

Numerical Evaluation of Harmful Consequences after Accidental Explosion at a Hydrogen Filling Station

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Abstract – This study aims to present computational technology that can be used to evaluate numerically the harmful environmental consequences caused by an accidental hydrogen release from failed high-pressure dispensing cylinders and its explosion at a vehicle hydrogen filling station. A coupled problem of a hydrogen explosion products expansion in the atmospheric ground layer and a harmful explosion pressure wave shock impact on service personnel and infrastructure buildings at an accident site is solved by means of computer experiment simulation series. A spatial time-dependent model of compressible hydrogen-air mixture flow is used to obtain pressure history in calculation area in order to assess maximum overpressure in control points of human possible locations and on building surfaces exposed to hydrogen blast wave impact. A deterministic impact consequences model is based on comparing maximum overpressure values extracted from the mathematical model with threshold ranges corresponding to certain degrees of human damage and infrastructure destruction. The presented computer technology allows safety experts to identify potentially dangerous zones by means of mathematical modelling and recommend effective protection measures to mitigate negative consequences of explosions.

Keywords – Explosion wave front; human health impact degree; hydrogen explosion; maximum excessive pressure; structure destruction level.

Nomenclature

x, y, z	Right system coordinates along width, height, and length	–
K	Number of destroyed high-pressure cylinders	–
τ	Time of gas mixture movement physical process	sec
P	Gas mixture pressure	Pa
ΔP_+	Maximum overpressure at explosion wave front	kPa
I_+	Explosion wave compression phase impulse	kPa s
r	Combustion products cloud radius	m
B	Conditional damage probability	%
Pr	Probit function of injury caused by explosion wave	–

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1. INTRODUCTION

Hydrogen is a very valuable modern source of energy that can replace hydrocarbon fuels in various areas of the economy: transport, metallurgy, household services etc. On the other side, it is very dangerous flammable chemical substance that can easily explode when mixed with air in case of accidental release into atmosphere as a result of hydrogen storage or dispensing equipment failure (Fig. 1) [1].

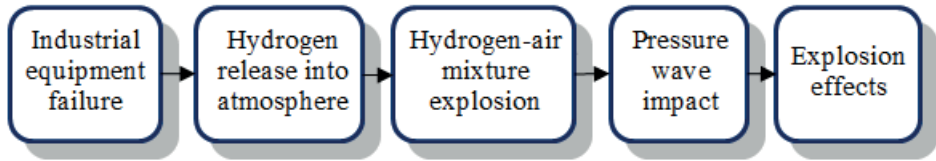


Fig. 1. Structural scheme of accident development.

Hydrogen explosion is accompanied by temporary atmospheric baric changes in comparison with ambient conditions. This pressure field disturbance forms shock wave overpressure which can be harmful to environment. Explosion intensity during accident depends on amount of released and reacted hydrogen and influences on level of consequences on human health and surrounding infrastructure buildings. The aim of this study is to identify such influence of explosion power on overpressure loading on human and infrastructure building not far from an explosion epicenter at a hydrogen filling station during accidental failure of several high-pressure hydrogen dispensing cylinders with total release of gaseous substance into the atmosphere. The expansion of combustion products generates pressure shock wave that moves away from explosion epicenter. Overpressure at the front of the wave affects service personnel and buildings. Its value can be compared with threshold limits for different levels of human injury and building destruction in order to evaluate accident consequences and recommend some mitigation equipment. The protection wall is considered as such a safety enhancing device, and its efficiency is assessed.

2. REVIEW OF LITERATURE

The environmental consequences of hydrogen explosions and protection measures efficiency can be evaluated by means of physical experiments [2]. During field experiment scientists can arrange any configuration of measurement equipment in order to validate their hypothesis about emergency release and chemical interaction of hydrogen with atmospheric air, and assess the environmental consequences caused by explosion [3]. However, a specific physical experiment is adapted to specific conditions and cannot take into account all possible circumstances associated with an uncontrolled explosion of a highly flammable gas, which makes it of little use in the engineering practice of safety experts. Simulation of various emergency scenarios using mathematical modelling tools [4]–[6] allows one to overcome the limitations of a physical experiment, provided that the model is adequate to real physical processes that are relevant in case of emergency emissions at high-risk industrial enterprises. The adequacy of the model must be confirmed by its validation in relation to the physical process [7], and its implementation in the form of a computer model must be verified in terms of stability with respect to different computational grids, initial and boundary conditions, etc. In addition, the mathematical model must meet the needs of the scientific and technical problem being solved and take into account such specific conditions as the complex terrain

of the emergency area [8], the buoyancy of the impurity relative to atmospheric air [9], the chemical activity of the impurity gas mixed with atmospheric oxygen [10], changing environmental conditions [11]–[12], scenarios and intensity of emergency release of impurities into the atmosphere [13], sometimes flow viscosity [14], etc. And the computer model, in turn, should be convenient and reliable to use in engineering practice [15].

