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RECENT PROGRESS IN THE JOINT VELOCITY-SCALAR PDF METHOD

M.S. Anand
Allison Engine Company
Indianapolis, Indiana

N95- 27890

- o TURBULENCE
- o REACTION (treatment, kinetic schemes, emissions)
- o TURBULENCE/CHEMISTRY INTERACTIONS
- o ATOMIZATION
- o SPRAY EVAPORATION

SIMULATION ISSUES:

- o NUMERICS (accuracy, convergence)
- o GEOMETRY (body-fitted grids, unstructured grids)
- o COMPUTATIONAL RESOURCES (Time, Storage)

JOINT VELOCITY-SCALAR PDF METHOD

SIGNIFICANT MILESTONES AND RECENT PROGRESS

o 2-D and 3-D time dependent flows (with finite-volume method)
  (Anand et al. 1987, Haworth & El Tahry 1989)

o Stochastic dissipation model development and validation
  (Pope & Chen 1990, Pope 1991, Anand et al. 1993)

o 2-D Elliptic flows (mean pressure algorithm), swirling flows
  (Anand et. 1989, 1993)

o Spray treatment
  (Anand 1990)

o Manifold methods for reaction kinetics
  (Maas & Pope 1992, 1994; Norris & Pope 1994; Norris & Hsu 1994)

o Solve Poisson equation for mean pressure: $$\frac{\partial^2 \langle p \rangle}{\partial x_j \partial x_j} = - \frac{\partial^2}{\partial x_i \partial x_j} \langle \rho U_i U_j \rangle$$

o Satisfy continuity by solving for velocity correction potential, velocity correction:

$$\frac{\partial^2 \phi}{\partial x_i \partial x_i} = - \frac{\partial}{\partial x_i} \langle \rho U_i \rangle \quad ; \quad \Delta U_i = \frac{1}{\langle \rho \rangle} \frac{\partial \phi}{\partial x_i}$$

o Solution algorithm is consistent with B-spline representation of mean fields

o Same descretized form: $\underline{\underline{A}} \cdot \underline{s} = \underline{b}$

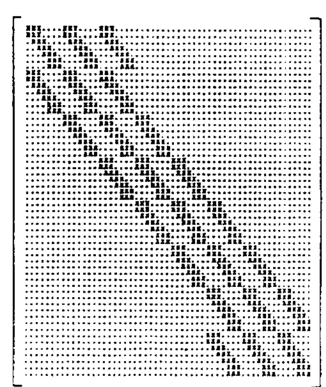
o $\underline{A}$ is a banded matrix, constant and same for both <p> and ϕ

o LU decomposition only once

o Special band solver economizes storage and computational effort

o Judicious implementation of the algorithm results in significant economy in computer resource requirement

$\underline{A}$ =



M = 7, N = 8, $\underline{A}$ (56 x 56)

TURBULENT COMBUSTION MODELING ISSUES

(FOR GAS TURBINE COMBUSTORS)

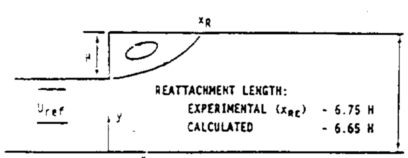
o Most promising method for turbulent reacting flows

ATTRIBUTES OF DIFFERENT PDF METHODS

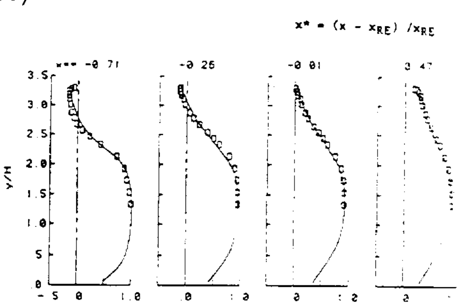
Method	**Attributes**	**Limitations/shortcomings**
Joint PDF of $\underline{\phi}$	Reaction treated exactly	Assumes gradient-diffusion, Does not give velocityfield (requires e.g, k-ε) Turbulence/chemistry interactions not fully simulated
Joint PDF of $\underline{U}$ and $\underline{\phi}$	Reaction exact, Convection (mean and turbulent) exact, Variable-density effects exact	Needs ε equation (or equivalent)
Joint PDF of $\underline{U}$, $\underline{\phi}$, and ω	... In addition Provides complete closure, Treats turbulent streams of different scales, Can account for effects of large scale structures	

PDF CALCULATIONS FOR A RECIRCULATING FLOW

(Anand et al. 1989)

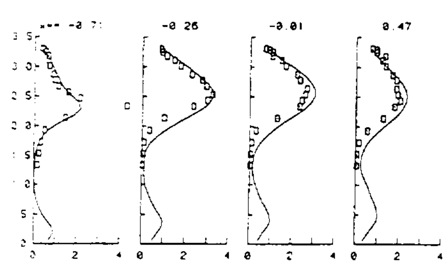


Backward-facing step
Pronchick and Kline (1983)

