MODELING OF TURBULENT SUPERSONIC REACTING SHEAR FLOWS USING POINT IMPLICIT FINITE VOLUME METHOD

M. Deepu*, S. S. Gokhale** and S. Jayaraj***

*Department of Mechanical Engineering, N S S College of Engineering, Palakkad-678 008, Kerala, India.
**Prof. and Director, ***Prof. in Mechanical Engineering, National Institute of Technology Calicut-673601, India.

Corresponding author: email: m.deepu@rediffmail.com, Ph: 91-4912553720, Fax 91-4912555900

Keywords: Supersonic Combustion, Scramjet, Reduced Chemistry, FVM

Abstract
Numerical simulation of two-dimensional turbulent reacting flows has been done using point implicit finite volume method. This method treats all chemical species terms implicitly and all other terms explicitly. Solver is based on the solution of unsteady, compressible, turbulent Navier-Stokes equations, using Unstructured Finite Volume Method (UFVM) incorporating RNG based $k$-$\varepsilon$ two equation model and time integration using three stage Runge-Kutta method. Reaction of hydrogen with air is modeled using an eight-step reaction mechanism. The preconditioning has found to be effective in overcoming the stiffness in chemically reacting flows. The method is validated against a standard coaxial jet hydrogen-air combustion experiment. The predicted values of temperature and species production were in good agreement with experimental results.

1 Introduction
Considerable fundamental research has been conducted in the development of scramjet propulsion systems. The performance of any supersonic combustor system depends on efficient injection and accurate burning. Future hypersonic vehicles are expected to have the performance and operability benefits from air breathing propulsion systems. The use of supersonic combustors in such vehicles requires efficient supersonic combustion within combustor lengths, short enough to be compatible with practical engine sizes. Micro scale mixing is essential as it promotes rapid reaction, but mixing alone doesn't initiate combustion process. Hydrogen has proven its role as fuel in such applications. The present work is an attempt towards the accurate prediction of heat release and species production in Hydrogen-Air mixing layers. The developed solver is based on two-dimensional Navier Stokes equation governing compressible turbulent flows. The time integration is done using three stage Runge-Kutta method. For modeling Hydrogen-Air reaction, an eight-step reaction mechanism proposed by Evans and Schexnayder [1] has been used. Flows involving finite rate chemistry are often found to be stiff, hence it is very difficult to solve them numerically using simple explicit methods. The point implicit method suggested by Bussing and Murman [2] is based on the implicit treatment of the chemical species in the source term and is effective in dealing the phenomena with differing time scales simultaneously. The implicit treatment of the chemical species in the source term reduces the stiffness considerably and higher CFL almost equal to that of non-reacting situations has been obtained.

Comparison of the numerical result has been compared with the standard axisymmetric reacting free shear flow experimental measurements of Cheng et al. [3]. The predicted heat release and species production rates are found to have reasonable agreement with the experimental results.
2 Formulations

Navier-Stokes equation for an axisymmetric flow can be written as
\[
\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{1}{r} \frac{\partial (rG)}{\partial r} = S
\]
(1)

Where
\[
U = \begin{bmatrix}
\rho \\
\rho u \\
\rho v \\
\rho \nu \\
\rho \nu v + \sigma_{sx} \\
\rho \nu^2 + \sigma_{sr} \\
\rho \nu u + \sigma_{sx} v - K \frac{\partial T}{\partial x} \\
\rho \nu \kappa - \mu_k \frac{\partial \kappa}{\partial x} \\
\rho \nu e - \mu_e \frac{\partial e}{\partial x} \\
\rho u Y_i
\end{bmatrix}
\]

\[
G = \begin{bmatrix}
\rho v \\
\rho \nu v + \sigma_{sx} \\
\rho v^2 + \sigma_{sr} \\
(\rho E + \sigma_{sr}) v + \sigma_{sx} u - K \frac{\partial T}{\partial r} \\
\rho \nu \kappa - \mu_k \frac{\partial \kappa}{\partial r} \\
\rho \nu e - \mu_e \frac{\partial e}{\partial r} \\
\rho u Y_i
\end{bmatrix}
\]

\[
S = \begin{bmatrix}
0 \\
0 \\
\frac{1}{r} (P + \sigma_{oo}) \\
0 \\
H_k = 2 \mu_k E_{yy} - \rho e \\
0 \\
H_k \\
H_k \\
\sigma_{xx} = P + \frac{2}{3} \rho \kappa - \mu_{eff} \left[ 2 \frac{\partial u}{\partial x} - 2 \left( \frac{\partial u}{\partial x} + \frac{1}{r} \frac{\partial v}{\partial r} \right) \right] \\
\sigma_{sr} = \sigma_{sx} = -\mu_{eff} \left[ \frac{\partial u}{\partial r} + \frac{\partial v}{\partial x} \right]
\end{bmatrix}
\]

Here
\[
k_{eff} = k_i + k_r
\]

From Sutherland’s law
\[
\mu_j = 1.458 \times 10^{-6} \frac{T^{1.5}}{T+110.4}
\]
and \( \mu_i \) is found from turbulence model

For the present analysis modified \( \kappa-\epsilon \) model called Renormalisation Group (RNG) model was used. Yakhot et al [4] proposed this model, which systematically removes all the small scales of turbulence motion from the governing equation by expressing their effects in terms of large scales and a modified viscosity.

