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Three-Dimensional Calculation of Supersonic Reacting Flows Using an LU Scheme

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ABSTRACT

A new three-dimensional numerical program incorporated with comprehensive real gas property models has been developed to simulate supersonic reacting flows. The code employs an implicit finite volume, Lower-Upper (LU) time-marching method to solve the complete Navier-Stokes and species equations in a fully-coupled and very efficient manner. A chemistry model with nine species and eighteen reaction steps are adopted in the program to represent the chemical reaction of H_2 and air. To demonstrate the capability of the program, flow fields of underexpanded hydrogen jets transversely injected into supersonic air stream inside the combustors of scramjets are calculated. Results clearly depict the flow characteristics, including the shock structure, separated flow regions around the injector, and the distribution of the combustion products.

PREVIOUS WORK

- Develop fluid dynamic code to study the mixing and chemical reactions inside the combustors of ramjets.

- A two-dimensional computer code (RPLUS) using LU scheme to simulate chemical reacting flows has been developed:
  - Fully coupled and very efficient.
  - Finite rate chemistry.
  - A fast equilibrium chemistry package.

- Previous work done by using RPLUS 2D code:
  - Hypersonic inlet flows at Mach 10 and 13.
  - The combustion of a hydrogen jet transversely injected into a supersonic air stream.
  - Hydrogen air mixture passing a 10^o ramp.

ANALYSIS

- 3D Navier-Stokes and N_s-1 species equations.
- Brabbs' finite rate chemistry model.
  - 9 species: H_2, H, OH, H_2O, O, O_2, HO_2, H_2O_2, and N_2.
  - 18 reaction steps.
- Implicit treatment of source terms in species equations.
- No source term in energy equation for either exothermic or endothermic reactions.
- Temperature and pressure are calculated iteratively from the following equations:

$$e = \sum_{i=1}^{N_s} Y_i h_i - \frac{p}{\rho} + \frac{1}{2}\left(u^2 + v^2 + w^2\right)$$

$$h_i = h^o_{fi} + \int_{T_{ref}}^{T} C_{pi} dT$$

$$p = \rho R_u T \sum_{i=1}^{N_s} \frac{Y_i}{M_i}$$

THERMODYNAMIC AND TRANSPORT PROPERTIES

- C_p, thermal conductivity, and viscosity of individual species are obtained from fourth order polynomial of T.
- Binary mass diffusivity is calculated using the Chapman-Enskog theory with Lennard-Jones intermolecular potential energy functions.
- Wilke's mixing rule is used for the transport properties of gas mixture.
- Mass concentration weighing is used for the C_p of gas mixture.

TURBULENCE MODEL

- Baldwin-Lomax model.
- $Sc_t = Pr_t = 0.9$

NUMERICAL SCHEME

- Time-marching LU scheme.
- Implicit treatment of source terms.

$$\frac{\partial Q}{\partial t} + \frac{\partial}{\partial x}\left(E^n + A^n \Delta Q\right) + \frac{\partial}{\partial y}\left(F^n + B^n \Delta Q\right) + \frac{\partial}{\partial z}\left(G^n + C^n \Delta Q\right)$$
$$= \frac{\partial E_v^n}{\partial x} + \frac{\partial F_v^n}{\partial y} + \frac{\partial G_v^n}{\partial z} + H^n + T^n \Delta Q$$

$$A = \frac{\partial E}{\partial Q}, \quad B = \frac{\partial F}{\partial Q}, \quad C = \frac{\partial G}{\partial Q}, \quad T = \frac{\partial H}{\partial Q}$$

$$A = A^+ + A^-$$
$$B = B^+ + B^-$$
$$C = C^+ + C^-$$
$$A^+ = 0.5(A + \gamma_A I)$$
$$A^- = 0.5(A - \gamma_A I)$$
$$B^+ = 0.5(B + \gamma_B I)$$
$$B^- = 0.5(B - \gamma_B I)$$
$$C^+ = 0.5(C + \gamma_C I)$$
$$C^- = 0.5(C - \gamma_C I)$$
$$\gamma_A \geq \max(|\lambda_A|)$$
$$\gamma_B \geq \max(|\lambda_B|)$$
$$\gamma_C \geq \max(|\lambda_C|)$$

$$\left[I + \Delta t\left(D_x^- A^+ + D_x^+ A^- + D_y^- B^+ + D_y^+ B^- + D_z^- C^+ + D_z^+ C^- - T\right)\right] \Delta Q$$
$$= \Delta t RHS$$

$$RHS = -\frac{\partial E^n}{\partial x} - \frac{\partial F^n}{\partial y} - \frac{\partial G^n}{\partial z} + \frac{\partial E_v^n}{\partial x} + \frac{\partial F_v^n}{\partial y} + \frac{\partial G_v^n}{\partial z} + H^n$$

