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Computational Estimation of Protection Wall Height Impact on Hydrogen Explosion Consequences

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***Abstract* – The purpose of the study is to determine numerically the height of a wall designed to protect people from the negative effects of a blast wave, ensuring a specified level of safety. An accidental explosion of a hemispherical hydrogen-air stoichiometric cloud is considered. Near the epicenter of the accident, a person is subjected to shock-impulse loading as the blast wave front passes. A protective wall is installed between the accident's epicenter and the person's location to mitigate the explosion's impact on human health. The wall's transverse size (width) is sufficiently large to ensure that it does not affect the safety of a person whose location remains unchanged. The required height of the protective wall can be determined by solving an inverse problem in gas dynamics, focusing on the movement of a multi-component mixture of hydrogen combustion products through the surface layer of the atmosphere at the accident site. The gas flow disturbed by the explosion collides with the wall barrier, partially reflects off the wall, and moves around it in a vertical longitudinal plane, exerting a baric effect on a person. Solving the combined gas-dynamic and safety problem of human damage by a blast wave helps determine whether the current height of the protective wall is sufficient to ensure a safe level of conditional probability of human damage. A series of computational experiments were conducted for different heights of the protective structure using the mathematical model of a gas explosion and probit analysis. As a result, the relationship between the conditional probability of human injury and the vertical size of the wall was established in the form of a plot. Using this plot, a safety expert can determine the required wall height to ensure a sufficient level of human safety in the event of a hydrogen explosion accident.**

***Keywords* – Blast wavefront; environmental consequences; gas dynamics direct problem; hydrogen explosion; overpressure; probit analysis; shock-impulse load.**

Nomenclature		
X, Y, Z	Coordinates along the Right system axes	–
H	Protective wall height	m
P	Local atmospheric pressure	Pa
ΔP_+	Local atmospheric maximum overpressure	kPa
I_+	Blastwave impulse	kPa·s
P_1	Lethal probability	%
P_2	Eardrum rupture probability	%

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1. INTRODUCTION

The negative consequences of human activity lead to pollution of the planet's atmosphere [1], global warming, rapid melting of glaciers, and rising sea levels, which pose a real threat to humanity's future existence. This encourages scientists to search for alternative energy sources that could replace traditional fossil fuels and not harm the environment [2]. One such alternative is using hydrogen, which is a very energy-intensive fuel. In addition, it is safe in terms of the harmfulness of its combustion products to the planet's atmospheric layer. However, hydrogen is a very explosive gas with a wide range of concentration limits for flammability. Its accidental release into the air leads to the formation of a hydrogen-air mixture with a high probability of explosion. In the event of an explosion, the blast wave quickly spreads through the space of a man-made object, destroying infrastructure and harming the health of people in the area of the epicenter of the accident (Fig. 1) [3].

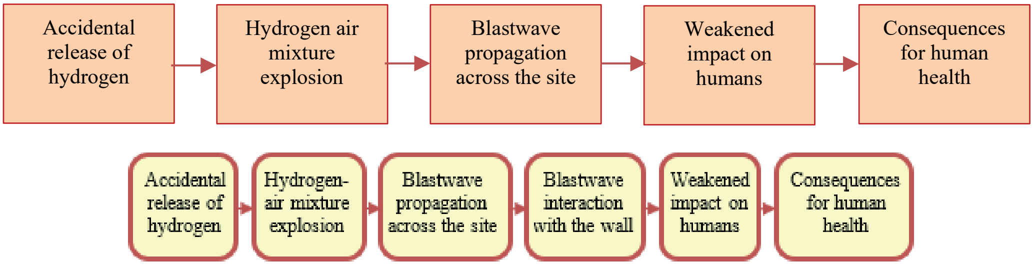

Fig. 1. Blast wave mitigation process flowchart.

Various types of protective structures, such as solid walls and screens of various designs, can significantly reduce the risk of destruction of buildings and injuries to personnel of industrial facilities [4]. Their purpose is to partially reflect the blast wave, thereby reducing the maximum excess pressure and impulse of the compression phase in the front of the blast wave and mitigating the shock-impulse load on the environment. The creation of effective protective structures, the development of their design, the selection of sufficiently strong materials for their manufacture, and their location in the right places to protect personnel during possible accidental release and explosion of hydrogen is a very important scientific and technical problem, which makes it possible to operate potentially dangerous industrial facilities with an acceptable level of explosion risks and a lower probability of negative consequences [5].

To solve this problem more effectively, the use of mathematical modeling of complex physical processes that accompany emergency releases of hydrogen into the atmosphere with the subsequent explosion of a hydrogen-air mixture can help. Adequate models of a hydrogen explosion allow for various computational experiments in which it is possible to change atmospheric conditions [6], the scale of an admixture release, various scenarios of it entering the atmosphere [7], the power of the explosion, check the effectiveness of protective structures and test the correctness of their location. All of the above confirms the relevance of this study, the purpose of which is to numerically determine the height of a solid protective wall that will provide an acceptable probability of human damage by a blast wave based on a mathematical model of a hydrogen explosion.

