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A COUPLED IMPLICIT SOLUTION METHOD FOR  
TURBULENT SPRAY COMBUSTION IN PROPULSION SYSTEMS

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OBJECTIVES

- Develop an efficient and robust algorithm for multi-phase chemically reacting flows at all speeds, with emphasis on low Mach number flows.
- Calculate turbulent spray combustion flow in a gas turbine combustor.

## MOTIVATION

- Many reacting flows in propulsion devices cannot be efficiently calculated by modern compressible flow CFD algorithms, e.g.,
  - rocket motor — wide range of Mach numbers, from near zero velocity at closed end to supersonic at nozzle exit.
  - gas turbine combustor — low subsonic velocity, but large density variation precludes incompressible approach.
- Most low-speed reacting flow codes based on TEACH-type technologies – inefficient and lack of robustness for complex flows.
- Tremendous progress made in high-speed compressible flow CFD in past two decades. Extending application range to low-speed flow regime highly desirable.

## OUTLINES

- GOVERNING EQUATIONS
  - Gas-Phase Equations
  - Liquid-Phase Equations
- NUMERICAL ALGORITHM
- NUMERICAL TEST RESULTS
- CONCLUSION
- FUTURE PLAN FOR ALLSPD CODE

# GOVERNING EQUATIONS

## • Gas-Phase Equations

$$\Gamma \frac{\partial \hat{Q}}{\partial \tau^*} + \frac{\partial \tilde{Q}}{\partial \tau} + \frac{\partial(\tilde{E} - \tilde{E}_v)}{\partial \xi} + \frac{\partial(\tilde{F} - \tilde{F}_v)}{\partial \eta} = \tilde{H}_c + \tilde{H}_l, \quad (1)$$

$$\hat{Q} = \frac{y^\delta}{J} \begin{pmatrix} p_g \\ u \\ v \\ h \\ \kappa \\ \epsilon \\ Y_1 \\ Y_2 \\ \cdot \\ \cdot \\ Y_{N-1} \end{pmatrix}, \quad \Gamma = \begin{bmatrix} 1/\beta & 0 & 0 & 0 & 0 & 0 & \cdot & \cdot & \cdot & \cdot & 0 \\ u/\beta & \rho & 0 & 0 & 0 & 0 & \cdot & \cdot & \cdot & \cdot & 0 \\ v/\beta & 0 & \rho & 0 & 0 & 0 & \cdot & \cdot & \cdot & \cdot & 0 \\ h/\beta - 1 & \rho u & \rho v & \rho & 0 & 0 & \cdot & \cdot & \cdot & \cdot & 0 \\ \kappa/\beta & 0 & 0 & \cdot & \rho & \cdot & \cdot & \cdot & \cdot & 0 & 0 \\ \epsilon/\beta & 0 & 0 & \cdot & \cdot & \rho & \cdot & \cdot & \cdot & 0 & 0 \\ Y_1/\beta & 0 & 0 & 0 & \cdot & \cdot & \rho & \cdot & \cdot & \cdot & 0 \\ Y_2/\beta & 0 & 0 & 0 & 0 & \cdot & \cdot & \rho & \cdot & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & 0 & \cdot & \cdot & \rho & \cdot & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & 0 & \cdot & \cdot & \rho & 0 \\ Y_{N-1}/\beta & 0 & 0 & \cdot & \cdot & \cdot & \cdot & 0 & \cdot & \cdot & \rho \end{bmatrix},$$

$$\mathbf{H}_c = \begin{pmatrix} 0 \\ -\frac{2}{3}\delta \frac{\partial(\mu_\epsilon v)}{\partial x} \\ \delta[p - \tau_{\theta\theta} - \frac{2}{3}\frac{\partial(\mu_\epsilon v)}{\partial y}] \\ -\frac{2}{3}\delta[\frac{\partial(\mu_\epsilon uv)}{\partial x} + \frac{\partial(\mu_\epsilon v^2)}{\partial y}] \\ y^\delta(\Psi - \rho\epsilon) - \frac{2}{3}\delta\mu_\epsilon v(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}) \\ y^\delta[(c_1 f_1 \Psi - c_2 f_2 \rho\kappa)\frac{\epsilon}{\kappa} + \Lambda] - \frac{2}{3}\delta\mu_\epsilon v(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y})c_1 f_1 \frac{\epsilon}{\kappa} \\ y^\delta S_1 \\ \cdot \\ \cdot \\ y^\delta S_{N-1} \end{pmatrix},$$

