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Computational and Experimental Study of the Structure of Diffusion Flames of Jet Fuel and its Surrogrates at Pressures up to 40 atm

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Outline

- Overview of completed work 2/06-11/08
- Discussion of work during no-cost extension
- Brief description of current project

Objectives (1)

- Examine flame structure of single component, JP-8 surrogate and JP-8 flames in a counterflow configuration
- Determine extinction values
- Model the surrogate(s) with semidetailed chemical kinetics
- Reduce chemical kinetics

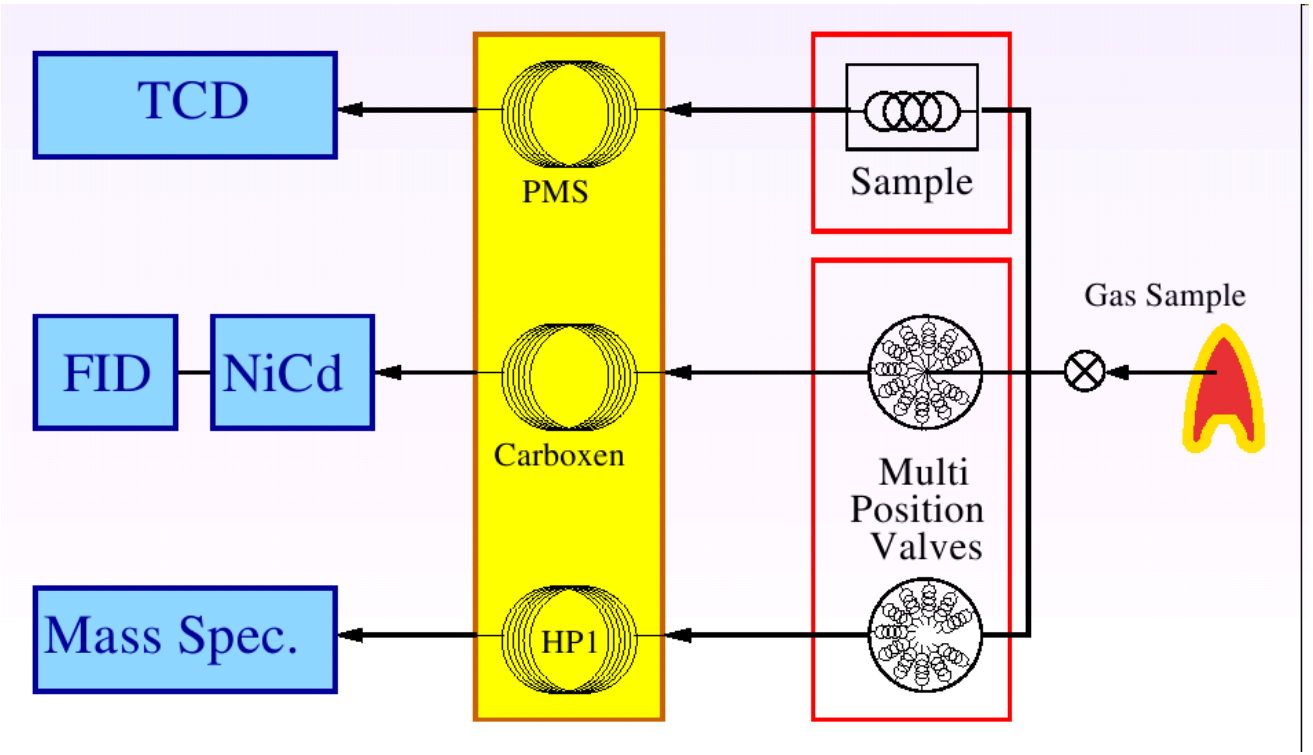
JP-8 Surrogate

- JP-8 is modeled as a six-component surrogate mixture (Violi, *et al.*, 2001)

  10% Iso-octane (C_8H_{18}), 20% Methylcyclohexane (C_7H_{14}), 5% Tetralin ($C_{10}H_{12}$), 30% Dodecane ($C_{12}H_{24}$), 20% Tetradecane ($C_{14}H_{30}$), 15% m-Xylene (C_8H_{10})

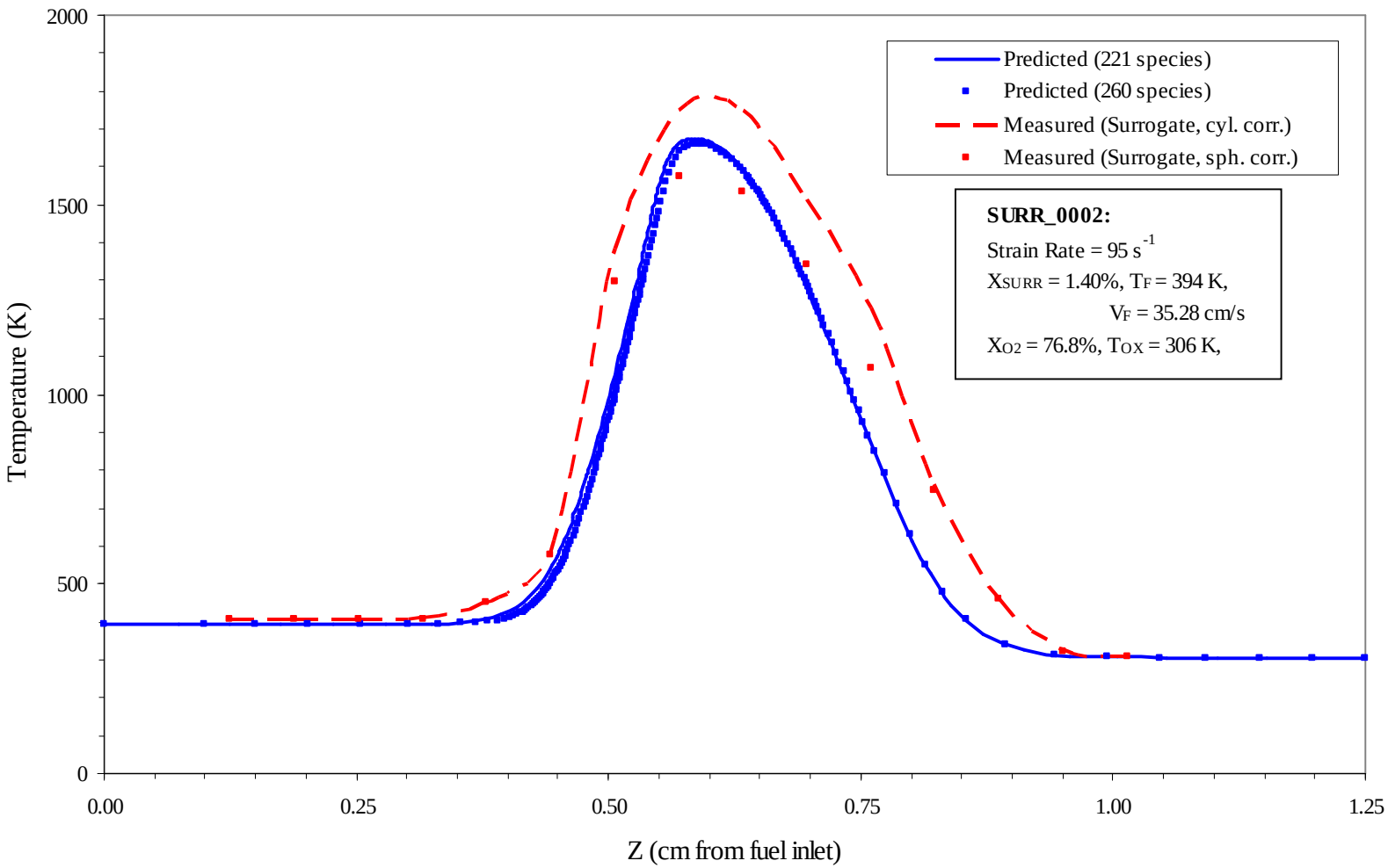
- Surrogate kinetics are modeled using <u>two</u> semi-detailed mechanisms
  - Initial studies use a 221-species mechanism containing 5032 reactions
  - Selected flames are modeled with a 260-species mechanism containing 7001 reactions

