Calculation of continuous spin detonation of a hydrogen-oxygen mixture in an annular combustor with oxygen ejection

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Abstract. A closed mathematical model of continuous spin detonation in a H₂-O₂ mixture with oxygen ejection from the environment has been developed. The model takes into account the inverse effect of pulsation processes in the combustor on oxygen ejection. A numerical study was performed for a 10 cm diameter ramjet annular combustor with geometric dimensions corresponding to experiments. One-wave modes of continuous spin detonation were calculated and the flow structure was analyzed with variation in the specific hydrogen flow rate from 3 to 3.75 kg/(s·m²). Decreasing the flow rate of ejected hydrogen during continuous detonation in the combustor is found to lead to a monotonic decrease in the detonation velocity, wave front height, average static pressure, and equivalence ratio, but to an increase in the oxygen ejection coefficient. The results are validated against experimental data.

1. Introduction
The results of studies of continuous spin detonation (CSD) according to Voitsekhovskii’s scheme are presented in [1, 2]. CSD of a hydrogen-oxygen mixture with oxidizer ejection was first obtained experimentally in [3, 4], and the calculations of CSD were performed in [5] using the Abramovich classical ejector flow model [6] at the combustor entrance. The objectives of this study were to develop a closed mathematical model of CSD in the O₂ ejection mode without using the simplifying assumption of [5], to numerically study the CSD dynamics of a H₂-O₂ mixture in the O₂ ejection mode in a ramjet annular combustor with a diameter of 10 cm, and to compare the results with experiments [4].

2. Formulation of the problem
2.1. Mathematical model
Mathematical modeling of the initiation and propagation of CSD in a H₂-O₂ mixture in the O₂ ejection mode was carried out in a ramjet annular combustor (diameter d, length L, expansion of the annular combustor channel from δ to Δ and then to Δexit) and an attached entrance section in the form of an annular converging nozzle (length L₀, contraction of the channel from Δ₀ to δ), which was initially filled with oxygen. For experimental annular combustors [3, 4], the following inequalities hold: δ < Δ << d/2, Δ₀ << d/2, and Δexit << d/2. Therefore, by expanding the annular region into a rectangular solution domain Ω₀ ∪ Ω (see figure 1), we can formulate a quasi-three-dimensional mathematical problem in a similar manner as was done in [2].
Figure 1. Solution domain of the periodic problem $\Omega_0 \cup \Omega$.

The $\text{H}_2\text{-O}_2$ mixture flow in the computational domain $\Omega_0 \cup \Omega$ is described by the following system of equations of non-stationary gas dynamics with chemical reactions:

\[
\begin{align*}
\rho_t + S^{-1} (\rho u S)_x + (\rho v)_y &= f_1^{\text{H}_2}, \\
(\rho u)_t + S^{-1} (\rho u^2 S)_x + (\rho uv)_y + p_x &= f_2^{\text{H}_2}, \\
(\rho v)_t + S^{-1} (\rho uv S)_x + (\rho v^2)_y + p_y &= 0, \\
(\rho E)_t + S^{-1} [\rho u (E + \frac{p}{\rho}) S]_x + [\rho v (E + \frac{p}{\rho})]_y &= f_4^{\text{H}_2}, \\
(\rho Y)_t + S^{-1} (\rho u Y S)_x + (\rho v Y)_y &= \rho f_5, \\
(\rho u)_t + S^{-1} (\rho u S)_x + (\rho v)_y &= \rho f_6 + f_6^{\text{H}_2}, \\
(\rho z)_t + S^{-1} (\rho u z S)_x + (\rho v z)_y &= 0.
\end{align*}
\]

Here $t$ is time, $x$ and $y$ are the spatial variables of the orthogonal coordinate system, $\rho$ is the density; $u$ and $v$ are the velocity components, $p$ is the pressure, $E = U + (u^2 + v^2)/2$, $U(T, \mu)$ is the total internal energy of the gas, $T$ is the temperature, $\mu$ is the current molar mass of the mixture, $Y$ is the fraction of the chemical induction period, $z$ is the mass fraction of oxygen, $S = S(x)$ is channel cross-sectional area in the domain $\Omega_0$ and the combustor, which varies along the $x$ coordinate as

\[
S(x) = \begin{cases}
\Delta_0 \cdot l, & -L_0 < x < -L_0 / 2 \\
[(\Delta_0 - \delta) \sin(-\pi / L_0) + \delta] \cdot l, & -L_0 / 2 < x < 0 \\
\delta \cdot l, & 0 < x < L_1 / 2 \\
[(\Delta - \delta) \sin(-\pi / L_1 - \pi / 2) + \delta] \cdot l, & L_1 / 2 < x < L_1 \\
[\Delta + (\Delta_{exit} - \Delta) \cdot (x - L_1)] \cdot l, & L_1 < x < L
\end{cases}
\]

