Cellular Structure of Spray Detonation

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Abstract

On the basis of the mathematical model of a two-phase two-velocity medium, detonation of a cryogenic (T_0 = 80 K) mixture (gaseous hydrogen-drops of liquid oxygen) was studied numerically. The dynamics of formation and the special features of the structure of the two-dimensional reaction zone of the detonation wave are discussed. The cellular structure of detonation is modeled for the first time for cryogenic hydrogen-oxygen spray.

Introduction

Cellular structures of detonation in gases are well known in experiments [1]. Cells in gas-droplet systems were found only in sprays of small ($d_0 \approx 5$ μm) droplets of decan [2]. The stability of detonation waves (DW) in homogeneous explosives is studied theoretically and numerically [3-8]. These waves may be described using the model of mechanics of one-velocity medium. The stability of DW for multivelocity heterogeneous reactive media [9], for example, sprays, has not yet been studied analytically. Therefore, the only constructive tool for solving the problem of stability of a DW in heterogeneous multivelocity medium is direct numerical simulation. Thus, the one-dimensional instability of detonation in a cryogenic hydrogen-oxygen spray was studied in [10], where, in particular, self-sustained one-dimensional autooscilatory regimes of spray detonation were obtained. Results of a numerical study of the two-dimensional instability of detonation in a cryogenic hydrogen-oxygen spray are described in the present report.

Statement of the problem

Let a plane channel of width y_0 contain a mixture of liquid oxygen droplets (with a diameter d_0, true density ρ_2^0, and volume concentration α_{20}) in gaseous hydrogen with an initial pressure p_0 and temperature T_{10}. A DW propagates along the channel. We have to find its dynamics and structure depending on the channel width, droplet diameter, and initial composition of the mixture.

Within the framework of the model of mechanics of a two-phase multivelocity medium [9], we consider a two-dimensional unsteady motion of monodispersed oxidizer droplets in a gaseous fuel. A combustion region is formed in the gas-droplet mixture behind the shock wave (SW) after a chemical delay of ignition. The rates of chemical reactions in this region are much greater than the mass-transfer rate between the phases. We use the following assumptions in the mathematical model: 1) there is no energy release in the zone of chemical induction; 2) chemical processes at each point behind the ignition front proceed instantaneously, and the composition of the gas phase is in chemical equilibrium; 3) the energy-release rate in the gas-droplet mixture is limited by the phase-transition velocity, and the thermal effect of chemical reactions per unit mass of evaporated droplets and the molar weight of the gas are variable quantities. The equations of two-dimensional unsteady two-phase flow, initial and boundary conditions, numerical method of solution in moving grids are lead in [11].

Calculation results

The numerical study was performed for a cryogenic hydrogen-oxygen mixture, which was a monodispersed spray of oxygen droplets in gaseous hydrogen ($2H_2+O_2$) for the initial temperature of the phases $T_{10} = T_{20} = 80$ K. The solution of the problem depends on three governing parameters: initial pressure of gaseous hydrogen p_0 and two scale factors - oxygen droplets diameter d_0 and channel width y_0. For a fixed value of p_0, the initial mean densities of gaseous hydrogen ρ_{10} and oxygen droplets $\rho_{20} = \alpha_{20}\rho_2^0$ are determined unambiguously. In particular, for $p_0 = 1$ atm, we have $\rho_{10} = 0.305$ kg/m^3 and $\rho_{20} = 2.44$ kg/m^3; the velocity of the ideal Chapman-Jouguet detonation is $D_{CJ} = 2.97$ km/sec.

It is known [10] that detonation of cryogenic hydrogen-oxygen spray in the one-dimensional formulation (in contrast to heterogeneous detonation of hydrocarbon-oxygen sprays) is unstable and propagates in a pulsing (autooscillatory) mode. The unstable element in the wave structure, which leads to periodic oscillations of parameters in the reaction zone, is the ignition front.

The numerical algorithm and the code developed for solving the two-dimensional unsteady problem allow one to study the dynamics of propagation of a heterogeneous DW in a plane channel with varied channel width and oxygen droplet diameter. First we consider the influence of the channel width y_0 on the dynamics of the detonation process for fixed values $p_0 = 1$ atm and $d_0 = 50$ μm. As the DW (initially one-dimensional) propagates, a crossflow instability of the ignition front develops in the reaction zone, which leads to transverse oscillations of gas-dynamic parameters of the flow. The flow pattern becomes two-dimensional, and the shock-front velocity experiences irregular oscillations. By varying channel width y_0, we show that oscillations of the SW velocity can appear are regular with respect to the x axis and have identical amplitudes on the opposite walls of the channel. There exists a minimum value of the channel width $y_0 = y_* = 10.55$ mm for which the SW velocity along the x axis at a distance $x/y_0 > 70$ in each longitudinal section changes periodically with a time period $\Delta t = 11.67$ μsec and a spatial period $b = 36.07$ mm. A regular transverse perturbation is formed in the DW structure, which is alternatively reflected from the channel walls so that the SW velocity and other gas-dynamic parameters on the opposite walls change in the same manner but in the opposite phase (shifted by half a period). The calculated values of D_{max} and D_{min}, and the wave velocity averaged over the period $\langle D \rangle = b/\Delta t$ are listed in Table. The quantity y_* , which will be called the eigenvalue of problem, orders the two-dimensional instability of a heterogeneous DW in the form of regular periodic solution and corresponds to half of the transverse size of the detonation cell $a/2$.

