Effect of an inert gas layer on an initiation of detonation in a hydrogen-air mixture.

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Abstract

The problem on screening of the initiation source by an inert gas layer is studied numerically. A finite difference method based on the Godunov scheme is used for computations. The results of solving the problem on explosion of a spherical trinitrotoluene charge surrounded by a stoichiometric hydrogen-air mixture containing a spherical layer of a pure air are presented. In the case, when the layer is in contact with the charge, for various values of the charge radius, the values of the critical dimension of the layer such that no self-sustaining detonation occurs when the dimension of layer exceeds this critical value are calculated. A linear dependence of the critical radius of the layer on the charge radius is revealed and theoretically substantiated. An analytic expression that demonstrates the validity of this linear relation for any explosives is obtained. In the case, when the layer is inside the mixture, it is established that the critical thickness of the air layer monotonically decreases, as the distance of the layer from the charge increases, until it reaches the value independent of the charge dimension. On the basis of the results of calculations, the approximate analytic relations for the critical parameters are obtained. They allow one to determine, for a fixed charge, the critical thickness of the layer as a function of its spatial position and, vice versa, to determine the critical energy of the charge for a layer of given thickness that is situated at a given distance from the charge.

Introduction

As is known, in order for the detonation to be initiated by an explosion in a combustible gas mixture, it is necessary that the released energy exceeds a certain critical value. When the energy is lower than the critical value, an overdriven detonation arising immediately after the explosion is gradually destroyed, and the chemical reactions occur in a slow combustion wave. Experimental and theoretical investigations of explosions of various nature have shown that the value of the critical energy depends on the manner and duration of energy release, geometrical dimensions of the source, and the initial parameters of the state of a combustible mixture [1-8]. If the mixture is inhomogeneous and the fuel is distributed over the space according to a certain law, the possibility of implementation of a self-sustaining detonation wave requires additional analysis. For example, the following three types of the flow development are possible in the air medium where hydrogen is distributed by the Gaussian law [9]: a rise of detonation followed by its destruction, the realization of combustion alone for any explosion energy, and the generation of a quasi-detonation mode when the combustion is localized behind a leading shock wave that propagates at the velocity much lower than the Chapman-Jouguet velocity under given conditions. According to the results obtained in [10,11], detonation also may occur for subcritical values of the explosion energy if a certain perturbation is introduced into the gas flow by a rigid shell that envelops an explosives charge and is destroyed in a certain period after its collision with a leading shock wave. The problem on screening of the initiation source by an inert gas layer is of essential interest. In this case the blast wave is damped after passing through the inert medium and its intensity may be insufficient to initiate self-sustaining detonation on entering the combustible mixture. The results of solving the problem on explosion of a spherical trinitrotoluene charge surrounded by a stoichiometric hydrogen-air mixture containing a spherical layer of a pure air are presented below.

Statement of the problem

Suppose that an explosion of a spherical charge of a solid explosive with radius r_0, density ρ_T and specific heat release Q_T occurs at the initial moment $t = 0$. It assumed that the explosive is immediately transformed into gaseous state with high pressure p, temperature T, and specific enthalpy h, which are related by the following equation of state [12]:

$$h = p\gamma/(\gamma - 1)\rho, \quad \gamma = 1 + (0.09 + 2.0\rho^2)/(0.3 + \rho^2), \quad [\rho] = g/cm^3$$

It is assumed that a part of space outside the charge in the form of a spherical layer with the internal radius R_1 and external radius R_2 is filled by air, whereas the remaining part is filled by a stoichiometric hydrogen-air mixture. The model of an ideal and perfect gas is used to describe the medium. In the usual notation, the system of equations describing flow with spherical waves is applied in the form:

$$\frac{\partial(\rho \mathrm{r}^2)}{\partial t} + \frac{\partial(\rho v r^2)}{\partial r} = 0$$

$$\frac{\partial(\rho r^2 v)}{\partial t} + \frac{\partial((\rho v^2 + p) r^2)}{\partial r} = 2pr$$

$$\frac{\partial((\rho v^2/2 + \rho h - p) r^2)}{\partial t} + \frac{\partial((v^2/2 + h)\rho v r^2)}{\partial r} = 0$$

$$\frac{\partial(\rho n_i r^2)}{\partial t} + \frac{\partial(\rho n_i v r^2)}{\partial r} = \rho\omega_i r^2$$

The equations of state for the hydrogen-air mixture have the usual form:

$$p = \rho RT/\mu, \quad h = \sum n_i h_i(T), \quad \mu^{-1} = \sum n_i = \sum \alpha_i m_i^{-1}, \quad i = 1, 2, ..., 7$$

Under the conditions in question it is necessary to take into account the following elementary stages of the hydrogen oxidation reaction [13]:

$H_2 + O_2 = OH + OH$,	$H + H + M = H_2 + M$,	$H + O_2 = OH + O$
$HO_2 + H = OH + H$,	$O + H_2 = OH + H$,	$H + OH + M = H_2O + M$
$OH + H_2 = H_2O + H$,	$H + O_2 + M = HO_2 + M$,	$O + H_2O = OH + OH$

where M denotes a third particle. The corresponding rate constants of the forward and backward reactions have been taken from the paper [13] and the values of the partial enthalpies $h_i(T)$, from [14].

