CHAPTER IX

COMPUTATIONAL STUDY OF SUPERSONIC COMBUSTION USING HYDROGEN

9.1 INTRODUCTION

In order to test the ability of clover nozzle to support supersonic combustion, numerical simulation of supersonic combustion is carried out using DCR configuration. Fuel used in the simulation is hydrogen. Simulation of combustion, particularly that of high speed flow is the most difficult work in FLUENT. Various challenges faced are

1) Difficulty of monitoring species involved in combustion that depends on nature of fuel. For example in the case of kerosene, at least five species have to be monitored. But in the case of hydrogen only three species are to be monitored. These equations for species will give rise to simultaneous equations which have to be solved in addition to continuity, momentum and energy equations. So analysis usually ends up with large number of simultaneous equations there by analysis becomes computationally more expensive.

2) Proper reactive model has to be selected since the analysis has to consider flow properties as well as reaction chemistry.

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3) Usually reactive flows are highly sensitive to initial turbulence (turbulence calculated based on the intensity given along with boundary conditions) and the type of turbulence model used.

4) A proper cold flow solution is needed; otherwise chemical reaction rate tends to get fluctuated abruptly. This fluctuation is very sensitive to temperature fluctuations during iterations. Occasionally iterations tend to get fluctuated which is known as spiking. Spiking is shown in Fig 9.1.

5) Even cold flow solutions are very sensitive to turbulent interactions.

9.1.1 Hydrogen as Fuel

Hydrogen is one of the most promising fuels in supersonic combustion as far as research is concerned. Hydrogen has got a wide range of flammability limit and ignition energy needed is minimum. Being a gas it can easily mix with supersonic jet much better than hydrocarbon fuels there by supersonic
combustion can be sustained easily. Hydrogen has high energy release. Numerical analysis using hydrogen is also simple since only three chemical species are to be monitored other than nitrogen (present if reaction is with air) if reaction considered is single step. Only disadvantage is that its density is very less.

9.1.2 Numerical Analysis

Numerical model used for the analysis of conical nozzle is shown in Fig. 9.2. Primary jet consists of hydrogen and air mixed at stoichiometric ratio supplied at total temperature of 450K. Secondary jet is air alone which is at a total temperature of 300K. Primary jet is supplied at Mach 1.5 to supersonic combustor after expanding it from 5 bar absolute.

![Numerical model for the analysis of conical nozzle.](image)

In the case of clover nozzle three dimensional sector model was preferred as three lobed clover nozzle exhibited symmetry with respect to two planes- major and minor such that the included angle between them is 60°. The flow domain used for the analysis with clover nozzle is shown in Fig.9.3.
The grid system used for conical model was quadrilateral as shown in Fig. 9.4.

Similarly grid system used for the analysis using clover nozzle is shown in Fig.9.5. In this case hybrid mesh scheme was used. One of the major challenges faced in the analysis is that combustor calculations are very sensitive to initial boundary conditions and turbulent boundary layer that develops at convergent section of nozzle, so flow simulation was done from throat.
Numerical simulation of high speed flow needs a cold flow solution to start with. In cold flow solution flow is analyzed without considering chemical reaction. Cold flow solution helps the flow field to settle to a steady value which will form as a good foundation for starting reactive flow. Cold flow solution was found to be very sensitive to turbulent interactions and initial values of turbulent parameters. To overcome this difficulty, first strategy was to simulate primary jet flow from throat of primary nozzle which helps to overcome the influence of turbulent parameters with flow as explained before. Second strategy was to run cold flow using inviscid flow. When analysis using inviscid flow converged, k-ε turbulence model was used to complete cold flow solution. During analysis by k-ε model, material properties were changed from calorically perfect to thermally perfect and viscosity variation was also taken into account. The analysis procedure is shown in Fig. 9.6.
During analysis of high speed reactive flow, properties of mixture were calculated using weighted mass fraction. For individual fluids, specific heat was calculated by using 5th order polynomial of temperature (thereby it was assumed thermally perfect) and viscosity was calculated by using Sutherland law. Once converged cold flow solution was obtained, chemical reaction was initiated by patching the combustion chamber with a temperature of 500K.