NUMERICAL SCHEME

- Two operators for 3D calculation.
- Operation count comparable to explicit schemes.

$$
\begin{aligned}
&N\Delta Q_{ijk} - \Delta t T_{ijk}\Delta Q_{ijk} + \\
&\frac{\Delta t}{\Delta x}\left(A^{-}_{i+1,j,k}\Delta Q_{i+1,j,k} - A^{+}_{i-1,j,k}\Delta Q_{i-1,j,k}\right) + \\
&\frac{\Delta t}{\Delta y}\left(B^{-}_{i,j+1,k}\Delta Q_{i,j+1,k} - B^{+}_{i,j-1,k}\Delta Q_{i,j-1,k}\right) + \\
&\frac{\Delta t}{\Delta z}\left(C^{-}_{i,j,k+1}\Delta Q_{i,j,k+1} - C^{+}_{i,j,k-1}\Delta Q_{i,j,k-1}\right) \\
&= \Delta t RHS
\end{aligned}
$$

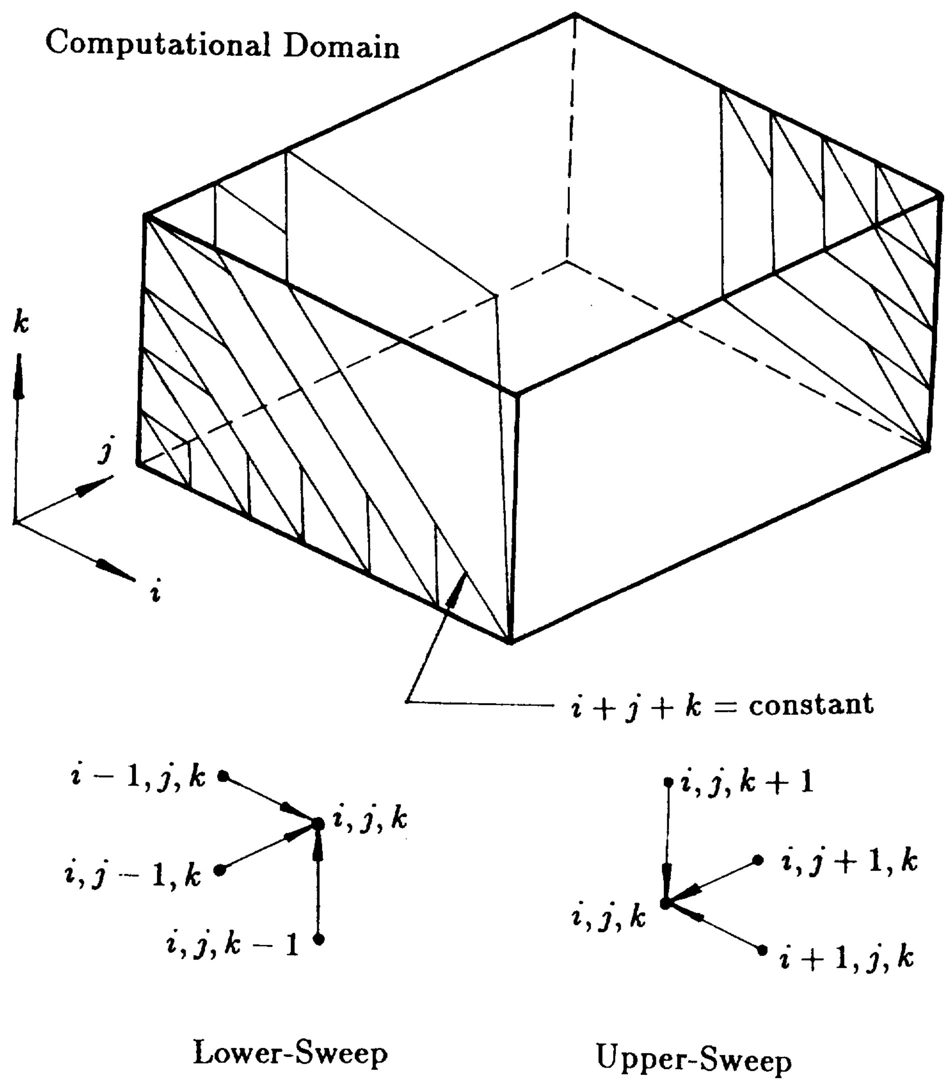
$$
N = I + \frac{\Delta t}{\Delta x}\left(A^{+}_{i,j,k} - A^{-}_{i,j,k}\right) + \frac{\Delta t}{\Delta y}\left(B^{+}_{i,j,k} - B^{-}_{i,j,k}\right) + \frac{\Delta t}{\Delta z}\left(C^{+}_{i,j,k} - C^{-}_{i,j,k}\right)
$$

