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PDF METHODS FOR TURBULENT REACTIVE FLOWS

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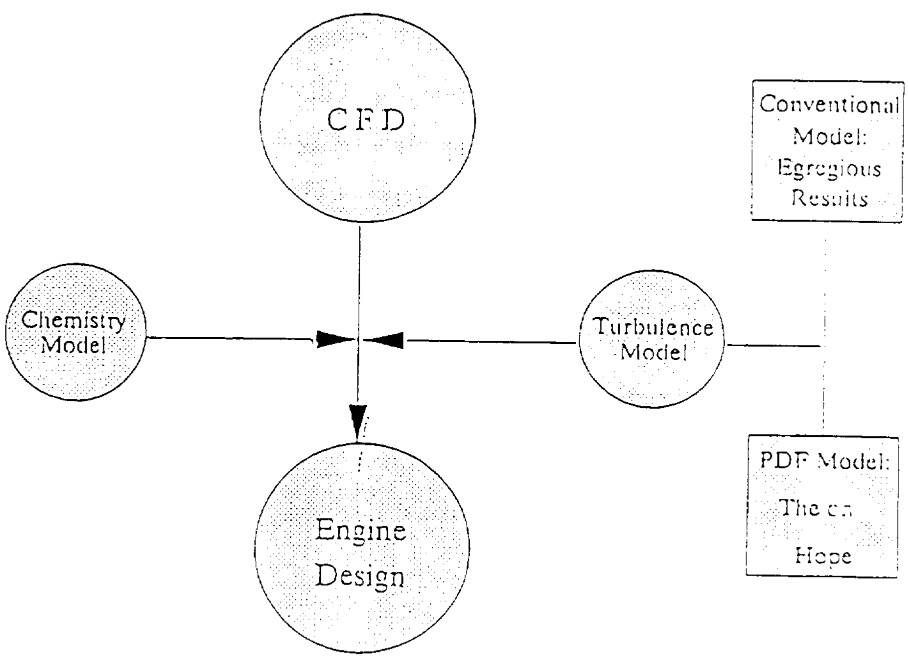
OUTLINE

- Motivation
- PDF modeling of reactive flows
- The Lewis PDF module
- Validations and applications
- Current research
- Technology transfer

COMPUTATION OF TURBULENT COMBUSTION



GOVERNING EQUATIONS

$$\rho_{,t} + (\rho u_i)_{,i} = 0$$
$$(\rho u_i)_{,t} + (\rho u_j u_i)_{,j} = -p_{,i} + \tau_{ij,j}$$
$$(\rho E)_{,t} + (\rho u_j E)_{,j} = -q_{i,i} + \Phi$$
$$(\rho Y_k)_{,t} + (\rho u_j Y_k)_{,j} = (\rho D Y_{k,j})_{,j} + \omega_k$$

$$A_{,t} \equiv \frac{\partial A}{\partial t}$$

$$A_{,j} \equiv \frac{\partial A}{\partial x_j}$$

CLOSURE PROBLEM:

$$u_i = \overline{u_i} + u'_i,$$
$$Y_i = \overline{Y_i} + Y'_i,$$

$\overline{u''_i u''_j}$ — Turbulence Modeling

$\overline{Y''_i u''_j}$ — Analogy of shear stress: diffusion model.

$\overline{\rho w_i}$ — ???

$$\rho w_i = \rho w_i(Y_1, ..., Y_n, T)$$

But in general:

$$\overline{\rho w_i} \neq \bar{\rho} w_i(\overline{Y_1}, ..., \overline{Y_n}, \overline{T})$$

PDF Modeling of Turbulent Reactive Flows
Current status

- Assumed PDF (Spalding, 1971; Gosman & Lockwook, 1973; ...)
  - ◇ Advantage: simple, fast.
  - ◇ Disadvantages: Need unique mixture fraction; assumed shape may not be real.
- Composition PDF (Pope, 1976; Dopazo & O'Brian, 1974)
  - ◇ Advantage: Reaction rate treated exactly; existing moment closure codes easily adapted.
  - ◇ Disadvantages: Turbulent diffusion needs model.
- Velocity-Composition joint PDF (Pope & Chen 1980, Pope 1981)
  - ◇ Advantage: Reaction rate treated exactly; no diffusion model needed.
  - ◇ Disadvantages: Models for velocity field relatively untried; Require more computer resource.

