Numerical study of continuously rotating detonation in two-fuel gaseous mixture

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Abstract. Numerical simulation of continuously rotating detonations of stoichiometric two-fuel mixture with air has been carried out for the cylindrical annular detonation chamber (DC) of the rocket-type engine. The syngas \((1-\alpha)\text{CO}+\alpha\text{H}_2\), a binary mixture of hydrogen \(\text{H}_2\) and carbon monoxide \(\text{CO}\), is taken. We studied the global flow structure in DC, and the detailed structure of the transverse wave (TW) front in the continuous rotating regime. 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 region of existence of stable continuous detonation regime in coordinates of the stagnation pressure - temperature in injection manifold (receiver) and the geometric limit of stable TW have been determined.

1. Introduction
At present, there are several different concepts of detonation propulsion engine. In the first concept, unsteady combustion of the mixture occurs in rotating transverse detonation waves (TDWs) in an annular cylindrical detonation chambers (DC) [1, 2]. This concept of engine can be realized as rocket-type or as flow-type of DC. In another way, this process is often called continuous spin detonation or continuously rotating detonation (CRD). The second concept only applies to flow-type detonation engine and uses steady oblique detonation waves (ODW) formed over the surface of the different compression bodies of various geometries in supersonic inflow of reacting mixture. The third concept based on periodically initiation of unsteady propagating DW in DC channel of pulse detonation engine (PDE). PDE implementation is possible both for the rocket-type and for the flow-type version of the fresh mixture supply.

To date, numerical studies of the detonation process have been limited to gas mixtures of one fuel with oxygen, sometimes with inert diluents (nitrogen for modeling air mixtures, argon). Apparently, this can be explained by the lack of appropriate models of chemical kinetics that do not require expensive computations. However, multifuel gas mixtures are widely used in the chemical industry and in the power industry (for example, syngas, a binary mixture of hydrogen \(\text{H}_2\) and carbon monoxide \(\text{CO}\)). In our works a two-stage generalized model of detonation kinetics for a multi-fuels mixtures has been proposed. Based on this kinetics, a numerical simulation of a two-dimensional (2D) structure of the propagating DW in syngas with air mixtures at normal initial condition has 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 transverse sizes of the detonation cell for studied mixture have been determine. The cell sizes are in
good quantitative agreement with experimental data [5] in a wide range of the H₂ concentration $\alpha$ in a stoichiometric mixtures $\alpha H_2+(1-\alpha)CO+Air$ syngas with air.

In present paper, based on the fundamental study of multi-front (cellular) structure of the classical propagating DW in two-fuel mixtures, numerical simulation of continuously rotating detonation of stoichiometric syngas-air for $\alpha=0.1$ has been carried out in the cylindrical annular DC of the rocket-type engine. The main goal was to study the possibility of detonation-type combustion of this rather difficult-to-detonate mixture (the calculated by us cell size under standard initial conditions is 25 mm and this value is very close to experimental data [5]).

2. Governing equations and chemical kinetics model

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 stage and main heat release stage) for two-fuel reacting mixtures first proposed by us in [3, 4]. For the first, induction stage, we proposed an original semi-empirical formula for determining the duration of the induction period in a two-fuel mixture, based on kinetic data in empirical Arrhenius-type formulas for the induction time in an individual mixture of each component of the binary fuel with an oxidizer.

The main heat release takes place after the induction period. The value of heat release and all thermodynamic parameters of the reacting gas is described by equations of the generalized kinetic model [3, 4]. This heat release 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 simulations.

Numerical investigations of CRD in a cylindrical annular DC have been conducted according to 2D approach [1, 2]. It is assumed that the size of the annular gap $\Delta$ is much smaller than the DC average diameter $d_{DC}$, $\Delta << d_{DC}$.

3. Numerical method

The resultant systems of equations were solved numerically using the 2D code based on the Godunov-type finite-volume scheme with the fourth-order MUSCL TVD reconstruction and the advanced HLLC algorithm for an approximate solution of the Riemann problem. In implementation of this algorithm for the case of a chemically reacting mixture, the “energy relaxation method” was used. Integration in time was performed with second-order accuracy by using additive semi-implicit Runge-Kutta methods. All details of these numerical algorithms can be found in [6, 7].