GC/MS Configuration

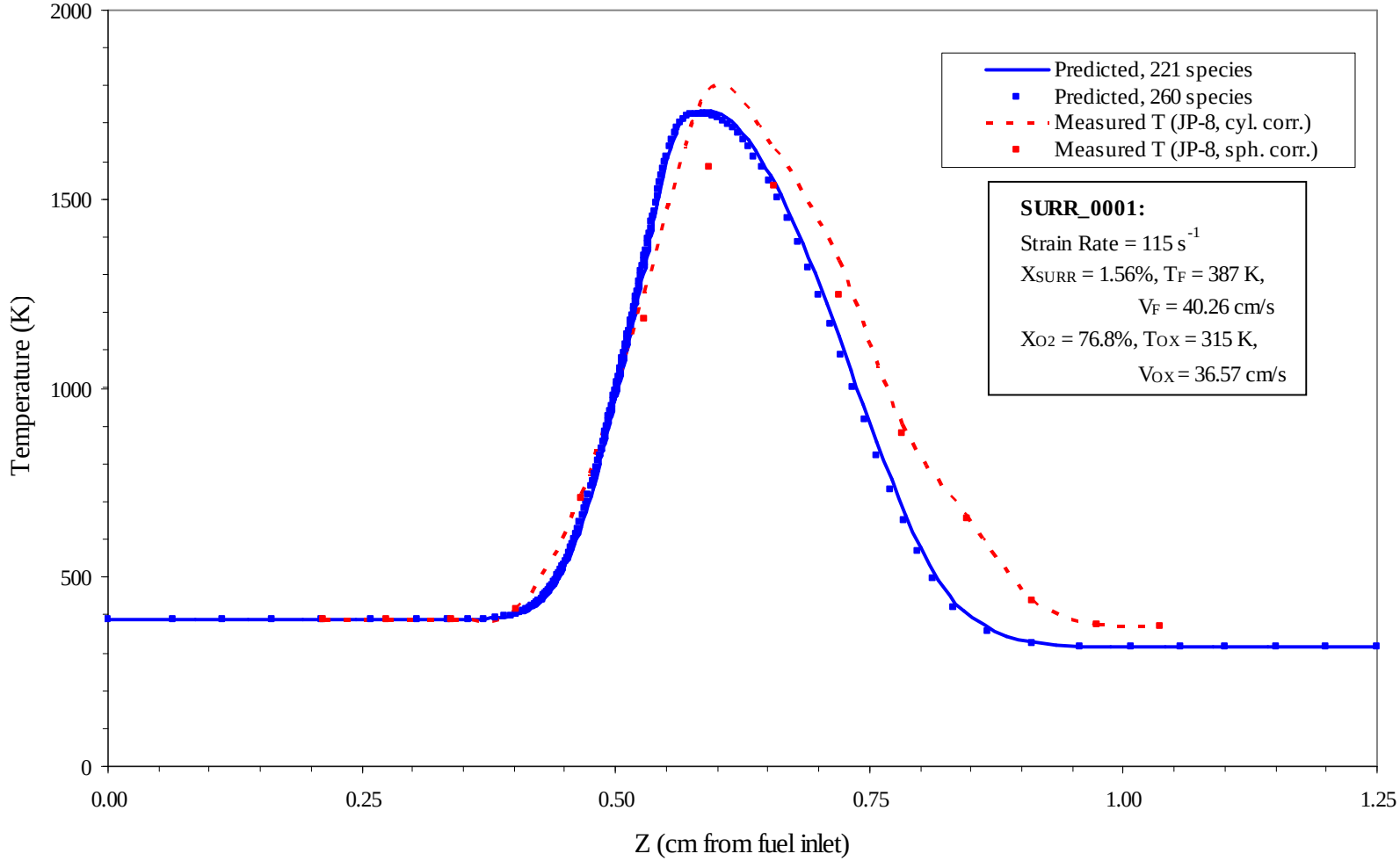


3 hours of flame burning and 30 hours of off-line analysis

Results: Surrogate Flames
Comparison of Temperature Profiles



Results: JP-8 Flames
Comparison of Temperature Profiles



Results: JP-8 Surrogate Flames Comparison of Rich Extinction Limits

- Rich extinction limits have been determined for two surrogate flames via continuation methods.
- Extinction limits for JP-8 flames with the same fuel flow rate have been measured and are identical to the surrogate extinction limits.
- The effects of kinetic mechanism on the rich extinction limit are examined for each surrogate flame

Inlet Surrogate Mole Fraction	Inlet Oxygen Mole Fraction	Strain Rate (s^{-1})	Mechanism	Predicted Rich Extinction Limit (% O_2 by mole)	Measured Rich Extinction Limit (% O_2 by mole)	% Variation (relative to measurement)
0.0156	0.768	115	221 Species	0.5512	0.594	7.21
			260 Species			
0.014	0.768	95	221 Species	0.6185	0.602	2.74
			260 Species	0.643		6.81

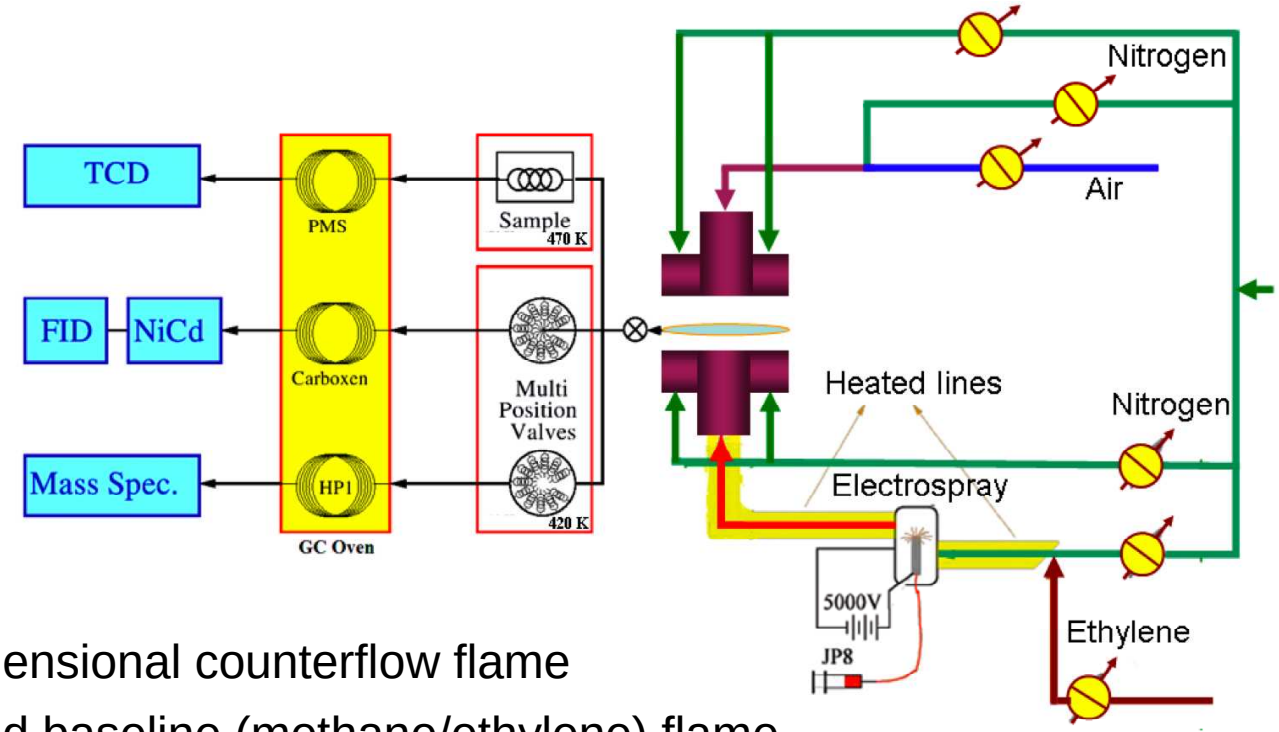
Summary of Completed Counterflow Work (1)

- Results were generated for lean, non-sooting counterflow diffusion flames with *n*-dodecane, methylcyclohexane, iso-octane, and the surrogate blend as fuels
- Single-solution methods provide computational temperature profiles for experimental comparison and a basis for future validation of velocity and species profiles
- Arc length continuation is used to predict rich extinction limits for each flame
- Predicted and measured temperature profiles and rich extinction limits are presented for each flame
  - Measurements are corrected for radiative losses
  - Especially good agreement is noted between computational results and experimental JP-8 flames
  - Rich extinction limits agree within 10%

Objectives (2)

- Examine flame structure of JP-8 doped flames
- Compare and contrast with promising surrogate candidates
- Model the surrogate(s) with semidetailed chemical kinetics
- Reduce chemical kinetics

Experimental System

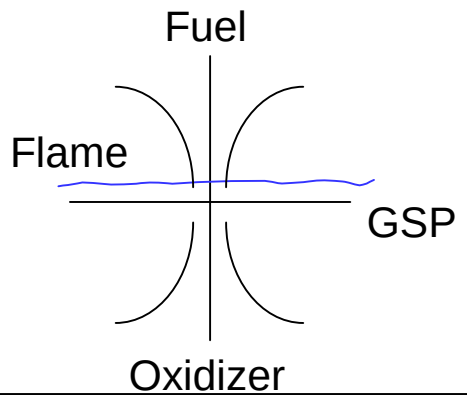


- One-dimensional counterflow flame
- Perturbed baseline (methane/ethylene) flame
  - Use flame as a “controlled” reactor by maintaining a fixed time-temperature baseline and constant stoichiometric mixture fraction and add O(1000) ppm liquid fuel
- Liquid dispersion by the electrospray, followed by spray evaporation in the fuel line
- Flame burning ~3 hrs, off-line analysis at least 30 hrs

Selection of Flames Spanning a Broad Range of Conditions

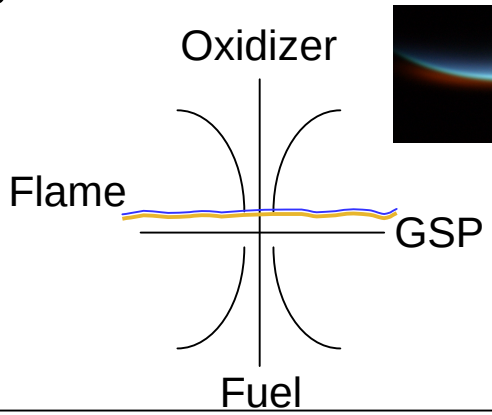
Non-sooting Flame Set

- Max. Temp= 1750K
- Strain Rate= 102 s^{-1}
- Stoich. mixture fraction Z_f= 0.77
- Fixed temperature profile
- Flame on fuel side of stagnation plane



Sooting Flame Set

- Max. Temp= 1989K
- Strain Rate= 69 s^{-1}
- Z_f= 0.18
- Fixed temperature profile
- Flame on oxidizer side of stagnation plane



