Parameters of shock waves during detonation and deflagration of fuel-air clouds

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Abstract. Methods for calculation of shock wave (SW) parameters used in industrial safety to assess the effects of explosions are considered. It is shown that existing methods do not provide the necessary accuracy of calculations. For the correct calculation of wave parameters, it is proposed to use high-accuracy CFD methods. The dimensionless dependences of pressure on distance are obtained for estimation of SW parameters, which allow to improve prediction of the effects of accidental explosions.

1. Introduction
Calculation of the parameters of the SW generated by the explosion of fuel-air clouds formed in the atmosphere after emergency release is a necessary element in the assessment of the consequences and in the risk analysis. There are various approaches to estimating the parameters of such SW: from experimental studies [1] to numerical calculations [2-5]. In recent years, the development of numerical methods and hardware has allowed to create computational technologies [6-8], which allow to simulate the generation of shock waves in various conditions. The main problem in this case is the achievement of high accuracy in the calculation of SW parameters. Accuracy of a few percent in SW overpressure can be considered acceptable.

It should be understood that high-accuracy calculations of multidimensional problems of SW propagation in a cluttered space for various energy release modes, including non-stationary deflagrations, require large computational resources and calculation time. Therefore, such calculations can be implemented, as a rule, in individual situations when it is required to investigate specific loading schemes.

More simpler methods are required to categorize objects or to make serial risk indicator calculations (such calculations within the framework of one project may require tens of thousands runs). In this case, simple parametric dependences are required, usually connecting the amount of released energy with excess pressure at a given distance. Examples of such approaches are [9-11]. The pressure dependences on the distance used in these approaches were obtained either in experiments (including the detonation of condensed explosives) or by one-dimensional numerical calculations. These and similar approaches were put into practice decades ago.

Today, there is a need to update these techniques, and first of all, the methodology [11], which is widely used in our country. It is necessary to clarify the formulas [11], primarily in terms of the range
modern requirements oblige to calculate the SW parameters in a wider range of overpressures. On the other hand, of interest is not only the overpressure determination, but also the knowledge of the velocity behind the wave (which is especially important for assessment of the effect of waves on mast structures, power lines).

Today there are no applied tools to perform such work. The development of such tools is the subject of this work.

2. Problem statement
The problem is solved in the following one-dimensional formulation.

The considered flows during detonation or deflagration of a spherical cloud of a fuel-air mixture in air are characterized by both smooth flow regions and discontinuities. Regions of smooth flow can be described by a system of equations in Lagrangian mass coordinates, expressing the laws of conservation of mass, momentum and energy:

\[ V = r^{\alpha - 1} \frac{\partial r}{\partial m}, \]  
\[ \frac{\partial u}{\partial t} = -r^{\alpha - 1} \frac{\partial p}{\partial m}, \]  
\[ \frac{\partial E}{\partial t} = -\frac{\partial (r^{\alpha - 1} pu)}{\partial m}. \]  

Here \( r \) – spatial coordinate (radius), \( t \) – time, \( V = 1/\rho \) – specific volume, \( \rho \) – density, \( u \) – velocity, \( m \) – lagrangian coordinate, \( \alpha \) – geometry factor (\( \alpha \)), \( p \) – pressure, \( E \) – the specific total energy equal to the sum of the thermal component and kinetic energy.

The system of equations (1) - (3) is closed by the equation for pressure calculation using specific internal energy.

The combustion processes of deflagration and detonation are characterized by a change in temperature and composition in the process of chemical preemptions, and this should be taken into account in the mathematical model. There are various ways to take this factor into account. The most fundamental approach is the kinetic modeling of chemical reactions (detailed kinetic schemes, globally kinetic schemes). This approach requires reliable knowledge of the constants of chemical reactions and the corresponding computational algorithms. However, there is a simpler approach to such modeling. This is a calculation of thermodynamically equilibrium or partially equilibrium compositions when the gas dynamics is considered [12].

