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A COMPOSITION JOINT PDF METHOD FOR THE MODELING OF SPRAY FLAMES

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INTRODUCTION

- THE COMPOSITION JOINT PDF METHOD HAS BEEN USED TO MODEL A WIDE CLASS OF GASEOUS TURBULENT REACTIVE FLOWS. (S.B. POPE)
- NONLINEAR CHEMICAL REACTION RATES COULD BE EVALUATED WITHOUT ANY APPROXIMATION.
- AN EXTENSION OF THE PDF METHOD TO THE MODELING OF SPRAY FLAMES.
- EVALUATE THE LIMITATIONS AND CAPABILITIES OF THIS METHOD IN THE MODELING OF GAS- TURBINE COMBUSTOR FLOWS.

Composition Joint Pdf Transport Equation

$$\bar{\rho}\tilde{p}_{,t} + \bar{\rho}\tilde{u}_i\tilde{p}_{,x_i} + [\tilde{\rho}w_\alpha(\underline{\psi})\tilde{p}]_{,\psi_\alpha} =$$

$$\{Mean\ convection\} \quad \{Chemical\ reactions\}$$

$$-[\bar{\rho} < u_i'' \mid \underline{\psi} > \tilde{p}]_{,x_i} - [\bar{\rho} < \frac{1}{\rho} J^\alpha_{i,x_i} \mid \underline{\psi} > \tilde{p}]_{,\psi_\alpha}$$

$$\{Turbulent\ convection\} \quad \{Molecular\ mixing\}$$

$$-[\bar{\rho} < \frac{1}{\rho} s_\alpha \mid \underline{\psi} > \tilde{p}]_{,\psi_\alpha}$$

$$\{Liquid - phase\ exchange\}$$

- $\tilde{p}$ = Density-weighted joint pdf.
- w_α = chemical source term for the α-th composition variable.
- $< u_i'' \mid \underline{\psi} >$ = conditional average of Favre velocity fluctuations.
- $< \frac{1}{\rho} J^\alpha_{i,x_i} \mid \underline{\psi} >$ = conditional average of scalar dissipation.
- $< \frac{1}{\rho} s_\alpha \mid \underline{\psi} >$ = conditional average of liquid-phase source term for the α-th composition variable.

- $< u_i'' \mid \underline{\psi} >$ is modeled using a gradient-diffusion model.
- $< \frac{1}{\rho} J_{i,x_i}^{\alpha} \mid \underline{\psi} >$ is modeled using a variant of Curl's model.
- The new term $< \frac{1}{\rho} s_\alpha \mid \underline{\psi} >$ involving the conditional average of liquid-phase source term is modeled based on the average values of species and enthalpy:

$$< \frac{1}{\rho} s_\alpha \mid \underline{\psi} >= \frac{1}{\bar{\rho} \Delta v} \sum n_k m_k (\epsilon_\alpha - \phi_\alpha)$$

$$for \;\; \phi_\alpha = Y_\alpha, \alpha = 1, 2, ..., s = \sigma - 1$$

$$< \frac{1}{\rho} s_\alpha \mid \underline{\psi} >= \frac{1}{\bar{\rho} \Delta v} \sum n_k m_k (-l_{k,eff} + h_{ks} - \phi_\alpha)$$

$$for \;\; \phi_\alpha = h.$$

MODELING ASPECTS

- THE MODELED PDF TRANSPORT EQUATION PROVIDES THE SOLUTION FOR THE SPECIES AND TEMPERATURE FIELDS WITH THE MEAN VELOCITY AND THE TURBULENT DIFFUSIVITY AND FREQUENCY PROVIDED AS INPUTS FROM THE CFD SOLVER AND THE SPRAY SOURCE TERMS FROM THE LIQUID–PHASE SOLVER.
- THE MEAN FLOW AND TURBULENCE EQUATIONS ARE SOLVED BY A CONVENTIONAL CFD SOLVER WITH THE MEAN SPECIES AND TEMPERATURE FIELDS PROVIDED AS INPUTS FROM THE PDF SOLVER AND THE SPRAY SOURCE TERMS FROM THE LIQUID–PHASE SOLVER.
- THE LIQUID–PHASE EQUATIONS ARE FORMULATED IN LAGRANGIAN COORDINATES WITH APPROPRIATE CONSIDERATION TAKEN INTO ACCOUNT OF THE EXCHANGES OF MASS, MOMENTUM, AND ENERGY BETWEEN THE TWO PHASES.