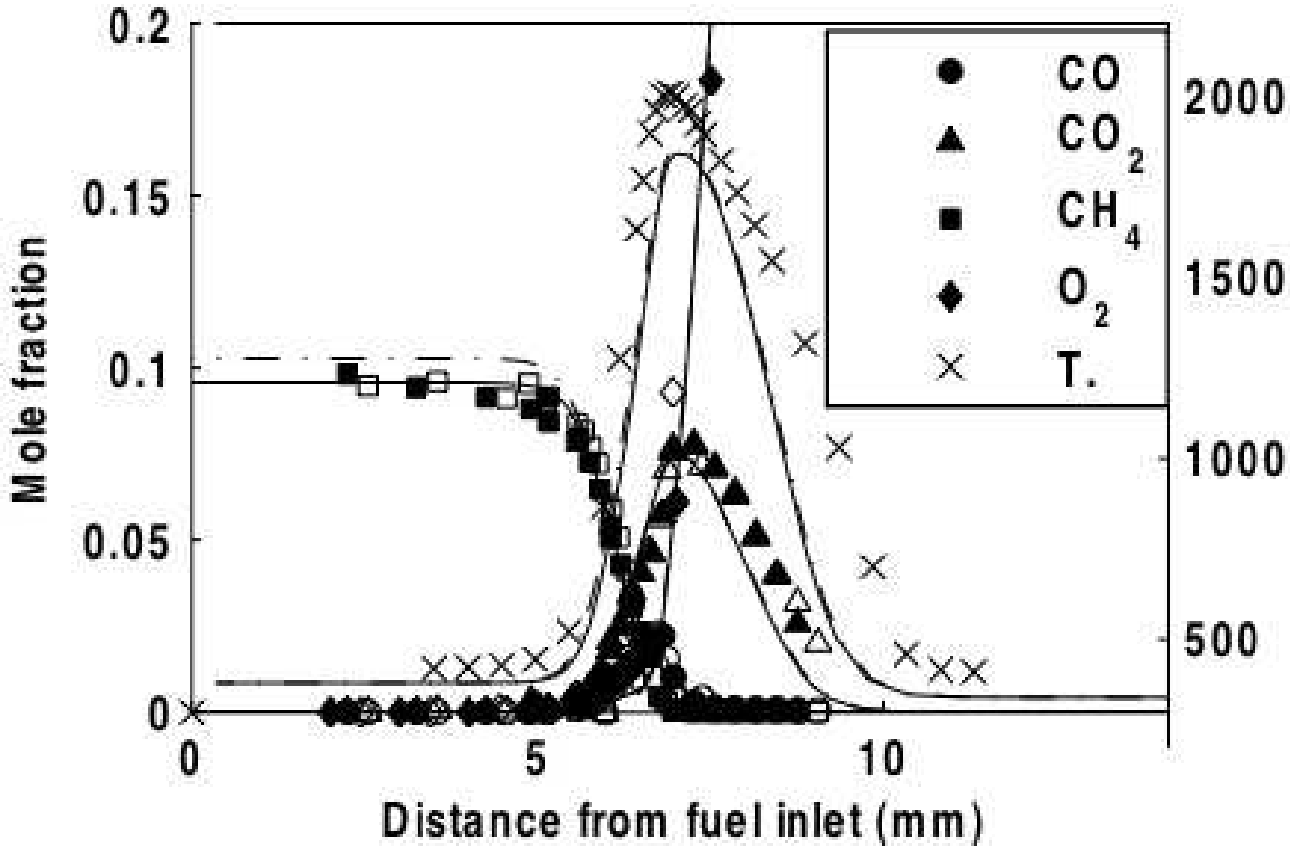
Experimental Conditions: Nonsooting Flames

		Flame A	Flame B	Flame C
Fuel Side	Molar Composition			
	N_2	0.897	0.902	0.902
	CH_4	0.103	0.097	0.097
	C2-C5 alkane impurities	232 ppm	232ppm	219 ppm
	JP-8 ($C_{11}H_{21}$)		992 ppm	
	Methyl-Cyclohexane			200 ppm
	Iso-Octane			100 ppm
	m-Xylene			150 ppm
	Tetraline			50 ppm
	Dodecane			300 ppm
	Tetradecane			200 ppm
	Mass Flux (g/min/cm^2)	2.80	2.97	2.97
	Temperature (K)	379		
Oxidizer Side	Molar Composition			
	N_2	0. 227		
	O_2	0. 773		
	Mass Flux (g/min/cm^2)	3.19	3.42	3.42
	Temperature (K)	340		
	Strain Rate (s^{-1})	110	117	117
	z_f	0.76		

Experimental Conditions: Sooting Flames

		Flame A Baseline	Flame A* Equal Carbon	Flame B Jet Fuel	Flame C Utah/Yale Surrogate	Flame D Aachen Surrogate
Fuel Side	Molar Composition					
	N_2	0.7278	0.7280	0.7340	0.7339	0.7339
	C_2H_4	0.2722	0.2719	0.2641	0.2641	0.2641
	C2 (Ethane) impurities	637 ppm	636 ppm	618 ppm	618 ppm	618 ppm
	Jet Fuel† ($C_{11}H_{21}$)			1953 ppm		
	Methyl-cyclohexane				394 ppm	
	Iso-Octane				197 ppm	
	m-Xylene				295 ppm	
	Tetralin				98 ppm	
	n-Dodecane				591 ppm	
	n-Tetradecane				394 ppm	
	Total=				1970 ppm	
	1,2,4-trimethylbenzene					450 ppm
	n-Decane					1520 ppm
	Total=					1970 ppm
	Mass Flux (g/(cm^2.min))	1.619	1.683	1.684	1.683	1.682
	Temperature (K)	407	407	407	407	407
Oxidizer side	Molar Composition					
	N_2	0.8070	0.8070	0.8070	0.8070	0.8070
	O_2	0.1843	0.1843	0.1843	0.1843	0.1843
	Mass Flux (g/(cm^2.min))	1.891	1.925	1.925	1.925	1.925
	Temperature (K)	370	370	370	370	370
	Strain Rate (s^{-1})	89.9	85.2	92.3	92.3	92.3
	z_f	0.18	0.18	0.18	0.18	0.18

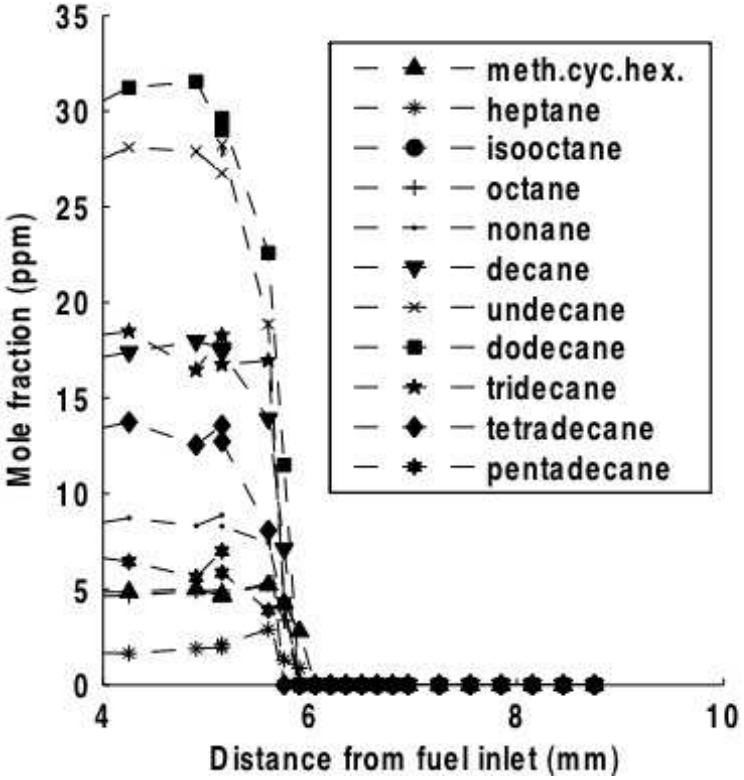
Non-sooting Flames: Major Species and Temp



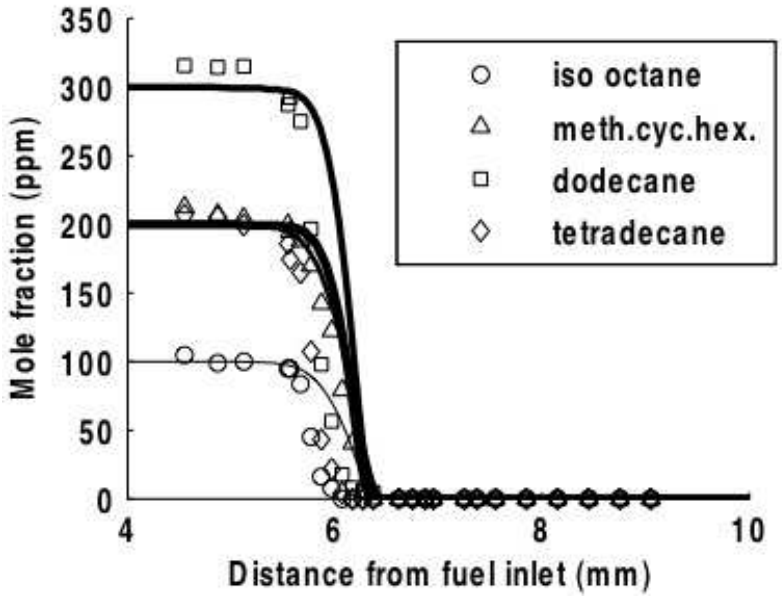
JP-8 doped - Full Symbols; Surrogate doped - Open Symbols; Line - computations