For a complete understanding of the properties and features of the mathematical model, with the help of which it is supposed to solve the formulated scientific and applied problem of obtaining excess pressure fields in the area of an emergency hydrogen explosion in order to assess the degree of impact on the environment, it is necessary to structure the main functional blocks of the solution process (Fig. 2).

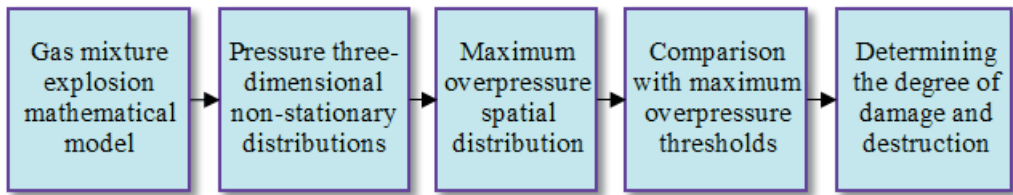


Fig. 2. Hydrogen explosion consequences assessment process functional scheme.

To analyze existing mathematical models of the movement of gas mixtures, let us turn to the model classification (Fig. 3) made in [16].

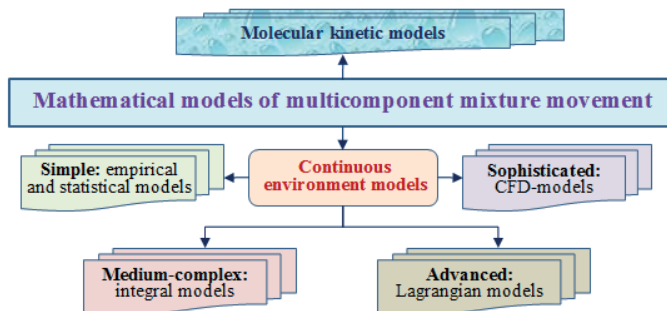


Fig. 3. Classification of models of dispersion of gas impurities.

Molecular kinetic models are the most accurate [17]–[19], but cannot be used for large computational areas due to a lack of computer resources. The first three large groups of continuum models (simple [20], [21], medium-complex [22], [23] and advanced [24], [25]) cannot be used in this study, because do not correspond to at least one of the requirements put forward to the model, the satisfaction of which together makes it possible to solve the posed scientific and applied problem. The only suitable group is a set of CFD-models that are based on the use of the Navier-Stokes equations, for example [26]–[31]. The use of these complex models, in turn, is hampered by their high requirements for computer resources, user qualifications, selection of specific turbulence models, etc. In addition, some mathematical models of the movement of impurities are time-independent [32], others are adapted to predict the impact on the environment of only toxic (non-explosive) chemicals [33], some models are designed to use a probabilistic approach [34], which is also unacceptable for this study.

Therefore, based on the analysis of available mathematical and computer models of gas dynamics of mixtures, it was decided to use a CFD model of a two-component flow of a mixture of air and hydrogen combustion products without taking into account viscosity (which does not play a significant role in the core of the flow) [5], which meets all the requirements for studying the movement of a blast wave in the area of a gas station in order to obtain overpressure fields in personnel locations, assess the consequences of the impact of the blast load on people and surrounding buildings, and identify the effectiveness of using a stationary protective wall to mitigate the consequences.

3. HYDROGEN EXPLOSION PROBLEM FORMULATION

The dispersion of hydrogen combustion products in the spatial computational domain is considered (Fig. 4). The blast wave spreads from the initial impurity cloud, gradually losing its intensity. The domain is a parallelepiped in the Cartesian coordinate system (axis OY is associated with the height, OZ – with the length, and OX – with the width of the domain). Harmful for human and infrastructure maximum overpressure, which is generated under the influence of explosion pressure wave propagation, can be considered as a main harmful parameter the value of which is inside limits of specific thresholds associated with some level of human injury and building destruction.

