NATIONAL ENERGY TECHNOLOGY LABORATORY

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Transported PDF Methods for Simulations of Oxy-Coal Combustion

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Acknowledgements

Xinyu Zhao, Penn State

Dave Huckaby, NETL

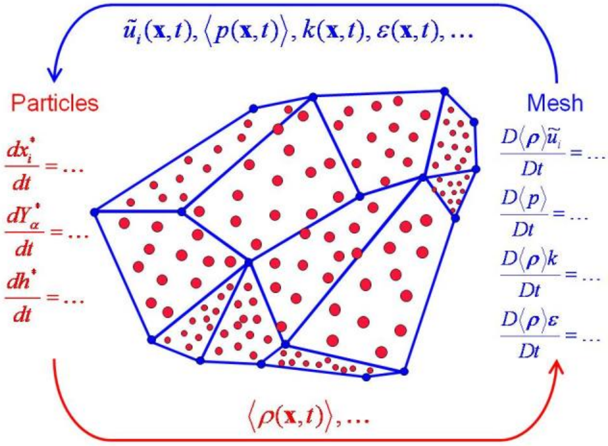
Mike Modest, University of California Merced

Transported Probability Density Function (PDF) Methods

Accommodating realistic chemistry, detailed soot and particle models, spectral radiation heat transfer and complex nonlinear interactions.

PDF methods offer compelling advantages for modeling chemically reacting turbulent flows.

- Model and solve an equation for the one-point, one-time joint PDF of quantities that determine the local thermochemical and/or hydrodynamic state of a reacting system
  - Composition PDF: species mass fractions and enthalpy
- Advantages
  - Resolves closure problems that arise from averaging or filtering highly nonlinear chemical source terms: $\langle S_\alpha \; \underline{Y},T,p \rangle \neq S_\alpha \; \langle \underline{Y} \rangle, \langle T \rangle, \langle p \rangle$
  - Realistic chemistry can be implemented with minimal further modeling
- Computational strategy
  - Lagrangian particle Monte Carlo methods
- Physical models required (composition PDF)
  - Turbulent velocity fluctuations (“turbulent diffusion”)
  - Molecular transport (“mixing”)
- Origins
  - Lundgren (1969) *Phys. Fl.* 12:485-497
  - Pope (1985) *PECS* 11:119-192



Hybrid Lagrangian particle/finite-volume PDF methods are the current mainstream approach.

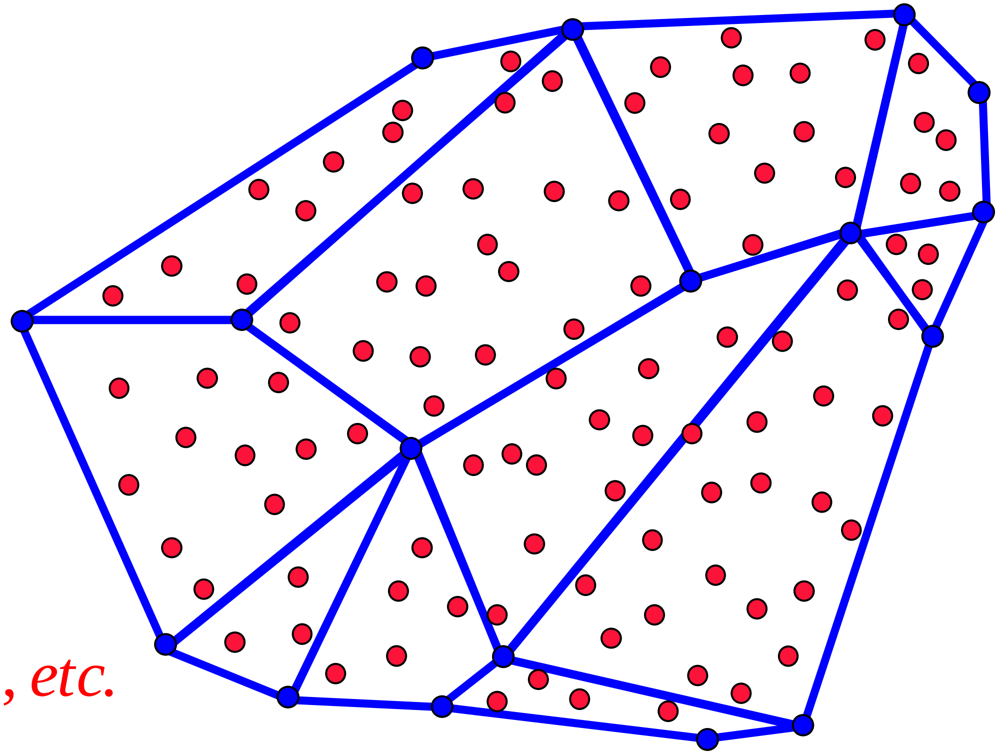
$$\tilde{u}_i(\underline{x},t),\ \langle p(\underline{x},t)\rangle,\ k(\underline{x},t),\ \varepsilon(\underline{x},t),\ \ldots$$

$$\frac{d\underline{x}^{(i)}}{dt} = \ldots$$

$$\frac{d\underline{Y}^{(i)}}{dt} = \ldots$$

$$\frac{dh^{(i)}}{dt} = \ldots$$

form $\langle \rho(\underline{x},t)\rangle$, *etc.*



$$\frac{D\langle\rho\rangle\tilde{u}_i}{Dt} = \ldots$$

$$\frac{D\langle p\rangle}{Dt} = \ldots$$

$$\frac{D\langle\rho\rangle k}{Dt} = \ldots$$

$$\frac{D\langle\rho\rangle\varepsilon}{Dt} = \ldots$$

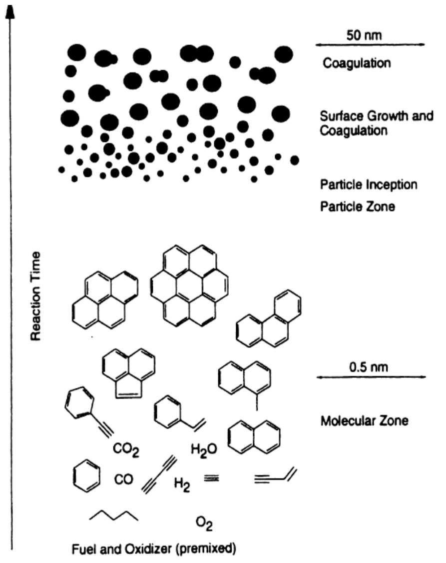
$$\langle \rho(\underline{x},t)\rangle,\ \tilde{\dot{\omega}}(\underline{x},t),\ \ldots$$

Radiation and turbulence-radiation interactions (TRI)

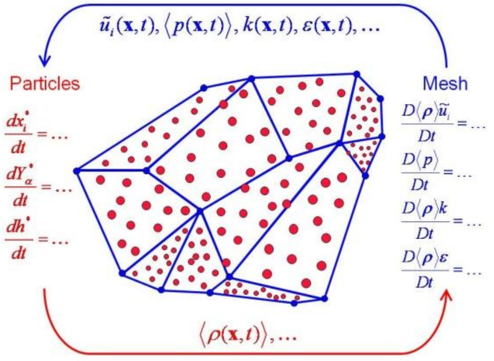
- Radiation is an Important Mode of Heat Transfer in Many (Most?) Turbulent Combustion Systems
- Radiation Often Has Been Ignored Altogether or Has Been Treated Using Simple Models
  - e.g., optically thin approximation
- Difficulties
  - Strong temperature dependence (T^4)
  - Spectral radiation properties
  - Solution of the radiative transfer equation (RTE)
  - Turbulence/radiation interactions (TRI)

Different levels of soot modeling are used in CFD.