$$\mathbf{H}_l = \begin{pmatrix} \sum_p n_p \dot{m}_p \\ \sum_p n_p \dot{m}_p u_p - \frac{4\pi}{3} \rho_p r_p^3 n_p \frac{du_p}{dt} \\ \sum_p n_p \dot{m}_p v_p - \frac{4\pi}{3} \rho_p r_p^3 n_p \frac{dv_p}{dt} \\ \sum_p n_p \dot{m}_p h_{fs} - 4\pi r_p^2 n_p h \Delta T \\ 0 \\ 0 \\ \sum_p n_p \dot{m}_p \\ \cdot \\ \cdot \\ 0 \end{pmatrix},$$

## ALLSPD MAIN FEATURES

### Present Capabilities

- 2-D and Axisymmetric geometries
- Second-order central difference for both inviscid and viscous terms
- Fully coupled, fully implicit algorithm
- Efficient convergence for wide range of Mach numbers (from  $M \leq 10^{-10}$  to supersonic)
- Finite-rate chemistry, realistic thermophysical properties
- Multi-block and body-fitted curvilinear coordinates for complex geometries
- $\kappa - \epsilon$  turbulence model
- Stochastic liquid spray model (dilute spray), vortex model for droplet internal circulation and diffusion
- Still a research code, require experience and knowledge of CFD and flow physics to use.

### Future Plans

- Development of a more efficient solver
- Extension to 3-D
- PDF model for turbulence/chemical reaction closure
- Thermal radiation model
- Detailed soot and NO<sub>x</sub> kinetic models
- Multi-grid and unstructured grid capabilities
- Dense spray and high pressure (near-/super-critical) spray models

## **Difficulties with Compressible Flow Algorithms at Low Mach Numbers**

- Disparities among system's eigenvalues (stiffness),  $u$ ,  $u + c$ ,  $u - c$ , resulting in significant slowdown in convergence rate.
- Singular behavior of pressure gradient term in momentum equations as Mach number approaches zero,

$$\rho^* u^{*2} + \frac{p^*}{\gamma M_r^2}$$

As Mach number is decreased, pressure variation ( $\Delta p^* \propto M^2$ ) becomes of similar magnitude as roundoff error of the large pressure gradient term ( $p^*/\gamma M_r^2$ ).

## METHOD OF APPROACH

### Pressure Singularity Problem

- Pressure decomposed into two parts:

$$p = p_o + p_g$$

$p_g$  replaces  $p$  in momentum equations and retains  $p_o$  as one of the unknowns.

- Employs conservative form of governing equations, but uses primitive variables

$$(p_g, u, v, h, Y_i)$$

as unknowns. Conservation property preserved and pressure field accurately resolved for all Mach numbers.

### Eigenvalue Stiffness Problem

- Pressure rescaled so that all eigenvalues have the same order of magnitude. Physical acoustic waves removed and replaced with pseudo-acoustic waves which travel at speed comparable to fluid convective velocity.

## EIGENVALUES RESCALING

$$\lambda = U, U, \frac{1}{2} \left[ U \left( 1 + \frac{\beta}{c^2} \right) \pm \sqrt{U^2 \left( 1 - \frac{\beta}{c^2} \right)^2 + 4\beta(\alpha_1^2 + \alpha_2^2)} \right], U, U \dots$$

$$\alpha_1 = \xi_x, \quad \alpha_2 = \xi_y, \quad U = \alpha_1 u + \alpha_2 v.$$

For well-conditioned eigenvalues, scaling factor  $\beta$  taken to be

$$\beta = u^2 + v^2.$$

## LIQUID-PHASE EQUATIONS

### • Droplet Motion Equations

$$\frac{dx_p}{dt} = u_p, \quad (2)$$

$$\frac{dy_p}{dt} = v_p, \quad (3)$$

$$\frac{du_p}{dt} = \frac{3}{16} \frac{C_D \mu_g Re_p}{\rho_p r_p^2} (u_g - u_p), \quad (4)$$

