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

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Project Overview

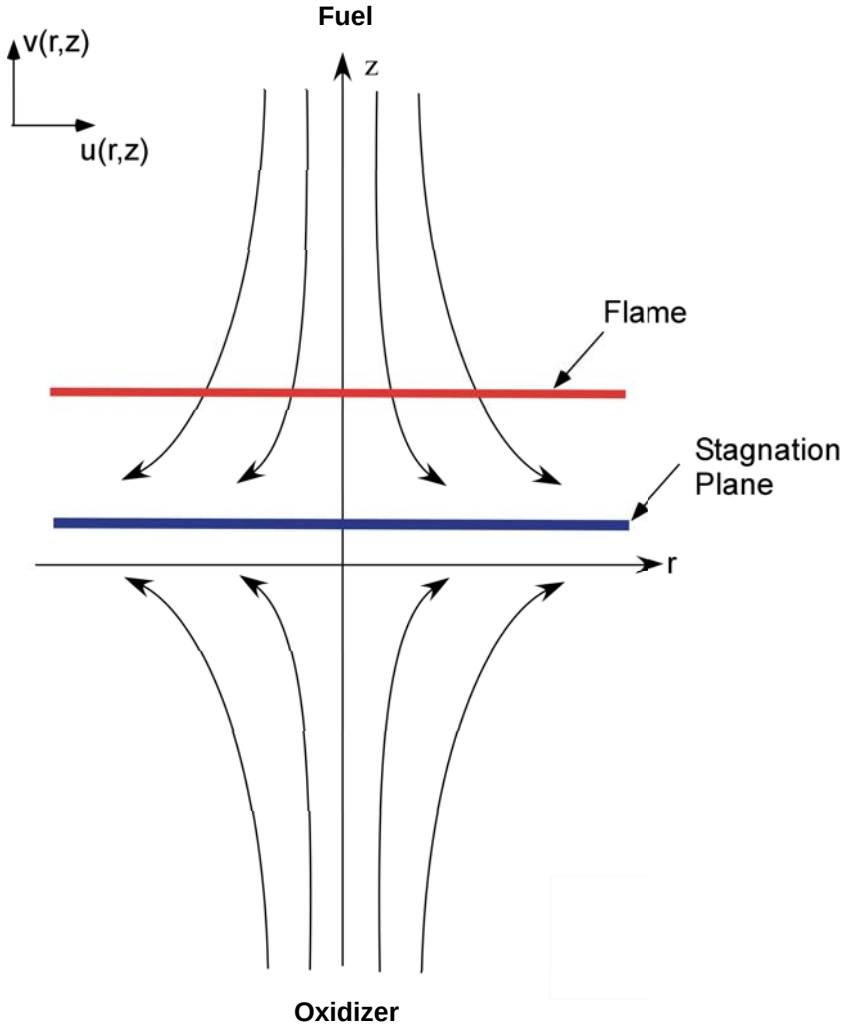
- Utilize surrogates and individual fuel components in a computational and experimental flame study of counterflow and coflow flames

  - Use the counterflow flame as a doped flame reactor
  - Design and test a high-pressure chamber to perform at pressures up to 40 atm
  - Implement a high-pressure soot formation model
  - Thermophoretic sampling and OH LIF flame thickness analysis
  - Develop a parallel computing methodology
  - Chemistry reduction techniques

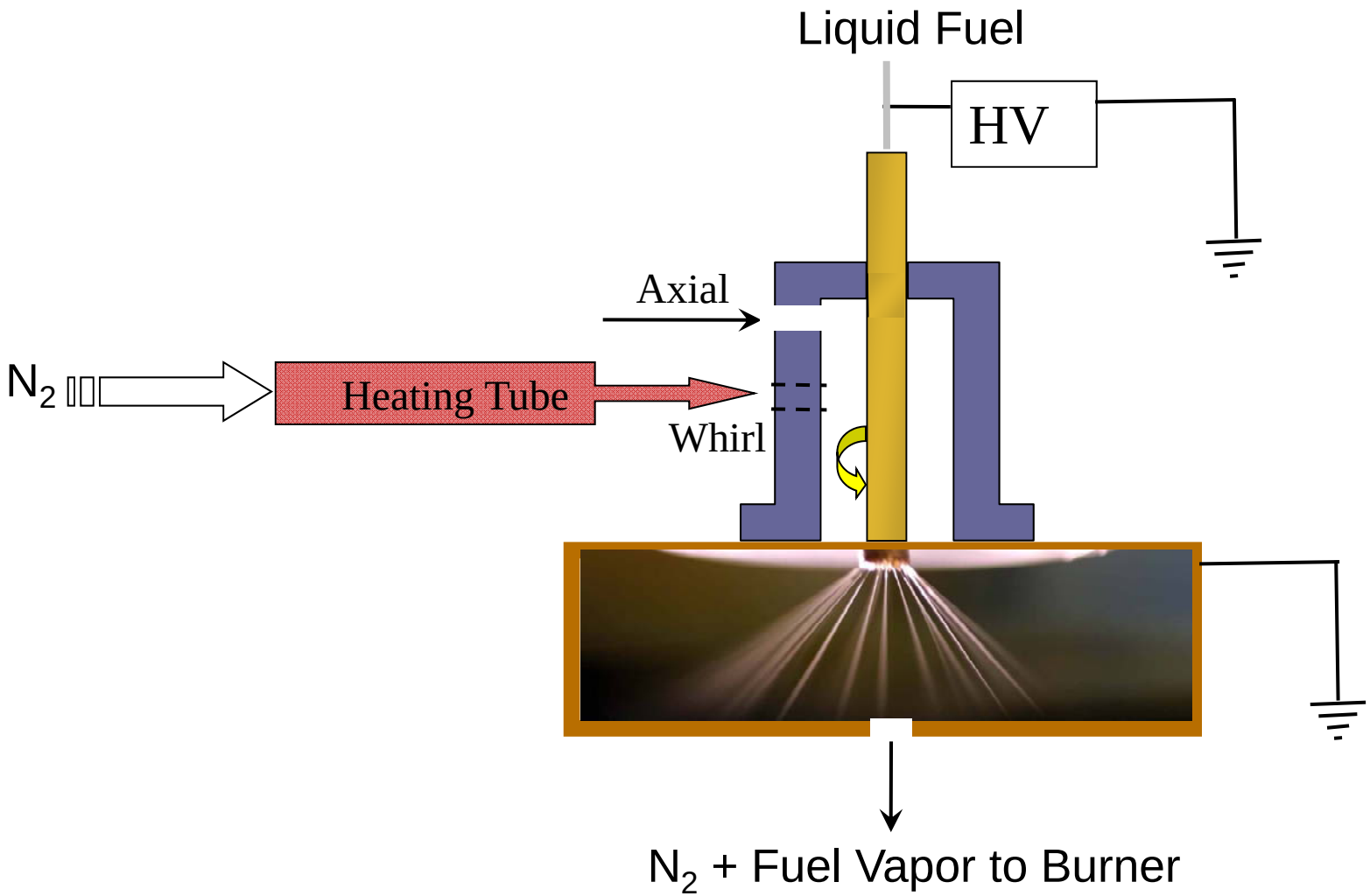
- Curate data

Counterflow Flames

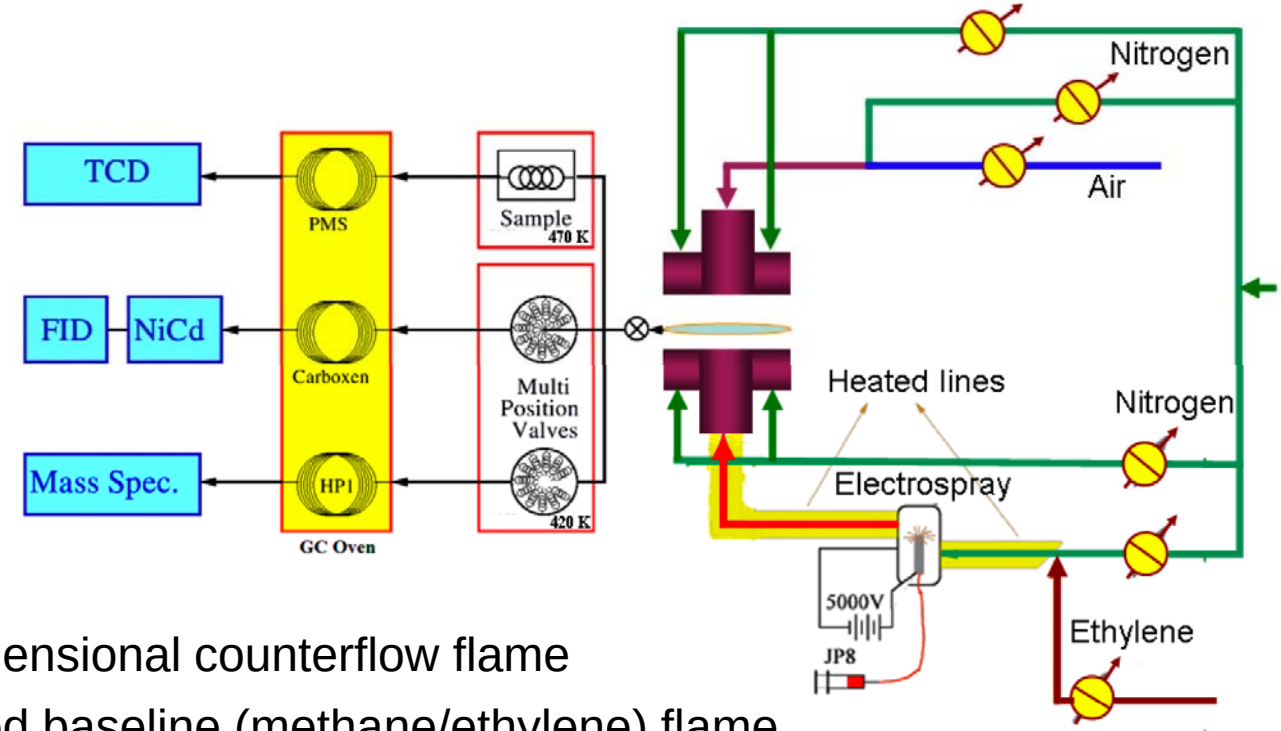
- Single Component – e.g., TMB, decane, iso-octane, dodecane, MCH
- Surrogates – e.g., Aachen, SERDP, 6-component (Violi et al.)
- Base CH4 and C2H4 flames as doped reactors
- High Pressure



Electrospray Vaporizer



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

Computational Approach

- Single-solution methods provide computational temperature, species and velocity profiles

- Arc length continuation is used to vary the strain rate, inlet conditions and pressure
  - -Automatically adjusts mesh to follow flame
  - -Determines critical points