- Correlation-Based
  - Soot volume fraction specified as a function of local equivalence ratio and temperature
- Two-Equation Models
  - Modeled equations solved for soot volume fraction and number density
- Detailed Models
  - Account explicitly for each key physical process
  - Require consideration of soot aerosol dynamics
- Soot Aerosol Dynamics
  - Method of moments with interpolative closure (MOMIC)
  - Discrete sectional method (DSM)
  - Variants and hybrids
- Implementations in PDF Methods
  - Correlation-based, two-equation and MOMIC

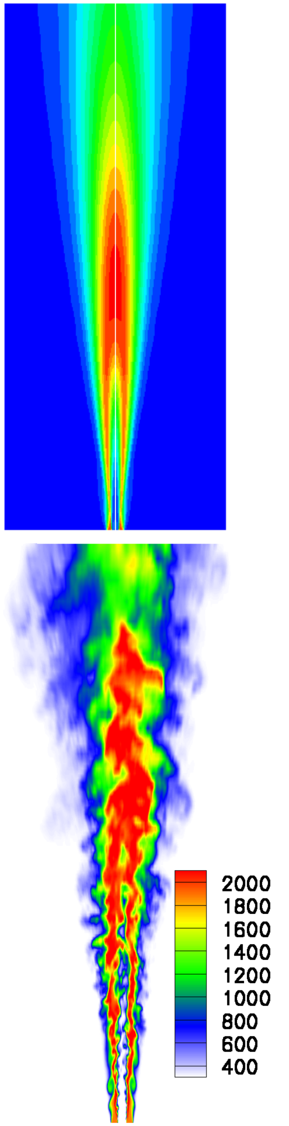


Bockhorn (Ed.)
Soot Formation in Combustion (1994)



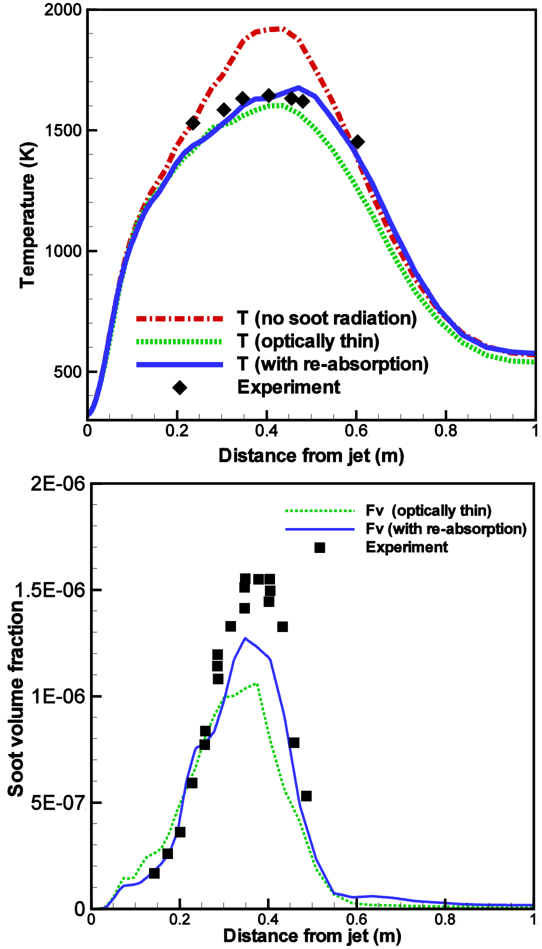
Comprehensive tools are being developed for simulating chemically reacting turbulent flows.

- Reynolds-Averaged and Large-Eddy Simulations
  - PDF-based models for unresolved fluctuations
- Skeletal-Level Gas-Phase Chemistry
  - 10-100 species
  - ISAT for chemistry acceleration
- Detailed Soot Models
  - Method of moments with interpolative closure
- Accurate and Efficient Radiative Transfer Equation Solvers/Spectral Radiation Treatments
  - Photon Monte Carlo (PMC)/line-by-line
  - High-order spherical harmonics/*k*-distribution methods
- Modular Approach
  - Finite-volume CFD, stochastic Lagrangian particle PDF, ray-tracing PMC, spectral radiation properties, soot models
- Parallelization
  - Multiple strategies

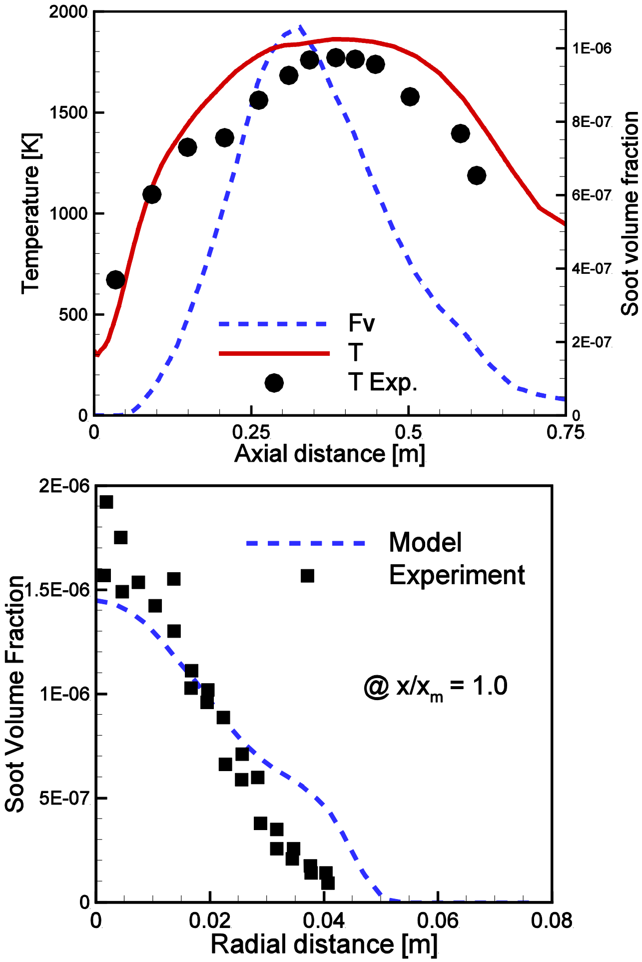


The C_2H_4-air flames of Kent & Honnery (1987) and Coppalle and Joyeux (1994) have been simulated.

