CFD Analysis of Supersonic Combustion at Mach 2 with K-E Turbulence Model

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Abstract. This In this paper combustion of hydrogen under unsteady and supersonic conditions has been presented. The combustor having an injector for injecting fuel parallel to the base. The main flow is also parallel to the base. Modeling of this supersonic combustion has been done using K-ε model with Finite rate chemistry combustion model. In supersonic combustion time available is very short for proper mixing. Intensity of heat release, duct geometry, injection techniques, and mixture (fuel + oxidizer) quality and flow regime are the predominating parameter which decides the flame stabilization. This numerical result demonstrates that flamelet approach is suitable in supersonic flows. Combustion characteristics for injected fuel and supersonic air flow in combustor are presented in this paper. The result shows that the mixing quality increases flame speed almost linearly. The stagnation temperature reaches up to 2420 k in the combustor.

1. Introduction
A new generation air breathing vehicles may use supersonic combustion in their propulsion system. Supersonic combustion is the essential requirement for supersonic/hypersonic flights. Generally in scramjet engines the combustor length is of the order of a meter, and the total time for mixture to be in combustor is in the order of few milliseconds. The major issues in combustion are mixing of fuel and oxidizer, flame initiation, stabilization and completion of combustion. These issues are difficult to address due to supersonic flow of air and limited combustor length. The complexity of flow pattern is very high in this combustor. At low flight speeds, the kinetic energy of the air is not sufficient for proper compression. Hence forth compression of air is required i.e turbojet engine. At higher flight speed the air flow speed is already supersonic at the entry to the combustor and will remain in supersonic condition even after diffusion. Hence forth the combustion will be taken place in supersonic flow regime. The scramjet (ramjet) which is a kind of air-breathing engine having supersonic/ hypersonic flight speeds and the combustion takes place in supersonic flow condition. Combustion efficiency in this type of combustors depends on high velocity flow, completeness in combustion and losses in pressure. [1]. Intensity of heat release, duct geometry, injection techniques, and mixture quality and flow regime are the predominating parameter which decides the flame stabilization. A stable supersonic combustion of hydrogen at mach 2 speed is performed by Aso & Hakim et al [2] resulting temperature is 2800 k and pressure is 3.5 bar. This study shows that strong bow shock is being generated due to increase in injection pressure which creates pressure losses. Different methods of fuel ignition and combustion have been reviewed [3] at low static temperatures for higher efficiency. It has been found common in experiments that inlet temperatures are higher than practical to sustain flame in low temperature hypersonic flow. But this is possible by designing the designing the combustor in a proper way. Low entry temperature is needed to compensate the intake and nozzle limitations. Scalar / scalar-velocity-turbulent frequency PDF (probability density functions) has been used in supersonic combustion by Gerlinger & Mobus et al[4]. CFD tools can be used to simulate the combustion conditions during supersonic regimes, which is having challenges of fast ignition and
reduce combustor length and weight. Hydrogen is also preferred as a fuel due to its short ignition delay. Moreover high quality experimental data is not available for the evaluation of supersonic combustion parameters. Efficient mixing of fuel and air is difficult and losses in total pressure have been reported Gerlinger & Stoll et al [5] in their numerical study of mixing and combustion enhancement at Mach 2, it is due to the extremely small residence time of air in supersonic combustors. Multi step chemistry in supersonic combustion gives higher spread heat release than single step chemistry. Moreover it gives intricate details of combustion i.e. ignition distance. Kumaran & Babu [6] used a chemistry model having 37 reactions and 9 species, to investigate its effect in the supersonic combustion of hydrogen. It is required in understanding the combustion process. The front tracking method has been used for studying numerically the atomization and spray formation by Xuxk & Ohzk et al [7]. This study shows that supersonic flow in the nozzle will initiate cavitation due to liquid-vapor region formation. During numerical study Lagrangian model for turbulent combustion in supersonic flows are generally used with RANS–AMA model to simulate these supersonic co-flowing jets. GRUENIG & Mayinger [9] experimentally investigated the supersonic combustion of Kerosene at Mach 2.15 in scramjet combustor. They observed that once the combustor has ignited, the air stream temperature could be reduced below the combustor ignition level.

NUMERICAL SOLUTION: MODEL:

Figure 1 Supersonic combustor having co-flow jets.

