A numerical study on the physics of mixing in two-dimensional supersonic stream

Mohammad Ali\textsuperscript{a}, Toshi Fujiwara\textsuperscript{b} & Anwar Pervez\textsuperscript{c}

\textsuperscript{a} Department of Mechanical Engineering, Bangladesh University of Engineering and Technology, Dhaka 1000, Bangladesh
\textsuperscript{b} Department of Aerospace Engineering, Nagoya University, Japan
\textsuperscript{c} Department of Mechanical Engineering, Bangladesh Institute of Technology, Khulna 9203, Bangladesh

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A numerical investigation has been performed on the physics of mixing for better understanding about the penetration and mixing mechanism, and eventually to find out the means of increasing the mixing efficiency. The two-dimensional full Navier-Stokes equations with an explicit Harten-Yee Mon-MUSCL Modified-flux-type Total Variation Diminishing (TVD) scheme have been used. A zero-equation algebraic turbulence model has been used to calculate the eddy viscosity coefficient. For this study the air of Mach number 5.0 is considered as main flow. Hydrogen gas at sonic condition is injected perpendicularly into it. The effects of molecular and turbulent diffusion coefficients, and that of boundary layer on mixing have been analyzed and discussed. The results show that upstream recirculation plays an important role to increase the mixing of side jet with the main flow of high Mach number. It has been found that the mixing is only possible by incorporating the molecular diffusion terms in the Navier-Stokes equations. The use of turbulence model increases the penetration height of hydrogen in the mixing field.

The study of the physics of mixing and combustion is very important to find out the physical mechanisms that can increase their efficiencies. Particularly, the mixing of reactants and their complete combustion in Supersonic Combustion Ramjet (Scramjet) engines have drawn special attention of present scientists of Aerodynamics. In fact, in supersonic combustion, high penetration and mixing of injectant with main stream is difficult due to their short residence time in combustor. In an experimental study, Brown and Roshko\textsuperscript{3} showed that the spreading of a plane turbulent mixing layer decreased remarkably with increasing the Mach number of supersonic jet. A similar conclusion was drawn by Papamoschou and Roshko\textsuperscript{7} on the basis of a theoretical analysis of shear-layers. These investigations showed that difficulty exists in achieving better mixing in high Mach number flows. Therefore, it is necessary to find out all the physical mechanisms that affect the mixing and combustion to analyze and optimize a supersonic combustor.

Several other investigations\textsuperscript{3,4,5,6,7,8,9,10,11} have been performed to analyze the mixing characteristics, and find out the means of increasing the mixing efficiency. In these investigations the authors showed a number of parameters that can affect on penetration and mixing. In an experiment, Rogers\textsuperscript{3} showed the effect of ratio between jet dynamic pressure and freestream dynamic pressure on the penetration and mixing of a sonic hydrogen jet injected normal to a Mach 4 airstream. In a similar flow arrangement, Kraemer and Tiwari\textsuperscript{4} found that the relative change in jet momentum was directly proportional to the relative size between the flow field disturbance and the upstream separation distance. The downstream injectant penetration height is directly proportional to the upstream separation distance, and, thus, the downstream mixing is dependent on the relative change in jet momentum. Similar conclusions were drawn by Thayer III and Corlett\textsuperscript{5}. They also found that the injectant concentration in the separated flow region was high when the temperature of both the injectant and freestream was taken as investigation parameter. Yokota and Kaji\textsuperscript{6,9} searched the enhancement of mixing by varying: (i) the angle of a finite length slit\textsuperscript{6} (when slit length is smaller than the width of computational domain) and (ii) slit aspect ratios\textsuperscript{7}. Besides, they examined the effects of injection methods\textsuperscript{8}, and the existence of pressure wave in the injecting flow field\textsuperscript{9} on mixing and total pressure loss.

In an experimental investigation, Moussa \textit{et al}.\textsuperscript{10} found that the geometric configuration of the boundaries of jet exit plays an important role on the mixing and its development process. Andreopoulos and Rodi\textsuperscript{11} searched the penetration of jet into the cross flow for the jet to cross flow velocity ratio of 0.5, 1.0 and 2.0. Also the authors discussed some other flow characteristics such as wakes, vortex motion, velocity gradient in shear layers near the jet exit.
Inlet conditions of Air
Pressure = 0.101 MPa
Temperature = 800.0 K
Mach = 5.0

Inlet conditions of Hydrogen
Pressure = 1.818 MPa
Temperature = 1128.0 K
Mach = 1.0

Fig. 1—Schematic diagram of the calculation domain.