$$\frac{dv_p}{dt} = \frac{3}{16} \frac{C_D \mu_g Re_p}{\rho_p r_p^2} (v_g - v_p), \quad (5)$$

$$Re_p = 2 \frac{r_p \rho_g}{\mu_g} [(u_g - u_p)^2 + (v_g - v_p)^2]^{1/2},$$

$$C_D = \begin{cases} \frac{24}{Re_p} \left(1 + \frac{Re_p^{2/3}}{6}\right) & \text{for } Re_p < 1000, \\ 0.44 & \text{for } Re_p > 1000. \end{cases}$$

### • Droplet Heat and Mass Transfer Equations

$$\frac{\dot{m}_p'' d_p}{\rho D_f} = 2N_s \ln(1 + B), \quad (6)$$

$$\frac{h d_p}{k} = \frac{2N_p \ln(1 + B)^{Le^{-1}}}{[(1 + B)^{Le^{-1}} - 1]} \quad (7)$$

$$N_s = 1 + \frac{0.276 Re_p^{1/2} Pr^{1/3}}{\left[1 + \frac{1.232}{Re_p Pr^{1/3}}\right]^{1/2}} \quad N_p = 1 + \frac{0.276 Re_p^{1/2} Sc^{1/3}}{\left[1 + \frac{1.232}{Re_p Sc^{1/3}}\right]^{1/2}},$$

$$B = \frac{Y_{f_{gp}} - \bar{Y}_{fg}}{1 - Y_{f_{gp}}} \quad Y_{f_{gp}} = \frac{X_{f_{gp}} W_f}{X_{f_{gp}} W_f + (1 - X_{f_{gp}}) W_a}$$

- Droplet Internal Temperature Equations  
(Vortex Model)

$$\frac{\partial T_p}{\partial t} = 17 \frac{k_l}{C_{pl}\rho_l r_p^2} \left[ \alpha \frac{\partial^2 T_p}{\partial \alpha^2} + (1 + C(t)\alpha) \frac{\partial T_p}{\partial \alpha} \right] \quad (8)$$

$$C(t) = \frac{3}{17} \left( \frac{C_{pl}\rho_l}{k_l} \right) r_p \frac{dr_p}{dt}$$

$$\begin{aligned} t &= t_{inj}, \quad T_p = T_{inj}, \\ \alpha = 0, \quad \frac{\partial T_p}{\partial \alpha} &= \frac{1}{17} \left( \frac{C_{pl}\rho_l}{k_l} \right) r_p^2 \frac{\partial T_p}{\partial t}, \\ \alpha = 1, \quad \frac{\partial T_p}{\partial \alpha} &= \frac{3}{16} r_p \frac{\partial T_p}{\partial r}, \end{aligned}$$

### NUMERICAL ALGORITHM

- Gas-Phase - ALLSPD code
- Liquid-Phase
  - Droplet motion equations (ODE) - Runge-Kutta method.
  - Droplet internal equations (PDE) - implicit method (Thomas algorithm).
  - Determination of spray time step for integration.
  - Stochastic separate flow model.
- Interaction Between Two Phases

## SPRAY TIME STEP

- Droplet Velocity Relaxation time ( $t_r$ )

$$t_r = \frac{16}{3} \left( \frac{\rho_l}{\rho_g} \right) \left( \frac{r_p^2}{\nu} \right) (C_D Re_p)^{-1}.$$

- Droplet Life Time ( $t_l$ )

$$t_l = \frac{r_p}{3\dot{m}_p'' \rho_l}.$$

- Droplet Surface Temperature Constraint Time ( $t_s$ )

$$t_s = \ln\left(\frac{1}{1 - \frac{\Delta T_p}{A}}\right) / A'$$

$$\frac{dT_p}{dt} = \frac{6}{\rho_l C_v d_p} [h(\bar{T} - T_p) - \dot{m}_p'' h_{fg}]$$