9.1.3 Grid Independence Study

In order to prove the repeatability of numerical result, grid independence study was carried out by increasing number of grids. The general trend is that as grid size increases, computation time also increases provided similar mesh schemes were used. In the case of conical nozzle, analysis was done using cells 54000 and 75000. By increasing cell number to 75000, it took a large number of iterations to converge. In the case of clover nozzle analysis was done by using cell numbers 80000 and 120000. Changing the number of grids never affected the results of high speed reactive flow.
9.1.4 Limitation on the Amount of Fuel Used

As the mass flow rate of fuel is increased, the amount of heat released to supersonic jet also increases if combustion is perfect. If the mass of fuel is large enough so that the amount of heat released is higher than the value needed for thermal choking, strong shock wave would be developed at combustor inlet on nozzle exit. So the amount of fuel used is limited as heat addition in this analysis is done at Mach 1.5. Using balanced chemical equations (called combustion equations), the stoichiometric mass fraction of hydrogen-air mixture was calculated. From this, individual mass flow rates of each reactant species were calculated as total mass flow rate through nozzle is already known and is fixed to be maximum. This helped to calculate the equivalence ratio of fuel during combustion. Another important fact is that mach number during heat addition is 1.5 which could get choked easily. This was delayed by providing a gradual divergence angle of 1° to combustor wall as per various references. Too large wall divergence is better to delay thermal choking but could cause flow separation.

9.2 RESULTS AND DISCUSSION

9.2.1 Mach Number along Combustor Axis

Here Mach number variation is drawn along the axis of combustor. This plot indicates whether main flow remains supersonic or choked. The result is shown in Fig.9.7 which compares clover nozzle with conical when operated as primary nozzle.
From Fig.9.7 it is clear that Mach number of main flow remains greater than unity for clover and conical nozzle. In the case of conical nozzle lowest Mach number obtained was 1.09 around the location x/L=0.6 where as in the case of clover nozzle it was unity. This lower magnitude of Mach number may be due to addition of excessive heat which is also clear from stagnation temperature plot. From graph the trend is that Mach number decreases unevenly as flow takes place through combustor. Finally as flow exits through combustor to free stream Mach number increases as flow further expands from high pressure in combustor (static pressure is high due to heat addition) to lower ambient pressure. This fact is evident from graph that Mach number starts to increase slowly after x/L=0.6 - 0.8.

9.2.2 Static Pressure along Combustor Axis

Addition of heat causes static pressure to increase in the case of supersonic flow. The variation in the magnitude of static pressure along the central axis of
combustor is shown in Fig. 9.8 which compares clover and conical nozzle when hydrogen fuel was used for combustion.

![Static Pressure along central axis](image)

Fig. 9.8. Static pressure variation along central axis of combustor.

Fig. 9.8. indicates uneven rise in the magnitude of static pressure. Both clover and conical nozzle indicated a large static pressure rise around the middle of combustor. Maximum magnitude of static pressure was 2.34 bar and 2.2 bar respectively in the case of clover and conical nozzle. So conclusion regarding static pressure is that clover nozzle is able to sustain supersonic combustion at static pressure higher than that of conical nozzle.

9.2.3 Shock Pattern along Combustor Axis

In Fig 9.8. static pressure variation along combustor axis is shown which indicates overall trend of increase but through fluctuations particularly near combustor inlet. The mesh scheme used was able to capture weak shock train
structure along radial plane. Fig 9.9. shows shock pattern captured along radial plane for conical nozzle. In the case of clover nozzle shock pattern captured by major and minor plane is shown in Fig 9.10.

9.2.4 Stagnation Temperature along Combustor Axis

Addition of heat causes stagnation temperature to rise. The comparative graph regarding stagnation temperature variation is shown in Fig.9.11.

Fig. 9.11 Stagnation temperature variation along central axis.
Stagnation temperature is the indicator of the amount of total thermal energy content in the fluid. Fig. 9.11 indicates that stagnation temperature of primary stream increased from 450K in the case of both clover and conical nozzle. Peak stagnation temperature obtained was 644.3K and 569.28K in the case of clover nozzle and conical nozzle respectively. Another important point is that clover nozzle was able to maintain the stagnation temperature at jet centre line almost consistently within 620K-630K between x/L=0.2 to x/L=0.8. This near consistency in the temperature distribution suggests that combustion is more favourable in the case of clover nozzle. Stagnation temperature in the jet centre line in the conical nozzle was consistent at 460K-465K up to x/L=0.36 thereafter temperature increased steadily to 569.28K around x/L=0.6. Fig. 9.11 suggests that jet centerline temperature of combustor is high when clover nozzle is used.