In this paper, we use the assumption of the existence of thermodynamic equilibrium in the reaction products. For this, the thermodynamic code TDS [13] is used. Calculations by this code allow to obtain detonation and deflagration characteristics. For example, for a stoichiometric mixture of propane with air, the parameters in the Chapman-Jouguet (CJ) plane obtained by the thermodynamic calculation of [13] are as follows:

- detonation velocity – 1761.87 m/c;
- pressure in the CJ plane – 1.757 MPa;
- density in the CJ plane – 2.16 kg/m³;
- mass velocity in the CJ plane – 784.162 m/c;
- adiabatic index in CJ plane – 1.181;

It should be noted that the adiabatic exponent in detonation products may change during their expansion, which in the general case must be taken into account in the model. In this paper, to take into account this fact, we used the approximate assumption of a change in the adiabatic renderer by the isentropic expansion. For example, for the mixture of propane and air mentioned above, according to
thermodynamic calculations, the adiabatic exponent for isentropic expansion from the CJ plane can be described by the following equation:

\[ \gamma = -0.0045 \rho^3 + 0.0379 \rho^4 - 0.1303 \rho^5 + 0.273 \rho^2 - 0.2417 \rho + 1.2978. \]  

(4)

As noted above, in the problems under consideration there are discontinuity surfaces. Such discontinuities include: contact discontinuities, shock waves, combustion fronts and detonations.

These discontinuities are considered as surfaces on which the integral laws of conservation of mass, momentum and energy are satisfied in the form of:

\[ \rho_b u_b = \rho_a u_a, \]  

(5)

\[ p_b + \rho_b u_b^2 = p_a + \rho_a u_a^2, \]  

(6)

\[ \frac{u_b^2}{2} + i_b + Q = \frac{u_a^2}{2} + i_a. \]  

(7)

Here \( \rho_b, u_b, p_b, i_b \) - the density, velocity, pressure, and enthalpy in front of the discontinuity surface, and \( \rho_a, u_a, p_a, i_a \) - the density, velocity, pressure, and enthalpy after the discontinuity surface, \( Q \) - discontinuity.

Relations (5) - (7) are written for the coordinate system in which the front is at rest. Accordingly, \( u_b \) is the velocity of the discontinuity relative to the medium before the discontinuity. For detonation, this is the detonation velocity; in the problems under consideration, the detonation velocity in the CJ mode. For deflagration, this is the flame velocity specified either by laminar or by turbulent flow characteristics. For a shock wave, this velocity is determined by the parameters of the medium before and after the rupture.

The system of written equations is supplemented by boundary and initial conditions. As the boundary conditions, the center of symmetry and stationary air in the standard state were chosen (the last condition was valid until a disturbance from the point of energy release arrived at a remote point on the boundary). As the initial conditions, we selected the standard conditions for air and unburned mixture and the detonation parameters of deflagration in the initiation region.

3. Numerical method

The solution of the system (1) - (3) in the one-dimensional case is carried out according to the “cross” scheme [14]. When one can use the scheme [14], contact discontinuities are calculated without distortion: the boundary of the difference cells exactly coincides with the contact discontinuity, therefore, the density jump is infinitely thin. The calculation of shock and detonation waves according to [14] is performed with distortions: the solution contains oscillations, front smearing. For calculation of the combustion fronts, scheme [14] is not intended at all.

To obtain more accurate solutions in the case of modeling flows with various kinds of discontinuities, we used the explicit localization method [2, 3].

In this case, the discontinuity is considered as the boundary of two neighbor difference cells, in one of which the initial mixture is located, and in the other - “products”, the initial mixture that was transformed during the transition through the boundary: compressed in the shock wave, burned in the flame front, or reacted at the detonation front. This boundary moves with a certain speed and through this discontinuity part of the mass from the cell before the front passes into the cell behind the front, along with the mass, both momentum and energy pass through the front also.

The speed of this discontinuity is determined:

- for CJ detonation, as the detonation velocity obtained, for example, from a thermodynamic calculation;
• for a shock wave, as a result of solution of the problem of a discontinuity decay with states before and after the discontinuity (standard Riemann problem);
• for the flame front, as a result of solution of the problem a discontinuity decay at the combustion front with states before and after it; in this case, the resulting solution includes a consideration of a flame front (at which relations (5) - (7) are satisfied), a wave traveling over the initial mixture before the front, and a wave traveling over the products after the flame front.

Accordingly, the flows of mass, momentum and energy are calculated according to (5) - (7) with those parameters before and after the rupture that arise during decay, i.e., in the general case, this parameters are different from the initial parameters in the cells.

