Numerical modelling of continuous spin detonation in rich methane-oxygen mixture

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Abstract. A numerical simulation of a two-dimensional structure of the detonation wave (DW) in a rich (equivalence ratio $\phi=1.5$) methane-air mixture at normal initial condition has been conducted. The computations have been performed in a wide range of channel heights. From the analysis of the flow structure and the number of primary transverse waves in the channel, the dominant size of the detonation cell for studied mixture has been determined to be 45÷50 cm.

Based on the fundamental studies of multi-front (cellular) structure of the classical propagating DW in methane mixtures, numerical simulation of continuous spin detonation (CSD) of rich ($\phi=1.2$) methane-oxygen mixture has been carried out in the cylindrical detonation chamber (DC) of the rocket-type engine. We studied the global flow structure in DC, and the detailed structure of the front of the rotating DW. Integral characteristics of the detonation process — the distribution of average values of static and total pressure along the length of the DC, and the value of specific impulse have been obtained. The geometric limit of stable existence of CSD has been determined.

1. Introduction

Detonation waves (DWs) in reacting gaseous mixtures have the complex three-dimensional and time-dependent multifront (cellular) structure. A geometrical parameter of this structure is the transverse size of the elementary cell of the DW — $a_0$. Based on this value, it is possible to determine such critical parameters of detonation as the critical conditions of detonation combustion, the critical energy of initiation, geometrical limits of steady detonation propagation, etc., i.e. to estimate the detonation hazard of gaseous mixture and to evaluate the possibility of using detonations in various schemes of advanced detonation-based propulsion systems.

A very regular cellular DW structure in hydrogen–oxygen mixtures was studied in our previous 2D numerical simulation [1]. A good agreement was obtained between the numerical results and experimental data on the size $a_0$ over a wide range of initial pressures and degrees of mixture dilution by argon. In the subsequent studies we have simulated the irregular detonation structure in stoichiometric methane–air [2] and methane–oxygen [3] mixtures.

The objectives of this work are further development of the proposed approximate model of chemical kinetics of methane to describe the detonation combustion of rich methane based gaseous mixtures, to perform a numerical simulation of the 2D irregular cellular structure of propagating DW in a rich methane–air mixture, and to study the flow structure in cylindrical DC with continuous rotating DW in a rich methane-oxygen mixture.
2. Governing equations and model of chemical kinetics

The dynamics of the compressible chemically reactive medium is described by the two-dimensional Euler equations.

The chemical reaction in the DW is described according to the two-stage model of the detonation kinetics (induction period and main heat release stage) first proposed in [4]. In the framework of this idea, a two-stage model of the kinetics of detonation combustion of methane-based mixtures \( \text{CH}_4 + a_1\text{H}_2 + a_2\text{O}_2 + a_3\text{N}_2 + a_4\text{Ar} + a_5\text{H}_2\text{O} \) has been developed and described in more detail in our paper [5]. The duration of the induction period is determined by known empirical formula [6] for methane mixtures. Constants of the approximate kinetic model have a clear physical meaning and are calculated from the tabulated thermochemical parameters of the mixture before the two-dimensional numerical calculation of the DW structure.

In this study, we adopt proposed model to describe a rich methane mixtures. The preliminary thermodynamic calculations of Chapman-Jouget (CJ) point and Von Neumann spike parameters by this kinetics in rich (equivalence ratio \( \phi = 1.5 \)) methane-air mixture \( 1.5\text{CH}_4 + 2\text{Air} \) reveal that this model is accurate. The comparison has been done with CEARUN (NASA) numerical code calculations. The model is useful for multi-dimensional numerical simulations of detonation processes and is currently the only simple model kinetics with high accuracy to calculate the irregular structure of the detonation wave.

The system of governing equations was closed by the well-known thermal equation of state for an ideal gas.