- 
- Local Grid Time Scale ( $t_g$ )
  - Turbulent Eddy-Droplet Interaction Time ( $t_i$ )

$$t_i = t_e, \quad \text{if } L_e > \tau |\vec{u}'' - \vec{u}_p''|$$

$$t_i = \min(t_e, t_t), \quad \text{if } L_e < \tau |\vec{u}'' - \vec{u}_p''|$$

where

$$L_e = C_\mu^{3/4} \kappa^{3/2} / \epsilon$$

$$t_e = L_e / (2\kappa/3)^{1/2}.$$

$$t_t = -\tau \ln[1 - L_e / (\tau |\vec{u}'' - \vec{u}_p''|)]$$

- Spray Time step -  $\Delta T_{spr}$

$$\Delta t_{spr} = \alpha \min(t_r, t_l, t_s, t_g, t_i)$$

## INTERACTION BETWEEN TWO PHASES

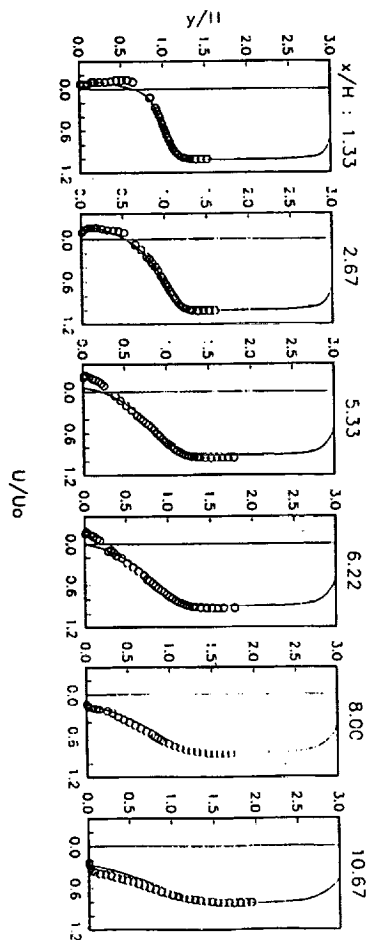
1. Initialize gas and liquid phase variables.
2. Solve liquid-phase equations.
3. Evaluate spray source term,  $H_l$ .
4. Solve gas-phase equations and update gas-phase variables.
5. Update spray source term,  $H_l$  ?  
    No, go to step 4.  
    Yes, go to step 2.

## NUMERICAL TEST RESULTS

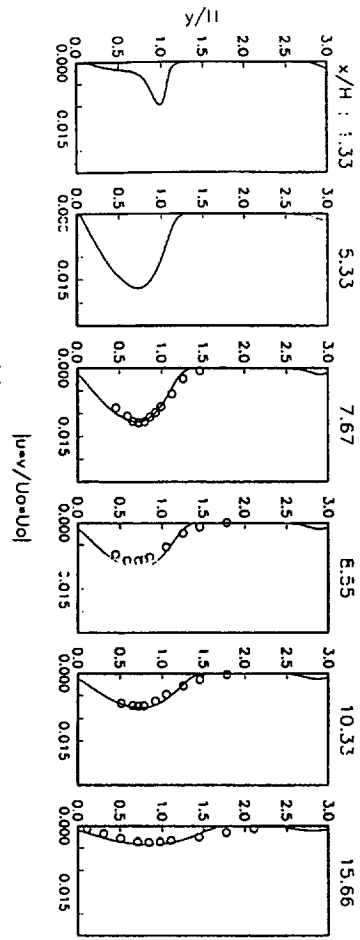
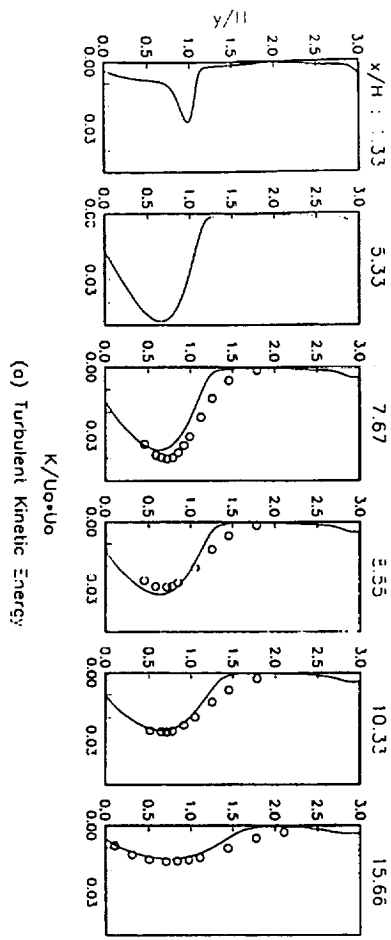
- Turbulent Backward-Facing Step Flow - non-reacting.
- Evaporating Turbulent Spray Flow.
- Gas Turbine Spray Combustion Flow.

