Numerical modelling of detonation combustion of hydrogen-air mixture in a supersonic annular chamber

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Abstract. The flow structure for various detonation regimes is numerically studied in a new flow-type supersonic annular detonation combustor. In the combustor with a new design, detonation burning of the reacting mixture is organized by using a compression body, shaped as a continuous monofilar helix with a constant pitch angle. Numerical simulations are performed for a supersonic flow of a stoichiometric hydrogen-air mixture with Mach number $M_0=3$ at the combustor entrance. A mathematical model of the reacting flow in the combustor is developed in a two-dimensional unsteady formulation. The flow dynamics at the beginning of combustor operation and the structure of the steady flow in the combustor are numerically studied. Simulations are performed for various helix angles and combustor sizes. A bifurcation of the steady flow structures with respect to the initial conditions of combustor operations is detected for some combinations of the geometric parameters of the combustor.

1. Introduction

A flow-type combustor with a new design was proposed in our previous publication [1]. The combustor is an annular channel located between the inner and outer cylindrical walls. A supersonic flow of a uniformly mixed stoichiometric hydrogen-air mixture with Mach number $M_0$ higher than the Mach number $M_{CJ}$ of the detonation wave in the Chapman-Jouguet (CJ) regime enters the combustor. The reacting mixture is burned in a steady oblique detonation wave (ODW). The ODW is formed at the ceiling above a compression surface, which is an infinitely thin solid monofilar helix. This helix overlaps the entire cross section of the annular channel from the inner to the outer wall of the combustor (see Fig. 1 in [1]). The helix has a constant angle $\alpha$ with respect to the combustor axis. The width of the annular channel is assumed to be much smaller than the combustor radius; therefore, the gas flow over the combustor radius is assumed to be uniform. As a result, the flow in the combustor can be modeled in a two-dimensional formulation, as it is usually done in studying rotating DWs in annular combustors [2].

The detonation flow structure in this combustor was studied in [1] for the Mach number $M_0=5$ (hypersonic flow) and varied geometric parameters of the combustor (length $L$, height $H=2\pi r_c$, and helix angle $\alpha$). The main intriguing result was detected effect of bifurcation of the steady structure of the detonation flow in the combustor over the initial vector of the solution at certain combinations of the geometric parameters of the combustor.

The present paper describes further investigations of the flow structure and steady flow regimes with a steady ODW in the annular combustor based on the new concept. Two-dimensional numerical
simulations are performed at the flow Mach number $M_0=3$ at the combustor entrance (supersonic regime) for different combustor geometries.

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 by 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 hydrogen mixtures. The main heat release takes place after the induction period. Changes in internal energy and all thermodynamic parameters of the gas are described at this stage by equations of the approximate kinetic model [6, 7]. The model is highly accurate and consistent with the second law of thermodynamics. The constants of the model have a clear physical meaning and are calculated from the tabulated thermochemical parameters of the mixture before the two-dimensional numerical calculation. This two-stage kinetic model was already used for numerical simulation of the two-dimensional cellular DW structure in hydrogen–oxygen mixtures in our previous study [8]. 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 dilution with argon.

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 are 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] is 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 is performed with second-order accuracy by using additive semi-implicit Runge-Kutta methods [13]. The time step is determined at each time layer of the solution from the stability condition [9]. In the present simulations, the values of the Courant number are CFL=0.3–0.4. A uniform fixed grid is used in both directions.

At the inlet boundary $x=0$ of the solution domain, incoming unperturbed supersonic flow parameters are specified. In the external peripheral grid cells at the outlet boundary $x=L$, low counterpressure for the guaranteed critical gas flow from the DC outlet into the surrounding virtual space is specified. At the upper and lower boundaries, periodic boundary conditions are defined at $x\leq L_1$ as well as the conditions of an impervious solid wall at $x>L_1$.

The code is parallelized with MPI library using the domain decomposition technique.

4. Results and Discussion

The present numerical simulations are performed for a stoichiometric hydrogen-air mixture. A uniform flow of the mixture with a static pressure $p_0=0.166$ atm and static temperature $T_0=850$ K is set at the combustor entrance ($x=0$). The geometric parameters $L$, $H$, and $\alpha$ were varied. For these initial parameters of the mixture, the Mach number of a self-sustained DW is $M_{CJ}=2.73$.

Preliminary numerical calculations show that it is more difficult to obtain flow regimes with an ODW stabilized at the helix at $M_0=3$ than at $M_0=5$ (see [1]). The simulation results obtained up to now can be in advance classified in the following way by considering the helix angle $\alpha$ as the governing parameter.

4.1. Supercritical helix angle
Figure 1. Stationary structure of flow field in a detonation chamber for $H=24$ cm and $\alpha=24^\circ$. Start from: (a) a uniform supersonic flow; (b) a motionless mixture.

