Numerical Simulation of Transverse H_2 Combustion in Supersonic Airstream in a Constant Area Duct

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Reacting flow field of H_2-air combustion behind a backward facing step in a constant area combustor is simulated numerically by solving three-dimensional Navier Stokes equations along with K-ε turbulence model and fast rate chemistry. Simulation captures all the essential features of the flow field. The computed surface pressures match extremely well with the results of other numerical computations for non-reacting flow. For reacting case, although a good match obtained in the downstream, present computation over predicts the surface pressure.

Keywords : Numerical simulation; Supersonic airstream; Area duct

NOTATION

A	:	coefficient matrix
d_1, d_2	:	dia of the upstream and downstream injectors, respectively
h	:	step height
H	:	enthalpy (also height of the combustor at inlet)
K	:	turbulent kinetic energy
L	:	length of the combustor
M	:	Mach number
P	:	pressure
Pr	:	Prandtl number
q	:	heat flux
R	:	residue
S	:	Sutherland constant
S_K, S_ε	:	source terms for K and ε
t	:	time
T	:	temperature
u	:	velocity
x, y, z	:	coordinate axes
Z	:	species mass fraction
W	:	width of the combustor

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Greek Letters

ρ	:	density
τ	:	shear stress
ε	:	turbulent kinetic energy dissipation rate
μ	:	dynamic viscosity
$\sigma_K, \sigma_\varepsilon, \sigma_c$	:	coefficients for K, ε and Z equations
λ	:	thermal conductivity
γ	:	ratio of specific heats

Suffix

i, j, k	:	axial direction
ref	:	reference value
l	:	laminar
t	:	turbulent
fs	:	free stream static value

INTRODUCTION

The success of efficient design of a hypersonic air breathing cruise vehicle depends largely on proper choice of propulsion system. This type of vehicle, according to current proposal, uses scramjet propulsion system with hydrogen fuel. A vital part of the effort to develop the scramjet combustor is the ability to understand the mixing and combustion process inside the combustor.

Due to the high supersonic flow speed in the combustion chamber, problems arise in the mixing of the reactants, flame anchoring and stability and completion of combustion within the limited combustor length. The flow field in the scramjet combustor is highly complex. An overview of basic concept in fuel/air mixing and mixing controlled supersonic combustion has been proposed by Heiser and Pratt[1].

One of the popular configurations often employed in scramjet combustor is backward facing step[2]. Fuel is injected perpendicular to the air flow through small dia orifices placed behind the backward facing step. The flow in the vicinity of the fuel injector is three dimensional, turbulent, chemically reacting, accompanied by flow separation and recirculation between the step and fuel injector. The spatial flow characteristics behind a backward facing step with normal injection are not well understood. The flow properties have been measured using pitot tubes shadowgraph[3], gas sampling[4] and static wall pressure[4-6]. Yet, these studies failed to address all the issues of the complex flow phenomenon and backward facing step flow field with normal injection, remain one of the interesting problems to study.

Transverse injection of an underexpanded sonic or supersonic jet into a supersonic free stream produces several flow structures. The schematic representation of the field is shown in Figure 1. The supersonic flow undergoes expansion at the corner of the base. As the free stream is blocked partially by the secondary flow, a strong bow shock wave is formed in front of the injection point followed by a barrel shock. Also ahead of the injection point, the boundary layer separates due to the interaction between shock waves and boundary layer. Downstream of the injection point, the boundary layer reattaches and a recompression shock wave is generated. Hence, this flow field is quite complicated and various shock waves/boundary layer interactions exist in the whole region.

With the advent of powerful computer, robust and efficient numerical algorithm, the CFD is being used increasingly to understand the complex flow structures of normal injection behind backward facing step.