The quantities $f_i^{\text{H}_2}$ ($i = 1, 2, 4, 6$) describe the injection of $\text{H}_2$ through the supply system located in the initial part of the domain $\Omega$ ($0 < x < L_1/2$). The supply of $\text{H}_2$ was carried out through a set of Laval micro nozzles uniformly distributed around the combustor circumference with total throat area per unit length $S_{cr}$. Under the assumption of instantaneous mixing of the components over the combustor cross
section, the right sides of system (1), expressing the mass, momentum, and energy fluxes of H2 in the combustor, are uniquely determined using the formulas of [2].

As in [7, 5], the quantities \( f_5 \) and \( f_6 \) describe the energy release within the framework of the two-stage kinetic model. The induction stage \( (0 < \chi < 1, \ f_5 = -1/T_{ind} \), \( f_6 = 0) \), where energy release is absent; the induction period was calculated using the White formula [8]:

\[
t_{ind} = \frac{K_a \left( \mu_{O2} \mu_{H2} \right)^{1/2}}{\rho \zeta(1-z)} \exp\left( \frac{\varepsilon_a}{RT} \right),
\]

where \( \varepsilon_a = 18.1 \text{ kcal/mol} \) is the activation energy, \( K_a = 4.17 \times 10^{-11} \text{ (mol-s/l)} \) is the pre-exponential factor, \( R \) is the universal gas constant, \( \mu_{O2} \) is the molar mass of oxygen, and \( \mu_{H2} \) is the molar mass of hydrogen. Chemical transformation stage \( (\chi = 0, f_5 = 0, f_6 \neq 0) \), where the rate of energy release is determined by the rate of chemical reactions [7]:

\[
f_6 = 4K_a [W_1(\mu)p^2 - W_2(T, \mu)p], \ W_1(\mu) = \frac{(1 - \mu)}{\mu_{max}}^2, \ W_2(T, \mu) = K_c \left( \frac{\mu}{\mu_{min}} - 1 \right) \left( \frac{T}{T_0} \right)^{\beta} \left[ 1 - \exp \left( -\frac{T}{T_0} \right) \right] \exp \left( -\frac{E_{d}}{RT} \right),
\]

where \( K_c \) is the generalized recombination rate constant, \( K(z) \) is the equilibrium constant, \( T_0 \) is the initial temperature of the mixture, \( \beta(z) = 1 + \sigma_{max}(\mu_{max}/\mu_{min} - 1) \), \( \sigma_{max}(z) \) is the molar fraction of triatomic molecules in the ultimately recombined state, \( \mu_{min}(z) \) and \( \mu_{max}(z) \) are the molar masses of the gas in the ultimately dissociated and ultimately recombined states. The quantity \( K(z) \) was calculated in accordance with the equation of chemical equilibrium for the corresponding composition, and the dependence of the remaining quantities on \( z \) are described in detail in [2].

System (1) was supplemented by the equations of state

\[
p = \rho RT/\mu, \ U = U_{inh} + U_{cb} \tag{5}
\]

where \( U_{inh} \) and \( U_{cb} \) are the thermodynamic and chemical components of the internal energy, respectively, which were determined in a similar manner as in [7].

System (1–5) is closed and completely determines the unsteady motion of the H2-O2 reaction mixture with variable heat release in the reaction zone behind the detonation wave.

### 2.2 Boundary conditions

a) at the nozzle entrance (boundary \( \Gamma_0: x = -L_0; \ 0 \leq y \leq L \) and at the combustor exit (boundary \( \Gamma_1: x = L; \ 0 \leq y \leq L \), the boundary fluxes of mass, momentum, and energy due to the interaction of the gas with the environment at pressure \( p = p_a \) were determined using the method of [9].

b) on the left and right boundaries of the domains \( \Omega \) and \( \Omega_0 \), the condition of the periodicity of the solution (with period \( L \)) was used:

\[
F(x, 0, t) = F(x, l, t), \ -L_0 \leq x \leq L. \tag{6}
\]

### 2.3 Initial constants of the model

The following initial constants of the model were specified (1)-(6):

\[
\begin{align*}
\mu_{O2} &= 2 \text{ kg/kmol}, \mu_{H2} = 32 \text{ kg/kmol}, \gamma = 1.4, \\
R &= 8.3144 \times 10^5 \text{ J/(kmol-K)}, \ E_d = 110 \text{ kcal/mol}, \\
K_a &= 6.0 \times 10^{-8} \text{ m}^2/(\text{kmol}^2\cdot\text{s}), \ T_0 = 300 \text{ K}, \ p_0 = 1.013 \times 10^5 \text{ Pa}
\end{align*}
\]