For computations we used a finite difference method based on the Godunov scheme [15]. The leading shock wave and the contact discontinuities are separated explicitly and the moving computational grid is used.

Results of calculations

We performed the calculations for a stoichiometric hydrogen-air mixture with the initial pressure $p_0 = 1bar$, temperature $T_0 = 300K$, and various values of the charge. As an explosive, we chose trotyl with the density $\rho_T = 1.6g/cm^3$ and the caloricity $Q_T = 1000kcal/kg$. It is supposed that the explosion products represent a perfect gas with the ration of specific heats $\gamma = 2.8$. According to the results of [8], the use of a constant value of γ instead of variable one defined by the formula presented above is fairly justified for the problem considered and allows one to substantially reduce the computing time.

Air layer is in contact with charge

Suppose that a layer of air directly adjoins the charge, i.e., $r_0 = R_1$. The calculations were made for $r_0 = 1, 2, ..., 10cm$, which are greater than the critical radius $r_0^* = 0.7cm$ [16]. For each charge radius the critical radius R_2^* of a layer such that a blast wave do not initiate a self-sustaining detonation wave after passing this layer was calculated. It turns out that the critical radius linearly depends on the charge radius; this dependence is well described by the relation $R_2^* = 12r_0$. The calculations showed when the intensity of the blast wave at the entry to the combustible mixture after passing through the air layer is lower than a certain threshold value, no detonation occurs.

The linear dependence of R_2^* on r_0 directly follows from the existence of the threshold value of the blast wave intensity. To prove this fact, we can employ the general functional dependence $p_s - p_0 = f\left(G^{1/3}/r_s\right)$ (G is the weight of the charge, p_s and r_s are the shock wave pressure and its radius respectively) proposed by Sadovskii [16] for determining the excess pressure at the shock wave front under the explosion.

Since $G = 4/3\,\pi\rho_B r_0^3$ the above equation yields: $p_* - p_0 = \Phi(r_0/R_2^*)$.

According to the theory of dimension and similarity [17], the following relation holds for a fixed pressure jump under the explosion of the explosive with ρ_B and Q_B:

$$(R_2^*/r_0)_B = (R_2^*/r_0)_T(\rho_B Q_B/\rho_T Q_T)^{1/3}.$$

Finally, taking into account the linear dependence established, we obtain

$$(R_2^*/r_0)_B = 12(\rho_B Q_B/\rho_T Q_T)^{1/3},$$

This formula determines the critical size of the air interlayer for an arbitrary explosive under the atmosphere pressure. With the similar reasoning for the plane and cylindrical symmetries, we can show that the linear dependence between the charge size and the critical size of the inert gas interlayer is preserved.

Air layer is inside combustible mixture

Now, suppose that the air layer is situated inside the hydrogen-air mixture, i.e., $r_0 < R_1 < R_2$. In this case, the development or the destruction of detonation may depend not only on the thickness $d = R_2 - R_1$ of the layer but also on its position with respect to the charge, i.e., for example, on R_1. The dependence of the critical thickness d^* on the internal radius R_1 was calculated. It is noteworthy that d^* first linearly decreases in the interval (r_0, R_1^L) as R_1 increases and then gradually reaches a constant value for $R_1 = R_1^C$. According to the calculations, the value d^* does not depend on r_0 for $R_1 > R_1^C$, where $R_1^C = 19.42r_0$ and in addition, $R_1^L = 8.7r_0$. It appears the results of calculations are well approximated by the formulas for the critical value of external radius R_2^* and the thickness of the layer d^*

$$R_2^* = 11,9r_0 + 0,1R_1, \qquad d^* = 11,9r_0 - 0,9R_1 \qquad ,$$

at the stage when the effect of combustion on the flow is not yet essential. These formulas can be used to determine the critical radius of the charge, i.e.,

the maximal radius of the charge at which the detonation does not restitute after passing through the air layer with given values of R_1 and R_2.