NUMERICAL METHOD

- Mean–Flow and Turbulence Equations
  - Axisymmetric, Unsteady.
  - Incompressible Navier–Stokes (Variable–Density).
  - A Standard Two–Equation k–ε Turbulence Model.
  - A Pressure–Based CFD Solver Based on the SIMPLE Algorithm of Patankar and Spalding.
- Liquid–phase Equations
  - The Spray Model (Raju and Sirignano).
  - Dilute Spray Assumption.
  - The ODE's for the Particle Size, Velocity, and Location are Solved Using a R–K Method.
  - The PDE's for the Internal Droplet Distribution (Vortex Model) are Solved by an Implicit Method.
  - Droplet Regression Rate is Based on Either a Gas–Phase Boundary Layer–Analysis or Low–Reynolds Correlation.

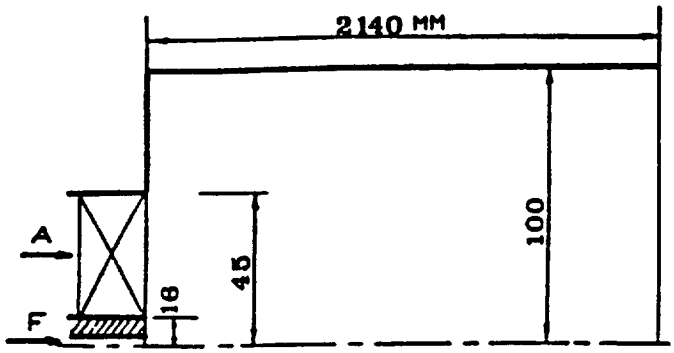
NUMERICAL METHOD

- The PDF Transport Equation
  - A Fractional Step Monte–Carlo Method (Pope).
  - Spatial Transport, Molecular Mixing, Liquid–Phase Source Terms, and Chemical Kinetics are advanced in a Series of Sequential Steps.
  - Vectorization
- Interaction Between the Two Phases
  - Interpolation of the Gas–Phase Properties at the Particle Location Using an Area–Weighted Averaging.
  - The Source Terms Evaluated at the Particle Location are redistributed among the surrounding Computational Nodes Using an Area–Weighted Averaging.

CHEMICAL KINETICS MODEL

- IT IS BASED ON A SINGLE STEP GLOBAL MECHANISM OF WESTBROOK AND DRYER FOR N-DECANE/OXYGEN COMBUSTION.

- THIS GLOBAL COMBUSTION MECHANISM WAS SHOWN TO PROVIDE ADEQUATE REPRESENTATION OF TEMPERATURE HISTORIES IN FLOWS NOT DOMINATED BY LONG IGNITION DELAY TIMES.



Geometry of the combustion chamber.
(El Banhawy and Whitelaw)

EXPERIMENTAL DETAILS

- The experimental data corresponds to the following inflow conditions:

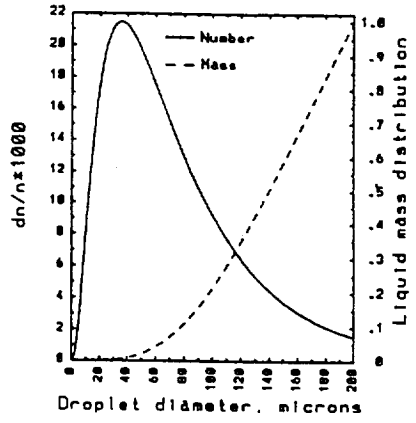
  inflow temperature = 310 K,
  air mass flow rate = 355 kg/h,
  air/fuel ratio =20.17,
  swirl vane angle = 45 deg,
  swirl number =0.721.

- The reported error in the measurements is about 10 to 15 % for the temperature and about 15% for the velocity.