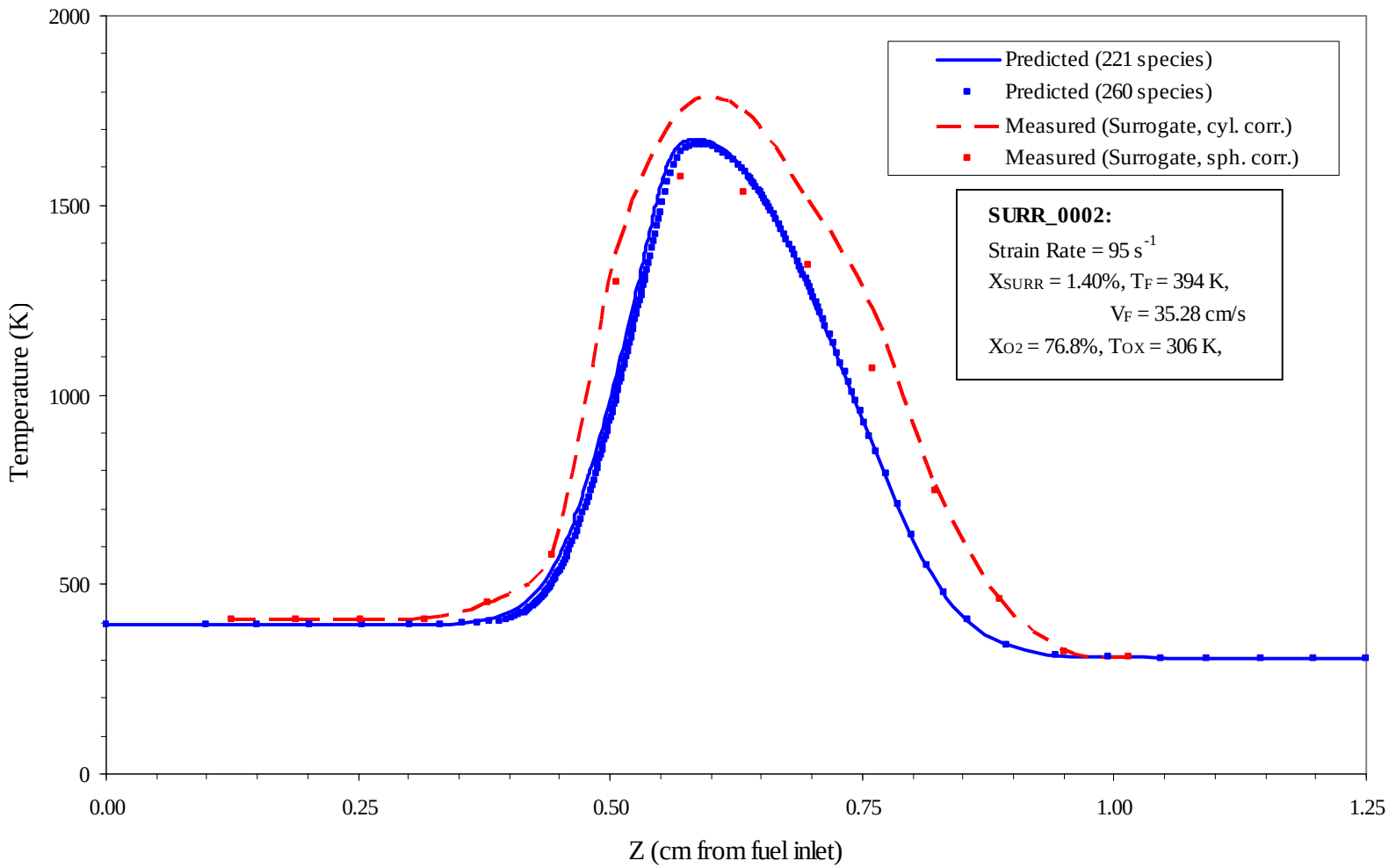
JP-8 Surrogate

- 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

Results: Surrogate Flames
Comparison of Temperature Profiles



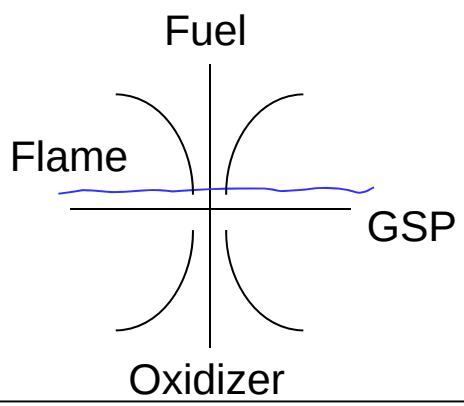
Doped Flames

- Probing of diffusion flames as flow reactors to study kinetics of critical surrogate components
- Examination of soot formation under conditions of incipient sooting
- Compare results using kinetic mechanisms, e.g., Ranzi C16, Wang (C1-C4) etc.
- Extension to high pressures

Selection of Flames Spanning a Broad Range of Conditions

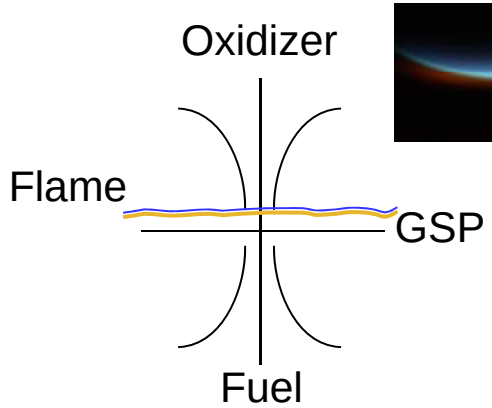
Non-sooting Flame Set

- Max. Temp= 1750K
- Strain Rate= 102 s^{-1}
- Stoich. mixture fraction Z_f= 0.76
- Fixed temperature profile
- Flame on fuel side of stagnation plane



Sooting Flame Set

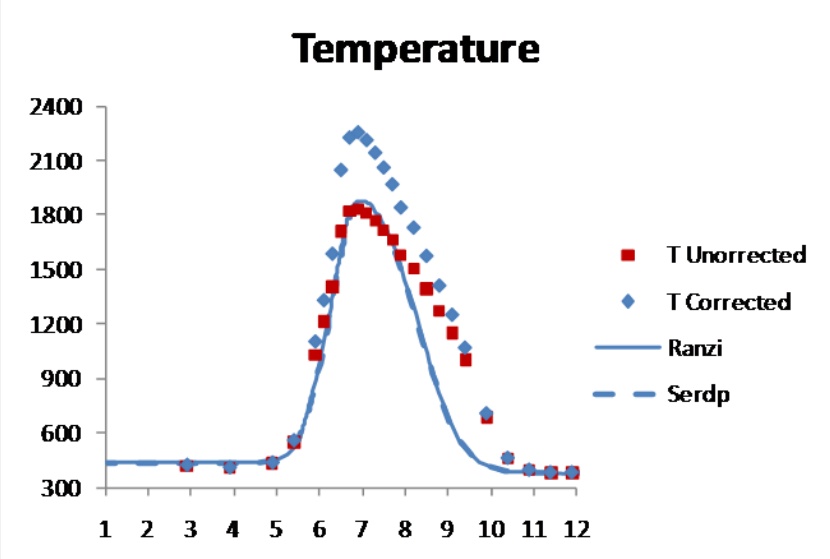
- Max. Temp= 1989K
- Strain Rate= 69 s^{-1}
- Z_f= 0.18
- Fixed temperature profile
- Flame on oxidizer side of stagnation plane

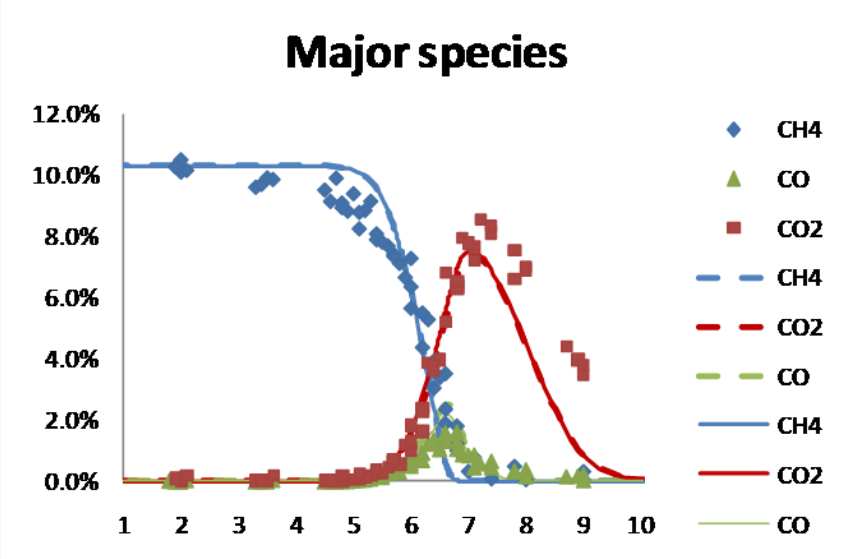


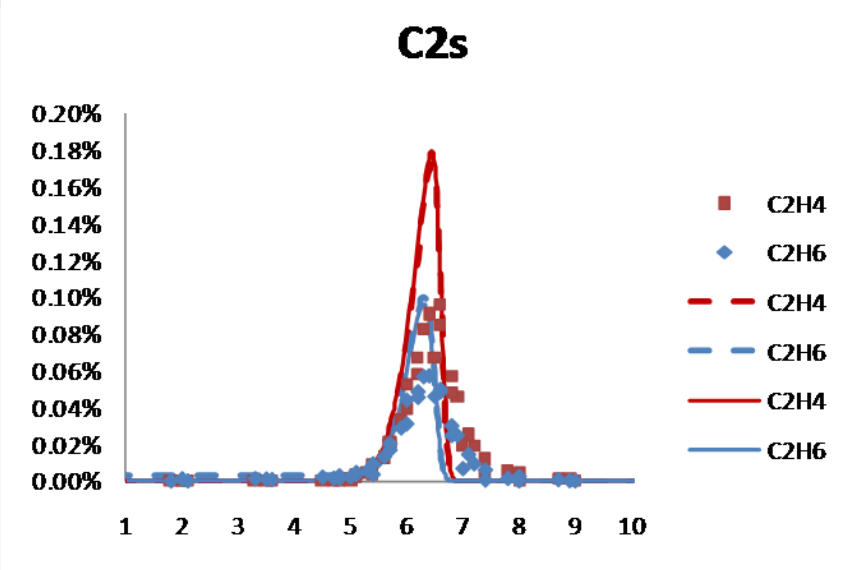
Experimental Conditions

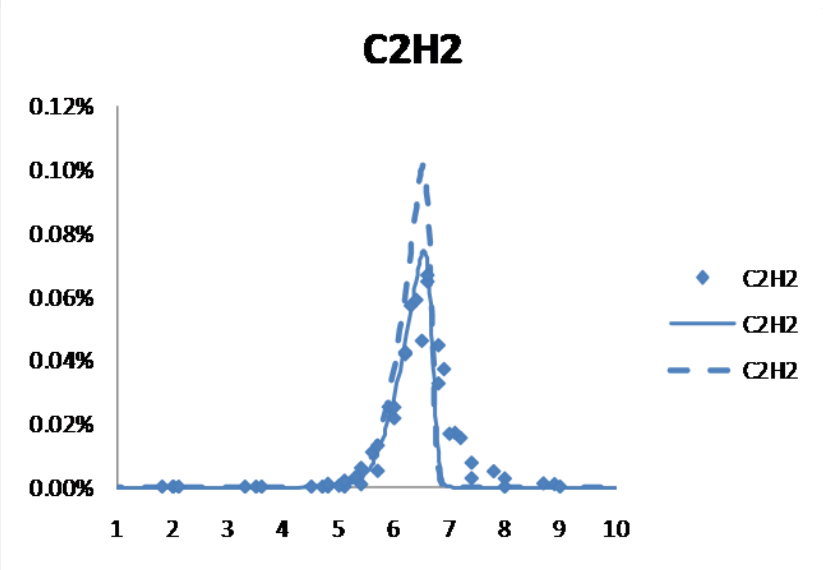
	CH_4 Baseline	CH_4 Decane	CH_4 TMB	CH_4 Achen	C_2H_4 Baseline	C_2H_4 + Achen	C_2H_4 + Decane	C_2H_4 + TMB
Molar Composition								
N_2	0.897	0.897	0.897	0.897	0.728	0.734	0.733	0.729
CH_4	0.103	0.103	0.103	0.103				
C_2H_4					0.272	0.2641	0.2641	0.2641
Impurities	232 ppm	232 ppm	232 ppm	232 ppm	660 ppm	660 ppm	660 ppm	660 ppm
,2,4-trimethylbenzene			229	229		450 ppm		450 ppm
n-Decane		774		774		1520 ppm	1520 ppm	
ass Flux (g/(cm^2·min))	2.8	2.93	2.84	2.97	1.62	1.68	1.67	1.63
Temperature (K)	435	435	435	435	407	407	407	407
Molar Composition								
N_2	0.227	0.227	0.227	0.227	0.8070	0.814	0.814	0.814
O_2	0.773	0.773	0.773	0.773	0.1843	0.186	0.186	0.186
ass Flux (g/(cm^2·min))	3.19	3.37	3.24	3.42	1.89	1.93	1.92	1.90
Temperature (K)	380	380	380	380	370	370	370	370
Strain Rate (s^{-1})	110		120		89.9		92.3	
z_f		0.76				0.18		