C&J 1994



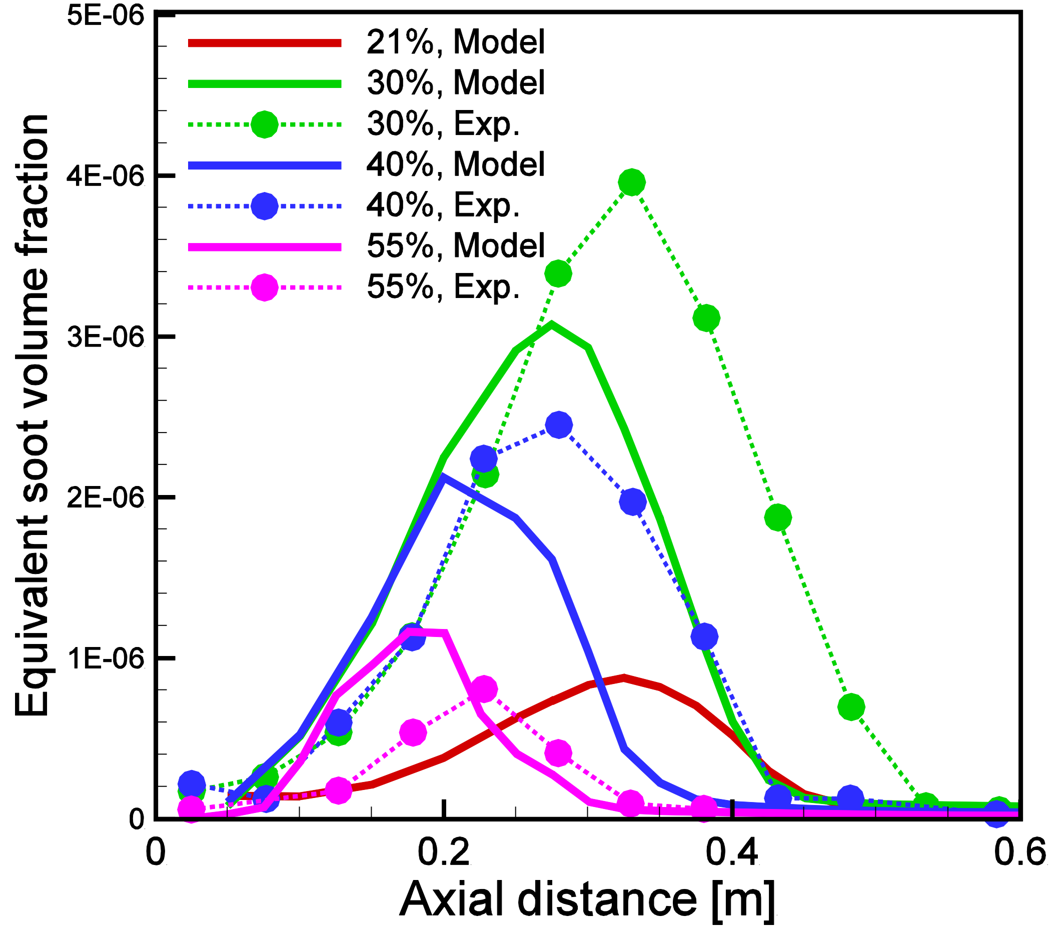
K&H 1987

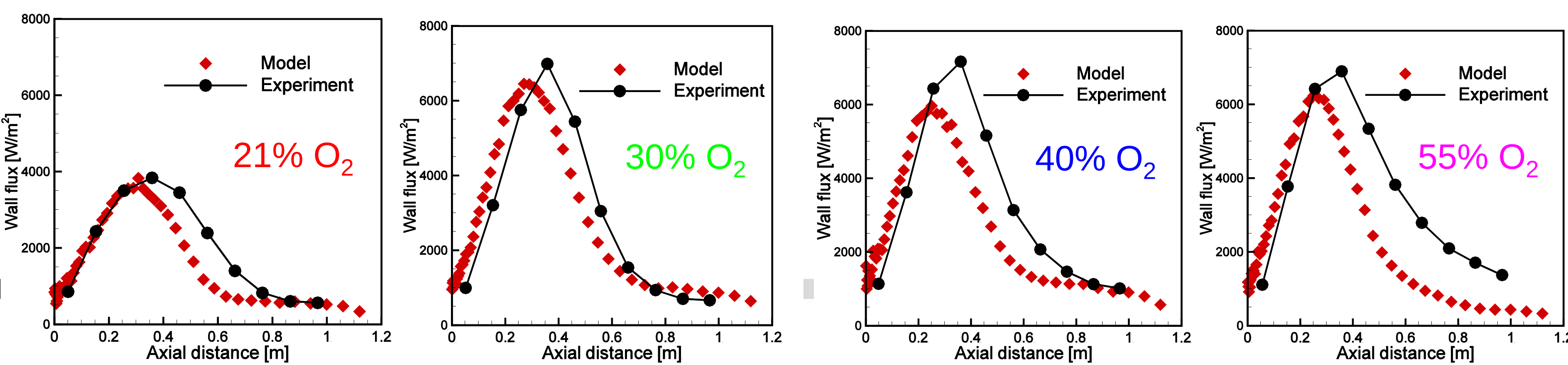


R.S. Mehta, D.C. Haworth & M.F. Modest (2010) Combust. Flame 157:982.

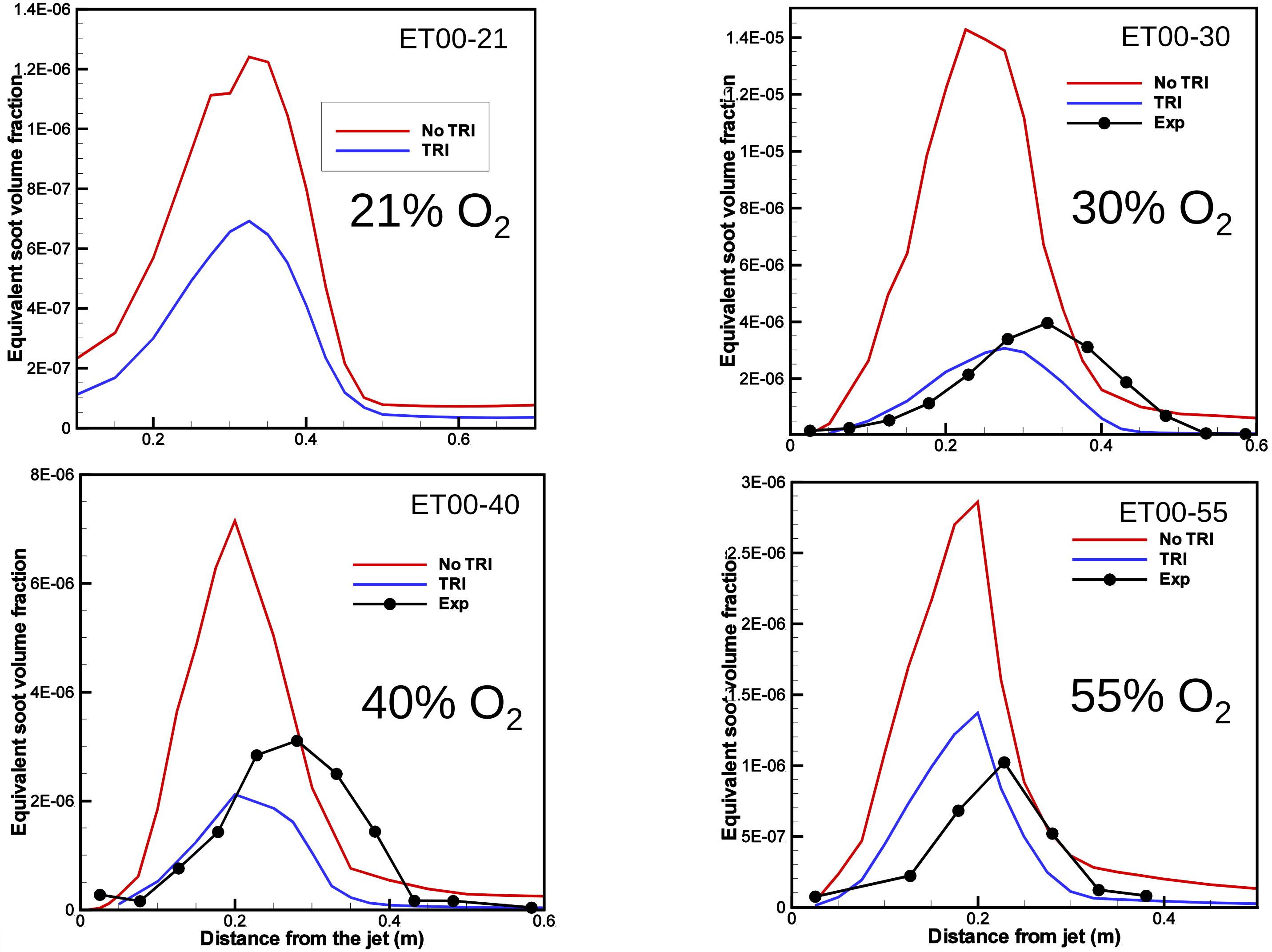
The model captures variations in soot and radiant heat flux with O_2 in oxygen-enriched CH_4/C_2H_4 flames, using the same models.

R.S. Mehta, D.C. Haworth & M.F. Modest (2010)
Combust. Flame 157:982.





Computed soot levels can decrease by more than a factor of three with consideration of TRI.



R.S. Mehta, M.F. Modest & D.C. Haworth (2010) Combust. Theory Model.14:105.

PDF-Based Simulations of Turbulent Syngas Flames

A step toward thermochemical environments that are representative of those in oxy-coal combustion systems.

Xinyu Zhao, Penn State

Dave Huckaby, NETL

Two TNF Workshop 40% CO, 30% H_2, 30% N_2 flames have been simulated.