$$
\begin{aligned}
&\left[N + \frac{\Delta t}{\Delta x}\left(A^{-}_{i+1,j,k}\right) + \frac{\Delta t}{\Delta y}\left(B^{-}_{i,j+1,k}\right) + \frac{\Delta t}{\Delta z}\left(C^{-}_{i,j+1,k}\right)\right] N^{-1} \\
&\left[N - \Delta t T_{i,j} - \frac{\Delta t}{\Delta x}\left(A^{+}_{i-1,j,k}\right) - \frac{\Delta t}{\Delta y}\left(B^{+}_{i,j-1,k}\right) - \frac{\Delta t}{\Delta z}\left(C^{+}_{i,j,k-1}\right)\right]\Delta Q \\
&= \Delta t RHS
\end{aligned}
$$

$$
N = \left(1 + \frac{\Delta t}{\Delta x}\gamma_A + \frac{\Delta t}{\Delta y}\gamma_B + \frac{\Delta t}{\Delta z}\gamma_C +\right) I
$$

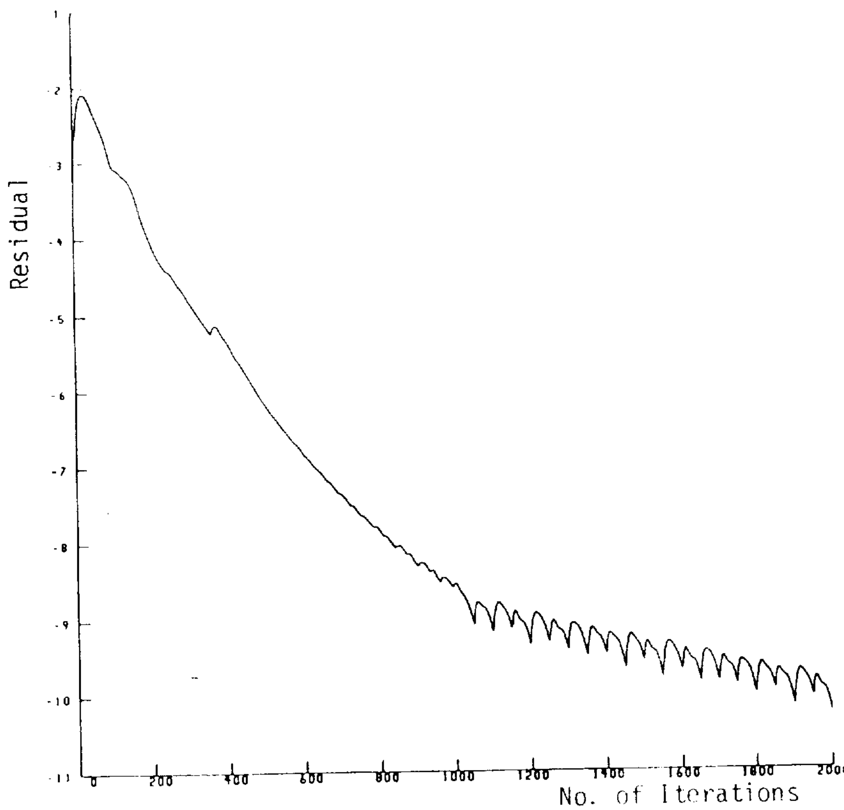
PROGRAM VECTORIZATION

- LHS can be vectorized on planes normal to the sweeping direction.