Baseline Methane

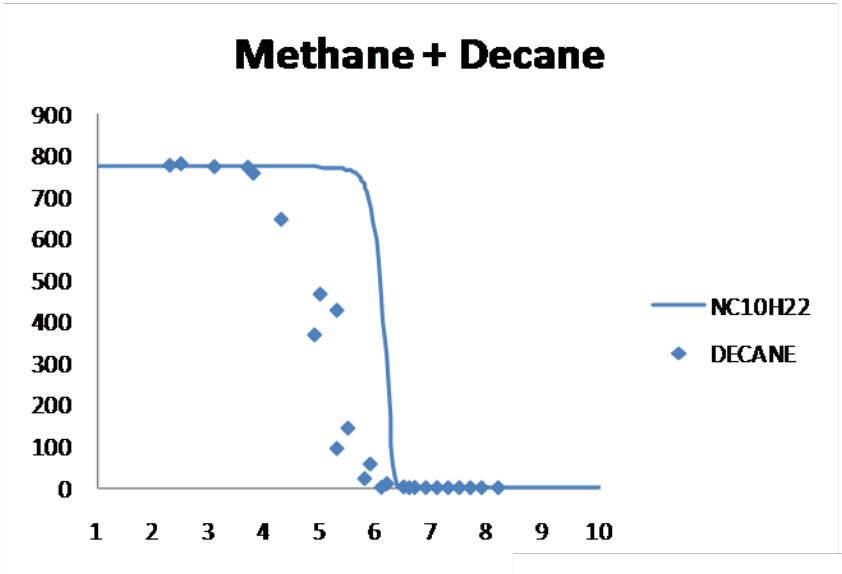


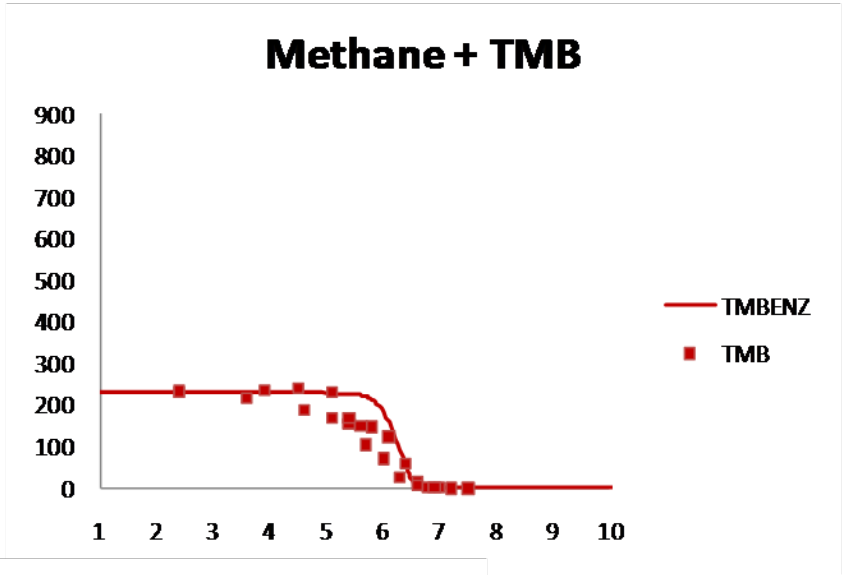


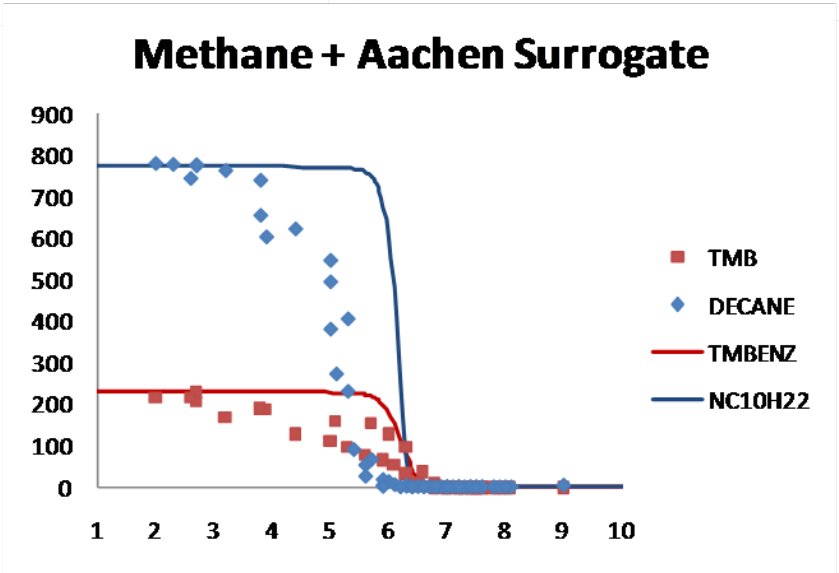




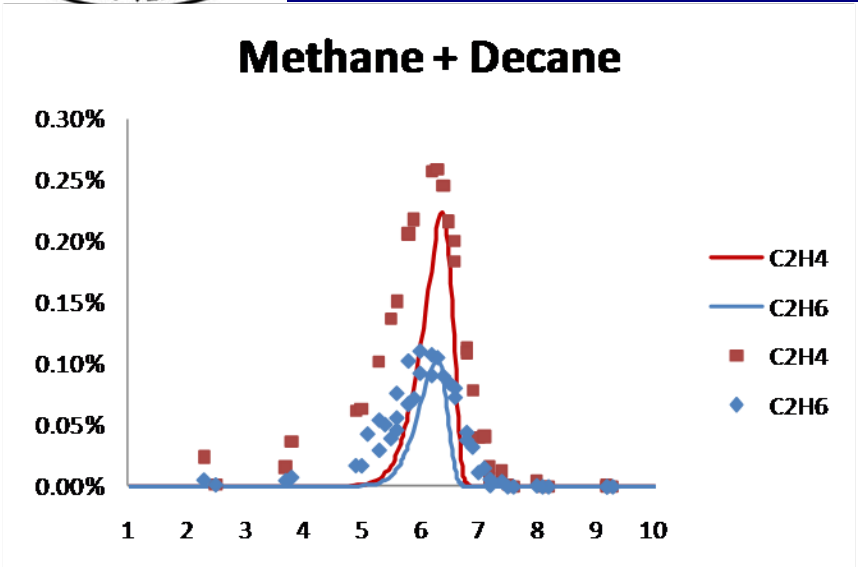
Primary Dopant(s)

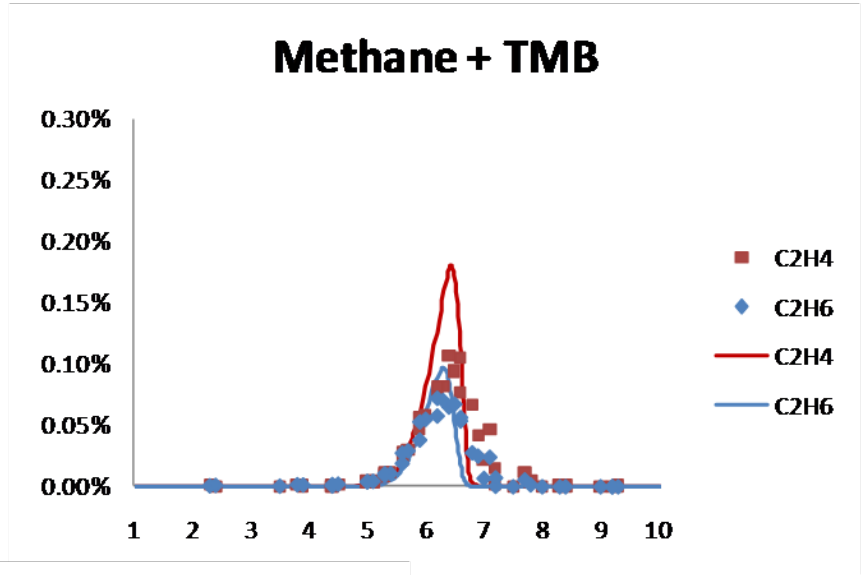


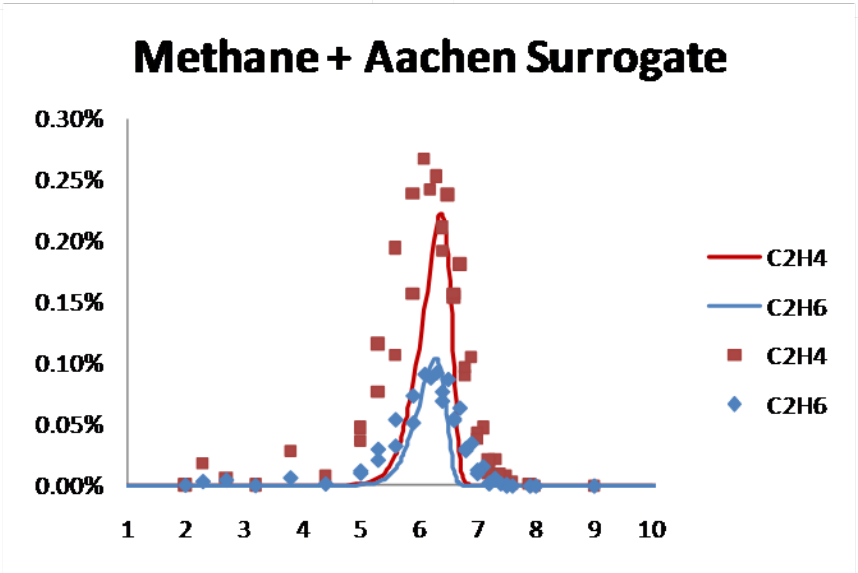




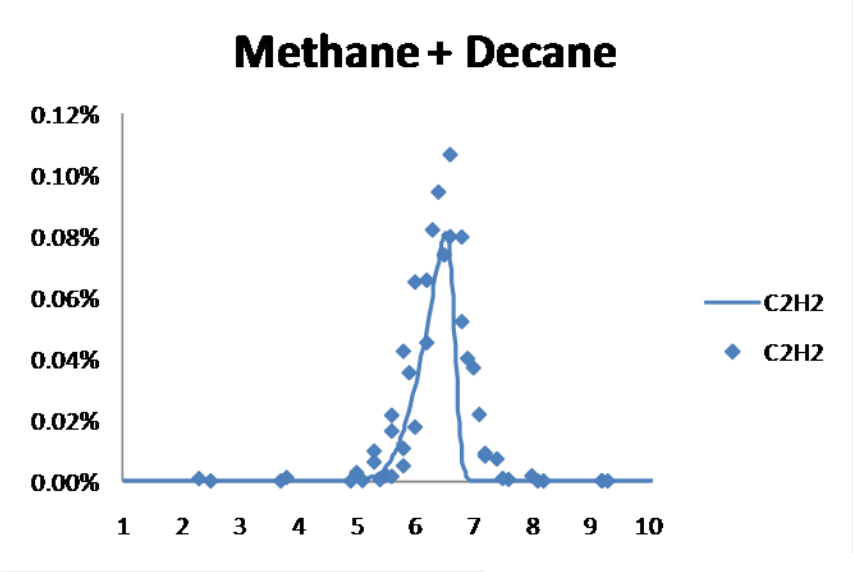
C2 Species


Methane + Decane
0.30%
0.25%
0.20%
0.15%
0.10%
0.05%
0.00%
1 2 3 4 5 6 7 8 9 10
C2H4
C2H6
C2H4
C2H6


Methane + TMB
0.30%
0.25%
0.20%
0.15%
0.10%
0.05%
0.00%
1 2 3 4 5 6 7 8 9 10
C2H4
C2H6
C2H4
C2H6