PDF Modeling of Turbulent Reactive Flows

- Objective:
  - ◇ Develop models that can accurately simulate finite rate chemical reactions in turbulent flows.
  - ◇ Develop and validate independent PDF modules.
  - ◇ Technology transfer.
- Criteria
  - ◇ Accuracy and robustness.
  - ◇ Practical in terms of today's computing power.
  - ◇ Easy integration with existing industry computational platform.

PDF Modeling of Turbulent Reactive Flows

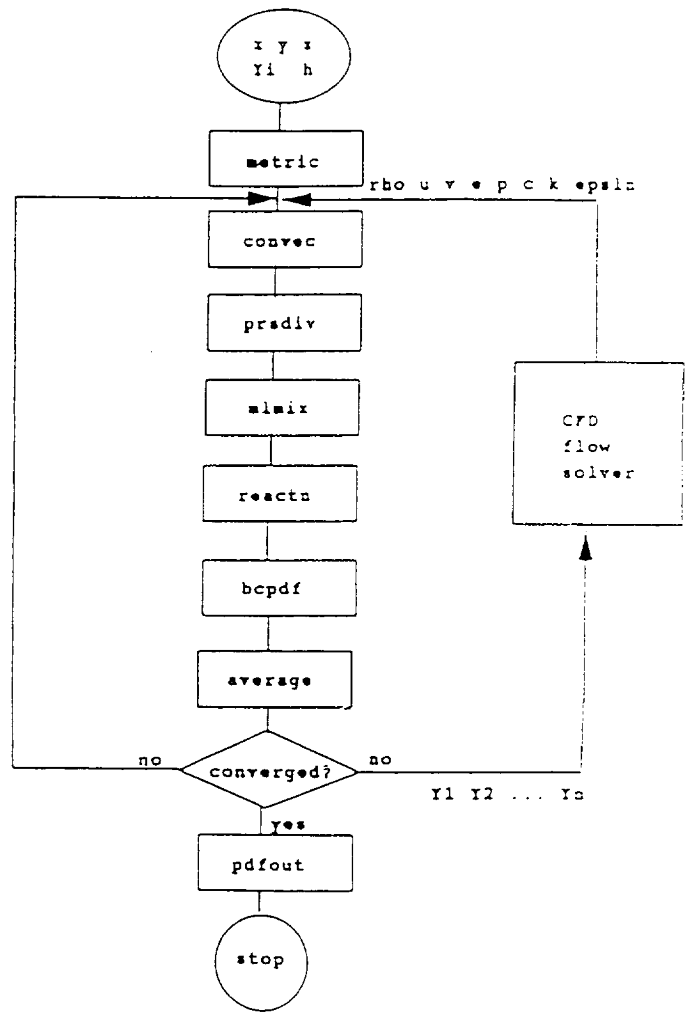
- Approach:
  - ◇ Joint pdf method for scalar compositions.
  - ◇ Moment closure schemes for velocity field.
  - ◇ Develop hybrid solver consisting of Monte Carlo method and finite-difference/finite-volume method.

PDF Modeling of Turbulent Reactive Flows

- Current status (Lewis)

$$
\begin{aligned}
&(\rho P)_{,t} + (\rho < u_j | Y_i, h > P)_{,j} + (\rho w_j P)_{,Y_j} \\
&= (D_t P_{,j})_{,j} + M(P) - (S_p P)_{,h}.
\end{aligned}
$$

  - ◇ Continuous mixing model developed.
  - ◇ Model for compressibility effect proposed.
  - ◇ 2D and 3D Monte Carlo PDF module developed.
  - ◇ Validation studies.
  - ◇ Code released to industry during a workshop.



Validation Cases

- Scalar field in homogeneous turbulence.
- Oblique shock.
- 2D supersonic hydrogen combustor.
- Axisymmetric supersonic combustor.
- Piloted flame near extinction.

Scalar field in homogenous turbulence pdf compared with Gaussian distribution

Current model

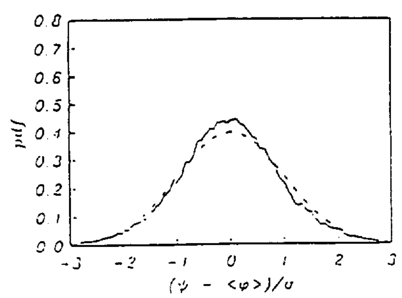


Figure 2. Asymptotic pdf distribution for a scalar in homogeneous turbulence. — present model; - - - Gaussian.

