Influence of channel geometrical properties and turbulence on propellant ignition in hypersonic ramjet combustion chamber

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Abstract. In this paper a method for simulation of combustion of hydrogen in supersonic air flow is developed. Obtained results are in a good agreement with experimental data. A model hypersonic ramjet engine is considered at 35 km altitude at M=6 and different factors impacting on combustion are analyzed.

1. Introduction
During design of new aircraft, a typical problem of optimization often arises. Prototyping and testing at the stage of structural appearance design are financially demanding, time-consuming and require complex and expensive experimental equipment. Sometimes it is simply impossible to recreate the needed external parameters within a test facility. Currently, these problems are being resolved through the use of numerical simulations, owing to the development of CFD software systems and growth of hardware computing power.

This work is aimed at developing and testing a mathematical model of chemically nonequilibrium turbulent flows in the high-speed ramjets under typical operating conditions. Particular attention is paid to the question of determining the moment of ignition of the combustible mixture.

2. Mathematical model
Problems of gas dynamics are described via the system of Navier-Stokes equations The basic system of equations includes the equations of continuity, momentum, conservation of the mass of chemical components and total energy:

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j) = 0, \\
\frac{\partial}{\partial t} (\rho u_j) + \frac{\partial}{\partial x_j} (\rho u_j u_i + \delta_{ij} \rho - \tau_{ij}) = 0, \\
\frac{\partial}{\partial t} (\rho C_s) + \frac{\partial}{\partial x_j} (\rho u_j C_s + J_{ij}) = \dot{w}_j, \quad s = 1, 2, ..., N_c - 1, \\
\frac{\partial}{\partial t} E_{\text{tot}} + \frac{\partial}{\partial x_j} [u_j (E_{\text{tot}} + p) + q_j - u_j \tau_{ij}] = 0
\]

In these equations: \( \rho \) - mixture density; \( u_j \) - velocity vector; \( p \) - pressure; \( \tau_{ij} \) - shear stress tensor; \( E \) - specific total energy; \( h_s \) - specific enthalpy; \( \rho_s \) - density of the component; \( V_{s,i} \) -
diffusion speed; \( q_j \) - heat flux; \( C_s = \rho_s / \rho \) - mass fraction; \( \dot{\omega}_s \) - production rate; \( N_C \) – number of gas mixture components, index \( s \) corresponds to the \( s \)-th component.

The equation of state is used to relate density of gas with pressure within the system:

\[
p = \rho \frac{R}{M_x} T
\]  

(2)

To account for effects of non-equilibrium, a separate equation for vibrational energy should be added (for more details, see [3]):

\[
\frac{\partial}{\partial t} (E_{v,m}) + \frac{\partial}{\partial x_j} \left( E_{v,m} H_j + q_{v,m,j} + E_{v,m} V_{m,j} \right) = S_{v,m}, \quad m = 1, 2, ..., N_M,
\]

(3)

where \( E_{v,m} \) is the specific (per unit volume) vibrational energy, \( q_{v,m,j} \) is the heat flux density of the vibrational energy, \( S_{v,m} \) is the source of vibrational energy due to energy transitions, the rate of formation of vibrational energy as a result of chemical reactions, and vibrational energy loss by spontaneous radiative deactivation, \( N_M \) is the number of vibrational energy modes; and \( V_{m,j} \) is the diffusion rate. Indices \( m \) and \( j \) mean mode number and direction correspondingly.

In turbulent flows extra mass, energy and stress fluxes are added. For their calculation \( K-\varepsilon-V_n \) turbulence model was used [1], as well as standard \( K-\varepsilon \) and SST models. For calculation of the formation rates of the chemical components, two models of chemical kinetics of hydrogen combustion are considered: the reduced one, presented in Table 1, and the complete system of reactions, described in detail in [2].

| Table 1: Reduced system reaction of hydrogen combustion. |
|---------------------------------------------------------|
| H + O\(_2\)→OH + O                                      |
| O + H\(_2\)→OH + H                                     |
| OH + H\(_2\)→H\(_2\)O + H                             |
| OH + OH→H\(_2\)O + O                                  |
| H + H + M→H\(_2\) + M                                |
| H + OH + M→H\(_2\)O+ M                                |

3. Numerical method

For numerical solution of the governing partial differential equations, the numerical method described in [4] and the Universe CFD program developed in the Department of aviation and space heat engineering of Moscow Aviation Institute were used.