Methane + Aachen Surrogate
0.30%
0.25%
0.20%
0.15%
0.10%
0.05%
0.00%
1 2 3 4 5 6 7 8 9 10
C2H4
C2H6
C2H4
C2H6

C_2H_2


Methane + Decane
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C2H2
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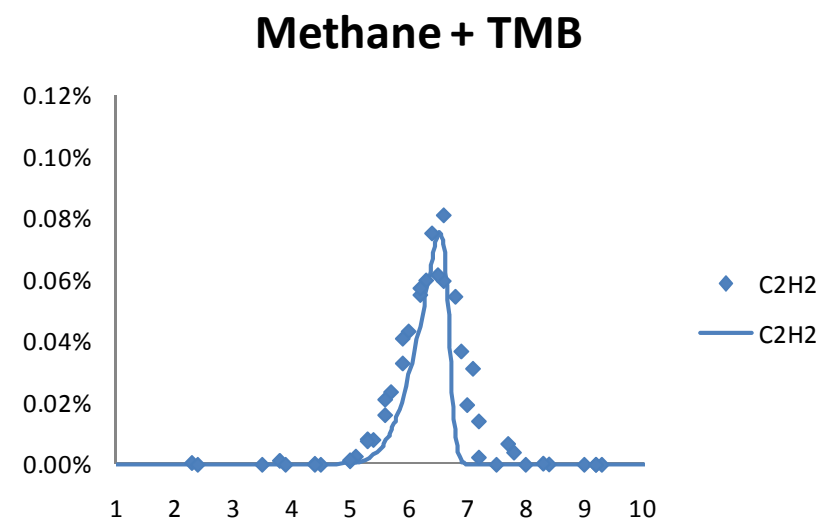
Methane + TMB
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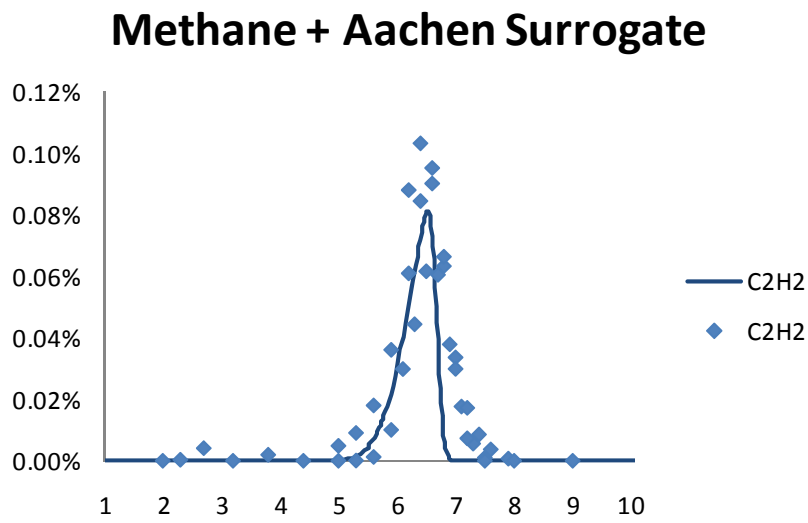
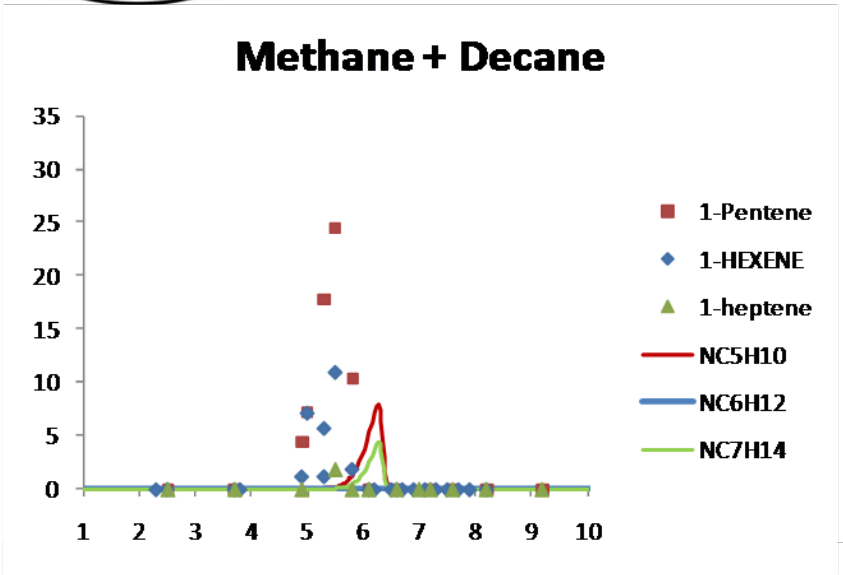
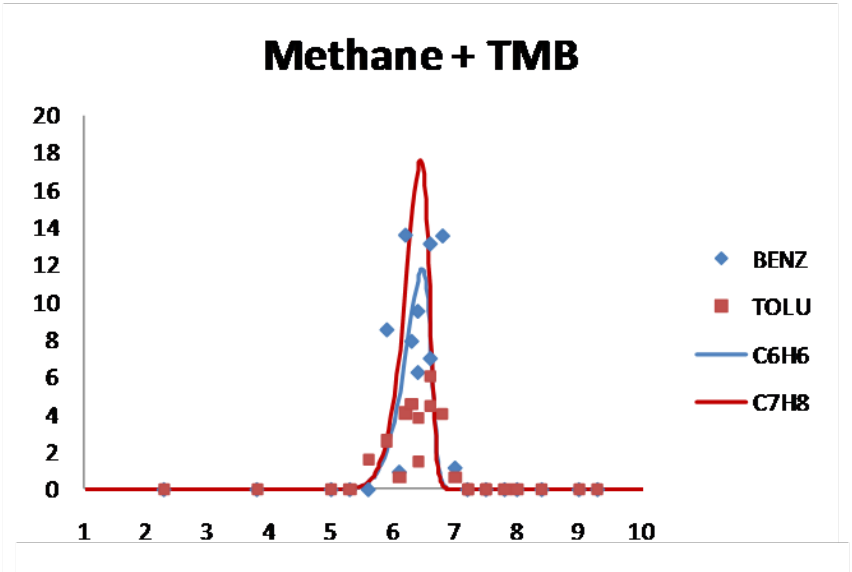
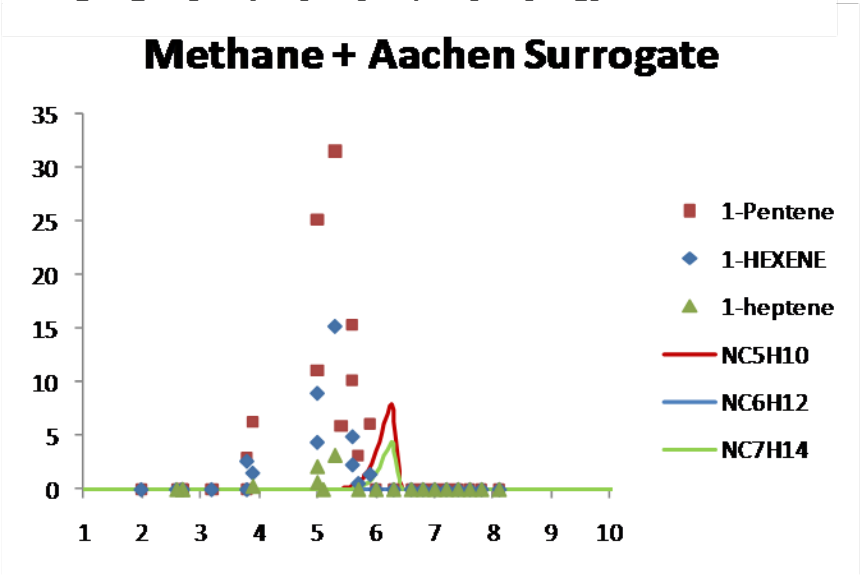
C2H2
C2H2

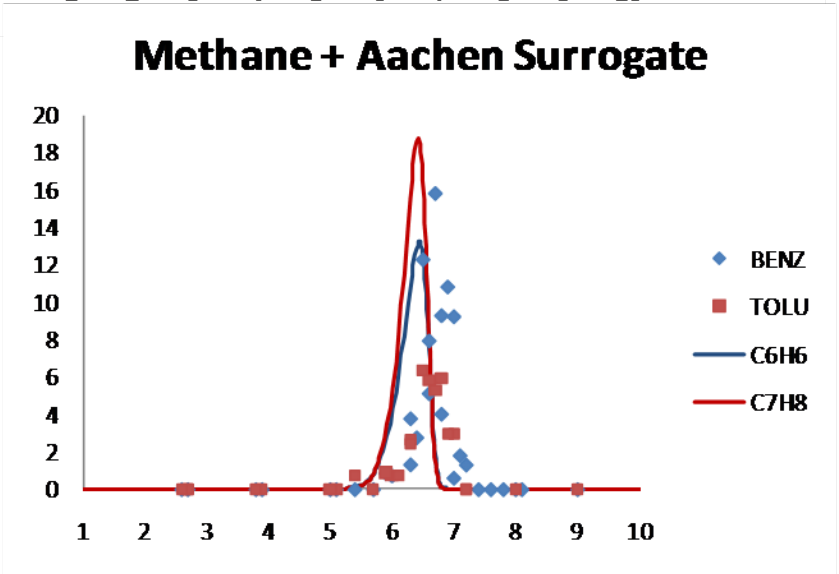

Methane + Aachen Surrogate
0.12%
0.10%
0.08%
0.06%
0.04%
0.02%
0.00%
1 2 3 4 5 6 7 8 9 10
C2H2
C2H2

Alkenes - Aromatics



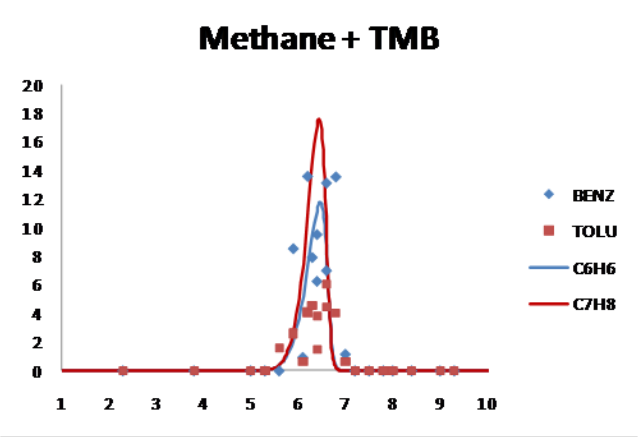


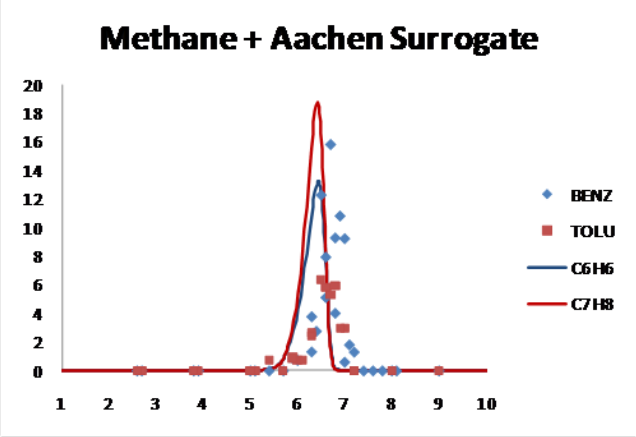




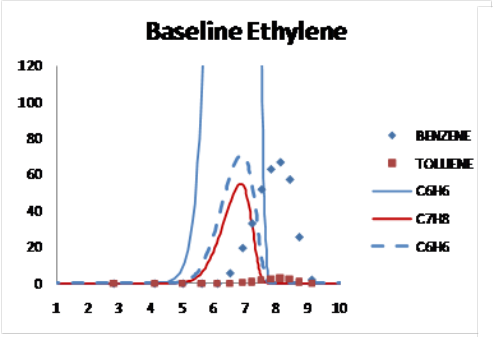
Aromatics

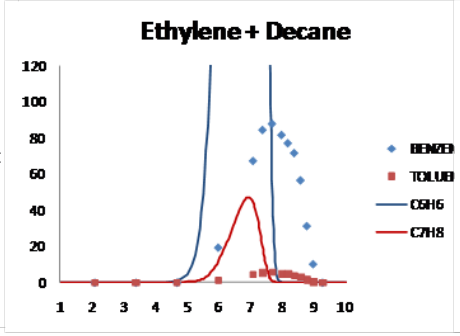
Nonsooting Methane Flame (z_f=0.18)