The angle of the helix (wedge), at which a detached ODW from the tip of the compression body arises is called the critical angle $\alpha_{cr}$. Within the framework of the simplest DW model in the CJ regime with instantaneous heat release (where the induction and heat release times are equal to zero), the critical helix angle for the chosen mixture is estimated as $\alpha_{cr}=19.4^\circ$ [3]. For detonation models with finite times of induction and heat release, it is necessary to perform two-dimensional calculations. Such calculations [3] showed that the value of $\alpha_{cr}$ is in the range from 19° to 20°. According to our calculations, the value of $\alpha_{cr}$ varies between 22° and 24°. These values were obtained in flow calculations in a semi-infinite space along the $y$ axis, i.e., in the absence of the rarefaction wave (RW) or any other waves at the upper boundary of the domain. In reality, the computations were performed in a finite-size two-dimensional domain with specially imposed numerical non-reflecting boundary conditions at the upper boundary, which formally corresponded to the condition $H=\infty$. The difference in the value of $\alpha_{cr}$ from that obtained in [3] can be explained by the difference in the detonation kinetics used and in the computational grid size (the grid in [3] was much rougher).

Figure 1 shows the normalized density field for the combustor with $H=24$ cm, $L=20$ cm, and $\alpha=24^\circ$. Figure 1a corresponds to a steady flow that originates from the uniform mixture with $\mathbf{u}=(M_0, c_0, 0)$ everywhere in the entire domain at the beginning ($t=0$) [1]. Here $\mathbf{u}$ is the two-dimensional vector of the bulk velocity of the gas and $c_0$ is the initial velocity of sound. Physically, this process corresponds to instantaneous insertion of the examined compression body into the initial uniform supersonic flow, followed by the formation of an unsteady shock-wave structure around the body at later times. Figure 1b shows the final flow pattern for the case with a motionless mixture $\mathbf{u}=(0,0)$ at the beginning. This initial state leads to the formation of a plane shock wave (SW) at $t=0$ in the vicinity of $x=0$, its propagation over the domain of the solution from left to right, and its interaction with the compression body. It is seen that a detached overdriven ODW is formed in both cases of combustor operation at the beginning. In this flow regime, effective operation of the flow-type combustor is impossible. It is seen in the central flow region that the ODW has a multifront (cellular) structure in this region.

An attempt was made to obtain a stable ODW inside the combustor channel at $\alpha=24^\circ > \alpha_{cr}$. For this purpose, a series of computations was performed with a decreasing value of $H$: 20, 18, 10, 8, and 6 cm. The computations were based on the following idea: as the domain height $H$ decreases, the RW, which starts to form with time behind the rarefaction surface of the helix (upper boundary of the domain), begins to interact with the bow SW [1, 3] formed above the compression surface of the helix (lower boundary of the domain). There is no heat release behind the bow SW yet; therefore, the pressure behind this SW is lower than the pressure behind the ODW front. This fact was expected to result in stabilization of the forming ODW inside the combustor channel.
Figure 2. Stationary structure of flow field in a detonation chamber for $H=6$ cm and $\alpha=24^\circ$. Start from: (a) a uniform supersonic flow; (b) a motionless mixture.

It turns out, however, that a detached overdriven ODW is formed for all values of $H$. As an example, figure 2 shows the final structure of the flow for $H=6$ cm for the case of process beginning from the flow with $\mathbf{u}=(M_0c_0, 0)$ (figure 2a) and for the motionless mixture ($\mathbf{u}=(0,0)$) at the beginning (figure 2b). As was mentioned above, the calculation with the formal value $H=\infty$ at $\alpha=24^\circ$ also predicts the formation of a detached ODW.

Thus, the RW formed at the upper boundary at the initial stage of flow evolution cannot stabilize the overdriven ODW inside the combustor channel if the helix angle is greater than $\alpha_{cr}$. However strange it may seem, an oblique SW is formed at the upper boundary instead of the RW at later times, after interaction with the ODW. This SW is fairly strong, and it is clearly visible in the upper part of the flow in Figs. 1 and 2. Thus, we obtain a steady oblique SW above an obstacle shaped as a backward-facing step in a supersonic flow, which is an extremely unusual flow configuration.

Figure 3. Stationary structure of temperature (K) flow field in a detonation chamber for $L=25$ cm and $\alpha=22^\circ$. Start from a uniform supersonic flow. (a) $H=\infty$; (b) $H=25$ cm.

4.2. Subcritical helix angle
Let us now consider the flow with the helix angle $\alpha=22^\circ < \alpha_{cr}$. The results of computations in the domain with $H=25$ cm and $L=25$ cm are presented in figure 3. The flow field with non-reflecting boundary conditions on the upper boundary (formally, $H=\infty$) is shown in figure 3a. Here one can see the classical so-called $\lambda$–structure with the bow SW, triple point, and oblique detonation wave [1, 3].
Figure 4. Stationary structure of flow in a detonation chamber for \( L=20 \) cm and \( \alpha=22^\circ \). Start from a uniform supersonic flow. (a) normalized density; (b) temperature (K).

Figure 3b shows the flow structure in a finite-size combustor, i.e., with the solid-wall boundary conditions on the upper surface of the helix. There was a uniform flow \( \mathbf{u}=(M_0\cdot c_0, 0) \) at the beginning of combustor operation. It is seen that the flow structure consists of a detached overdriven ODW in the lower part of the domain and a short nonreacting oblique SW in the upper part of the domain. Approximately the same type of the flow is formed in the case of computations with the SW at the combustor entrance \( \mathbf{u}=(0,0) \) at \( t=0 \); there are only minor differences of no principal importance.

