Numerical simulation of hydrogen combustion in oxidizer supersonic flow in flowpaths of various configurations

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Abstract. The paper deals with the numerical simulation of the combustion of a hydrogen-air mixture in a supersonic flow in channels of various configurations. Axisymmetric and plane type flows are considered. The simulation is based on solving the complete system of Navier-Stokes equations with closure using a turbulence model and detailed chemical kinetics. To validate the results, Beach-Evans-Schexnayder and Burrows-Kurkov experimental data are used. The influence of various kinetic mechanisms, models of turbulence, and boundary conditions on the solution obtained is considered. The boundaries of the methods are shown.

1. Introduction

Today in the world there is an increased interest in the development of a hydrogen scramjet which is considered as part of a combined powerplant for hypersonic civil aircraft and the first stages of space systems for outputting payload to orbit. Such engines are developed in the framework of international projects HEXAFLY-INT, HIKARI, SKYLON [1-2].

In the development of high-speed hydrogen combustion chambers, much attention is paid to improving the efficiency of the organization of the mixing of the fuel-air mixture. In the case of high-speed flows, when the residence time of the fuel-air mixture in the flow path is small, the combustion efficiency is determined not only by the quality of mixing the components, but also by chemical kinetics.

For mathematical modeling of the processes of the hydrogen-air mixture mixing and burning during the high-speed flow of components, various computational schemes, models of turbulence, and chemical kinetics mechanisms are used, which can lead to significantly different results. Important for the simulation of high-speed reactive flows is the model of combustion-turbulence interaction (TCI). In [3], a significant effect of the used TCI models on the results of calculations performed for known experimental configurations of flow paths was shown. Thus, the question arises of the limits of applicability of mathematical models for describing the combustion of hydrogen in high-speed flows at different velocities, flow temperatures, turbulence levels, and flow path configurations. To answer this question, the results of numerical simulation are validated according to accurate physical experiments.

As applied to the problem of hydrogen combustion in a high-speed flow of an oxidizing medium, a large amount of experimental data has been accumulated. Thus, in the experiment of Burrows-Kurkov [4], the flow of a hydrogen jet in the near-wall layer of a supersonic air flow in a flat expanding channel is considered. Another classic experiment is considered to be the Andersen experiment [5], in which hydrogen was injected companionably and perpendicularly to a supersonic air flow, which flowed in an expanding path. As part of the experiments conducted in more complex geometric configurations (the presence of niches, ledges, flame stabilizers), first of all, it is necessary to note the
experiments in “HOLOD” program [6-7]. From modern experiments, it is possible to mention studies using the HyShot program [8–9], which studied the effect of the height of a rectangular channel on the characteristics of hydrogen combustion in a shock-wave structure of a flow.

2. Beach-Evans-Schexnayder experiment

The setup of the experimental facility is shown in figure 1. In the experiment, hydrogen was supplied through a circular nozzle with a Mach number \( M = 2 \) into the vitiated air from the fired heater, which was supplied to the nozzle to \( M = 1.9 \). In the experiment, measurements of pressure, temperature, mixture composition in the direction perpendicular to the axis of symmetry at different distances from the place of hydrogen supply were made[10]. The parameters of the hydrogen jet and the free flow are presented in table 1.

| Table 1. Beach-Evans-Schexnayder experiment parameters |
|-----------------------------------------------|
| Parameter | Hydrogen | Free jet |
| Mach number | 2 | 1.9 |
| Temperature, K | 251 | 1495 |
| Velocity, m/s | 2432 | 1510 |
| Pressure, MPa | 0.1 | 0.1 |
| Mass fractions: | | |
| \( \text{H}_2 \) | 1 | 0 |
| \( \text{O}_2 \) | 0 | 0.241 |
| \( \text{N}_2 \) | 0 | 0.478 |
| \( \text{H}_2\text{O} \) | 0 | 0.281 |

Figure 1. Beach at al. experiment scheme.

The mass concentration of water was chosen as a parameter for validation. In numerical modeling, the models of turbulence (Sekundov [11], Menter [12] and \( \gamma-\text{Re}\Theta \) [13] models), the mechanisms of chemical kinetics (Dimitrov [14], Hanson-Hong [15], Starik [16]), TCI models were varied (laminar finite rate, eddy-dissipation concept, flamelet). Also, due to the lack of data on the level of turbulence at the inlet, the relative turbulent viscosity parameter (the ratio of turbulent viscosity to molecular viscosity) was varied.