It should be noted that when, for example, detonation approaches the cloud boundary, a restructuring of the difference grid is necessary. The algorithm for this adjustment is shown in Figure 1. From Figure 1 it is seen that before the detonation approaches the cloud boundary (see Figure 1 (a)), there are two cells with detonation products (purple) and the initial mixture (gray) in the vicinity of the discontinuity.

As the discontinuity moves, new mesh cells join to the cell before the front, and another cells separate from the cell behind the front. This allows cells before the discontinuity not to decrease in size smaller than a certain size. And this procedure allows cells after the discontinuity not to increase in size larger than a certain size. In this work, two cells before and after the front are formed from three ordinary cells.

Using the method of explicit localization described above (and especially the explicit localization of shock waves) allows one to calculate with high accuracy the parameters of SW, especially at a far distance, where the waves have relatively small overpressure.

4. Verification of the developed method
To verify the developed method, the following experimental data were selected [1]. In these experiments, the parameters of the shock waves generated by detonation of spherical hydrogen-air clouds with a volume of 10-15 m$^3$ were investigated. The following data set was chosen as a test:
• a stoichiometric mixture of hydrogen with air in a spherical rubber shell;
• volume 10 m$^3$;
• cloud radius 1.34 m.

The results of comparing the calculation with the experiment are presented in Figure 2.

As one can see from the comparison, the proposed approach describes the real physical processes with good accuracy.
5. Calculations of various combustion modes and detonation

KAs noted above, one of the urgent tasks is to develop simple prognostic models for assessing the effects of accidental explosions. One of such models is presented in [11]. According to [11], the pressure during combustion/detonation of a cloud can be defined as a dimensionless function of overpressure versus a dimensionless distance. These dependencies are shown in Figure 3.

Each of the deflagration lines in Figure 3 consists of two sections: the real part used in the calculations (solid line) and the fictitious part, unused in the calculations, corresponding to the unified formal record of the graphical dependence in Figure 3 (dashed line). The fictitious section is cut off from the real one by the fact that it is impossible to exceed the pressure in SW from detonation compare to deflagration. The dependence of the overpressure in the SW generated by detonation on the distance acts as such a “dividing line”. In Figure 3, this line is dark blue. According to [1], the dependence corresponding to this line is valid up to a dimensionless distance of 24. Further, the shape of this dependence is incorrect: in Figure 3, this appears as a bend of the dark blue line up.

Using the approach developed in this paper, new dependencies were proposed. They are based on the approximation of many different types of fuel-air mixtures used in calculations. The approximation is constructed so that all the calculated curves are below the proposed approximation.

The constructed approximations are as follows:
\[ \ln(P_x) = -0.9274 - 1.5415 \ln(R_x) + 0.1953(\ln(R_x))^2 - 0.0285(\ln(R_x))^3, \quad 0.2 \leq R_x \leq 50 \] (8)

\[ \ln(I_x) = \begin{cases} 
-3.3228 - 1.3689 \ln(R_x) - 0.9057(\ln(R_x))^2 - 0.4818(\ln(R_x))^3, & 0.2 \leq R_x \leq 0.8 \\
-3.2656 - 0.9641 \ln(R_x) - 0.0108(\ln(R_x))^2, & 0.8 < R_x \leq 50 
\end{cases} \] (9)

Dependence (8) is shown in Figure 3 by a light blue line.

The constructed dependencies (8-9) can be used in regulatory documents for the assessment of consequences and risk analysis.

6. Conclusions
An approach to calculation of parameters of shock waves generated by combustion or detonation is proposed and implemented in the form of computational technology. The approach is implemented in one-dimensional geometry, while all gas-dynamic discontinuities — the detonation wave, the deflagration front, and the shock wave — are considered explicitly as infinitely thin discontinuities on which the conservation laws in the integral form are satisfied. This approach allowed us to calculate the parameters of shock waves with maximum accuracy. Using the proposed approach, universal dependences of dimensionless pressure and dimensionless pressure impulse in shock waves on the dimensionless distance during detonation or combustion of fuel-air clouds were obtained. The obtained dependencies can be used in regulatory documents in the field of industrial safety.

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