Non-sooting Flames: C7-C15 Alkanes

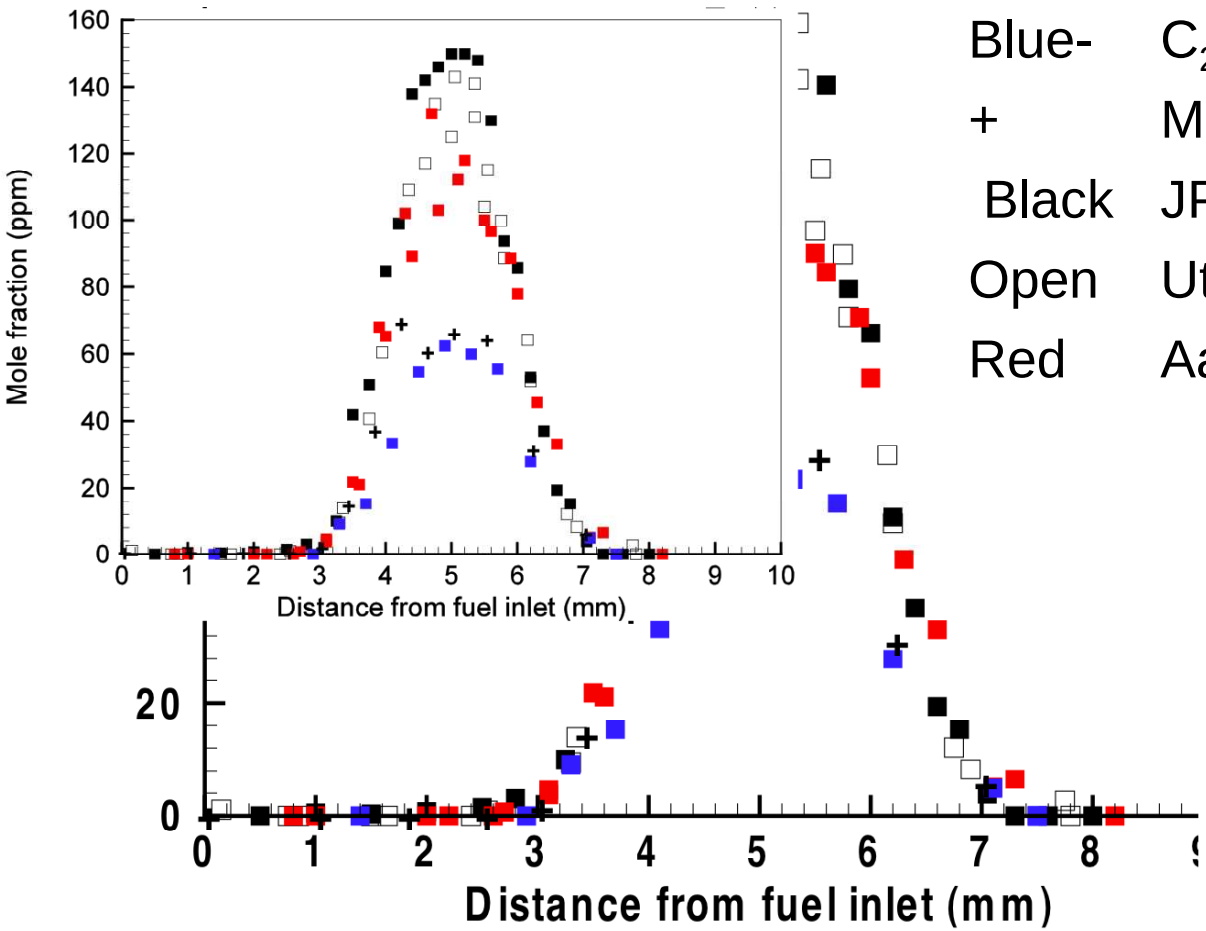
JP-8 doped



Surrogate doped (line-computational)

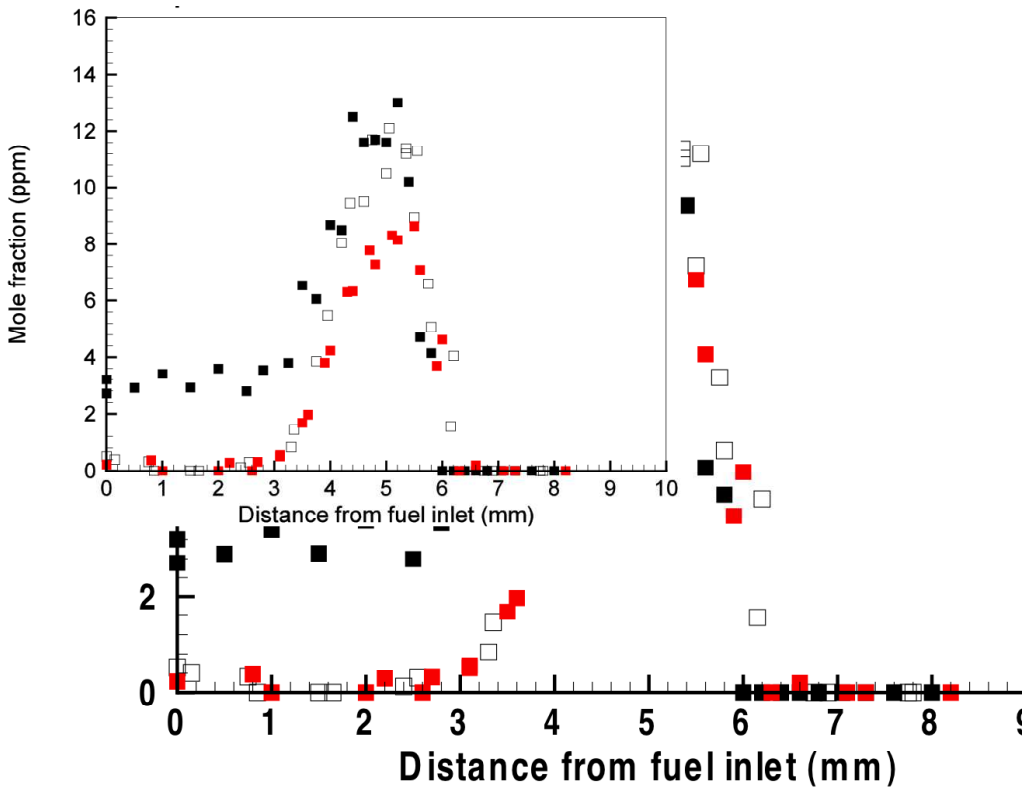


Sooting Flames: Benzene Profiles



Blue-	C_2H_4 Baseline (A)
+	Modified C_2H_4 Baseline (A*)
Black	JP-8-doped (B)
Open	Utah/Yale-doped (C)
Red	Aachen-doped (D)

Sooting Flames: Toluene Profiles



Black JP-8-doped (B)

Open Utah/Yale-doped (C)

Red Aachen-doped (D)

Summary of Completed Counterflow Work (2)

- Baseline flames were identified spanning a broad range of stoichiometric mixture fractions, including nonsooting and incipiently sooting conditions, to test the perturbation from the addition of O(1000) ppm JP-8 and surrogates
- The addition of jet fuel to these flames flame leads to the fragmentation of heavier alkanes to smaller ones, down to C2-hydrocarbons and the appearance of peak aromatic concentrations surviving further into the high temperature region.
- A 6-component surrogate captures the pyrolysis and oxidation behavior of JP-8 reasonably well, with the most significant discrepancy for benzene, toluene and ethylene under non-sooting conditions.
- The computational results using a semi-detailed kinetic mechanism are in reasonably good agreement with the experiments.

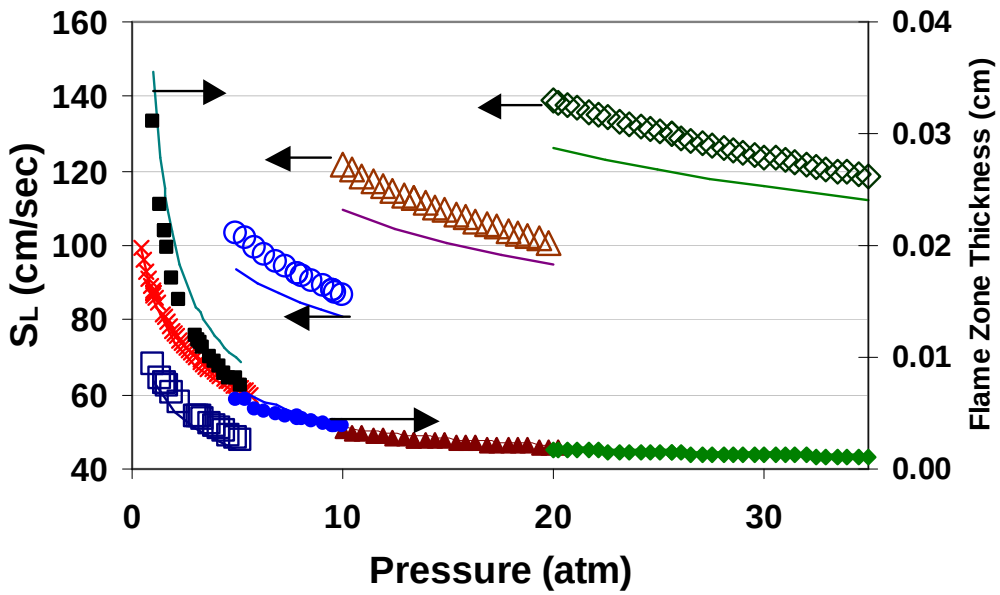
Summary of Completed Counterflow Work (2)

- Experiments on an incipiently sooting doped flame show good agreement between surrogates and JP-8 even with respect to benzene and toluene, as soot precursors.
- A procedure was demonstrated to reduce the experimental time to operate the burner for a complete flame scan to approximately 4 hours, with 30 hours of automated off-line GC/MS/FID chemical analysis.
- The JP-8 chemical analysis is invariably incomplete and accounts for roughly only 15-20% of the overall carbon introduced as liquid fuel.

Freely Propagating Flames

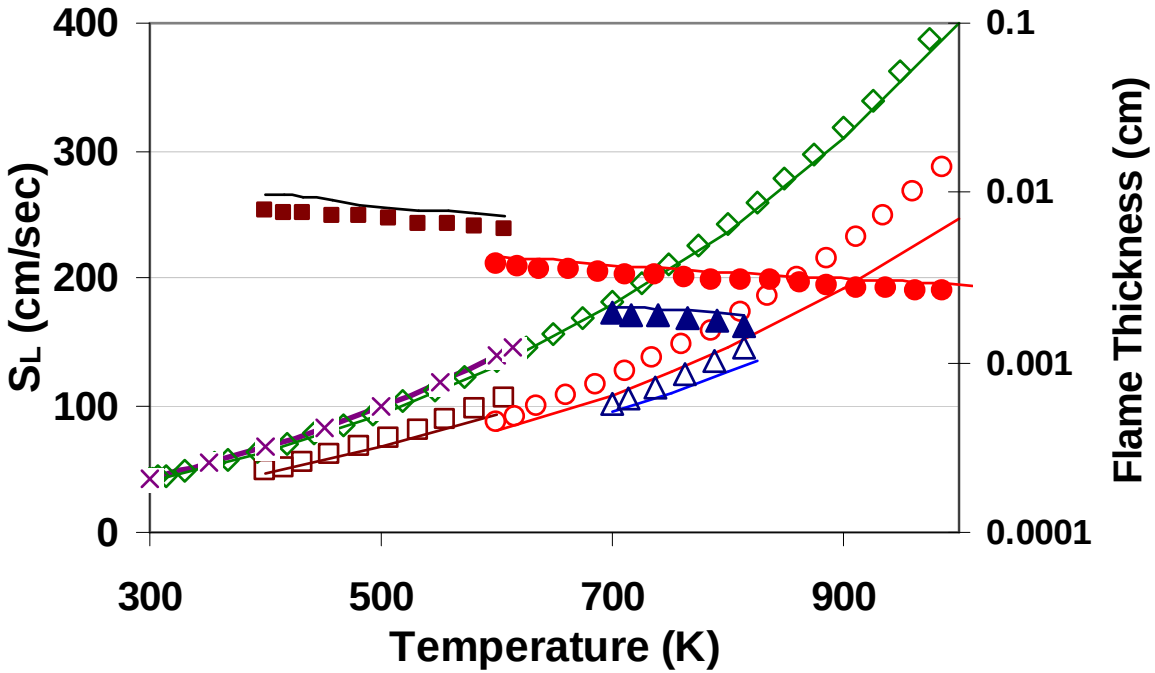
- Freely propagating JP-8/Air premixed flames were computed for
  - Pressures ranging between 0.5 to 35 atmospheres
  - Equivalence ratios varying between 0.4 – 2.7
  - Inlet temperatures ranging from 300 K to 1000 K
  - Vitiation equivalence ratio ranging from 0.0 – 0.3