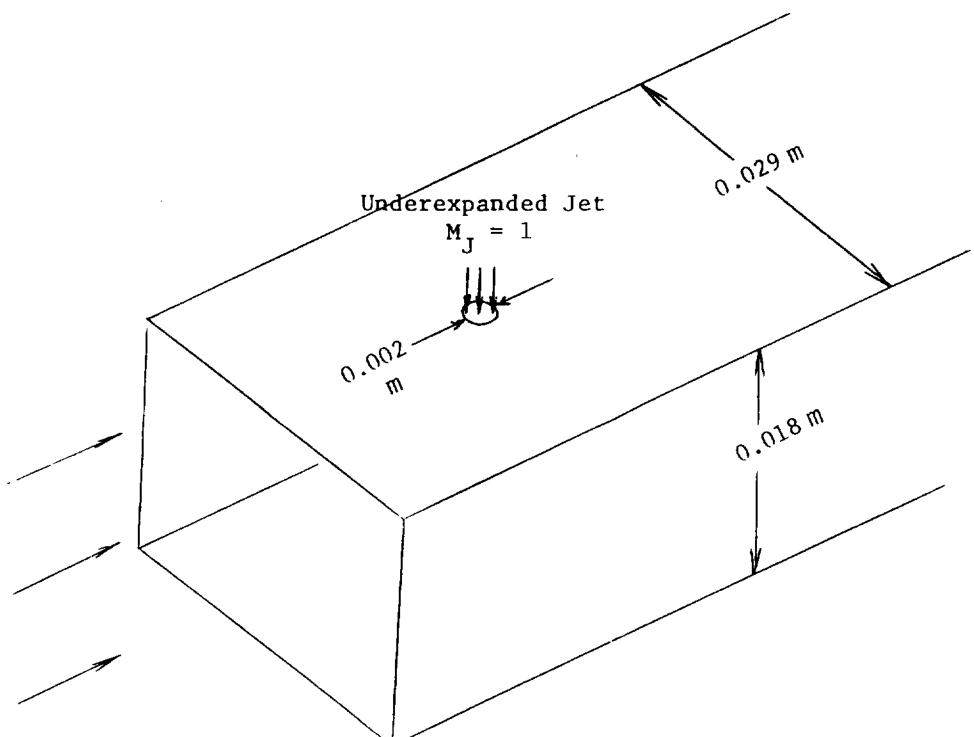
CONVERGENCE HISTORY

- Coarse grid (30x25x30)



- Present calculation:
  - Residuals reduced by 4 orders of magnitude.
  - Single injection case: (61x39x43) 8 MW, 5 hrs on Cray 2.
  - Dual Injection case: (81x39x43) 11 MW, 6 hrs on Cray 2.

