RECENT ADVANCES IN PDF MODELING OF TURBULENT REACTING FLOWS

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MOTIVATION

Accurate and Efficient Prediction of Emissions

1. Accurate Prediction of Emissions From Combustion Devices Requires Treatment of Finite-Rate Kinetics
2. The Effect of Turbulent Fluctuations in Velocity, Energy, Composition, etc. on Finite-Rate Chemical Kinetics Must be Modeled

TURBULENCE/CHEMISTRY INTERACTIONS
Possible Approaches

- Neglect Fluctuations
  - + Simple
  - – Ignores Effect of Turbulence
- Eddy Break Up
  - + Simple
  - – Assumes Fast Chemistry
  - – Mean Density, Temperature Must Still Be Modeled
- Prescribed PDF
  - + Efficient
  - – Limited to Fast Chemistry or Single Step Reaction
- Composition PDF
  - + Finite-Rate Multi-Step Kinetics
  - – Expensive
  - – Gradient Diffusion
- Velocity-Composition PDF
  - + More Accurate
  - – More Expensive

PARTICLE REPRESENTATION
A Solution Method for a Large Number of Independent Variables

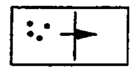
- Computational Requirements Increases Exponentially With Dimensions for Finite Difference Methods
- Computational Requirements Increase Linearly With Dimensions for Monte Carlo Methods

COMPOSITION PDF SOLUTION

Stochastic Lagrangian Particle Simulation

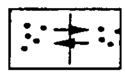
Particle Composition and Position Changed to Model Transport of Joint PDF

- Mean Convection
  - Move Particles Between Cells



- Chemical Reactions
  - Lookup Table Holds Composition Change

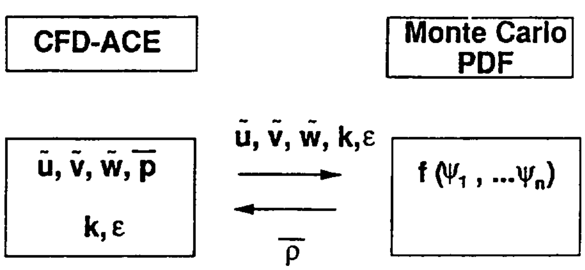
- Turbulent Diffusion
  - Exchange Particles Between Cells



- Molecular Mixing
  - Particle Interaction Changes Composition

COUPLING

PDF Solution is Separate Module



CHEMICAL KINETICS

Reduced Models are Used

Hydrogen: $2H_2 + O_2 \Leftrightarrow 2H_2O$

CO: $CO + H_2O \Leftrightarrow CO_2 + H_2$
$2H_2 + O_2 \Leftrightarrow 2H_2O$

Methane: $CH_4 + 2H + 2H_2O \rightarrow CO + 4H_2$
$CO + H_2O \Leftrightarrow CO_2 + H_2$
$2H_2 + O_2 \rightarrow 2H_2O$
$3H_2 + O_2 \Leftrightarrow 2H_2O + 2H$

Hydrocarbon: $C_nH_{2n+2} + (\frac{n}{2})O_2 \rightarrow n\ CO + (n+1)\ H_2$
$C_nH_{2n+2} + n\ H_2O \rightarrow n\ CO + (2n+1)\ H_2$
$CO + H_2O \Leftrightarrow CO_2 + H_2$
$2H_2 + O_2 \Leftrightarrow 2H_2O$

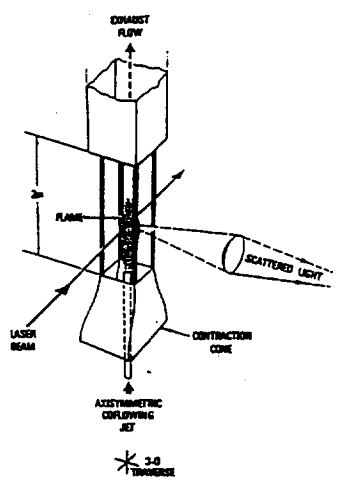
Thermal NO: $N_2 + O \Leftrightarrow NO + N$
$N + O_2 \Leftrightarrow NO + O$
$N + OH \Leftrightarrow NO + H$

RESULTS TO BE PRESENTED

- Jet Diffusion Flame (Hydrogen with Helium Dilution)
- Bluff Body Stabilized Flame (H$_2$/CO)
- Piloted Jet Diffusion Flame (Methane)
- Generic Gas Turbine Combustor (Propane)