Stagnation temperature along planes at five different axial locations(x/L=0, 0.25, 0.50, 0.75, 1.00) is presented in Fig. 9.12. Fig.9.12. indicates that maximum temperature inside supersonic combustor run by clover nozzle reached around 2150K near minor plane around x/L=0.75. At this point Mach number was unity and was thermally choked. But this Mach number increased to supersonic values as flow expanded towards the exit of combustor. Numerical result clearly indicates that Mach number there after continuously increased and stagnation temperature dropped. This fact is evident in Fig.9.7 and Fig. 9.11. This reduction in stagnation temperature may be due to mixing of jet which caused chemical reaction to cease.
9.2.5 Stagnation Pressure along Combustor Axis

Addition of heat will cause stagnation pressure to decrease whether it is subsonic or supersonic flows. The graphical plot is presented as Fig. 9.13. Addition of heat causes stagnation pressure to drop sharply in the case of clover nozzle whereas reduction is gradual in the case of conical nozzle. Conclusion regarding the study of stagnation pressure variation along combustor axis is that supersonic combustor run by clover nozzle exhibits higher stagnation pressure loss which is due to heat addition as well as mixing enhancement by vortices.
9.2.6 Combustion Efficiency

In order to evaluate the thermodynamic performance of supersonic combustor, combustion efficiency is calculated. Combustion efficiency is defined as the ratio of Actual stagnation temperature rise of primary jet to theoretical stagnation temperature rise. Actual stagnation temperature rise is calculated based on numerical result. Theoretical stagnation temperature rise is calculated based on the balanced chemical equations once equivalence ratio is determined. Thus combustion efficiency is,

\[ \text{combustion efficiency} = \frac{(\Delta T_0)_{\text{actual}}}{(\Delta T_0)_{\text{theoretical}}} \]

Based on the equivalence ratio of 0.41 theoretical stagnation temperature rise is calculated as 2800K. In the case of clover nozzle maximum temperature during analysis was obtained as 2150K. This value was obtained around x/L=0.7
in between major plane and minor plane but close to minor plane. In this region flow is chocked. In the case of conical nozzle maximum stagnation temperature was 596K inside combustor. Magnitude of combustion efficiency is calculated and tabulated in Table. 9.1.

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<tr>
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<th>Clover nozzle</th>
<th>Conical nozzle</th>
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<tr>
<td>Combustion Efficiency</td>
<td>67%</td>
<td>18.68%</td>
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Table. 9.1. Comparison of Combustion Efficiency.

Higher combustion efficiency in the case of clover nozzle is primarily due to better mixing and uniformity in the distribution of stagnation temperature. Higher combustion efficiency indicates better chemical to thermal energy conversion.

9.2.7 Role of Vortices in Supersonic Combustion

As in the case of thermal mixing result vorticity dynamics plays a vital role in supersonic combustor application using clover nozzle. The mesh scheme used was able to capture vortex in the exit plane of clover nozzle (which is combustor inlet). Vector plot at nozzle exit plane is shown in Fig. 9.14. The presence of vortex not only causes primary hot jet to interact and mix with secondary cold jet but also distributes hydrogen from primary fuel inside combustor much more effectively than conical nozzle. Conical nozzle depends on small scale turbulence and wall shear stress to enhance mixing of supersonic jet which is not very effective as per numerical results. The role of vorticity based mixing enhancement technique is effective in high speed flow.
Fig. 9.14. Vortex pattern at exit plane of clover Nozzle.

Fig. 9.14 indicates path lines of flow at clover nozzle exit (combustor inlet).

Path line pattern once again confirms the vortical movement of fluid flow at combustor inlet.

Fig. 9.15. Path lines drawn at combustor inlet.

9.2.8 Arrhenius Reaction Rate

Arrhenius reaction rate is compared along jet centre-lines of combustors run by clover and conical nozzle are presented in Fig. 9.16. Arrhenius equation
indicates the fundamental expression for a chemical reaction rate in terms of temperature.

Fig. 9.16. Comparison Arrhenius reaction rate for combustion supported by clover and conical nozzle.

From Fig. 9.16. it is clear that the rate of chemical reaction is higher for clover nozzle compared to conical nozzle along most of the entire combustor axis. This suggests that the clover nozzle is capable of supporting chemical reaction at high speeds much better than conical nozzle. The reason for enhanced chemical reaction rate by clover nozzle is due to following reasons.

1) Clover nozzle provides better mixing of jet than conical nozzle. There by the temperature distribution is more uniform which is one of the requirements for combustion process. The role of vortices in this aspect is already explained. By enhancing better mixing of jet, clover nozzle
ensures that hydrogen is more uniformly distributed in the high speed flow than that of conical nozzle.

2) Higher temperature also causes exponential rise in the reaction rate. It is already proved that clover nozzle maintains almost consistent stagnation temperature at jet centre line along combustor which is higher than conical.

Another notable point is that Arrhenius reaction rate sharply falls towards the end of combustor. The reason for this reduction has been related to stagnation temperature reduction. As stagnation temperature decreases the reaction rate also drops. It is due to increase in the magnitude of Mach number as flow exits from supersonic combustor which may affect flame stability as well.