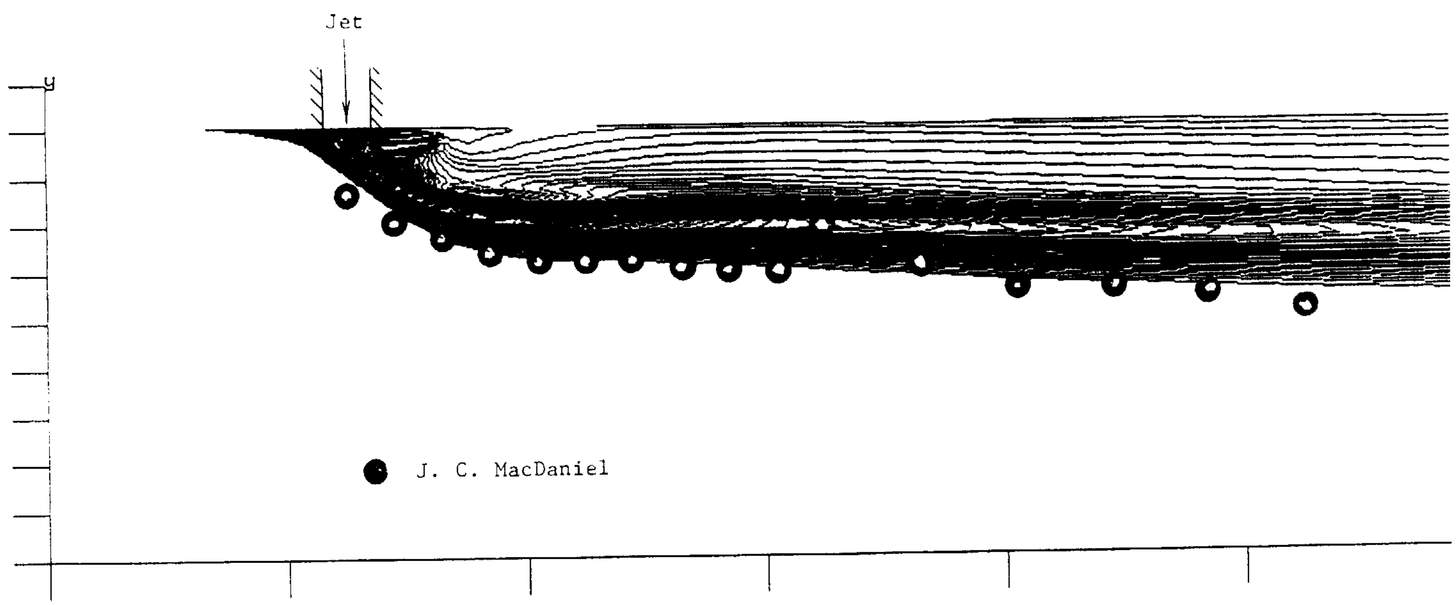
GEOMETRY AND FLOW CONDITION



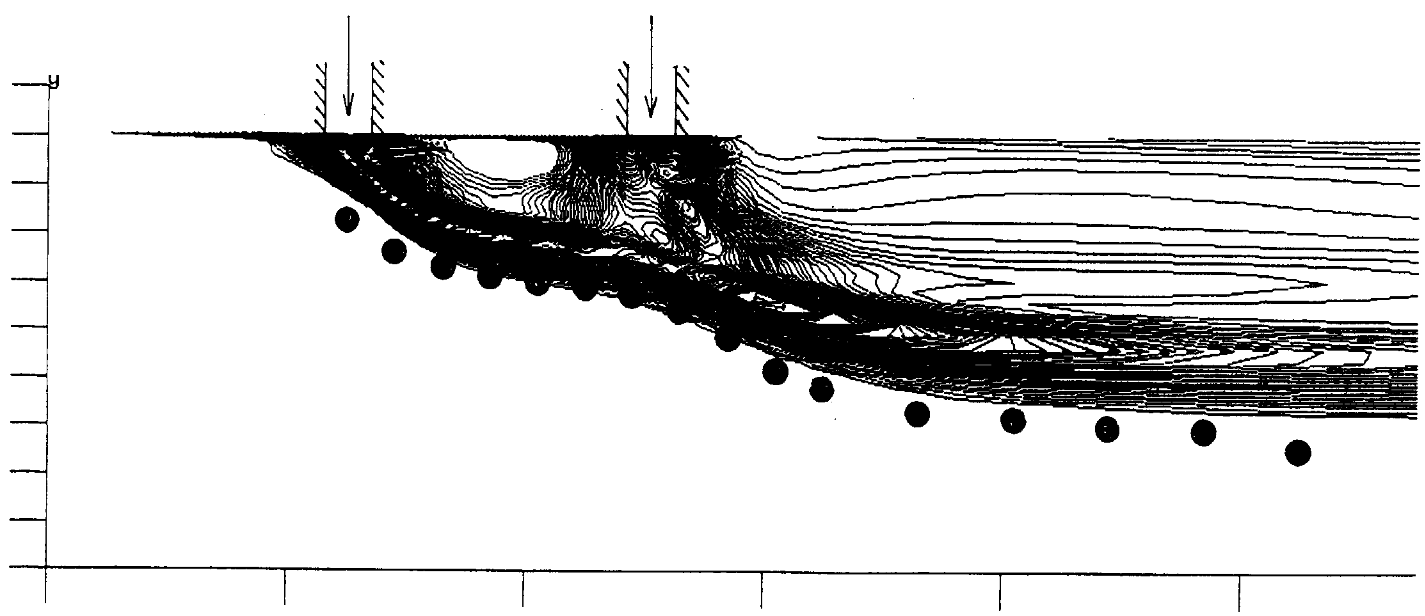
$M_{FS} = 2.07$
$P^o_{FS} = 310$ kPa
$T^o_{FS} = 298$ K

