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# MODELING OF TURBULENT CHEMICAL REACTION



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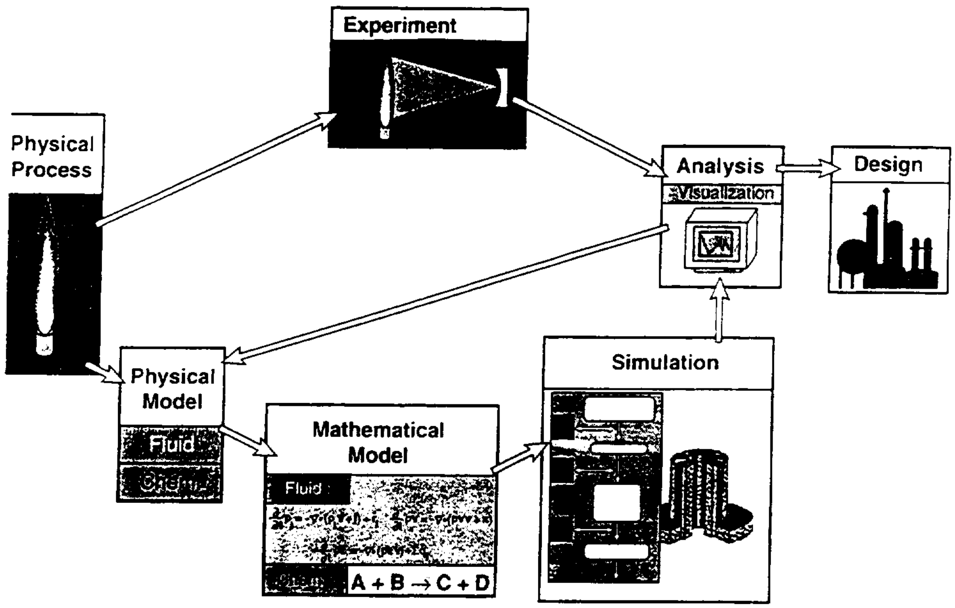
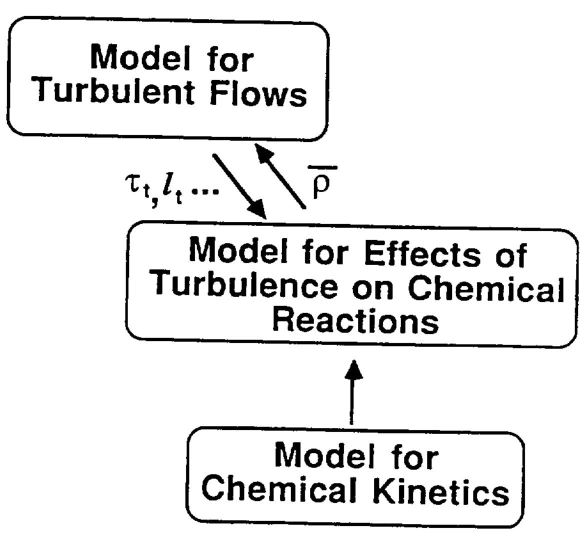
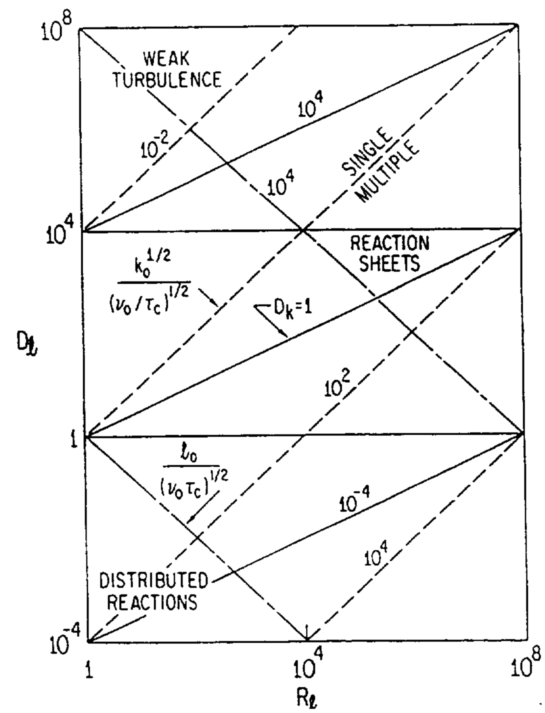



## *Modeling Turbulent Reacting Flows*

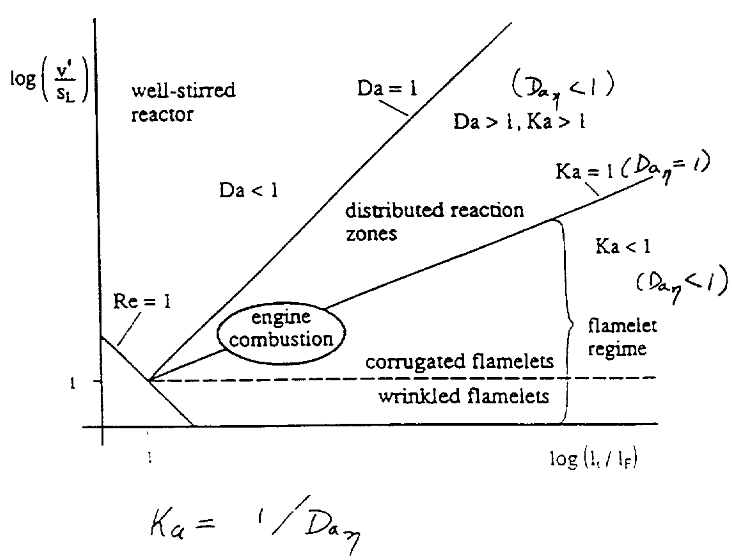


## Regimes of Turbulent Combustion




Turbulent Reactive Flows edited by P.A. Libby and F.A. Williams (1994)