# PARTICLE TRACES

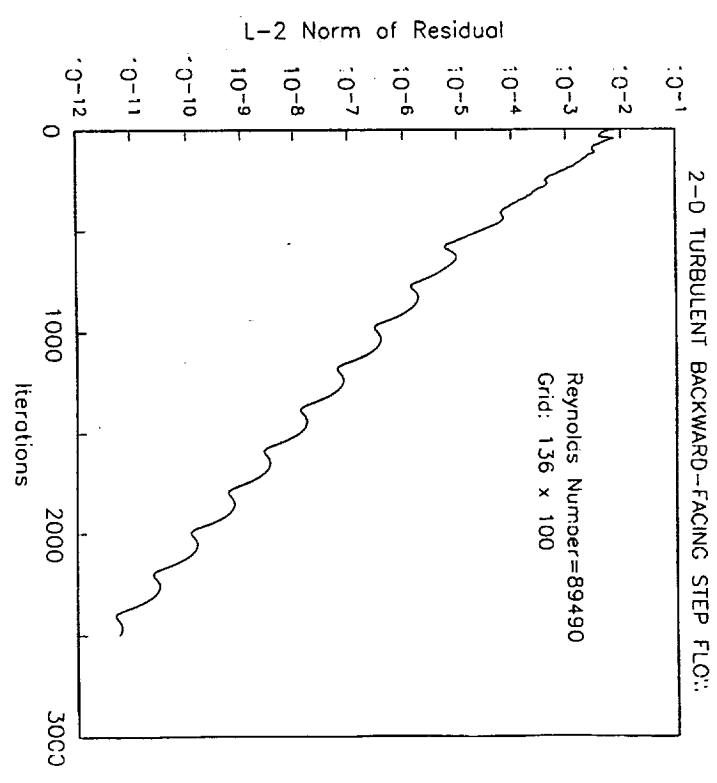
0.052 MACH  
89490.00 DEG ALPHA  
136 x 100 GRID