For modeling Hydrogen-Air reaction, an eight-step reaction mechanism proposed by Evans and Schexnayder [1] has been used for which the reaction steps and reaction rates are summarised in table 1.

From the law of mass action applicable for any chemical reaction
\[
\sum_{i=1}^{N} \gamma_{ji} C_i \leftrightarrow \sum_{i=1}^{N} \gamma_{ji} C_i
\]
(2)

Where \( i=1,2,3,\ldots \) represents species and \( j=1,2,3\ldots \) represents reactions.

Net change in concentration of any species can be found as
\[
\dot{C}_i = \sum_{j=1}^{N} (\dot{C}_{ji})
\]
(3)

And the net production of species is given by
\[
\dot{\omega}_i = \dot{C}_i W_i
\]
(4)

Reaction rates in the above equation can be found from Arrhenius law.
Table 1. Reaction steps and reaction rates [1]

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Forward Rates</th>
<th>Backward Rates</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>A</td>
<td>n</td>
</tr>
<tr>
<td>H₂+M</td>
<td>5.5×10^{18}</td>
<td>-1.0</td>
</tr>
<tr>
<td>O₂+M</td>
<td>7.2×10^{18}</td>
<td>-1.0</td>
</tr>
<tr>
<td>H₂O+M</td>
<td>5.2×10^{21}</td>
<td>-1.5</td>
</tr>
<tr>
<td>OH+M</td>
<td>8.5×10^{18}</td>
<td>-1.0</td>
</tr>
<tr>
<td>H₂O+O</td>
<td>5.8×10^{13}</td>
<td>0.0</td>
</tr>
<tr>
<td>H₂O+H</td>
<td>8.4×10^{13}</td>
<td>0.0</td>
</tr>
<tr>
<td>O₂+H</td>
<td>2.2×10^{14}</td>
<td>0.0</td>
</tr>
<tr>
<td>H₂+O</td>
<td>7.5×10^{13}</td>
<td>0.0</td>
</tr>
</tbody>
</table>

Reaction rates are expressed in Arrhenius law form 

\[
\frac{k}{RT} = \exp \left( -\frac{E_{\text{a}}}{RT} \right)
\]

where \( M \) is a third body.

For each species two sets of coefficients are used for the temperature intervals, one applicable from 300K up to 1000K and the other applicable from 1000K up to 3000K. Total energy of flow field is given by

\[
E = \sum_{i=1}^{N} Y_i h_i - \frac{P}{\rho} + \frac{1}{2} \left( u^2 + v^2 \right)
\]

Temperature is worked out from the following equation using the Newton-Raphson method from the modified energy equation. The pressure is calculated from the resulting temperature as follows

\[
p = \rho R \sum_{i=1}^{N} \frac{Y_i T}{W_i}
\]

The point implicit scheme in which all the six chemical species (H₂, O₂, OH, H, O and H₂O) terms are treated implicitly and all other terms explicitly. This is carried out using a preconditioning Matrix.
differential equation. For obtaining the solution this has to be integrated with respect to time.

A method of successive iteration is used to integrate the governing equation. Space discretisation technique converts the partial differential equations into ordinary differential equation. Next step is to integrate this equation with respect to time. The variables are updated after each sweep of computational domain. The method is only conditionally stable as it is an explicit method. Here to accelerate the convergence, local time stepping is employed. That is each control volume marches with its own maximum allowable time step specified by the explicit stability criteria.

\[
\Delta t_i \leq \frac{\Delta l_i}{q_i + c}
\]

(13)

Where \( q_i \) is the fluid velocity of \( i^{th} \) cell, \( q_i = \sqrt{u_i^2 + v_i^2} \)

and \( c = \sqrt{\gamma RT} \), the sound velocity and \( \Delta l_i \) is the characteristic dimension of the hexahedral element.

\[
\Delta t_i = CFL \times \frac{\Delta l_i}{q_i + c}
\]

(14)

CFL is the Courant, Friedrichs and Lewis number

The developed program is mainly consisting of following steps.

- Storing the nodal connectivity and elemental connectivity
- Calculation of resultant flux after obtaining viscous flux and applying suitable boundary conditions.
- These results are modified with respect to boundary conditions and updating the flow variables in all cell centers of the domain for each step.