Numerical modeling was carried out on a two-dimensional block-structured grid with a total number of cells 40000. At the first stage, a series of calculations were carried out in a quasistationary approximation to describe the effect of the initial level of turbulent viscosity, and a kinetic scheme [16] was used to describe combustion. Figure 2 shows the distribution of the mass concentration of water vapor in the section \( x/d = 8.26 \), for two different turbulence models (Secund and Menter) and different values of relative turbulent viscosity at the inlet \( \mu/\mu = 100; 1000 \), as well as for the case of laminar flow. The interaction model in the presented calculation series is laminar finite rate. From the results presented in the graph, the following conclusions can be made.

- The laminar finite rate interaction model predicts well the concentration of combustion products, but the mixing layer is incorrectly solved;
- the initial level of turbulence has a significant impact on the decision;
- Secundov and Menter's turbulence models provide similar results when specifying the same turbulent viscosity at the inlet to the computational domain.

At the second stage, the influence of chemical kinetics mechanisms on the simulation results was evaluated. Comparison of the results in the control cross sections showed insignificant differences in the results for the mechanisms of Dimitrov, Starik and Hanson-Hong. The reason is that ignition in the conditions of this experiment occurs before the 1st control section. Let us follow the evolution of the layer of mixing downstream using the example of the mechanisms of Dimitrov and Starik. Figure 3
shows the graphs of the distribution of the mass fraction of water in sections x/dj = 1.15; 3.04; 7.35. In the section x/dj = 1.15, a layer of mixing of the hydrogen jet and vitiated air was formed; no ignition occurred, and the profiles are identical. In the section x/dj = 3.04, there is a difference in the results caused by various ignition delays in the Dimitrov and Starik mechanisms. When calculating by the Dimitrov mechanism, the mass fraction of water at the maximum reaches mH2O = 0.4, while in the calculation with Starik mechanism ignition just occurs. In the section x/dj = 7.35, the maximum of the mass fraction of water reaches the limiting value, and the mechanisms of Dimitrov and Starik provide almost identical results. The same picture is observed in the control sections located downstream. The difference in the ignition delay length of the case is Δx = 4 mm or in relative coordinates Δx/dj = 0.42.

Figure 2. The distribution of the mass fraction of water in cross section with a longitudinal relative coordinate x/dj = 8.26 r/dj = 0 corresponds to axis

Figure 3. The distribution of the mass fraction of water in cross section with a longitudinal relative coordinates: 1) x/dj = 1.15; 2) x/dj = 3.04; 3) x/dj = 7.35. [1] – Dimitrov chemical kinetics, [2] – Starik chemical kinetics

Figure 4 shows the distribution of the mass concentration of molecular hydrogen near the symmetry axis when calculated using different kinetic schemes. As you can see the use of the Starik mechanism gives the result closer to the experimental curve.

From the presented results it can be concluded that the main role in this problem is played by the turbulent transfer of momentum. All used mechanisms of chemical kinetics in the control sections gave the same result. At the same time, the development of the flame front along the axis demonstrates the difference in the results for various mechanisms, namely, different ignition delay lengths. Thus, we conclude that for the parameters of the experiment, the choice of the mechanism of chemical kinetics is not essential. In this case, using the data of the Beach-Evans-Schexnayder experiment for the validation of the mechanisms of chemical kinetics in terms of predicting the ignition delay is impossible.

At the next stage, a series of calculations was performed with the flamelet interaction model. A detailed description of the mathematical approaches used in this model can be found, for example, in [17]. In the model, the reaction zone is considered as a set of laminar elementary flames (flamelets) in a turbulent flow. The main assumption is that chemical reactions are localized in the region of the

Figure 4. Distribution of the mass fraction of hydrogen on axis. [1] – Dimitrov chemical kinetics, [2] – Starik chemical kinetics
stoichiometric ratio of components. The approach allows us to separate the calculation of chemical transformations and the calculation of turbulent flow. The distribution of the mass fraction of water in the control section according to the results of calculations with the flamelet interaction model, the chemical kinetics of Hanson-Hong and the $\gamma$-Re$\Theta$ turbulence model and variation of the relative turbulent viscosity $\mu_t / \mu = 100; 1000; 10000$ are shown in figure 6. This formulation provided the best fit between calculated and experimental data. In contrast to the quasilaminar approach, the flamelet model satisfactorily describes the position of the maximum mass fraction of water in all control sections. As in the previous calculations, it is necessary to note the significant influence of the boundary turbulent viscosity.