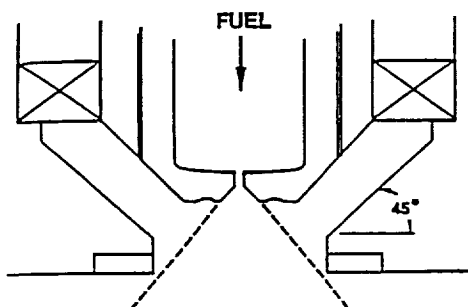


o Experiment of Kim et al., 1980  
— Computations



Experiment of Kim et al., 1980  
Computations





**OPERATING MODE 1**  
NO ATOMIZING AIR

LIQUID FLOW RATE : 1.26 grams / sec

AIR FLOW RATE : 0.00 grams / sec

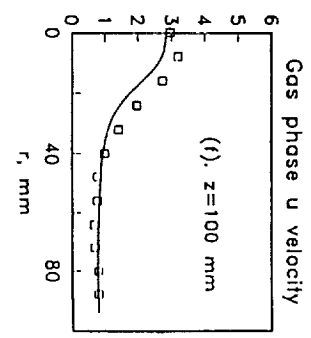
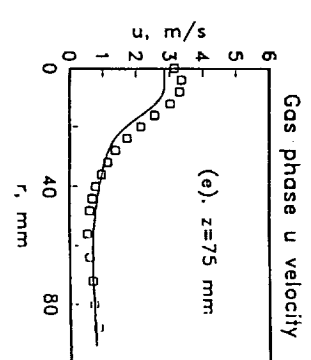
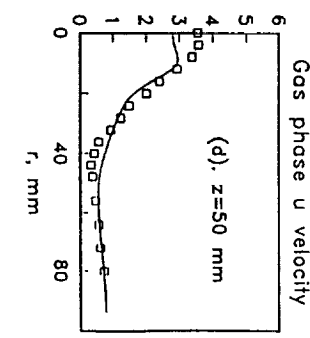
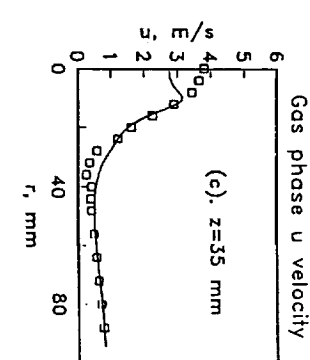