The following geometric parameters were used:

\[
\begin{align*}
L_0 &= 10 \text{ cm}, \ L_1 = 1 \text{ cm}, \ L = 10 \text{ cm}, \ S_0/S_\Lambda = \delta/\Delta = 0.338, \\
S_{x0}/S_\Lambda = S_{x0}/S_\Delta = 3.36, \ S_{y0}/S_\Lambda = S_{y0}/\Delta = 3.
\end{align*}
\]
2.4 Governing parameters of the model

For fixed geometric dimensions of the domains \( \Omega_0 \) and \( \Omega \) and the relations for \( S(x) \), the solution of the non-stationary CSD problem (1–8) depends on the governing parameters:

\[
\frac{p_{H_2}^*}{T_{H_2}^*}, \frac{S_{cr}}{p_a}, l.
\]

Here \( p_{H_2}^* \) and \( T_{H_2}^* \) are the pressure and stagnation temperature in the \( H_2 \) supply system, \( p_a \) is the ambient pressure, and \( l \) is the period of the problem along the \( y \) axis.

3. Calculation results

In the computational domain \((-10 \text{ cm} < x < 10 \text{ cm}, 0 < y < l)\), the following two-dimensional non-stationary periodic problem with a period \( l = \pi(d_c - \Delta) = 29.845 \text{ cm} \) and parameters in the \( H_2 \) supply system: stagnation pressure \( \frac{p_{H_2}}{p_0} = 3.133 \), stagnation temperature \( \frac{T_{H_2}}{T_0} = 1 \), initial specific hydrogen flow rate \( g_{H_2} = \frac{G_{H_2}}{S_{\Delta}} = 3.75 \text{ kg/(s}\cdot\text{m}^2) \), which corresponds to experiments [4], was solved. Here \( x = 0 \) is the coordinate of the combustor entrance, \( S_{\Delta} = \pi(d_c - \Delta)\Delta = 14.9 \text{ cm}^2 \) is the cross-sectional area at a distance of 1 cm from the combustor entrance. At the combustor end, a counterpressure \( \frac{p_a}{p_0} = 1 \) was specified. Oxygen at rest in the domain \( \Omega_0 \) and the stoichiometric \( H_2\text{-O}_2 \) mixture at rest in the domain \( \Omega \) were used as initial parameters. First, over \( \approx 1 \text{ ms} \), we calculated the purging of the combustor: supplying \( H_2 \) to the initial part of \( \Omega \) led to \( \text{O}_2 \) ejection from \( \Omega_0 \), resulting in the formation of a detonable mixture in the combustor.

The calculations of the initiation of a transverse detonation wave (TDW) and the dynamics of its formation show that by the time \( t \approx 11.2 \text{ ms} \) after the initiation, self-sustained CSD of the TDW is established. The time dependence of the dimensionless pressure \( P = \frac{p}{p_0} \) at a fixed point \( x = 0.5 \text{ cm}, y = 0 \) and the average combustor pressure are presented in figure 2. One can see periodic oscillations with a period \( \Delta t \approx 0.127 \text{ ms} \), which corresponds to a rotation frequency of the TDW \( f \approx 7.87 \text{ kHz} \) and a detonation velocity \( D \approx 2.35 \text{ km/s} \). The height of the TDW front is \( h \approx 1.8 \text{ cm} \).

Figure 2. Dependence of the dimensionless pressure \( P = \frac{p}{p_0} \) on time \( t \) (ms) at the point with coordinates \((x = 0.5 \text{ cm}, y = 0)\) (solid line) and the mean pressure (dashed line) at a distance \( x = 0.5 \text{ cm} \) from the combustor edge.

The distribution of the dimensionless temperature \( T/T_0 \) (a) and the equivalence ratio \( \phi = 8(1/z - 1) \) (b) in the computational domain at the time \( t = 11.2 \text{ ms} \) are presented in figure 3. It is evident from the temperature field that the TDW front moves from left to right along the triangle of the incoming cold mixture formed by mixing of the ejected hydrogen and oxygen ejected from the environment \((x < 0)\). An oblique shock wave (train) moves down to the left. Figure 3.b clearly shows a light zone of an
elevated $H_2$ content in the mixture ($\phi > 1.5$) behind the TDW front. Note that photo records [4] also showed a low-temperature zone in the TDW structure, presumably due to the inflow of low-temperature hydrogen at high pressure.