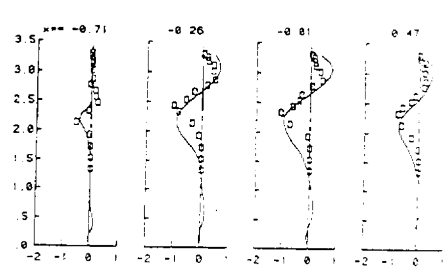


Storage: 1.3 Mwords
CPU Time: 6 min. Cray YMP

$\langle U\rangle/U_{ref}$



$10^2 \langle u'^2\rangle/U^2_{ref}$



$10^3 \langle u'^2v'\rangle/U^3_{ref}$

STOCHASTIC DISSIPATION MODEL

o Provides complete closure of the PDF equation (joint velocity-frequency-scalar)

o More realistic than a mean dissipation model. Dissipation (rather, turbulent frequency) is also a random variable and included in the joint PDF.

o Treats multiple scales in the flow

o Accounts for internal intermittency

o Accounts for effects of large scale structures, and influence of origin and history of the fluid particles

$$\boxed{d\omega^* = -\omega^* \langle\omega\rangle (S_\omega + C_\chi \Omega)\, dt + \langle\omega\rangle^2 h\, dt + \omega^* (2C_\chi \langle\omega\rangle \sigma^2)^{1/2}\, dW}$$

$$\boxed{dU_i^* = -\frac{1}{\rho}\frac{\partial \langle P \rangle}{\partial x_i} dt + D_i dt + (C_0 \tilde{k}\, \omega^*)^{1/2}\, dW_i}$$

SWIRLING FLOWS

o No theoretical limitations

o Additional production terms due to non-zero mean swirl velocity

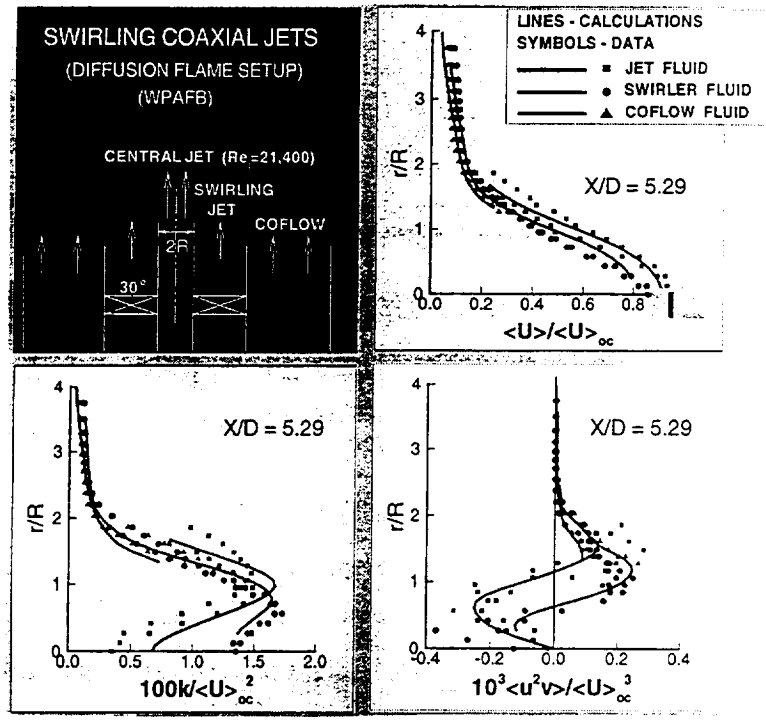
o Additional terms in calculating the mean pressure (or mean pressure gradients)

- Boundary layer flows:
  > radial pressure gradient
  > axial pressure gradient also included

- Elliptic flows
  > additional terms in the Poisson equation for pressure

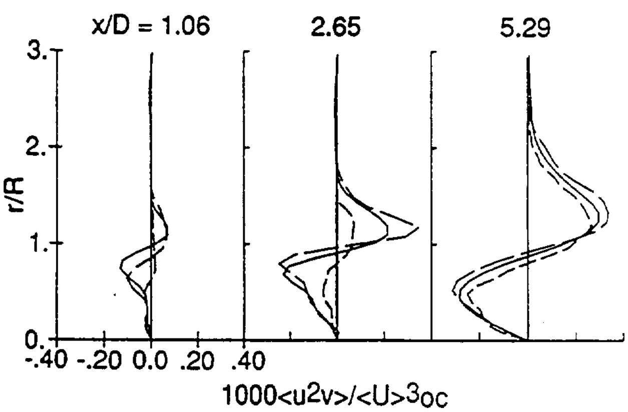
o Validation of the stochastic dissipation model and first calculation of swirling flows with the joint PDF method (Anand et al. 1993)