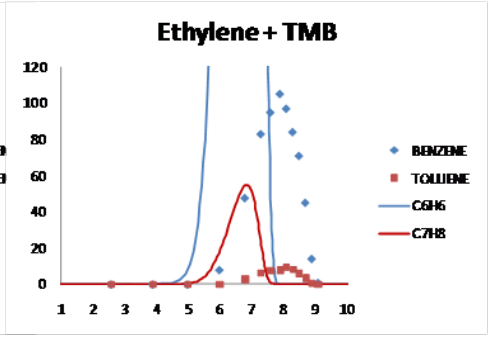


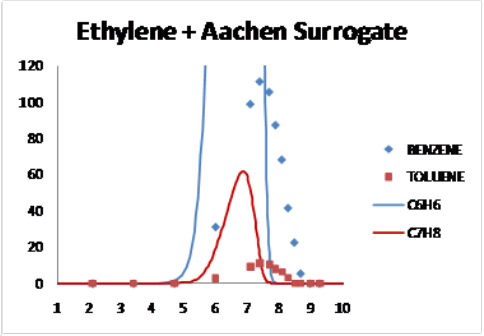


Sooting Ethylene Flame (z_f=0.76)









Principal Observations

- Experimental testbed for validation of kinetic mechanism in flames to account for diffusive-reactive effects
- Major species are modeled well by Ranzi's kinetics, but are based on simple (CH_4, C_2H_4) fuels, showing that the model "degenerates" appropriately to simple hydrocarbons
- Minor species are in reasonable agreement, which may deteriorate if concentrations are very small (<50 ppm)

High-Pressure Fames

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.

Critical Scaling

•Laminar Flow

$$Re = \frac{Ud}{\nu} < 2{,}000$$

•Suppression of buoyancy instabilities

Counterflow

$$\frac{Gr}{Re^2} = \frac{gl^3\Delta T}{8\nu^2\overline{T}} \cdot \frac{\nu^2}{U^2d^2} = \frac{gl^3\Delta T}{8\left(\frac{al}{2}\right)^2 d^2\overline{T}} = \frac{gl\Delta T}{2a^2d^2\overline{T}}$$

Coflow

$$\frac{Gr}{Re^2} = \frac{gl^3\Delta T}{8\nu^2\overline{T}} \cdot \frac{\nu^2}{U_0^2d^2}$$

Here the critical difference is in the length scale l that in coflow flames is larger and enters with the third power. In couterflow l is the burner separation and is of the same order of magnitude as d

Spatial Resolution Issues

Mixing layer thickness decreases with $p^{-1/2}$

$$\delta \approx \sqrt{\frac{D}{a}} \propto \sqrt{\frac{1}{p \cdot a}}$$

Inert substitution to compensate for the reduced thickness of the temperature profile

$$\frac{\delta_T\big|_{He}}{\delta_T\big|_{N_2}} = \sqrt{\frac{\alpha_{He} \cdot a_{N_2}}{\alpha_{N_2} \cdot a_{He}}} \approx \sqrt{8.9 \cdot \frac{a_{N_2}}{a_{He}}} = 3.0 \cdot \sqrt{\frac{a_{N_2}}{a_{He}}}$$

and of the species profile

$$\frac{\delta_m\big|_{He}}{\delta_m\big|_{N_2}} = \sqrt{\frac{D_{He} \cdot a_{N_2}}{D_{N_2} \cdot a_{He}}} \approx \sqrt{3.4 \cdot \frac{a_{N_2}}{a_{He}}} = 1.8 \cdot \sqrt{\frac{a_{N_2}}{a_{He}}}$$

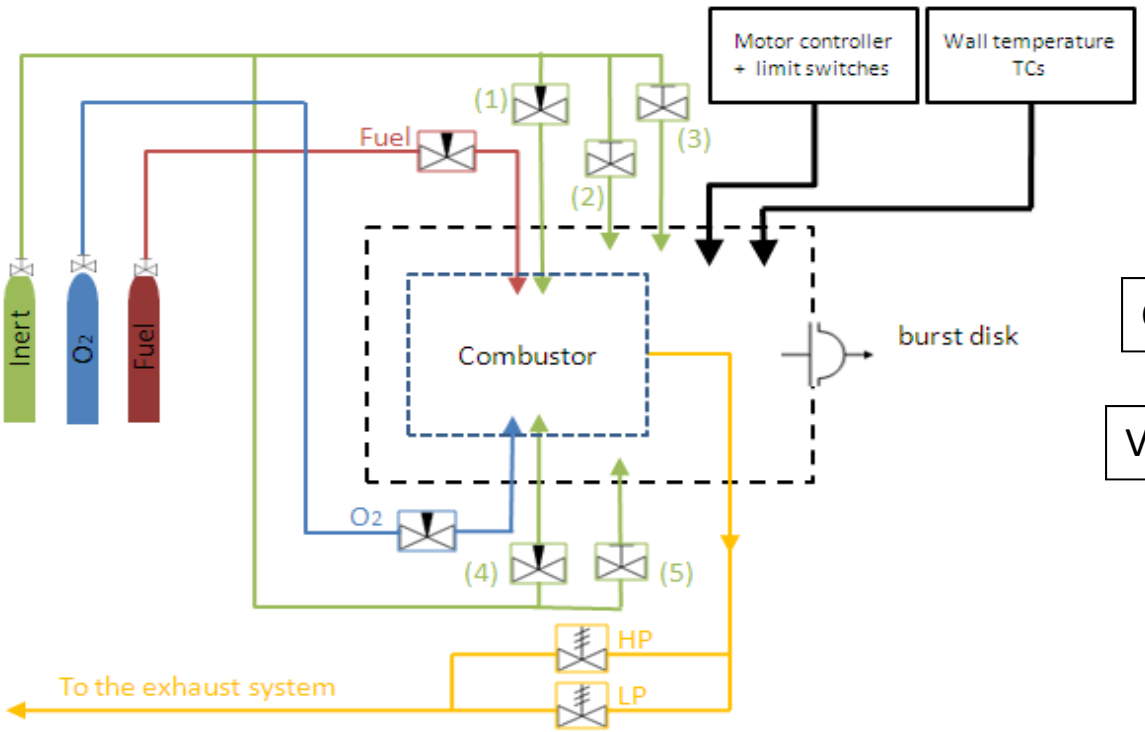
Computational Estimates

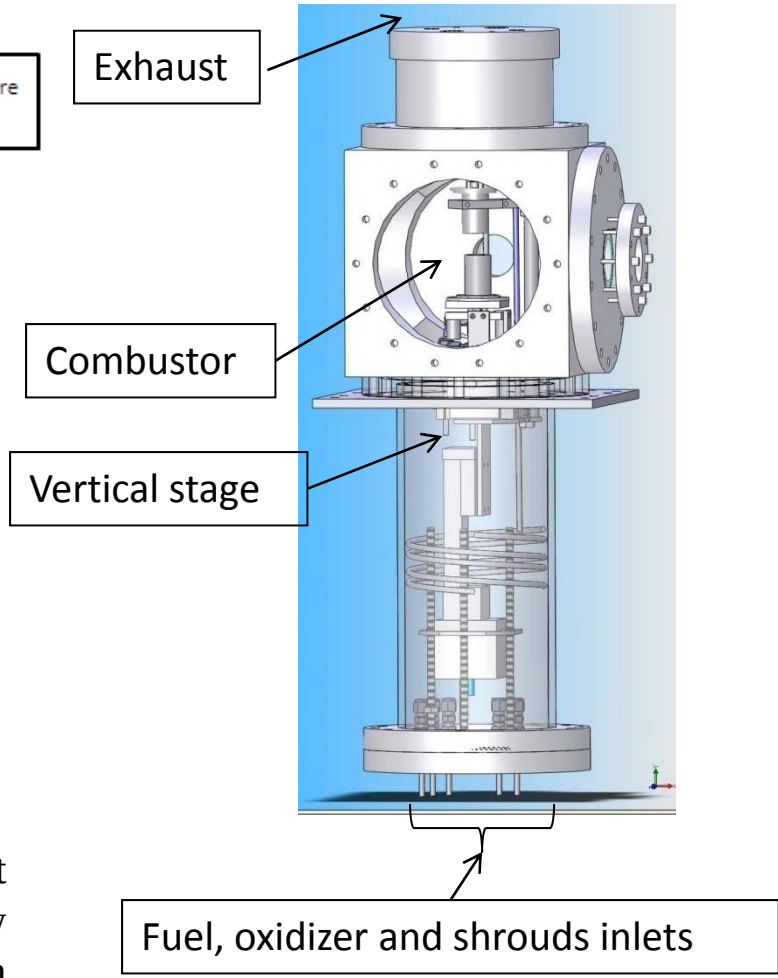
P (atm)	Inert	δ (mm)	a (s^{-1})	Re	Gr/Re^2
1	N_2	4	95	$2.0\ 10^2$	0.15
10	He	3.3	95	$2.8\ 10^2$	0.15
20	He	2.4	95	$5.6\ 10^2$	0.15
40	He	1.7	95	$1.1\ 10^3$	0.15

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

System Overview

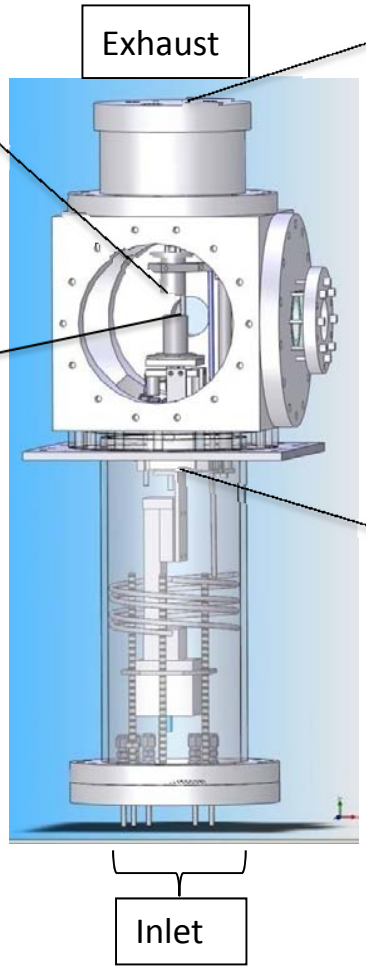




Fuel: fuel flow controller, O2: oxygen flow controller, (1): inert flow controller for fuel dilution, (2): auxiliary inert rotameter, (3): inert rotameter for fuel shroud, (4): inert flow controller for oxygen dilution, (5): inert rotameter for oxygen side shroud, LP: low pressure back-pressure regulator, HP: high pressure back-pressure regulator.

He-Diluted 25 atm Flame

Stable He-diluted blue flame at 25 atm



No impediments to reach higher pressures, up to 40 atm, except for flow meter limitations

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 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

Soot Concerns

- Soot formation increases rapidly as pressure rises
- Previous soot models were based upon one atmosphere submodels
- Diagnostic Difficulties
  - Use of gas sampling by ultrafine quartz microprobes for off-line GC/MS analysis
  - Application of optical diagnostics (e.g., OH LIF)

Modified Aerosol Equations for High Pressure Simulations

From atmospheric flames (free molecular regime) to practical aero engine combustion (transition to continuum regime), the mean free path, λ, (and Knudsen number, $Kn = 2\lambda/dp$) decrease dramatically.