2. Review of Literature

For analyzing the effectiveness of a protective structure [8], it is necessary to obtain initial information about the change in time of the disturbed pressure state of the atmosphere around the epicenter of the accidental explosion [9], namely at the potential location of the personnel of an industrial facility that has been affected by the shock wave [10], which moves from the epicenter of the accident and gradually loses its intensity [11]. The indicators of the disturbed pressure state of the atmosphere are usually considered to be the maximum overpressure (MO) and the impulse of the compression phase (ICP) in the explosion wavefront [12]. They are factors of negative impact on objects in the path of the shock wave propagation, which must be obtained to assess the consequences of varying degrees of this impact in terms of injuries to people and destruction of structures of infrastructure facilities [13]. This initial information about the pressure disturbance of the flow in the accident zone is contained in the non-stationary pressure field. It can be obtained in two ways: by measuring pressure during a large-scale physical experiment on a model of an industrial facility with the reproduction of a real hydrogen release and explosion under specific climatic conditions or by calculating on the basis of an adequate mathematical model of the explosion [14] taking into account the non-stationary nature of the physical process, the complex terrain [15], the compressibility of the gas-air mixture, etc. Field experiments [16], of course, most accurately correspond to real processes but have a number of shortcomings that do not allow researchers to widely use them in engineering practice for the entire range of possible studies, but rather only to check the adequacy of mathematical models (their validation [17]). The means of mathematical modeling of physical processes associated with the study of the propagation of a blast wave significantly exceed the capabilities of large-scale physical experiments, because they do not have their shortcomings. They are able to reproduce almost infinite variations of atmospheric conditions [6], the complexity of the terrain [15], the power of the explosion [18], scenarios of the release of flammable gas into the atmosphere [3], the design and dimensions of protective structures, the structural materials of their manufacture [18], etc. It is enough to have an adequate mathematical model of a physical process that takes into account all possible nuances of its occurrence and development, and its reliable computer implementation, which is verified [17] and convenient for calculation in the hands of a user who is an expert in the safety of an industrial facility.

Therefore, to determine the safe height of the protective wall at a hydrogen refueling station for vehicles, where an accidental release of hydrogen occurs due to the failure of high-pressure storage vessels and its explosion [19], it was decided to use a mathematical model of the explosion of a gas-air mixture, which meets all the requirements for obtaining initial information about the disturbance of atmospheric parameters during an explosion [10]. The model generates a blast wave that moves from the explosion's epicenter toward the refueling worker's location, gradually losing its power. At the control point where a person is located, it is necessary to control the non-stationary pressure and accumulate information about the damage factors (MO and ICP) to assess numerically human damage's conditional probability. It is obvious that the maximum negative impact will be in the absence of a protective wall [20]. Installing a wall in the path of the shock wave propagation leads to its partial reflection from this obstacle, partial bypassing of the structure, and the continuation of its gradual movement towards the person in a weakened state. Installing the wall will mitigate the shock-impulse load on a person and, therefore, reduce the consequences of the explosion [21]. Thus, by comparing the degree of damage obtained from the model with its permissible level [18], it will be possible to conclude the protective structure's effectiveness (Fig. 2).

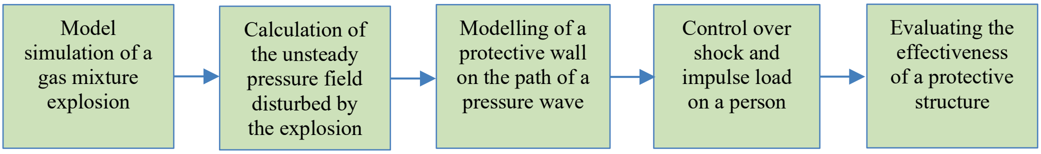

Fig. 2. Flow chart of numerical detection of protection effectiveness.

Numerical studies of the impact of protective structures on the safety of an industrial facility were conducted in [22]. A detailed analysis of the expansion of the flow during the passage of a blast wave around a wall of various designs was conducted in [23]. In [18], a deterministic prediction of the strength of a solid protective wall was conducted to obtain recommendations for selecting structural materials for the wall. The combined problem of the gas-dynamic state in the explosion area and the strength state in the root section of the wall was considered, considering the stress of the bending moment under the influence of gas pressure forces from the explosion [20]. The study is carried out from the point of view of the impact of the explosion power on the consequences for the environment and the strength of the protective wall. In [15], a protective cavity in the ground in the form of a parallelepiped is explored, and the effect of its depth on reducing the probability of human damage by the blast wave is investigated.