3. Numerical method

The resultant systems of equations were solved numerically using the code based on the Godunov-type finite-volume scheme [7] with the fourth-order MUSCL TVD reconstruction [8] and the advanced HLLC algorithm [9] for an approximate solution of the Riemann problem. In implementation of HLLC algorithm for the case of a chemically reacting mixture, the “energy relaxation method” [10] was used. This method eliminates the problem of numerical solution of the Riemann problem for a medium with a complicated nonlinear equation of state (including that with a variable ratio of specific heats). Integration in time was performed with second-order accuracy by using additive semi-implicit Runge-Kutta methods [11]. The time step was determined at each time layer of the solution from the stability condition [7]. In the present simulations, the values of the Courant number were CFL=0.3–0.4.

In numerical simulations of propagating 2D detonation wave in the straight channel we use an adaptive moving grids technique in \( x \) direction with local refinement in the vicinity of a leading shock front. In more details it was described in [1-3].

The codes are parallelized with MPI library using the domain decomposition technique.

4. Physical background: 2D structure of DW in a rich methane–air mixture in channel

Numerical simulation was performed for a rich methane–air 1.5 \( \text{CH}_4 + 2\text{Air} \) at normal initial conditions with the equivalence ratio \( \phi = 1.5 \). This value of \( \phi \) corresponds to the mole fraction of methane in mixture \( c = 0.136 \), which is on the upper (rich) limit for detonability and near the upper limit for combustion of the methane–air mixtures [12]. The DW propagation in a 2D straightline channel was studied. The boundary conditions and the method of DW initiation are described in [1-3].

In this study we have modelled the DW structure in channels with a height \( H = 40 \) cm, 45 cm, 50 cm, 60 cm, 65 cm, 70 cm. The total number of numerical cells in the \( x \) and \( y \) directions were \( N_x=2000, N_y=2000 \) respectively. Calculations with varying \( H \) showed that the cellular structure of the DW with two main (primary) transverse waves exists in sufficiently wide range of \( H \). This range is much wider than for hydrogen-oxygen mixtures [1].

To study grid convergence of the numerical solutions the calculations have been performed with twice as many number of numerical cells \( N_x=4000, N_y=4000 \) for channel height \( H = 45 \) cm, 50 cm, and 65 cm as in regular simulations. The simulations revealed a flowfield with two approximately equal
primary transverse waves for $H = 45$ cm and 50 cm. Based on these results of the calculations, we conclude that grid convergence of the numerical solutions was obtained in our study.

From the analysis of the flow structure with varying $H$, the transverse size of the dominant detonation cell for rich ($\varphi = 1.5$) methane-air mixture determines to be $a_0 = 45 \div 50$ cm. The dominant cell is the cell formed by a pair of primary transverse waves that are nearly identical intensity and symmetric. For other values of the channel height $H$ the two primary transverse waves have different intensity and reveal a chaotic uncoordinated movement. Empirical data on the size of the cell $a_0$ for a given mixture composition are not known to the author, is necessary to conduct large-scale experiments for this mixture.

5. Simulation of continuous rotating DW in a rich methane-oxygen mixture

Numerical investigation of continuous spin detonation (CSD) in a rich methane-oxygen $1.2 \text{CH}_4 + 2 \text{O}_2$ ($\varphi = 1.2$) in the annular cylindrical detonation chamber (DC) has been conducted according physical and mathematical 2D model, see [13,14]. The described above kinetics model of detonation combustion of methane mixtures has been used. In order to compare numerical simulation results with experiments in annular cylindrical DC (average diameter $d_c = 3.5$ cm, the annular gap $\Delta = 0.5$ cm, DC length $L_c = 9$ cm) [18], two-dimensional time-dependent calculations have been done under the same geometric and input governing physical parameters, as in the experiments [14], see Chapter 2, Table 2.1. Total mass flow rate of a fresh $1.2 \text{CH}_4 + 2 \text{O}_2$ mixture from manifold (receiver) in the experiment was $G_0 = 85$ g/s, which ensure the specific mass flow rate in the annular channel of the DC $g_\Sigma^0 = G_0/S_c = \rho \cdot u_y = 154.6$ kg/s$\cdot$m$^2$ on the inlet boundary $y = 0$. In the experiments the stagnation pressure and temperature in injection manifold (receiver) were $p_m = 6.81$ atm, $T_m = 293.15$ K, and $S_*/S_c = 0.1026$. Here $S_c$ – DC annular channel cross-sectional area, $S_*$ – the total throat area of Laval micro-nozzles at the inlet wall of DC [13], $\rho$ – mixture density, $u_y$ – velocity on $y$ axis. In experiments [14] with this mixture a single rotating DW has been obtained in the given DC, respectively a two-dimensional computational domain width has been selected $W = \pi d_c = 10.9956$ cm. A periodic boundary conditions have been set at the left and right boundaries $x=0$ and $x=W$ [13]. On the outlet boundary $y = L_c$ a value of counterpressure $p_{out} = 1$ atm has been set.