Modified curl's model

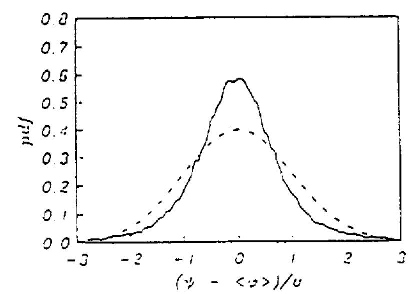
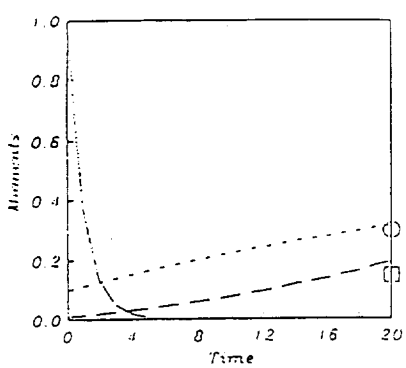


Figure 1. Asymptotic pdf distribution for a scalar in homogeneous turbulence. — modified Curl model; - - - Gaussian.

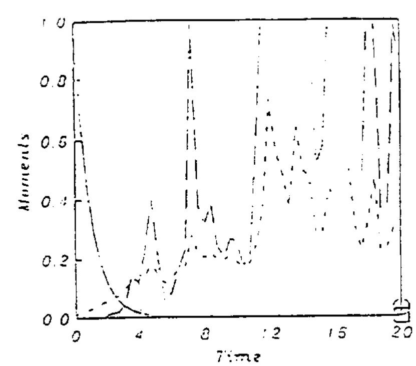
Scalar field in homogenous turbulence 3rd and 4th moments compared with Gaussian

Current model



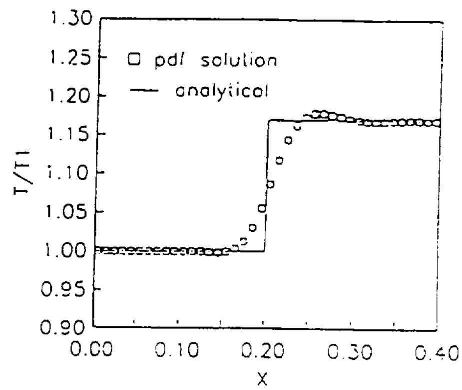
Evolution of moments from the present model. — standard deviation, - - - 0.1 × fourth central moment, – – 0.01 × sixth central moment, o 0.1 × fourth moment for Gaussian distribution, □ 0.01 × sixth moment for Gaussian distribution.

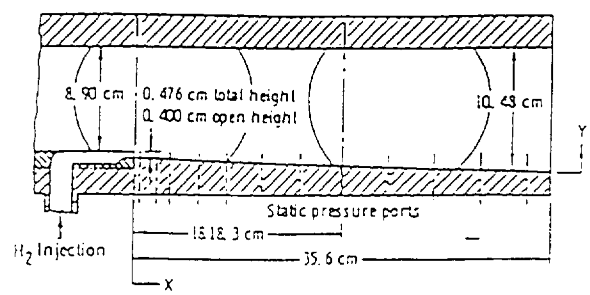
Modified curl's model



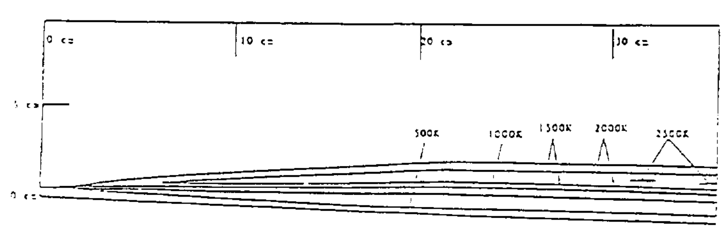
Evolution of moments from the modified Curl model. — standard deviation, - - - 0.01 × fourth central moment, – – 0.0001 × sixth central moment, o 0.01 × fourth moment for Gaussian distribution, □ 0.0001 × sixth moment for Gaussian distribution.

Temperature across an oblique shock: pdf solution compared with analytical prediction.



