Numerical simulation of classical and rotating detonation waves in methane mixtures

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Abstract. A numerical simulation of a two-dimensional multi-front irregular structure of the detonation wave (DW) in methane-based mixtures at normal initial conditions have been conducted. The computations have been performed in a wide range of channel height. From the analysis of the flow structure and the number of primary transverse waves in channel, the dominant size of the detonation cell for studied mixtures has been determined. We have simulated the cellular front structure in stoichiometric methane–air and methane–oxygen mixtures, and in a rich (equivalence ratio $\phi=1.5$) methane-air mixture. Based on the fundamental studies of front structure of the classical propagating DW in methane mixtures, numerical simulation of continuous spin detonation 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 continuous 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 rotating DW has been determined.

1. Introduction

One of the most important problems in the theory of dynamic systems is the formation and destruction of ordered gas-dynamic structures in a reactive medium. An example of such a self-organizing system is a multi-front (cellular) DW steadily propagating in a reacting gas mixture. The complex three-dimensional and time-dependent structure of the front of these waves propagating in constant cross-section channels shows some order, whose geometrical parameter is the size of the elementary cell of the DW $a_0$. Based on this value, it is possible to determine such parameters of detonation as critical conditions of detonation combustion, the critical energy of initiation detonation propagation limits, etc., i.e. to estimate the detonation hazard of gaseous mixture.

Depending on the chemical composition of the gas, DW in some mixtures have very regular cellular structure, whereas in other mixtures DW shows very irregular chaotic cell structure. A very regular cellular DW structure in hydrogen–oxygen–argon 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. Then 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 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]. The duration of the induction period is determined by known empirical formula [5] for methane mixtures. The main heat release starts after the induction period.

Within the framework of this concept, a kinetics model 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 in our paper [6]. It is assumed that during the induction period all the methane molecule is completely decomposed to form CO molecules. We replace the real multistep chemical processes by single \textit{brutto}--reaction of special form [6]. The molar mass of the gas \( \mu \) in the main heat release phase is described by the kinetic equation [7,8]. The thermal effect of the chemical reaction and thermodynamic parameters of the gas are described by explicit algebraic formulas on density and temperature [8]. Then we adopt proposed model to describe a rich methane mixtures.

The calculations of CJ parameters and Von Neumann spike parameters for methane mixtures showed that this model is highly accurate. The model is consistent with the second law of thermodynamics. Constants of the model have a clear physical meaning and are calculated from the tabulated thermochemical parameters for the given mixture before the two-dimensional numerical calculation of the DW structure. The model is useful for multi-dimensional numerical simulations of detonation processes and is currently the only approximate 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 [9] with the fourth-order MUSCL TVD reconstruction [10] and the advanced HLLC algorithm [11] 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” [12] 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 [13]. The time step was determined at each time layer of the solution from the stability condition [9]. 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 straight channel, we use an adaptive moving grids technique in the \( x \) direction with local refinement in the vicinity of a leading shock front. The code is parallelized with MPI library using the domain decomposition technique.

4. Simulation of 2D structure of propagating DW in a rich methane–air mixture
The DW propagation in a 2D straight-line channel was studied. The slip conditions (impermeable solid wall) [9] were imposed on the upper, lower, and left boundaries of the channel, and the right boundary was subjected to the condition of an undisturbed initial state of the gas. The DW was initiated near the left closed end of the channel and propagated from left to right along the \( x \) axis. The
size and energy of the initiation source [1-3] were chosen sufficiently large to ensure a supercritical regime of DW initiation in methane mixture.

The detonation cell size for the methane-based mixture was determined in a procedure similar to that used in the numerical study of stoichiometric hydrogen mixtures [1] with regular cellular structure. The initial height of the channel \( H \) was chosen rather arbitrarily; usually, it was assumed to be slightly higher than the presumed size of the cell \( a_0 \). Further variation of \( H \) in the calculations affected the number of primary transverse waves (TWs), remaining at the DW front after its initiation and the establishment of a self-sustained Chapman–Jouguet detonation regime, thus, the cell size was determined. The two transverse waves form the detonation cell.

According to this method, the dominant size of the detonation cell at normal initial conditions 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.

For a rich methane–air \( 1.5\text{CH}_4+2\text{Air} \) mixture at normal initial conditions numerical simulation has been performed for equivalence ratio \( \phi=1.5 \). This value of \( \phi \) corresponds to the mole fraction of methane in mixture \( c=0.136 \), which is near the upper (rich) limit for detonability. We have modeled 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 \( H \).