Numerical simulations have shown that for given manifold parameters ($p_m = 6.81$ atm, $T_m = 293.15$ K) a stable CSD regime with a single rotating transverse DW (TDW) cannot exist in DC with predetermined geometrical dimensions. After the numerous numerical calculations it has been found that self-sustained continuous rotating DW can exist with the following parameters in the manifold $p_m = 40$ atm, $T_m = 1000$ K, see Figures 1 and 2.

![Figure 1](a) Structure of rotating detonation wave in a detonation chamber of diameter $d_c = 3.5$ cm at $p_m = 40$ atm, $T_m = 1000$ K: (a) pressure (atm) flow field; (b) temperature (K) flow field.
Figure 1 shows the flow structure with a single TDW in this DC after the establishing of steady spinning regime. The pressure and temperature flow fields are shown for time moment $t=844.6 \mu s$, see Fig.2a. A white curve on these flow fields shows an instant position of Mach number $M=u_y/c=1.0$ isoline, where $c$ is a speed of sound. Figure 1 clearly shows the cellular (multifront) structure of the front of this TDW, that is similar to a multifront structure of TWs on the front of propagating DW. On Figure 1b one can see a number of the unburned pockets of gas. These pockets lead to variation in time of the value of the specific flow rate $g_{\Sigma, \text{Out}}$ on the outlet boundary.

**Figure 2.** Spin detonation parameters: (a) static pressure $p$ (atm) history at the point $x=0, y=0$, see Figure 1; (b) distribution of average static pressure <$p$> (curve 1) and total pressure <$p_0$> (curve 2) along the axial length of a detonation chamber.

Figure 2a shows the dependence of the static pressure (atm) on time (s) on the inlet boundary of the DC. This is a virtual pressure gauge data at a fixed point ($x=0, y=0$). Analysis of the obtained pressure history shows, that within 194.6 $\mu$s of the detonation process the TDW is on a steady rotation regime with an average time period of rotation $<\Delta t>=47.6 \pm 0.2 \mu s$.

Figure 2b presents the distribution of calculated values of the averaged on $t$ from 650 $\mu$s to 844.6 $\mu$s and on $0 \leq x \leq W$ the static <$p(y)$> and total <$p_0(y)$> pressures along the length of DC channel. The data for the drawing of these curves has been taken from the simulation of detonation process shown on Figure 2a. It is seen that the static pressure (curve 1) decreases along the length of the chamber. Moreover, in the main heat release zone ($0 < y < 2.0 \text{ cm}$) the rapid decline of pressure from about 10 atm to 6 atm is observed, and then it decreases slowly with minor fluctuations to a value of about 4 atm at the outlet of the channel ($y=L_c=9 \text{ cm}$). The length of the main heat release zone, obtained from these graphics correlates very well with the average height of TDW <$h$>, see Figure 1. The curve 2 shows, that the averaged total pressure determined as $p_0=p+\rho \cdot u_y^2$ is constant (with very minor fluctuations) along the length of the DC. This total pressure behavior is completely consistent with the laws of gas dynamics.