Details of Fuel Injection

- A fuel nozzle of swirl-atomization type was used.
- The liquid fuel injection is simulated by injecting a discretized parcel of liquid mass at the end of each $\Delta t_{injection}$
- The droplet-size distribution is given by:

$$\frac{dn}{n} = 4.21\ 10^6 \left[\frac{D}{D_{32}}\right]^{3.5} e^{-16.98\left(\frac{D}{D_{32}}\right)^{0.4}} \frac{dD}{D_{32}}$$

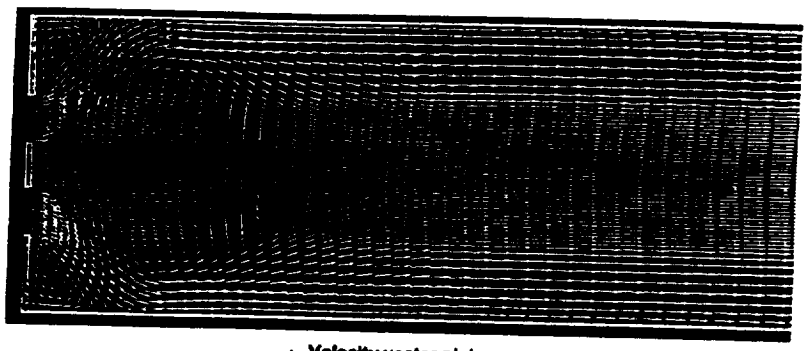


Droplet size Distribution

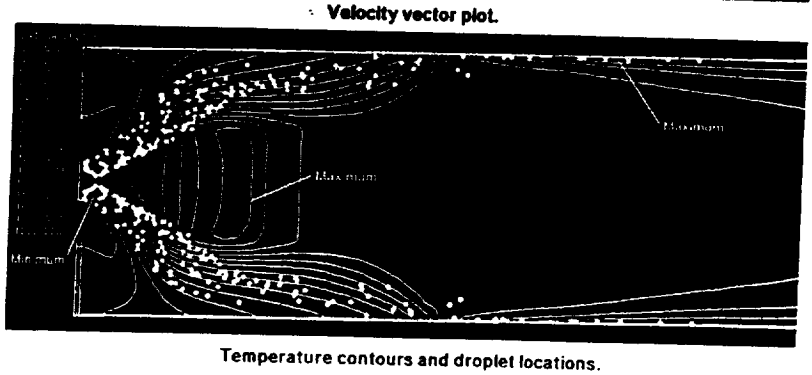
- The initial droplet injection velocity corresponds to: $u_k = 11.0$ m/s, $w_k = 6.1$, and $v_k = 0.5 - 2.5$.

PARAMETER SELECTIONS

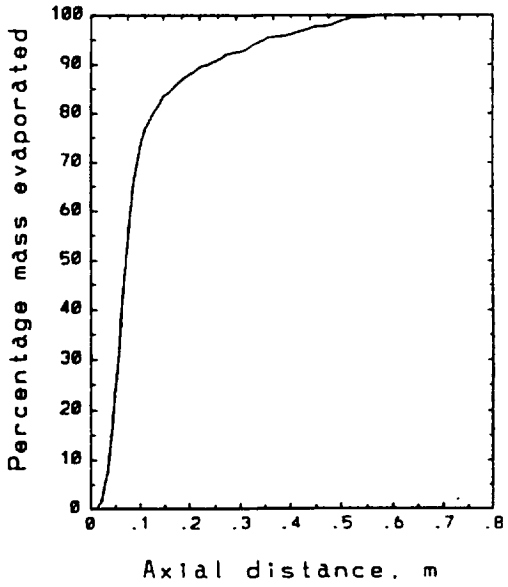
- The computations were performed on a grid with a mesh size of 60x60.
- The PDF solution is obtained by making use of 250 particles per cell.
- $Dt_g = Dt_{injection} = 1.5$ ms, $Dt_k = 0.0375$ ms, and $Dt_{Monte-Carlo} = 0.015$ ms.
- Two CPU seconds on a CRAY Y-MP per one Dt_g and about 2 to 3 CPU hours – 4000 time steps – for the solution to reach steady state.