As mentioned above, the mathematical model should adequately describe the real process of explosion and shock wave propagation through the space of an industrial site with acceptable accuracy. Mathematical models of the motion of gas mixtures based on the Navier-Stokes equations [24] are too complex, require an additional choice of the turbulence model [25], and require significant computer resources and high qualifications of the expert. In addition, the stated problem does not require detailed information about viscous flow in thin boundary layers near solid surfaces flowing around [26]. It is sufficient to consider the flow core, where the effects of viscosity are practically not manifested. This means that the spatial flow can be modeled using the equations of inviscid gas motion (Euler equations) [27], which significantly reduces the requirements for the density of the computational grid and the required computational resources [3]. Since achieving the goal of the work requires calculating the direct gas dynamics problem for different heights of the protective wall to obtain non-stationary pressure fields, assessing the state of human safety based on the probit analysis model in engineering-acceptable terms, it is considered that the use of a gas-air mixture flow model based on Euler equations is the most appropriate.

3. Blast Wave Propagation Problem Statement

The three-dimensional flow of a two-component gas mixture (combustion products of hydrogen and air) through the space of an industrial site in the XYZ coordinate system is considered (Fig. 3). The OZ axis coincides with the direction of movement along the length of the computational domain, OY – with the vertical direction, along the height of the domain, and the OX axis runs along the width of the site. It is assumed that a pre-formed hemispherical cloud of a stoichiometric mixture explodes so quickly that in its space, the parameters of the explosive mixture practically instantly change to the parameters of the combustion products (instantaneous explosion model [28]). Since the viscous flow in the boundary layers is not considered, the computational grid can be evenly divided along the coordinate axes to obtain identical cubic cells.

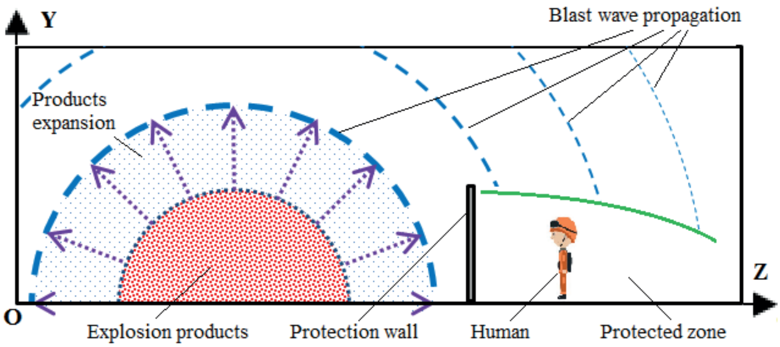

Fig. 3. Scheme of forming a safe zone during a gas explosion.

The shock wave generated by the expansion of compressed high-temperature hydrogen combustion products spreads across the site, gradually losing its power. At some point, it passes by the person's location, exerting a shock-impulse load on him. The consequences of this negative impact depend on the values of the MO and ICP in the front of the blast wave. The option without human protection is the most dangerous for him. Installing a protective solid wall between the explosion's epicenter and the person can mitigate the intensity of negative factors affecting the person. The probability of damage will correspond to an acceptable level of danger at a certain value of the wall height. In this work, the criterion for determining the state of human safety is the conditional probability of damage (fatal outcome and rupture of the eardrum), and its safe level is set at a probability level of 30%. Thus, a protective wall of a certain height can create a safety zone for a person behind the wall at the control point.

4. Methods and Procedures

4.1. Model Equations and Boundary Conditions

To obtain initial information about the disturbed state of atmospheric air pressure, a system of equations of motion of a mixture of ideal gases of hydrogen and air combustion products is considered. These equations reflect the laws of conservation of mass, momentum, and energy of the mixture, which are supplemented by the equation of conservation of the combustion products component. The equation of state of the mixture is used to close the system [3]. The Godunov integral-interpolation method, explicit in time [29], is used to solve the system of equations. Each direct gas dynamics problem calculation continues until the explosion wave leaves the actual space. The boundary conditions traditional for a predominantly subsonic flow are set: at the entrance to the calculation space - entropy function, flow velocity, direction angles of the velocity vector; at the exit – back pressure; on the surfaces of solid bodies (wall, ground) – no-flow conditions. The parameters of hydrogen combustion products with a hundred percent concentration are taken as the initial conditions in the cloud region. In the rest of the calculation area, the parameters of the atmosphere undisturbed by the explosion are specified (the gas-dynamic calculation is not performed in the area inside solid solids).

4.2. Gas Explosion Simulation

Within the framework of using the explicit Godunov method, the hydrogen explosion was simulated by setting the initial conditions in the hemispherical region of the hydrogen-air cloud with a stoichiometric hydrogen concentration. Considering the extraordinary speed of the chemical reaction, it was assumed that the combustion process occurs instantaneously. This allows, at the moment of explosion in the cloud cells, to replace the parameters of the explosive mixture with the parameters of the hydrogen combustion products, thereby generating a shock wave that moves from the epicenter of the accident and affects the environment. The explosion model was validated on experimental data and the results of other explosion models for hydrogen and propane [10].