Table.

p_0, atm	d_0, μm	D_{max}, km/sec	D_{min}, km/sec	$\langle D \rangle$, km/sec	a, mm	a/b
1	25	7.24	1.75	3.00	11.2	0.566
1	50	7.34	1.94	3.09	21.1	0.585
1	100	5.58	2.05	3.04	44.3	0.50
0.5	50	7.07	1.76	3.04	32.8	0.55
2	50	5.64	2.27	3.03	13.6	0.499

The calculated periodic two-dimensional DW structure ($y_0 = y_*$) in a heterogeneous mixture $2H_2 + O_2$ during one period is shown in Fig.1. [isochores of the condensed (R_2 =

ρ_2/ρ_{20}) and gaseous ($R_1 = \rho_1/\rho_{20}$) phases in the cell]. To control the reliability of the periodic solution found, we performed additional calculations, where the channel width was doubled ($y_0 = 2y_* = a$) for a fixed moment of time, and a mirror reflection of the distribution of the gas-dynamic parameters from the solution domain $0 < y < y_*$ was transferred to the region $y_* < y < 2y_*$. The initial data obtained in this way were used to calculate an unsteady problem. It is shown that a self-sustained heterogeneous DW propagates over the channel. The reaction zone of this DW has two-dimensional periodic solution with two opposing transverse waves, which is symmetric about the channel $y = y_*$. The internal structure of this DW coincides identically with that shown in Fig.1.

The cell size in a heterogeneous mixture should depend on the initial diameter of oxygen droplets. To determine this dependence, we performed calculations in which the initial diameter of the droplets was increased twice as compared to the basic variant. By varying the channel width for $d_0 = 100$ μm, we found the eigenvalue of problem $y_* = 22.15$ mm for which a two-dimensional periodic solution with a regular cellular wave structure is formed. The results obtained are listed in Table. It is seen that a twofold increase in d_0 leaves the mean detonation velocity $\langle D \rangle$ almost unchanged and increase the transverse size of the cell by almost a factor of 2. The cell shape also changes: $a/b = 0.5$, i.e., the cell becomes more extended in the longitudinal direction. Thus, a classical detonation cell was obtained for the first time in numerical simulation of heterogeneous detonation in a cryogenic hydrogen-oxygen gas-droplet mixture.

Analysis of the Cellular Structure of a Heterogeneous DW.

In a heterogeneous DW, as in gas detonation [1], collisions of transverse waves moving over the leading front in opposite directions lead to reproduction of the front structure in time. The main element of this structure is a triple configuration consisting of a Mach stem, an incident wave, and a reflected (transverse) wave adjacent to the first two elements at the triple point. Dynamics of interaction of transverse waves is demonstrated in Fig. 2. The calculated trajectory of the triple point is shown in Fig. 1 by the solid curve. The special feature of the cellular structure for a heterogeneous DW in a cryogenic mixture $2H_2+O_2$ is that the induction zone of chemical reactions l_{ind} has a finite length ($0.04 \div 0.2a$) at all times because of the low temperature of the gas phase behind the SW front. Therefore, the triple configuration at the leading front is always a shock-wave configuration. The location of the end of the induction period is clearly seen in Fig.1 in the regions of high gradients of the gas density, and the maximum in l_{ind} is always observed at the moment of arrival of the triple point at the cell axis. In contrast to the gas-phase parameters, the distribution of parameters of the condensed phase (R_2) in the reaction zone is more smooth. For the heterogeneous mixture $2H_2+O_2$, only 10 - 20% of the mass of liquid oxygen droplets are gasified by the end of the induction period of chemical reactions. The calculations show that the length of the zone of complete energy release in the heterogeneous DW is determined by the intensity of mass exchange (rate of mass addition from oxygen droplets to the gas phase). For oxygen droplets 100 μm in diameter, this length is an order of magnitude greater than l_{ind} and amounts to 2-2.5 a. It is of interest that the gas-phase velocity at the end of the energy-release zone at all times is supersonic relative to the mean wave velocity $\langle D \rangle$, and the Mach number $M = (\langle D \rangle - u_1)/c_1$ reaches 1.4. This means that the transition from subsonic to supersonic flow occurs in the reaction zone. The parameter characterizing the cell shape is usually the ratio of the transverse to the longitudinal size of the cell (a/b). In the case considered, we have $a/b = 0.5$

for p_0 = 1 atm and d_0 = 100 μm, i.e., the cell in a heterogeneous mixture may be more extended in the longitudinal direction than in reactive gases [1].