	Flame A	Flame B
Nozzle diameter	4.58 mm	7.72 mm
Jet velocity	76 m/s	45 m/s
Coflow velocity	0.7 m/s	0.7 m/s
Jet Reynolds #	16700	16700
Jet mass fractions $CO/H_2/N_2$	0.554/0.03/0.416	0.554/0.03/0.416
Coflow mass fractions $O2/N_2$	0.234/0.766	0.234/0.766
Jet and coflow temperatures	292 K	292 K

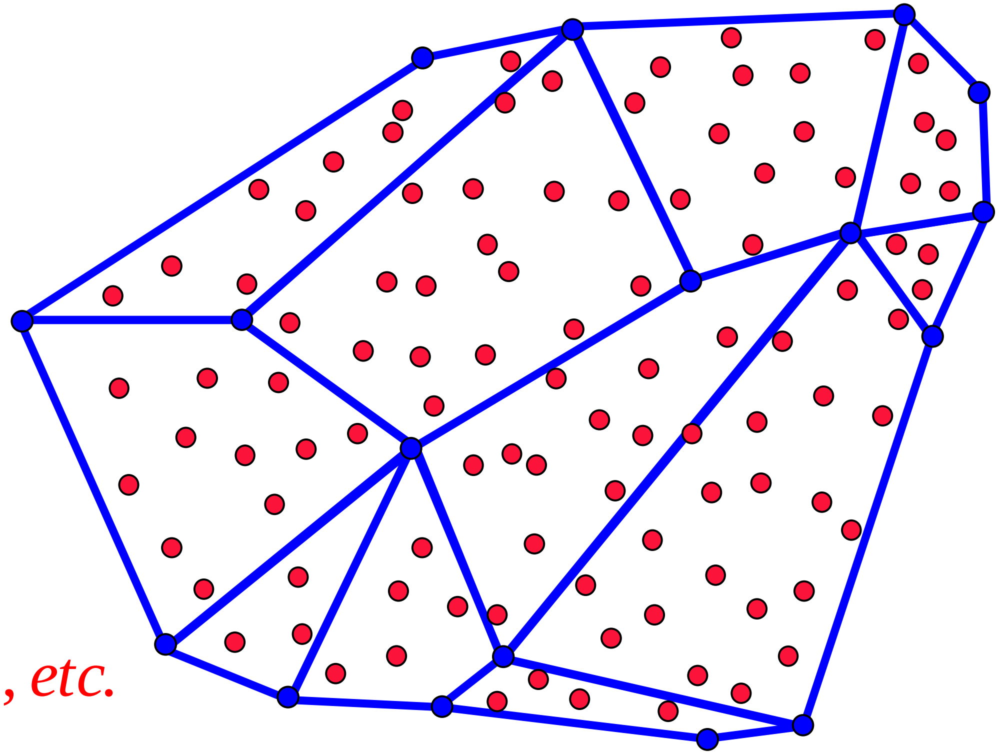
Experimental data including mean and rms temperature, species mass and mole fractions, and velocity fields can be found on the TNF website: http://www.sandia.gov/TNF/DataArch/SANDchn.html

A Hybrid Lagrangian particle/finite-volume PDF method has been implemented in OpenFOAM.

$$\tilde{u}_i(\underline{x},t),\ \langle p(\underline{x},t)\rangle,\ k(\underline{x},t),\ \varepsilon(\underline{x},t),\ \ldots$$

$$\frac{d\underline{x}^{(i)}}{dt} = \ldots \qquad \frac{d\underline{Y}^{(i)}}{dt} = \ldots \qquad \frac{dh^{(i)}}{dt} = \ldots$$

form $\langle \rho(\underline{x},t)\rangle$, *etc.*



$$\frac{D\langle\rho\rangle\tilde{u}_i}{Dt} = \ldots \qquad \frac{D\langle p\rangle}{Dt} = \ldots \qquad \frac{D\langle\rho\rangle k}{Dt} = \ldots \qquad \frac{D\langle\rho\rangle\varepsilon}{Dt} = \ldots$$

$$\langle \rho(\underline{x},t)\rangle,\ \tilde{\dot{\omega}}(\underline{x},t),\ \ldots$$

Sensitivity studies have been performed with variations in physical and numerical parameters.

- Chemical Mechanism
  - 10-species, 6-step syngas (including thermal NO)
  - GRI-Mech 2.11 (including detailed NOx)
  - Princeton C1 mechanism (courtesy of F.L. Dryer)
- PDF Mixing Model
  - Modified Curl with C_ϕ=1.5
  - EMST with C_ϕ=1.5 and variations (C_ϕ=1.0, 2.0, 8.0)
- Radiation Model
  - No radiation
  - Optically thin radiation (CO_2, H_2O, CO)
  - PMC spectral radiation with reabsorption (CO_2, H_2O)
- Flame Stabilization
  - Resolve recirculation zone
  - Local equilibrium in small zone close to nozzle
- Computational Acceleration
  - Parallelization and direct integration
  - Parallelization and ISAT

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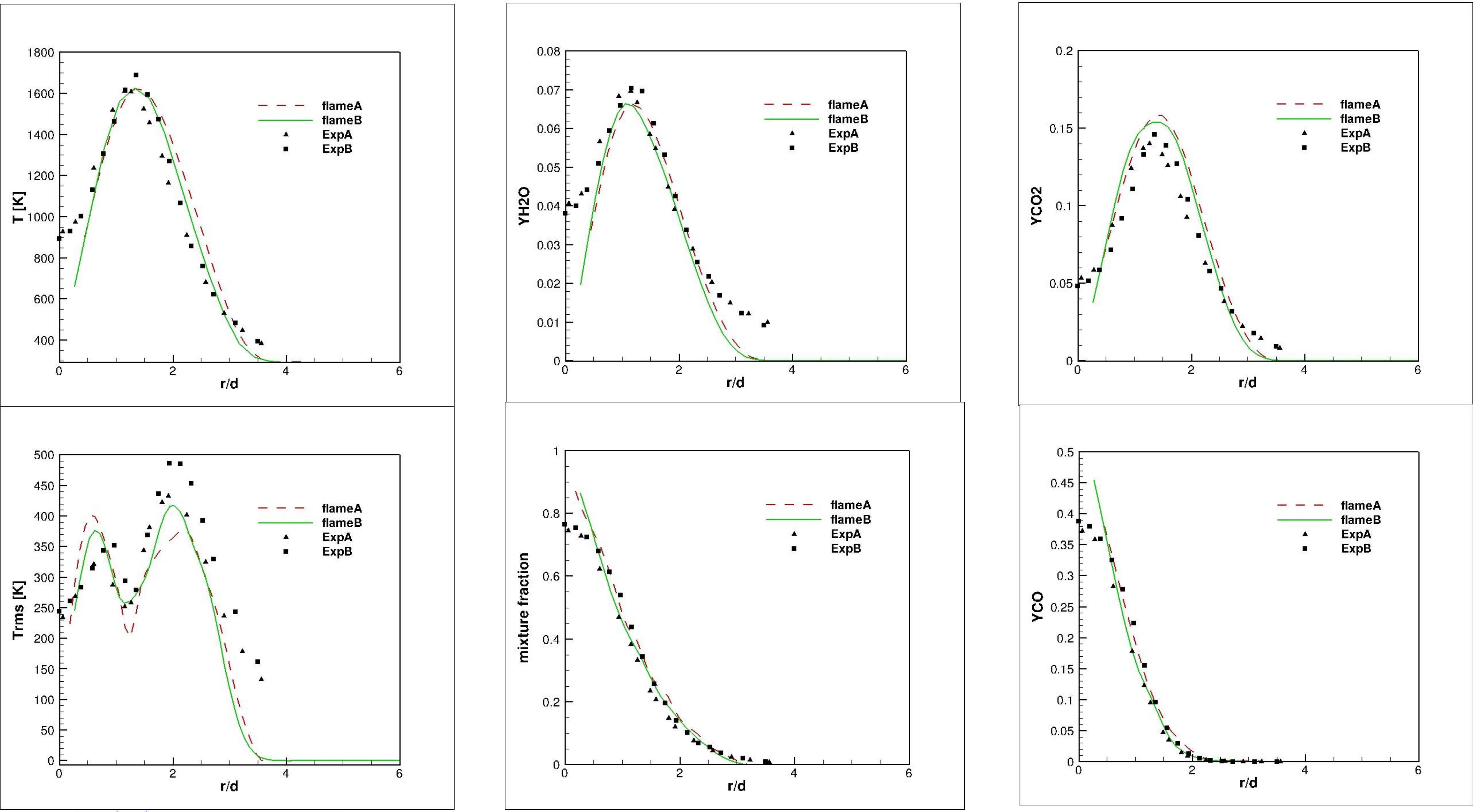
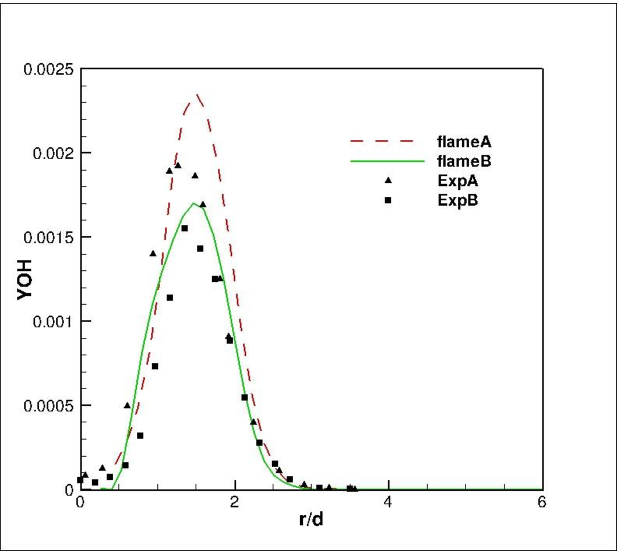
Baseline model