In comparison with [4], a block was added to the method for the case when the basic equations are strongly stiff. In this case, even using the implicit representation of the source, when integrating a differential equation numerically, one would expect the requisite step size to be relatively small. In connection with the stiffness, the actual value of the Courant number can rarely be chosen more than unity, and as a result, there is no need to use the implicit representation of the convective members.

The system of equations (1) in the transformed coordinate system \((\xi, \eta, \zeta)\) can be represented in the following vector form (see [1],[4]):

\[
\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{E}}{\partial \xi} + \frac{\partial \mathbf{F}}{\partial \eta} + \frac{\partial \mathbf{G}}{\partial \zeta} = \mathbf{S}
\]

(4)

To approximate the convective fluxes on the faces of finite volumes, the Roe method [8] and the explicit form are used. The source is written in an implicit form. Then the finite volume representation of equation (4) will be the following:

\[
\left( \frac{\partial \mathbf{U}}{\partial t} \right)_{i,j,k} + K(\mathbf{U}_{i,j,k}) = \mathbf{S}(\mathbf{U}_{i,j,k}^{n+1})
\]

(5)

where \( K(\mathbf{U}) \) is the finite-volume representation of convection and diffusion.
Applying the expansion in a Taylor series, we obtain from (5) the following system:

\[
\begin{bmatrix}
I & -\Delta t \left( \frac{\partial S}{\partial \mathbf{U}} \right)^{\ast} \\
1 & 0
\end{bmatrix}
\begin{bmatrix}
\mathbf{U}_{i,j,k}^{n+1} \\
\mathbf{U}_{i,j,k}^{n}
\end{bmatrix}
- \Delta t \mathbf{S}\left( \mathbf{U}_{i,j,k}^{n}\right) + \mathbf{S}^{n} = 0
\]

where \(\mathbf{S}^{n}\) is the explicit increment due to convective and diffusion fluxes; \(I\) is the identity matrix.

The proposed explicit-implicit numerical scheme is fully coupled. In this case, there is no need for repeated inversion of the 7-diagonal matrix at each time step. Thus, there is no more laborious part of the solution of the Navier-Stokes equations, which arises with the implicit representation of convective flux.

### 4. Verification of the mathematical model

To verify the simulation technique, the work of Burrows and Kurkov [5] was selected, which was devoted to the experimental study of supersonic vitiated air flow. In this experiment a parallel injection of hydrogen was carried out.

As described by Figure 1, a sonic jet of hydrogen is injected tangentially near the wall into a supersonic vitiated airstream flowing into a duct with diverging walls. The jet slot height is 0.4 cm and wall temperature is held fixed at 298K. The operating conditions are presented in Table 2.

![Figure 1. Geometry of Burrows, Kurkov experiment [5].](image)

| Substance | \(M\) | \(p, \text{ Pa}\) | \(T, \text{ K}\) | \(C_{\text{H}_2}\) | \(C_{\text{O}_2}\) | \(C_{\text{H}_2O}\) | \(C_{\text{N}_2}\) |
|-----------|------|-----------------|----------------|----------------|----------------|----------------|----------------|
| Air       | 2.44 | \(10^5\)        | 1270           | 0.0            | 0.258          | 0.256          | 0.486          |
| \(\text{H}_2\) | 1.0  | \(10^5\)        | 254            | 1.0            | 0.0            | 0.0            | 0.0            |

Figure 2 show the experimental and calculated profiles of some flow parameters in the outlet section of the channel at a distance of 0.356 m from the place where hydrogen is injected under various calculation conditions.

