Three-dimensional numerical simulation of continuous spin detonation in hydrogen-oxygen and hydrogen-air mixtures using OpenFOAM package

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Abstract. A mathematical model of continuous spin detonation for hydrogen-oxygen and hydrogen-air mixtures is developed within the framework of a nonstationary gas-dynamic formulation. An OpenFOAM package is used to carry out numerical calculations in an annular cylindrical combustor in order to compare the main solution parameters with experimental data for geometric dimensions of combustors 40 mm and 306 mm in diameter corresponding to the experiments for hydrogen-oxygen and hydrogen-air mixtures. Regimes with a single continuously rotating transversal detonation wave are obtained for given fuel mixtures. It is shown that the solution significantly depends on the coordinate along the radius. The results for the hydrogen-oxygen mixture are in good agreement with an experiment in terms of a wave velocity and satisfactory agreement relative to a front height and the number of waves (a 1.5- to 2-fold difference). The results for the hydrogen-air mixture are in satisfactory agreement with an experiment for the wave velocity and front height and significantly differ from it on a minimal flow rate of the mixture, in which the existence of continuous spin detonation is possible in the combustor.

1. Introduction

Continuous spin detonation (CSD) is currently under experimental and numerical studies based on a scheme proposed by B.V. Voitsekhovskii in 1960s in [1, 2]. Detonation regimes with CSD are described in detail in annular combustors (ACs), such as a liquid propellant engine (LPE) [3] and flow-type combustors [4, 5] for a series of fuel-oxygen and fuel-air mixtures.

The purpose of this study is to perform the three-dimensional nonstationary formulation of a closed mathematical model of CSD for hydrogen-oxygen and hydrogen-air mixtures, use the OpenFOAM package (www.openfoam.org) for developing a universal computational algorithm for three-dimensional simulation of the CSD of the above-mentioned mixtures in a wide range of original parameters for different types and sizes of ACs, numerically investigate the combustion dynamics of the hydrogen-oxidizer mixtures in transversal detonation waves (TDWs) in two annular ACs of the LPE type for two kinds of oxidizers (oxygen and air), and verify the constructed mathematical model by comparing the obtained results with experimental data [3, 4].
2. Formulation of the problem

2.1. Mathematical model

Within the framework of this model, a perfectly stirred mixture of hydrogen and oxidizer is injected into an AC with a specific flow rate $g_{in}$ via Laval micronozzles uniformly distributed over the entrance of the AC. The latter is a space bounded by two cylinders with an annular gap of width $A$. The AC length is $L_{ch}$ and its outer diameter is $D_{ch}$. The mixture is burned, and detonation products are released into the space with backpressure $P_{backpressure}$ and flow rate $g_{out}$. The gas-dynamic flow of the reacting hydrogen-oxidizer mixture in the solution domain is described by a three-dimensional system of equations of nonstationary gas dynamics with chemical transformations. At an initial instance, the energy required for detonation initiation is released in the small part of the AC.

\[
\frac{\partial \rho}{\partial t} + \text{div} \rho \vec{U} = 0
\]

\[
\frac{\partial \rho \vec{U}}{\partial t} + \text{div} \rho \vec{U} \vec{U} + \text{grad} P = 0
\]

\[
\frac{\partial \rho E}{\partial t} + \text{div} \rho E \vec{U} = 0
\]

\[
\frac{\partial \rho \mu}{\partial t} + \text{div} \rho \mu \vec{U} = F_{\mu}
\]

\[
\frac{\partial \rho I}{\partial t} + \text{div} \rho I \vec{U} = F_{I}
\]

Here $t$ is the time, $\rho$ is the density, $\vec{U}$ is the velocity vector, $P$ is the pressure, $E = U_p + \frac{|\vec{U}|^2}{2}$, $U_p$ is the total internal energy of the gas, $\mu$ is the current molecular mass of the mixture, and $I$ is the fraction of the chemical induction period.

The energy release is described by a two-stage kinetics model [6] using the Nikolaev chemical kinetics [7].