In this study, the physics of supersonic mixing and diffusion mechanisms have been investigated. The geometric configuration of the calculation domain and the inlet conditions of both main and injecting flows are shown in Fig. 1. Considering the same design-concept of an airframe-integrated Scramjet engine module, the configuration of fuel injection scheme has been varied. The length and height of present calculation domain are 10.0 cm and 5.0 cm, respectively. The upper and right boundaries are assumed open. Hydrogen is injected from the bottom wall through a slot of width 0.1 cm. The temperature and pressure conditions of main flow at the inlet are taken as Weidner and Drummond. In recent testing on Scramjet engine at Kakuda Research Center of National Aerospace Laboratory (NAL), Mach 4.0 and 6.0 were considered. Therefore, an average Mach number value 5.0 is chosen for the main flow. A backward-facing step as shown in Fig. 1 is used which can assist the increase of re-circulation region in upstream of injector. A rectangular grid system is used which consists of 194 nodes in the horizontal direction and 121 in the vertical direction. For better numerical simulation the grid points are clustered near the walls and around the injector. Particularly, 10 grid points are provided at the exit of injector. A zero equation turbulence model developed by Baldwin and Lomax has been introduced in the computer code and the effects of molecular and turbulent diffusion coefficients on mixing have been shown. Also the characteristics of the growing flow field and the mixing mechanisms in re-circulation are discussed.

**Governing Equations**

The flow field is governed by the two-dimensional full Navier-Stokes equations with conservation equations of species. Body forces are neglected. For non-reacting flow, these equations can be expressed by

\[
\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = \frac{\partial F_v}{\partial x} + \frac{\partial G_v}{\partial y}
\]

where

\[
U = \begin{bmatrix}
\rho \\
\rho u \\
\rho v \\
E \\
\rho_i 
\end{bmatrix}, 
F = \begin{bmatrix}
\rho u \\
\rho u^2 + p \\
\rho u v \\
(E + p) u \\
\rho_i u 
\end{bmatrix}, 
G = \begin{bmatrix}
\rho v \\
\rho u v \\
\rho v^2 + p \\
(E + p) v \\
\rho_i v 
\end{bmatrix}
\]

\[
F_v = \begin{bmatrix}
0 \\
\sigma_x \\
\sigma_y \\
\tau_{xy} \\
\sigma_x u + \tau_{xy} v + q_x \\
\sigma_y u + \tau_{xy} v + q_y \\
m_{ij}
\end{bmatrix}, 
G_v = \begin{bmatrix}
0 \\
\tau_{xy} \\
\tau_{xx} u + \sigma_y v + q_x \\
\tau_{yy} v + \sigma_x u + q_y \\
\tau_{yx} u + \tau_{xy} v + q_x \\
\tau_{xy} v + \tau_{yx} u + q_y \\
m_{ij}
\end{bmatrix}
\]

\[
p = \sum_{i=1}^{m} \rho_i R_i T = \sum_{i=1}^{m} \rho_i \frac{R_i}{W_i} T,
\]

\[
E = \sum_{j=1}^{n} \rho_j C_p T = \sum_{j=1}^{n} \rho_j \frac{R_i}{W_i} T + \frac{P}{2} \left[ \frac{u^2}{2} + \frac{v^2}{2} \right].
\]

The following terms are expressed as,

\[
\sigma_x = \lambda \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) + 2 \mu \left( \frac{\partial u}{\partial x} \right),
\]

\[
\sigma_y = \lambda \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) + 2 \mu \left( \frac{\partial v}{\partial y} \right),
\]

\[
\tau_{xy} = \tau_{xx} = \mu \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right),
\]

\[
q_x = \kappa \frac{\partial T}{\partial x} + \rho \sum_{i=1}^{m} D_{ni} H_i \frac{\partial Y_i}{\partial x},
\]

\[
q_y = \kappa \frac{\partial T}{\partial y} + \rho \sum_{i=1}^{m} D_{ni} H_i \frac{\partial Y_i}{\partial y},
\]

\[
m_{ix} = \rho D_{ni} \frac{\partial Y_i}{\partial x}, 
\]

\[
m_{iy} = \rho D_{ni} \frac{\partial Y_i}{\partial y}, 
\]

\[
\lambda = -\frac{2}{3} \mu.
\]
The values of \( C_p \) and \( H \) are considered as functions of temperature and determined from the polynomial curve fitting developed by Moss\(^{17}\). Temperature is calculated by Newton-Raphson method.