Variations in Flame Speed and Flame Thickness as a Function of Pressure



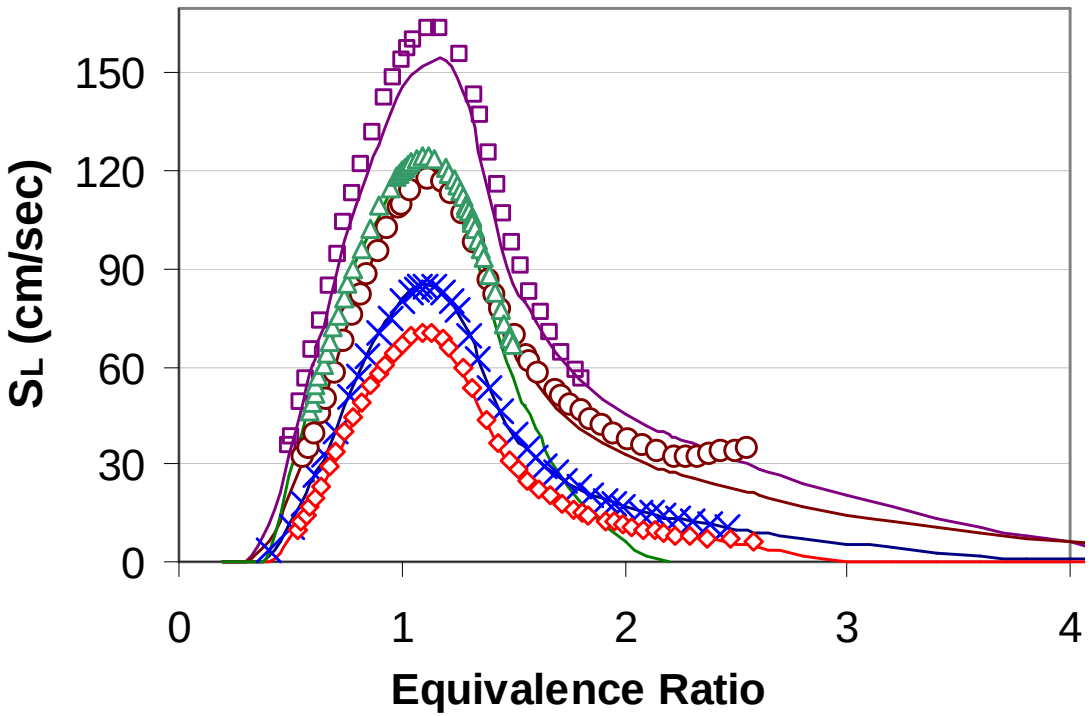
Flame speed (open symbols) and Flame Thickness (smaller solid symbols) at Stoichiometric Conditions. □ 400K, X 475K, ○ 600K, Δ 700K, and ◇ 800K. Solid lines are correlations.

Flame speeds and Flame thickness as a Function of Temperature



Flame speeds (open symbols) and Flame thickness (closed symbols) as a Function of Temperature at Stoichiometric Conditions. ◇ 1 atm, □ 5 atm, ○ 10 atm, Δ 20 atm. Solid lines are correlations.

Comparison of Flame Speeds as a Function of Equivalence Ratio



Comparison of Computations and Correlations of Flame Speeds for Selected Conditions as a Function of Equivalence Ratio. Symbols are computed flame speeds: □ 800K/10 atm, ○ 800K/35 atm, Δ 572K/1 atm, X 600K/10 atm, ◇ 500K/5 atm. Solid lines are correlations.

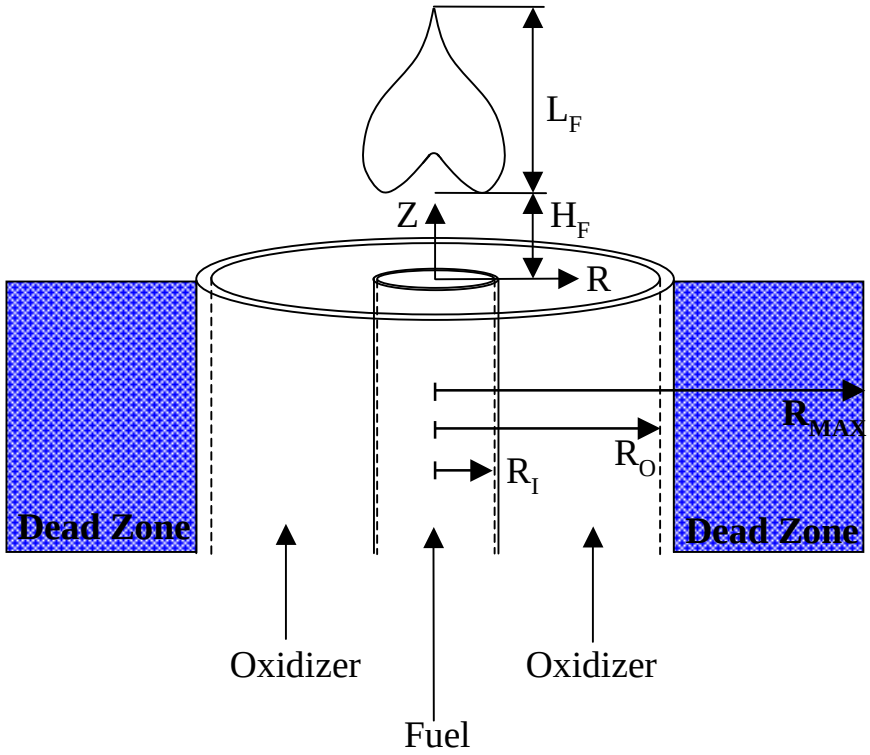
Parallel Simulation of Axisymmetric Coflow Laminar Diffusion Flames

- Goal is to develop a parallel algorithm that solves axisymmetric coflow diffusion flame problems across a distributed-memory computing cluster

- Motivation is to speed the simulation of combustion problems that are already tractable on a single processor
  - *e.g.*, steady-state and transient simulations of sooting flames using simple hydrocarbon fuels

  and to facilitate the simulation of complex combustion problems that were previously intractable on a single processor
  - *e.g.,* sooting, coflow/2-d counterflow diffusion flames using a six-component JP-8 surrogate blend

Axisymmetric Coflow Diffusion Flame Model



- Cylindrical coordinates
- Unconfined flow at atmospheric pressure
- Steady-state, (sooting), lifted diffusion flame
- Burner dimensions:

  R_I = 0.2 cm

  R_O = 2.5 cm

  R_{MAX} = 7.5 cm

Parallel Coflow Diffusion Flame Model

Issues needed to be addressed by parallel flame model

- ⇒ Domain decomposition of the computational tensor-product grid
- ⇒ Parallel implementation of a damped, modified, Newton's method
- ⇒ Parallel implementation of the block-line Gauss-Seidel preconditioned Bi-CGSTAB iterative solver

Domain Decomposition Techniques

Strategy

Uses a parallel computing model in which

- ⇒ Master and local processors perform computations
- ⇒ Master processor coordinates inter-processor communication and I/O
- ⇒ Large data structures are decomposed onto each processor (*e.g.,* Jacobian)
- ⇒ Small data structures are stored on each processor (*e.g.*, solution vector)

Simple, strip-domain decomposition techniques partition contiguous blocks of physical grid rows onto individual processors

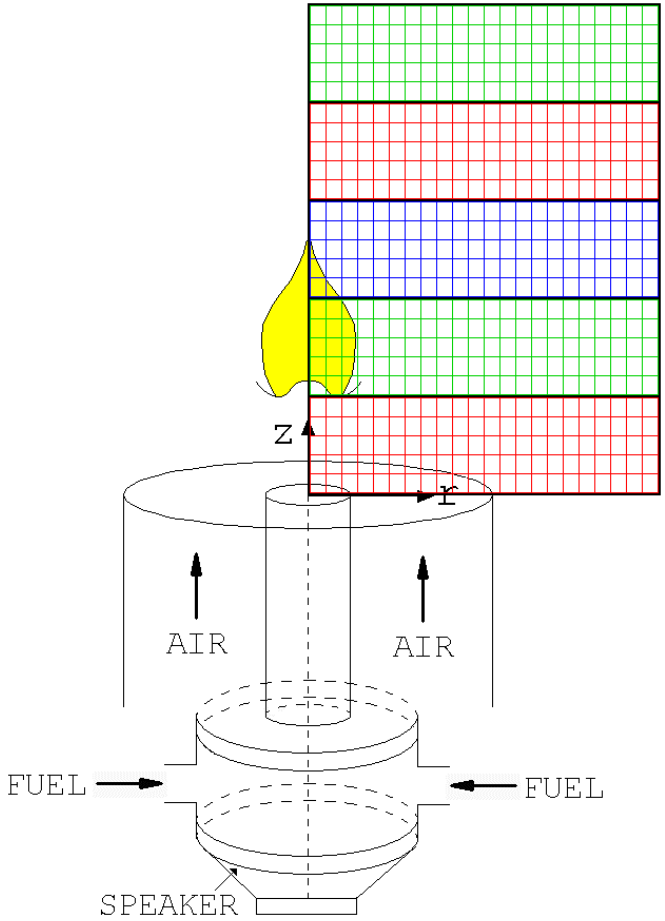
- ⇒ Evenly distribute the total number of N_{PZ} grid rows across the N_{PROC} processors of the cluster
- ⇒ Remaining grid rows are distributed amongst all local processors
- ⇒ Master processor receives fewest possible grid rows