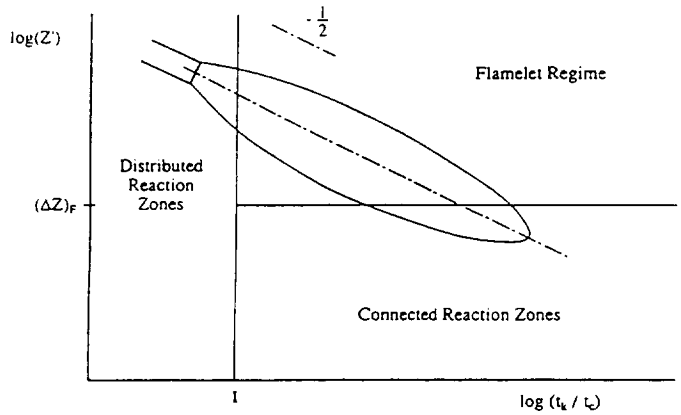
## Regimes of Premixed Turbulent Combustion




$Ka = 1/Da_\eta$

Turbulent Reactive Flows edited by P.A. Libby and F.A. Williams (1994)

## Regimes of Non-Premixed Turbulent Combustion




Turbulent Reactive Flows edited by P.A. Libby and F.A. Williams (1994)

## Chemical Closure Models

**(1) Laminar Chemistry**

$$<\rho w_i> = \rho w_i(\overline{Y}_i, \overline{T})$$

**(2) Fast Chemistry**

$$<\rho w_i> \approx -\frac{1}{2}\overline{\rho}\tilde{\chi}_f \frac{\partial^2 Y^e(f)}{\partial^2 f}$$

**(3) Flamelet model**

$$<\rho w_i> = \iint \rho w_i(\eta, \chi_f) P_{f,\chi_f}(\eta, \varepsilon_f) d\eta d\varepsilon_f$$

**(4) Assumed PDF:**

$$<\rho w_i> = \int .. \int \rho w_i(\phi_i) \cdot P_\phi d\phi_1 d\phi_2 .. d\phi_n$$

**Assumed the shape of $P_\phi$.**

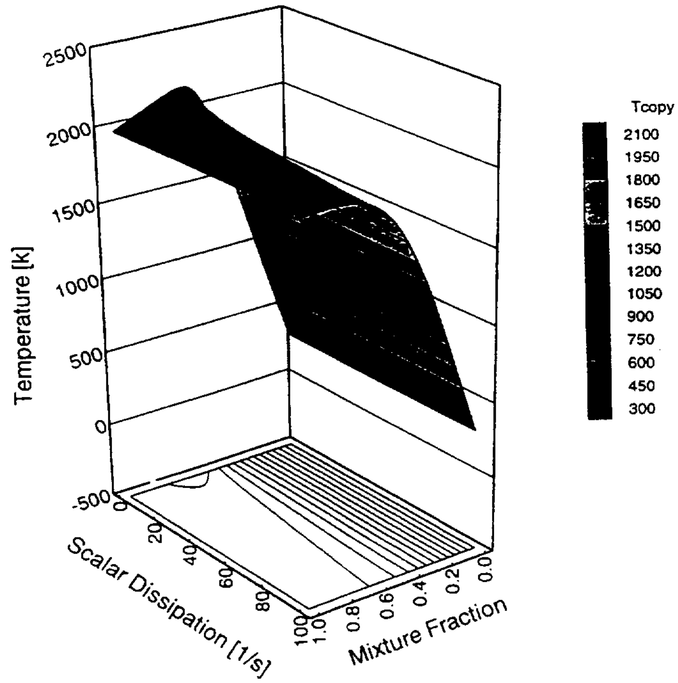
**(5) Scalar PDF method:**

**Solve for $P_\phi$ directly.**

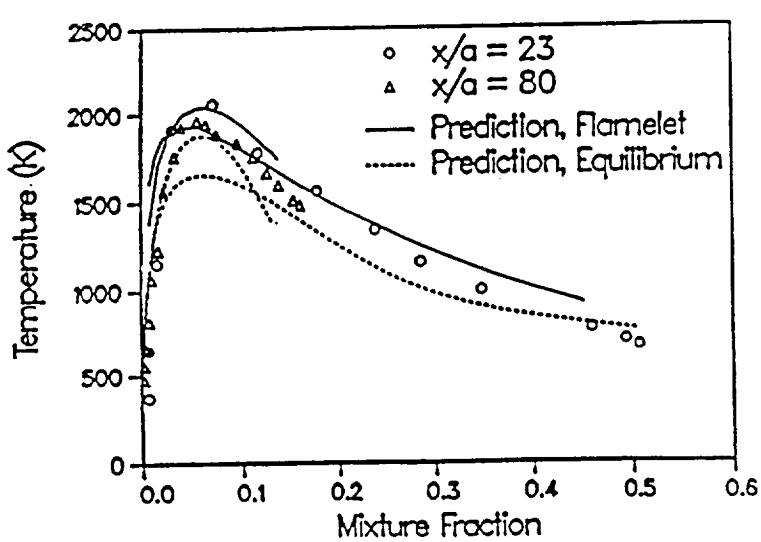
**(6) Conditional Moment Closure (CMC)**

$$<\rho w_i> = \int <\rho w_i | \eta> \cdot P_f(\eta) d\eta$$

Flamelet library with one side being burned premixed flame$\phi$=1.4




Flamelet Model: 69%H2+31%CH4
Turbulent Jet Flame, Rey.=10,000




Vranos, et al. "Nitric Oxide Formation and Differential Diffusion in a Turbulent Methane-Hydrogen Diffusion Flame," 24th Symposium(International) on Combustion/The Combustion Institute, 1992/pp 377-384

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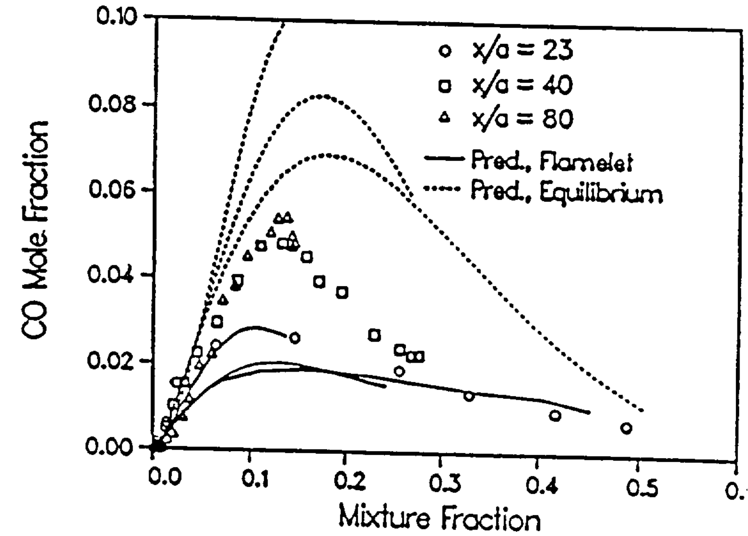