In present 2D numerical simulations a fixed grid, uniform in both directions, is used.

At the DC inlet boundary $y=0$ there are the system of Laval micro-nozzles that are feeding from injection manifold (receiver) with fresh pre-mixed gaseous mixture. The algorithm of micro-nozzles operation depending of stagnation pressure $p_m$ and stagnation temperature $T_m$ in manifold and the back pressure at the inlet boundary of the chamber has been described in detail in [1, 2]. At the outlet boundary $y=H_{DC}$ there are virtual external grid cells with low back pressure to guarantee critical gas flowout from this boundary into the surrounding virtual space.

At the left $x=0$ and right $x=W_{DC}=\pi d_{DC}$ boundaries, a periodic boundary conditions are defined.

The codes are parallelized with MPI library using the domain decomposition technique. At normal-resolution simulations the total number of numerical cells in the $x$ and $y$ directions were $N_x=1536$, $N_y=768$ respectively. At high-resolution simulations the total cells number were twice greater.

4. Results and Discussion

Numerous numerical simulations have shown that a stable CRD regime in the syngas-air mixture turned out to be possible only for sufficiently large DC sizes and rather high values of the stagnation pressure and temperature in the manifold. In this case, the effect of the influence of the length of the
DC on the stability of the detonation regime was obtained. This result is fully consistent with experimental observations [1].

Let us demonstrate this effect by the example of the detonation regime for DC with $H_{DC}=60$ cm, $W_{DC}=120$ cm, and $S_*/S_{DC}=0.1$, where $S_{DC}$ – DC annular channel cross-sectional area, $S_*$ – the total throat area of micro-nozzles. In all other our simulations, the value of $S_*/S_{DC}$ remained unchanged. The parameters of the mixture in the manifold are $p_m=15$ atm, $T_m=900$ K. For these DC and manifold parameters CRD regime is not sustained. Figure 1 shows the pressure history recorded by a virtual point-wise pressure gauge located at $x=0$, $y=0$. The values for static (red line) $p$ and 'total' pressure (blue line) $p_{tot}=p+p'u_y^2$ are given. Each peak on this record corresponds to the passage of the DW front over the pressure gauge; the time between the peaks is the TDW rotation period $\Delta t$. The difference in the magnitude of the pressure in the peaks is due to the internal multifront structure of the TDW (see figure 2) and the discreteness of reading data from the virtual gauge.

![Figure 1. Static pressure $p$ and total pressure $p_{tot}$ (atm) history at the point $x=0$, $y=0$ for $H_{DC}=60$ cm, $W_{DC}=120$ cm.](image1)

![Figure 2. Structure of rotating detonation wave in detonation chamber with $H_{DC}=60$ cm, $W_{DC}=120$ cm: temperature (K) flow field at $t=15$ ms.](image2)
Figure 3. Structure of rotating detonation wave in detonation chamber with HDC=60 cm, WDC=120 cm: numerical Schlieren-visualization flow field at t=18 ms.

Figure 4. Static pressure $p$ and total pressure $p_{tot}$ (atm) history at the point $x=0$, $y=0$ for $H_{DC}=100$ cm, $W_{DC}=120$ cm.

Figure 5. Structure of rotating detonation wave in detonation chamber with $H_{DC}=100$ cm, $W_{DC}=120$ cm: normalized density flow field at $t=20$ ms.
Figure 6. Structure of rotating detonation wave in detonation chamber with $H_{DC}=100$ cm, $W_{DC}=120$cm: temperature (K) flow field at $t=30$ ms.

In Figure 1, we see regular pressure peaks up to about the time moment $t=15$ ms, which indicates the stability of the CRD regime. The structure of the flow inside the DC at the time $t=15$ ms is shown in figure 2, the temperature flowfield is presented. Here we see a multifront TDW with a height of about $h=25$ cm and a classic "triangle" of fresh mixture in front of it. However, after this moment, the regularity of the pressure maxima is disrupted. Analysis of the flow fields shows that during this time interval there is a sharp irreversible increase in the length of the induction zone, separation of the heat release zone from the leading shock front of the TDW. This ultimately leads to the breakdown of the detonation regime, and the degeneration of the TDW into a weak oblique pressure jump, shown in figure 3 at $x=50$ cm for $t=18$ ms.