![Graph](image)

**Figure 5.** The distribution of the mass fraction of water in cross section with a longitudinal relative coordinate: a) $x/d_j = 8.26$; b) $x/d_j = 27.9$

3. Burrows-Kurkov experiment

The experiment setup is shown in figure 6. The main parameters of the experiment are shown in table 2. The pressure and component concentrations were measured at a distance of 35.6 cm from the supply pylons, and the delayed ignition of the fuel was measured at various flow parameters.

| Table 2. Burrows-Kurkov experiment scheme |
|------------------------------------------|
| Hydrogen       | Free jet        |
|----------------|-----------------|
| Mach number    | 1               | 2.44           |
| Temperature, K | 254             | 1270           |
| Velocity, m/s  | 1216            | 1764           |
| Pressure, MPa  | 0.1             | 0.1            |

![Diagram](image)

**Figure 6.** Burrows-Kurkov experiment setup

The calculation was carried out in 2D formulation in a quasi-stationary approximation to describe the combustion using kinetic schemes [14, 16], a model of turbulence [11], the grid consisted of 50,000 cells. Figure 7 shows the changes in the mass concentration profile of water at the outlet of the computational zone for different levels of free-stream turbulence and various kinetic schemes. An increase in the width of the reaction zone and a slight shift of the maximum of the water concentration profile to the right with increasing turbulent viscosity can be noted. And although it is not possible to achieve complete coincidence of concentration profiles with experiment, the data obtained confirm the conclusions made in the previous part of the article:
the laminar finite rate interaction model predicts well the concentration of combustion products, but the mixing layer is incorrectly solved;

- the initial level of turbulence has a significant impact on the decision;
- the use of various kinetic mechanisms does not have a significant effect on the distribution of concentration profiles in the cross section.

Using a different chemical kinetics scheme does not have a strong effect on the concentration profile. But at the same time, the results using different chemical kinetics schemes differ greatly in the length of the ignition delay. In the experiment, the dependence of the ignition delay on the main flow temperature was obtained, this dependence is shown in figure 8, the dots show the values of the ignition delay length from calculations using different kinetics schemes. As can be seen, although it is not possible to obtain complete agreement with the experimental data, it can be concluded that the use of a more modern kinetic mechanism [16] gives results closer to the experimental ones, the error lies within 10%.

**Figure 7.** The distribution of the mass fraction of water in cross section. [1] – Dimitrov chemical kinetics, [2] – Starik chemical kinetics.

**Figure 8.** Ignition delay length. [1] – Dimitrov chemical kinetics, [2] – Starik chemical kinetics.

### Conclusion

In this work, numerical simulation of hydrogen combustion in a supersonic vitiated air flow was carried out in the formulation of experiments [4], [10] with a variation of turbulence models, chemical kinetics mechanisms, turbulence interaction models with combustion, and inlet turbulence values. According to the results of computational research, the following conclusions can be done:

- The turbulence rate at the nozzle exit is an important factor that significantly influences the result, which leads to the need for a parametric specification of turbulent viscosity at the inlet to the computational domain;
- The best qualitative and quantitative agreement with experimental data on component concentrations in the cross section was obtained using the flamelet interaction model, Hanson-Hong chemical kinetics and γ-ReΘ turbulence model, in the developed combustion zone for control sections the average relative error range is 5-8%.
- The use of various chemical kinetics schemes does not have a strong effect on the concentration profiles of the components, but it also has a strong effect on the length of the ignition delay. The difference in the length of the delay, determined using different kinetic mechanisms, reaches 25%. The use of modern kinetic mechanisms gives the best agreement with experimental data; the error of the result lies within 10%.

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