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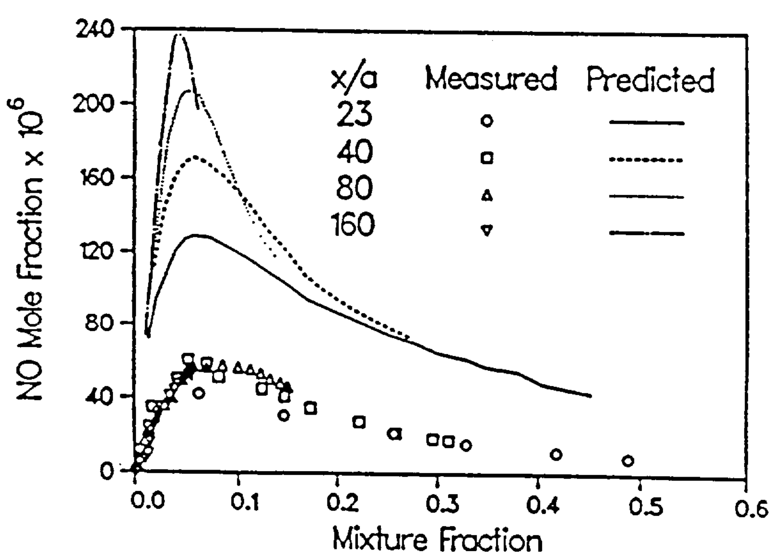
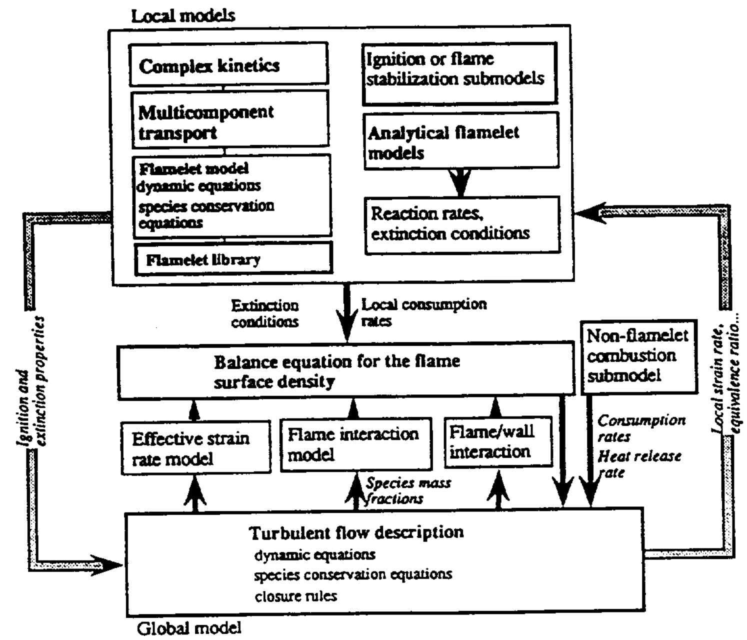



Vranos, et al. "Nitric Oxide Formation and Differential Diffusion in a Turbulent Methane-Hydrogen Diffusion Flame." 24th Symposium(International) on Combustion/The Combustion Institute, 1992/pp. 377-384

## Advanced Flamelet Approach




## Conditional Moment Closure (CMC)

Definition:

$$< Y_i | \eta > \equiv < Y (\bar{x},t) | f(\bar{x},t) = \eta >$$

Equation:

$$< \rho | \eta > \frac{\partial < Y_i | \eta >}{\partial t} + < \rho \tilde{u} | \eta > \cdot \nabla < Y_i | \eta > + \frac{\nabla \cdot \{ < \rho u' y' | \eta > P_f(\eta) \}}{P_f(\eta)}$$

$$= < \rho w_i | \eta > + < \rho D_i \nabla f \cdot \nabla f | \eta > \frac{\partial^2 < Y_i | \eta >}{\partial \eta^2}$$

Modeling:

$$< w_i | \eta > \approx w_i (< T | \eta >, < Y_i | \eta >, ..)$$

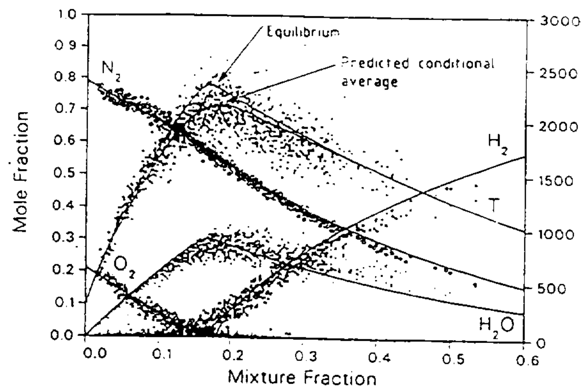
$$< \rho D_i \nabla f \cdot \nabla f | \eta > \approx < \rho D_i \nabla f \cdot \nabla f > \approx \frac{1}{2} \bar{\rho} \chi_f$$