The first stage is the induction stage ($0 < I < 1$): $F_{I} = -\frac{1}{t_{\text{ind}}}, F_{\mu} = 0$. Here $t_{\text{ind}}$ is the induction time for the corresponding mixture. Similarly to [3, 5], the induction time is described by the expression:

\[
t_{\text{ind}} = \frac{K_{\text{ind}}}{[C]} \exp \left( \frac{E_{\text{ind}}}{RT} \right)
\]

Here $[C] = \frac{\rho V_{O_2}}{\sigma} \cdot 1000$ is the oxygen concentration in [mol/m$^3$], $E_{\text{ind}} = 17.15$ kcal/mol is the activation energy, $K_{\text{ind}} = 5.38 \cdot 10^{-8}$ (mol·s/m$^3$) is the pre-exponent, $R$ is the universal gas constant, $\nu_{O_2}$ is the number of moles of the oxygen, $\sigma = \sum \mu_i \nu_i$, $\mu_i$ denotes the molar masses of the mixture components (H$_2$, O$_2$, N$_2$, Ar), and $\nu_i$ is the number of moles of the components.

The second stage is the energy release [7] ($I = 0$):

\[
F_{\mu} = \frac{4K_{\rho}^2}{\mu} \left( 1 - \frac{\mu}{\mu_{\text{max}}} \right)^2 - 4K_{\rho} \left( \frac{\mu}{\mu_{\text{min}} - 1} \right) \left[ \frac{T}{T_{0}} \right]^{\beta} \left( 1 - \exp \left( -\frac{0}{T} \right) \right) \exp \left( -\frac{E_{\mu}}{RT} \right),
\]

\[
U_p = U_{th} + U_{ch}, U_{th} = \frac{RT}{\mu} A(\mu, T), U_{ch} = E_{\mu} \left( \frac{1}{\mu} - \frac{1}{\mu_{\text{min}}} \right),
\]
\[
A(\mu, T) = \frac{3}{4} \left( \frac{\mu}{\mu_a} + 1 \right) + \frac{3}{2} \left( \frac{\mu}{\mu_a} - 1 \right) \frac{0/T}{\exp(0/T) - 1}
\]

Here \( \mu_{\text{min}}, \mu_{\text{max}} \), and \( \mu_a \) are the molar masses of gas in ultimately dissociated, ultimately recombined, and atomic states, respectively; \( \theta \) is the effective temperature of excitation of vibrational degrees of freedom of molecules; \( \bar{E}_d \) is the mean dissociation energy of the reaction products.

Constants of the model: \( \mu_{\text{H}_2} = 2 \text{ kg/kmol}, \mu_{\text{O}_2} = 32 \text{ kg/kmol}, \mu_{\text{N}_2} = 28 \text{ kg/kmol}, \mu_{\text{Ar}} = 40 \text{ kg/kmol}, \nu_{\text{H}_2} = 2, \nu_{\text{O}_2} = 1, R = 8.3144 \times 10^3 \text{ J/(kmol-K)}, K_a = 6 \times 10^2 \text{ m}^2/(\text{kmol}^2\text{s}), E_d = 109.68 \text{ kcal/mol}, \beta = 1.5, \theta = 3500 \text{ K}. \) For hydrogen-oxygen mixture: \( K = 1769 \text{ kmol/m}^3, \mu_{\text{min}} = 6 \text{ kg/kmol}, \mu_{\text{max}} = 18 \text{ kg/kmol}, \mu_a = 6 \text{ kg/kmol}, v_{\text{N}_2} = 0, v_{\text{Ar}} = 0. \) For hydrogen-air mixture: \( K = 3500 \text{ kmol/m}^3, \mu_{\text{min}} = 14.54 \text{ kg/kmol}, \mu_{\text{max}} = 24.62 \text{ kg/kmol}, \mu_a = 10.53 \text{ kg/kmol}, v_{\text{N}_2} = 3.7275, v_{\text{Ar}} = 0.0445. \)

2.2 Boundary conditions.
The condition of the mixture inflow from the Laval micronozzles is specified at the combustor entrance, and the backpressure \( P_{\text{backpressure}} \) is given at the combustor exit. Boundary parameters are calculated similarly to \([3, 5]\).