Modifications required for

- Particle diffusion
- Coalescence rates
- Thermophoresis
- Growth/oxidation surface reaction rates

Approach follows that described by M. Sitarski and J.H. Seinfeld, J. Coll. Int. Sci., Vol. 61, 261, 1977

Modified Aerosol Dynamical Equations

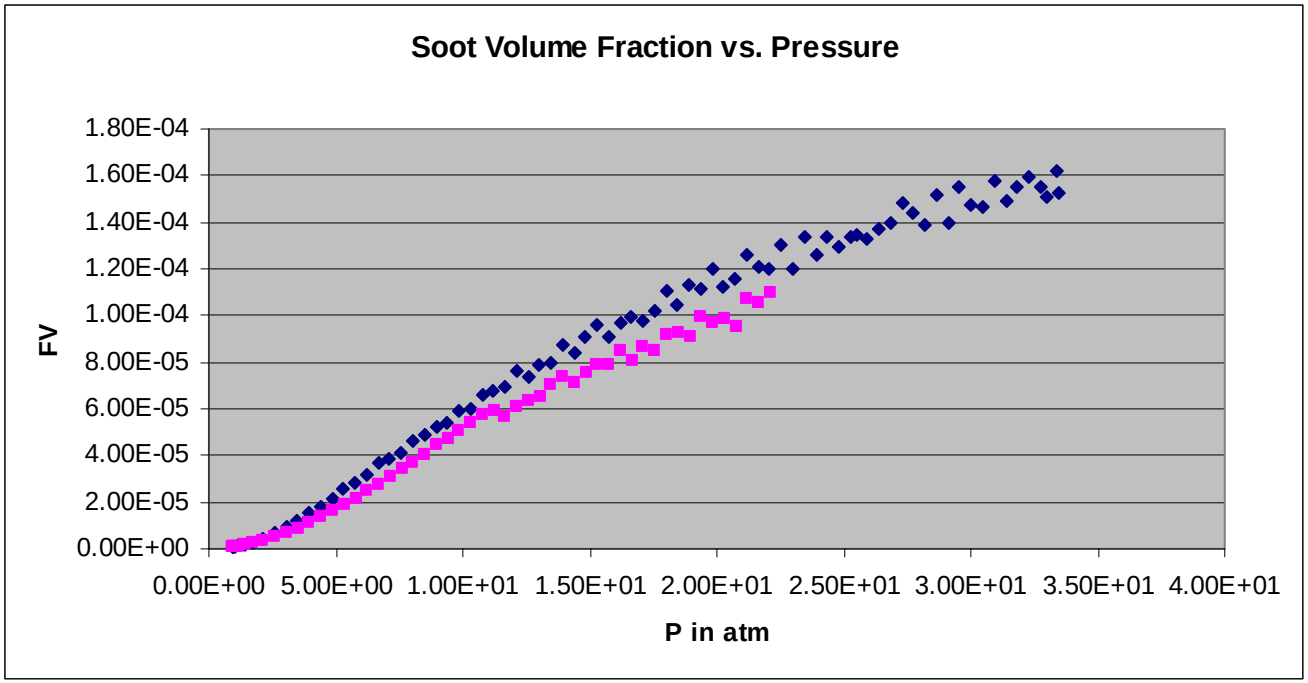
Diffusion: $D_m = ((kT)/(3\pi d_p \mu))(1.+Kn(1.257+.4exp(-1.1/Kn)))$

Thermophoresis: $V_{th} = - (1+AKn+BKn*exp(CKn))(Cp_g+C_tKn\lambda i)(2Cp_g\Delta T/5P)/$
$((1+3C_mKn)(2Cp_g+Cp_s+2C_iKnCp_s))$

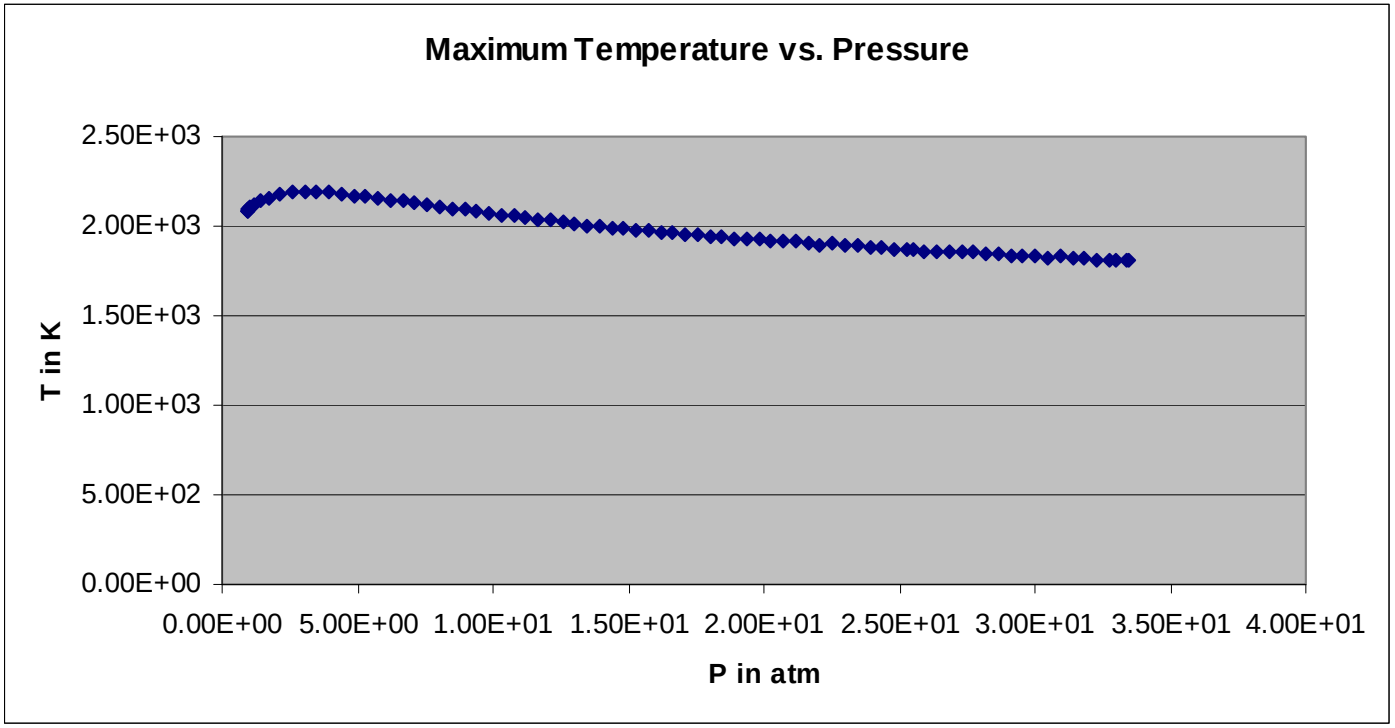
Coalescence: $\beta_{mn} = 2\pi(D_m+D_n)(d_{pm}+d_{pn})((d_{pm}+d_{pn})/(d_{pm}+d_{pn}+2g_{nm}) +$
$8(D_m+D_n)/((d_{pm}+d_{pn})(c_m^2+c_n^2)^{1/2}))$, where $c_m = (8kT/\pi m)^{1/2}$

- Most important for larger particles
- PSR comparisons with and without the high pressure corrections indicate the influence on the coalescence coefficients is most important (they are slowed down, allowing more soot formation).

Soot Volume Fraction in Ethylene-Air Counterflow Flames



Temperature Variation

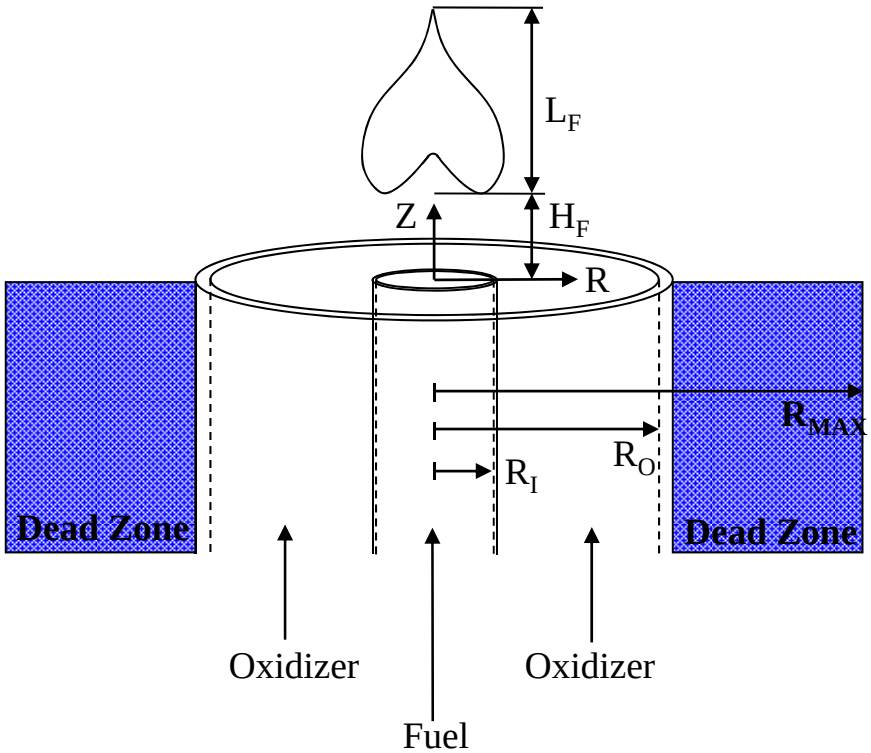


Parallel Simulation of Axisymmetric Coflow Laminar Diffusion Flames

- 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 and to facilitate the simulation of complex combustion problems that were previously intractable on a single processor
  - *e.g.,* sooting, coflow diffusion flames using JP-8 surrogate blends