4.3. Evaluation of the Explosion Consequences Degree

Sometimes, a deterministic approach is used to assess the effects of a blast wave on the environment. It consists of comparing the maximum values of excess disturbance parameters (for example, MO) obtained from the explosion model and comparing them with the threshold values of these parameters obtained experimentally for different degrees of damage (destruction). However, this approach does not allow assessing such characteristics as the risk of consequences, considering the total risk from a combination of emergencies (toxic substance release, explosion, fire). Therefore, it was decided to use a probabilistic approach [15], which is based on the probit analysis model. The essence of the approach is to obtain dangerous parameters from the explosion model (excess pressure and impulse of the compression phase of the shock wave), calculate dangerous factors in time (for an explosion, these are MO and ICP in the shock wave front in Fig. 4), which are components in the ratios for calculating probit functions for different levels of human damage consequences (bruise, RBP, lung rupture, fatality). This probit function allows for the calculation of the conditional probability of corresponding damage, which can be used in risk-based systems to assess the safety of industrial enterprises.

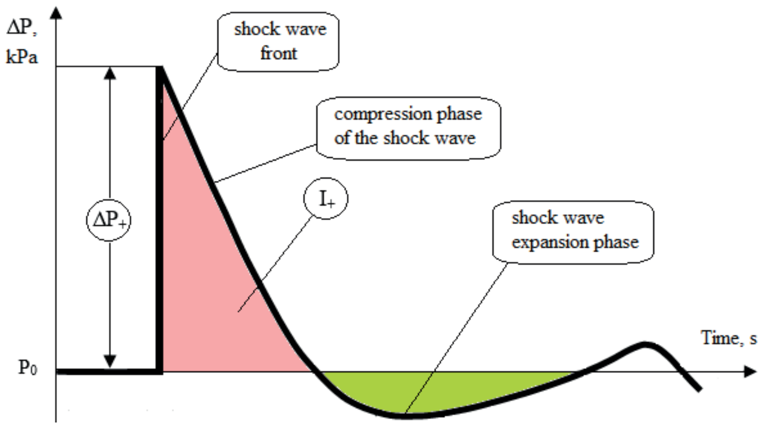

Fig. 4. Graphical representation of dangerous factors of the consequences of shock wave damage.

Calculations according to the probit analysis model are built into the computer explosion model, which solves the combined direct gas-dynamic problem of the flow of the gas mixture in the site's space and the safety problem of determining the consequences of damage to the environment by the blast wave. As a result, the solution represents the field of conditional probability of damage, which is used to extract the probability value at the point of personnel location. In this work, the values of the conditional probability of the RBP and the SN are used to assess the effectiveness of a protective wall of a certain height.

5. RESULTS

According to the task, the explosion occurs at the site of a hydrogen refueling station, where several high-pressure vessels for storing gaseous hydrogen fail. The location of the hemispherical cloud of hydrogen combustion products, the protective wall with a height of *H*, the human safety control point, the dimensions and distances to the epicenter of the explosion, and the center of the coordinates of the area are presented in Fig. 5. The initial parameters of the hydrogen combustion products in the cloud are as follows: 3450 K, 900 kPa adiabatic ratio is 1.24, and molar weight is 24.41 kg/kmol. A uniform computational grid with cells is used, all dimensions of which are 0.2 m. Evidently, the shock wave will go around the wall barrier not only in the vertical plane, where the height of the wall will have a significant effect but also in the horizontal plane, enhancing the damage at the control point. To avoid the wall width's influence on the safety state at control point C, its value is taken as the maximum for the computational space under consideration. Similarly, to minimize the influence of the wall thickness (the dimension along the OZ axis), its value is taken as the minimum possible for a given computational grid.

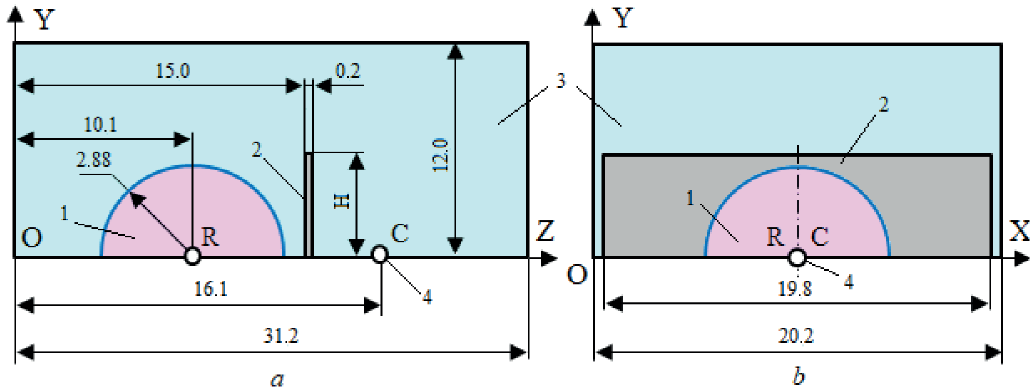

Fig. 5. Location of objects on the site: 1– initial chemical reaction products cloud; 2 – protective wall; 3 – undisturbed air; 4 – location of a person (a – central cross-section YOZ, b – frontal view in vertical plane XOY).