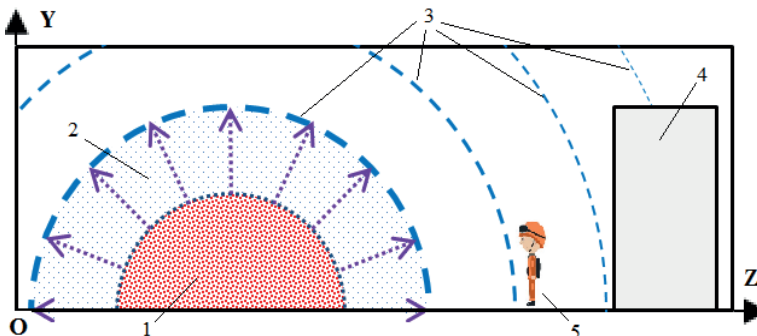


Fig. 4. Accident development scheme: 1 – explosion products cloud; 2 – pressure expansion process; 3 – explosion wave propagation; 4 – infrastructure building; 5 – overpressure exposed person.

The combustion products expansion model allows calculating pressure distribution in computational domain and extract from its maximum overpressure field which is used for determining the level of environmental consequences caused by an explosion (injury level of exposed human and destruction degree of infrastructure near the accident epicenter) at the site of filling station with different configuration (presence/absence of the protection wall and infrastructure building).

4. METHODS AND PROCEDURES

4.1. Model Basic Equations, Boundary and Initial Conditions

To obtain non-stationary three-dimensional pressure fields of a gas mixture of hydrogen combustion products with air, a complete system of conservation laws for the mixture without taking into account viscosity, supplemented by the law of conservation of mass of combustion

products, is used [5]. The system of equations is closed by the equation of state of the mixture. No-flow boundary conditions are set on the surfaces of the ground, building and protective wall. The system of equations is hyperbolic, therefore, at the entrance to the computational domain, the values of wind speed and angles of the velocity vector relative to the coordinate axes, as well as the full entropy function, are specified as boundary conditions. The flow is predominantly subsonic (the presence of supersonic zones is allowed). Therefore, at the exit from the computational domain, static pressure is specified as a boundary condition. The gas-dynamic parameters of hydrogen combustion products are set in the region occupied by the cloud as the initial condition. The system of differential equations is brought into integral form and solved by the end-to-end calculation method [14]. The method makes it possible to calculate not only the external flow, but also the internal flow of gases (for example, in a tunnel [35]), including in non-simply connected areas, makes it possible to consider the complex topography of the area [36], to integrate continuous impermeable objects of various design types into the calculation area [37].

4.2. Hydrogen Explosion Process Simulation

The instant explosion model is used to simulate the explosion physical process. It is assumed that released hydrogen forms the stoichiometric air-hydrogen cloud that is instantly chemically reacted with formation of combustion products at constant volume. The temperature and pressure of them are used to set initial conditions in the cloud [5]. The computation process of pressure wave propagation is stopped when the wave exits the computational domain [14].

4.3. Hydrogen Explosion Impact Evaluation Method

To understand how the shock-pulse load from a blast wave on the environment is formed, it is necessary to consider the diagram of a typical pressure wave profile (Fig. 5). The characteristic features of a blast wave are the presence of a pressure peak in the front, primary phases of compression and rarefaction. The magnitude of the difference between the peak pressure and the ambient pressure represents the main shock damaging factor – the maximum overpressure ΔP_+ . The integral of the primary compression phase gives the value of the second damaging factor I_+ – the impulse load on the environment.

There are two main approaches to evaluate the explosion consequences on environment: probabilistic and deterministic. The first one uses the explosion physical process model to extract both dangerous factors (maximum overpressure and impulse) and through probit analysis calculate the conditional probability of some level of human injury or infrastructure destruction. The probability B depends on so called probit-function of specific damage Pr , which itself is a function of maximum overpressure and impulse for every type of consequences for human or building. This approach is useful for risk-oriented methods of safety evaluation. It can be used for such dangerous physical processes as toxic gases dispersion, explosion wave propagation, high temperature combustion products thermal radiation etc.

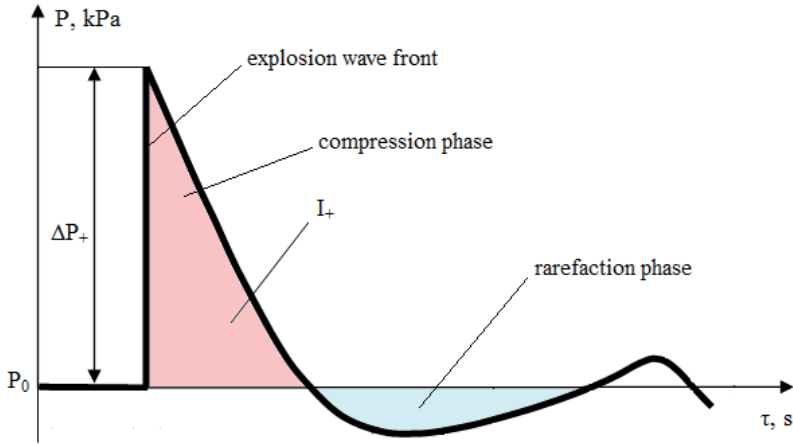


Fig. 5. The typical explosion wave profile.