$$\bar{q} = \frac{1}{2}\rho_J u_J^2 / \frac{1}{2}\rho_{FS} u_{FS}^2$$

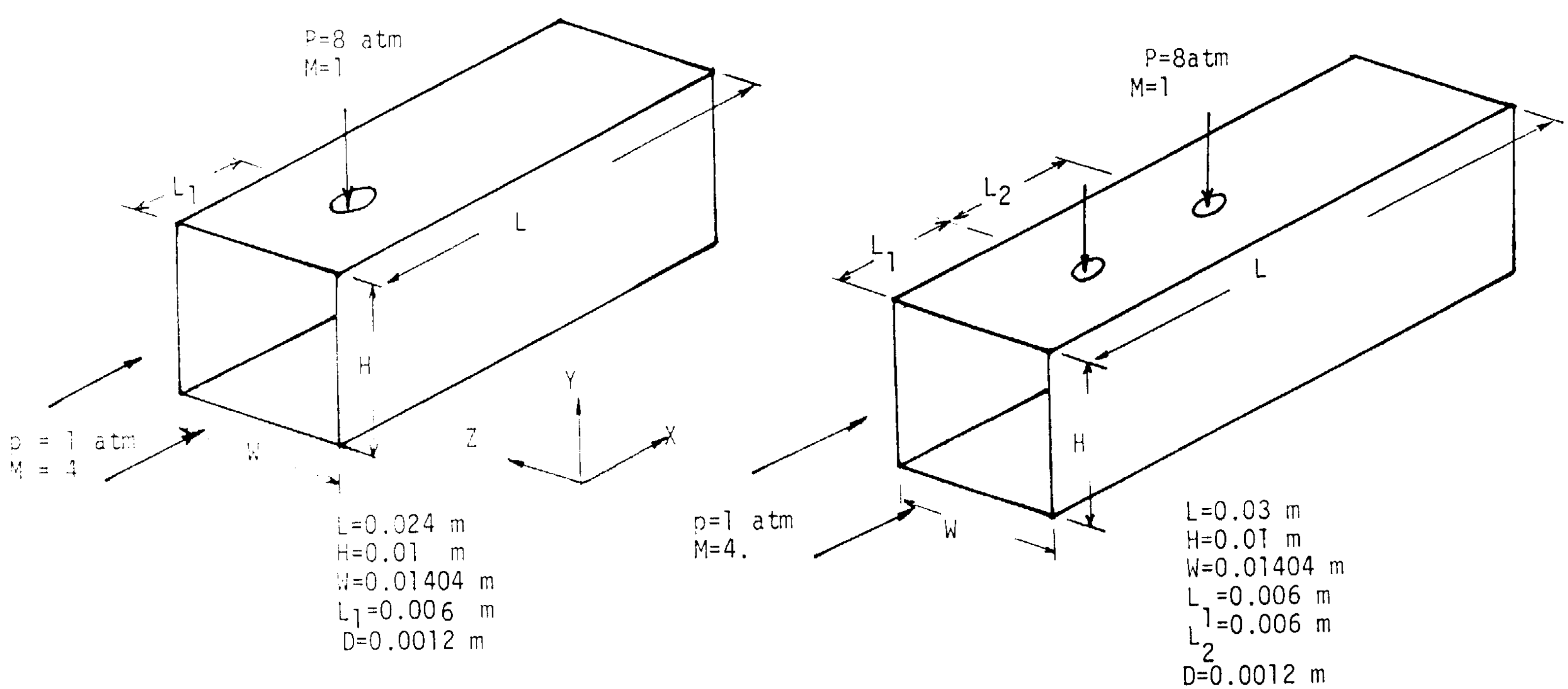
MASS-FRACTION CONTOUR ($\bar{Q} = 1.02, 60 \times 100 \times 50$)