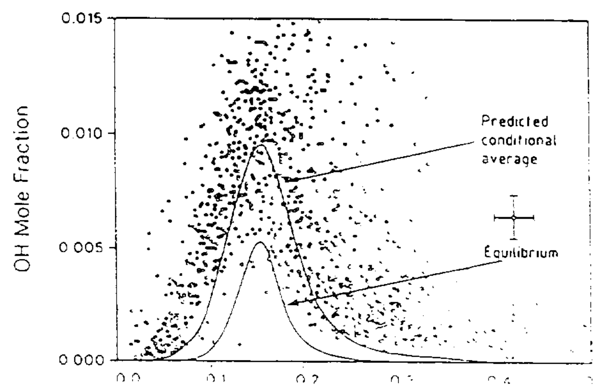
$$< \rho \tilde{u} | \eta > \approx \overline{\rho \tilde{u}}$$

$$< \rho u' y' | \eta > \approx 0$$

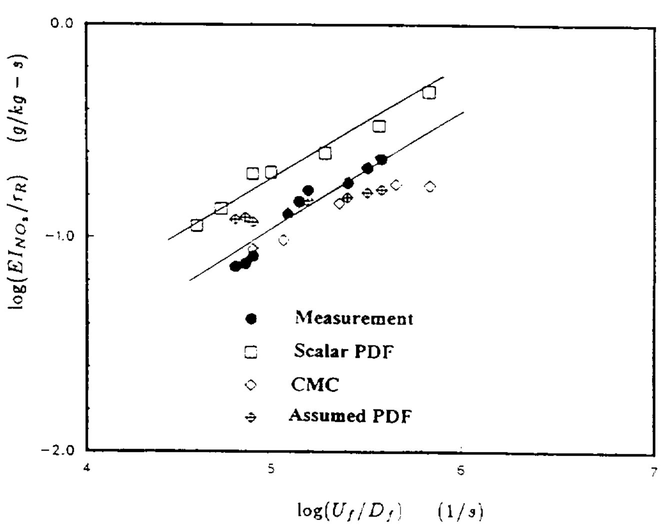
$$< \rho | \eta > \approx \rho (< Y_i | \eta >, < T | \eta >)$$

## Conditional Moment Closure (CMC)




## NOx Emissions from Turbulent H2 Jet Flames



## Conditional Moment Closure (CMC)

Applications:

- Incorporated into existing moment closure CFD codes for complex geometry flows
- Realistic Chemistry - Detailed or reduced

Research issues:

- Modeling of conditional statistics
- Preferential diffusion
- Parallel computing algorithms

## Probability Density Function (PDF)

Applications:

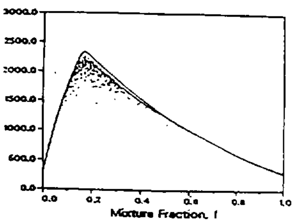
- $NO_X$ from methane jet flames with reduced chemistry
- Sooting flames
- 2-D flows

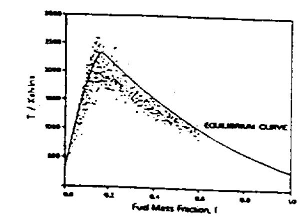
Research Topics:

- Mixing model
- Extension to droplet spray & particle laden flows
- Preferential diffusion
- Efficient stochastic algorithm
- Construction of chemical tables
- Parallel computing - 3D Flows or 2D flows with complex chemistry

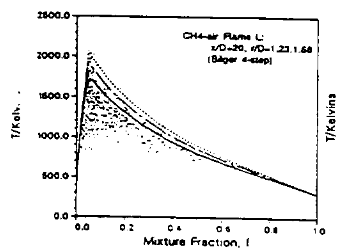
## Departures From Chemical Equilibrium

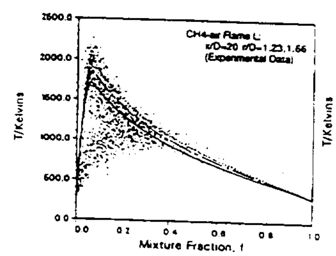
(PDF) Hydrogen (EXP.)



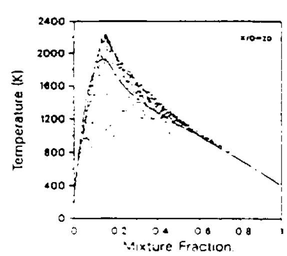



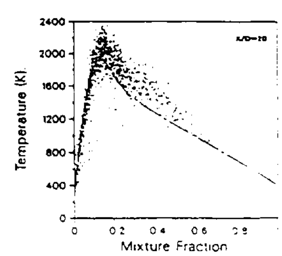
Methane




Methanol



## Mixing Models for PDF Methods

- Modified Curl's Model (stochastic)

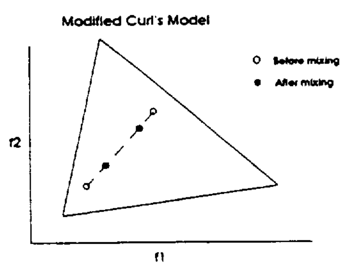
$$-\sum_{\alpha=1,\beta=1}^{k}\frac{\partial^2}{\partial\psi_\alpha\partial\psi_\beta}\left\{\left\langle\varepsilon_{\alpha\beta}|\bar{\phi}=\bar{\psi}\right\rangle\tilde{P}_{\bar{\phi}}(\bar{\psi},t)\right\}=$$

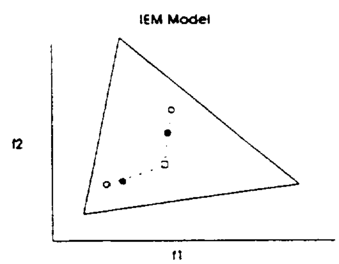
$$\frac{1}{\tau_{mix}}\left\{\iint_{\psi'\psi''}\left[\tilde{P}_{\bar{\phi}}(\psi',t)\tilde{P}_{\bar{\phi}}(\psi'',t)H(\psi',\psi''|\bar{\psi})-\tilde{P}_{\bar{\phi}}(\bar{\psi},t)\right]d\psi'd\psi''\right\}$$

- IEM (Interaction-by-Exchange-with-the-Mean) Model (deterministic)