The results of the simulation of the rich methane–air mixture are presented in Figure 1a. Figure 1a shows the DW structure in a channel of height \( H=45 \) cm with the wave front located at \( x_f=1500 \) cm. This is the numerical Schlieren visualization of the flow field. For comparison, the front structure for stoichiometric methane-oxygen mixture in a channel height \( H=a_0=0.35 \) cm at \( x_f=12 \) cm is shown on Fig. 1b. For both value of \( H \) there is a system of the two main (primary) TWs, denoted by AA and BB, that forms the detonation cell. At showed time, TWs have approximately equal size and intensity, and move in the opposite direction to each other, in antiphase.

Moreover, the DW front has a system of secondary (smaller) TWs, denoted by ‘aa’, ‘bb’, etc. of different size, intensity, and direction of motion. There are also the third order smaller TWs ‘a’a’’, ‘b’b’’, etc. on leading shock. The movement all these perturbations of the DW leading shock front is rather random.

Figure 2a shows a front-propagation velocity (solid line) as a function of DW front position after the initiation in a channel \( H=45 \) cm. Denotation has reached quasi-steady propagation regime at the last 9÷10 meters. The average DW velocity obtained on this base is \( D_{\text{aver}} =1876 \) m/s (dashed line). This value is slightly higher than the Chapman–Jouguet velocity (dash-dot line) \( D_{\text{CJ}}=1840 \) m/s derived from thermodynamic calculations. Approximately the same absolute difference in the velocity of the
multifront DW in a self-sustained CJ regime with $D_{CJ}$ was observed for hydrogen-oxygen mixtures with regular cell structure [1] and stoichiometric methane mixtures with irregular structure [2,3].

![Figure 2](image-url)

**Figure 2.** A rich methane-air mixture: (a) front-propagation velocity (solid line) as a function of front position in channel $H=45$ cm; (b) magnified fragment of the primary transverse wave AA in channel $H=50$ cm.

Figure 2b presents an enlarged fragment of the primary transverse wave AA in the position $y\approx38$ cm for DW channel $H=50$ cm. Figure 2b clearly shows the fine cellular structure of the front of the main transverse wave. The fine TWs on the front of primary wave AA are denoted as ‘a’‒‘a’′’, ‘b’‒‘b’′’. The multifront (cellular) structure of the transverse waves had been observed earlier experimentally on soot imprints [14]. The secondary transverse waves that form the fine structure of the leading DW front (see Fig.1), had been observed in the experiments [15]. Thus, this simulation reproduces a real characteristic feature of the detonation of hydrocarbon mixtures – instability of the front of the transverse waves itself and instability the leading shock front of the DW.

The fine (cellular) structure of the transverse waves has been found previously in our simulations of DW in stoichiometric methane‒air [2] and methane‒oxygen [3] mixtures. Furthermore, Figure 2b shows a significant amount of unburned pieces of gas at a considerable distance behind the DW leading shock front, denoted as P1 and P2. This phenomenon was not observed in simulations of regular mixtures based on hydrogen [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. The simulations revealed a flowfield with two approximately equal primary transverse waves for $H=45$ cm and 50 cm. Based on these calculation results, we conclude that grid convergence of the numerical solutions was obtained in our study. The transverse size of the dominant detonation cell for rich methane-air mixture determines to be $a_0=45\div50$ cm. Empirical data on the size of the cell $a_0$ for a given mixture composition are not available in literature, it is necessary to carry out 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 [16,17]. 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) [17], two-dimensional time-dependent calculations has been done under the same geometric and input governing physical parameters, as in the experiments [17], 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
$G_0 = 85 \text{ g/s}$, which ensure the specific mass flow rate in the annular channel of the DC $g_{\Sigma 0}$

$= G_0 / S_c = \rho \cdot u_y = 154.6 \text{ kg/s} \cdot \text{m}^2$ on the inlet boundary $y=0$. In the experiments the stagnation pressure and temperature in injection manifold (receiver) were $p_m=6.81 \text{ atm}$, $T_m=293.15 \text{ K}$. For given manifold data this value of $g_{\Sigma 0}$ at critical regime of inflow from the system of Laval micro-nozzles at the inlet wall of DC [17] is provided with the value of $S_c / S_* = 0.1026$, where $S_c$ - DC annular channel cross-sectional area, $S_*$ - the total throat area of micro-nozzles, $\rho$ - mixture density, $u_y$ - velocity on $y$ axe. In experiments [17] with this mixture a single rotating DW has been obtained in the given DC, respectively a two-dimensional computational domain width has been selected $W = \pi d_c = 10.9956 \text{ cm}$. A periodic boundary conditions have been set at the left and right boundaries $x=0$ and $x=W$ [16]. On the outlet boundary $y = L_c$ a value of counterpressure $p_{out} = 1 \text{ atm}$ has been set.