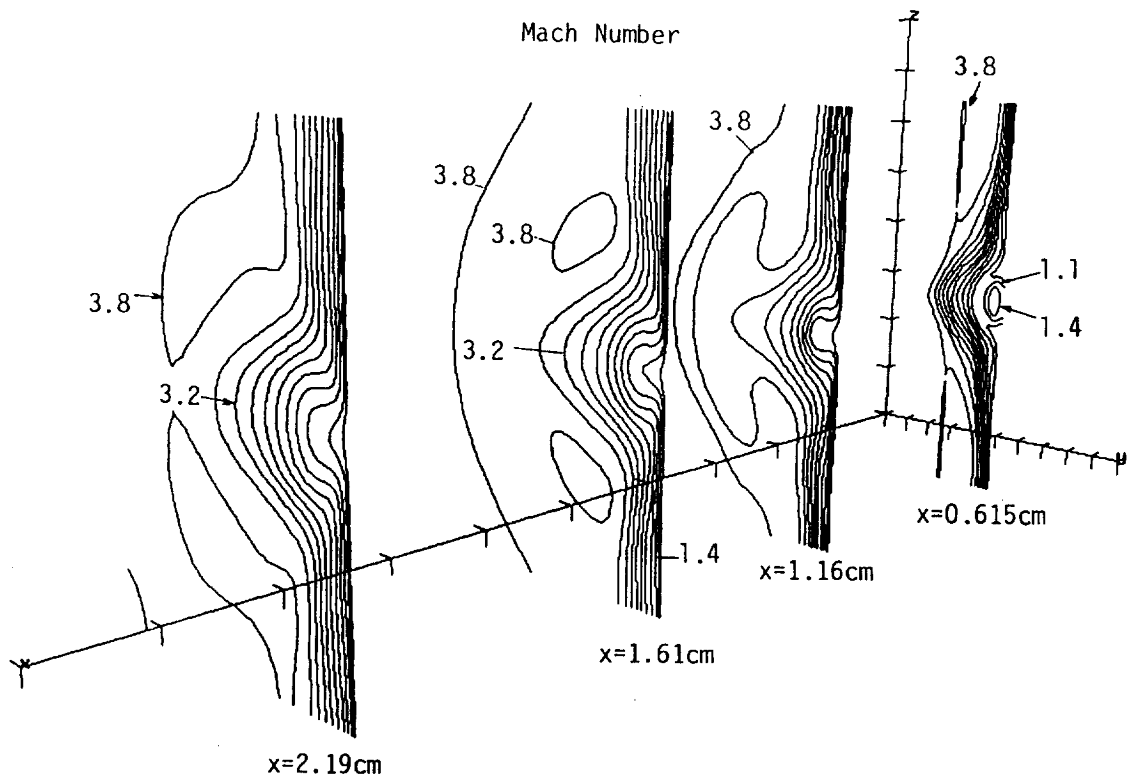


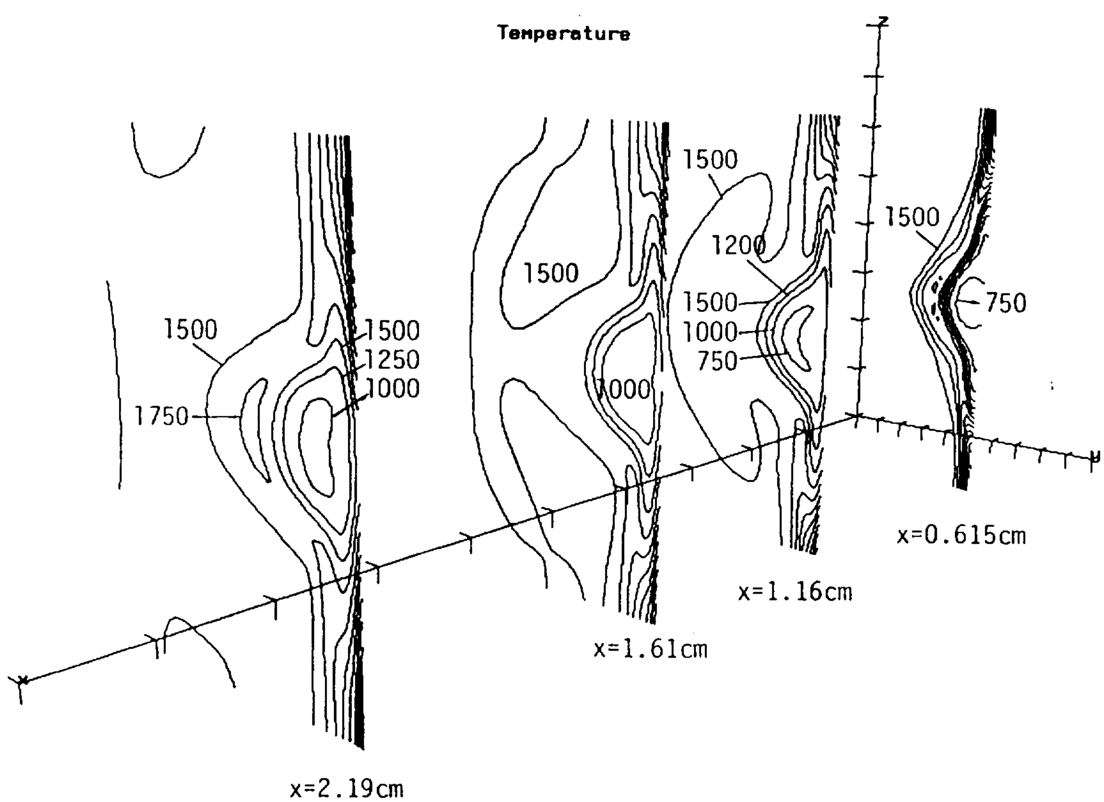
MASS-FRACTION CONTOUR (Two Ports, $\bar{Q} = 1.02$, $70 \times 100 \times 50$)