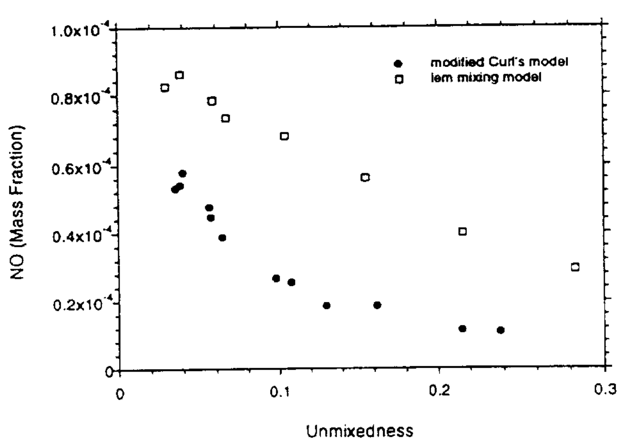
$$-\sum_{\alpha=1,\beta=1}^{k}\frac{\partial^2}{\partial\psi_\alpha\partial\psi_\beta}\left\{\left\langle\varepsilon_{\alpha\beta}|\bar{\phi}=\bar{\psi}\right\rangle\tilde{P}_{\bar{\phi}}(\bar{\psi},t)\right\}=\frac{C_\phi}{2\tau_{mix}}\frac{\partial}{\partial\psi_\alpha}\left[(\bar{\psi}-\tilde{\phi})\tilde{P}_{\bar{\phi}}(\bar{\psi},t)\right]$$

Mixing Frequency: $\omega_{mix} = 1/\tau_{mix}$



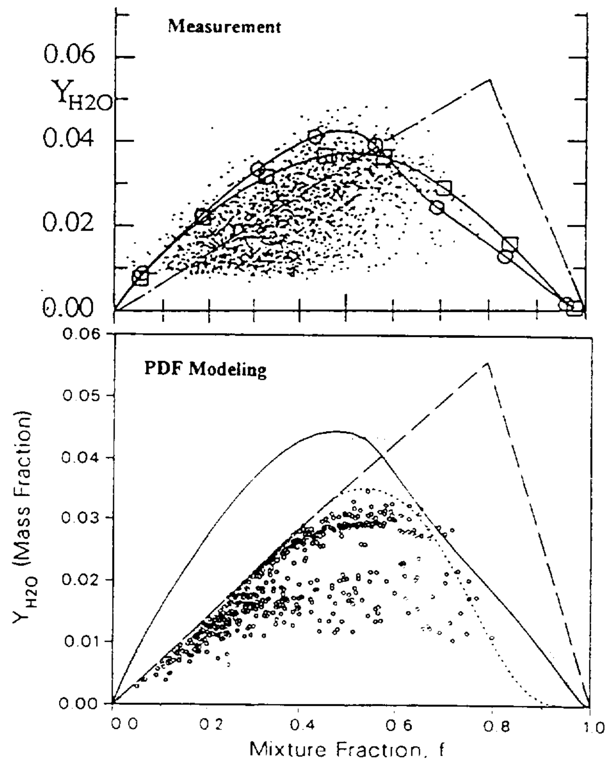

## PaSR: H2/NOx Detailed Chemistry $\phi$=1 $\tau$=1ms



## Comparison of Predicted and Measured H2O Mass Fractions

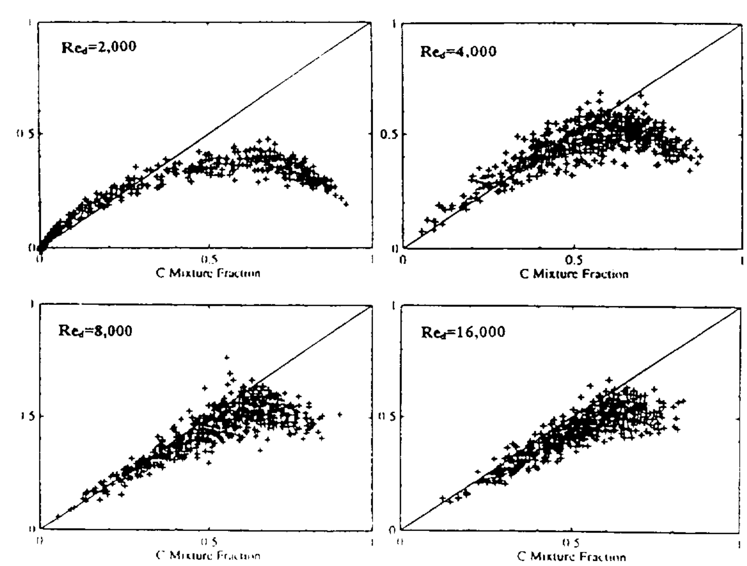
## Turbulent Nonpremixed Jet Flames

Fuel: (CO/H2/N2: 0.30/0.10/0.6 )



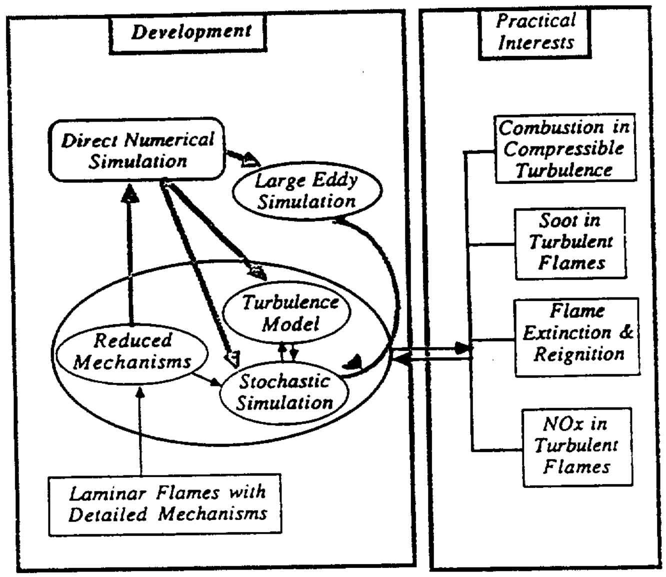

## Experimental Evidence of Preferential Diffusion in Turbulent Jet Flames

### (Fuel: 36%$H_2$+64% $CO_2$)




"Differential Molecular Diffusion in Reacting and Nonreacting Turbulent Jets of H2/CO2 mixing with Air," L.L.Smith Ph.D. Thesis, University of California at Berkeley (1994)

## Computation of Turbulent Reacting Flows



INTRODUCTION TO TURBULENCE SUBPROGRAM

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Institute for Computational Mechanics in Propulsion
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Cleveland, Ohio