Results in processor-specific subdomains each containing N_{PZL} contiguous grid rows

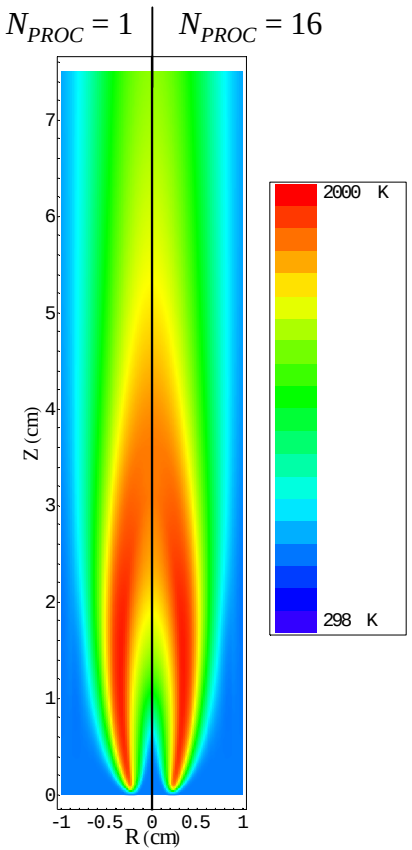
Ethylene-Air Test Case

Sooting ethylene-air diffusion flame

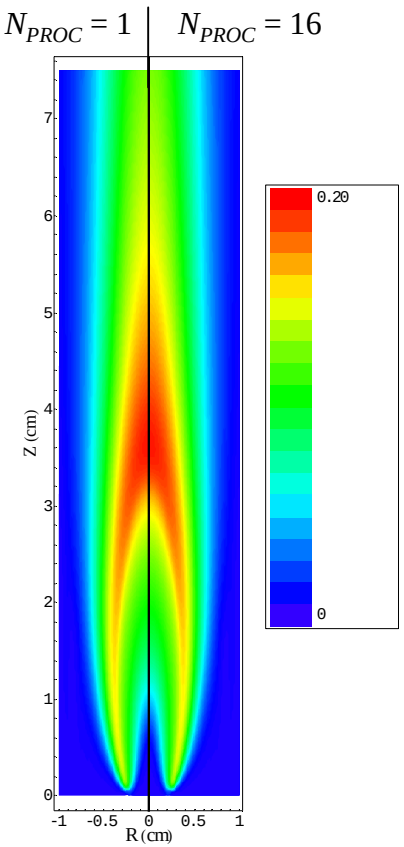
- ⇒ 66 chemical species
- ⇒ 20 soot sections
- ⇒ 476 reactions (Sun, Sung, Wang and Law, 1996)
- ⇒ Bridges gap between simple fuels and multicomponent surrogate blends



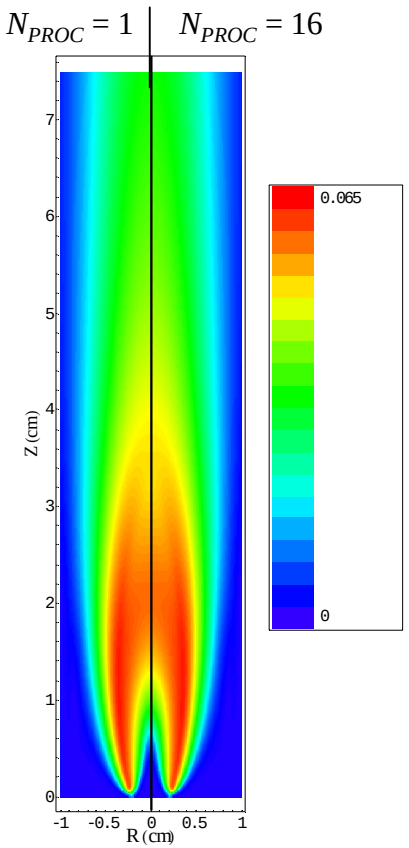
Results: Comparison of Serial and Parallel Solutions



Predicted Temperature

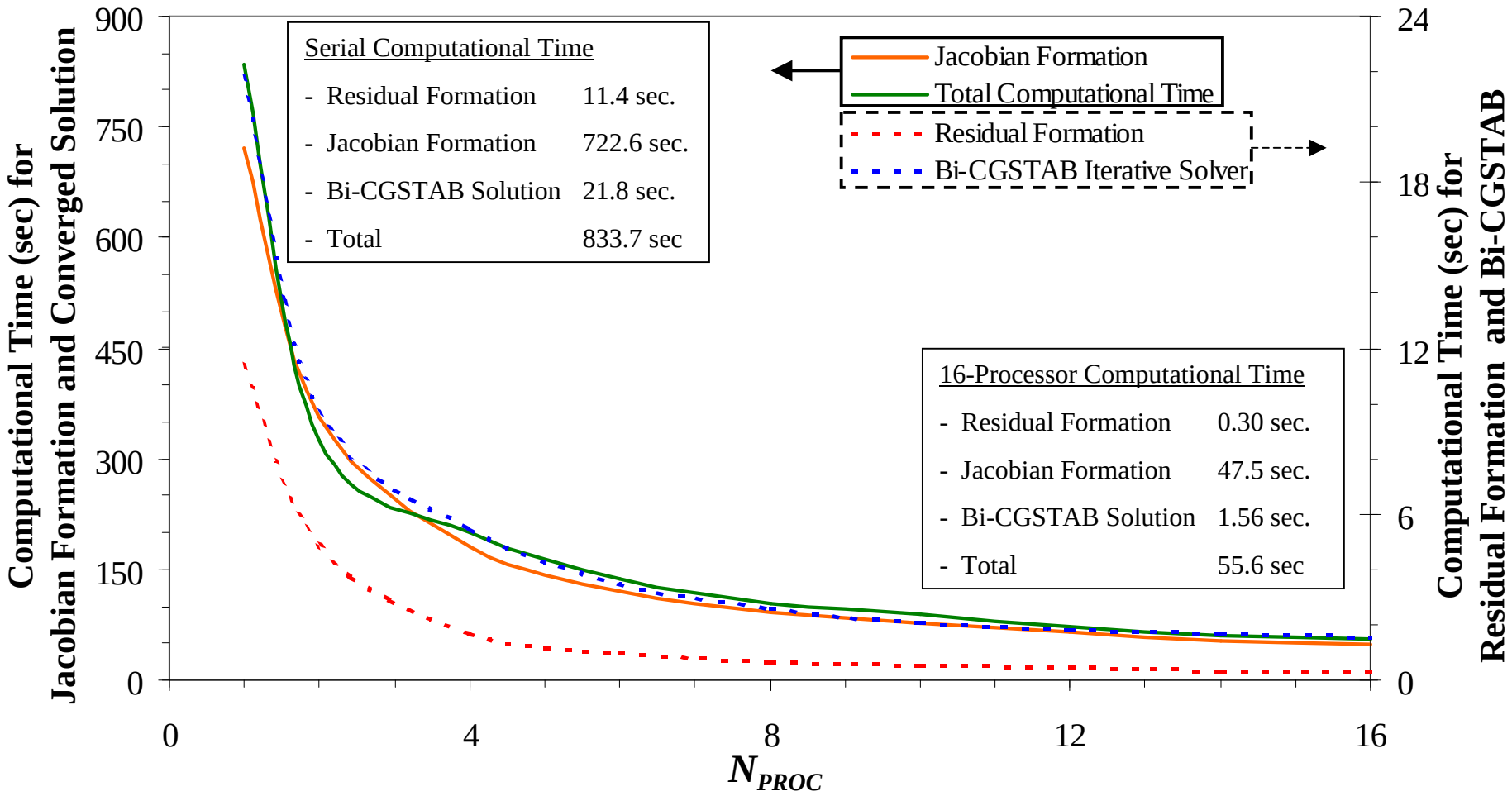


Predicted H_2O Mass Fraction



Predicted CO_2 Mass Fraction

Results: Reduction in Computational Time



JP-8 Coflow Diffusion Flame

•JP-8 is modeled as a six-component surrogate mixture (Violi, *et al.*, 2001)

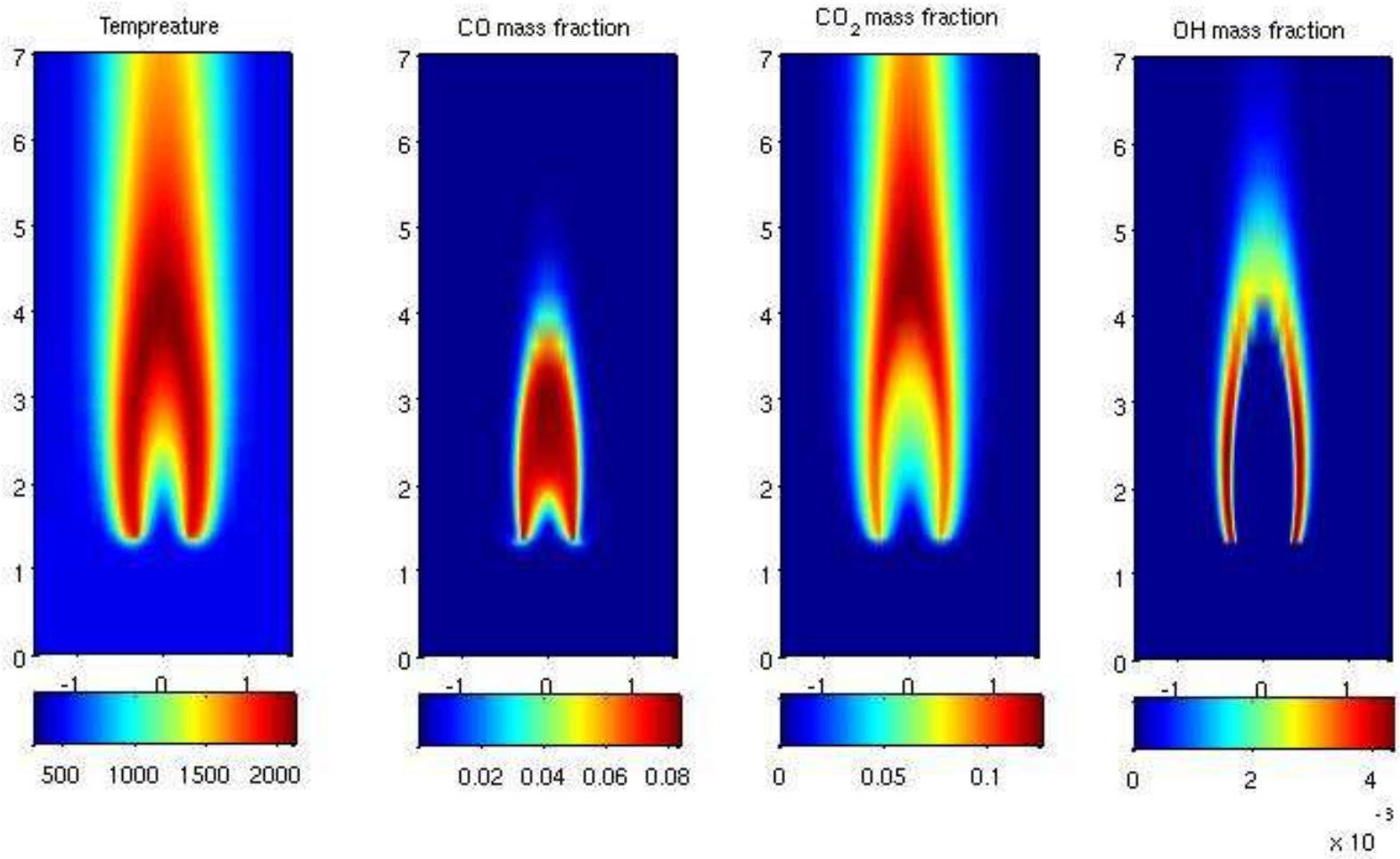
10% Iso-octane (C_8H_{18}), 20% Methylcyclohexane (C_7H_{14}), 5% Tetralin ($C_{10}H_{12}$), 30% Dodecane ($C_{12}H_{24}$), 20% Tetradecane ($C_{14}H_{30}$), 15% m-Xylene (C_8H_{10})