The methodology of a deterministic approach to finding the negative consequences of the impact of excess pressure on the environment involves calculating the magnitude of this damaging factor and comparing it with the scale of consequences [36]. Such a scale for damage to the human body is presented in Table 1.

TABLE 1. EXPLOSION OVERPRESSURE IMPACT ON PERSONNEL

Excessive pressure ΔP_+ , kPa	< 10	10–40	40–60	60–100	> 100
Consequences	Safe	Light	Average	Heavy	Lethal

Light impact on human health is associated with bruises and loss of hearing, average impact – with bleeding, heavy impact is accompanied by concussion. The degree of destruction of buildings can be determined from Table 2 by the amount of excess pressure depending on the structural material of their manufacture.

TABLE 2. EXPLOSION OVERPRESSURE IMPACT GRADE ON INFRASTRUCTURE BUILDING

Structure construction material	Destruction from overpressure, kPa			
	weak	medium	severe	total
Antiseismic concrete	25–35	80–120	150–200	> 200
Sectional ferroconcrete	10–20	20–30	–	30–60
Brick	8–15	15–25	25–35	35–45
Wood	6–8	8–12	12–20	20–30

In this paper we use the deterministic approach to evaluate the consequences of gaseous hydrogen explosion at vehicle filling station caused by accidental failure of several high-pressure hydrogen dispensing cylinders.

5. RESULTS

According to accident scenario at the hydrogen vehicle filling station, a certain volume of hydrogen gas quickly reacts with oxygen in the air to form a cloud of combustion products in the shape of a hemisphere with a radius r (Fig. 6). The center of hemisphere E will be considered the epicenter of the emergency explosion. There is complete calm on the site (the speed of the air mass at the entrance to the area is zero). The temperature of the gases of combustion products (a mixture of water vapour and residual nitrogen from the air, the oxygen of which has reacted) is 3177 °C, adiabatic ratio is 1.24, and molar weight is 0.02441 kg/mol.

The calculated volume is a parallelepiped 31.2 m long, 20.2 m wide, and 12 m high. The computational grid has 156 finite-difference cells along the OZ axis, 101 cells along the OX axis, and 60 cells along the OY axis, i.e., each cell is a cube with a side of 0.2 m.

One group of scenarios considers the installation of a solid protection wall between explosion epicenter and personnel and infrastructure building (Fig. 6). The wall is 10.2 m long (along the OX axis), 0.2 m thick (along the OZ axis) and 2.2 m high (along the OY axis).

The scale of emergency consequences depends on the number K of destroyed high pressure fuel dispensing vessels (Table 3). Five explosion intensity options O1–O5 are considered. They assume different combustion products cloud radius for each option.

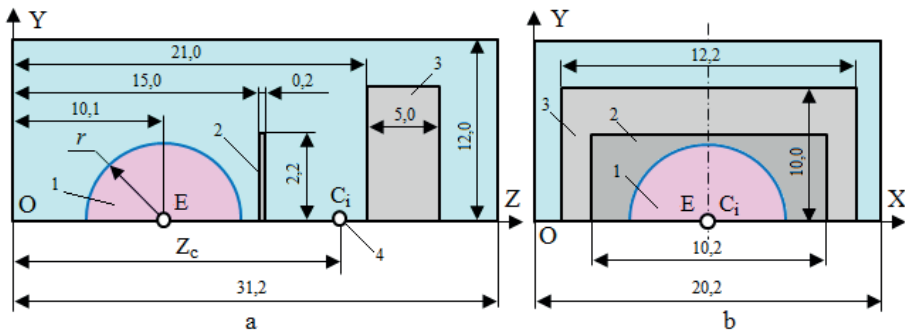


Fig. 6. Map of objects: 1– explosion products cloud; 2 – protection wall; 3 – infrastructure building; 4 – control point (a – central plane YOZ, b – front view plane XOY).

TABLE 3. EXPERIMENT MAIN OPTION PARAMETERS

Emergency parameter	Options				
Explosion power option identifier	O1	O2	O3	O4	O5
Number of failed containers K	1	2	3	4	5
Combustion products cloud size r , cm	200	252	288	317	342

Besides, for each option of explosion power three possible additional scenarios are considered (Table 4): 0 – there are no building and protection wall at the accident site (these experiments are identified by Ox.0 series); 1 – the building is present (Ox.1 series); 2 – the building and protection wall are both installed (Ox.2 series).