HYDROGEN JET DIFFUSION FLAME

Illustration of Experiment at Sandia National Lab



$Re \approx 10^4$

<u>Fuel</u>

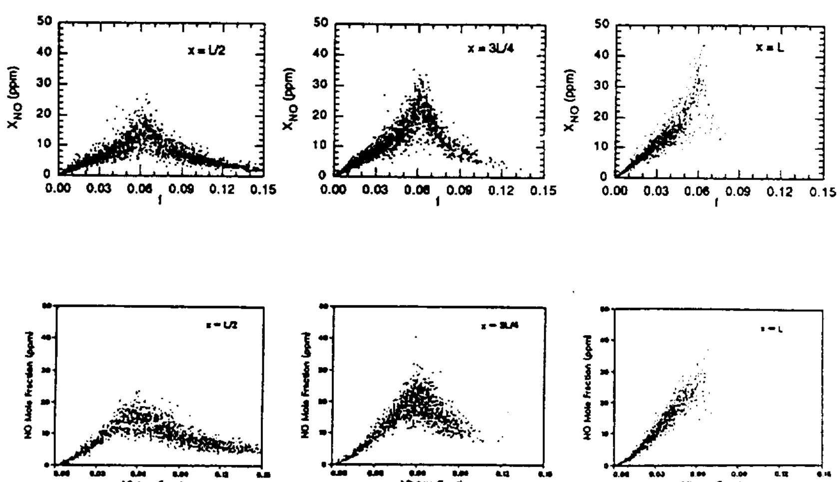
100% H_2

80% H_2, 20% He

60% H_2, 40% He

60% HYDROGEN FLAME

Scatter Plots of Mixture Fraction and NO Mole Fraction

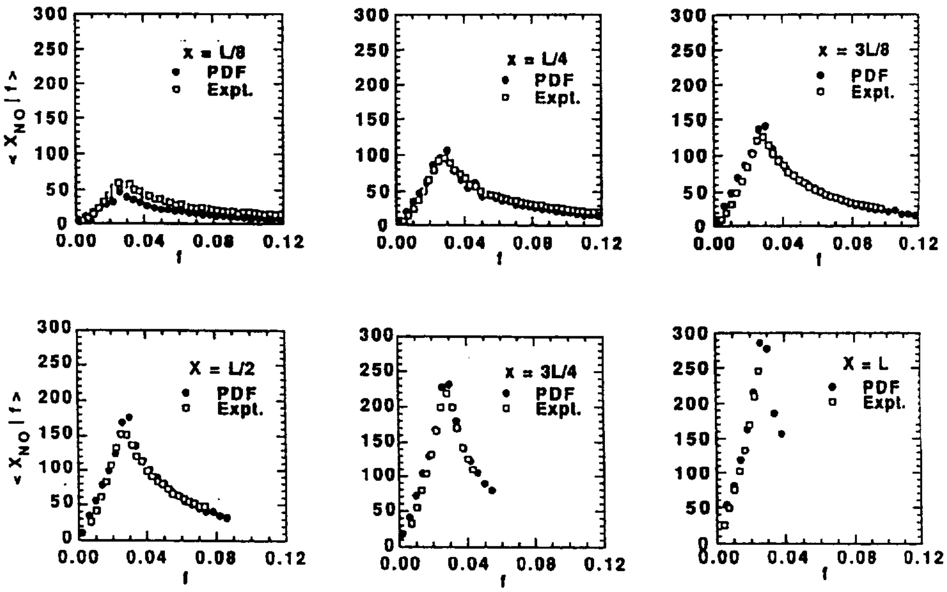


PDF Results

Experime Data

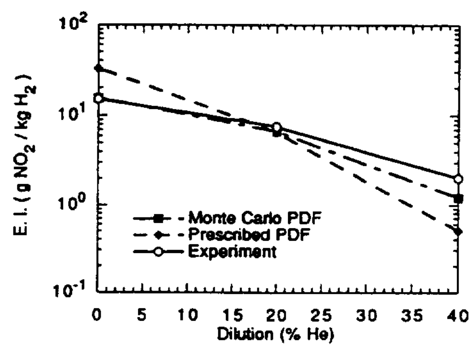
UNDILUTED HYDROGEN FLAME

Conditional Averged NO Mole Fraction



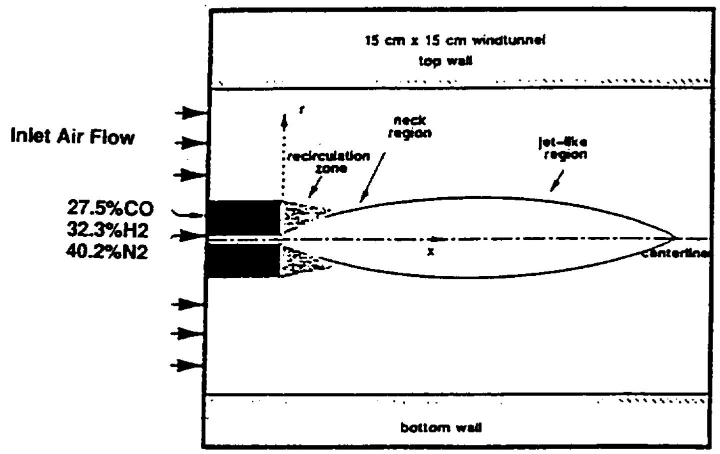
