Numerical simulation of the shock-wave structure of a reacting hydrogen-air mixture in a model channel

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Abstract. The paper deals with the results of numerical simulation of hydrogen-air combustion in a supersonic flow of a model channel of a known configuration, investigated in the “HyShot” project. The simulation is carried out by solving the Favre-averaged system of Navier-Stokes equations, supplemented by a turbulence and combustion model and a chemical-kinetic mechanism. The influence of different throat heights on the performance of the model due to combustion efficiency and total pressure loss coefficients is investigated.

1. Introduction

The investigation of the fuel-air mixture combustion in a shock-wave structure of a high-speed flow aims at solving the problem of the development of combined power engines for reusable aerospace systems [1, 2]. Due to the high flow speed in the combustor, there is a need to increase mixing and combustion of the fuel components [3–5]. Creating an efficient fuel combustion is possible using different methods of fuel supply, flame stabilizers, active external influences and other factors. Both hydrogen-air mixtures, providing a high specific impulse and corresponding high environmental characteristics, and mixtures based on various hydrocarbons, for example, ethylene [6, 7] are considered as working components.

Numerical simulation is one of the methods for studying the features of the process of mixing and burning of fuel and oxidizer in a supersonic flow and identifying effective ways of their development. In [8] mixing of fuel and oxidizer is numerically investigated when fuel is supplied from a hybrid coaxial hydrogen-air wall-mounted cylindrical jet injected into a supersonic flow. It is shown that the use of this type of feed provides high values of mixing and depth of fuel penetration into the combustor, due to an increase in the spiral feature of the hydrogen jet leading to jumps in mixing. In [9], studies continue with the use of a hybrid jet, but hydrogen is already supplied through a number of such jets. Different jets diameters and their effect on flow characteristics are considered. In [10], RANS modeling was carried out with a correction in the turbulence model to take into account the wall roughness for the development of combustion in a supersonic flow. It is shown that taking into account the roughness allows more accurately determining the pressure on the walls and predicting the experimental mode of operation. A number of well-known flight and ground experiments, as well as numerical work, were carried out in the HyShot project. For example, the paper [11] considers numerical calculations with different throat heights, which are based on the experiment described in [12]. A strong dependence on the choice of the RANS model of turbulence and the model of interaction between combustion and turbulence is revealed. In [13], the autoignition process is investigated on the basis of the model [14] using LES modeling. It is shown that, based on the
structure of the flame and the mass fraction of the HO$_2$, the autoignition process can be divided into 5 temporal parts before steady state and into 3 spatial parts in the steady state regime. It was determined that the maximum mass fraction of HO$_2$ can serve as one of the indicators of the steady state. In [15], the influence of the fuel ER on combustion in a supersonic flow is considered using LES and PaSR modeling.

2. Problem statement

2.1. Model description

Numerical simulations is carried out on the basis of the experimental model of the “HyShot” project [12] for different throat heights. A scheme of the model is shown in figure 1.

The model consists of an air intake, combustor, and nozzle and has horizontal and vertical symmetry planes. Model length = 625 mm width = 75 mm. The study considers configurations with throat heights = 20, 24 and 32 mm and with inlet heights = 82, 86, 94 mm.

2.2. Computational mesh

To begin with, a 2D computational mesh is constructed for a throat height = 20 mm. In view of the fact that, under the condition with no fuel supply ("cold" flow), the 3D effect is only in the corner walls of the model, then the use of a 2D computational domain will serve to estimate the mesh convergence. The number of cells in the longitudinal (Nx) and transverse (Ny) directions is presented in table 1, which also presents the values of the height of the minimum cell (Ymin) adjacent to the model wall and the maximum value of the parameter Y+. Figure 2 shows a part of the 2D view of the computational mesh for mesh No.-1 near the throat.

The mesh convergence is verified by the pressure and temperature distribution along the model wall (Figure 3). The experimental values are also presented for the pressure distribution [12]. The inflow conditions correspond to the mode from [16] for throat height = 20 mm. According to the data obtained, it may be seen that an increase in the number of cells in the longitudinal and transverse directions does not affect the result obtained.

It is also shown that the mesh with Ymin = 0.05 mm gives a similar pressure distribution compared to Ymin = 0.005 mm and Ymin = 0.0005 mm. However, when comparing the temperature results, it can be seen that the use of a wall function reduces the values along the combustor. The values of the Y + distribution along the model are shown in figure 3c. According to the results obtained, mesh No.-1 with a value of Ymin = 0.005 mm is used for creating the 3D computational mesh (Figure 4). The
mesh in the area of jets is presented in figure 4b. The 3D mesh contains \( \approx 5 \times 10^6 \) cells. The value of the \( \text{Y}^+ \) parameter for "cold" and "hot" flow is \(< 5.\)

![Figure 3](image1.png)

**Figure 3.** The mesh convergence along the model wall:
   a) pressure, b) temperature, c) \( \text{Y}^+ \) distribution.

![Figure 4](image2.png)

**Figure 4.** The 3D computational mesh: a) general view, b) view in the area of jets.

In the area of inlet and outlet, the computational mesh expands due to additional cells that take into account the evolution of the flow, as well as the independence of the resulting solution from the boundary conditions.

### 2.3. Boundary conditions and numerical models

The physical parameters of the inflow and fuel injection, which are used in numerical simulation [11], correspond to the experimental ones. The Mach number and static parameters are set as the boundary conditions at the inlet, the supersonic outlet condition at the outlet, the adiabatic condition on the walls and the symmetry condition on the planes. Numerical modeling is based on Favre-averaged Navier-Stokes equations. To describe the processes of turbulence, \( \gamma \text{-Re}\Theta \) model is used [17]. The mechanism [18] (Dimitrov) is used as a chemical-kinetic mechanism. The Laminar Finite-Rate / No TCI (LFR) model is used to describe combustion processes.
3. The results and discussion

3.1. The validation. The “cold” flow

The comparison of the results for 3D one-component air (Air) and multicomponent air (Dimitrov), consisting of 23% oxygen and 77% nitrogen, with experiments is presented (Figure 5).