Conclusion

We investigated the effect of a spherical layer of air that separates a explosive charge from a stoichiometric hydrogen-air mixture or is situated inside this mixture on the initiation of detonation. In the first case, for various values of the charge radius, we numerically calculated the values of the critical dimension of the layer such that no self-sustaining detonation occurs when the dimension of layer exceeds this critical value. We revealed and theoretically substantiated a linear dependence of the critical radius of the layer on the charge radius and obtained an analytic expression that demonstrates the validity of this linear relation for any explosives. In the second case, we established that the critical thickness of the air layer monotonically decreases, as the distance of the layer from the charge increases, until it reaches the value independent of the charge dimension. On the basis of the results of calculations, we obtained the approximate analytic relations for the critical parameters that allow one to determine, for a fixed charge, the critical thickness of the layer as a function of its spatial position and, vice versa, to determine the critical energy of the charge for a layer of given thickness that is situated at a given distance from the charge.

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References

[1] Ya. B. Zel'dovich, S. M. Kogarko, N. N. Simonov. Experimental study of spherical gaseous detonation. *Zhurn. Tekhn. Fiziki*, vol. 26, No. 8: 1744-1769, 1956. (In Rus.)

[2] S. M. Kogarko, V. V. Adushkin, A. G. Lyamin. Study of spherical detonation of gaseous mixtures. *NauchnoTekhn. Probl. Goreniya i Vzryva*, vol. 1, No. 2: 22-35, 1965. (In Rus.)

[3] R. Knystautas, J. H. Lee. On the effective energy for direct initiation of gaseous detonations. *Combust. and Flame*, vol. 27, No. 2: 221-228, 1976.

[4] J.H. Lee. Initiation of gaseous detonation. *Ann. Rev. Phys. Chem.*, vol. 28: 75-104, 1977.

[5] V. A. Levin, V. V. Markov. On initiation of detonation for concentrated input of energy. *Izv. Akad. Nauk SSSR. Mekhan. Zhidk. i Gaza*, No. 5: 89-93, 1974. (In Rus.)

[6] V. A. Levin, V. V. Markov. Initiation of detonation for concentrated input of energy. *Fizika Goreniya i Vzryva*, vol. 11, No. 4: 623-633, 1975. (In Rus.)

[7] V. A. Levin, V. V. Markov, S. F. Osinkin. Modeling of initiation of detonation in the combustible gas mixture by the electric charge. *Khimich. Fizika*, vol. 3, No. 4: 611-614, 1984. (In Rus.)

[8] V. A. Levin, V. V. Markov, S. F. Osinkin. Initiation of detonation in a hydrogen-air mixture by explosion of a spherical charge trinitrotoluene. *Fizika Goreniya i Vzryva*, vol. 31, No. 2: 91-95, 1995. (In Rus.)

[9] V. A. Levin, V. V. Markov, S. F. Osinkin. Initiation of detonation in an nonhomogeneous hydrogen-air mixture. *Report, Moscow University Institute of Mechanics, Moscow*, No. 4376, 1995. (In Rus.)

[10] V. A. Levin, V. V. Markov, S. F. Osinkin. Stabilization of detonation by a destructible shell. *Dokl. Akad. Nauk*, vol. 352, No. 1: 48-50, 1997. (In Rus.)

[11] V. A. Levin, V. V. Markov, S. F. Osinkin. Stabilization of detonation in supersonic flows of combustible gas mixtures. *Proc. 16th Int. Colloq. on dynamics of explosions and reactive systems, Krakov, Poland*, 529-537, 1977.

[12] G. L. Brode. *Computer analysis of blast.* Ed. Mir, Moscow. In Mechanics, No. 2. 1976. (In Rus.)

[13] R. Takai, K. Yoneda, T. Hikita. Study of detonation wave structure. *Proc. of the 15th symp. (intern.) on combustion (Pittsburgh)*, 69-78, 1975.

[14] A. V. Gurvich, V. A. Medvedev, G. A. Khachkuruzov, et. al. *Thermodynamic properties of individual substances.* Ed. Nauka, Moscow. vol. 2. 1982. (In Rus.)

[15] S. K. Godunov, A. V. Zabrodin, G. P. Prokopov. A difference scheme for two-dimensional problems of gas dynamics andcomputation of the flow by a detached shock wave. *Zh. Vychisl. Mat. Mat. Fiz.*, No. 6: 1020-1050, 1961. (In Rus.)

[16] M. A. Sadovskii. *Mechanical effect of air shock waves by the data of experimental investigation.* Ed. Akad. Nauk SSSR, Moscow. In Explosion Physics, No. 1. 1952. (In Rus.)

[17] L. I. Sedov. *Similarity and Dimensions Methods in mechanics.* Ed. Nauka, Moscow. 1967. (In Rus.)