Similar flow fields were obtained in the combustor with \( \alpha=15^\circ \), \( H=60 \) cm, and \( L=80 \) cm. In computations without the RW at the upper boundary, \( H=\infty \), a stable \( \lambda \)–structure with the ODW was formed in the combustor. In the case of a real finite-height combustor, a detached ODW was formed regardless of the conditions at the beginning.

Thus, it can be expected that there is a certain value of \( H \), possibly, very large, that initiates a transition from the detached ODW to the \( \lambda \)–structure in the finite-height combustor if the RW formation at the upper boundary and its interaction with the ODW formed at the lower boundary at early times are taken into account. This idea will be verified in further investigations.

Computations were also performed for a shortened combustor with \( \alpha=22^\circ \), \( H=25 \) cm, and \( L=20 \) cm. The following flow configurations were detected in this case, in contrast to the above-considered case with \( L=25 \) cm. Figure 4 shows the flow fields calculated for the case of a uniform flow at the beginning. It is seen that a stable classical \( \lambda \)–configuration with the ODW is formed inside the combustor. There is a cardinal difference from the case with \( L=25 \) cm (cf. figure 3b). Figure 5 shows the flow fields for the case with the SW at the combustor entrance. One can see a detached ODW above the compression surface of the helix in the lower part of the flow and an oblique inert SW at the upper boundary of the combustor above the rarefaction surface of the helix. Thus, there is a bifurcation of the steady solution in terms of the initial condition of the problem, which was observed in our previous work [1] at \( M_0=5 \). So, we have found that the steady flow structure depends on the starting conditions of detonation combustion in the combustor.

In computations for \( L=20 \) cm without the RW at the upper boundary, i.e., \( H=\infty \), a stable \( \lambda \)–structure with the ODW is formed inside the combustor, similar to the case with \( L=25 \) cm. The structure of the \( \lambda \)–configuration looks very much like the structure in figure 4; the only difference is the absence of the RW in the upper part of the flow.

For the flow type considered here, there is one more characteristic value of the helix angle. This is the angle \( \alpha_{CJ} \) at which oblique Chapman-Jouguet detonation arises on the helix (or wedge). If \( \alpha > \alpha_{CJ} \), as in all computations described above, then an overdriven ODW is formed near the compression body. The estimate of this angle based on the ideal detonation model [3] yields approximately 13°, \( \alpha_{CJ} < \alpha_\text{cr} \). In further investigations, it is planned to simulate detonation flows in the combustor at \( \alpha < \alpha_{CJ} \).
The classical initial and boundary conditions lead to a drastic change in the steady flow structure in the combustor. This phenomenon was observed in our previous study for the problem at certain geometric parameters of the combustor. This phenomenon was observed in our previous study for different initial conditions of the solution for different initial conditions of the ICW transforms of the solution for different initial conditions of the flow reconstruction for two different conditions at the beginning. A scale effect has been found in the case of formation of a steady overdriven oblique detonation wave at angles $\alpha < \alpha_c$. An increase in the combustor length $L$ for the same value of $\alpha$ and identical initial and boundary conditions leads to a drastic change in the steady flow structure in the combustor. The classical $\lambda$-structure with the ODW transforms to a detached DW from the helix tip in the case of a uniform flow at the beginning.

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References
[1] Trotsyuk A V 2017 J. of Phys.: Conf. Series 899 042010 doi:10.1088/1742-6596/899/4/042010
[2] Bykovskii F A and Zhdan S A 2013 Continious Spin Detonation (Novosibirsk: Lavrentyev Institute of Hydrodynamics Press) 422 p in Russian
[3] Berlyand A T, Vlasenko V V and Svisheev S V 2001 Combust. Explo. Shock Waves 37 82–98
[4] Korobeinikov V P, Levin V A, Markov V V and Chernyi G G 1972 Acta Astronaut. 17 529–37
[5] White D R 1967 Proc. 11th Symposium (Int.) on Combustion The Combustion Institute (Pittsburgh: Academic Press) 147–54
[6] Nikolaev Yu A and Fomin P A 1982 Combust. Explo. Shock Waves 18 53–8
[7] Nikolaev Yu A and Zak D V 1988 Combust. Explo. Shock Waves 24 461–4
[8] Trotsyuk A V 1999 Combust. Explo. Shock Waves 35 549–58
[9] Godynov S K 1976 Numerical Solution of the Multi-Dimensional Problems of Gaseous Dynamics (Moscow: Nauka Press) 400 p in Russian
[10] Yamamoto S and Daiguji H 1993 Comput. Fluids 22 259–70
[11] Batten P, Leschziner M A and Goldberg U C 1997 J. Comput. Phys. 137 38–78
[12] Coquel F and Perthame B. 1998 SIAM J. Numer. Anal. 35 2223–49
[13] Shen J W and Zhong X 1996 AIAA 27th Fluid Dynamics Conf., New Orleans, LA, June 17-20, 1996 AIAA Paper No.96–1969