Baseline model is in reasonable agreement with experiment and captures correct scaling.

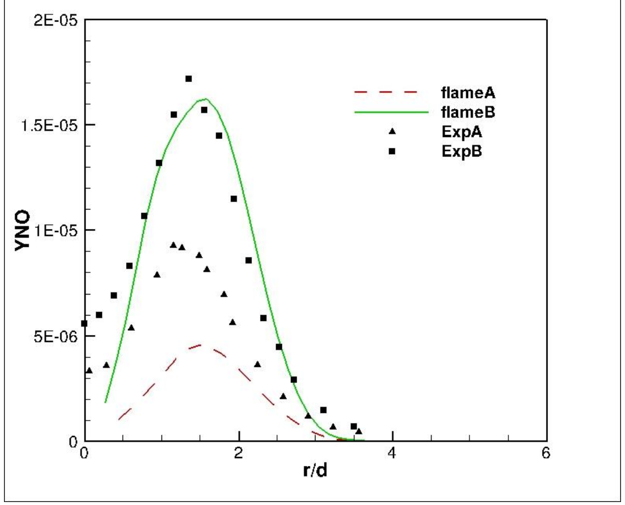


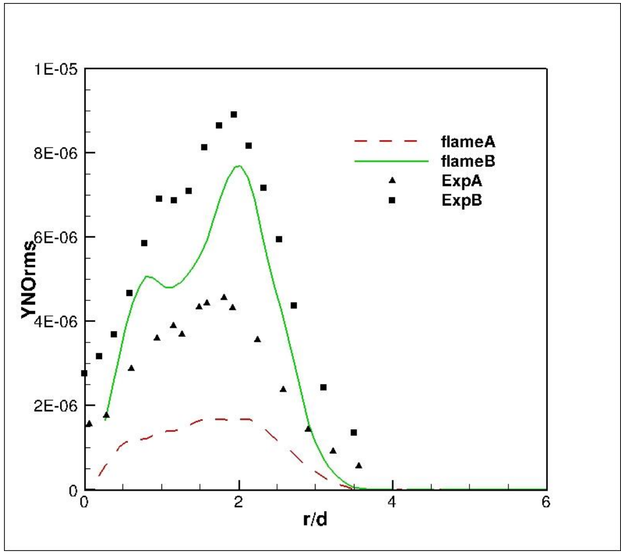
x/d = 20

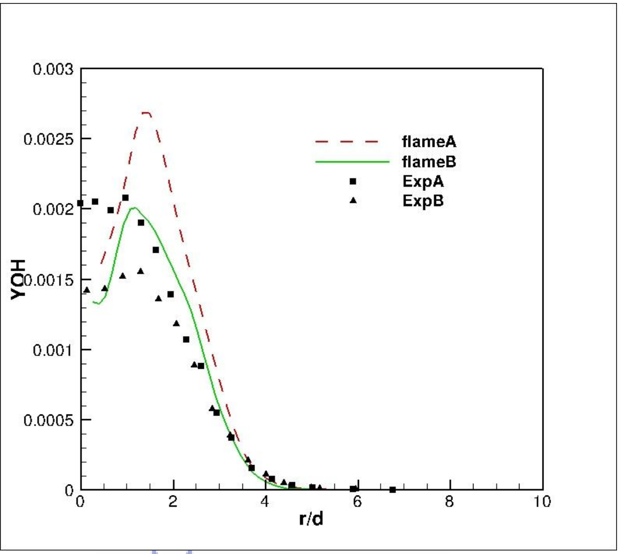
Baseline model (cont.)