![Figure 3](image.jpg)

**Figure 3.** Structure of rotating detonation wave in a detonation chamber of diameter $d_c=3.5 \text{ cm}$: (a) pressure (atm) flow field; (b) temperature (K) flow field.

![Figure 4](image.jpg)

**Figure 4.** Spin detonation parameters: (a) static pressure $p$ (atm) history at the point $x=0$, $y=0$, see Fig.3; (b) distribution of average static pressure $\langle p \rangle$ (curve 1) and total pressure $\langle p_0 \rangle$ (curve 2) along an axial length of a detonation chamber.

Numerical simulations have shown that for given manifold parameters ($p_m=6.81 \text{ atm}$, $T_m=293.15 \text{ K}$) a stable CSD regime with a single rotating transverse DW (TDW) cannot exist in the given DC. After the numerous numerical calculations it has been found that self-sustained continuous rotating DW can exist at the manifold parameters $p_m=40 \text{ atm}$, $T_m=1000 \text{ K}$.

Figure 3 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 $t=844.6 \mu\text{s}$, see
Figure 4a. A white curve on these flow fields shows an instant position of Mach number \( M=\text{Mach}/c=1.0 \) isoline, where \( c \) is a speed of sound. Figure 3 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, see Figure 2b. Analogous on Figure 3b one can see a number of the unburned pockets of gas. These pockets lead to variation in time the value of specific flow rate \( g_{\Sigma,\text{out}} \) on outlet boundary.

Figure 4a shows the dependence of 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 4b presents the distribution of calculated values of the averaged static \( <p(y)> \) and total \( <p_d(y)></p+\rho \cdot u_x^2> \) 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 in Figure 4a. It is seen that the static pressure (curve 1) decreases along the length of the chamber. Moreover, in the main heat release zone \((0 < y < 2.0 \text{ cm})\) it is observed rapid decline of pressure from about 10 atm to 6 atm, and then it with minor fluctuations decreases slowly to a value of about 4 atm at the outlet of the channel \((y=L_y=9 \text{ cm})\). The length of the main heat release zone, obtained from this graphics correlates very well with the average height of TDW \( \langle h \rangle \). The curve 2 shows that the average total pressure 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. Concluding Remarks

The two-stage model of the kinetics of detonation combustion of methane-based mixtures with an oxygen and air has been developed. The use of this kinetic model for modelling 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 \((\phi=1.5)\) methane-air mixture has been performed. The size of the detonation cell for this mixture determines to be \( a_c=45±50 \text{ cm} \).

The use of the proposed model of chemical kinetics and the same two-dimensional numerical code to calculate CSD in 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 [17] it was obtained that the primary control parameter, which determines the existence of the CSD regime is the specific mass flow rate \( g_{\Sigma,\text{in}} \) of fresh mixture at DC inlet boundary. In experiments [17] this value was \( g_{\Sigma,\text{in}}=154.6 \text{ kg/s·m}^2 \) for the manifold parameters \( p_m=6.81 \text{ atm}, T_m=293.15 \text{ K} \). In the numerical simulations the stable CSD regime with single TDW has been obtained at the substantially greater (in several times) value of \( g_{\Sigma,\text{in}}=470 \text{ kg/s·m}^2 \) \( (p_m=40 \text{ atm}, T_m=1000 \text{ K}) \) in the same DC, and the marginal regime has been realized at \( g_{\Sigma,\text{in}}=411.4 \text{ kg/s·m}^2 \) \( (p_m=35 \text{ atm}, T_m=1000 \text{ K}) \).

Numerical simulation also showed that in addition to the specific flow rate \( g_{\Sigma,\text{in}} \), the second governing parameter is the stagnation temperature \( T_m \). Indeed, reducing the stagnation temperature from \( T_m=1000 \text{ K} \) to \( T_m=900 \text{ K} \) at \( p_m=40 \text{ atm} \) leads to termination of the CSD.

A significant discrepancy has been obtained for the TDW velocity. In the numerical simulation the value of the average velocity is \( <D>/D_{\text{CF}}=0.931 \), and in experiment [17] this value is \( <D>/D_{\text{CF}}=0.75 \). In
our opinion, such low experimental value of the TDW velocity raises the question whether this shock is in a reality the detonation wave in the classical consideration according to the ZND theory. But the TDW height is in very good agreement with the experimental data.

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 for classical DW in a straight 2D channel. However, in the case of simulations of the rotating DW in the annular 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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