![Figure 5](image)

**Figure 5.** Pressure (a) and temperature (b) distribution for “cold” flow along of model wall.

The results show that there is a large difference in temperature values, as well as differences in the 4th and 5th pressure peaks. Further used multicomponent air (Dimitrov).

Figure 6 shows the pressure and temperature fields for "cold" flow (Dimitrov) with visible zones of increased pressure and temperature, which are favorable for the onset of autoignition.

![Figure 6](image)

**Figure 6.** The pressure (a) and temperature (b) fields for “cold” flow through plane of symmetry.

3.2. The validation. The “hot” flow.

Pressure and temperature distributions are shown for fuel supply conditions in figure 7 (“hot” flow). The pressure shows a good qualitative agreement between the simulation and experimental results for a throat height = 20 mm. The mean relative error is approximately 18%.
Figure 7. Pressure and temperature distribution for “hot” flow along the model wall.

Figure 8 shows the pressure, temperature and mass fraction of H₂O fields for "hot" flow. Figure 8a shows the region of pressure increase during hydrogen supply, as well as partial retention of the shock-wave structure of the flow in the combustor. The main temperature rise on the height of the model is observed at the end of the combustor, which is also consistent with figure 8c.

Figure 8. Pressure (a), temperature (b) and mass fraction H₂O (c) fields for “hot” flow through the plane of the jet.

3.3. The results with different throat heights
Pressure and temperature distributions of different throat heights are presented in figure 9. It is shown that with increasing throat heights, the pressure and temperature of the wall decrease along the model.

Figure 9. Pressure and temperature distribution for different throat heights.
The simulation results also allow obtaining the combustion efficiency and the mass fraction of water (figure 10), as well as the averaged Mach numbers along the model and the total pressure losses coefficient (figure 11). It is shown that for the throat height = 32 mm, the combustion efficiency becomes higher (\( \eta = 83.4\% \)) than for other values of the throat heights. At \( \text{Th} = 20 \) and 24 mm, the efficiency of combustion has approximately the same values at the nozzle exit, 75.9\% and 76.4\%, respectively.

**Figure 10.** Combustion efficiency and the mass fraction of \( \text{H}_2\text{O} \) distribution for different throat heights.

**Figure 11.** The averaged Mach numbers and the total pressure losses coefficient for different throat heights.

**Conclusions**

The 3D numerical simulation of the combustion process in a supersonic air flow of a model channel investigated in the "HyShot" project has been performed. The computational schemes and models have been validated based on the pressure distribution along the wall. It has been found that the use of computational models (the \( \gamma\text{-Re}\Theta \) model [17], Dimitrov [18]) can be used to solve combustion problems in a supersonic flow. Differences in the results are shown for different throat heights = 20 mm, 24 mm, and 32 mm that take into account the hydrogen combustion efficiency and total pressure loss coefficients. It is calculated that for a throat height of 32 mm, the combustion efficiency is higher than for other configurations of the model at the same values of total pressure losses.

**References**

[1] Zhang H, Guo J, Xu Y, Du B, Wang Y and She W 2017 *Proceedings of the 21th AIAA International Space planes and hypersonic systems and technology conference* 12
[2] Mehta U, Aftosmis M, Bowles J and Pandya S 2015 *20th AIAA International Space Planes and Hypersonic Systems and Technologies Conference* 21
[3] Seleznev R K, Surzikov S T and Shang J S 2019 *Progress in Aerospace Sciences* 106 43–70
[4] Choubey G, D Y, Huang W, Yan L, Babazadeh H and Pandey K M 2020 *International journal of hydrogen energy* 1–17
[5] Liu Q, Baccarella D and Lee T 2020 *Progress in Aerospace Sciences* 1–82
Kim K, Park G and Jin S 2019 *Acta Astronautica* 446–64
Kukshinov N V and Mamyshev D L 2018 *BMSTU Journal of Mechanical Engineering* 60–6
Zhang Y, Barzegar G M, Hosseini S, Abazari A M and Li Z 2021 *International Journal of Hydrogen Energy* 46 16048–62
Zhang Y, Rana P, Moradi R and Li Z 2021 *International journal of hydrogen energy* 19645-56
Pelletier G, Ferrier M, Vincent-Randonnier A, Sabelnikov V and Mura A 2020 *Journal of Propulsion and Power* 1–16
Xing F, Cai J, Huang Y and Yao Y 2017 21st *AIAA International Space Planes and Hypersonic Technologies Conference* 12
Odam J 2004 *Ph.D. Dissertation, Mechanical Engineering Dept.* (Univ. of Queensland, Brisbane, Australia)
Liu B, An J, Qin F, He G, Zhang D, Wu S, Shi L and Li R 2019 *International Journal of Hydrogen Energy* 11
Lorrain P, Brieschenk S, Capra B C and Boyce R R 2012 18th *AIAA/3AF International Space Planes and Hypersonic Systems and Technologies Conference* 18
Liu B, Xu J-ch, Qin F, He G-q, Zhang D and Shi L 2020 *International Journal of Hydrogen Energy* 1–9
Xing F, Zhang S and Yao Y 2012 *AIAA paper* 1–12
Langtry R B and Menter F R 2009 *AIAA Journal* 47(12) 2894–906.
Dimitrow V I 1977 *React. Kinetic Catal. Lett.* 7(1) 81–6