TABLE 4. ADDITIONAL SCENARIO OPTION IDENTIFICATION

Parameter	Options		
	Ox.0	Ox.1	Ox.2
Experiment option identifier	Ox.0	Ox.1	Ox.2
Infrastructure building presence	No	Yes	Yes
Protection wall presence	No	No	Yes

To analyze the efficiency of the protection wall, the overpressure is collected in control points C_i (C0–C4) at the distance $Z_c = \{16.1; 17.1; 18.1; 19.1; 20.1\}$ m from the origin of the computational domain is set on the ground along the OZ direction in the width center of the computational area (Fig. 6). These control points are considered as possible location places of service man. The points are located between the wall and the building in order to evaluate overpressure shock impact on human and loading on the exposed side of the building.

Initial conditions in the form of gas-dynamic parameters of combustion products are set in those calculation cells whose centers fell inside the cloud hemisphere [5].

During all the calculation experiments, pressure fields are controlled to analyze the effect of the protection wall and building presence (Fig. 7). The distribution of excess pressure at points of potential personnel location is determined (Fig. 8). It helps to extract the value of the main dangerous factor of maximum overpressure which is used during deterministic evaluation of the consequences caused by explosion wave on exposed serviceman (Fig. 9) and infrastructure building (Fig. 10).

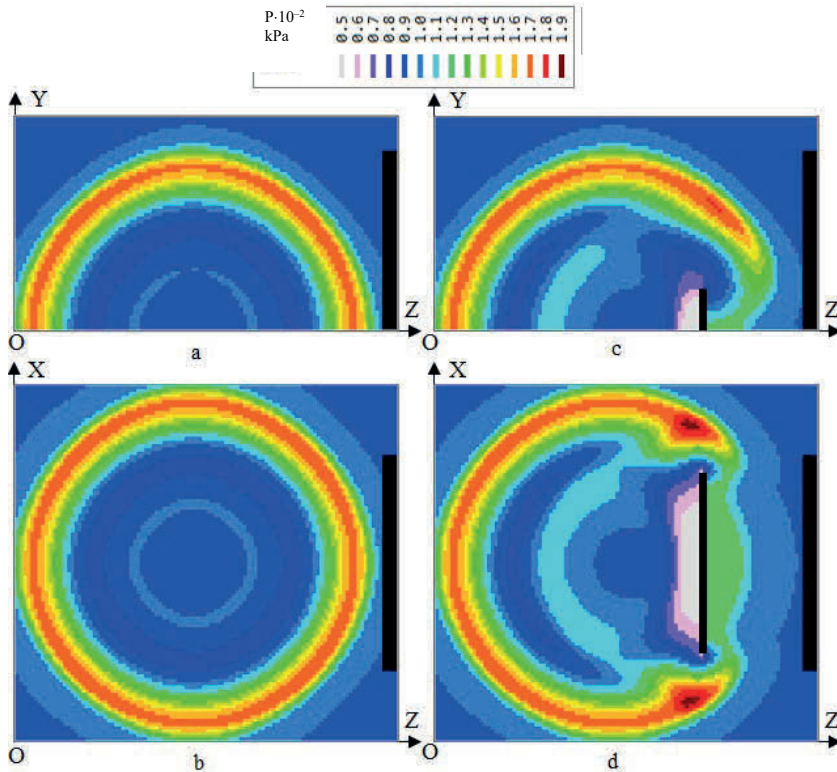


Fig. 7. Pressure fields after 0,0107 s: a, b – option O5.1, c, d – option O5.2 in planes YOZ (in the middle) and XOZ (near the ground) respectively.

The pressure fields show that the blast wave is moving away from the center of the accident, gradually losing its intensity (Fig. 7). In the absence of a protection wall, the wave front has a concentric shape until the moment it meets the surface of the building wall (Fig. 7(a&b)). In the case of installing a protection wall (Fig. 7(c&d)) the wave front is significantly distorted: a pressure wave reflected from the wall appears, a rarefaction zone is formed in front of the wall and a safer zone for humans is generated behind the wall. A pressure wave approaches the building, the intensity of which is significantly reduced by the protective wall.