2.3 Initial conditions.
A motionless combustible mixture is set as initial data in the AC.

3. Numerical results
The problem is solved numerically for the stoichiometric hydrogen-oxygen and hydrogen-air mixtures for the corresponding geometric dimensions of the AC and the parameters in the mixture injection system. The solution domain is covered by a stationary grid with uniform cell steps along all axes. The number of cells is 192 000 for the hydrogen-oxygen mixture and 240 000 for the hydrogen-air mixture. The Godunov finite-difference scheme is applied in the calculations with the help of the OpenFOAM package.

3.1 Geometric parameters
For the case where oxygen is used as an oxidizer, the geometric parameters of the AC are taken from \([3]\) (\( D_{\text{ch}} = 4 \text{ cm}, A = 0.5 \text{ cm}, \) and \( L_{\text{ch}} = 4 \text{ cm} \)); for air, the parameters are taken from \([4]\) (\( D_{\text{ch}} = 30.6 \text{ cm}, A = 2.3 \text{ cm}, \) and \( L_{\text{ch}} = 66.5 \text{ cm} \)).

3.2 Injection system parameters
The flow rate at the combustor entrance is set in accordance with the experiments \([3, 4]\): \( g_a \approx 46 \text{ kg/s/m}^2 \) and \( g_a \approx 75 \text{ kg/s/m}^2 \) for the calculations with oxygen and air, respectively. At the combustor exit, the backpressure is set as \( P_{\text{backpressure}} = 0.2 \text{ atm} \) for oxygen and \( 1 \text{ atm} \) for air.

3.3 Detonation initiation
At the initial time \( t = 0 \), the energy sufficient for detonation initiation is released in one section of the domain. Thus, a TDW begins propagating over the AC. In order to ensure that the TDW propagates only in a single direction (counterclockwise), the solution domain is temporarily blocked by a vertical solid wall.

3.4 Calculations in the hydrogen-oxygen mixture
The calculations of the initiation and propagation of the TDW for the stoichiometric hydrogen-oxygen mixture show that, for \( g_a \approx 46 \text{ kg/s/m}^2 \), by the time \( t \approx 8.2 \text{ msec} \) after the initiation, the CSD with a single TDW becomes quasistationary and self-supporting with a velocity \( D \approx 2.07 \text{ km/s} \) and a front height of \( \approx 3.2 \text{ cm} \). Figure 1 illustrates a three-dimensional temperature distribution (K) in the
combustor (a) and horizontal (b) (at a distance of 1 cm from the entrance) and vertical (c) (at a distance of 1 cm behind the TDW) cross sections of temperatures in the AC. Clearly, the TDW moves around the annular space of the combustor in a counterclockwise direction and occupies most of the AC by height. An oblique shock wave (tail) moves downstream from the TDW. Figure 1.b clearly shows the dependence of the solution on radius: the injected mixture inflows nonuniformly, filling up the space closer to the outer diameter of the combustor earlier than to the inner diameter. Directly behind the TDW (figure 1.c), the mixture stops inflowing, while the height of the layer of the fresh mixture at a distance of half the combustor perimeter is about half the AC height.

![Figure 1](image)

**Figure 1.** Calculated temperature distribution (K) in the AC for \( g_{\text{in}} \approx 46 \text{ kg/s/m}^2 \) at the time \( t \approx 8.2 \text{ msec} \).

The minimal flow rate \( g_{\text{min}} \) of the existence of CSD is determined by conducting calculations with decreasing flow rate of the mixture injection \( g_{\text{in}} \). It is shown that, as the flow rate drops below \( g_{\text{in}} \approx 40 \text{ kg/s/m}^2 \), the CSD is stopped. This means that the solution with a single TDW, obtained for \( g_{\text{in}} \approx 46 \text{ kg/s/m}^2 \), is physically admissible because it is located in the vicinity of \( g_{\text{min}} \) from the standpoint of the flow rate.

