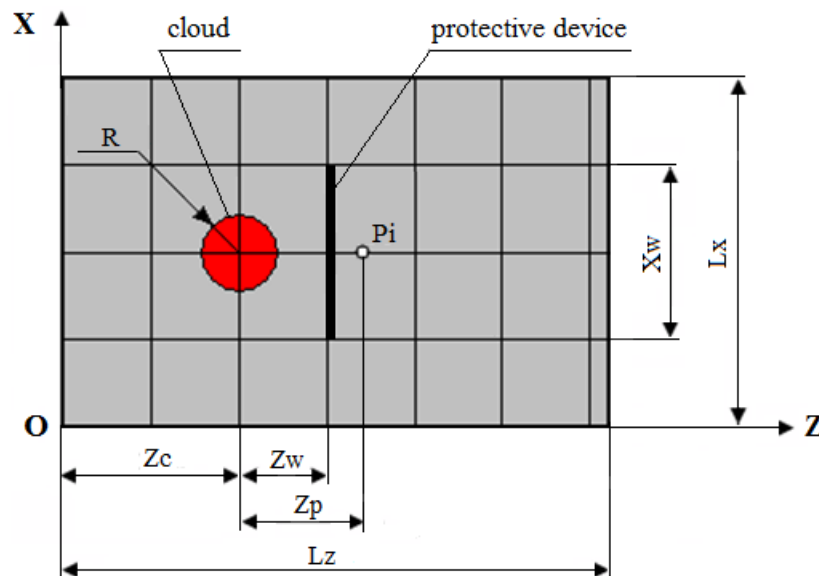


Fig. 2. The layout of hydrogen cloud, protection wall, and control points  $P_i$  near the earth.

The difference between the experiment options is in a different distance  $Z_w$  of the wall from the explosion epicenter. Variant V0 does not contain a protective wall at all.

Table 3. Options of the protective wall location.

Option number	V0	V1	V2	V3	V4
$Z_w$ [m]	–	5.0	6.0	7.0	8.0

During all the experiments the overpressure history in all the control points is collected (Fig. 3) and pressure distribution in all the planes can be obtained in order to analyze the influence of the wall on the pressure transformation (Fig. 4).

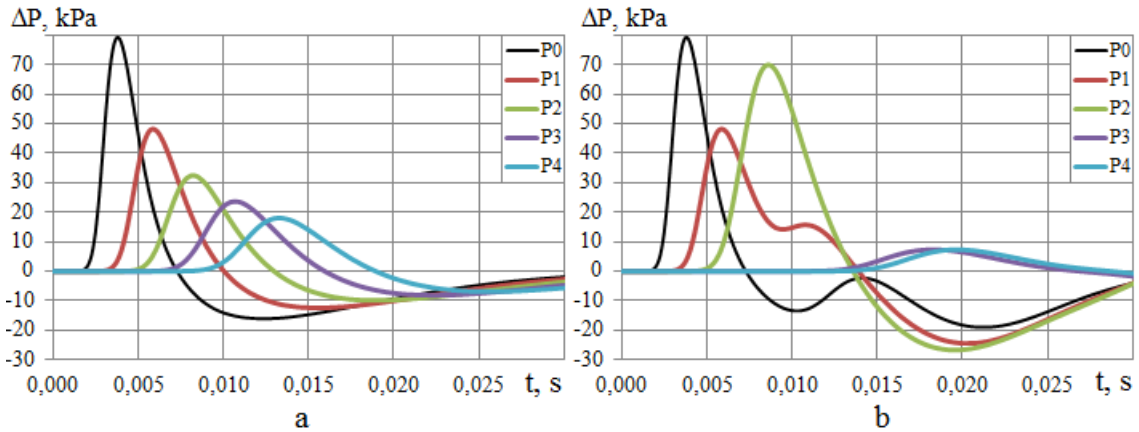


Fig. 3. Overpressure history in the control points P0-P4: a – without protection (option V0); b – with protection (option V2 of the wall location).

The model allows finding the distribution of pressure (Fig. 4). The overpressure history in every control point gives the information about maximum overpressure  $\Delta P_+$  and impulse  $I_+$  (Fig. 5) for each scenario of the wall location to analyze the probable damage to personnel (Fig. 6) and maximum overpressure on the wall surface exposed to explosion wave (Fig. 7). It allows assessing the overpressure loading and choosing appropriate material the wall to be made of.