Numerical simulations have shown that a reduction of the stagnation temperature to $T_m=900 \text{ K}$ at $p_m=40 \text{ atm}$ leads to a complete breakdown of detonation combustion process and disappearance of TDW in DC. The reduction of stagnation pressure to $p_m=35 \text{ atm}$ at $T_m=1000 \text{ K}$ still gives stationary in general detonation regime with rotating TDW. The TDW shape is significantly changing over time and has greatly distorted form with 1 or 2 transverse waves on its front. This mode can be considered as marginal, insofar further decrease of stagnation pressure to $p_m=30 \text{ atm}$ at $T_m=1000 \text{ K}$ leads to the complete destruction of the CSD regime.
6. Discussion and Conclusions
The two-stage model of the kinetics of detonation combustion of methane-based mixtures with an oxygen and air has been developed. The proposed model of the kinetics of detonation combustion of methane is highly accurate and consistent with the second law of thermodynamics. The use of this kinetic model for the simulation of the two-dimensional cellular structure of detonation wave provides realistic results. The dominant size of the detonation cell for stoichiometric methane-air mixture determines to be 34±1 cm, and 0.3±0.35 cm for methane-oxygen mixture [2,3]. These values are in good agreement with all available experimental data. A numerical simulation of 2D structure of the DW in rich (equivalence ratio $\phi=1.5$) methane-air mixture has been performed. From the analysis of the flow structure, the size of the detonation cell for this mixture has been determined to be $a_0=45\div50$ cm. This value is in a good agreement with the result of the analytical model of the detonation cell by Vasil’ev and Nikolaev [15] $a_0=38$ cm. The experimental values of the cell size for this rich mixture composition are not available in literature up to now.

The 2D simulations for these three gas mixtures were reproduced the DW irregular cellular structure with all its main features observed in the experiments [16,17] with stoichiometric methane-air and methane-oxygen mixtures: a chaotic uncoordinated movement of the main transverse waves; the presence of a fine (secondary) cell structure at the transverse waves themselves; the existence of numerous secondary transverse waves at the leading shock front, forming a hierarchy of the decreasing size DW front perturbations; and a significant number of pockets of the unburned mixture at a considerable distance behind the DW front, etc.

The use of the proposed model of chemical kinetics and the same two-dimensional numerical code to calculate CSD in a rich methane-oxygen mixture in the annular cylindrical DC produced very interesting results. It has been found that it is impossible to obtain a stable CSD regime with the parameters in the manifold, at which in experiment was obtained stably rotating single TDW. In [14] from the analysis of experimental data it was obtained that the primary control parameter, which determines the boundaries of the existence of the CSD regime and the main characteristics of detonation flow in DC, is the specific mass flow rate $g_{\Sigma,m}$ of fresh mixture at inlet boundary of DC. In experiments [18] this value was $g_{\Sigma,m}=154.6$ kg/s·m$^2$ for the manifold parameters $p_m=6.81$ atm, $T_m=293.15$ K. In the numerical simulations the stable CSD regime with single TDW has been obtained at the substantially greater (in several times) value of $g_{\Sigma,m}=470$ kg/s·m$^2$ ($p_m=40$ atm, $T_m=1000$ K) in the same DC, and the marginal regime has been realized at $g_{\Sigma,m}=411.4$ kg/s·m$^2$ ($p_m=35$ atm, $T_m=1000$ K).

Numerical simulation also showed that in addition to the specific flow rate $g_{\Sigma,m}$, the second governing parameter is the stagnation temperature $T_m$. Indeed, reducing the stagnation temperature from $T_m=1000$ K to $T_m=900$ K at $p_m=40$ atm leads to termination of the CSD. Although for this case, the specific flow rate $g_{\Sigma,m}=494.45$ kg/s·m$^2$ is even more than for the steady CSD mode $g_{\Sigma,m}=470$ kg/s·m$^2$.

A significant discrepancy has been obtained for the TDW velocity. In the numerical simulation the value of the average velocity is $<D>/D_C=0.931$ (see Figure 2a), and in experiment [14] this value is $<D>/D_C=0.75$. In our opinion, such low experimental value of the TDW velocity raises the question whether this shock is in reality the detonation wave in the classical consideration according to the ZND theory.

However, the height of the TDW is in the very good agreement with the experimental data. In 2D simulation the height is $h=18.7$ mm, $h=15\div20$ mm has been obtained in experiment [14].

Thus, the developed two-stage kinetic model and 2D numerical code give excellent results in the modelling of irregular cellular structures in methane-based mixtures in the case of DW propagation in the straight 2D channel. However, in the case of simulations of the rotating DW in the annular channel of cylindrical DC the significant discrepancies have been obtained between the calculated and experimental values of governing parameters under which the stable CSD regime is realized.
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