The overpressure history at control points (Fig. 8 for the most powerful blast option O5) gives a general picture of the blast wave propagation in the area of potential location of service personnel for all three configurations of the presence (or absence) of solid protection wall and infrastructure building objects in the actual calculation area. In the absence of a wall and building (option O5.0), the pressure wave gradually loses its impact load (maximum overpressure) without changing its classic appearance (Fig. 8(a)). In the absence of a protective wall and the presence of a building, the picture of the pressure wave dynamics is similar to the previous one, with the exception of its right part, where the appearance of a wave reflected from the building is visible, which is superimposed on the primary one (Fig. 8(b)). For the control point C4, which is the closest to the building, the peak of the reflected wave exceeded the peak of the primary wave, i.e., at point C4 the situation with the building is more dangerous for humans.

In the case of presence of both, a protective wall and a building, the picture of the dynamics of the pressure wave changes dramatically (Fig. 8(c)). The shock intensity of the primary pressure wave drops significantly. The safest zone for humans is now located at points C0–C3, and the peak of the reflected wave at point C4 now exceeds the peaks of the primary waves at other control points.

The overpressure history in all the control points (Fig. 8) helps to extract the value of the main dangerous factor of maximum overpressure which used during deterministic evaluation of the consequences caused by explosion wave on exposed serviceman in control points (Fig. 9) and infrastructure building (Fig. 10).

Comparing maximum overpressure values in control points (Fig. 9) with threshold limits for different human impact degree (Table 1), it is obvious that all options are not safe for human because ΔP_+ exceeds 10 kPa. At control point C0 (Fig. 9(a)) an explosion with power O1 without protection leads to average consequences (bleeding), O2 – to heavy consequences (concussion), and O3–O5 – to lethal effect. Protection with solid wall leads only to light consequences for all variants of explosion intensity O1–O5. At more distant from the accident epicenter E control point C2 (Fig. 9(b)) an explosion with power O1 without protection leads to light consequences (bruises, hearing loss), O2 – to average consequences, and O3–O5 – to heavy consequences. Installation of the wall leads to light consequences for all variants of explosion intensity O1–O5. At the most distant from the accident epicenter E control point C4, that is the closest to the building, (Fig. 9(c)) an explosion with power O1 and O2 without protection leads to light consequences, O3 and O4 – to average consequences, and O5 – to heavy consequences. Installation of the protection wall leads to light consequences for options of explosion power O1–O4 and to average consequences for option O5. Thus, the wall effectively protects a human from the consequences of average, heavy and lethal level.