## OBJECTIVES

- A means for CMOTT to interact with industry

- A vehicle for technology transfer to industry

## CONCEPT OF TURBULENCE MODULE

- Exact CFD equations:

$$\frac{D\rho U_i}{Dt} = \frac{\partial}{\partial x_j}[\mu(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3}\frac{\partial U_k}{\partial x_k}\delta_{ij}) - \rho\overline{u_i u_j}] - \frac{\partial P}{\partial x_i}$$

- Reynolds stresses will be recasted as:

$$-\rho\overline{u_i u_j} \equiv \mu_T(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3}\frac{\partial U_k}{\partial x_k}\delta_{ij}) + \underbrace{[-\rho\overline{u_i u_j} - \mu_T(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3}\frac{\partial U_k}{\partial x_k}\delta_{ij})]}_{T_{ij}}$$

$$\mu_T \equiv C_\mu \frac{k^2}{\varepsilon}$$

- CFD equations become:

$$\frac{D\rho U_i}{Dt} = \frac{\partial}{\partial x_j}[(\mu + \mu_T)(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3}\frac{\partial U_k}{\partial x_k}\delta_{ij})] + \frac{\partial T_{ij}}{\partial x_j} - \frac{\partial P}{\partial x_i}$$

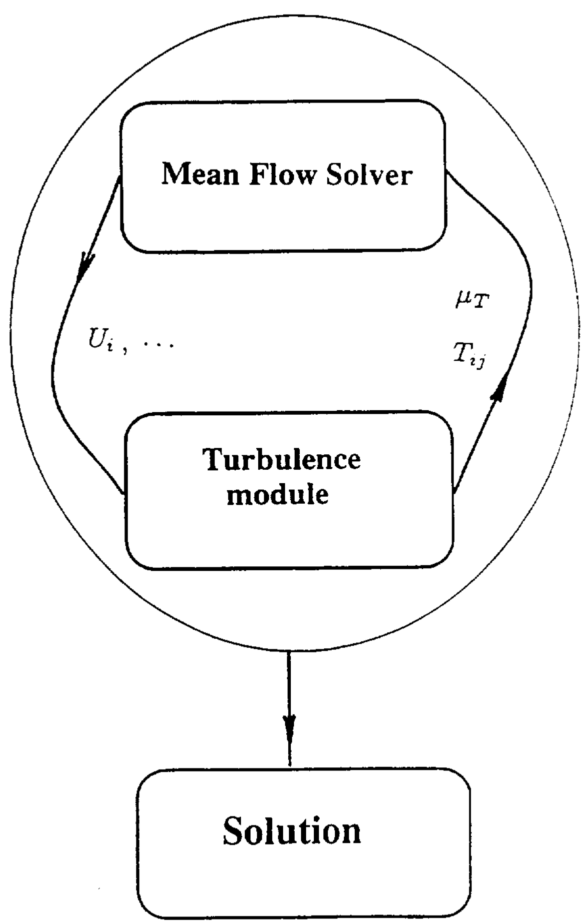
- The task of turbulence module: Provide $\mu_T$ and $T_{ij}$

- Turbulence Module:
  - ◇ Input: $U_i$, $\rho$ and $\mu$ … from the mean flow solver
  - ◇ Output:

$$\mu_T = C_\mu \frac{k^2}{\varepsilon} \quad [\frac{Dk}{Dt} = \ldots, \qquad \frac{D\varepsilon}{Dt} = \ldots]$$

$$T_{ij} = -\rho\overline{u_i u_j} - \mu_T(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3}\frac{\partial U_k}{\partial x_k}\delta_{ij})$$

  - ◇ Models for $\rho\,\overline{u_i u_j}$
    - One- and two-equation eddy viscosity models
    - Reynolds stress algebraic equation models
    - Reynolds stress transport equation models



## Module with CMOTT research code (incompressible)

- CFD equations in CMOTT research code:

$$\frac{D\rho U_i}{Dt} = \frac{\partial}{\partial x_j}[(\mu + \mu_T)(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i})] + \frac{\partial}{\partial x_j}T_{ij} - \frac{\partial P}{\partial x_i}$$

- Turbulence module: provide $\mu_T$ and $T_{ij}$
  - ◇ Built-in models without wall function:
    - - Launder-Sharma and Chien $k-\varepsilon$ models
    - - CMOTT $k-\varepsilon$ model
  - ◇ Built-in models with wall function:
    - - $k-\omega$ model, standard $k-\varepsilon$ model
    - - CMOTT $k-\varepsilon$ model
    - - CMOTT Reynolds stress algebraic equation model

## Module with NPARC code

- CFD equations in NPARC code:

$$\frac{D\rho U_i}{Dt} = \frac{\partial}{\partial x_j}[(\mu + \mu_T)(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3}\frac{\partial U_k}{\partial x_k}\delta_{ij})] - \frac{\partial P}{\partial x_i}$$

- Turbulence module (present time): provide isotropic $\mu_T$
  - ◇ Build-in models without wall function:
    - - Baldwin-Lomax model and Chien $k-\varepsilon$ model
    - - CMOTT $k-\varepsilon$ model
  - ◇ Further development:
    - - Models with wall function
    - - Reynolds stress algebraic equation models
    - - Reynolds stress transport equation models

## Joint Program with Industry
## on Turbulence Module

- For those who want to use the available modules:
  - ◇ Need interface program for particular industry codes
    - Grid informations, Boundary treatment, ...
- For those who want a module for their own codes:
  - ◇ Need modules exclusively for particular industry codes
- Maintain and update the turbulence modules along with model development.