**Transport Properties**

The molecular viscosity coefficient \( \mu \) and thermal conductivity \( \kappa \) of each species are determined by Sutherland formulae\(^{18}\) as:

\[
\frac{\mu_i}{\mu_0} = \left( \frac{T}{T_0} \right)^{1.5} \frac{T_0 + S_{u_i}}{T + S_{u_i}}
\]

\[\ldots \text{(2)}\]

and

\[
\frac{\kappa_i}{\kappa_0} = \left( \frac{T}{T_0} \right)^{1.5} \frac{T_0 + S_{u_i}}{T + S_{u_i}}
\]

\[\ldots \text{(3)}\]

and those of gas mixture by Wilke’s formulae\(^{18}\) and Wassiljewa’s equation\(^{19}\) as:

\[
\mu_i = \sum_{i=1}^{n} \frac{\chi_i \mu_i}{\sum_{i=1}^{n} \chi_i \phi_{ij}}
\]

\[\ldots \text{(4)}\]

\[\text{and } \phi_{ij} = \left[ 1.0 + \left( \frac{\mu_i}{\mu_0} \right)^{0.5} \left( \frac{W_j}{W_i} \right)^{0.25} \right]^p \left( 8 + 8 \frac{W_i}{W_j} \right)^{0.5}
\]

\[\ldots \text{(5)}\]

where \( \phi_{ij} \) is the ratio of the molecular mass of species \( i \) and \( j \) at a given pressure and temperature.

\[A_{ij} = 1.065 \phi_{ij}, \text{ and } z_i \text{ are the mole fractions, while } \mu_0, T_0 \text{ and } \kappa_0 \text{ are the reference values.}
\]

The effective molecular diffusion coefficient for each species is determined\(^{19}\) as:

\[
D_{mol} = \frac{1 - Z_i}{\sum_{j=1}^{n} Z_j / D_{ij}}
\]

\[\ldots \text{(6)}\]

\[\text{where } D_{ij} = \frac{0.001858 \cdot T^{1.3} \left( \frac{W_i + W_j}{W_i \cdot W_j} \right)^{0.5}}{p \cdot \sigma \cdot \Omega \cdot \sigma_0}
\]

\[\text{and } \Omega = \left( \frac{T}{T_{ij}} \right)^{-0.145} + \left( \frac{T}{T_{ij}} + 0.5 \right)^{-2.0}
\]

\[\text{where } T_{ij} = \left( \frac{T_u}{T_d} \right)^{0.5}
\]

\[\sigma_{ij} = \frac{1}{2} \left( \sigma_u + \sigma_d \right)
\]

\[T = \text{ absolute temperature (K)}
\]

\[p = \text{ pressure (atm)}
\]

A zero-equation algebraic turbulence model developed by Baldwin and Lomax\(^{16}\) is used to simulate boundary layer separation, re-circulation and shock-expansion regions near the injector. The primary advantage of using this model is that it does not need to calculate the boundary layer thickness, rather it calculates the eddy viscosity \( \mu_e \) based on the local vorticity, \( \omega \). This is very helpful because at the injection port and adjacent region it is difficult to define boundary layer thickness. Secondly, this model can successfully calculate the separated flows both over a flat plate and a compression corner. According to Baldwin and Lomax\(^{16}\), the eddy viscosity \( \mu_e \) is defined as:

\[
\mu_e = \begin{cases} 
\left( \frac{\mu_i}{\mu} \right)_{\text{inner}} & \text{if } y \leq y_{\text{crossover}} \\
\left( \frac{\mu_i}{\mu} \right)_{\text{outer}} & \text{if } y > y_{\text{crossover}}
\end{cases}
\]

\[\ldots \text{(7)}\]

where \( y \) is the normal distance from the wall and \( y_{\text{crossover}} \) the smallest value of \( y \) at which the value of viscosity in the outer region becomes less than or equal to the value of viscosity in the inner region.