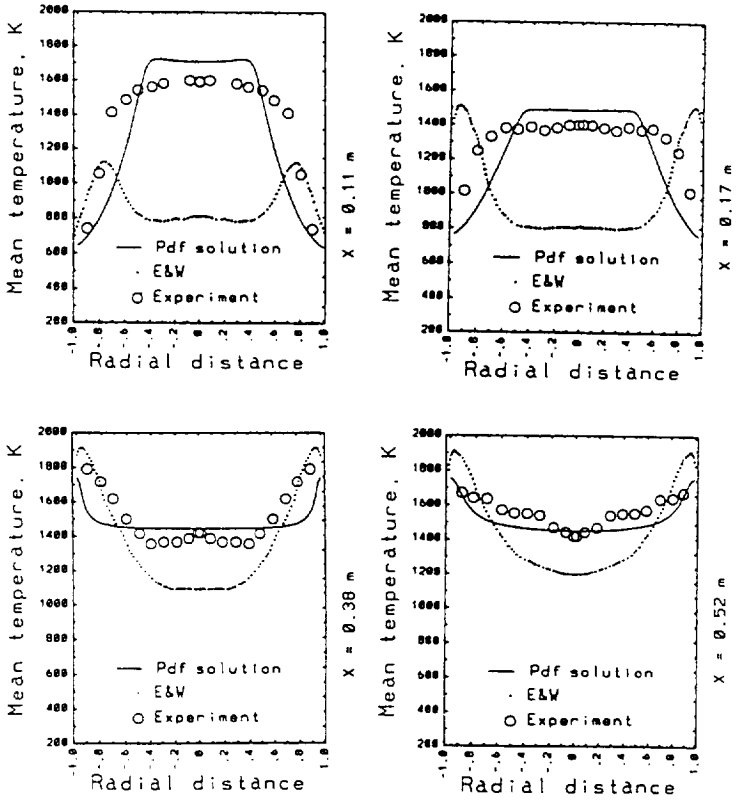
Velocity vector plot.



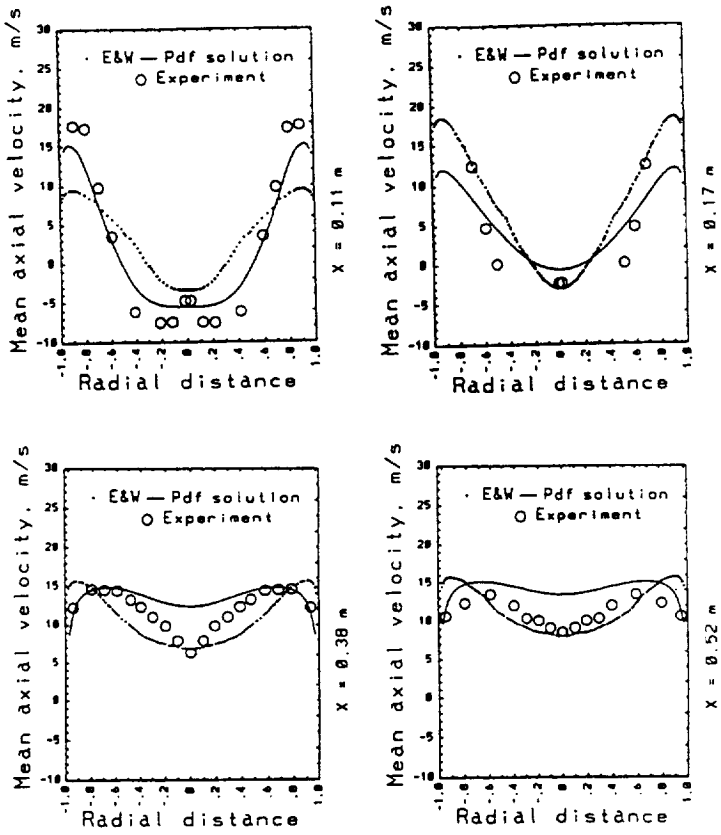
Temperature contours and droplet locations.



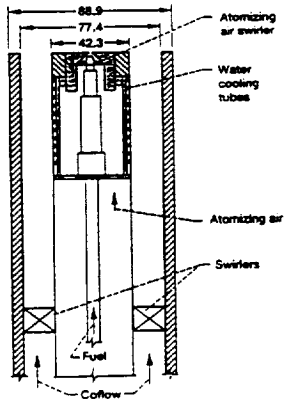
Spray evaporation rate.