Analysis of the data presented in Figure 2 shows that the results of simulation obtained using SST and \(K-\varepsilon\) turbulence models and nonequilibrium chemical kinetics agree satisfactorily with the experimental data of [5]. An exception is the cross profile of the volume fraction of hydrogen, especially when using the \(K-\varepsilon\) model of turbulence. This is probably due to the variability of Prandtl and Schmidt turbulent numbers. The importance of taking this factor into account is shown, for example, in [6] and [7]. In this paper constant values: \(Pr = Sc = 0.9\) were used.

However, if the variability of \(Pr, Sc\) is taken into account, the value of the turbulence intensity of the air flow at the entrance to the channel has a much greater effect on the further calculation results. In most calculations, the intensity value was \(T_i = 2\%\). For comparison, Figure 3 shows the calculation results for \(T_i = 5\%\). The results differ significantly from both the calculation presented in Figure 2 and the experimental data.

Figure 4 shows a comparison of the calculation results of the volume fraction of the main combustion product, \(\text{H}_2\text{O}\), using different models of nonequilibrium chemical kinetics. Obviously, the
difference is inappreciable. The same applies to other flow parameters (for brevity sake they are not given).

Figure 2. A comparison of the calculated cross profiles of the volume fractions of the components in the cross section at a distance of 0.356 m from the place of injection of hydrogen with the Burrows and Kurkov experiment [5]. Calculation with different models of turbulence and chemistry: 1 - SST, full chemistry; 2 - K-ε, full chemistry; 3 - SST, Eddy dissipation model. Experimental data are represented by symbols: circles, triangles and squares.

Figure 3. A comparison of the calculated cross profiles of the volume fractions of the components in a section of 0.356 m (with an increased turbulence intensity in the initial section of the air flow: $T_i = 5\%$) with the experiment [5].

Figure 4. The calculated cross profiles of the volume fraction of H2O at a cross section of 0.356m using different models of nonequilibrium chemical kinetics: 1 - full model, 2 - short model.

5. Numerical investigation of a model scramjet
To analyze the influence of geometric parameters, the choice of the chemical and thermal kinetics model, and also the choice of the turbulence model on the results of the calculation, the numerical simulation of supersonic combustion in a flat channel was performed. The geometry of the channel is presented in Figure 5.
tics were used, as well as various models of turbulent mixing of combustion. As criteria of combustion efficiency in the scramjet the following parameters were considered: the possibility of igniting the fuel and, accordingly, the exhaust velocity from the supersonic nozzle. It is possible that the increase in pressure and temperature will not be enough to ignite the fuel. At a distance X1 from the origin of the CC, a pylon of length X2 is located on the axis of flow, in which the flow decelerates, consists of two sections: the first one - with the angle of inclination to the axis equal to \( \alpha \), and the second one - with the angle of inclination \( \beta = (\beta > \alpha) \). Behind the input device there is a combustor chamber (CC) with length \( L_1 \). The wall of the CC can be parallel to the axis, or it may be inclined to the axis at a small angle \( \psi \).

The size of the output nozzle of the injector is 0.02 m. Next to the CC, there is a supersonic nozzle \( \psi \) degree equal to 10. A hydrogen gas is fed through the right flat end of the pylon with the following parameters: \( U_{inf} = 2048 \text{ m/s} \) - speed of \( H_2 \) at the outlet of the injector, \( T_{inf} = 151.5 \text{ K} \) - temperature of \( H_2 \) at the outlet of the injector, \( p_{inf} = 13725 \text{ Pa} \) - pressure \( H_2 \) at the output of the injector.

The purpose of this study is to check the effect of different geometric parameters of the channel on the possibility of igniting the fuel and, accordingly, the exhaust velocity from the supersonic nozzle. Various models of chemical kinetics were used, as well as various models of turbulent mixing of fuel and oxidizer. It was assumed that the walls of the channel are adiabatic and that the slip condition is ensured on them.

Table 3 shows the main results of the numerical. As criteria of combustion efficiency in the scramjet the following parameters were considered: \( L_e \) - the distance from the channel start to the point of ignition; \( p_{max} \) - the maximum pressure at the outlet from the CC; \( R_{sp} \) - vacuum specific impulse.