The viscosity in the inner region is given by:

\[
\left( \frac{\mu_i}{\mu} \right)_{\text{inner}} = \rho \cdot \frac{\mu}{l^2} \cdot |\omega|
\]

\[\ldots \text{(8)}\]

The mixing length in the inner region \( l \) is expressed as:

\[
l = k \cdot y \times [1 - \exp (-y^*/A^*)]
\]

\[\ldots \text{(9)}\]

where

\[
y^* = \frac{\rho \cdot u_{\tau} \cdot y}{\mu_w} \quad \frac{\sqrt{\rho \cdot u_{\tau} \cdot y}}{\mu_w}
\]

\[\ldots \text{(10)}\]

For two-dimensional flow, the magnitude of the vorticity is given by:

\[
|\omega| = \sqrt{\left( \frac{\partial u}{\partial y} - \frac{\partial v}{\partial x} \right)^2}
\]

\[\ldots \text{(11)}\]
For the outer region,
\[
\mu_{\text{outer}} = K \cdot C_{CP} \cdot \rho F_{\text{WAKE}} F_{\text{KLEB}}(y)
\]
where \( K \) is the Clauser constant, \( C_{CP} \) an additional constant, and
\[
F_{\text{WAKE}} = \min \left\{ \left( \frac{F_{\text{max}}}{y_{\max}} \right)^{2}, \left( \frac{C_{W} \cdot y_{\max} \cdot U_{\text{ag}}^{2}}{F_{\text{max}}} \right) \right\}
\]
where \( F_{\text{max}} \) is the maximum value of the potential
\[
F(y) = y[n] \left[ 1 - \exp(-y^{+} / A^{+}) \right]
\]
at each \( y \) station in the flow domain, and \( y_{\max} \) is the \( y \) coordinate at which this maximum occurs. The function \( F_{\text{KLEB}}(y) \) is the Klebanoff intermittency factor given by
\[
F_{\text{KLEB}}(y) = \left[ 1 + 5.5 \left( \frac{C_{\text{KLEB}} \cdot y}{y_{\max}} \right)^{-2} \right]
\]
\( U_{\text{ag}}^{2} \) is the difference between the magnitude of the maximum and minimum total velocity in the profile at a fixed \( x \) station, expressed as
\[
U_{\text{ag}}^{2} = \left( \sqrt{v^{2} + v^{2}} \right)_{\text{max}} - \left( \sqrt{v^{2} + v^{2}} \right)_{\text{min}}
\]
\( \left( \sqrt{v^{2} + v^{2}} \right)_{\text{max}} \) is taken to be zero along all \( x \) station.

The following are the constants used for this model and are directly taken from Baldwin and Lomax:
\[
A^{*} = 26, \quad C_{CP} = 1.6, \quad C_{\text{KLEB}} = 0.3, \quad C_{\text{KL}} = 0.25, \quad k = 0.4, \quad \kappa = 0.0168
\]

The values of the turbulent thermal conductivity of the mixture \( \kappa_{t} \) and turbulent diffusion coefficient of \( i \)-th species \( D_{i} \) are obtained from eddy viscosity coefficient \( \mu \) by assuming a constant turbulent Prandtl and Lewis number equal to 0.91 and 1.0, respectively. They can be expressed as
\[
\frac{\mu_{i} \cdot C_{P}}{k_{i}} = 0.91
\]

The final values of \( \mu, \kappa \) and \( D_{i} \) used in the governing equations are
\[
\mu = \mu_{i} + \mu_{t}, \quad \kappa = \kappa_{i} + \kappa_{t}, \quad D_{i} = D_{i} + D_{t}
\]

**Numerical Scheme**

The system of governing equations for non-reacting flow is solved using an explicit Harten-Yee Non-MUSCL Modified-flux-type TVD Scheme. The two-dimensional, rectangular physical coordinate system \((x, y)\) is transformed into the computational coordinate system \((\xi, \eta)\) in order to solve the problem on uniform grids. After applying the transformation, Eq. (1) can be expressed as
\[
\frac{\partial U}{\partial t} + \frac{\partial F}{\partial \xi} + \frac{\partial G}{\partial \eta} = \frac{\partial \hat{F}}{\partial \xi} + \frac{\partial \hat{G}}{\partial \eta}
\]
where
\[
\hat{U} = J^{-1}U, \quad \hat{F} = J^{-1}(\xi_{x}F + \xi_{\eta}G), \quad \hat{G} = J^{-1}(\eta_{x}F + \eta_{\eta}G)
\]
\[
\hat{F}_{\nu} = J^{-1}(\xi_{x}F_{\nu} + \xi_{\eta}G_{\nu}), \quad \hat{G}_{\nu} = J^{-1}(\eta_{x}F_{\nu} + \eta_{\eta}G_{\nu})
\]