GOVERNING EQUATIONS:

Navier-Stokes equations are not only useful for supersonic flight conditions and combustor geometries, but also for the determination of shock wave and shock layer. These equations are:

Continuity Equation: \[ \rho \frac{\partial u}{\partial x} + \rho \frac{\partial (u^2)}{\partial y} + \rho \frac{\partial (uv)}{\partial z} = 0 \]  \hspace{1cm} (1)

X-momentum Equation: \[ \rho \frac{\partial u}{\partial t} + \rho \frac{\partial (uu)}{\partial x} + \rho \frac{\partial (uu)}{\partial y} + \rho \frac{\partial (uv)}{\partial z} = \rho \frac{\partial P}{\partial x} + \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} + \frac{\partial \tau_{zx}}{\partial z} \]  \hspace{1cm} (2)

Y-momentum Equation: \[ \rho \frac{\partial v}{\partial t} + \rho \frac{\partial (uv)}{\partial x} + \rho \frac{\partial (uv)}{\partial y} + \rho \frac{\partial (vv)}{\partial z} = \rho \frac{\partial P}{\partial y} + \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} + \frac{\partial \tau_{zy}}{\partial z} \]  \hspace{1cm} (3)

Z-momentum Equation: \[ \rho \frac{\partial w}{\partial t} + \rho \frac{\partial (uw)}{\partial x} + \rho \frac{\partial (uw)}{\partial y} + \rho \frac{\partial (ww)}{\partial z} = \rho \frac{\partial P}{\partial z} + \frac{\partial \tau_{zx}}{\partial x} + \frac{\partial \tau_{zy}}{\partial y} + \frac{\partial \tau_{zz}}{\partial z} \]  \hspace{1cm} (4)

Energy Equation: \[ \frac{\partial (uE)}{\partial t} + \frac{\partial (uuE)}{\partial x} + \frac{\partial (uvE)}{\partial y} + \frac{\partial (uwE)}{\partial z} = \frac{\partial (Pv)}{\partial x} + \frac{\partial (\tau_{xx} v)}{\partial x} + \frac{\partial (\tau_{yx} v)}{\partial y} + \frac{\partial (\tau_{zx} v)}{\partial z} + \frac{\partial (Pw)}{\partial y} + \frac{\partial (\tau_{xy} w)}{\partial x} + \frac{\partial (\tau_{yy} w)}{\partial y} + \frac{\partial (\tau_{zy} w)}{\partial z} + \frac{\partial (Pw)}{\partial z} + \frac{\partial (\tau_{zx} w)}{\partial x} + \frac{\partial (\tau_{zy} w)}{\partial y} + \frac{\partial (\tau_{zz} w)}{\partial z} \]  \hspace{1cm} (5)

For the Newtonian fluid, the normal stresses \( \sigma_{xx}, \sigma_{yy}, \sigma_{zz} \) are the summation of pressure and normal stress (viscous) \( \tau_{xx}, \tau_{yy}, \tau_{zz} \). During supersonic combustion specific energy \( E \) is

\[ E = e + \frac{1}{2} (u^2 + v^2 + w^2) \]  \hspace{1cm} (6)

During supersonic combustion kinetic energy of flow contributes highly to the conservation of energy as shown in the above equation.

The equation of state assuming air as a perfect gas is,

\[ P = \rho RT \]  \hspace{1cm} (7)

Where - \( R \) is the gas constant.

And for the internal energy:

\[ e = c_v T \]  \hspace{1cm} (8)
Where - \( C_v \) - specific heat for constant volume.
Assuming Prandtl number is constant (approximately 0.71 for the perfect air), the thermal conductivity may be calculated as below:

\[
k = \frac{\mu C_v}{R} \quad (9)
\]

As per the Sutherland’s law viscosity \( \mu \) can be calculated as follows-

\[
\mu = \mu_0 \left( \frac{T}{T_0} \right)^{15} \left( \frac{T_0 + 120}{T + 120} \right) \quad (10)
\]

where subscript 0 refer for standard values at sea level.