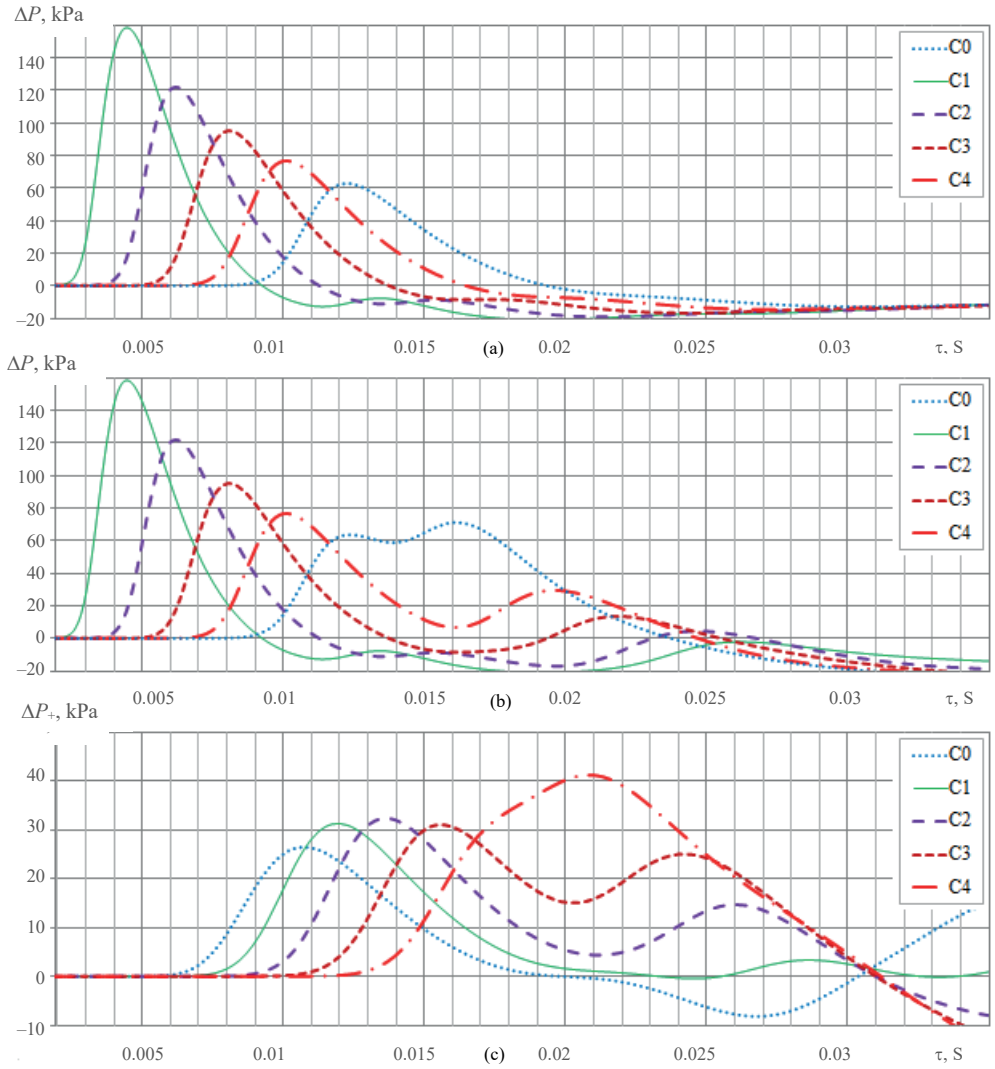


Fig. 8. Overpressure history for explosion power option O5 in control points C0–C4: (a) – variants with the absence of a wall and building; (b) – wall presence; (c) – with wall and building presence.

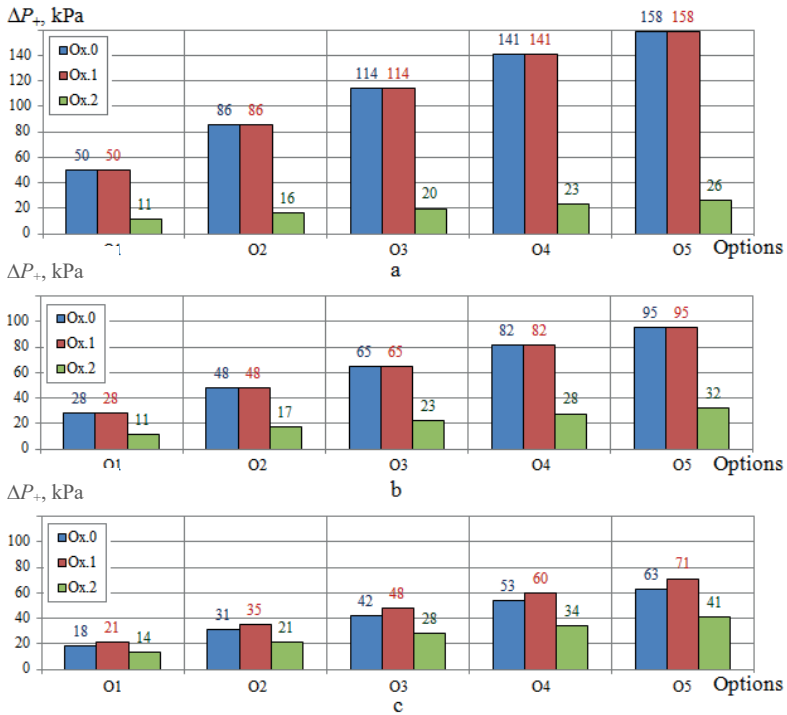


Fig. 9. Maximum overpressure in control points C0 (a), C2 (b), and C4 (c) for different explosion power options O1–O5.

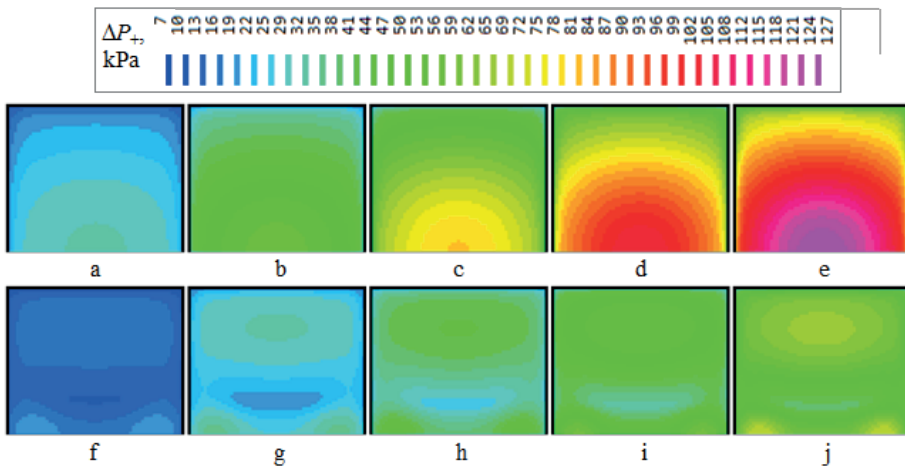


Fig. 10. Maximum overpressure fields on the exposed to an explosion side of the building: a–e options Ox.1; f–j options Ox.2.