The grid Jacobian \( J \) and metric terms are,
\[
J^{-1} = x_{\xi} \eta - x_{\eta} \xi, \quad \xi_{x} = J y_{\eta}, \quad \xi_{\eta} = -J x_{\eta}, \quad \eta_{x} = -J y_{x}, \quad \eta_{\eta} = J x_{x}, \quad \eta_{x} = J x_{\eta}, \quad \eta_{\eta} = J x_{x}
\]

For the left hand side of Eq. (22), the explicit Non-MUSCL TVD scheme can be written as
\[
U_{i,j}^{n+1} = U_{i,j}^{n} - \frac{\Delta t}{\Delta \xi} \left( F_{i+1/2,j}^{n} - F_{i-1/2,j}^{n} \right)
\]
\[-J_{i,j} \frac{\Delta t}{\Delta \eta} \left( G_{i,j+1/2} - G_{i,j-1/2} \right) \]  

(23)

The variables \( \hat{F} \) and \( \hat{G} \) can be described as

\[
\hat{F}_{i+1/2,j} = \frac{1}{2} \left( \hat{F}_{i,j} + \hat{F}_{i,j+1} + R_{i+1/2} \Phi_{i+1/2} \right) \]

(24)

The \( R_{i+1/2} \) is an eigen vector matrix and \( \Phi_{i+1/2} \) is a vector with the elements \( \Phi_{i+1/2} (i = 1, 2, 3, 4, 5) \). The variables used in the above equations are

\[
\Phi_{i+1/2} = \begin{pmatrix} \phi_{i+1/2} \\ \phi_{i+1/2} \end{pmatrix}
\]

(25)

\[
\begin{pmatrix} \psi_{i+1/2} \\ \psi_{i+1/2} \end{pmatrix} = \begin{pmatrix} \chi_{i+1/2} + \chi_{i+1/2} \\ \chi_{i+1/2} \end{pmatrix} - \begin{pmatrix} \chi_{i+1/2} + \chi_{i+1/2} \\ \chi_{i+1/2} \end{pmatrix} ; \\
\end{pmatrix}
\]

\[
\begin{pmatrix} \psi_{i+1/2} \\ \psi_{i+1/2} \end{pmatrix} = \begin{pmatrix} \chi_{i+1/2} + \chi_{i+1/2} \\ \chi_{i+1/2} \end{pmatrix} - \begin{pmatrix} \chi_{i+1/2} + \chi_{i+1/2} \\ \chi_{i+1/2} \end{pmatrix} ; \\
\end{pmatrix}
\]

\[
\begin{pmatrix} \psi_{i+1/2} \\ \psi_{i+1/2} \end{pmatrix} = \begin{pmatrix} \chi_{i+1/2} + \chi_{i+1/2} \\ \chi_{i+1/2} \end{pmatrix} - \begin{pmatrix} \chi_{i+1/2} + \chi_{i+1/2} \\ \chi_{i+1/2} \end{pmatrix} ; \\
\end{pmatrix}
\]

\[
\begin{pmatrix} \psi_{i+1/2} \\ \psi_{i+1/2} \end{pmatrix} = \begin{pmatrix} \chi_{i+1/2} + \chi_{i+1/2} \\ \chi_{i+1/2} \end{pmatrix} - \begin{pmatrix} \chi_{i+1/2} + \chi_{i+1/2} \\ \chi_{i+1/2} \end{pmatrix} ; \\
\end{pmatrix}
\]

(26)

(27)

\[
\delta_{i} = \delta \sqrt{U + |V| + \sqrt{c_{x}^{2} + c_{y}^{2} + \eta_{x}^{2} + \eta_{y}^{2}}} \]

(28)

(29)

\[
U = \xi_u + \xi_v, \quad V = \eta_u + \eta_v \]

(30)

The Courant number CFL is chosen as 0.7 to obtain rapid convergence and avoid unsteadiness in calculation.