Now the generalized form of Turbulence Equations is as below:

\[
\left( k \right) \frac{\partial^2 k}{\partial t} + \frac{\partial (\bar{u}k)}{\partial x} + \frac{\partial (\bar{v}k)}{\partial y} + \frac{\partial (\bar{w}k)}{\partial z} = \left( \frac{\partial \bar{u}}{\partial x} \right)^2 + \left( \frac{\partial \bar{v}}{\partial y} \right)^2 + \left( \frac{\partial \bar{w}}{\partial z} \right)^2 + \frac{\partial^2 \bar{p}}{\partial \bar{s}^2} + \frac{\partial \bar{q}}{\partial \bar{s}^2} + \frac{\partial \bar{r}}{\partial \bar{s}^2} + \frac{\partial \bar{t}}{\partial \bar{s}^2} + (S_e = P - D) \quad (11)
\]

Chemical Reaction Model:
For hydrogen-water reaction hydrogen combustion reactions module has been used.

\[
2H_2 + O_2 = 2H_2O
\]

Combustion Equilibrium Condition
To develop combustion equilibrium module we should know all the chemical species which are coming out from the reactions. It should also calculate the concentration of species during equilibrium condition. The main species are \( H_2, N_2, H_2O, OH, O \) and \( NO \).

This multi-step finite rate combustion reaction module chemical rate equations to model all reaction happening in the process. The chemical reaction rate may be calculate using the Arrhenius equation, having \( k \) as chemical reaction rate coefficient, \( A_p \) is exponential constant and \( E_a \) is the activation temperature exponent.

\[
k = A_p T^n e^{-\frac{E_a}{RT}}
\]

2. Result & Discussion
Local refinement and re-coarsening of the computational grid has been as shown in figure 2. The numerical analysis has been done for both steady and unsteady cases. The computational approach is validated by comparing experimental and numerical simulation result in case of the hydrogen combustion in steady case. The K-\( \varepsilon \) model having the specialty to capture the turbulent chemical interaction. Hence the variations predicted in the temperature flow field shows the good agreement with experimental data [36].

Figure 2 : Multiple adaptive grid
Table-1 Inlet flow conditions for the air and H$_2$ jet.

|       | Air          | H$_2$         |
|-------|--------------|---------------|
| Ma    | 2            | 1             |
| V[m/s]| 830          | 1560          |
| P[10^5Pa]| 1           | 1             |
| P[kg/m$^3$]| 1.002      | 0.097         |
| yO$_2$| 0.232        | 0             |
| yN$_2$| 0.736        | 0             |
| yH$_2$O| 0.032      | 0             |
| yH$_2$| 0            | 1             |
| K$_{m2/3}$| 10          | 2400          |
| E$_{m2/3}$| 650        | $10^8$        |

Figure 3 Comparison of computed Temperature result with experimental [deepu journal of combustion] data

Steady analysis is presented here to understand the mixing behavior. The cold flow without combustion has been investigated in this section. The validation test data is showing the capability of prediction for the code for the chemical reaction in supersonic flow field. The static pressure field shows that some spot localized within the local fuel rich zone. One can note also the presence of expansion waves followed by recompression shocks, which generated by the center-body profile and interaction between the main stream and fuel-jet. The expansion and shock waves travel downstream producing pressure fluctuation as in figure 4, it is observe that from figure 5, the deflection of path line and the accompanying density increases/decreases near the rich fuel zone. Pressure fluctuation are well reproduce in stream at x=0.205m and x=0.22m. Near the H$_2$ jet, figure 6, it can be seen that the pressure is more compared to the lower and upper wall of the combustion chamber. The XY plot presented for the pressure and velocity at y=0 i.e. in center of the jet in figure 8 and 9. Variations of X velocity are presented at different X location in figure 9 and 11. A decrease in temperature is seen due to the average non-reacting hydrogen concentration is decreasing along the wall.
Figure 6 Contour of Static pressure