# DESCRIPTION OF TURBULENCE SUB-PROGRAM

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## General Transport Equations

$$\frac{\partial}{\partial t}(rJ^{-1}\rho\phi) + \frac{\partial}{\partial \xi_i}(C_i\phi - D_{i\phi}) = rJ^{-1}S_\phi$$

- Non-dimensional form ($\mu$, $\mu_t$ $\Leftrightarrow$ $\mu/Re$, $\mu_t/Re$)
- Conservative form
- Cartesian velocity components
  1. Easy to transform (chain rule)
  2. No curvature terms

## Discretization

- Finite-volume method
- Source term

  $S_\phi = S_1 + S_2\phi, \quad S_1 \geq 0$ and $S_2 \leq 0$
- Transient term
  1. 1st-order fully implicit scheme
  2. 2nd-order three-level fully implicit scheme
- Diffusion term

  Standard central differencing scheme

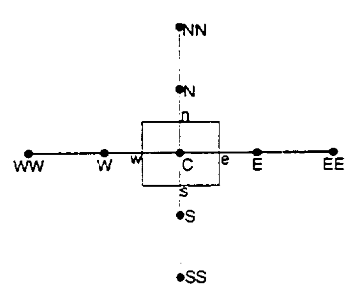
- Convection term: HLPA scheme

  (Hybrid Linear/Parabolic Approximation)

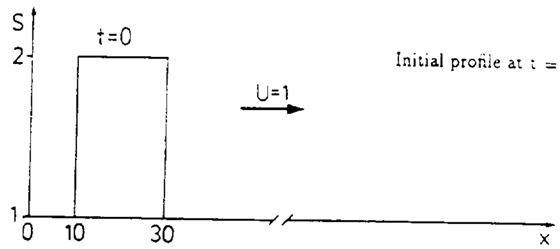
$$\phi_w = \phi_W + \gamma(\phi_C - \phi_W)\widehat{\phi}_W, \quad \widehat{\phi}_W = \frac{\phi_W - \phi_{WW}}{\phi_C - \phi_{WW}}$$

$$\gamma = \begin{cases} 1 & \text{if } |\widehat{\phi}_W - 0.5| < 0.5 \\ 0 & \text{otherwise} \end{cases}$$

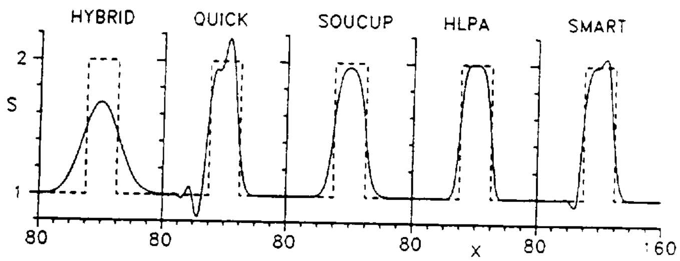
- Second-order accurate
- Bounded (non-oscillatory)
- Diagonally dominant matrix



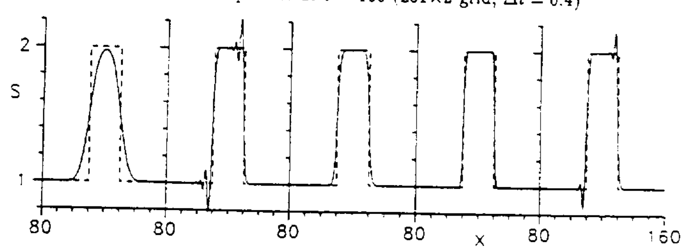
## Example 1




Initial profile at t = 0

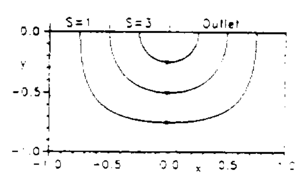


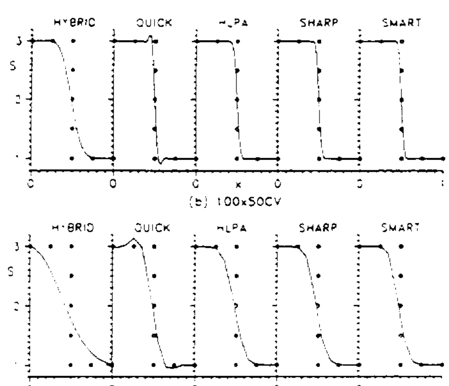

Predicted profiles at t = 100 (201×2 grid, $\Delta t = 0.4$)



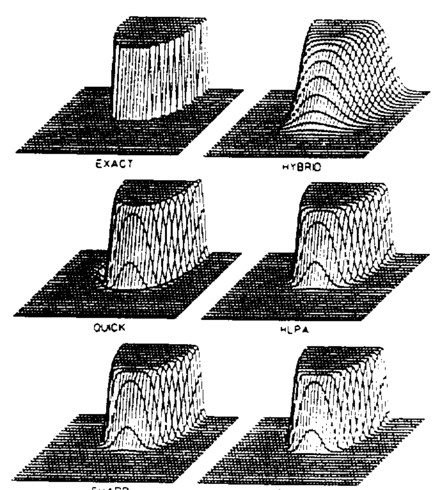

Predicted profiles at t = 100 (1001×2 grid, $\Delta t = 0.1$)

## Example 2




*S*-profiles at outlet (○, exact solution).




orthographic projection of *S*-field.

## Solution Procedure

- Non-delta form

  Positiveness ($\phi \geq 0$ but $\Delta\phi$ may $< 0$)

  Simple linearization

- Algebraic equations

  $A_C\phi_C = A_W\phi_W + A_E\phi_E + A_S\phi_S + A_N\phi_N + S$

  $A's, \; S \geq 0$

- Decoupled solution

- Alternating direction TDMA solver

## Boundary Conditions

- Inflow: $\phi$ specified

- Outflow: Fully-developed condition

- Symmetry: $\partial\phi/\partial n = 0$

- Wall:

  1. Low-Reynolds number turbulence models
  2. Standard wall-function approach

## Sub-Programs

- NPARC2D version

  Plane or axisymmetric, without swirling

  Compressible

  Non-vectorized

- FAST2D version

  Plane or axisymmetric, with or without swirling

  Incompressible

  Vectorized

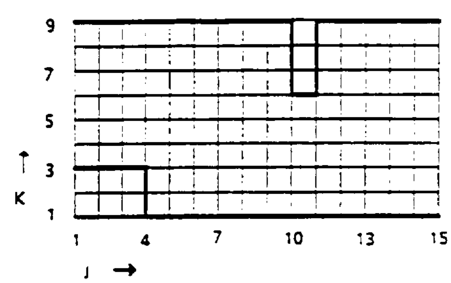
## NPARC2D Version

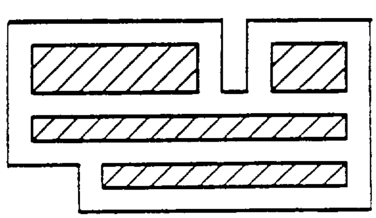
- Grid arrangement

  Control volume centers

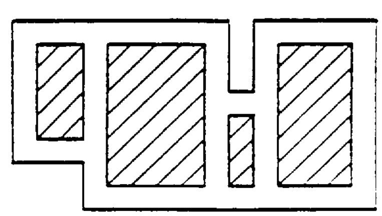
  Boundary nodes

  Embedded bodies



J-Patches



K-Patches

- Input from the main code
  1. Geometric quantities: $x,\ y,\ \xi_x,\ \xi_y,\ \eta_x,\ \eta_y,\ J$
  2. Flow variables: $\mu,\ J^{-1}\rho,\ J^{-1}\rho U,\ J^{-1}\rho V,\ J^{-1}E$
  3. Patch control: $5 \times 2$ parameters
  4. Boundary conditions: $7 \times 2$ parameters

- Output
  1. To the main code: $\mu_t$
  2. For post-processing: $K,\ \epsilon,\ y^+,\ y_n,\ f_\mu$

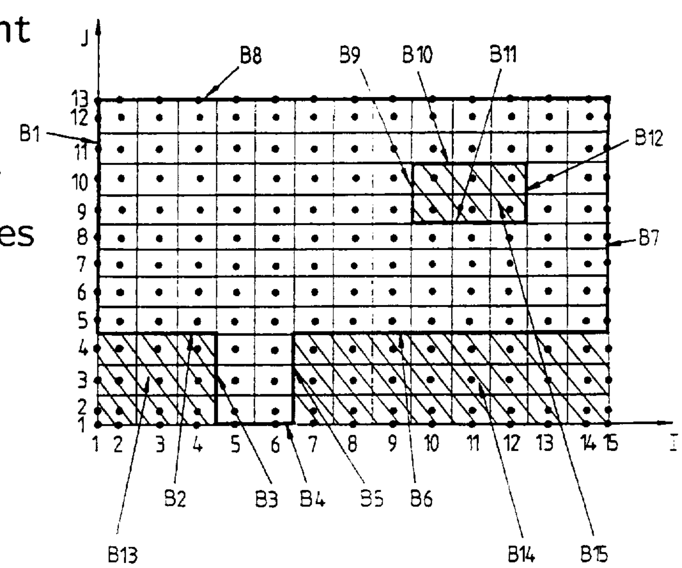
## FAST2D Version

- Grid arrangement

  CV centers

  Boundary nodes

  Embedded bodies



- Vectorization

  Single-index:

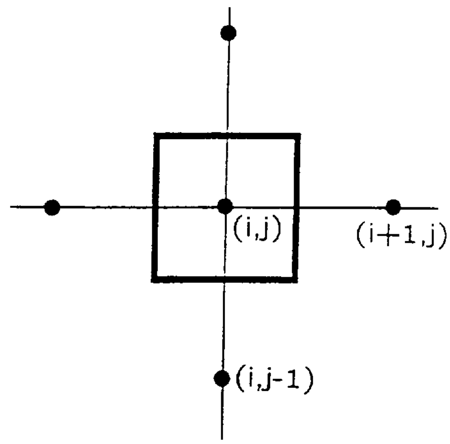
  ii=i+(j-1)ni

  $\phi$(i,j)=$\phi$(ii)

  $\phi$(i+1,j)=$\phi$(ii+1)

  $\phi$(i,j-1)=$\phi$(ii-ni)

  Control parameter:




$$\text{KBLK} = \begin{cases} 1 & \text{for computational nodes} \\ 0 & \text{otherwise} \end{cases}$$

$$\phi=\text{KBLK}\cdot\phi_c+(1-\text{KBLK})\phi_b$$

- Input from the main code
  1. Geometric quantities: $x,\ y,\ x_\xi,\ x_\eta,\ y_\xi,\ y_\eta,\ J$
  2. Flow variables: $\mu,\ \rho,\ U,\ V,\ W,\ C_w,\ C_s$
  3. Vectorization parameters
  4. Boundary parameters

- Output
  1. To the main code: $\mu_t,\ T_{ij}$
  2. For post-processing: $K,\ \epsilon,\ y^+,\ y_n,\ f_\mu$

OVERVIEW OF PROBABILITY DENSITY FUNCTION (PDF) MODELING AT LeRC

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**OBJECTIVE**

Accurately model the effect of turbulence on chemical reactions in a fluid flow

**APPROACH**

Use Probability Density Function (PDF) model - Express dependent variables as functions representing statistically realizable events

**POSSIBLE MODELING STRATEGIES**

1. Evolution PDF - solve for function
   a. Joint PDF for velocities and chemical species
   b. Joint PDF for only chemical species & energy

2. Assumed PDF - function prescribed
   Limited range of applicability - reaction time << or >> turbulence time scale

## CURRENT APPROACH

- Develop evolution PDF model for compressible reacting flows & extend to spray combustion
- Solve for joint PDF for species and energy using Monte-Carlo technique
- Couple with conventional CFD codes

## AREAS OF IMPACT

- NOx Prediction - HSCT and AST application
- Spray combustion - swirling turb. reacting flows
- Scramjet flow path analysis
- Ignition kinetics - prediction of blow-off, etc.
- Combustion instability studies

## CODE FEATURES

- Modular - can be coupled with any CFD code
- Applicable for compressible flows with discontinuities
- Monte-Carlo solver for generalized curvilinear coordinate system
- Easily adaptable for parallel computation (currently under progress)

## CURRENT STATUS

- 2-D and axisymmetric version released
  (default H2-air chemistry - 5 species)
  - parallel version to be released
- 3-D version demonstrated for supersonic combustion (jet in cross flow)
  - validation planned for HSCT-type configurations
- General chemistry (CHEMKIN)
  - Hydrocarbon spray combustion case currently under study
- CFD codes used - RPLUS, ALLSPD, & SIMPLE-type

## FUTURE PLANS

- Further application/validation of 3-D model
- Improved closure models - mixing and turbulence (use available DNS data)
- Parallel processing - workstation clusters
- Unsteady applications - long-term
- Extend scope of impact