HYDROGEN DIFFUSION FLAME

Dilution Effects on Emmisions Index



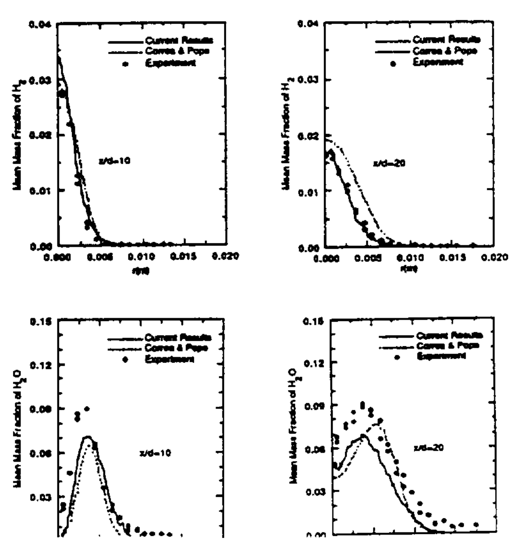
BLUFF BODY STABILIZED DIFFUSION FLAME

Illustration of Experiment of Correa and Gulati



BLUFF BODY STABILIZED DIFFUSION FLAME

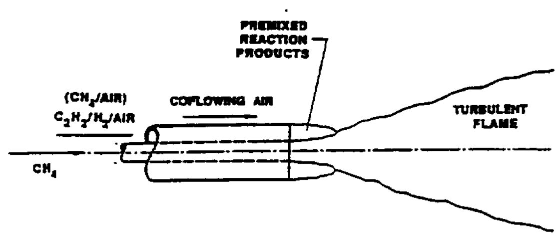
Composition PDF Predicts Mean Values as well as Velocity-Composition PDF



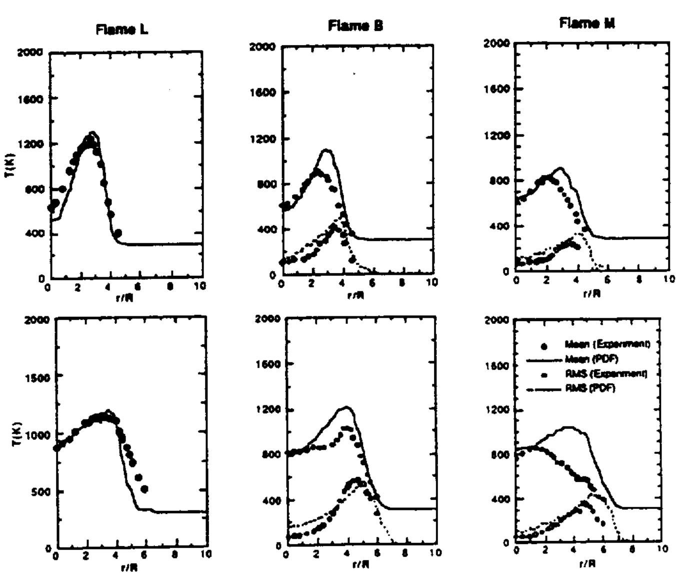
PILOTED JET DIFFUSION FLAME
Illustration of Experiment of Masri et.al.