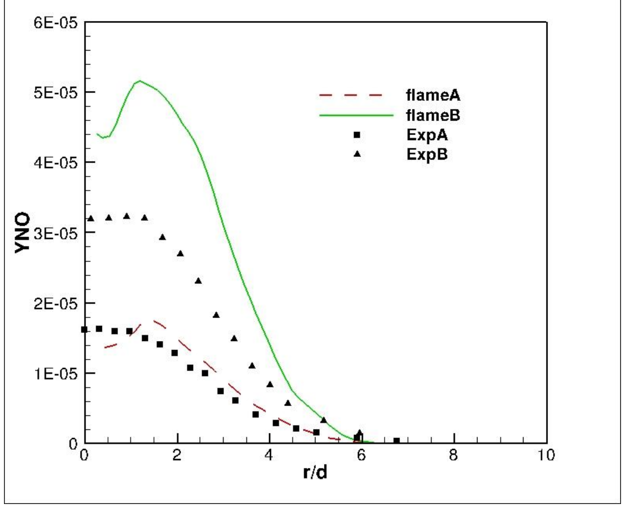
x/d = 20

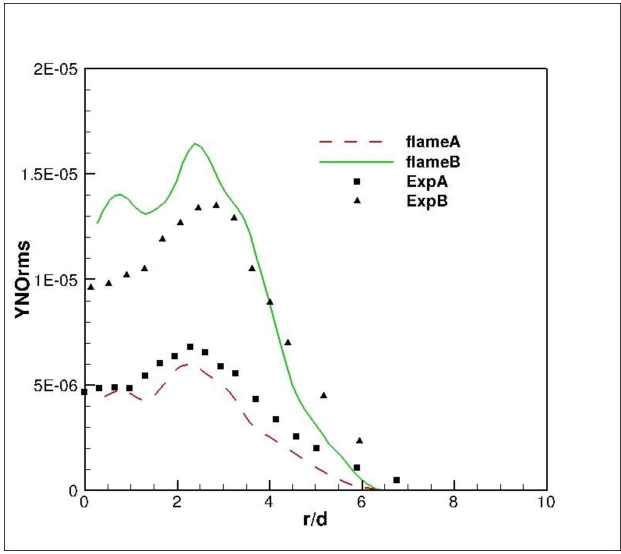






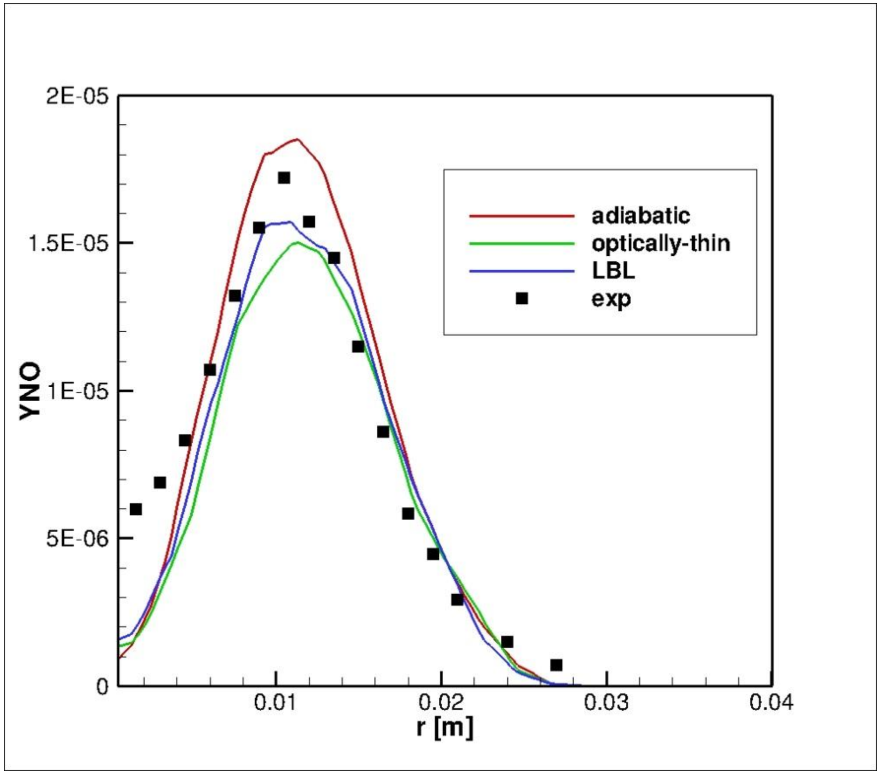
x/d = 40



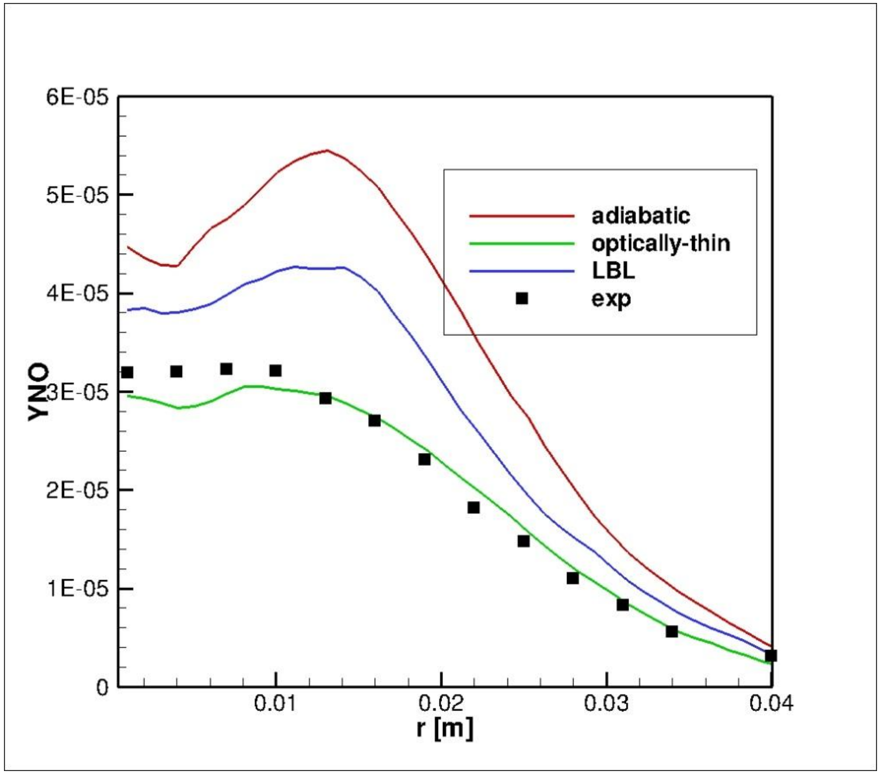


Radiation effects are relatively small, but are discernable – especially for NO.

x/d = 20



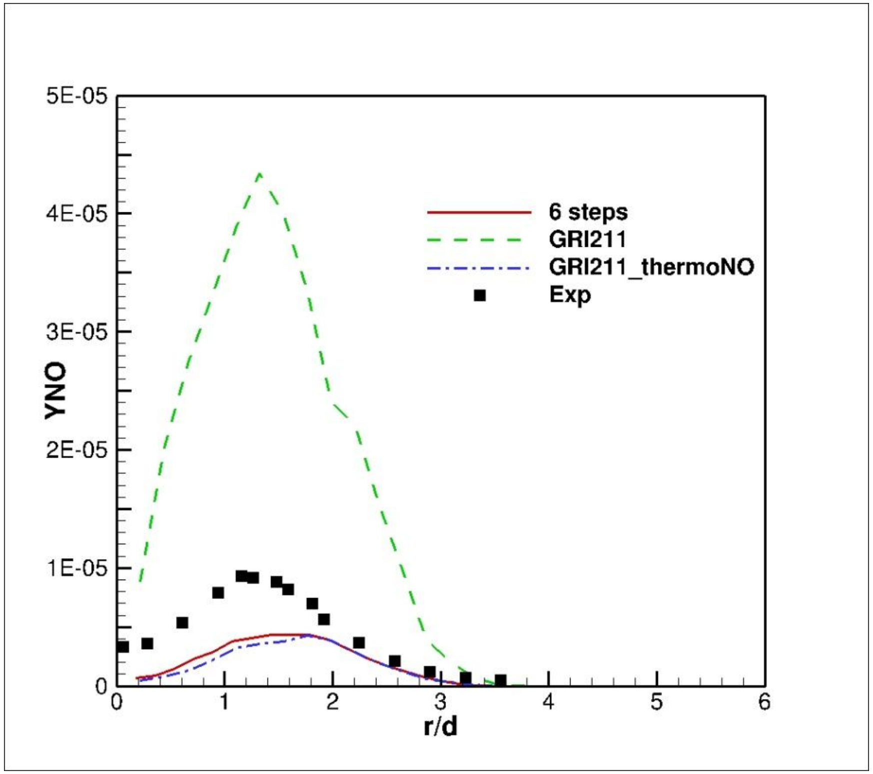
x/d = 40



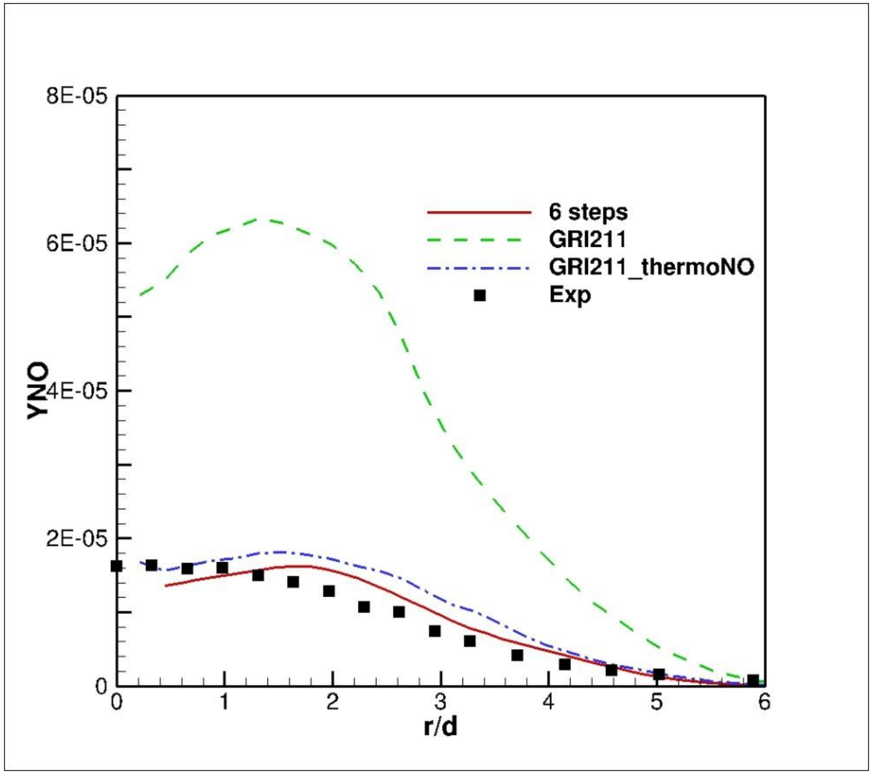
Flame B

Chemistry effects are most pronounced in CO and NO predictions.

