Estimating the applicability of kinetic schemes in hydrogen combustion simulation in combustion chambers of aircraft engines

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Abstract. This paper presents the results of numerical simulation of hydrogen combustion in a supersonic flow of an oxidizing medium in a model combustion chamber using various models of chemical kinetics. The best scheme, which most accurately describes the combustion processes, is revealed. Comparison of the calculated distribution of molar fractions with experimental data is carried out, and relative deviations for the piloted mode of operation of the chamber are obtained.

1. Introduction
The study of hydrogen combustion in a supersonic air flow is of interest for the creation of combined power plants for aerospace systems and aerospace aircraft. Such horizontal launch systems are an alternative to the existing means of launching a payload into orbit.

It is especially difficult to obtain fields of temperatures, pressure, velocities and other parameters, according to the distributions of which it is possible to more confidently judge about the processes occurring in the chamber [1-2]

It is possible to reduce the number of real experiments by using numerical simulation, which allows obtaining a three-dimensional picture of the flow parameters at various operating modes of the propulsion system. To obtain correct data, it is necessary to use models that most accurately describe physical processes, such as turbulence and mixing of flows [3] and combustion in a supersonic flow [4].

Combustion in a supersonic or transonic air flow is among the processes that are difficult to simulate, since the problems associated with chemical reactions are closely related to the calculation of changes in the parameters of a high-speed air flow [5-8].

In this regard, there is a need for numerical modeling using various combustion schemes in order to test them and to establish the reliability of the calculations obtained.

In this paper, we numerically simulate the combustion of hydrogen in a model combustion chamber with a sudden expansion. Hydrogen is chosen as the most promising fuel, since it has a high rate of heat release, is non-toxic, does not form soot in the flow of combustion products, and is easy to dispose of in the event of a spill into the environment [9-11].

2. Statement of the Problem
The aim of this work is to test the chemical-kinetic combustion schemes of Hanson-Hong, Dimitrov, and Yakimovsky using the example of numerical modeling of hydrogen combustion in a combustion chamber for various types of fuel injection with further comparison of the results.
2.1. Mathematical Models
To simulate the combustion process and then compare its parameters in this work, we used the chemical-kinetic scheme of Hanson, Dimitrov and Yakimovsky.

The Hanson-Hong model [12] includes 10 reactions with high activation energy and has very high reaction rates for the production of water. The following substances are involved: H$_2$, O, H, O$_2$, H$_2$O, HO$_2$, H$_2$O$_2$, OH, N$_2$, Ar. According to the analysis of the activation energy, in a diffusion flame [13], the reaction rate is maximum in the position with the temperature peak. A decrease in temperature on either side of the peak leads to a rapid drop in the rate of the chemical reaction. Three reactions contain temperature indices, which add a power-law dependence on temperature to the rate equation. Therefore, the Hanson-Hong model may be called one of the fastest.

Yakimovsky's scheme [14] includes 33 reactions, 13 components and has reactions for the formation of nitrogen compounds such as HNO, NO$_2$, and NO.

Dimitrov's scheme includes 9 components and 30 reactions; nitrogen does not participate in the reactions and acts as a buffer gas.

The k-ω SST turbulence model developed by Menter [15] was used as a turbulence model. The main advantage of the model is its low sensitivity to the boundary conditions of the external flow, which allows counting the jet flows [16]. To take into account the interaction of turbulence with combustion, the laminar finite rate model was used. The finite velocity laminar model computes the chemical source terms using the Arrhenius equations and ignores the effects of turbulent fluctuations. This model is accurate for laminar flames, but inaccurate for turbulent flames due to the highly nonlinear chemical kinetics of Arrhenius. The laminar model can be suitable for combustion with relatively slow chemistry and low turbulence of chemical interaction, for example, when burning in a supersonic flow.

The AUSM method was used to solve the general system of conservation equations [17, 18]. We used the second order of approximation of convective fluxes at the boundaries of the cells and the Courant number equal to unity.

2.2. Computational domain
An experiment was carried out at NASA Langley Research Center [16] to obtain data for the validation of computational hydrodynamic codes used in the design of supersonic combustion chambers. An investigation of the flow was made in a supersonic combustion chamber consisting of a diverging channel with an angular injector wall located downstream. The input Mach number of the combustion chamber was 2. The main measurement method was coherent anti-Stokes Raman spectroscopy, and the surface pressures were obtained.

The heater located in front of the combustion chamber is shown in Figure 1.