**Table 3. Simulation results**

| Test no. | Turb. model | Chem. model | Therm. equiv. | \( \alpha^\circ \) | \( \beta^\circ \) | \( \psi^\circ \) | \( L_{b0} \) [m] | \( \theta^\circ \) | \( L_{a1} \) [m] | \( p_{max} \) [Pa] | \( R_{sp} \) [m/s] | Ign. |
|----------|-------------|-------------|---------------|-----------------|----------------|-----------------|-----------------|----------------|----------------|-----------------|----------------|-------|
| 1        | k-\( \varepsilon \) | full        | +             | 15              | 25             | 0               | 6               | 15             | 6.0            | 58,000          | 12,110          |       |
| 1a       | k-\( \varepsilon \) | full        | -             | 15              | 25             | 0               | 6               | 15             | 6.2            | 53,000          | 12,850          | +     |
| 1b       | k-\( \varepsilon \) | reduced     | -             | 15              | 25             | 0               | 6               | 15             | 6.8            | 80,000          | 17,320          | +     |
| 2        | k-\( \varepsilon \) | full        | +             | 15              | 25             | 1               | 6               | 15             | 5.2            | 5,260           | 13,400          | -     |
| 3        | k-\( \varepsilon \) | full        | -             | 15              | 25             | -0.25           | 6               | 15             | 4.9            | 66,000          | 14,810          | +     |
| 4        | k-\( \varepsilon \) | full        | -             | 15              | 25             | 0               | 5.2             | 15             | 6.2            | 50,000          | 14,810          | +     |
| 4a       | k-\( \varepsilon \) | reduced     | -             | 15              | 25             | 0               | 5.2             | 15             | 5.2            | 12,000          | 14,810          | -     |
| 5        | k-\( \varepsilon \) | full        | +             | 15              | 20             | 0               | 6               | 15             | 9.1            | 9,000           | -               |       |
| 6        | k-\( \varepsilon \) | full        | -             | 15              | 30             | 0               | 6               | 15             | 3.2            | 51,000          | 17,650          | +     |
| 7        | k-\( \varepsilon \) | full        | -             | 15              | 30             | 0               | 4               | 15             | 3.2            | 51,000          | 20,500          | +     |
| 8        | k-\( \varepsilon \) | full        | -             | 15              | 30             | 0               | 4               | 20             | 3.2            | 51,000          | 21,730          | +     |
| 9        | k-\( \varepsilon \)-\( V_n \) | full | -             | 15              | 30             | 0               | 4               | 20             | 3.2            | 56,000          | 20,700          | +     |
| 10\( ^b \) | k-\( \varepsilon \)-\( V_n \) | full | -             | 15              | 30             | 0               | 4               | 20             | 3.2            | 46,000          | 22,320          | +     |

\(^a\)This column denotes whether ignition occurred in the configuration or not.

\(^b\)Different air-fuel ratio is implemented.
Analysis of the calculation results displayed in Figure 6 shows that taking into account the thermal nonequilibrium has a negligible effect on the temperature distribution (compare curves 1 and 2).

An essential difference is manifested when using the short model of chemical kinetics (curve 3). Ignition occurs at a greater distance from the entrance, and passes more intensively.

![Figure 6](image)

**Figure 6.** Temperature distribution along the channel axis for test 1. 1 - calculation using full chemical kinetics and taking into account thermal non-equilibrium; 2 - calculation using the full chemical kinetics and without taking into account thermal non-equilibrium; 3 - calculation using short chemical kinetics and without taking into account thermal nonequilibrium.

Test 2 shows that even a small expansion of the combustor chamber (angle of inclination of 1°) can lead to the fact that ignition does not occur. This result is obtained for all physical models.

