Modelling of mixing and ignition of a cold hydrogen jet in a supersonic hot air flow

O S Vankova¹ and N N Fedorova¹,²

¹ Khristianovich Institute of Theoretical and Applied Mechanics, Siberian Division of Russian Academy of Sciences, 4/1 Institutskay st., Novosibirsk, 630090, Russia
² National Research Novosibirsk State University, 1 Pirogova st, Novosibirsk, 630090, Russia
vankova@itam.nsc.ru

Abstract. The paper presents the results of numerical studies of self-ignition and supersonic combustion of cold hydrogen jet supplied to the M=2 vitiated air flow. The calculations are carried out using the ANSYS Fluent on the basis of the full Favre-averaged Navier-Stokes equations supplemented by the κ-ω SST turbulence model and several kinetic mechanisms including 1, 16 and 38 reactions. The results of calculations of mixing of a cold hydrogen jet and a hot inert mixture are in good qualitative and quantitative agreement with experimental data. The results obtained for the reactive flow show that in the calculation the combustion layer is closer to the channel bottom wall than in the experiment, and the temperature of the reaction product is by 10 % lower.

1. Introduction
Turbulent combustion is one of the most important issues in systems such as rockets, internal combustion engines, industrial burners and furnaces [1]. Therefore, the study of the phenomenon is a key task for the development and improvement of practical systems in terms of increasing efficiency, reducing fuel consumption and the formation of pollutants.

After validation on verified experimental data and available theoretical formulas, simulation methods allow one to better understand impact of various physical mechanisms participating in combustion, to analyze the stability of the process and to predict the formation of pollutants. The structure of the turbulent flame in the combustion chambers is controlled by turbulence, chemical kinetics, acoustics, and radiative heat transfer. The choice of the turbulence model, the kinetic mechanism, and the description of the Turbulence and Combustion Interaction (TCI) are the key points in the numerical simulation of supersonic combustion processes [1][2][4].

The usage of models based on detailed kinetic mechanisms requires huge computer resources, especially in the case of a large number of chemical reactions. The flamelet concept based on the assumption that the chemical reaction times are shorter than the turbulent time scales help to significantly reduce the necessary computer resources. This approach allows chemical reactions to be calculated independently of the main flow calculations using special tables containing the values of chemical parameters for various values of scalar quantities.

Most of works on supersonic combustion uses simplified / reduced chemical mechanisms and the explicit transfer of chemical components involved in the process. In the framework of this approach, closure is necessary for the ensemble-averaged source term in the transport equations of chemical
components. This can be achieved using a simple but less accurate model based on using the Arrhenius law for averages, as well as using the Eddy Dissipation Concept (EDC) or algebraic or transport equations for the probability density function (PDF). Due to the strong nonlinearity of the source term and a wide range of scales due to combustion, the transport equations are rigid and therefore difficult to solve.

At present, hydrogen is considered as one of fuels of the future. In order to control hydrogen self-ignition and stable combustion, a full understanding of these processes is vital. The study of hydrogen combustion in supersonic flows presents great difficulties, both theoretically and experimentally. A theoretical study is complicated by the fact that the laws of combustion at supersonic speeds are determined by the intensity of the processes of turbulent exchange, the rates of chemical reactions in the stream, and the influence of gas-dynamic effects accompanied by heat generation. Moreover, each of these factors can have a significant impact on the processes of mixing and combustion [5].

The purpose of the research is to present a numerical study of the processes of mixing, self-ignition and combustion of cold hydrogen jet supplied into a supersonic (M=2) flow of hot vitiated air. We use a laminar combustion model that does not take into account subgrid fluctuations in the composition and temperature of the mixture. The simplicity of this approach explains its application for obtaining the first approximation for further more complex models.

As a test case, the problem is chosen of mixing and ignition of a cold hydrogen jet supplied into the supersonic flow (M=2) in an expanding channel. The case was experimentally investigated in [6] both for a non-reactive flow with the inert main flow gas and a reactive flow in which the hot vitiated air was supplied to the channel. These experimental data were used for mathematical model validation in [7] where a good agreement was obtained between the experimental and computed profiles of composition and Pitot pressure.

2. Problem setup and methods
The problem is computed with the same geometry as in the experiments [6] (Figure 1 (a)). The length of the combustion chamber is \( L = 0.406 \) m, its height at the inlet is \( H_{\text{inlet}} = 0.089 \) m and at the outlet \( H_{\text{outlet}} = 0.1048 \) m. The hydrogen is injected parallel to the channel bottom wall at a distance of 0.2 m from the channel inlet. The height of the slot for hydrogen injection is \( h = 0.004 \) m, the lip thickness is \( h_j = 0.00076 \) m. The scheme of 2D computation domain is presented in Figure 1 (b) where the positions of inlet, outlet sections and the origin of the coordinate system are shown. In the computations, the direction of \( x \)-axis coincides with the channel bottom wall.