•Surrogate kinetics are modeled using a 221-species mechanism containing 5032 reactions

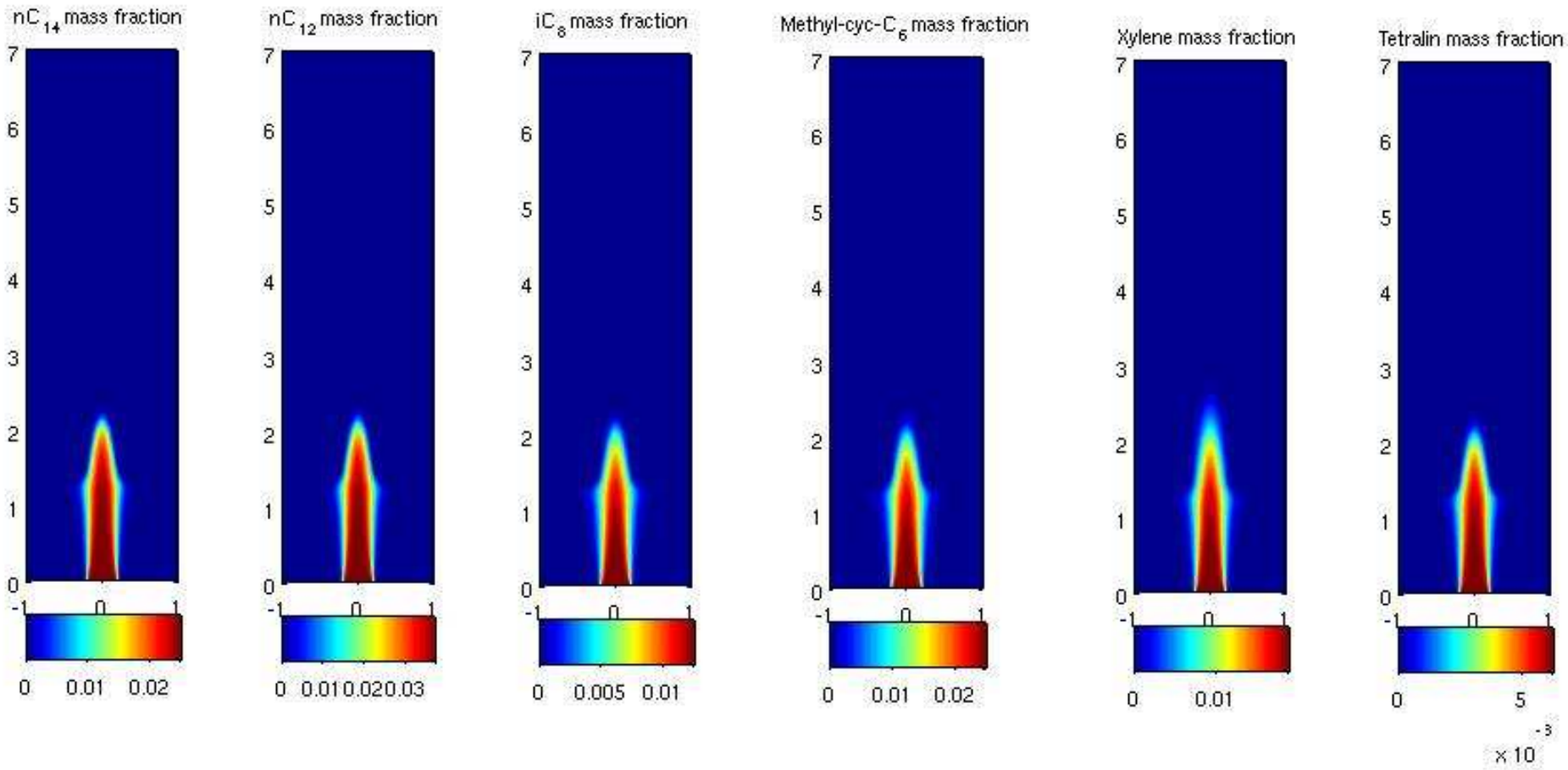
•VF= 35 cm/sec (average) VOX=35 cm/sec (plug)