**Boundary Conditions and Convergence Criterion**

The Navier-Stokes analysis imposes that the normal and tangential velocity components are zero on the walls. The walls are assumed to be thermally adiabatic, so that \( \partial T/\partial n \) = 0. For non-catalytic walls, the normal derivative of species mass fraction also vanishes, and consequently the gradient of total density becomes zero. The pressure is determined from the equation of state. The temperature, pressure and density at inflow boundary are assumed steady. At outflow boundary the variables are determined by first-order extrapolation due to supersonic character of flow. Throughout the present study, the following convergence criterion has been set on the variation of density:

\[
\left( \frac{\Delta \rho_{\text{new}} - \rho_{\text{old}}}{\rho_{\text{old}}} \right)^{2} \leq 10^{-3} \]

(31)

where \( JJ \) and \( KK \) are the total number of nodes in the horizontal and vertical directions, respectively.

**Program Verification**

To verify the present code, a comparison has been made with the experimental data published by Weidner et al. [13]. The geometry of the experiment is shown in Fig. 2, where helium gas was injected at sonic condition from a 0.0559 cm slot into a rectangular duct of 25.4 cm long and 7.62 cm high. The slot was located 17.8 cm downstream of the duct entrance. The flow conditions of helium at the slot exit were \( P = 1.24 \) MPa, \( T = 217.0 \) K and \( M = 1.0 \). At the entrance of the duct, the airstream conditions were \( P = 0.0663 \) MPa, \( T = 108.0 \) K and \( M = 2.9 \). Using the same geometry and flow conditions, the flow field was computed for...
Results and Discussion

Study on numerical diffusion

The numerical diffusion, might be incorporated by the computer code, was checked by (i) reducing the mesh size, i.e., grid refinement study, and (ii) using different kinds of limiters in TVD scheme.

Grid refinement study

The present investigation adopted a grid system consisted of 194 nodes along the horizontal direction and 121 nodes along the vertical direction. Using twice of this grid system, i.e., 387 nodes along the horizontal direction and 241 nodes along the vertical direction, the flow field was calculated. The compari-
son of mixing between the two grid systems is shown in Fig. 5(a, b) where no significant difference can be found in penetration and distribution of hydrogen both in upstream and downstream of injector. Therefore, it has been concluded that the grid system 194×121 is a reliable one for present analysis.

Effect of 'Limiters' in TVD scheme

Significant numerical diffusion can be found when the limiter in TVD scheme has been changed from 'minmod' to 'superbee'. Fig. 6(a, b) compare the numerical diffusion between minmod and superbee limiters. The solid lines are for exact solution and symbols for numerical solution. It is evident from these two figures that due to limitations of the Limiters numerical diffusion occurs in both cases. However, it is significantly lower in the result computed by superbee limiter. Fig. 7(a, b) show the effects of
limiters on mole fraction contour of hydrogen in present investigation. Fig. 7b shows that the use of superbee limiter in TVD scheme reduces the numerical diffusion significantly appeared by the use of minmod limiter, as shown in Fig. 7a. In upstream of injector, the penetration height of hydrogen is same for both limiters whereas in downstream, penetration height of hydrogen is higher for minmod limiter caused by numerical diffusion. For both limiters, in upstream and on the top of injectors the contour lines are concentrated and in downstream they are spreading in similar manner. Other characteristic phenomena of the flow field, such as the pattern of shock waves and their positions, pressure distributions, can be observed by pressure contours shown in Fig. 8(a, b). The separation shock of main air stream caused by upstream recirculation is clear to see in the flow field calculated by superbee limiter. By observing the separation shock of main flow it can be understood that in upstream of injector, the superbee limiter predicts higher pressure compared to the minmod limiter. In downstream both cases show the recompression shock clearly, but the superbee limiter calculates slightly lower pressure than the minmod limiter. No significant difference in the pattern of shocks and their positions can be found between the two limiters, and for both cases similar trend of pressure distributions exists all over the flow fields. However, the significant difference in hydrogen penetration height leads us to perform the calculation using superbee limiter as it can reduce the numerical diffusion in present solution of mixing problem.