Various numerical simulations of transverse sonic jet injections into supersonic cross flows have been described in recent literature. Two-dimensional mixing flow calculations[7-9] show results that qualitatively predict the whole flow pattern. However, the quantitative prediction of the separated region is not so encouraging. Sun, *et al*[10] have carried out two-dimensional and three-dimensional Navier Stokes simulation of supersonic turbulent flow field with transverse sonic injection through a flat plate using weighted essentially non-

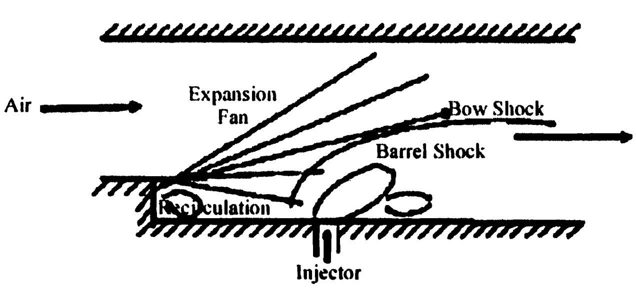


Figure 1 Flow characteristics in a backward facing step supersonic combustor

oscillating (WENO) scheme and Jone-Launder K-ε turbulence model. Although, computed surface pressures match well with the experimental value[11] for two-dimensional case, no comparisons with the experimental results are presented for 3-D case.

Lee and Mitani[12] have studied the comparative performance of three transverse injectors for mixing augmentation in scramjet combustor using a three-dimensional Navier Stokes equation along with K-ω SST model. Edwards low diffusion flux splitting upwind difference scheme was used for discretization. It has been observed that the mixing characteristics are strongly related to jet to cross flow momentum ratio. In case of higher values of momentum ratio, slower mixing rates, higher penetration, and more losses of stagnation pressure are shown.

Hao and Yu[13] have conducted numerical simulation of the flow field created by sonic transverse injection through a circular nozzle into a supersonic flow. Three-dimensional equations are solved using extended Conservation Element and Solution Element (CESE) method and the injectant penetrations are computed. Qualitative features of vorticity, injectant concentration at various cross-sections of the flow field have been presented. Backward facing step and staged injection is employed generally in the scramjet combustor to avoid intake combustor interaction. Numerical simulation of sonic transverse injection in supersonic flow in confined environment has not been reported adequately in the literature.

Chakraborty, *et al*[14] carried out non-reacting simulation of staged transverse sonic injection behind backward facing steps in a confined environment using three-dimensional Navier Stokes equations using Cartesian grid along with K-ε turbulence model with wall functions and obtained reasonable agreement with the experimental value of injectant penetration and various flow profiles at various axial locations of the combustor.

Uenishi, *et al*[15] carried out three-dimensional Navier Stokes calculations with Baldwin - Lomax turbulence model[16] for transverse sonic H_2 injection in a supersonic reacting flow in a constant area combustor[17] using MacCormack's explicit method and obtained qualitative agreement with the experimental results. Combustion of H_2 in supersonic air-stream is modelled by two-step reaction mechanism proposed by Rogers and Chinitz[18].

In the present study, turbulent reacting flow field with transverse H_2 injection behind backward facing step is simulated in a constant area combustor[17] by solving three-dimensional Navier Stokes equations along with K-ε turbulence model and infinitely fast rate chemical kinetics using a commercial CFD software CFX-TASC flow[19].

The computed results were compared with other numerical results[15].

METHODOLOGY

The CFX TASCflow[19] is an integrated software system capable of solving diverse and complex multi-dimensional fluid flow and heat transfer problems. The software solves three dimensional Navier Stokes equations in a fully implicit manner. It is a finite volume method and is based on a finite element approach to represent the geometry. The method retains much of the geometric flexibility of finite element methods as well as the important conservation properties of the finite volume method. It utilizes numerical upwind schemes to ensure global convergence of mass, momentum, energy and species. It implements a general non-orthogonal, structured, boundary fitted grids. In the present study, the discretization of the convective terms is done by first order upwind difference scheme. The turbulence model used was K - ε model with wall functions. The turbulence chemistry interaction is modelled using an infinitely fast rate kinetics based eddy dissipation model.

Governing Equations

The appropriate system of equations governs the turbulent flow of a compressible gas may be represented as under.