The maximum overpressure distribution on the exposed wall of a building provides information about the impact load on the structure and the degree of its destruction, depending on the structural material of its manufacture (Fig. 10). Explosion loads for a series of experiments with a building Ox.1 (without a protective wall) are shown on Fig. 10(a–e), and a series Ox.2 (with the wall) are represented on Fig. 10(f–j). For example, in the absence of

a protective wall (O1.1), the option of using antiseismic concrete will lead to partial weak damage of the building (Table 2), sectional ferroconcrete – significant weak and partially medium damage, brick – significant medium and partially severe damage, and wood – significant severe and partially total destructions (Fig. 10(a)). With the increase of explosion power, the level of destruction is more severe. For instance, for option O3.1 (Fig. 10(c)), the use of antiseismic concrete leads to weak damages of the building, sectional ferroconcrete, brick, and wood – total destructions. For option O5.1 (Fig. 10(e)) use of antiseismic concrete leads to medium building damages, any other material – total destructions.

Installing a protective wall (Ox.2) significantly reduces the load on the building. For example, for the lightest power explosion (O1.2), the option of using antiseismic concrete causes any damages to the building, use of sectional ferroconcrete and break leads to partially weak damages, wood – significant medium and partially severe damages (Fig. 10(f)). With the increase of explosion power, the level of destruction is not as severe as without the protection wall. For instance, for option O3.2 (Fig. 10(h)) use of antiseismic concrete leads to weak damages of the building, sectional ferroconcrete – to severe damages, brick, and wood – to the total destructions. For option O5.2 (Fig. 10(j)) use of antiseismic concrete leads to weak damages, sectional ferroconcrete, brick, and wood – to the total destructions. Such deterministic analysis can be used by safety experts during building construction material choice [38] while projecting the building near the filling station or to forecast the level of destruction of existing building.

6. DISCUSSION

The shock loads on the surface of a building in the zone of an emergency hydrogen explosion obtained as a result of a numerical experiment are significantly enhanced due to the occurrence of a pressure wave reflected from the wall of the building [8], which in general corresponds to expert expectations. Although, for a more detailed analysis and forecast of a building's resistance to blast loads, it is necessary to consider the detailed design of the building and the entire complex of bending and shear stresses in the critical sections of the building, and compare them with the limit values for the structural materials used [37].

The resulting impact loads in places where a person might be located are probably underestimated due to the absence of the human body itself in the calculation area. By approximating it into a solid object (like a building and a protective wall), it is possible to calculate the maximum excess pressure on the surface of the body, taking into account the occurrence of a reflected wave. In this case, one can expect an increase in the impact load on a person.

The installation of a protective wall undoubtedly significantly increased safety at control points and reduced the load on the building. But the protective wall itself is an object of increased maximum overpressure and needs to evaluate the strength, determine the safe thickness and select the manufacturing material [36], which will allow the wall not to collapse.

In the deterministic approach to assessing the level of consequences of a blast wave, only one damaging factor is used – the maximum excess pressure in the blast wave front. Most likely, taking into account the impulse component of the load will lead to an increase in the negative impact on the environment, especially since the probabilistic method [35] makes it possible to take into account both harmful factors when assessing damage to people and buildings in the emergency explosion zone.

Thus, promising directions for further improvement of the proposed methodology are the development of a deterministic approach to assessing the consequences of an explosion by

taking into account the impulse component of the blast load and expanding the map of objects in the computational domain by adding the human body, which will make it possible to obtain more accurate blast loads on it by taking into account the reflected pressure wave.

7. CONCLUSION

Pressure disturbance of the atmosphere at the site of a hydrogen filling station caused by an emergency explosion of hydrogen gas is being studied. A time-dependent spatial hydrogen explosion model based on the system of hyperbolic conservation law equations solved by first order accurate in both space and time Godunov's method is used. A deterministic analysis of the of explosion power influence on level of environmental consequences is performed. The efficiency evaluation of stationary located protection wall is accomplished. Basing on calculated maximum overpressure values at serviceman potential locations and overpressure distribution on the exposed wall surface of the infrastructure building, the conclusions about the degree of injury to personnel and the level of the building destruction are made. It has been shown that the choice of structural material of a building can reduce the degree of destruction, and the installation of a protective wall significantly increases the level of safety in the area of an accident.

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