![Figure 1. The experimental scheme [6] (a) and computation domain (b).](image)

The initial data for the free flow and hydrogen jet are given in Table 1. Experimental data set [6] includes two runs, the first for the inert mixture with a low oxygen concentration, and the second for the reactive mixture with a high oxygen concentration.

Mathematical modeling of flows in the combustion chamber is carried out using the ANSYS Fluent software on the basis of the Favre-averaged Navier-Stokes equations of viscous heat-conducting gas, supplemented with the \( k-\omega \) SST turbulence model and the conservation law equations for multispecies mixture. A density–based solver and the AUSM scheme [8] of third order approximation are applied.
To simulate the combustion process of a hydrogen-air mixture the detailed kinetic schemes including 1, 16, and 38 reactions ([9], [10]) are used. Previously, in [11], [12] these kinetic schemes were verified by the authors using the experimental data [7].

### Table 1. Initial data.

|          | Mach number | Static temperature, K | Velocity, m/s | Static Pressure, MPa | Species mass fraction |
|----------|-------------|-----------------------|---------------|----------------------|----------------------|
| Jet      | 1           | 254                   | 1216          | 0.1                  | H₂  1  O₂  0  N₂  0  H₂O 0 |
| Inert flow | 2.44        | 1270                  | 1764          | 0.1                  | 0.0005  0.0509  0.7324  0.2162 |
| Reactive mixture | 2.44    | 1270                  | 1764          | 0.1                  | 0  0.258  0.486  0.256 |

Structured computational grids are constructed in ANSYS Meshing using sizing instruments. The coarse, medium and fine grids consist of about 2·10^5, 3·10^5 and 5·10^5 cells, respectively. For the “cold” case, a grid convergence study has been performed to ensure the results of computations on various grids differ by no more than 5 percent. Most of the computational results presented below are obtained using the medium grid. The y^* values do not exceed 30 for the upper channel wall. For the bottom wall, it lays in a range of 1 ÷ 5 that allows resolving the laminar sublayer of the turbulent boundary layer.

At the inlets, the static pressure, static temperature, Mach number and species mass fraction are prescribed in accordance with data of Table 1. At the outlet, static pressure and temperature are applied corresponding to standard atmospheric conditions. Since the main part of the flow at the outlet is supersonic, this conditions works only a very narrow subsonic part of the boundary layer. At the walls, the no-slip conditions for velocity are applied, and for temperature, cold wall condition Tw=300K is applied in accordance to experiments [6].

### 3. Results and discussion

The solution of the problem is implemented in several stages. First, the flow of inert/reactive mixture is simulated in a plane channel without hydrogen injection. The profiles of gas-dynamic and turbulent parameters are obtained having the boundary layer thickness equal to that in the experiments. These profiles are recorded and set at the inlet when computing flows in the combustion chamber.

At the second stage, the "cold" flow is simulated in which the mixing of hydrogen and in the inert gas mixture is studied. At the third stage, the “hot” flow is computed taking into account a hydrogen ignition in the wet air supersonic flow.

#### 3.1. “Cold” case results

Figure 2 shows the profiles of dimensionless total temperature T0/Tref, Tref = 2380K, in the x = 0 cm cross-section. The graph shows that the thickness of the boundary layer on the channel walls is approximately equal to δ ≈ 1 cm, and a good agreement between the calculated curve and the experimental points has been obtained.

In Figure 3, the computed distributions of static pressure are presented on the upper and lower walls of the combustion chamber for the “cold” case. The graph shows that at the inlet to the channel, the pressure does not change significantly. At x = 0, the pressure drop occurs on the lower wall which is due to the jet. Then the pressure rises sharply up to the level of P ≈ 95 000 Pa and remains practically constant till the outlet. Within 1 < x < 7, small pressure drops are visible on the bottom wall. On the upper wall, in the region 13 < x < 18, the pressure drop occurs due to action rarefaction wave originated at the injection slit, after which pressure are recovered and remain approximately constant P ≈ 88 000 Pa till the exit.

Figure 4 shows the calculated static pressure field for the “cold” case. The picture shows that two rarefaction waves emanate form on the lip. The first wave propagates downstream, then falls on the upper wall and reflects from it. Namely this wave causes the pressure fall that is seen in Figure 3. The
second rarefaction wave falls and reflects from the bottom wall and the contact surface formed by the upper jet boundary. These results in a formation of a reflected compression wave expanding to the upper wall and a series of weak expansion/compression waves that can be seen in the transonic near-wall regions near the bottom wall (Fig. 4 (b)).