Figure 3. Calculated two-dimensional structure of CSD in the $H_2$-$O_2$ mixture in the $O_2$ ejection mode for $g_{H_2} = 3.75$ kg/(s·m$^2$): (a) – temperature field $T/T_0$; (b) – equivalence ratio $\phi$.

Comparison with experiments for a flow rate $g_{H_2} = 3.75$ kg/(s·m$^2$) shows complete agreement on the number of waves in the combustor (one TDW in the combustor), good agreement on the composition of the mixture: the calculated equivalence ratio $<\phi>$ of the mixture in the combustor is 5% higher than the experimental estimates. Note that the calculated TDW velocity $D \approx 2.35$ km/s was 1/3 higher than that in experiments [4]. This may be due to the ideal model of mixing of the components of the mixture.

We performed calculations of CSD in the $O_2$ ejection mode for the specific hydrogen flow rate varied in the range $g_{H_2} = 3 - 3.75$ kg/(s·m$^2$). Some results are presented in table 1. Here $<p>/p_a$ is the average static pressure at a distance of 5 mm from the combustor entrance and $n = G_{O_2}/G_{H_2}$ is the oxygen ejection coefficient.

Table 1. Calculated parameters of CSD in the $H_2$-$O_2$ mixture with oxygen ejection.

| $g_{H_2}$, kg/(s·m$^2$) | $<p>/p_a$ | $h$, cm | $D$, km/s | $<\phi>$ | $n$ |
|------------------------|-----------|---------|-----------|----------|-----|
| 3.75                   | 1.19      | 1.18    | 2.35      | 0.88     | 9.09|
| 3.5                    | 1.19      | 1.75    | 2.31      | 0.83     | 9.64|
| 3.25                   | 1.18      | 1.7     | 2.28      | 0.76     | 10.53|
| 3                      | 1.17      | 1.6     | 2.19      | 0.69     | 11.6 |

It follows from the calculations that decreasing the specific hydrogen flow rate $g_{H_2}$ leads to a monotonic decrease in the velocity and rotation frequency of the TDW, the front height $h$, and the average static pressure $<p>/p_a$. There is also a noticeable drop in the parameter $<\phi>$, which directly depends on $g_{H_2}$. The obtained numerical results agree with the experimental data of [4], where a decrease in $g_{H_2}$ from 3.75 to 2.25 kg/(s·m$^2$) also led to a decrease in TDW velocity (from 1.76 to 1.57 km/s) and equivalence ratio (0.84–0.47).
We also calculated the average specific impulse per unit mass of fuel $I_{sp,f} = (<p_0> - p_a)S_{exit}/(gH_2 \cdot g)$. Here $<p_0> = \frac{1}{l} \int_0^l (p(L,y,t) + \rho u y(L,y,t))dy$ is the total pressure at the combustor exit, $S_{exit}$ is the combustor exit area, and $g$ is the acceleration due to gravity.

For all calculation variants listed in table 1, the specific impulse changed slightly and was approximately $I_{sp,f} \approx 1300 \pm 100$ s. For $g_{H_2} < 3$ kg/(s$^2$m$^2$) in the combustor with a specified period $l = 29.845$ cm, there was a disruption and attenuation of the TDW with the subsequent establishment of the one-dimensional (without energy release) classical mode of $O_2$ ejection from the environment due to $H_2$ supply to the chamber entrance.

4. Conclusions
A quasi-three-dimensional non-stationary mathematical model of continuous spin detonation in a hydrogen-oxygen mixture in the mode of oxygen ejection from the surrounding space was developed. Numerical simulation was performed for geometric dimensions of the combustor corresponding to the experiment. At a specific hydrogen flow rate $g_{H_2} = 3.75$ kg/(s$^2$m$^2$), a periodic solution with one transverse detonation wave moving at a velocity $D \approx 2.35$ km/s was obtained. The structure of the gas-dynamic flow was analyzed. The results show agreement with the experiment for the number of waves in the combustor and the composition of the mixture and satisfactory agreement for the velocity and rotation frequency of the detonation wave. Monotonic dependence of the main parameters of the solution on $g_{H_2}$ was found by varying $g_{H_2} = 3$–3.75 kg/(s$^2$m$^2$) in calculations, which agrees with experimental data. It is shown that in continuous spin detonation of the hydrogen-oxygen mixture in the oxygen ejection mode, the calculated specific impulses per unit mass of fuel are approximately equal to $I_{sp,f} \approx 1300 \pm 100$ s.

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