Initiation of Detonation in Confined Volume by Converging Shock Wave

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Abstract

The problem of a direct initiation of spherical and cylindrical detonation in a stoichiometrical hydrogen-air mixture under normal conditions in the space, confined by rigid shell, as result of low pressure domain (cavity) collapse is under consideration. The investigation of the flow with taking into account the detail mechanism of chemical reactions is done by a finite-difference method based on the Godunov's scheme with a moving difference grid and explicit capture of the leading shock and the contact surface. It is obtained, that under given low pressure in the cavity and its radius being equal or greater the known radius for the case of unconfined space, there exists the minimal critical radius of the shell, starting from which the detonation wave is formed into the flow field under consideration.

Introduction

It is well known, that for a direct initiation of detonation in a combustible gas mixture it is requires a sufficiently quick energy release, for example, as result of explosion of condensed explosive or of exploding wire, by an electric discharge, by a laser spark, etc. Moreover, the value of released energy must exceed some critical value depending on method of energy release and initial parameters of a combustible mixture. When the energy is less than critical one, the initiation is failed [1-8]. Nevertheless, some conditions may arise in the nature, when the initiation of a detonation will possible without any additional supply of an energy. The fundamental condition of a self-sustained detonation wave formation is an arising of sufficiently strong shock wave, which is capable to ignite a combustible mixture [9].

The problem of a direct initiation of spherical and cylindrical detonation in a stoichiometrical hydrogen-air mixture without any external energy input but only as a result of a decomposition of a low pressure ball domain was considered in [10]. As result of the discontinuity decomposition on the boundary of the spherical or cylindrical domain the rarefaction wave propagates in the external space and the converging shock wave is formed in this domain. In the case of inert gas the converging shock wave goes to the self-similar regime approaching to the centre of symmetry [11,12]. After the shock wave reflection from the centre symmetry the diverging shock wave, which propagates through the disturbed gas and rapidly decays, is formed [13]. In the case of combustible mixture the conditions for ignition may arise. The various situations may take place depending on the values of defining parameters. When the difference of the pressures is sufficiently small the ignition does not

take place because of small time period during which the gas mixture particle is in suitable conditions for ignition. More over even if the gas mixture ignites near the centre of symmetry, the detonation will not take place due to the fast decaying of the reflected shock wave which much more than in homogeneous medium [12]. On the other hand, when the difference of the pressures is sufficiently high and the size of the cavity is relatively large, there can be suitable conditions for ignition both behind the converging and diverging shock waves. The reflected shock wave moving into pre-heated gas mixture may transform in a detonation wave, which does not decay after interaction with the contact surface and propagates in opened space. The qualitative analysis shows that some critical values of initial parameters for initiation of detonation exist. As was shown in [10] even for atmospheric pressure in the external space the self-sustained detonation wave may arise after reflection from the centre of symmetry. It was appears the some minimal critical radius of the domain under which the detonation is realised exists for every fixed low pressure value. The proper dependencies ware obtained for both kinds of flow symmetry.

Statement of the problem

Suppose that inside of the spherical or cylindrical rigid shell (with radius R_s) filled by stoichiometrical hydrogen-air mixture at rest under normal conditions there is the coaxial cavity (with radius R_L) at initial time moment. The pressure in cavity, P_L , is less than pressure P_0 outside it. The uniform temperature and molar fractions of mixture components are in the considered domain. The wave picture of the flow arising due to the discontinuity decomposition on the boundary of the spherical or cylindrical cavity is shown schematically in the Fig.1. In case of the unlimited space, according to [10], the selfsustained detonation wave is formed, if radius of cavity is not less the certain critical value dependent on pressure in the specified domain. It is obvious, that the presence of a rigid shell will not affect formation of a detonation, if shell radius is more than radius of a diverging rarefaction wave at the moment of a beginning of propagation of a detonation in a selfsustained mode in the unlimited space. The question is of interest on at what minimal radius of a shell and given radius of the cavity inside the region, limited to a shell, there will be a selfsustained detonation.