Effect of molecular diffusion coefficient on mixing

Fig. 9a shows that though the diffusion-flux terms in the governing equations [Eq. (1)] are inactivated, hydrogen reaches to a certain distance along the vertical direction from the bottom wall in both upstream and downstream of injector. This spreading of hydrogen is caused by stretching and folding of fluid layers in the flow field. Recalling the species continuity equations in Eq. (1), we can see that even if the diffusion terms are inactivated, hydrogen can spread in the flow field due to the flux terms. The non-mixing
characteristics can be proved by taking the hypothesis that without the inclusion of molecular diffusion terms in [Eq. (1)], the mole fraction of hydrogen does not change along a streamline of the spreading region of hydrogen. From Fig. 9b, it can be seen that the mixing of hydrogen is occurring due to inclusion of molecular diffusion terms in the governing equation resulting in higher penetration along the vertical direction than that in Fig. 9a.

Figs 10 and 11 prove the above hypothesis. In these figures the solid line represents for mole fraction contour and dotted line for streamline. In both figures total number of streamlines and their starting positions are same, and also the total number of mole fraction contour lines are same. Obviously, every contour line shows the same value of hydrogen mole fraction. In Fig. 10, if we follow the 5th streamline, we can understand that the top most line of mole fraction
contour matches with it, which means that the mole fraction of hydrogen is approximately same along the 5th streamline. Again in downsteam of injector the 7th streamline shows that it is followed by one mole fraction contour line without any significant deviation and no other contour line crosses it. On the other hand, Fig. 11 shows that on left side of the domain the 4th streamline is away from the topmost mole fraction contour line, whereas in downsteam the topmost two contour lines cross-over the 4th stream line. Besides in Fig. 10, the 5th streamline matches with the farthest line of hydrogen contours, whereas in Fig. 11, the 5th streamline is in deep of the mole fraction contours of hydrogen. Thus, the investigation shows that mixing between the ingredients, particularly hydrogen with other species, cannot occur without the action of molecular diffusion.

Effect of turbulent model on mixing

The use of turbulence model increases the transport coefficients, i.e., viscosity coefficient, thermal conductivity and diffusion coefficient. The enhancement of viscosity coefficient enlarges the size of recirculations as well as boundary layer thickness in both upstream and downsteam of injector as they are directly proportional to the viscosity. The injection into the thick boundary layer enhances the mixing region. These phenomena can be understood by the comparison between the Figs 12a and 12b. In Fig. 12a, we can see that in upstream of injector, the contour lines are accumulated on the edge of the separated turbulent boundary layer, whereas in Fig. 12b, they are more uniformly distributed. In downsteam, the turbulence model moves the corresponding contour lines further away from the bottom wall, which means that the enhancement of diffusion coefficient causes higher penetration and mixing of hydrogen.

Characteristics of the growth of interaction and mixing

Fig. 13 shows the characteristics of the flow field when there is no injection. A turbulent boundary layer can be found in the flow field which starts from the upper end of backward-facing step. Besides, there exists a strong shock caused by the bottom wall and boundary layer separation. The side injection causes a hindrance of mainstream and consequently makes a thicker boundary layer and a steeper shock. In Fig. 14, it can be found that initially (t = 0.6 and 1.0 μs) the mixing layer of hydrogen is growing symmetrically. In fact, within turbulent boundary layer the mixing layer can grow symmetrically due to the lower velocity of mainstream. As soon as the mixing layer interacts with the edge of the turbulent boundary layer it losses the symmetric nature and spreads more in downsteam due to the high momentum of mainstream. At the interaction region the contour lines are concentrated but in both upstream and downsteam...
they are scattered. The spread of hydrogen is the highest in downstream. The shock-front, caused by the expansion of injector, is evident in temperature contour of the growing flow field shown in Fig. 14b. When mixing layer grows sufficiently, the hindrance of side jet causes to generate an upstream re-circulation and makes early separation of upstream boundary layer. This early separation thickens the turbulent boundary layer resulting rapid growth of hydrogen mixing layer. The growing shock-front interacts with the shock of main stream making the separation shock steeper and eventually helps thickening the upstream boundary layer as well as enlarging the upstream re-circulation region. Thus, the boundary layer increases the mixing of injectant in the flow field.