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

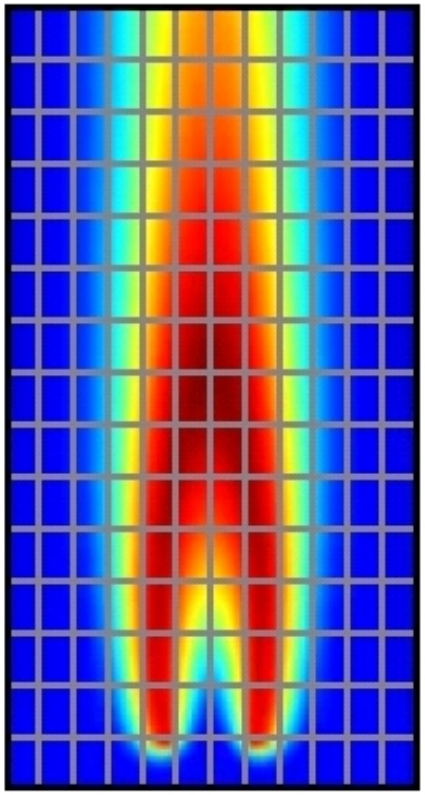
  R_{MAX} = 7.5 cm

Block Domain Decomposition

1. **Computational grid**

2. Generate Subdomains

3. Define Halo regions (domain overlap for data transfer)



Block Domain Decomposition

1. Computational grid

2. **Generate Subdomains**

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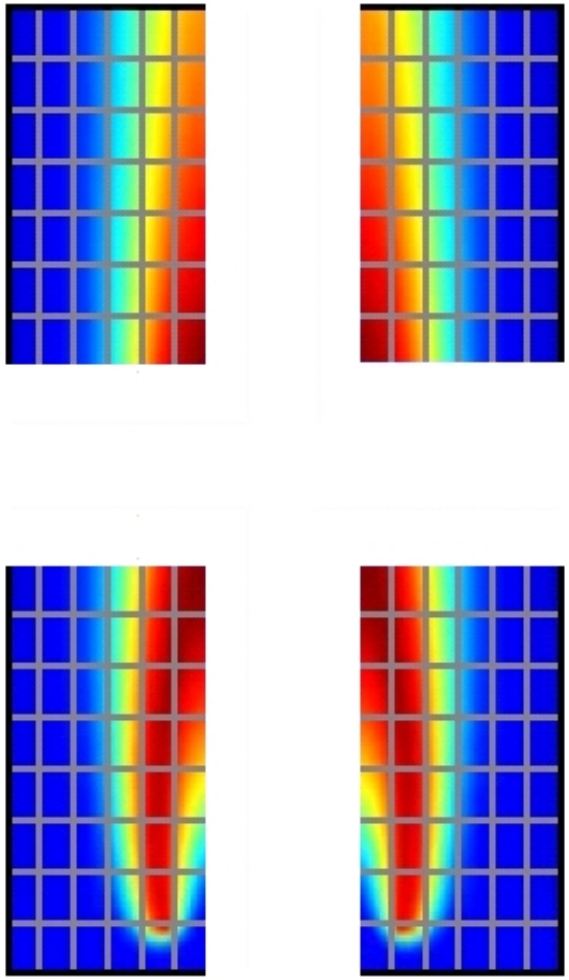
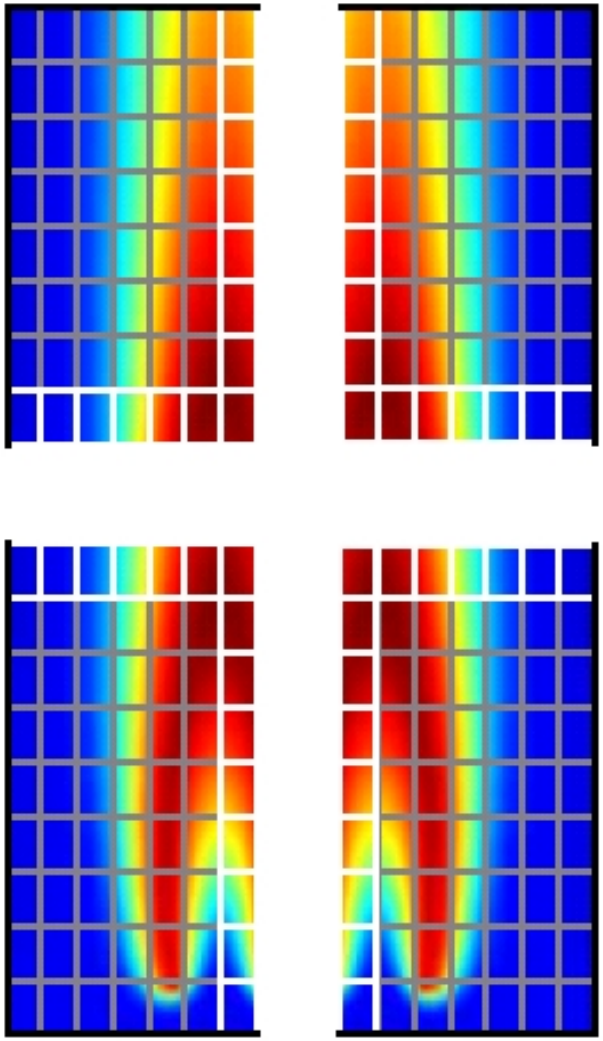


Block Domain Decomposition

1. Computational grid

2. Generate Subdomains

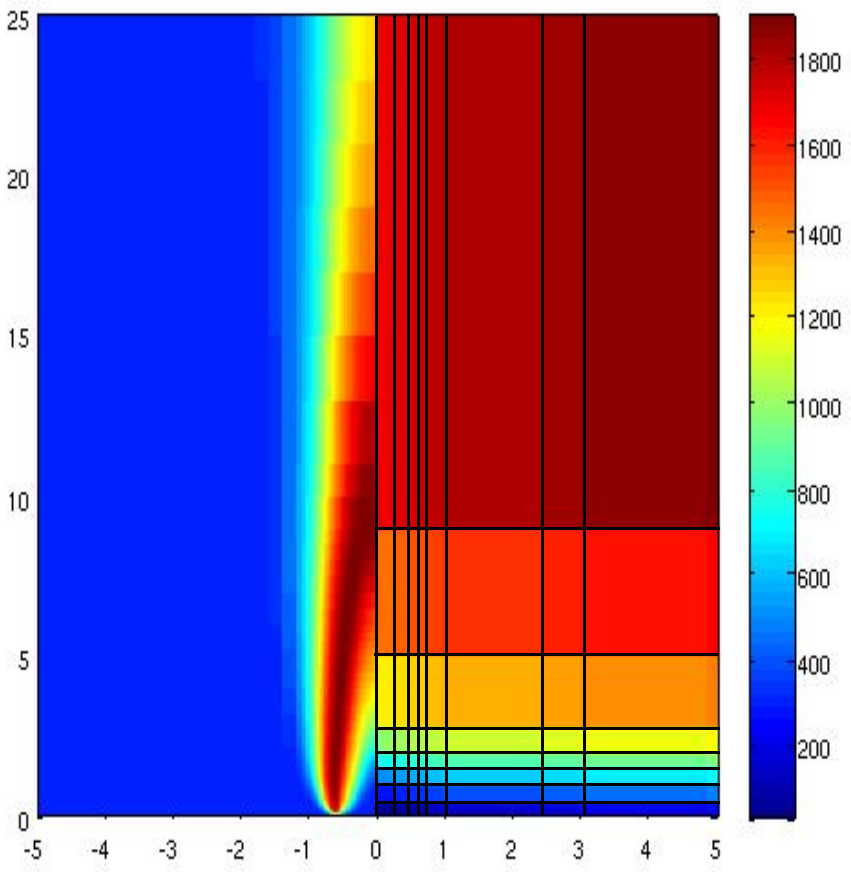
3. **Define Halo regions (domain overlap for data transfer)**



Block Domain Decomposition

Decomposition of an ethylene flame on 64 cores:

- Balance number of grid points across cores
- Balance number of grid points between r and z directions to minimize communication



JP-8 Coflow Diffusion Flame

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

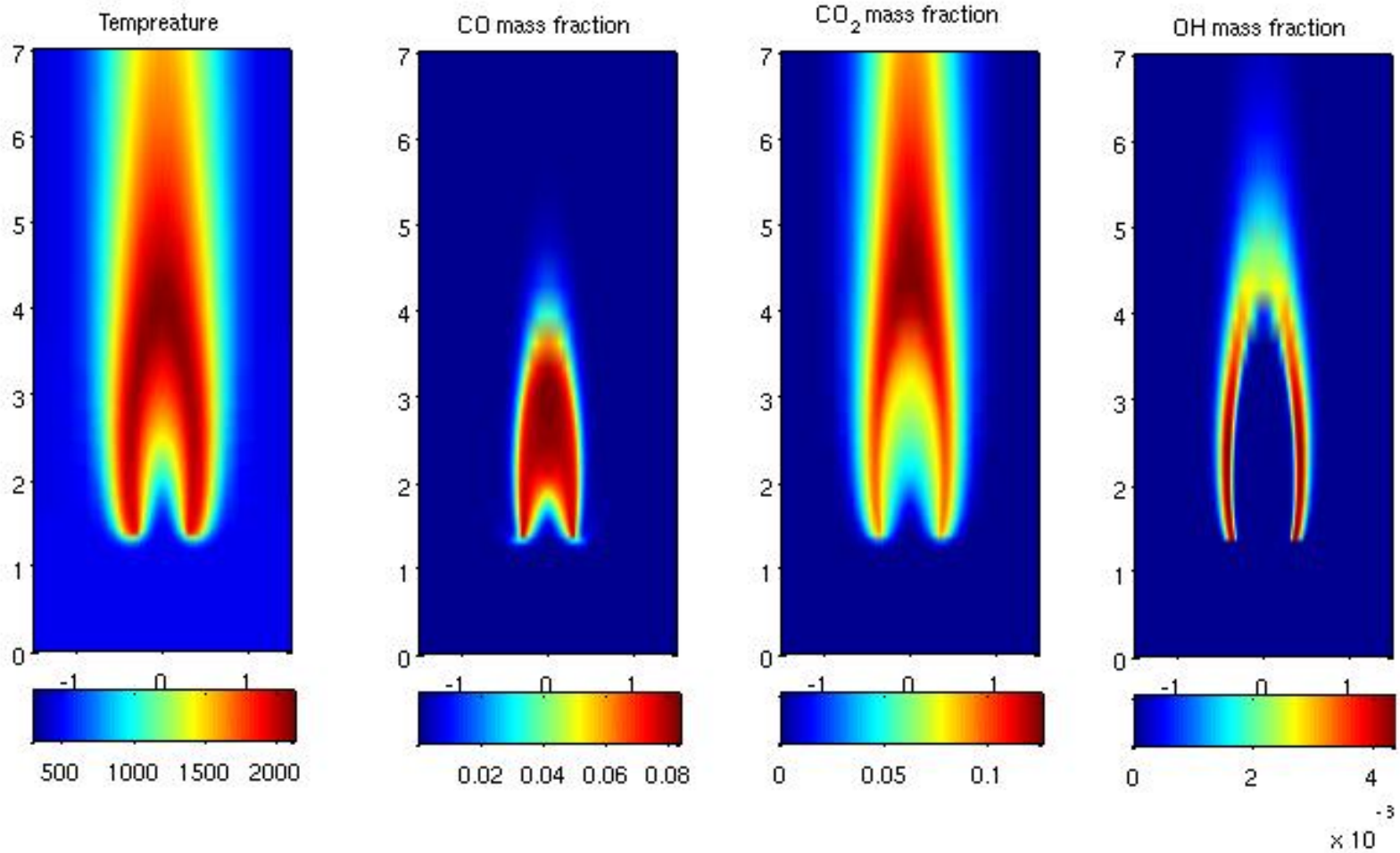
10% Iso-octane (C_8H_{18}), 20% Methylcyclohexane (C_7H_{14}), 5% Tetralin ($C_{10}H_{12}$), 30% Dodecane ($C_{12}H_{24}$), 20% Tetradecane ($C_{14}H_{30}$), 15% m-Xylene (C_8H_{10})

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

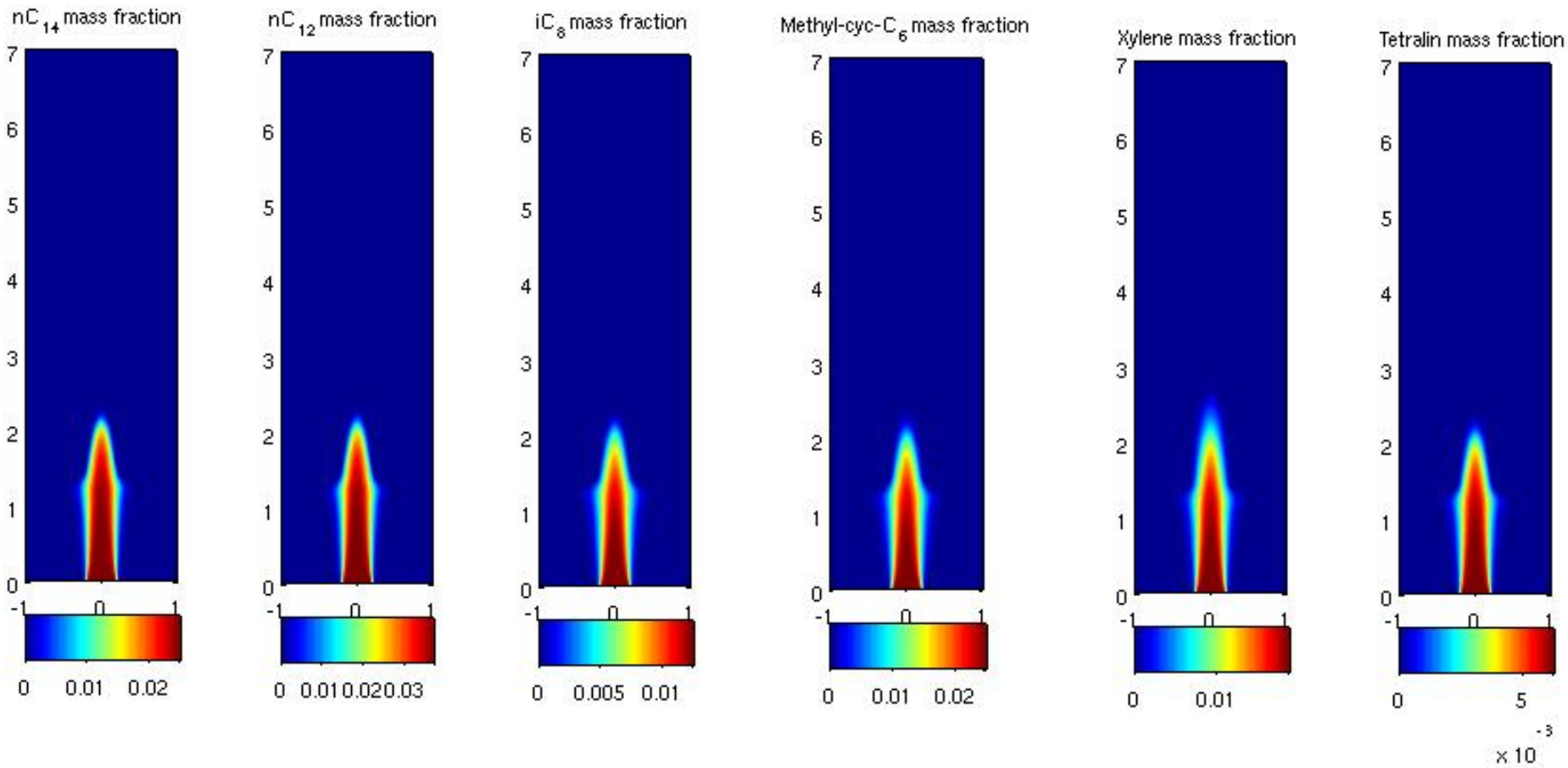
•VF= 35 cm/sec (average) VOX=35 cm/sec (plug)