<u>*x/d* = 20</u>



<u>*x/d* = 40</u>



Flame A

PDF-Based Simulations of a 0.8 MW Oxy-Methane Burner

Next step toward thermochemical environments that are representative of those in oxy-coal combustion systems.

Xinyu Zhao, Penn State

Dave Huckaby, NETL

Simulations are underway for OXYFLAM-2.

Experiment	Furnace and burner configurations	Experimental program
OXYFLAM-1 December 1995 –January 1996	Water-cooled furnace – Single coaxial-jet diffusion flames	Input/output + Detailed in-flame measurements including laser sheet visualization + Calibration of the HTS† pyrometer
OXYFLAM-2 April–May 1996	Refractory-lined furnace – Single coaxial-jet diffusion flames	Input/output + Detailed in-flame measurements
OXYFLAM-3 December 1996	Refractory-lined furnace – Staged and premixed flames	Input/output + Detailed in-flame measurements
1997–1998	N/A	Analysis of the OXYFLAM-1, -2 and -3 experiments – Calibration of the HTS-pyrometer

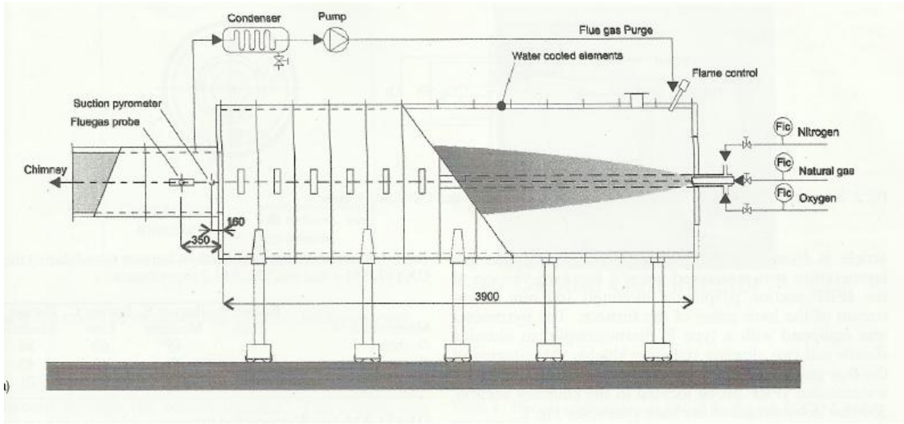
*N/A = Not applicable
†HTS = High-Temperature Suction

N. Lallemant, F. Breussin, R. Weber, T. Ekman, J. Dugue, J. M. Samaniego, O. Charon, A. J. Van Den Hoogen, J. Van Der Bemt, W. Fujisaki, T. Imanari, T. Nakamura and K. IINO. Flame Structure, heat transfer and pollutant emissions characteristics of oxy-natural gas flames in the 0.7-1 MW thermal input range. Journal of Institute of Energy, 73, pp. 169-182

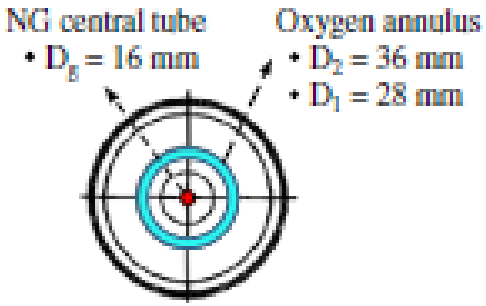
This is a pilot-scale burner with small fuel and oxidizer jets.

Properties	Jet	Coflow
Velocity	105.4 m/s	109.7 m/s
Reynolds #	162600	128600
Composition	0.8869 CH_4 0.0463 C_2H_6 0.00094 C_3H_8 0.0032 C_4H_{10} 0.0009 C_5H_{12} 0.0379 N_2 0.0152 CO_2 0.02 O_2	99.5% O_2
Temperature	298 K	298 K
K	627.9 J/kg	850.16 J/kg
Epsilon	4.617E6	2.9094E6
Wall Temperature	Specified as $T_w(y) = 1700.6 + 212.59y - 46.669y^2$	