Figure 7 Contour of Static pressure

Figure 8 Contour of Static pressure

Figure 9 Contour of velocity

Figure 10 Contour of X velocity

Figure 11 Contour of X velocity
3. Reactions during flow

The static pressure, density, Mach number and Stagnation temperature have shown in the computational results in figure 12, 13, 14 and 15 respectively. For this reacting flow the static pressure is different on lower and upper walls as compared to the fig 1. This rise in pressure is mainly due to the combustion is not very high because of low global equivalence ratio. Shock-wave-boundary-layer interactions play a vital role at the inlet. When these boundary layers are sufficiently strong, these shock waves impinge on the boundary layers that are sensitized by adverse pressure gradients caused by a pressure raise in the combustion chamber, which leads to flow separations and produces other adverse effects on the inlet operation. Moreover the inlet flow structure also get modified due to the new structure of shock waves induced by the local boundary-layer distortion. Some transonic spot near to fuel rich zone has been identified in this supersonic flow field. A fine balance is needed in between the flame propagation speed and the fluid velocity for the sustainability of flame. The fluid velocity is more than the flame speed in supersonic combustion region hence this flame sustainability can be solved only by the generation of recirculation region which provide sufficient residence time for the fuel-air mixing, ignition and chemical-reaction propagation. The heat releases and the flame spreads is showing upward as it moves along the wall as shown in the static temperature contour. The pressure distribution at the centre of flow and near to the upper and lower wall given in the figure 16 and 17 shows good agreement with the experimental data. The profiles of the stream wise velocity component at two different locations are presented in the figure 18 and 19. The position of the computed minimum of the velocity inside the jet tends to be shifted upward and after jet exits at x=0.2m, the maximum speed followed by the expansions waves is higher compare to x=0.32m.
1. Unsteady Analysis

In unsteady calculations, the mixing and flame front propagation integrated over time has been shown. On each time step the fluid regime properties have been calculated. The path of the jet can be predicted by the unsteady equations and its intensification and attenuation can be predicted. Along the time line the shock dissipates completely and further temperature field and the shock wave produced by the combustion becomes steady state as shown in figure 15 and figure 21. The temperature also rises sharply and within a very short time combustion takes place and it reaches up to 23.9e+03 K. It can be easily visualized that some form of shock wave has created near the flame front in the contour of temperature. It can only understand by transient numerical calculation because these waves are not present in steady state calculations. At a different time step the temperature field and also some fluid properties are presented here. At 2.0e-04 s time step the flame properties is quite different to previous one and also the flame temperature reaches up to 28.1e+03 K which is quite high. The flame front at different time step and various crosswise x location are presented in the figure 29, 30 and 31. The temperature profile at 2.24e-03s is quite similar to steady state calculation that means combustion is taking very minimal time. Velocity profile at a different time step presented here for various x location. From figure 32 and 33 it is clear that as the flame front increases, the velocity at different X cross-location is also increases. At a time step 2e-04 and 2.24e-03 pressure and velocity contour is depicted. In both figure 24 and 25 the static pressure field shows that some spot localized due to adverse pressure gradient within the local fuel rich zone in the combustion chamber. This phenomenon leads to flow separations and produces other adverse results on the inlet operation. Fig 25 shows the profiles of numerical and experimental shock waves densities. This shocks wave and jet flows shows the increasing density as the flow behind the shock wave slows further for particular time step 24µs. The comparison shows that the shock stand-off is slightly in acceptable range.
Figure 22 contour of Velocity profile at .0002s

Figure 23 contour of velocity profile at 2e-04 s

Figure 24 contour of Pressure profile at 2e-04 s

Figure 25 contour of Pressure profile at 2.24e-03 s

Figure 26 contour of Density profile at 2e-04 s

Figure 27 contour of Density profile at 2.24e-03 s
Figure 28 contour of velocity profile at 2.24e-03 s

Figure 29 contour of temperature profile at 3.2e-05 s

Figure 30 contour of Temperature profile at 2.224e-03 s

Figure 31 contour of Temperature profile at 2e-04

Figure 32 contour of Velocity profile at 3.2e-05 s

Figure 33 contour of velocity profile at 2e-04 s
4. Conclusion

This computational analysis of supersonic regime combustion is very much in line with the unsteady analysis of H₂ and air combustion. The results show that the flamelet combustion approach is feasible in supersonic regime, which is being demonstrated by the results though few other parameters are still to be evaluated. Some parameters such as Mixing, penetration and combustion characteristics of injected fuel in air during combustion have been shown. The increment of jet penetration to free stream happens due to increment of jet to free stream momentum flux ratio. The results shows that better mixing of air and fuel in the combustion chamber is due to more extreme shear layers and stronger shocks, which are induced during the flow. These phenomena will leads to losses in total pressure of the supersonic stream. Moreover results shows that the k-ε model is quite compatible to predict the fluctuation in pressure and turbulence which is reasonably isotropic. These results are also in line with the mathematical results which were using during designing of a nozzle, and experimental data is also in agreement with the computational data.

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