Continuity equation

$$\frac{\partial \rho}{\partial t}+\frac{\partial}{\partial x_k}(\rho u_k)=0, \qquad k = 1, 2, 3$$

Momentum equation

$$\frac{\partial}{\partial t}(\rho u_i)+\frac{\partial}{\partial x_k}(\rho u_i u_k)+\frac{\partial P}{\partial x_i}=\frac{\partial(\tau_{ik})}{\partial x_k}, \qquad i, k = 1, 2, 3$$

Energy equation

$$\frac{\partial}{\partial t}(\rho H)+\frac{\partial}{\partial x_k}(\rho u_k H)=-\frac{\partial}{\partial x_k}(u_j \tau_{jk})+\frac{\partial q_k}{\partial x_k}, \qquad j, k = 1, 2, 3$$

Turbulent kinetic energy (K) equation

$$\frac{\partial}{\partial t}(\rho K)+\frac{\partial}{\partial x_k}(\rho u_k K)=\frac{\partial}{\partial x_k}\left(\left(\frac{\mu_l}{\Pr}+\frac{\mu_t}{\sigma_K}\right)\frac{\partial K}{\partial x_k}\right)+S_K$$

Rate of dissipation of turbulent kinetic energy (ε) equation

$$\frac{\partial}{\partial t}(\rho \varepsilon)+\frac{\partial}{\partial x_k}(\rho u_k \varepsilon)=\frac{\partial}{\partial x_k}\left(\left(\frac{\mu_l}{\Pr}+\frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_k}\right)+S_\varepsilon$$

Species mass fraction (Z)

$$\frac{\partial}{\partial t}(\rho Z)+\frac{\partial}{\partial x_k}(\rho u_k Z)=\frac{\partial}{\partial x_k}\left(\left(\frac{\mu_l}{\Pr}+\frac{\mu_t}{\sigma_c}\right)\frac{\partial Z}{\partial x_k}\right)$$

where, ρ, u_i, p, H are the density, velocity components, pressure and total enthalpy, respectively and $\mu=\mu_l+\mu_t$ is the total viscosity; μ_l, μ_t being the laminar and turbulent viscosity and Pr is the Prandtl number. The source terms S_k and S_ε of the K and ε equation are defined as

$$S_K=\tau_{ik}\frac{\partial u_i}{\partial x_k}-\rho\varepsilon \text{ and } \tau_{ik}=\mu_t\left(\frac{\partial u_i}{\partial x_k}+\frac{\partial u_k}{\partial x_i}\right)$$

where turbulent shear stress is defined as

$$\tau_{ik}=\mu_t\left(\frac{\partial u_i}{\partial x_k}+\frac{\partial u_k}{\partial x_i}\right)$$

Laminar viscosity (μ_l) is calculated from Sutherland law as

$$\mu_l=\mu_{ref}\left(\frac{T}{T_{ref}}\right)^{3/2}\left(\frac{T_{ref}+S}{T+S}\right)$$

where T is the temperature and μ_{ref}, T_{ref} and S are known coefficients. The turbulent viscosity μ_t is calculated as

$$\mu_t=c_\mu\frac{\rho K^2}{\varepsilon}$$

The coefficients involved in the calculation of μ_t are taken as

$$c_\mu=0.09, \quad C_{\varepsilon 1}=1.44, \quad C_{\varepsilon 2}=1.92$$
$$\sigma_k=1.0, \quad \sigma_\varepsilon=1.3, \quad \sigma_c=0.9$$

The heat flux q_k is calculated as

$$q_k=-\lambda\frac{\partial T}{\partial x_k}$$

where λ is the thermal conductivity.

Combustion Modelling

The eddy dissipation combustion model is used to simulate the reactions in flames. The eddy dissipation model, used extensively for its simplicity and robustness in predicting reactive flows, is based on the concept that chemical reaction is very fast relative to the transport process in the flow. The products are formed instantaneously as the reactants mix at the molecular level. The model assumes that the reaction rate may be related directly to the time required to mix reactants at molecular level. In turbulent flows, this mixing time is dictated by the eddy properties and, therefore, the burning rate in proportional to the rate at which turbulent kinetic energy is dissipated, that is, reaction rate $\alpha\ \varepsilon / K$, where K is the turbulent kinetic energy and ε is its dissipation rate. The chemistry of the combustion reaction of hydrogen in air is represented on a molar basis by