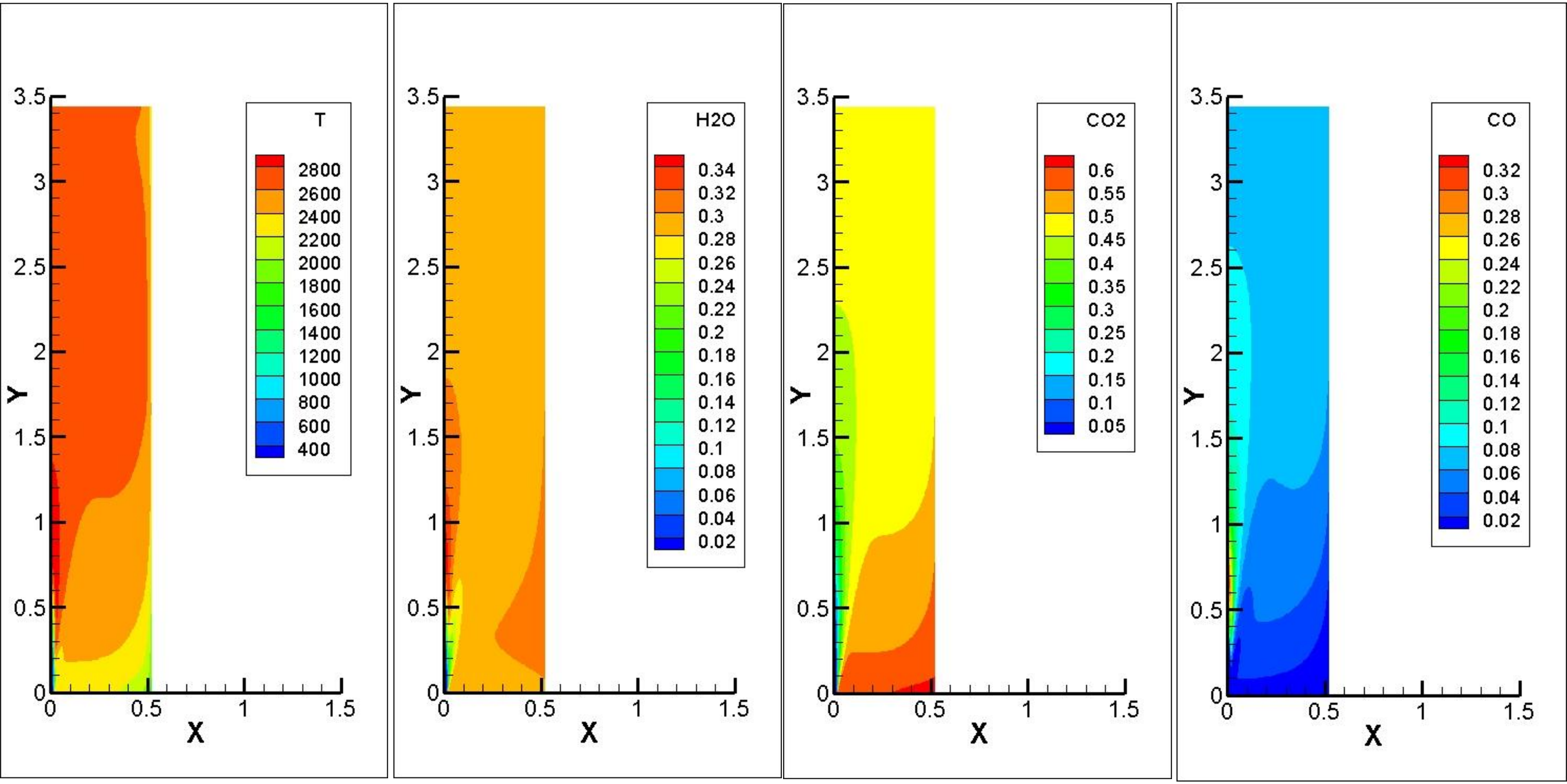
Burner schematic

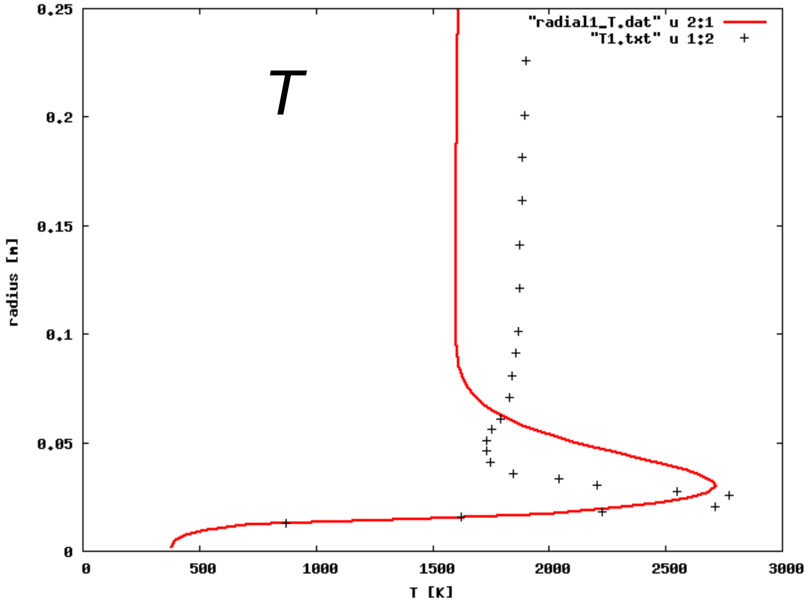


Nozzle dimensions



Initial non-PDF results are obtained using a steady-state solution algorithm.

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"T1.txt" u 1:2
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T [K]
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2000
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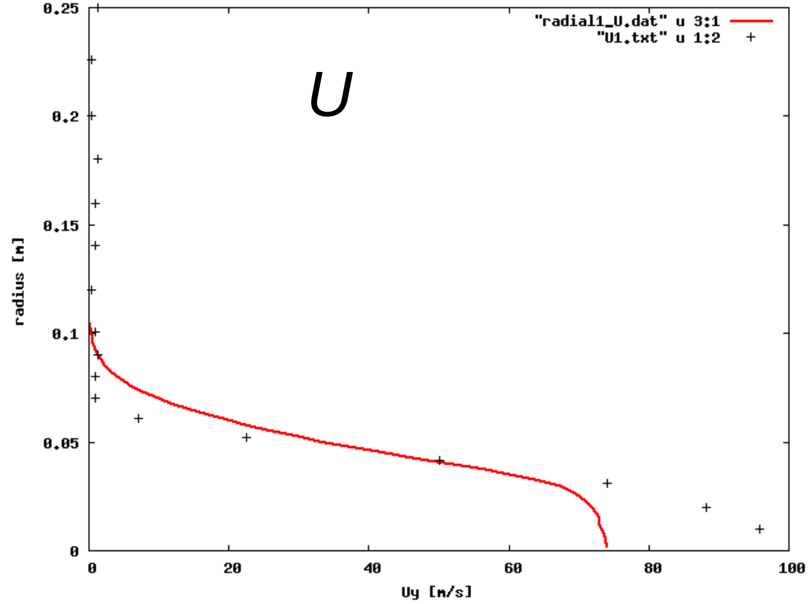
3000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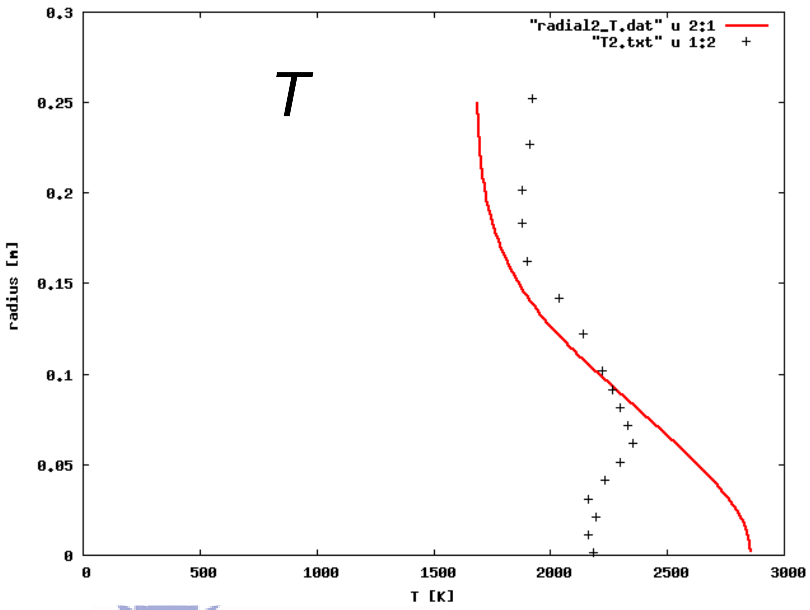
x = 0.22 m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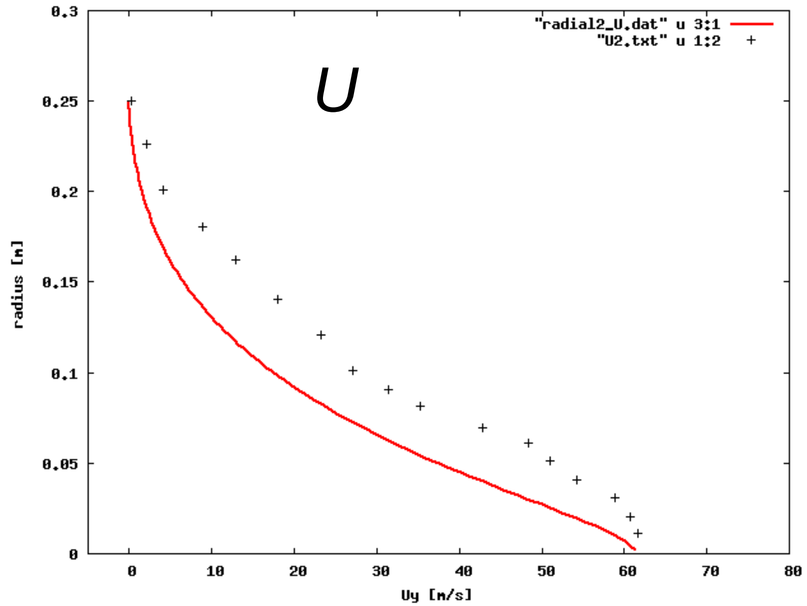
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0.25
0.3
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10
20
30
40
50
60
70
80

x = 0.82 m

Concluding Remarks

PDF methods offer compelling advantages for modeling chemically reacting turbulent flows.

- Realistic chemistry, soot and radiation models are required to predict temperatures, heat transfer rates and pollutants
- Turbulence-chemistry interactions (TCI) and other complex nonlinear interactions significantly change the global and local flame behavior
  - Expected to become increasingly important in next-generation combustion systems for power generation and other applications
- Transported PDF methods are a particularly appealing approach for dealing with TCI and other complex nonlinear interactions
  - Resolve key closure problems
  - Accommodates realistic chemistry, multi-phase systems with radiation
  - Rational approach that minimizes need for further modeling to account for effects of turbulent fluctuations
- Encouraging results have been obtained in environments approaching those of oxy-coal combustion
  - Results are at least as good (if not better) than any reported to date for the TNF syngas flames

Next steps

- Continue simulations of oxy-methane burners
  - Initiate transported PDF method
  - Enable radiation models
- Move to particle-fueled systems
  - Use a separate stochastic Lagrangian formulation to model coal particles
  - Couple with transported PDF and radiation models
  - Follow approaches developed for liquid fuel/PDF coupling in turbulent spray flames