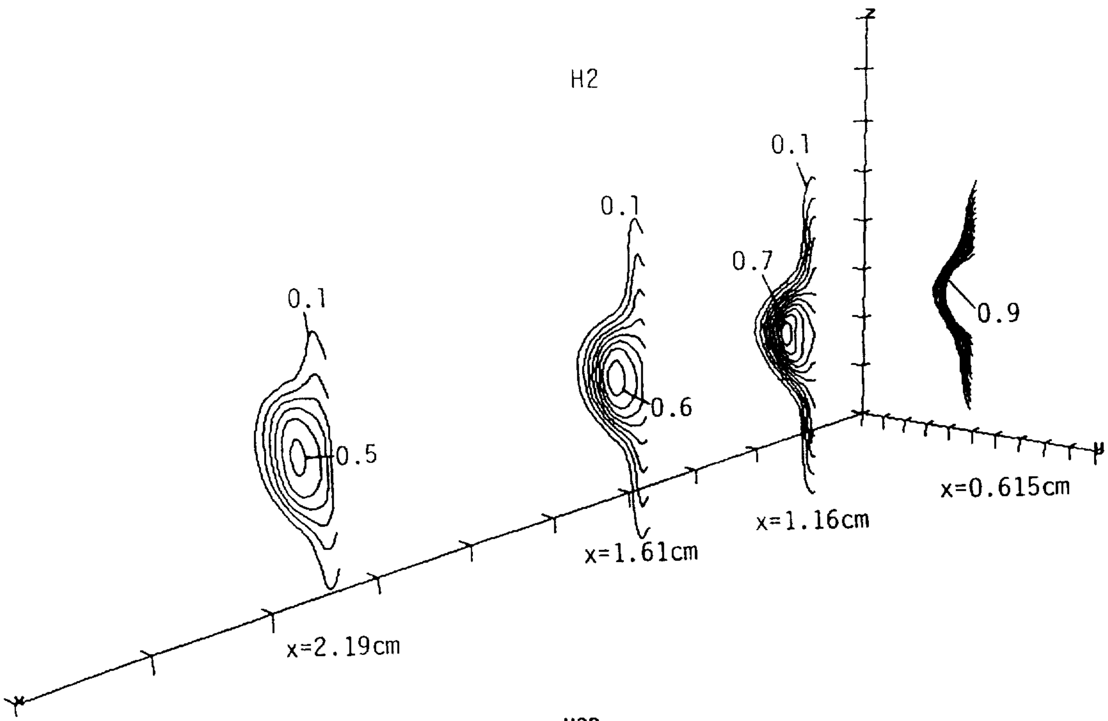


FLOW CONFIGURATION

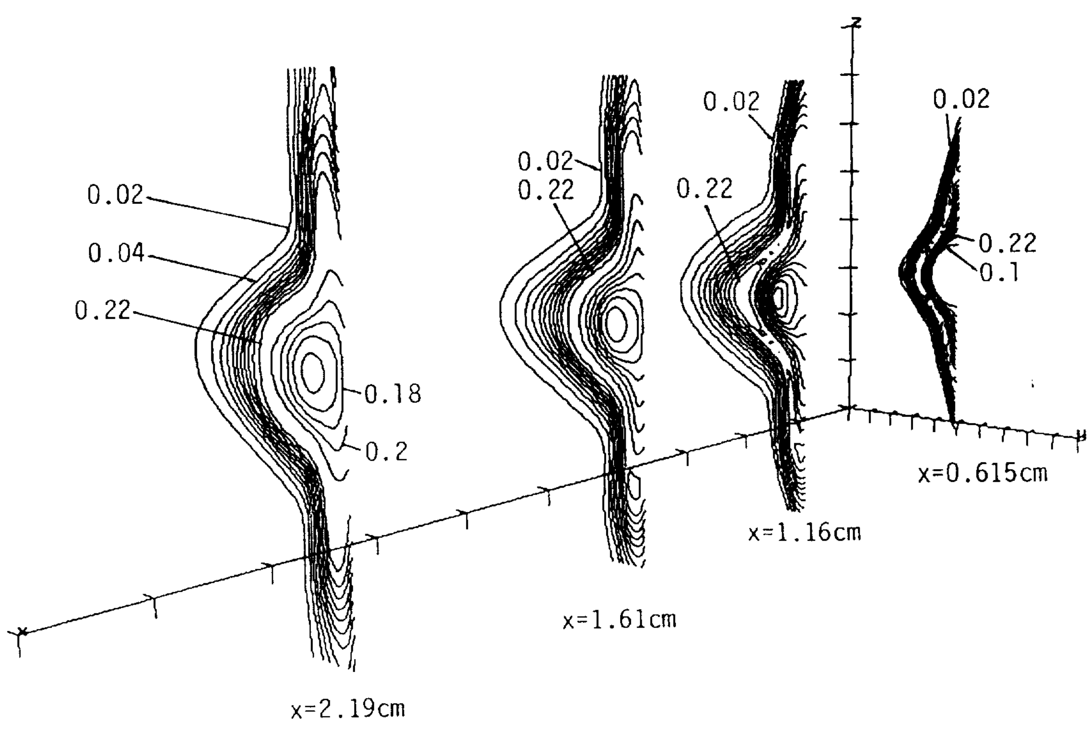



Mach Number
3.8
3.8
3.8
3.8
3.8
1.1
1.4
3.2
3.2
1.4
x=1.16cm
x=0.615cm
x=1.61cm
x=2.19cm


Temperature
1500
1500
1200
1500
750
1500
1500
1000
1500
750
1500
1250
1000
1000
1750
x=0.615cm
x=1.16cm
x=1.61cm
x=2.19cm


H2
0.1
0.1
0.1
0.7
0.9
0.6
0.5
x=0.615cm
x=1.16cm
x=1.61cm
x=2.19cm

H2O


0.02
0.02
0.02
0.22
0.22
0.02
0.04
0.22
0.22
0.1
0.18
0.2
x=0.615cm
x=1.16cm
x=1.61cm
x=2.19cm

CONCLUDING REMARKS

- A new three-dimensional computer code for high speed reacting flows has been successfully developed.

- The code is very efficient because the LHS can be vectorized on the planes normal to the sweeping directions.

- The validity of the code is assessed by the comparison between the calculated results and MacDaniel's experimental data for non-reacting mixing flows.

- The code is applied to chemically reacting flows of H_2 jets transversely injected into hot airstream.
  - Results clearly depict the shock structure, recirculations, and species distribution due to chemical reaction.
  - Two-hole injection allows deeper penetration of the fuel jet and more complete combustion of H_2 and air.