Experimental Conditions

Flame	Fuel Jet Velocity
L	41 m/s
B	48 m/s
M	55 m/s



PILOTED JET DIFFUSION FLAME
Good Agreement with Experimental Data



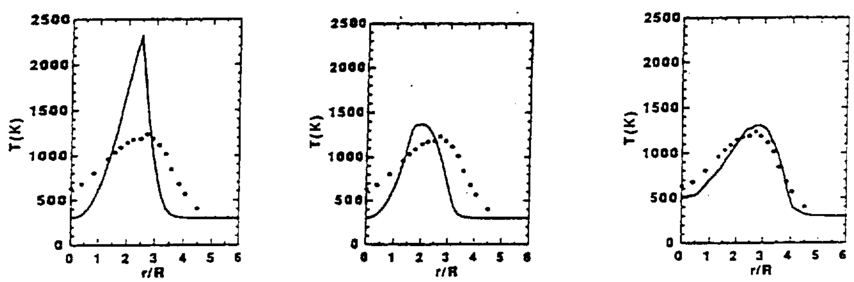
x/D = 20

x/D = 30

PILOTED JET DIFFUSION FLAME

More Accurate Prediction with Monte Carlo PDF

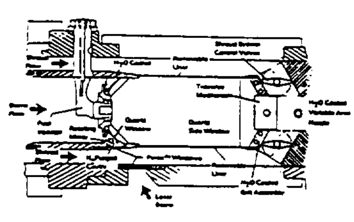
No PDF | Prescribed PDF | Monte Carlo PDF

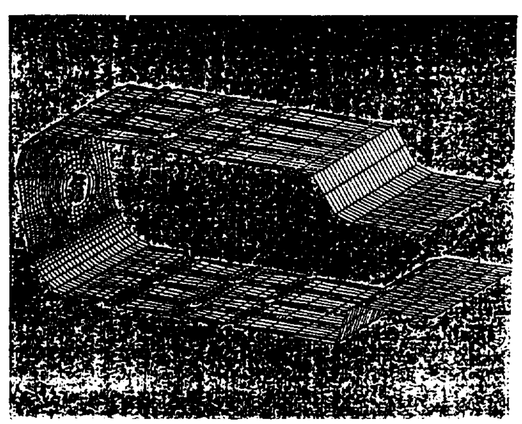


Flame B at x = 20D

GENERIC GAS TURBINE COMBUSTOR

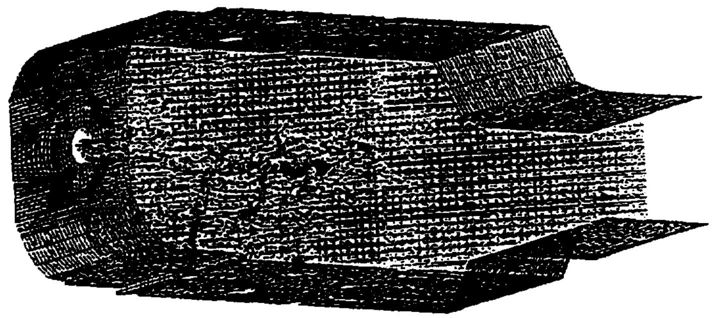
Pratt & Whitney Four-Nozzle Sector Combustor Tested at Wright Laboratory



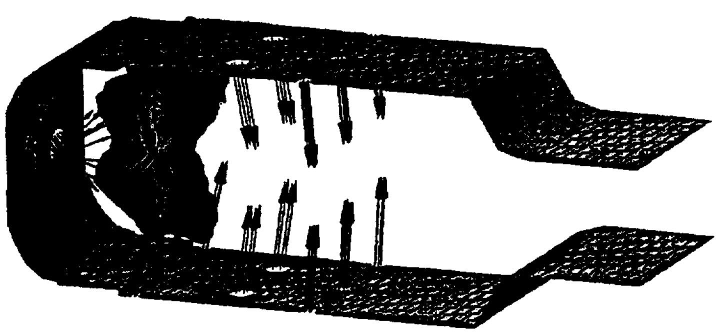


67,840 Cells

MONTE CARLO PDF COMBUSTOR CALCULATION
Stochastic Particle Traces



VERTICAL PLANE THROUGH CENTER OF FUEL INJECTOR
Mean CO Mass Fraction Countours



RUN TIME AND MEMORY

3D Combustor Calculation (68,000 cells)

Conventional CFD

CPU Time	20 hours
Memory	80 MBytes

Monte Carlo PDF

CPU Time	100 hours
Memory	120 MBytes

Parallel PDF (Projected)

CPU Time	25 hours	25 hours	25 hours	25 hours
Memory	30 MBytes	30 MBytes	30 MBytes	30 MBytes

CPU Time for IBM RS/6000 Model 560

CONCLUSIONS

- Monte Carlo PDF Solution Successfully Coupled with Existing Finite Volume Code
  - Minor Changes to Finite-Volume Code
  - Can be Coupled with Other Codes
- PDF Solution Method Applied to Turbulent Reacting Flows
  - Good Agreement with Data for 2D Case
  - Demonstration of 3D Elliptic Flow
- PDF Methods Must be Run on Parallel Machines for Practical Use