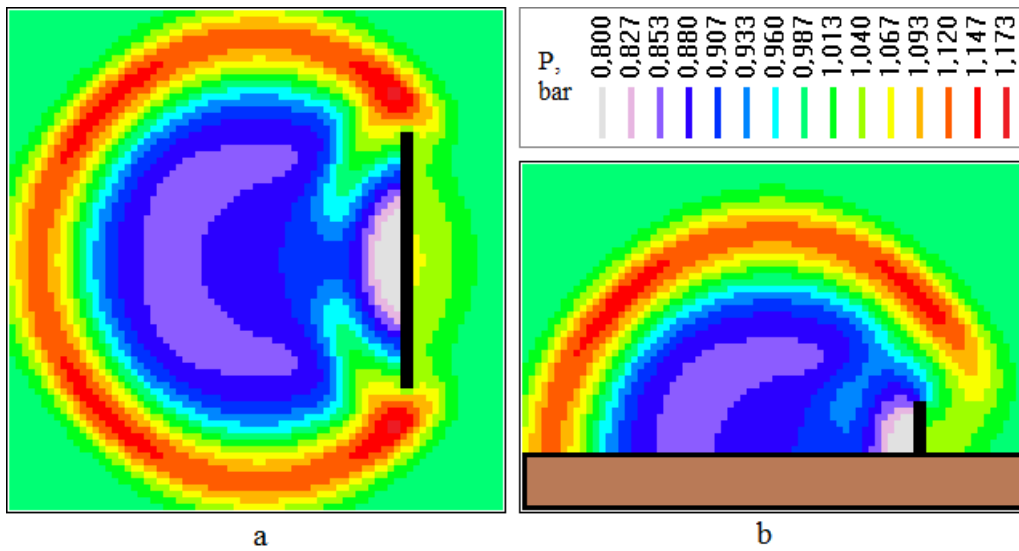


Fig. 4. Pressure [bar] distribution at 0.0107 s after explosion for protection option V2: a – XOZ plane (near the ground); b – plane YOZ

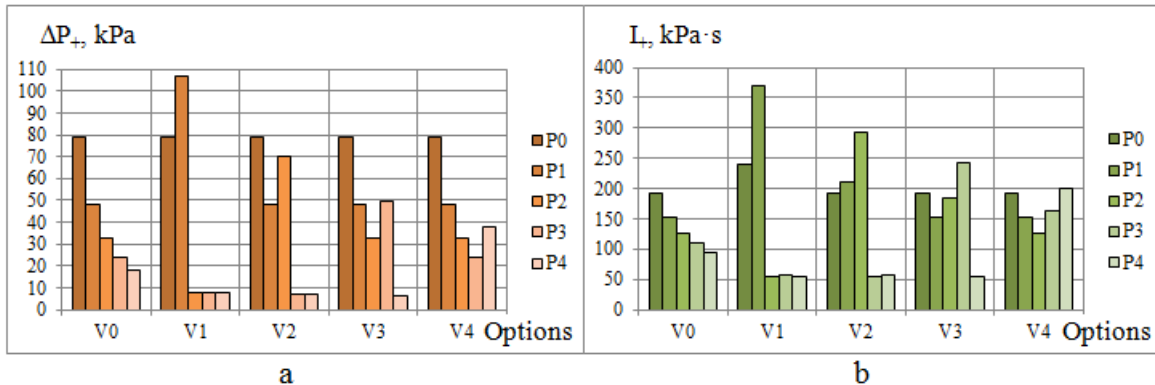


Fig. 5. Shock-impulse load distribution in the control points P0-P5 for different options of the wall location V0-V5: a – maximum overpressure  $\Delta P_+$ ; b – impulse  $I_+$

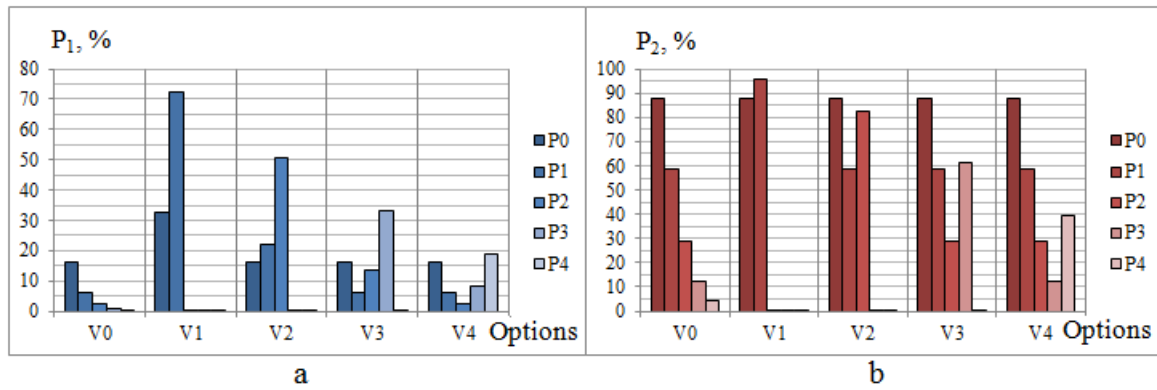


Fig. 6. Damage conditional probability [%] distribution in the control points P0-P5 for different options of the wall location V0-V5: a – lethal injury  $P_1$ ; b – eardrum rupture  $P_2$