JOINT PDF CALCULATIONS FOR SWIRLING FLOWS



JOINT PDF CALCULATIONS FOR SWIRLING FLOWS

COMPARISON WITH REYNOLDS-STRESS MODEL RESULTS AND ASSESSMENT OF GRADIENT DIFFUSION MODELING



RS MODEL:

$$< u^2 v > = -C_s \frac{k}{<\varepsilon>} < v^2 > \frac{\partial < u^2 >}{\partial r}$$

$C_s = 0.22$

——— PDF CALCULATIONS
– – – RS MODEL WITH RSM RESULTS
— — RS MODEL WITH PDF RESULTS

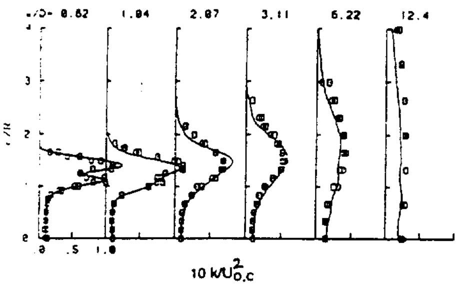
SPRAY CALCULATIONS

(Anand 1990)

o Advanced spray models (stochastic Lagrangian, Monte Carlo) naturally compatible with the joint PDF method

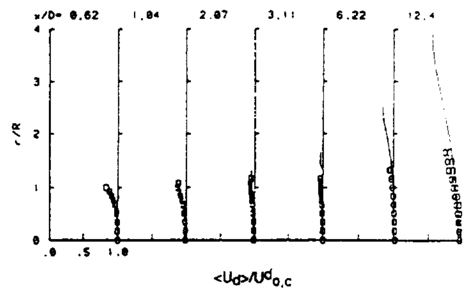
o Assumptions about turbulent kinetic energy partition avoided

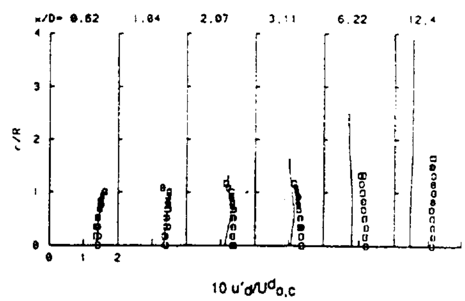
o Effects of gas phase turbulence structure (velocity cross-correlation) included



Computed profiles of normalized turbulent kinetic energy of air compared against data.

105 micron glass beads, NASA HOST C data

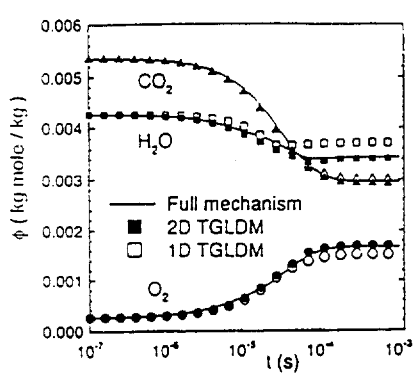




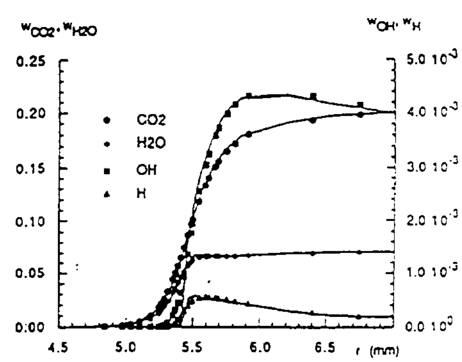
REDUCED KINETICS / MANIFOLD METHODS

o Low dimensional manifold methods (ILDM, TGLDM)

- Given detailed kinetcs, they provide low-dimensional description (e.g., 1-D, 2-D, 3-D) in multidimensional composition/scalar space
- Use dynmical systems theory to determine the low. dim. manifold
- Avoid ad hoc assumptions, e.g, partial equilibrium of some of the reactions Implications for ignition and lean blow-off
- Not fuel specific like conventional reduced kinetic schemes



Perfectly Stirred Reactor (Pope & Maas 1993)



Laminar Premixed Flame (Maas & Pope 1994)

PARALLEL PROCESSING

o Objective: Turnaround time of 1day or less for 3-D combustor calculations

o Particle partitioning, domain decomposition (multigrid, multi-block)

o Preliminary results for 2-D flow with particle partitioning (Pope 1994)

- 16 nodes, 128 MB each, IBM SP1
- 12.8 million particles (800,000 per processor)
- 50 time steps
- 44 minutes/processor (45 minutes clock time)

Extrapolation to 3-D combustor calculations
- 6.5 hours clock time with 32 processor SP1

JOINT PDF FOCUS AREAS

o 3-D Flows, Improved solution algorithms

o Parallel processing

o Reduced kinetics / Low Dimensional Manifolds

o Evaporating / reacting sprays

o Emphasis on emissions and performance predictions