Governing equations

In the usual notations the system of equations describing flow with cylindrical and spherical waves was used in the form:

$$\frac{\partial(\rho r^{\nu-1})}{\partial t} + \frac{\partial(\rho v r^{\nu-1})}{\partial r} = 0,$$

$$\frac{\partial(\rho v r^{\nu-1})}{\partial t} + \frac{\partial((\rho v^2 + p) r^{\nu-1})}{\partial r} = (\nu - 1) p r^{\nu-2},$$

$$\frac{\partial((\rho v^2 / 2 + \rho h - p) r^{\nu-1}}{\partial t} + \frac{\partial((v^2 / 2 + h) \rho v r^{\nu-1})}{\partial r} = 0,$$

$$\frac{\partial(\rho n_i r^{\nu-1})}{\partial t} + \frac{\partial(\rho n_i v r^{\nu-1})}{\partial r} = \rho \overline{\varpi}_i r^{\nu-1}$$

v = 2;3 for the cylindrical and spherical case respectively.

Under the conditions in question it is necessary to take into account the following elementary stages of the hydrogen oxidation reaction [14]:

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

where M denotes a third particle. The corresponding rate constants of the forward and backward reactions have been taken from the paper [14].

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

$$P = \frac{\rho RT}{\mu}, h = n_i h_i(T), \mu^{-1} = n_i = \alpha_i m_i^{-1}, i = 1,2 \text{ K 8}.$$

The values of the partial enthalpies $h_i(T)$ have been taken from the paper [15]. The initial and boundary conditions were also established for the problems under consideration. The equations of gas dynamics were solved jointly with the equations of chemical kinetics by a finite-difference method based on the Godunov's with a moving difference grid and explicit capture of the leading shock and, moreover, the contact surface [16].

Results of calculations

The calculations were made for fixed initial values of the thermodynamic parameters of the combustible mixture surrounding the cavity: $P_0 = 10^5 \Pi a$, $T_0 = 300^\circ K$ and the molar fractions $r_{H_2} = 0.286$, $r_{O_2} = 0.143$, $r_{N_2} = 0.571$ ($n_i = r_i / m_k r_k$).

The numerical research has shown, that at the given pressure in the cavity and its radius, not smaller critical radius for the unlimited space, there is a minimal critical radius of a shell R_s^* , since which in the limited space the detonation wave is formed. The wave pictures illustrating the failure and formation of detonation are given in Fig.2a-c. According to calculations, critical radius of a shell depends on the radius of the cavity, and the difference between them aspires to the certain final limit (see Fig.3a,b).

Discussion

The considered statement of a problem allows to estimate value of the minimal critical energy E_* , which initiates a detonation at collapse of a cavity. It is obvious, that the flow arises at the expense of a part of internal energy of a spherical layer limited to a shell and a cavity, which is calculated on a difference of pressure in it and cavity. At equality of these pressures the internal energy is equal to zero and the gas remains in a condition of rest. According to calculations, the critical energy has a minimum at the certain value of the radius of a cavity (see Fig.4), which on the order surpasses critical energy of initiation of a detonation by a charge TNT in the unlimited space.

Conclusions

The process of initiation of a detonation in volume limited to a rigid shell, in result of collapse of the low pressure domain located inside it is investigated. Is established, that at fixed radius of a cavity and pressure inside it, the detonation is formed in considered region, if radius of a shell is not less the certain minimal critical value, which depends on radius of a cavity and pressure inside it, and the difference between radiuses of the shell and cavity aspires to the certain final value. Is shown, that the minimum of critical energies of a spherical layer on the order surpasses energy of initiation of a detonation by a charge TNT in the unlimited space [8].

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Fig.4 The dependence of the critical energy on the cavity radius.





Fig.2 The wave picture in the case of the detonation failure (a, b) and formation of the spherical detonation (c) under $P_L = 0.2 * 10^5 Pa$ and $R_L = 0.6m$.