To obtain the value of the height of the protective wall that will ensure an acceptable level of human safety at the control point ($P_C < P_a = 30$ %), a series of computational experiments were conducted, each of which was a solution to the combined direct problem "gas dynamics-safety" for a protective wall of a certain height (Table 1) from 0.0 m to 3.0 m with a step of 0.2 m.

TABLE 1. CALCULATION SERIES DESIGNATION

Calculation characteristics	Series of calculations		
Calculation ID	C0	C1	C2 … C15
Height of protective wall, m	0.0	0.2	0.4 … 3.0

In fact, the inverse problem of finding the safe height of the wall was solved by solving a series of direct “gas dynamics-safety” problems (Fig. 6).

Obtaining one solution took approximately 20′ of the central quad-core Intel Core™ i7 processor with subsequent graphical processing of the obtained results in spreadsheets.

During each solution of the direct problem "gas dynamics-safety" for one of the options for the wall height C0–C15, a non-stationary pressure field was calculated (Fig. 7 and Fig. 8). It is obvious that in the vertical plane, the shock wave goes around the protective wall, partially reflecting from it (Fig. 7). In the horizontal plane near the ground, it is visible how the shock wave, colliding with the wall, spreads to the sides, trying to bypass it (Fig. 8). But the width of the wall is large enough to prevent the wave from going around the wall from the sides, in order to minimize this impact on the state of human safety at the control point behind the wall.

Initial information about the non-stationary spatial distribution of pressure serves as the basis for searching for fields of negative factors: MO and ICP.

The values of the negative factors of the influence of pressure disturbances due to a hydrogen explosion are used in probit analysis to calculate the consequences of human injury in the zone of an accidental explosion, namely the conditional probability of rupture of the eardrums (Fig. 9).

The resulting fields of probability of damage can be further used to calculate the risks of damage by multiplying the probability values by the frequency of occurrence of this type of accident.

A comparative graph of overpressure history at the control point R for all variants of the height of the protective wall C0–C15 is presented in Fig. 10.

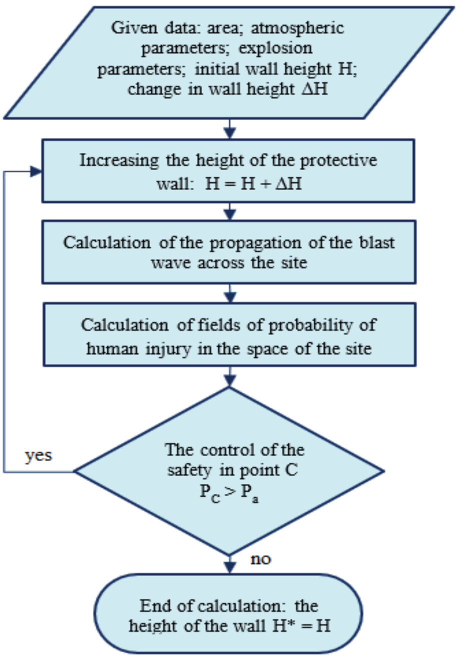

Fig. 6. Scheme for calculating the safe height of a protective wall.

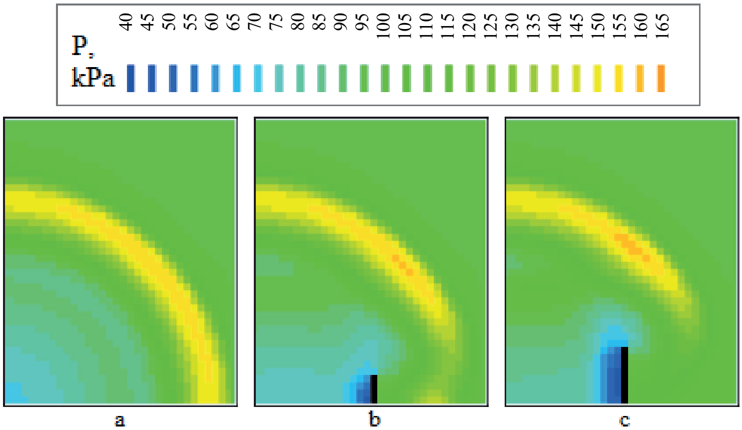

Fig. 7. Static pressure 0.011046 seconds after the accident start (YOZ): a, b, and c – tests C0, C6, and C12.