![Heater of the test setup with the subsequent nozzle.](image)

Molecular oxygen and air are premixed and H$_2$ is burnt in this oxygen-enriched air. The flow rate is chosen so that the mass fraction of O$_2$ is the same as that of standard air. The setup is designed to test
the combustion chamber of a ramjet engine for supersonic combustion by directly connecting the outlet of the setup nozzle to the inlet to the combustion chamber. Gas consumption for the heater is $0.915 \pm 0.008$ kg/s for air, $0.0284 \pm 0.0006$ kg/s for $\text{H}_2$ and $0.300 \pm 0.005$ kg/s for $\text{O}_2$. Heater stagnation pressure is $0.765 \pm 0.008$ MPa. Nominal design conditions are heater stagnation temperature of $1827 \pm 75$ K; outlet temperature of $1187 \pm 60$ K; outlet pressure of $100 \pm 1.5$ kPa; and the Mach number at the exit of 1.989.

The test model is shown in Figure 2.

![Test facility for supersonic combustion NASA (NASA Langley Direct-Connect Supersonic Combustion Test Facility): (a) scheme of the model of the combustion chamber of a jet engine; (b) injection area.](image)

Figure 2.

3. Calculation and analysis of results

Comparison of the data obtained by numerical methods with experimental values gives a good result for the study of a piloted case. Figure 3 shows distributions of concentrations (molar fractions) for $\text{N}_2$, $\text{O}_2$, and $\text{H}_2$ in the 6th section of the combustion chamber at $y = 33.5$ mm, using various kinetic schemes: the Henson-Hong, Yakimovsky scheme, as well as the Dimitrov scheme. The last two schemes give the best results in terms of concentrations, since at the entrance to the chamber, in addition to oxygen and nitrogen, water was supplied, and in Hanson's scheme, argon was supplied.
Figure 3. Distributions of $N_2$, $O_2$, and $H_2$ concentrations in the 6th section of the combustion chamber at $y = 33.5$ mm for the Hanson, Yakimovskiy and Dimitrov schemes, unpiloted case.

This fact also affects the distribution of pressures on the centerline of the upper and lower walls, respectively (Figures 4-7). Pressure peaks in the area of up to 0.5 m are caused by a shock-wave system created by injectors and steps; combustion occurs in this area when the fuel interacts with this system. The pressure drops smoothly downstream due to the divergence of the channel; this is explained by the Hugoniot equation.

Figure 4. Distribution of pressure on the centerline of the upper wall of the duct for an unpiloted case.

Figure 5. Distribution of pressure on the centerline of the lower wall of the duct for an unpiloted case.
Figure 6. Pressure distribution on the centerline of the upper wall of the duct for a piloted case.

Figure 7. Pressure distribution on the centerline of the lower wall of the duct for a piloted case.

For an unpiloted case, the deviation is 13.8% for nitrogen for Hanson's chemistry, 12.0% for Yakimovsky's chemistry, and 12.0% for Dimitrov's chemistry. For hydrogen, the corresponding values are: 38.2%, 36.0%, 36.1%. For oxygen: 28.4%, 13.9%, 11.4%. These deviations are due to the large scatter of the experimental data obtained by the CARS method. Since there are a large number of experimental points with a large scatter, where one coordinate z corresponds to several values, and the values are located on both sides of the calculated graph, the relative deviations take large values. It is obvious that if we calculate the average values of the experimental data at each point and compare them with the calculated graphs, the deviations will significantly decrease. It may be concluded that the best scheme describing the kinetics of a hydrogen-air mixture as it moves through a straight-through channel at supersonic speed is the Dimitrov scheme.

Conclusion
A numerical study of the parameters of supersonic flows has been carried out in the NASA Langley Direct-Connect Supersonic Combustion Test Facility (NASA). The aerodynamic characteristics of the flow have been calculated with hydrogen supply at an angle of 30° to the flow with the Mach number $M = 2$.

These parameters have been determined using the Ansys software. The solution has been obtained in a three-dimensional setting. As a result of the study, the distributions of molar fractions of $N_2$, $O_2$, $H_2$ have been compared with experimental data.

It has been found that combustion is the most intense in the upper and lower parts of the duct. Pressure peaks in the area up to 0.5 m are caused by a shock-wave system created by injectors and
steps; combustion occurs in this area when the fuel interacts with this system. The pressure drops smoothly downstream due to the divergence of the channel. The minimum value of the molar fraction of N\textsubscript{2} increases from 1 section to 7, which may be expected from the flow, the intensity of mixing of the components of which increases along the length of the air duct.

For the unpiloted case, the deviation is 26.8% for Hanson's chemistry, 20.6% for Yakimovsky's chemistry and 19.8% for Dimitrov's chemistry. The best scheme describing the kinetics of a hydrogen-air mixture as it moves through a straight-through channel at a supersonic speed is the Dimitrov scheme.

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