•TF=480 K TOX = 480 K

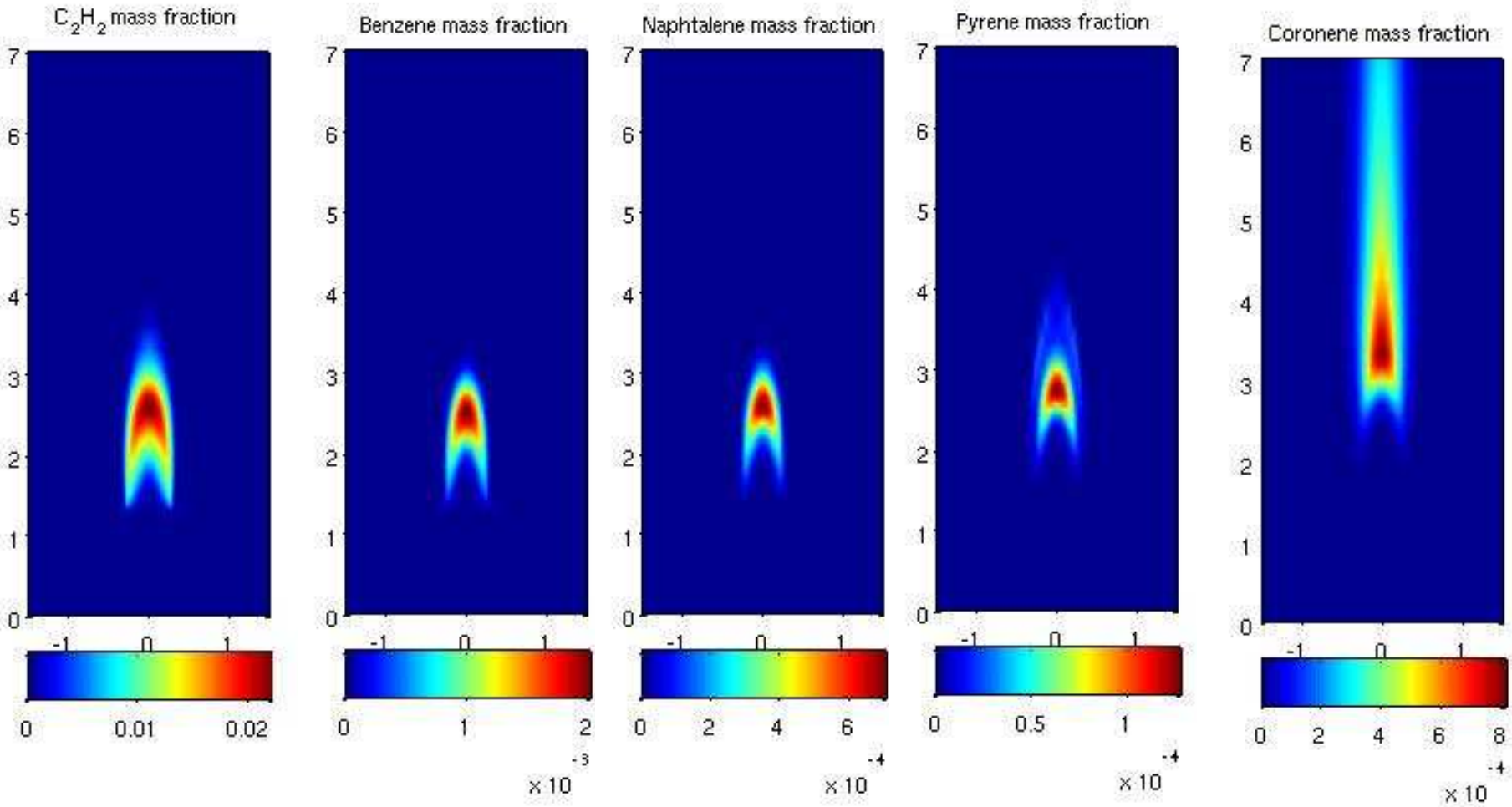
Temperature and Major Species



Surrogate Components



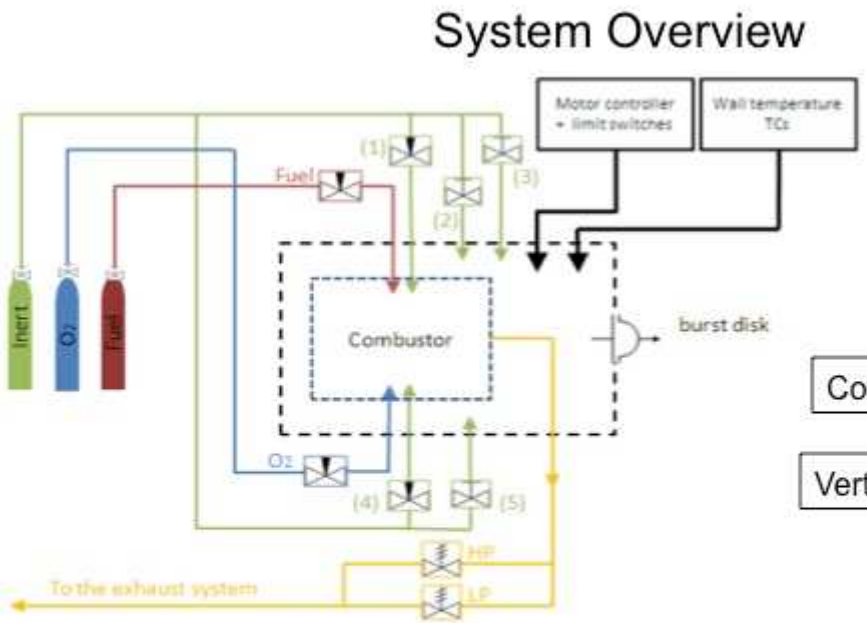
Soot Related Species

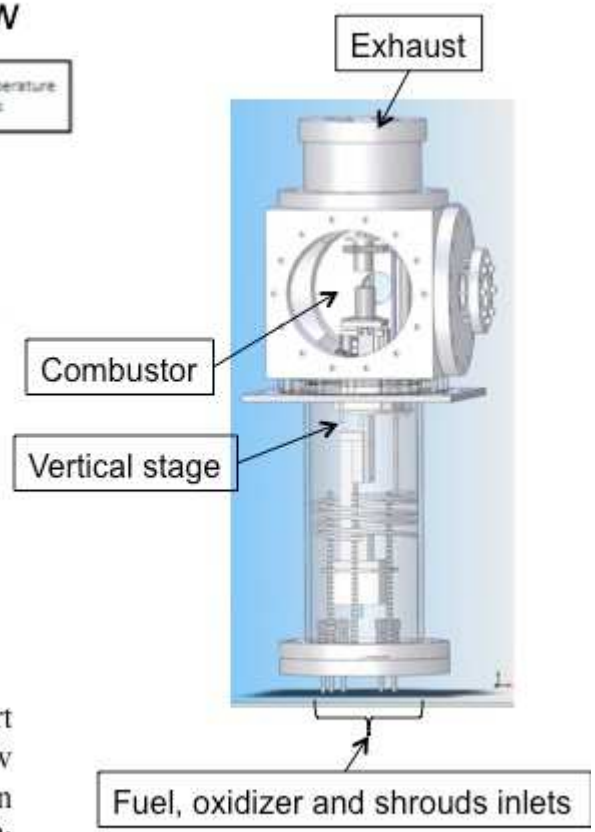


High Pressure Flames

- Examine systematically individual components of surrogate(s) and model their chemical kinetics (collaboration with Charlie Westbrook);
- Design and test a high-pressure chamber to perform similar work at high pressures (up to 40 atm);
- Model two-dimensional flame configurations using parallel methodology
  - -Coflow flames
  - -Counterflow
- Employ various chemistry reduction techniques

System Overview

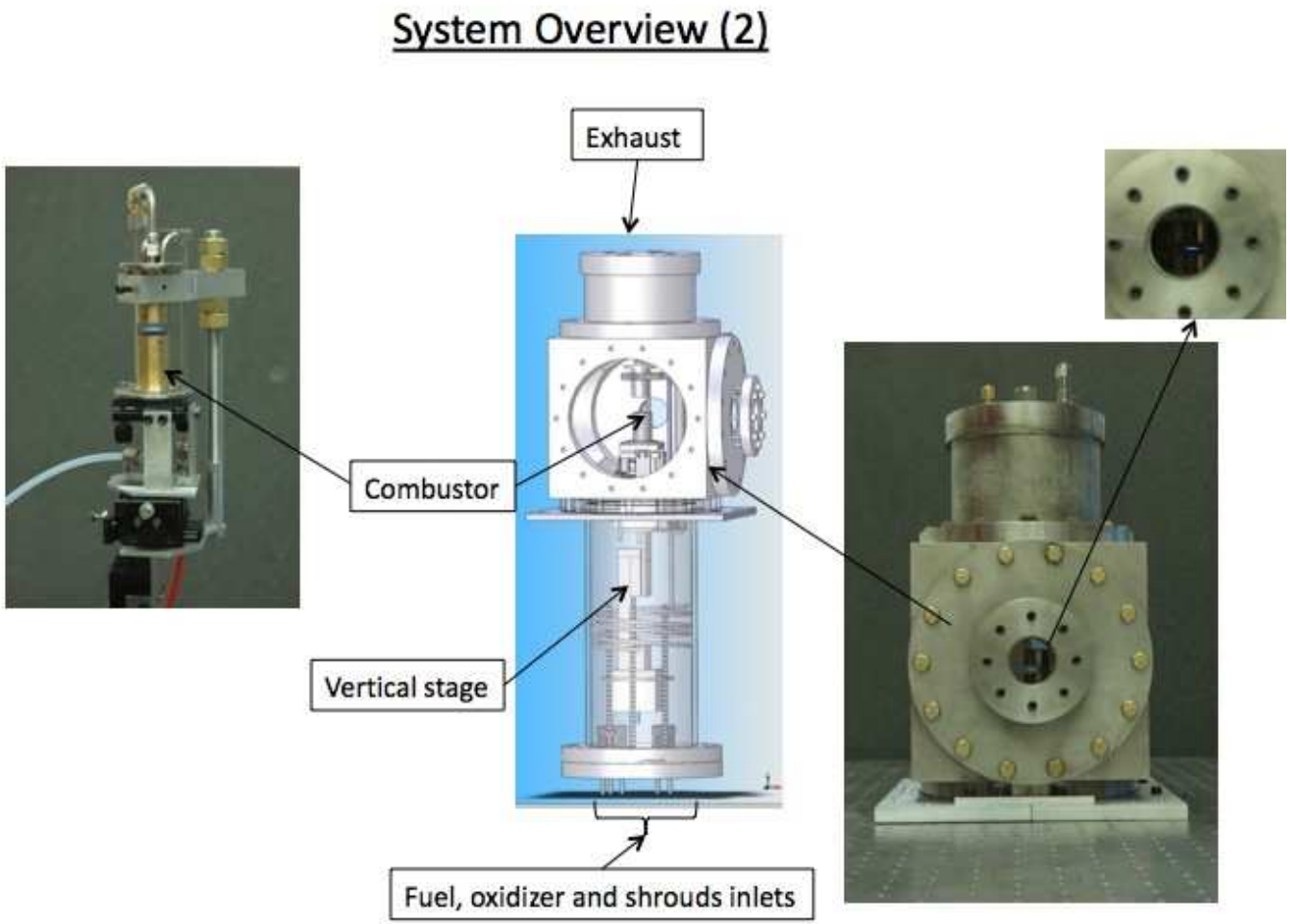




•Fuel: fuel flow controller, O2: oxygen flow controller,

•(1): inert flow controller for fuel dilution, (2): auxiliary inert rotameter, (3): inert rotameter for fuel shroud, (4): inert flow controller for oxygen dilution, (5): inert rotameter for oxygen side shroud, LP: low pressure back-pressure regulator, HP: high pressure back-pressure regulator.

Burner and Flame



System Overview

- The chamber is an 8x8x8 in^3 stainless steel cube bored with 6 in holes
- The system is controlled by a Labview interface to ease the monitoring of safe chamber operation
- Chamber pressure and wall temperature are automatically checked for anomalous values
- Visual interface controls the mass flow controllers to set automatically the experimental conditions (strain rate, fuel mass fraction and stoichiometric mixture fraction)
- A glow coil allows flame ignition at high pressure
- 20 different flow controllers are necessary to set accurately the flow rates in the pressure range 1 to 40 atm. A system of valves controls the switching between the set of flow controllers depending on pressure range

Scaling Considerations

The selection of the counterflow configuration was based upon

-the anticipated suppression of buoyancy instabilities at elevated pressures compared to coflow flames

-the use of the temperature-time history to control soot formation by strain rate and dilution

-the use of an inert such as helium to maintain the Reynolds number within the laminar range and to compensate for the pressure-induced reduction in flame thickness by stretching the Convective-Diffusive and Reactive-Diffusive zones.

Computational Estimates

P (atm)	Inert	δ (mm)	a (s^{-1})	Re	Gr/Re^2
1	N_2	4	95	$2.0\ 10^2$	0.15
10	He	3.3	95	$2.8\ 10^2$	0.15
20	He	2.4	95	$5.6\ 10^2$	0.15
40	He	1.7	95	$1.1\ 10^3$	0.15

Preliminary Results

•Preliminary testing demonstrated that stable flames could be established at pressures up to 25 atm without any buoyancy instability or turbulence. The flames were operated under either nonsooting or lightly sooting conditions at stoichiometric mixture fractions between 0.24 and 0.5 and strain rates between 20 s^{-1} and 150 s^{-1}, regardless of pressure.

•Scaling considerations suggest that by experimenting with a high-diffusivity diluent such as Helium, sufficiently thick flames can be stabilized, despite the high-pressure conditions, for subsequent probing of the flame structure with adequate resolution.

•Future work includes

- Implementing optical diagnostics (OH LIF) to check the thickness of the reacting layer (Lewis number effect);

- Gas sampling by ultrafine quartz microprobes for off-line GC/MS analysis.

Acknowledgements

- Luca Tosatto, Hugo Bufferand and Saeed Jahangirian performed the bulk of the experiments; Lorenzo Figura designed and tested the high-pressure chamber; and Bruno Coriton helped with OH LIF experiments.
- Dr. James (Tim) Edwards (WPAFB) supplied the JP-8.
- Research supported also by
  - ARO DURIP (Grant # W911NF-07-1-0231, Dr. Ralph Anthenien, Program Manager)