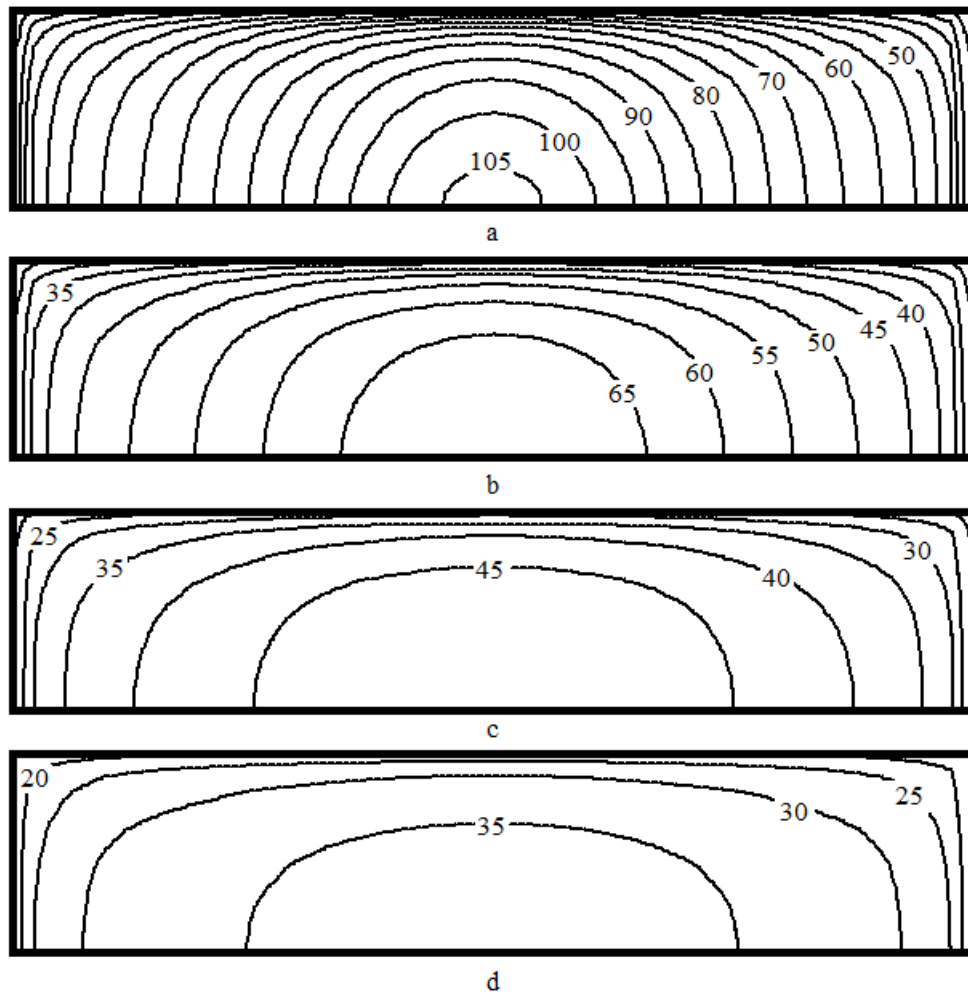


Fig. 7. The fields of maximum overpressure [kPa] on the wall surface: a, b, c, d – for options V1, V2, V3, and V4 of the wall location, respectively

## Results Discussion

During the scenario V0 (there is no wall) the pressure wave is spreading along the computational domain (Fig. 3, a) smoothly losing its shock intensity (Fig. 5, a), impulse loading (Fig. 5, b) with the distance from the explosion epicenter. This pressure wave doesn't cause lethal danger (Fig. 6, a) and heads to significantly probable eardrum rupture in points P0 and P1 (Fig. 6, b). Installation of the protective wall changes the safety state drastically (Fig. 6). The pressure wave mostly reflects from the wall amplifying a pressure phase in front of the wall (Fig. 3, b) and decreasing it behind the wall (Fig. 5). Reflected pressure wave can cause high lethal risk in options V1 and V2 (Fig. 6, a)

and eardrum rupture risk in all the options except V4 (Fig. 6, b). The situation behind the wall can be considered as fully safe (Fig. 6). On the other hand, the surface of the wall is exposed to the significant overpressure loading and can cause the destruction of the wall (Fig. 7). Using the destruction thresholds for different wall materials (Table 2) it can be decided that for all the scenarios all the materials except antiseismic concrete are not allowed to make the protective wall because of the total destruction risk (Fig. 7).

### Summary

An explosion of emergently released hydrogen at the fueling station is numerically evaluated. A three-dimensional mathematical model of instantaneous gas mixture explosion based on the Euler equations solved by Godunov method is used. A comparative analysis of the effectiveness of differently located protective wall that is made of different materials is carried out. Basing on maximum overpressure control and conditional damage probability at critical points and comparative analysis of the overpressure distribution on the wall surface the most effective location of the protective wall and the material it is made of can be recommended taking into account the personnel safety and the ability of the wall to withstand the overpressure loading without destruction.

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