3 The Computational Domain

A schematic of the experimental facility developed by Cheng et al. [3] is shown in Fig. 1. Measurements for of temperature and composition have been carried out using ultra-violet Raman scattering and laser induced predissociative fluorescence techniques. The inner jet and outer jet inflow conditions were specified from experimental measurements and is given in Table 1.

![Fig. 1: Experimental facility developed by Cheng et al.](image)

<table>
<thead>
<tr>
<th></th>
<th>( H_2 ) Jet</th>
<th>( Air ) Jet</th>
<th>Ambient Air</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diameter (mm)</td>
<td>2.36</td>
<td>17.8</td>
<td>120</td>
</tr>
<tr>
<td>Mach Number</td>
<td>1.0</td>
<td>2.0</td>
<td>0</td>
</tr>
<tr>
<td>Pressure (MPa)</td>
<td>0.112</td>
<td>0.107</td>
<td>0.101</td>
</tr>
<tr>
<td>Temperature (K)</td>
<td>545</td>
<td>1250</td>
<td>300</td>
</tr>
<tr>
<td>Mass Fraction</td>
<td>( Y_{H_2} = 1.0 )</td>
<td>( Y_{O_2} = 0.245 ), ( Y_{H_2,O} = 0.175 )</td>
<td>( Y_{H_2,O} = 0.0233 ), ( Y_{H_2,O} = 0.01 )</td>
</tr>
</tbody>
</table>

The Details of computational domain is given in Fig. 2. The left face of the computational domain is given with a supersonic inflow condition in the region of supersonic air stream. Hydrogen jet with above mentioned conditions is introduced at respective position as separate boundary condition. Remaining portion in left face is considered as no slip wall. Top face is a no slip wall. A supersonic out flow condition is maintained at outlet. Since the entire flow field is symmetrical about axis of the coaxial jet, a symmetry condition is utilized there.

The entire computational domain was divided in to 112000 control volumes. An enlarged view of the grid near mixing region of the jets is shown in Fig. 3. More grid points are placed in the mixing region of two jets and relatively less for region far in ambient air.
The entire flow field is initialized with ambient conditions and the solution is marched in time. After 22500 iterations, at CFL equal to 0.5, convergence has been observed.

4 Results and Discussion

The introduction of point implicit technique has found to be effective in dealing chemical source terms. CFL almost equal to that of compressible turbulent flow (without reaction) could successfully demonstrate this phenomenon.

Vector plot for the mixing region near jet outlets is shown in Fig.4. Low velocity regions can be found in mixing layer with recirculations near lip region, this leads to enhanced mixing of the jets.

Fig. 2: Details of computational domain

Fig. 3: Grid near mixing region

Fig. 4: Velocity vectors near jet outlets

Fig. 5: Mach field view of the flow near jet outlets

The Mach field view for the mixing layers near to the jet outlet is shown in Fig. 5. Alternate compression and expansion takes place for the jet and is not enough to perturb the flow field much in the region near to the jet outlets. The thickness in the lip region, separating the two flows, creates small expansions that are further suppressed by latter stream. Comparison of the predicted value of temperature at exit of the computational domain (101mm from jet outlet) with experiment is shown in Fig.6. Reasonable match has been obtained inside core region of the jet and a slight difference in the mixing layers. The difference is due to the value of initial turbulence level given at the inlet and also due to the numerical dissipation effects.

The temperature plot for the entire domain is given in Fig 7. The mixing becomes more predominant in the region far from the jet outlets and heat release gradually increases in the mixing layer between hydrogen and air. Non reacting fuel core extends up to 30mm from jet outlets. Outer layer between supersonic air stream and ambient has almost same temperature through out the length.

Fig. 6. Temperature and H₂O profiles at exit
5 Conclusions
Future hypersonic vehicles are expected to have the performance and operability benefits from air breathing propulsion systems. The use of supersonic combustors in such vehicles requires efficient supersonic combustion within combustor lengths, short enough to be compatible with practical engine sizes. Micro scale mixing is essential as it promotes rapid reaction, but mixing alone does not initiate combustion process. Hydrogen has proven its role as fuel in such applications. Thus the developed numerical method is highly useful in predicting heat release and species production rates in practical engine systems.
Introduction of large number of variables has lead to consumption of more CPU time per iteration. This will set a real challenge while applying this method for three dimensional or lengthy domains.
A point implicit finite volume solver has been developed and tested for the supersonic mixing and reaction of coaxial streams of Hydrogen and air. The implicit treatment of the chemical species in the source term reduces the stiffness considerably and higher CFL almost equal to that of non-reacting situations has been obtained. Reasonable match has been obtained with experiment for the temperature inside core region of the jet and a slight difference in the mixing layers.

6 Acknowledgements
The first author thank Dr. T. Jayachandran, Head of Fluid Mechanics and Heat transfer Division of Propulsion group, Vikram Sarabhai Space Centre, Thiruvananthapuram, India, for sharing his expertise in the progress of this work.

7 References