An increase in the length of the DC from $H_{DC}=60$ cm to $H_{DC}=100$ cm leads to stabilization of the CRD regime. The values of $p_m=15$ atm, $T_m=900$ K value remain the same. Figure 4 shows a pressure history that shows time-regular pressure peaks from $t=15$ ms to $t=30$ ms. In total, the TDW made 18 full circulations. The average rotation period of the TDW is $\Delta t=810.7$ $\mu$s, which corresponds to the average detonation velocity $D_{\text{aver}}=1480$ m/s. Figure 5 shows the field of normalized density in the DC at time $t=20$ ms, and figure 6 shows the temperature field (K) at time $t=30$ ms. These figures show a stable multifront TDW structure with internal transverse waves at its front. Note only an insignificant decrease in the TDW height from $h\approx 28$ cm for the moment $t=20$ ms to with $h=25.5$ cm for the moment $t=30$ ms. The time-averaged specific mass flow rate $<\rho \cdot u_y>$ into the DC on the inlet boundary is $<\rho \cdot u_y>=200$ kg/s$\cdot$m$^2$, averaged value of specific impulse on outlet boundary is $<I>=115$ s.

Further two-dimensional studies have shown that with an increase in the DC diameter, stable detonation modes are possible at a lower stagnation pressure, $p_m=10$ atm. For the DC parameters $H_{DC}=100$ cm, $W_{DC}=200$cm, $p_m=10$ atm, $T_m=900$ K, a stable regime of TDW rotation was obtained. Figure 7 shows the pressure history from $t=30$ ms to $t=44$ ms. The average rotation period of the transverse DW is $\Delta t=1350.7$ $\mu$s, the average detonation velocity is $D_{\text{aver}}=1481$ m/s. Figure 8 shows the temperature flowfield in a DC with a steadily rotating multifront TDV with a height of $h\approx 45$ cm. At the TDW front, approximately 4–5 internal transverse waves are observed. For this mode, the average specific flow rate is $<\rho \cdot u_y>=133.3$ kg/s$\cdot$m$^2$ and the average specific impulse is $<I>=88.1$ s.

Conclusions
In this study, the two-stage generalized model of detonation kinetics developed for modeling multifront DWs in two-fuel mixtures was applied to study the phenomenon of continuously rotating detonation in this mixture. The first stage of the study showed that the phenomenon of CRD is possible for a mixture of syngas with air at a hydrogen content of $\alpha=0.1$ in this binary fuel. It has been
shown that for a stable CRD mode, sufficiently large DC sizes and high values of pressure and temperature in the manifold are required. At present, numerical experiments are being carried out to find stable CRD regimes at lower parameters in the fresh mixture supply system, especially temperature, for more convenient use of the detonation mode of combustion of syngas mixture in industrial burners or in a detonation engine.

![Figure 7](image1.png)

**Figure 7.** Static pressure \( p \) and total pressure \( p_{\text{tot}} \) (atm) history at the point \( x=0, y=0 \) for \( H_{\text{DC}}=100 \text{ cm, } W_{\text{DC}}=200 \text{ cm} \).

![Figure 8](image2.png)

**Figure 8.** Structure of rotating detonation wave in detonation chamber with \( H_{\text{DC}}=100 \text{ cm, } W_{\text{DC}}=200 \text{ cm} \): numerical Schlieren-visualization flow field at \( t=44 \text{ ms} \).

The above average specific mass flow rate and specific impulse values should be considered as indicative values, since they are obtained for a chamber of a rather arbitrary \( W_{\text{DC}} \) size, which simply provides a sustained state of rotating detonation. In the future, we plan, for each of the stable regimes mentioned above, to search for the minimum value of \( W_{\text{DC min}} \), at which a stable mode is still possible. This value of \( W_{\text{DC min}} \) correlates with the minimum distance \( \Delta l_{\text{min}} \) [1] between two adjacent TDWs in a set of TDWs rotating in the same direction in a chamber of sufficiently large diameter. The value of \( \Delta l_{\text{min}} \) is an analogue of the transverse size of the detonation cell in a DW propagating in a straight channel for the case of a CRD in a cylindrical DC. It is more correct to determine all the parameters of the stable regime of the CRD at \( W_{\text{DC}=W_{\text{DC min}}} \).
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