$$H_2 + ½ O_2 = H_2O.$$

Discretization of Governing Equations

The CFX-TASCflow solver utilizes a finite volume approach, in which the conservation equations in differential form are integrated over a control volume described around a node, to obtain an integral equation. The pressure integral terms in the momentum integral equation and the spatial derivative terms in the integral equations are evaluated using finite element approach. An element is described with eight neighbouring nodes. The advective term is evaluated using upwind differencing with physical advection correction. The set of discretized equations form a set of algebraic equations as below

$$A\vec{x} = b$$

where $\vec{x}$ is the solution vector. The solver uses an iterative procedure to update an approximated x_n (solution of x at nth time level) by solving for an approximate correction x' from the equation $A\vec{x}'=\vec{R}$ where $\vec{R} = \vec{b} - A\vec{x}_n$ is the residual at nth time level. The equation $A\vec{x}'=\vec{R}$ is solved approximately using an approach called Incomplete Lower Upper Factorization method. An algebraic multigrid method is implemented to reduce low frequency errors in the solution of the algebraic equations. Maximum residual $[=\phi_i^{n+1} - f(\phi_i^{n+1}, \phi_i^n)] < 10^{-4}$ is taken as convergence criteria.

RESULTS AND DISCUSSION

Numerical simulations were carried out in the present study to simulate transverse H_2 combustion in scramjet combustor geometry[17]. The sketch of the combustor geometry is shown in Figure 2. Uenishi, *et al*[15] have done the numerical investigation of the same geometry with two minor modifications to the geometry and boundary conditions and those are as follows.

- ❑ Injectors were assumed to be equally spaced over the duct, and;

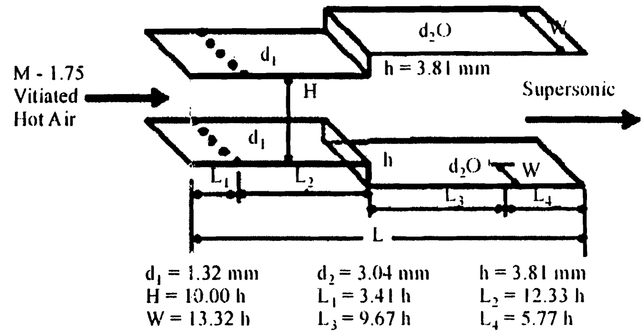


Figure 2 Schematic representation of the computational domain

- ❑ Symmetry rather than wall boundary conditions were imposed at side boundaries (y = 0.0 and y = W).

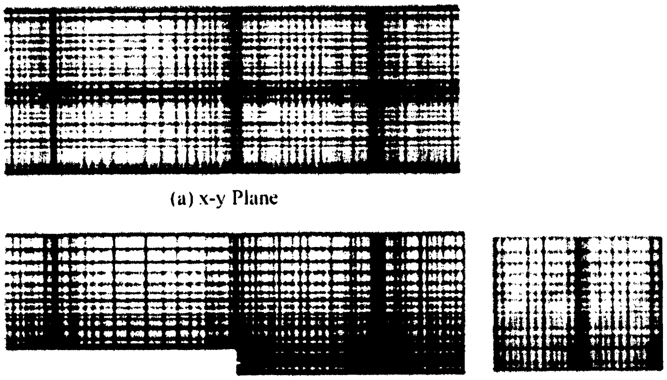
These modifications meant that the computations considered the flow around a single primary fuel injector in a row of injectors across the duct, and ignored the side wall effects. The same geometry and boundary conditions as applied by Uenishi, *et al* are considered for the present computation. The total length of the combustor is 118.8 mm with a backward facing step of 3.8 mm height is provided on both the walls at 60.0 mm downstream from the inlet plane. The height of the combustor is 38.1 mm at inlet and 45.7 mm at exit plane. The width of the combustor is 50.8 mm (W).

The hot vitiated air of 1.75 Mach number enters the combustor. Oxygen is replenished in the vitiated air, that is, it contains oxygen in a volume fraction equal to that of air, but is contaminated by a significant fraction of water. In the present case, vitiated air contains 17% of water (by mass). The sonic H_2 injectors were employed at the upstream and downstream section of the combustor. The upstream injectors, which are having 1.32 mm dia each, are placed at 13.0 mm downstream from the inlet. The distance between two consecutive injectors along the width is 12.7 mm. The primary injectors are 3.04 mm in dia each and employed at 71.4 mm downstream from the inlet. The details of the flow conditions of the upstream and downstream injectors and vitiated air stream are given in Table 1. The mass flow rates of H_2 are 2.7 gm/s and 20.6 gm/s from upstream and downstream injectors, respectively.