Near wake radial profiles of temperature.

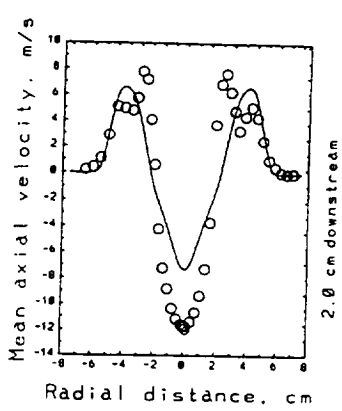


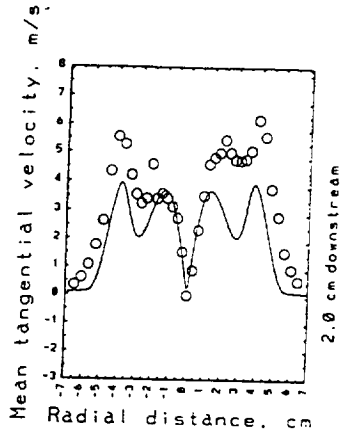
Near wake radial profiles of velocity.

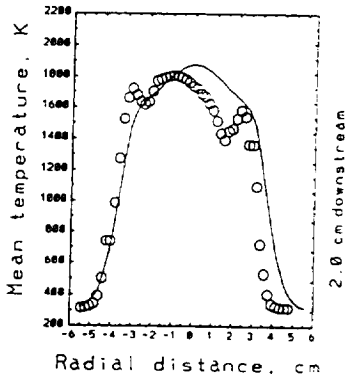


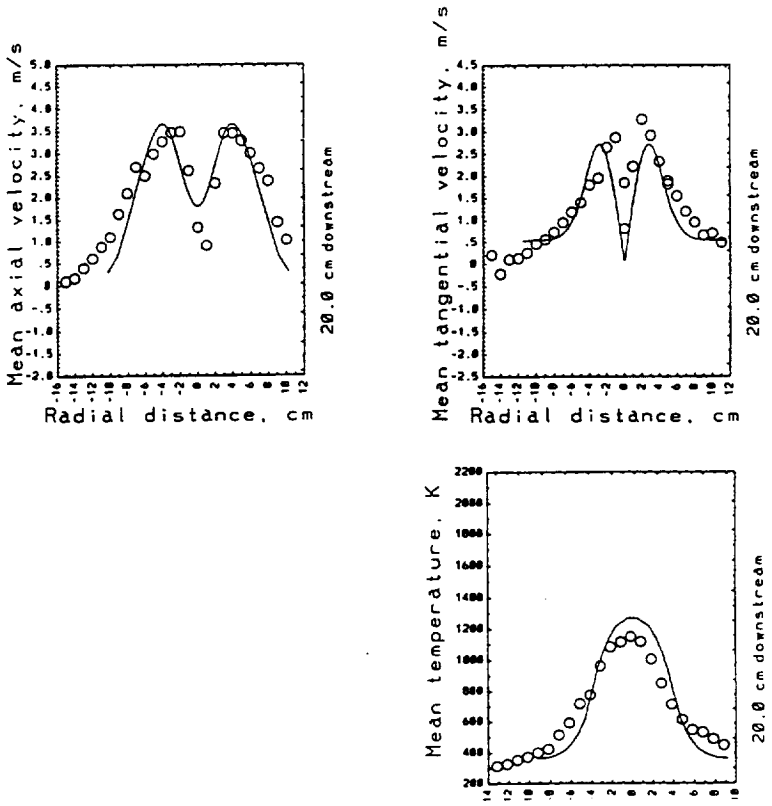
Schematic of an open spray burner.
(Dan Bulzan of IFMD at LeRC)

Photograph of swirl-stabilized, spray flame.









CONCLUDING REMARKS

- The comparisons show that the general features of the flowfield are correctly predicted by the present solution procedure.
- The present solution appears to provide a better representation of the temperature field, particularly, in the reverse-velocity zone.
- The overpredictions in the centerline velocity could be attributed to the following reasons:
  - The use of k-ε turbulence model is known to be less precise in highly swirling flows.
  - The swirl number used here is reported to be estimated rather than measured.