A very small restriction of the combustor chamber at 0.25° (test 3) leads to a substantial shift of the ignition point to the left. This is due to the additional compression of the flow in the CC. The values of $p_c$ and $R_{sp}$ slightly increase compared to test 1. Since ignition of fuel in test 1a occurs far enough from the beginning of the nozzle, a shorter CC is used in test 4. This increases the length of the nozzle, since the length of the entire channel remains unchanged. As a result, the specific impulse is higher than in test 1. As expected, in the case of using short chemistry (test 4a), ignition does not occur.

When the angle of inclination of the second section of the input device $\beta$ decreases from 25° to 20° (test 5), ignition does not occur. Apparently, this is due to the fact that the pressure and temperature in the input device are not sufficiently increased.

Test 9 used $k\cdot\varepsilon \cdot V_n$, which accounts for compressibility. However, as the results of calculations show, the compressibility practically does not affect the beginning of the ignition of the fuel (compare the results of tests 8 and 9a). Nevertheless, it is obvious that the nature of turbulent mixing changes significantly: when the effect of compressibility is taken into account, the mixing layer becomes narrower.

In tests 1-9, the air–fuel ratio was close to the stoichiometric (equivalence ratio was ~ 0.96). To test the effect of this factor, test 10 was carried out, in which the hydrogen mass flow was reduced by 20%. This led to a reduction in combustor pressure and engine thrust, but also to a certain increase in the specific impulse. Further tests are devoted to the analysis of the effect of the preliminary injection of a certain fraction of the fuel in the engine input device. Hydrogen was supplied in the first section of the input device at a distance of 0.3 m from the beginning of the channel. The results of calculations under various conditions are shown in Table 4.

**Table 4.** Simulation results with various air-fuel ratio

| Test No. | $L_k$, [m] | $k = \frac{m_{H_2}}{m_{H_2}}$ | $L_c$, [m] | $p_c$, [Pa] | $R_{sp}$, [m/s] |
|---------|-----------|-----------------|-----------|------------|----------------|
| 11      | 4         | 0.231           | 2.4       | 58,000     | 20,520         |
| 12      | 4         | 0.174           | 2.4       | 61,000     | 20,048         |
| 13      | 2         | 0.174           | 2.4       | 50,000     | 19,750         |
| 14      | 3         | 0.174           | 2.4       | 60,600     | 20,820         |
| 15      | 3         | 1.0             | 1.3       | 54,000     | 19,800         |
| 16$^b$  | 3         | 0.231           | 2.3       | 60,000     | 20,585         |

$^a$ Geometric parameters of the channel: $\alpha = 15°$, $\beta = 30°$, $\varphi = 0°$, $\theta = 20°$

$^b$ Hydrogen mass flow is increased (the equivalence ratio is 1.15)
Analysis of the results shows that the preliminary injection of a small amount of fuel significantly accelerates the ignition of the combustible mixture (the point of ignition shifts upstream). This allowed to reduce the length of the combustor chamber, which is very important in terms of the overall dimensions of the engine.

An interesting result is obtained if we compare tests 8 and 12. The geometry of the channel is completely identical for both of them. In test 12, the pressure in the CC is higher, but the specific impulse is somewhat lower than in the case of feeding all fuel through the central pylon. This is due to the fact that during the preliminary injection the quality of combustion improves (less unburned hydrogen). As a consequence, the molar mass of the gas mixture increases, and owing to this, exhaust velocity from the nozzle decreases.

6. Conclusion

A computational model for simulation of hydrogen combustion in supersonic air flow was developed.

It is shown that the combustion performance substantially depends on the geometric characteristics of the input device, the combustion chamber and the nozzle. Using the full system of chemical reactions allowed to obtain more accurate data on the determination of the moment of ignition of the combustible mixture.

It was shown that taking into account the influence of high-speed compressibility in the turbulence model leads to some slowing down of the mixing of the fuel and the oxidizer (the angle of expansion of the mixing layer decreases), but practically does not affect the instant of ignition, the maximum combustion temperature and the specific impulse.

It is shown that the preliminary injection of a small amount of fuel significantly accelerates the ignition of the combustible mixture (the point of ignition shifts upstream). This allowed to reduce the length of the combustor chamber, which is very important in terms of the overall dimensions of the engine.

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