Taking the advantage of the geometrical symmetry, only one-fourth of the geometry has been considered for the simulation. In the simulation, x axis is taken along the length of the combustor while y and z axes are taken along the width

Table 1 Combustor inflow conditions

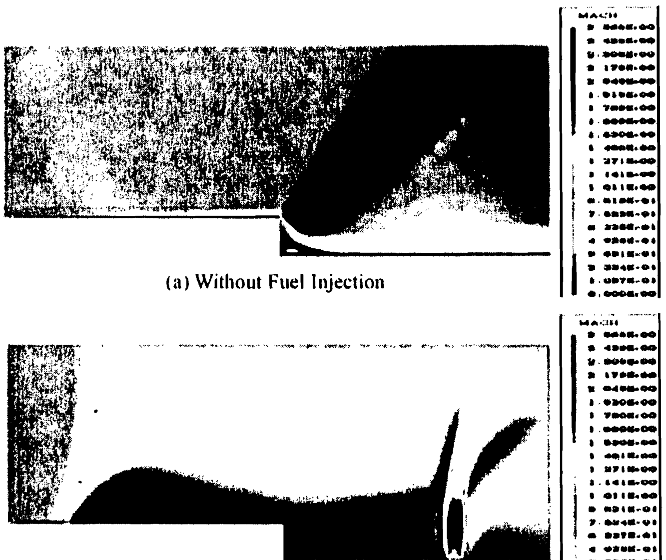
Flow	M	Pressure, *bar*	Temperature, K
Upstream H_2 injectors	1.00	2.13	250
Primary H_2 injectors	1.00	12.16	250
Vitiated air stream	1.75	1.23	1212



(a) x-y Plane

(b) z-x Plane (c) y-z Plane

Figure 3 Grid structure in the computational domain (111 × 41 × 32)



(a) Without Fuel Injection

(b) With Fuel Injection

Figure 4 March number distribution (at y = W/2)

and height of the combustor. And the origin of the *x*, *y* and *z* axis is placed at the bottom corner of the step. A total number of 111 × 41 × 32 grids are used in the simulation. The grid structures of the computational domain in *x-y*, *z-x* and *y-z* plane are shown in Figure 3(a), Figure 3(b) and Figure 3(c), respectively. Grids are fine near the injector, step and wall regions and are relatively coarse in rest of the domain.

The qualitative features of the non-reacting (without fuel injection) and reacting flow field are presented by Mach number, pressure, temperature, H_2O mass fraction and H_2 mass fraction distribution in the plane of primary injectors ($y=W/2$ in *x-z* plane) and different axial locations shown in Figure 4 – Figure 6.

The difference of flow features with and without fuel injection is shown in Figure 4 and through the Mach number distribution in the plane of injection ($y = W/2$) near the lower

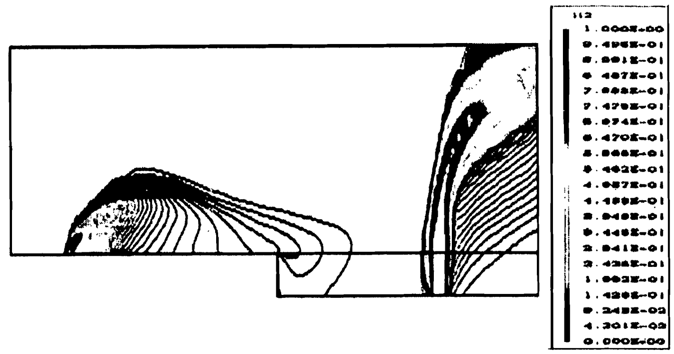
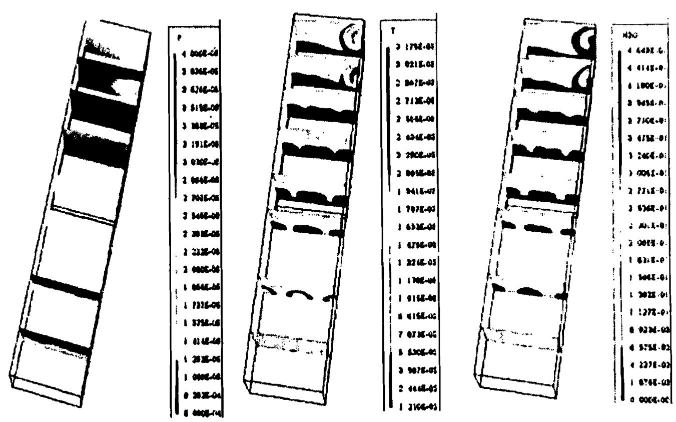