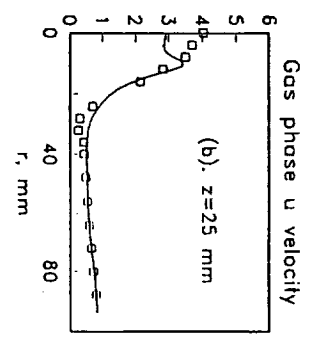
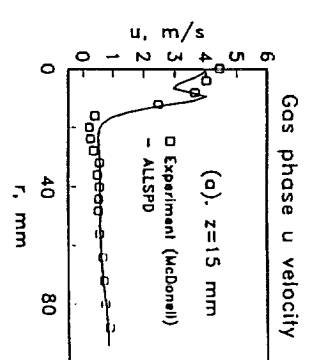
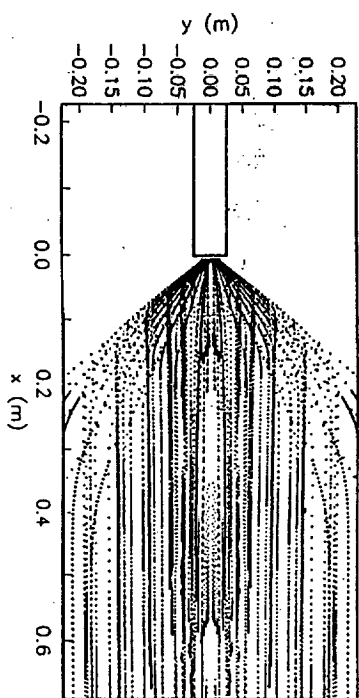
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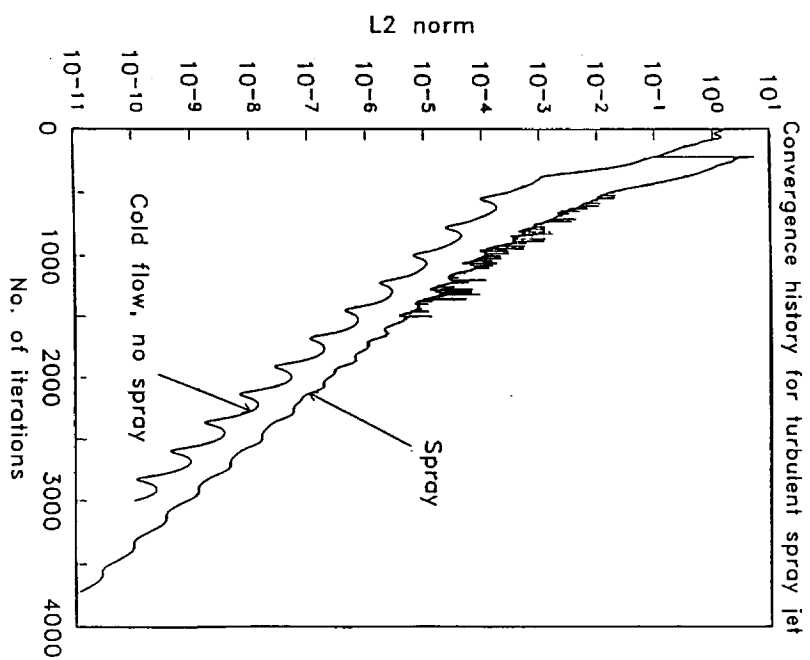
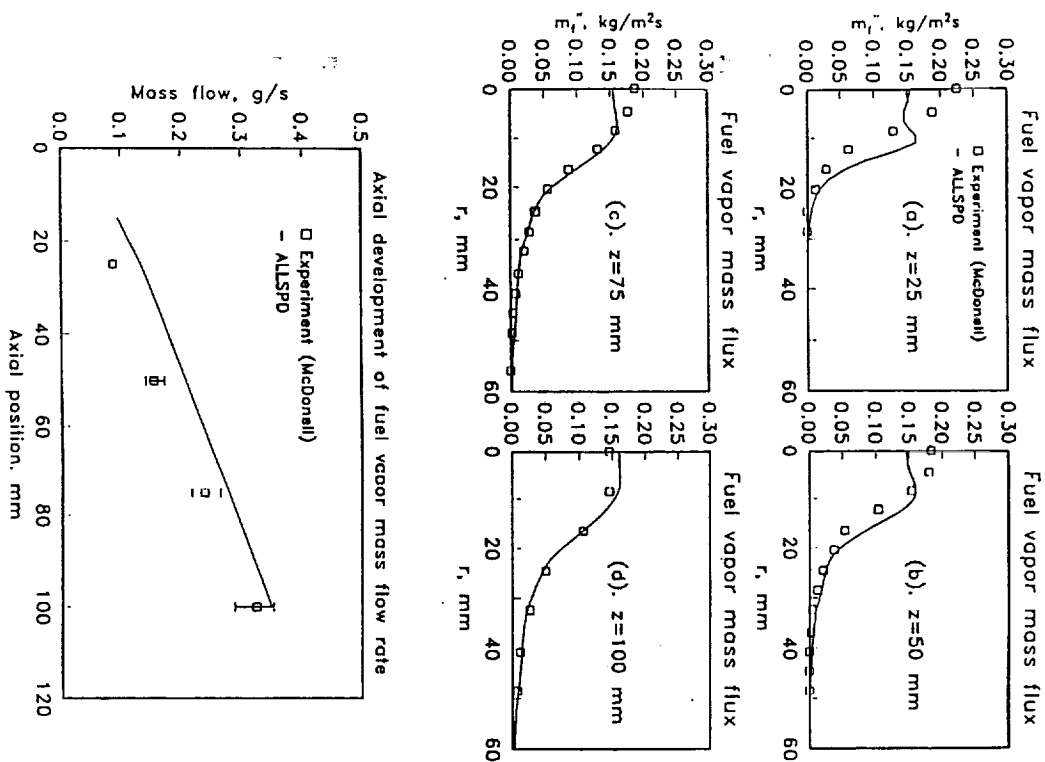
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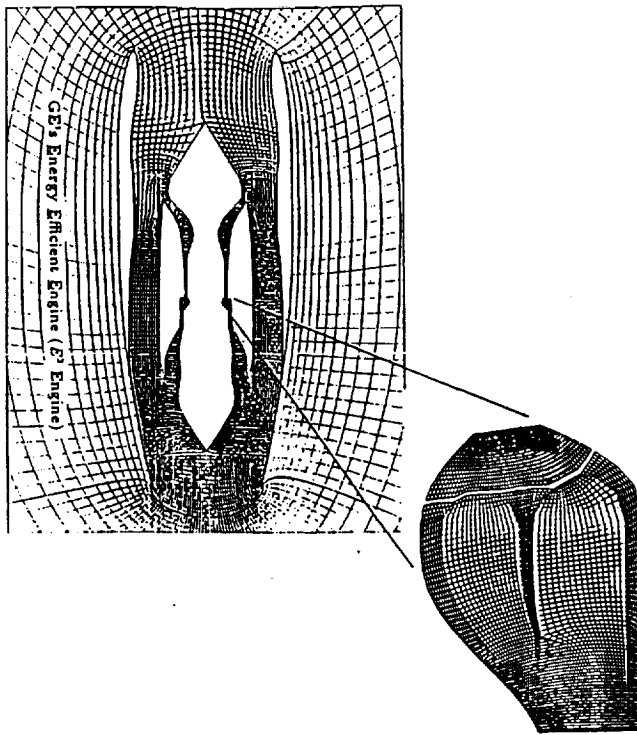
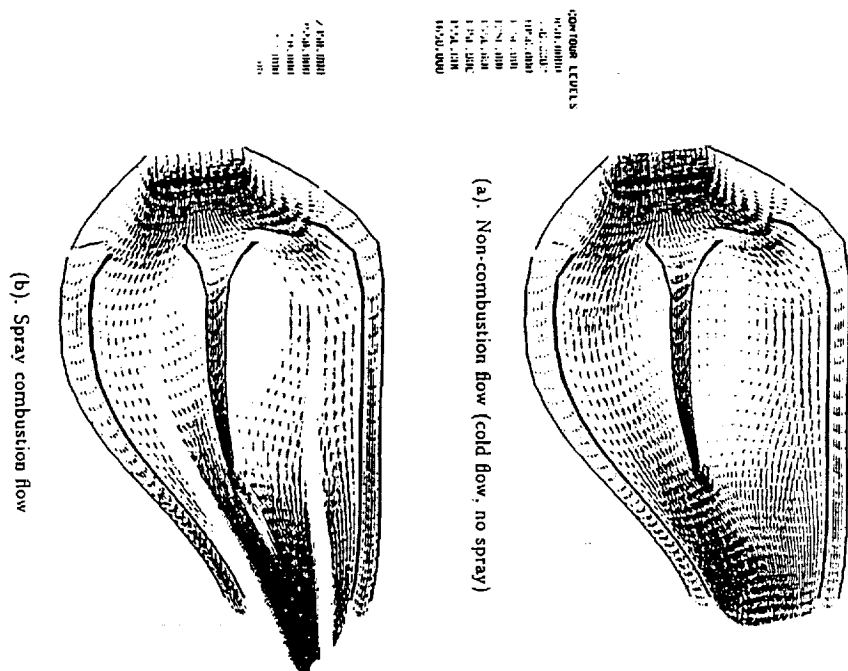