**Mixing by flow re-circulation**

Fig. 15 shows the velocity vector near injector of the developed flow field. To analyze the mixing mechanisms, the flow field is divided into three sections; (i) upstream region of injector, (ii) top of injector and the adjacent region, and (iii) downstream region. In upstream there are two re-circulations; (a) one primary large re-circulation, elongated up to backward-facing step, and clockwise in direction, and (b) one secondary small re-circulation and anticlockwise in direction, caused by the primary re-circulation and suction of side injection. Due to interaction between main and injecting flows, the air is slowed down and enters the re-circulation which creates large gradient of hydrogen mass concentration in re-circulation near side jet as well as causes easy diffusion of hydrogen. When this mixture, containing higher mass concentration of hydrogen, comes to the upper side of the re-circulation, it causes large gradient of hydrogen mass concentration which enhances the mixing with air. By this mechanism, hydrogen can reach up to the backward-facing step as well as surrounding regions of upstream primary re-circulation. As on the top of injector there exists a high mass concentration of hydrogen, therefore around the injector, mixing is caused by both diffusion and convection of injection. Immediately downstream of injector there is another re-circulation which enhances mixing by diffusion as described earlier. In far downstream where no re-circulation exists, mixing is occurred mainly by diffusion. In fact, due to re-circulation in upstream region, high amount of hydrogen can mix with air which is carried downstream by velocity of flow, mixes with more air and spreads in large region by expansion and diffusion phenomena.

**Conclusions**

The physics of diffusion and mixing of hydrogen in supersonic airstream has been studied using two-dimensional full Navier-Stokes equations with zero-equation turbulence model. It has been found that the
high penetration and mixing of injectant is not easy due to short residence time of flow in combustor. The upstream re-circulation plays an important role for diffusion and mixing, specially when the Mach number of main stream is high. Investigation shows that the backward-facing step causes early separation of turbulent boundary layer and increases the upstream re-circulation region which can enhance mixing in upstream caused by increasing the mass concentration gradient of injectant. On the other hand, around the injector, mixing is dominated by convection due to injection and re-circulation while at far downstream mixing is occurred mainly by diffusion. The boundary layer thickness has a significant effect on mixing and by thickening boundary layer penetration and mixing can be enhanced in both upstream and downstream of injector. The enhancement of mixing causes more uniform distribution of hydrogen in downstream of the injector.

Nomenclature

c = sound speed, m/s  
$C_p$ = specific heat at constant pressure, J/(kg.K)  
$D_i$ = turbulent diffusion coefficient, m$^2$/s  
$D_{ij}$ = binary-diffusion coefficient for species $i$ and $j$, m$^2$/s  
$E$ = total energy, J/m$^3$  
$F$ = flux vector in $x$-direction  
$\tilde{F}$ = transformed flux vector in $\xi$-direction  
$\tilde{G}$ = flux vector in $y$-direction  
$\tilde{G}_i$ = transformed flux vector in $\eta$-direction  
$H$ = enthalpy, J/kg  
$J$ = transformation Jacobian  
$K$ = number of grid points in $x$-direction  
$M$ = Mach number  
$m$ = mass flux of species, kg/s  
$p$ = pressure, Pa  
$q$ = energy flux by conduction, W/m$^2$  
$R$ = universal gas constant, J/(kg.mol.K)  
$S_a$ = Sutherland constant for viscosity, K  
$S_b$ = Sutherland constant for thermal conductivity, K  
$T^*$ = temperature, K  
$T_{ef}$ = effective temperature, K  
$t$ = physical time, s  
$u$ = horizontal velocity, m/s  
$U$ = vector of conservative variables  
$\tilde{U}$ = transformed vector of conservative variables  
$V$ = contravariant velocity in $\xi$-direction  
$\gamma$ = vertical velocity, m/s  
$\eta$ = transformed coordinate in $\eta$-direction  
$\xi$ = transformed coordinate in horizontal direction  
$\rho$ = mass density, kg/m$^3$  
$\sigma$ = normal stress, Pa  
$\sigma_{\alpha\beta}$ = effective collision diameter, Å  
$\tau$ = shear stress, Pa  
$\mu$ = coefficient of dynamic viscosity, kg/(m.s)  
$\kappa$ = thermal conductivity, W/(m. K)  
$\Omega_0$ = diffusion collision integral  
$\omega$ = vorticity, s$^{-1}$  

Superscripts

$ns$ = number of species

Subscripts

$i,j$ = index for species  
$l$ = laminar case  
$m$ = mixture  
$t$ = index for turbulence  
$\nu$ = viscous term  
$x$ = horizontal direction  
$y$ = vertical direction  
$xy$ = reference plane  
$0$ = reference value

References