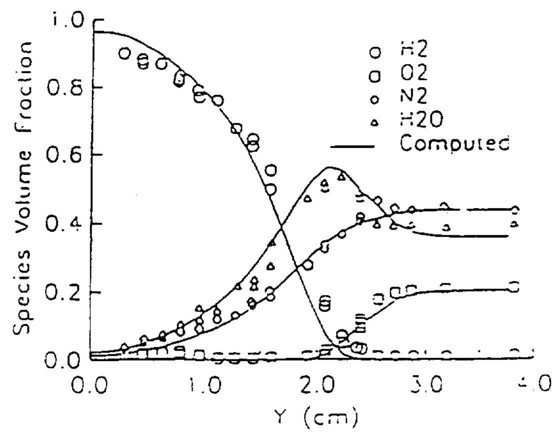


Supersonic hydrogen combustor
(Exp. Burrows & Kurkov, 1973)



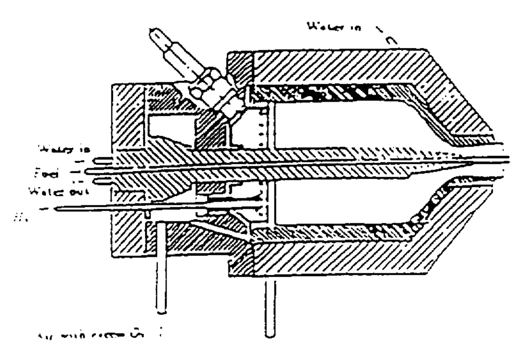
Temperature Contour (pdf solution)

Supersonic hydrogen combustor
Mole fraction:
pdf solution compared with exp. data

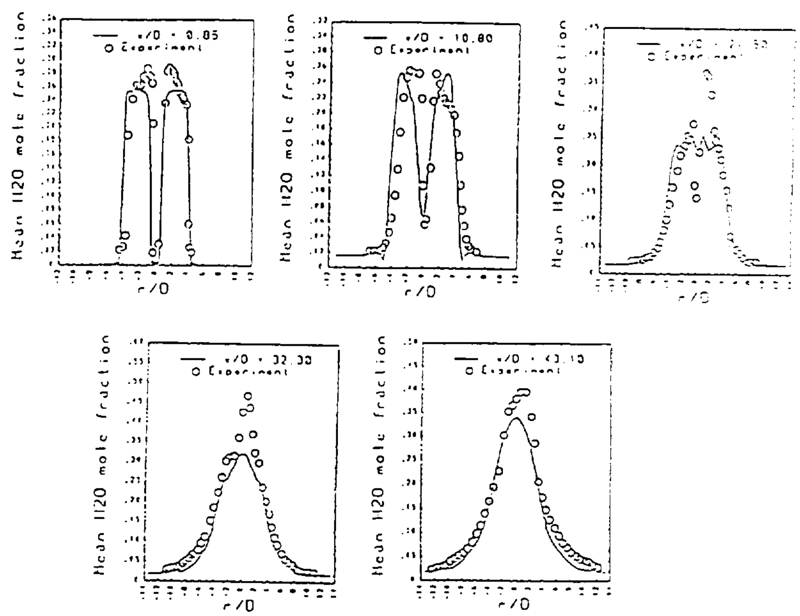


Coaxial burner: geometry and test condition
(Exp. Cheng, et al. 1991)

Exit Conditions	Hydrogen Jet	Outer Jet	Ambient Air
Mach Number	1	2	0
Temperature, K	545	1250	300
Velocity, m/s	1780	1417	0
Pressure, MPa	.112	.107	.101
Mass Fraction			
Y_{H_2}	1.	0.	0.
Y_{O_2}	0.	.245	.233
Y_{N_2}	0.	.35	.757
Y_{H_2O}	0.	.175	.01