Conclusions

The following results were obtained by numerical simulation of spray detonation in a plain channel. Transverse instability of the two-dimensional reaction zone of heterogeneous DW was obtained for the first time for a cryogenic mixture $2H_2+O_2$ in the form of cellular structures with cell size depending on the droplet diameter and the initial pressure. It was found that the heterogeneous DW reaches a periodic regime with a regular cellular structure only for certain discrete values of the channel width (eigenvalues of the problem). The special features of dynamics of the transverse wave and gas-dynamic parameters in the reaction zone of the heterogeneous DW during one period are analyzed. The cell size is calculated, which increases almost linearly with increasing initial diameter of oxygen droplets. The initial pressure dependence of the cell size can be approximated by a power function as $a \sim p_0^{-2/3}$.

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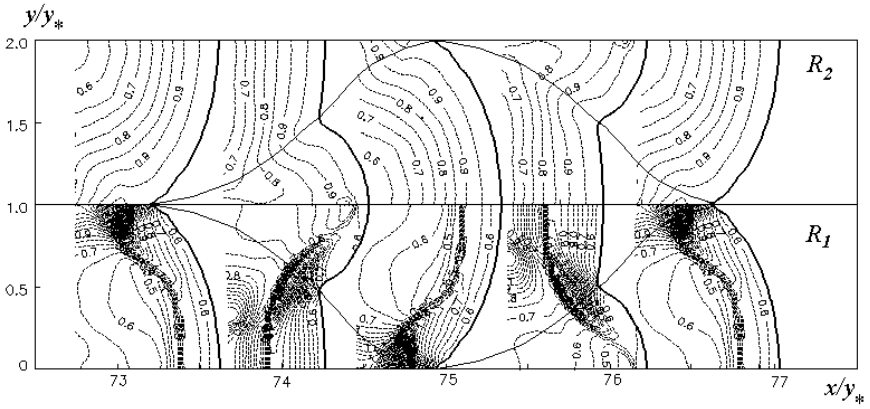

Fig. 1. Cellular DW structure in the heterogeneous mixture $2H_2+O_2$ for one period (d_0 = 50 μm and a = 21.1 mm).

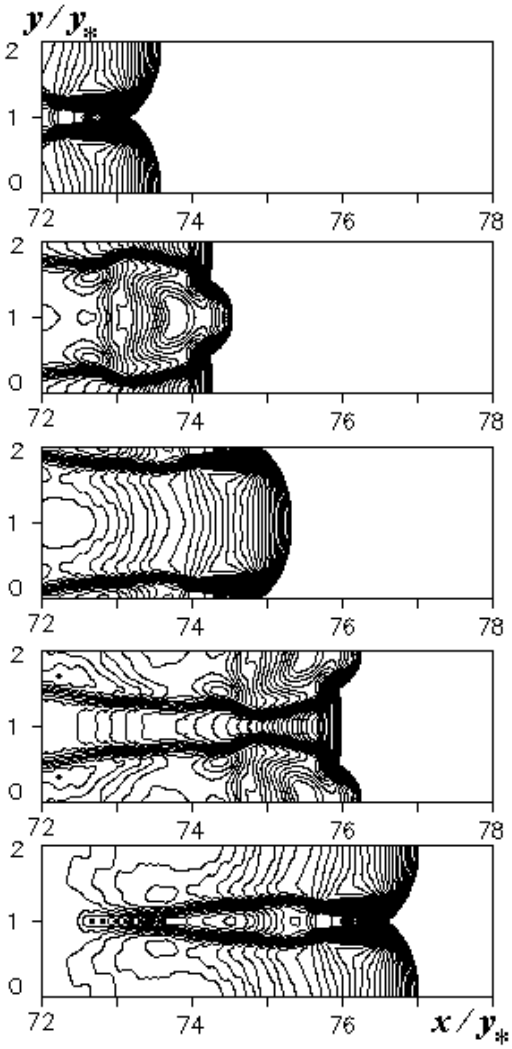

Fig. 2. The evolution of isobars in the heterogeneous mixture $2H_2+O_2$ for one period (d_0 = 50 μm and a = 21.1 mm).