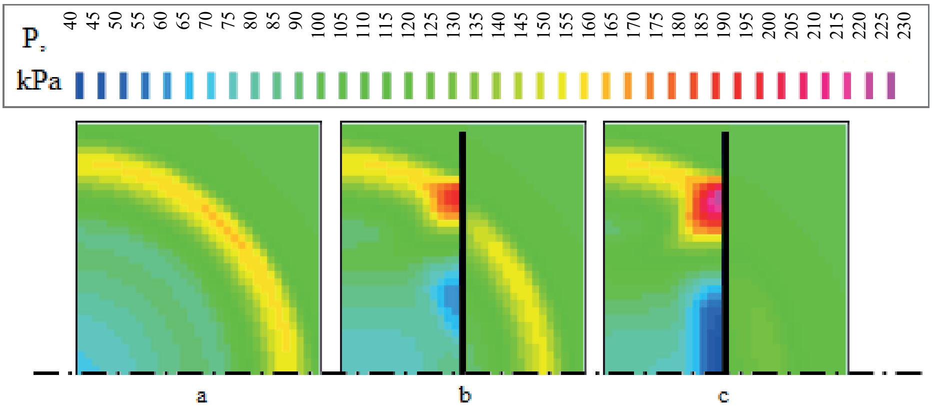

Fig. 8. Static pressure 0.011046 seconds after the accident start (XOZ): a, b, and c – tests C0, C3, and C9.

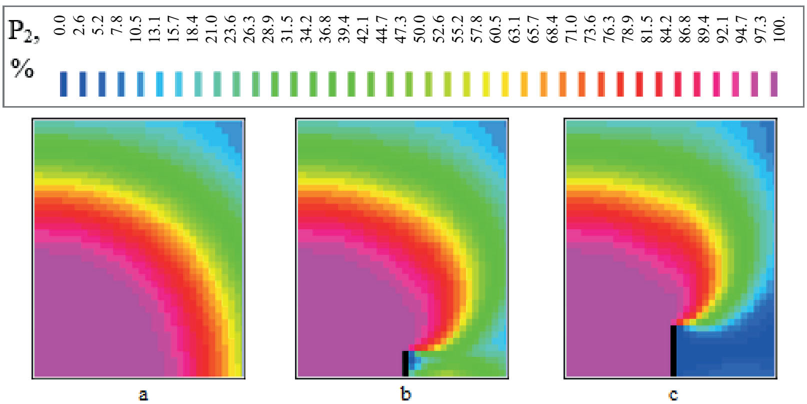

Fig. 9. Eardrum rupture probability (YOZ): a, b, and c – tests C0, C6, and C9.

Information on the change in pressure at the control point allows finding the maximum excess pressure as seen in Fig. 11 and the impulse of the compression phase at the control point as depicted in Fig. 12, and, using probit analysis, to construct comparative diagrams of the probability of human damage for eardrum rupture probability (see Fig. 13) and lethal probability (see Fig. 14).

Analysis of the fields of conditional probability of damage allows for the observation that with the increasing height of the protective wall, the protected zone where it is safe for a person to be during an emergency hydrogen explosion becomes larger.

The pressure change graph in Fig. 10 and comparative diagrams of dangerous factors at the control point (for MO in Fig. 11 and ICP in Fig. 12) indicate a significant influence of the wall height on their values: an increase in the height of the protective structure obviously reduces MO and ICP from the maximum values for the variant without protection C0 to their safe values in the latest calculation variants.

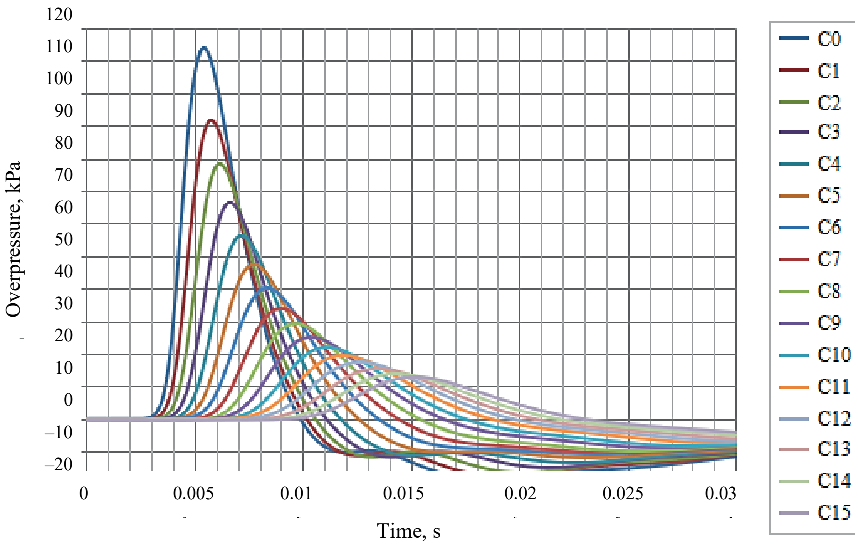

Fig. 10. Time distribution of excess pressure at the control point for different heights of the protective wall.

Since the values of dangerous factors of the impact of the blast wave on the human body are components for calculating the probability of damage, it is obvious that with increasing wall height, the conditional probability of rupture of the eardrums (Fig. 13), which depends only on MO, and the probability of lethal outcome (Fig. 14), which also depends on the ICP in the blast wave front, gradually decreases.