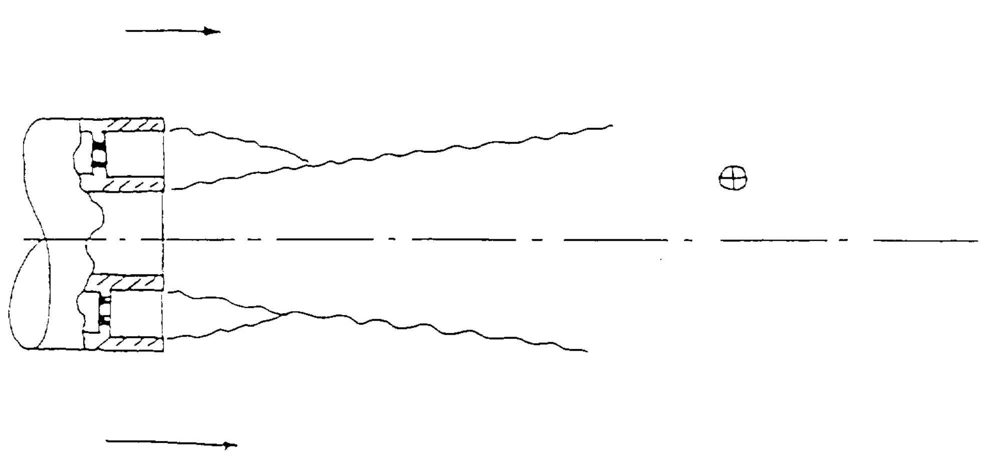


Mean H2O mole fraction
Coaxial burner
pdf solution compared with exp. data



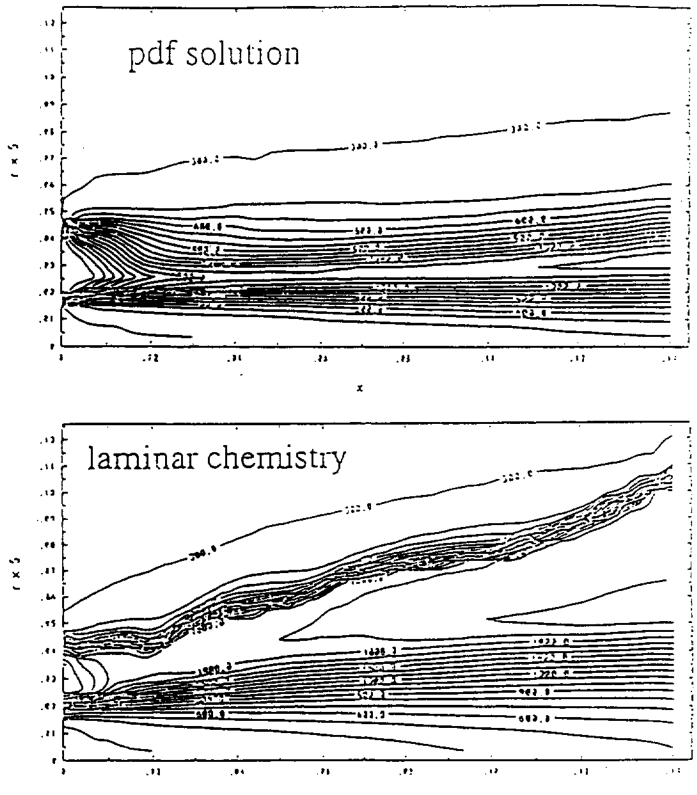
Piloted flame (Masri et al., 1994)

Fuel: 45% CO, 15% H2, and 40% N2
Flame close to extinction



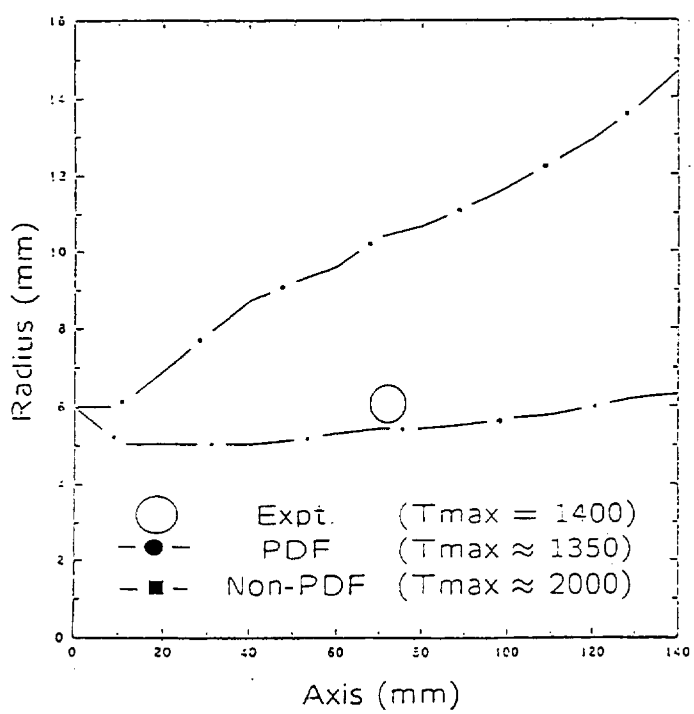
Piloted Flame

Mean Temperature



Piloted Flame

Flame Location



Current Projects

◇ Application of PDF module to emission predictions

◇ Incorporate general chemistry procedure.

◇ Incorporate spray models.

◇ Use parallel computing for the PDF module.

Collaboration with industry and technology transfer

- Features of independent pdf module:
  - ◇ Easily coupled with any existing industry flow codes.
  - ◇ Novel averaging scheme to reduce memory requiement.
  - ◇ General chemistry package.
  - ◇ Parallelized workstation version.
- Technology transfer: workshops
  - ◇ July, 1993; code released to 15 US institutions.
  - ◇ October, 1994.