### 3.5 Calculations in the hydrogen-air mixture

Similarly to the calculations from the previous part of the study, the CSD of the hydrogen-air mixture is performed. Figure 2 shows the pressure-time dependence at a point \( R = 15 \text{ cm}, Z = 64 \text{ cm} \). Periodic pressure pulsations associated with the arrival of the TDW at this point are visible. Knowing the time interval \( \Delta t \) between the pulsations and the AC perimeter \( D_{\text{ch}} \pi \), one can calculate the detonation velocity \( D \approx 1.57 \text{ km/s} \). With time, the flow rate \( g_{\text{out}} \) at the AC exit is compared with \( g_{\text{in}} \approx 75 \text{ kg/s/m}^2 \), which indicates that the TDW becomes quasistationary. The height of the TDW front is \( \approx 14 \text{ cm} \). The structure of the TDW for the hydrogen-air mixture is similar to that obtained for the hydrogen-oxygen mixture. As in the calculations with oxygen, the injected mixture flows nonuniformly along the radius.
Figure 2. Pressure P versus the time t.

Figure 3 and 4 below illustrate the dependences of the velocity and rotation frequency of the TDW on the specific flow rate of the mixture (green points). Red points indicate a disruption of the TDW and the end of the CSD regime. Clearly, the velocity drops along with the flow rate, which can be related to a decrease in the height of the inflowing layer, thereby reducing the energy release behind the TDW front.

Figure 3. TDW velocity D (km/s) versus the flow rate (kg/s/m²).

Figure 4. TDW rotation frequency f (kHz) versus the flow rate (kg/s/m²).

4. Results and Discussion
The calculation results for the hydrogen-oxygen mixture are in good agreement with the experiments on the TDW velocity [3] and in satisfactory agreement in terms of front height and the number of waves (in the experiment, with this flow rate of the mixture, a two-wave regime with a front height lower than 2-2.5 times is implemented). Satisfactory agreement is obtained for the hydrogen-air mixture in terms of the TDW velocity (the estimated velocity is 25% higher than that in the experiments) and front height (40% lower than the experimental one). There is a significant difference from the experiment in the minimum flow rate $g_{\text{min}}$ of the hydrogen-air mixture, with which CSD can exist in the combustor. In the experiment [4], $g_{\text{min}} \approx 46$ kg/s/m²; in this calculation, $g_{\text{min}} \approx 25-30$ kg/s/m², indicating an approximately 1.5-fold difference from the experimental data. A significant
decrease in $g_{\text{min}}$ relative to the experiments is presumably related to a simplified mixture injection system in the presented mathematical model.

The analysis shows that three-dimensional effects strongly influence the inflow of the fresh mixture, which induces the formation of a complex shape of the contact boundary between the detonation products and the cold mixture. The fact that the fresh mixture nonuniformly fills the space along the radius can reduce the energy release behind the TDW front, thereby causing a decrease in the TDW propagation velocity in comparison with the quasi-three-dimensional calculation [5]. Thus, the constructed mathematical model and the algorithm for solving the three-dimensional problem allow describing the CSD in combustors of the LPE type and analyze three-dimensional effects that are not observed in two-dimensional calculations.

5. Conclusions
A closed mathematical model of continuous spin detonation is described in a three-dimensional nonstationary formulation for hydrogen-oxygen and hydrogen-air mixtures. The OpenFOAM package is used for these mixtures for the combustor sizes and parameters in the mixture injection system corresponding to the experiments to numerically obtain the solution with a single transverse detonation wave. Comparison with the experimental data is performed. For the hydrogen-oxygen mixture, there is good agreement with the experiment in terms of the wave velocity and satisfactory agreement in terms of the number of waves and the front height. For the hydrogen-air mixture, there is satisfactory agreement related to the wave velocity and front height and the 1.5-fold difference in the minimum flow rate $g_{\text{min}}$ of the existence of the continuous spin detonation. For both mixtures, the significant three-dimensional effects that influence the processes in the combustor are revealed.

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