Figure 5 Reacting flow H_2 mass fraction contours (at y = W/2)



(a) Pressure (b) Temperature (c) H_2O Mass Fraction

Figure 6 Pressure, temperature and H_2O mass distribution at different axial locations (x/h = – 12.0, – 7.63, – 2.02, 1.1, 5.14, 8.6, 11.7 and 15.13)

wall. For without fuel injection case, expansion fan from the step shoulder and recirculating flow behind the step are observed, whereas, for the reacting case, precombustion shockwave caused due to reaction has made the flow field subsonic in the step and the injector locations. The H_2 injected from the upstream injectors are fully consumed (Figure 5) whereas significant amount of H_2 injected from the downstream injectors remains unburnt at the outlet of the combustor. More amount of H_2 is injected from the downstream injectors and less distance available for the reaction of this H_2 are the causes for less burning of H_2 fuel with mainstream.

The distribution of pressure, temperature and H_2O at different axial locations in the combustor (x/h = -12.0, -7.63, -2.02, 1.1, 5.14, 8.6, 11.7 and 15.13) has been shown in Figure 6. The maximum temperature in the combustor has been found to about 3100 K. Rise in pressure due to the combustion has been observed and found to increase along the axial distance of the combustor. The development of the reaction zone along the combustor length is also seen clearly from the figure.

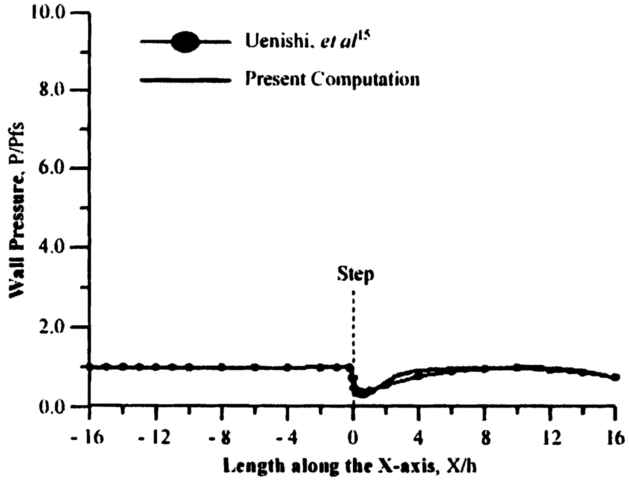


Figure 7 Wall pressure distribution [at y = W/2 (without fuel injection)]

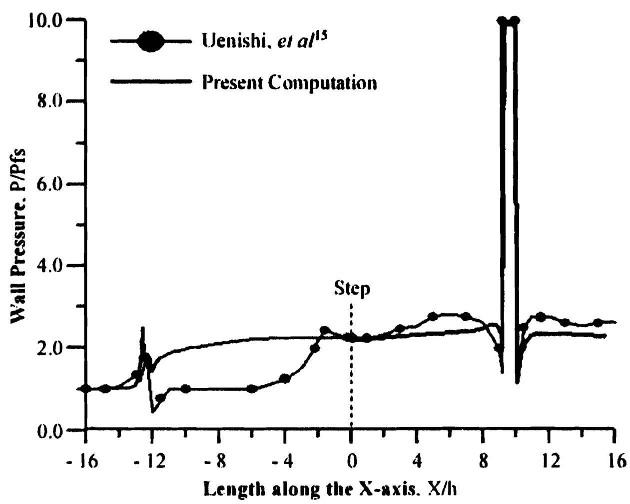


Figure 8 Wall pressure distribution at [y = W/2 (with fuel injection)]