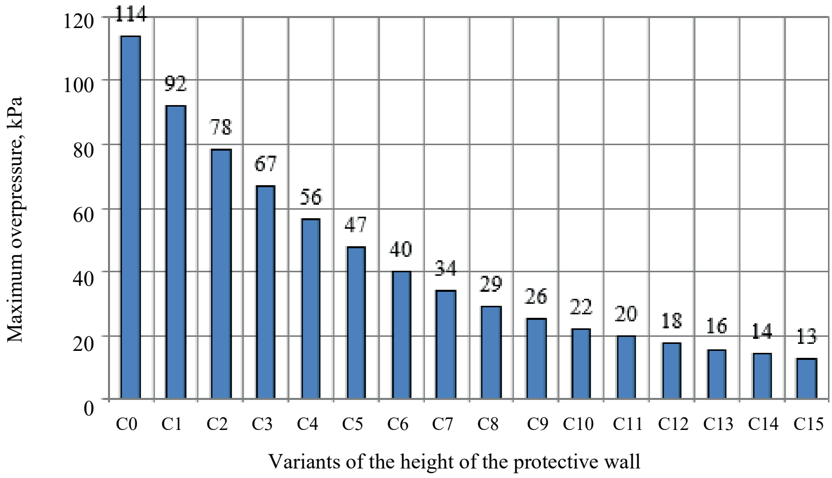

Fig. 11. Maximum overpressure distribution at the control point for different protective wall heights.

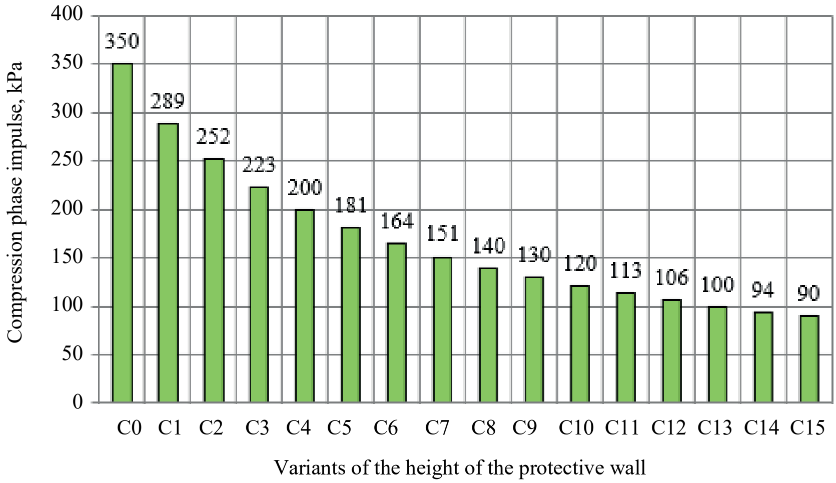

Fig. 12. Explosion wavefront impulse distribution at the control point for different protective wall heights.

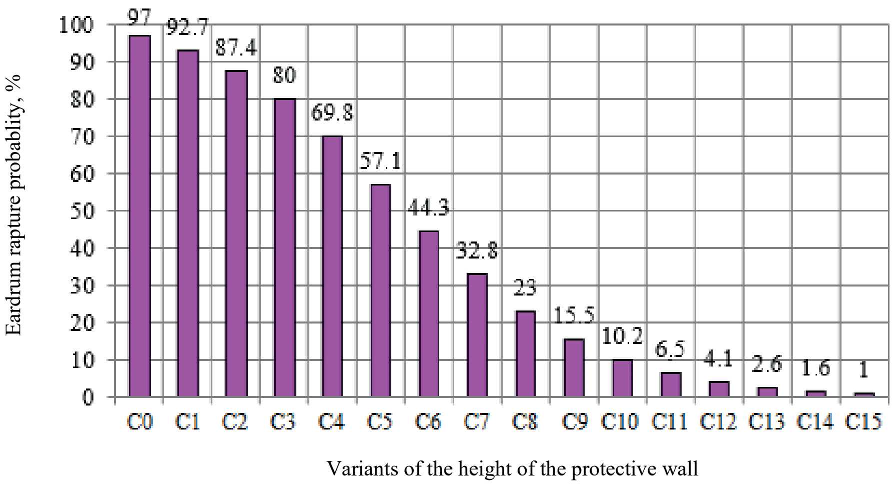

Fig. 13. Eardrum rupture probability distribution at the control point for different protective wall heights.