Fig. 9 Center-plane cut for GE's EEE gas turbine engine and the grid for the combustor.



**Fig. 11 Velocity vectors (colored by temperature) for (a) non-combustion and (b) spray combustion cases for the gas turbine spray combustion flow.**

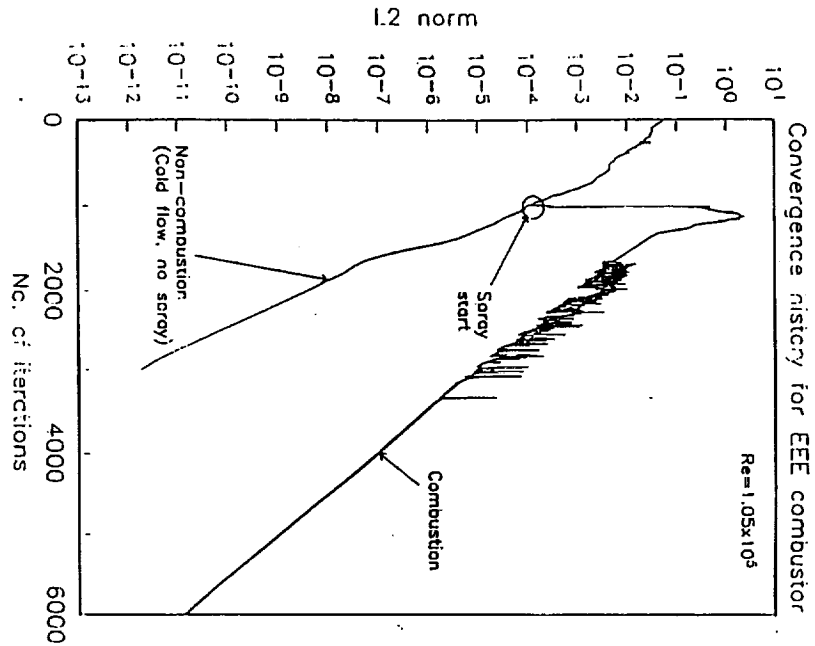


Fig. 13 Convergence history for both non-combustion and spray combustion cases for the gas turbine spray combustion flow.

## CONCLUSION

- ALLSPD code efficiently coupled with the SSF spray model.
- Satisfactory convergence property for flows with and without spray.