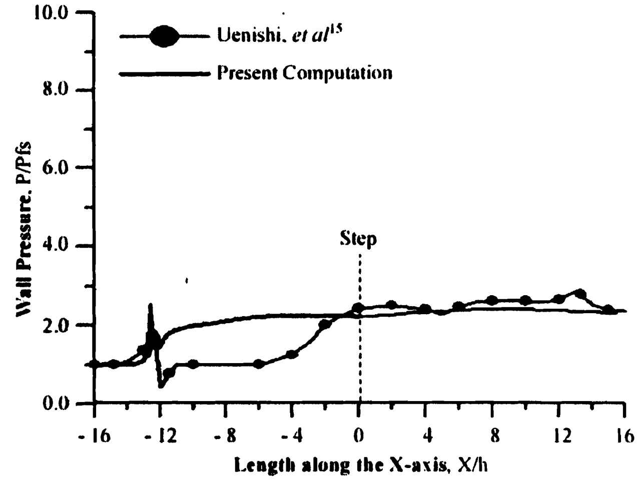


Figure 9 Wall pressure distribution at [Y = W/4 (with fuel injection)]

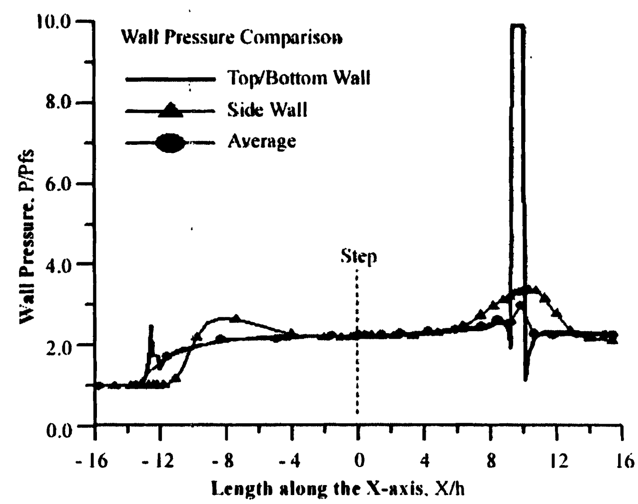


Figure 10 Wall pressure comparison (with fuel injection)

The axial distribution of the non-dimensional non-reacting surface pressure at midplane ($y = W/2$) of the combustor is compared with the computational results suggested by Uenishi, *et al*[15] as shown in Figure 7. The pressure is normalized with free stream static pressure while the axial distance has been normalized with the step height. A very good match has been obtained.

The axial distribution of non-dimensional reacting surface pressure at $y=W/2$ (midplane) and $W/4$ is shown in Figure 8 and Figure 9, respectively. The present computation shows a higher value of surface pressure at the near field zone of the upstream injectors. As the fast rate kinetics is assumed in the simulation, the resulting instantaneous heat release has over-predicted the surface pressure in the near field zone while the surface pressure matches well with the results of Uenishi, *et al*[15] in the far field zone. It is to be noted that a two step chemical kinetics has been used in the numerical simulation of Uenishi, *et al*[15]. A finite rate chemistry may be required to get a better match in the near field. Also, it can be observed that due to low equivalence ratio for the upstream injectors, the pressure rise is moderate. A comparison of the top/bottom wall, side wall and average surface pressure has been shown in Figure 10.

CONCLUSION

Numerical simulations have been carried out for reacting flow field of transverse H_2 injection in a supersonic airstream behind a backward facing step in a scramjet combustor. Three-dimensional Navier Stokes equations are solved along with K-ε turbulence model and infinitely fast kinetics using a commercial CFD software CFX-TASCflow. The simulation captures all the important features of the reacting flow field behind backward facing step which includes the bow shocks due to injection, recirculating flow behind step, reaction zone, etc. The computed surface pressure matches very well with the numerical results of Uenishi, *et al*[15] for the non-reacting case. For the reacting case, although a very good match has been obtained for the downstream region, the present computation overpredicts the surface pressures in the near field. The higher pressure rise associated with instantaneous heat release assumed in the combustion modelling may be the cause for this discrepancy.

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