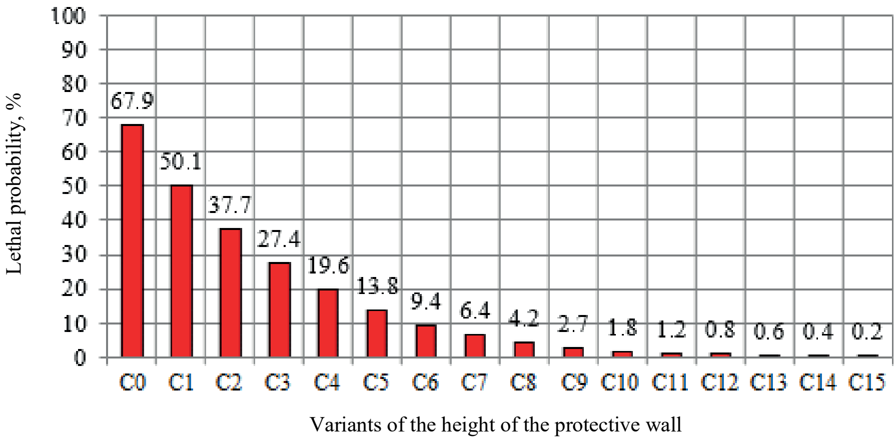

Fig. 14. Lethal probability distribution at the control point for different protective wall heights.

Suppose the dependence of the conditional probability of human injury for both types of consequences is presented on a general graph, and an allowable level of injury of 30 % is imposed. In that case, the required minimum height of the protective wall can be determined from the plot. Thus, to ensure acceptable safety from the point of view of the conditional probability of rupture of the eardrums, the wall should be higher than 1.45 m. In contrast, from the point of view of the conditional probability of a fatal outcome, the height of the wall should be higher than 0.55 m (see Fig. 15).

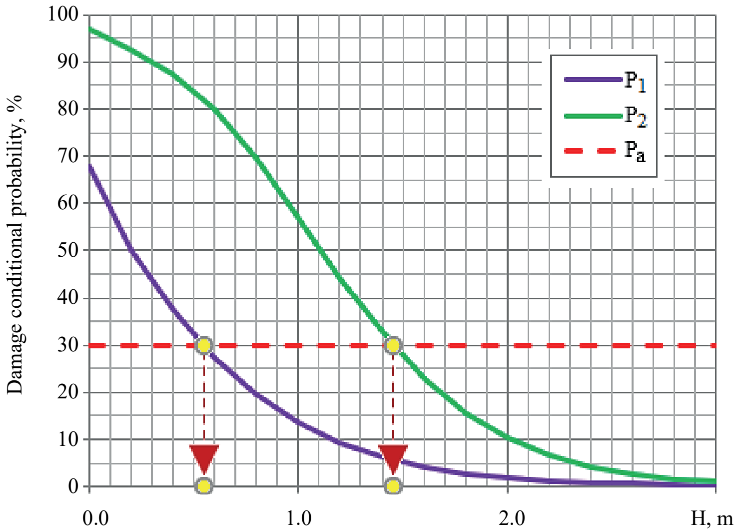

Fig. 15. Determining the safe height of a protective wall at a given minimum permissible probability of damage: P_1 – lethal probability; P_2 – eardrum rupture probability; P_a – a given acceptable probability.

6. Discussion

The computational technology presented in the paper for determining the height of a protective wall to achieve a given level of safety at the control point of a potential human location during an emergency hydrogen explosion at a man-made facility has the characteristics of an inverse problem, which is solved by finding solutions to numerous direct problems "gas dynamics-safety". Suppose you have a sufficiently fine computational grid. In that case, this algorithm for finding the height of the wall can be automated using, for example, the method of simple iterations so that the solution converges to one root. The calculation of the MO does not cause any difficulties when calculating the flow by the Godunov method explicit in time, one of the properties of which is a small-time step, which is due to its limitation under the Courant-Friedrichs-Lewy (CFL) convergence condition. If, for the settlement calculations, this is a disadvantage that increases the convergence time to the solution, then for the non-stationary calculation "gas dynamics-safety" it is useful because it helps to more accurately calculate the MO by searching for the maximum value during the iteration process and integrate (for example, by the method of rectangles) the ICP in the front of the explosion wave. If the algorithm for determining dangerous factors for probit analysis does not cause difficulties for open space because the shape of the shock wave does not differ much from the classical one, then for calculations of the internal flow (explosions in tunnels [28]) the proposed calculation of the ICP can lead to unpredictable results, since the presence of reflection waves can distort the compression phase of the total pressure wave.

7. Conclusion

The paper proposes a computational technology for finding the height of a wall to protect a person from the negative impact of a shock-impulse load due to the passage of an explosion wave that occurred at an industrial site of a gas station as a result of an emergency release of hydrogen into the atmosphere with its subsequent explosion. The technology essentially allows you to find a wall that is so high that it is installed between the explosion's epicenter and the person's location, which would provide an acceptable level of safety. In fact, the solution to the inverse problem is found by searching for a number of solutions to direct compatible problems "gas dynamics-safety" of a non-stationary gas mixture flow after an explosion and probit analysis. The developed technology can be used by risk experts to assess the safety of industrial enterprises where explosive gases are involved and to develop and verify the effectiveness of structures to protect personnel from the effects of emergency explosions.

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