Figure 5 presents the computed profiles of the molar fraction of the mixture components (H2, N2, and H2O) in the cross-section \( x = 35.6 \, \text{cm} \) together with experimental points. The graph shows good qualitative and quantitative coordination of data.

Thus, as a result of calculations of the “cold” flow, it is found that the mathematical model quite accurately describes the process of mixing a cold hydrogen stream with a supersonic external stream of moist hot air.

**Figure 2.** Profile of dimensionless total temperature in the \( x = 0 \) cross-section.

**Figure 3.** Computed static pressure distributions along the top (red line) and bottom (blue line) walls.

**Figure 4.** Static pressure field in the whole computation domain (a) and in the vicinity of the jet injection slit (b).

**Figure 5.** Computed and experimental mole fraction profiles of the mixture components in the cross-section \( x = 35.6 \, \text{cm} \).
3.2. “Hot” case results

After getting the cold flow field, the blocks of chemical kinetics containing 1, 16 and 38 reactions for hydrogen combustion in air are activated in the computation model, and the “hot” flow is computed taking into account a hydrogen ignition in the wet air supersonic flow.

Figure 6 shows the calculated static temperature in this case. The figure shows that almost constant temperature is maintained in the most part of the channel except the region of the weak expansion and compression waves generated at the injection slit. The formation of a mixing layer at the periphery of the cold jet can be seen. A significant increase in temperature up to \( T_{st} \approx 1500 \) K testifies on the hydrogen self-ignition. At the same time, an area with a low temperature and high hydrogen concentration remains near the wall till the exit section. In Figure 7, the profiles of dimensionless temperature \( T_0/T_{ref} \) are presented at the \( x = 0 \) cm and \( x = 35.6 \) cm cross-sections. The calculated data are in a rather good qualitative and quantitative agreement with the experiment except the combustion region \( 1 < y < 3 \) cm in which the total temperature is 10% underpredicted.

![Figure 6. Computed static temperature field in “hot” case.](image)

![Figure 7. Profiles of dimensionless total temperature at the inlet (\( x = 0 \) cm) and outlet (\( x = 35.6 \) cm) of the combustion chamber.](image)
experimental data. It should be noted that the peak concentration of the main reaction product is well predicted by kinetic schemes containing 1 and 16 chemical reactions, while the most detailed scheme with 38 reactions, underestimates the maximum value of H2O concentration by 20%.

4. Conclusion

The processes of mixing, ignition, and combustion of a cold hydrogen jet supplied parallel to the main hot wet supersonic air flow in are simulated using ANSYS Fluent. The calculated data are compared with the experimental data [6]. The results of calculations of mixing of a cold hydrogen jet and a hot inert mixture are in good qualitative and quantitative agreement with experimental data.

![Figure 8. Profiles of the H2 (a) and H2O (b) mole fraction for the “hot” case at x = 35.6 cm.](image)

The results obtained for the reactive flow show that in the calculation the combustion layer is closer to the lower wall than that in the experiment. Differences in the calculated and experimental data can be due to insufficient grid resolution of wave structures in the flow, three-dimensional effects, and also due to neglecting the processes of interaction of turbulence and combustion. All these factors will be taken into account in future work.

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References

[1] Poinsot T, Candel S and Trouvé A 1995 Prog. Energy Comb. Scien. 21 531–76
[2] Gonzalez-Jueza E D, Kerstein A R, Ranjanc R and Menone S 2017 Prog. Energy Comb. Scien. 60 26-67
[3] Kong D, Eckhoff R K and Alfert F 1995 J. Hazard. Mater. 40 69 – 84
[4] Kong S C and Reitz R D 2002 Trans. Amer. Soc. Mech. Eng. 124 702 - 7
[5] Curran E T, Heiser W H and Pratt D T 1996 Ann. Rev. Fluid Mech. 28 323-60
[6] Burrows M C and Kurkov A P 1973 Analytical and Experimental Study of Supersonic Combustion of Hydrogen in a Vitiated Airstream NASA TM X-2828 (34 pp)
[7] Evans J S and Schexnayder C J Jr 1980 AIAA Jour. 18 188-93
[8] Liou M S and Steffen C J Jr 1993 J. Comp. Phys. 107 23–39
[9] Tien J H and Stalker R J 2002 Combust. Flame. 130 329–48
[10] Ladeinde F 2009 A Critical Review of Scramjet Combustion Simulation AIAA Paper 2009-127 13 pp
[11] Bedarev I A and Fedorov A V 2006 Combust. Expl. Shock Waves 42 19–26
[12] Fedorov A V, Fedorova N N, Vankova O S and Tropin D 2018 AIP Conf. Proc. 1939 020019