•TF=480 K TOX = 480 K

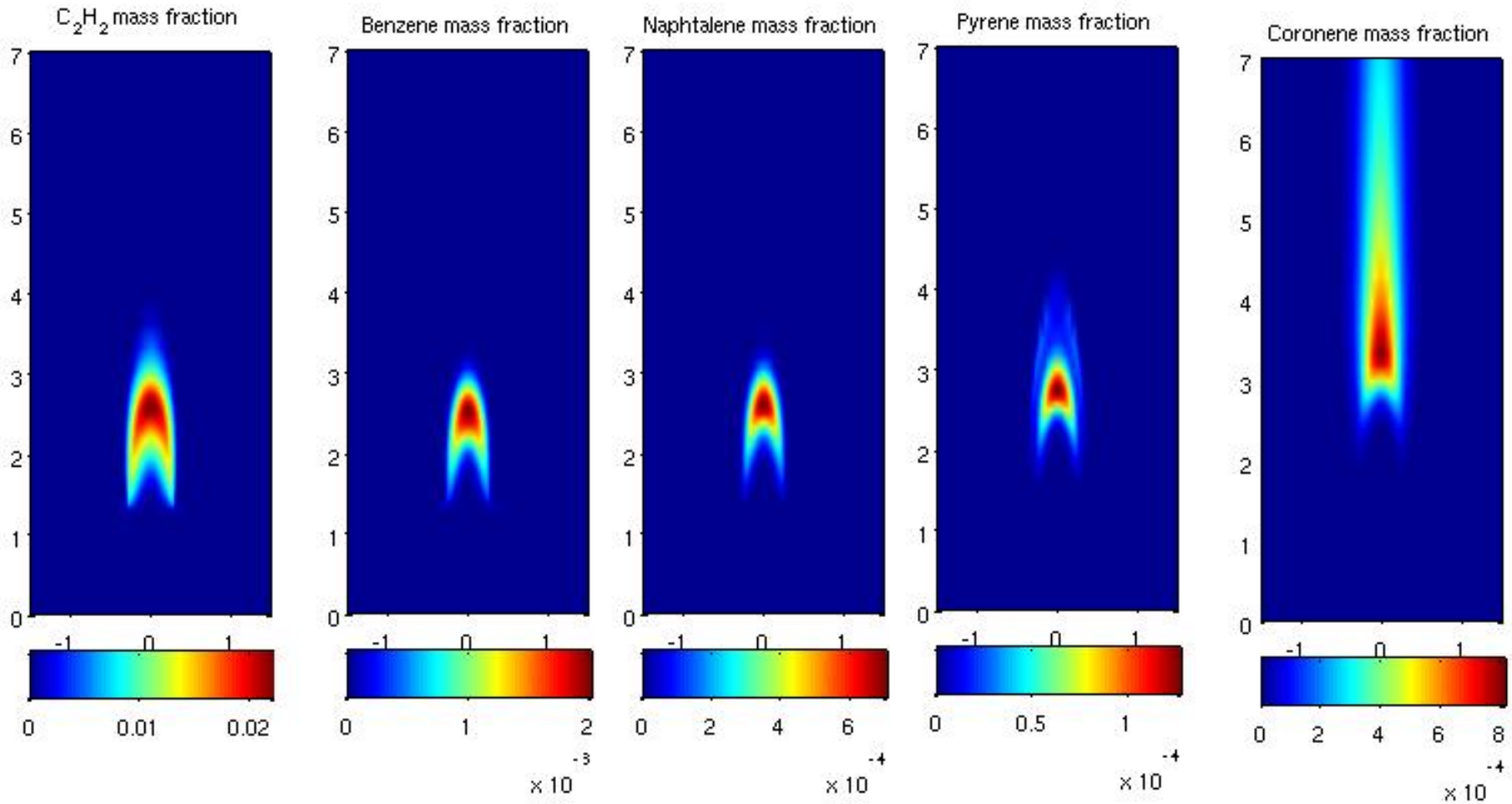
Temperature and Major Species



Surrogate Components

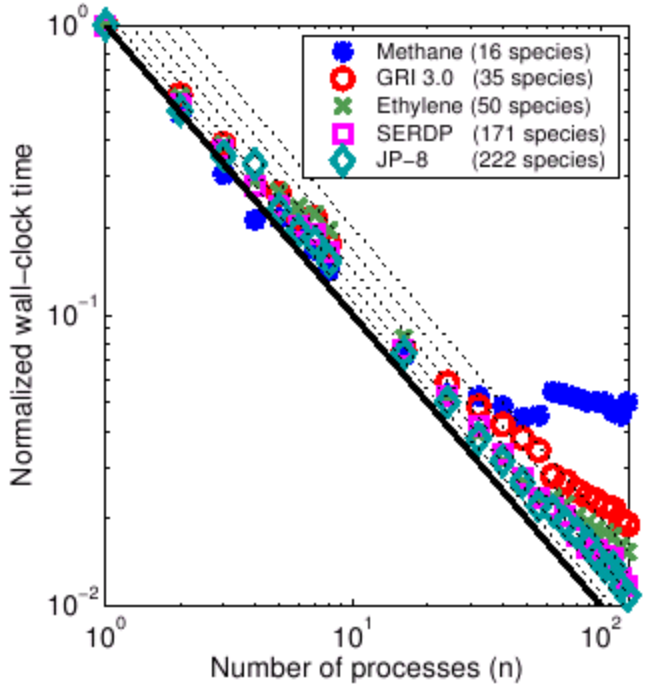


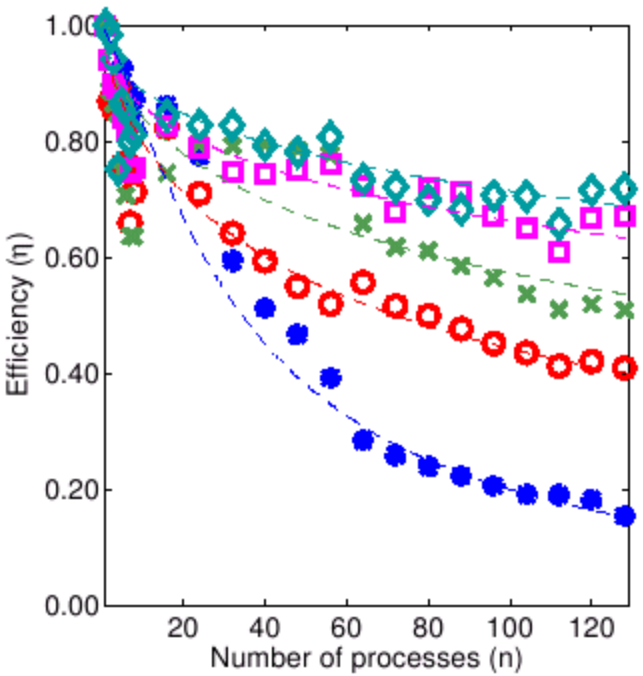
Soot Related Species



Scalability: Mechanism Size

Fixed grid size. Chemical mechanisms range form 16 species to 222 species

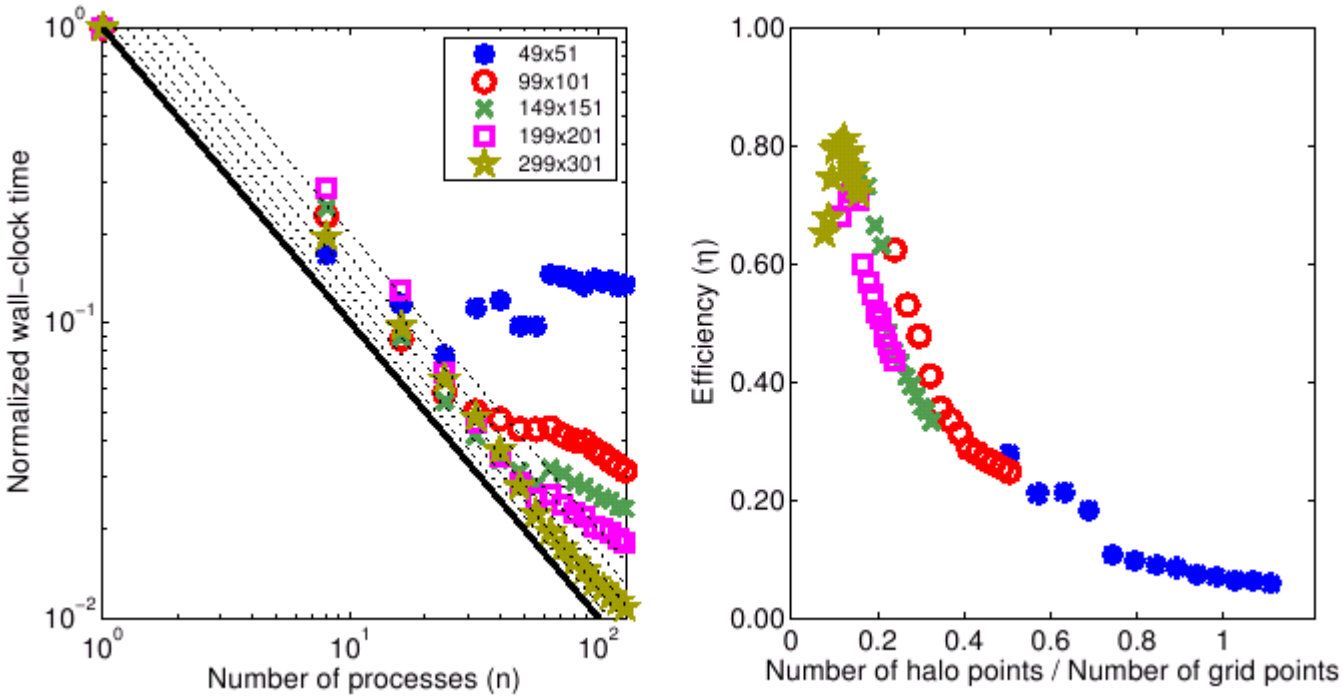




- Large mechanisms have higher parallelization efficiency
- Scalability up to 128 cores demonstrated for JP-8

Scalability: Grid Size

Small 16-species mechanism: grid size variable from 49x51 to 299x301



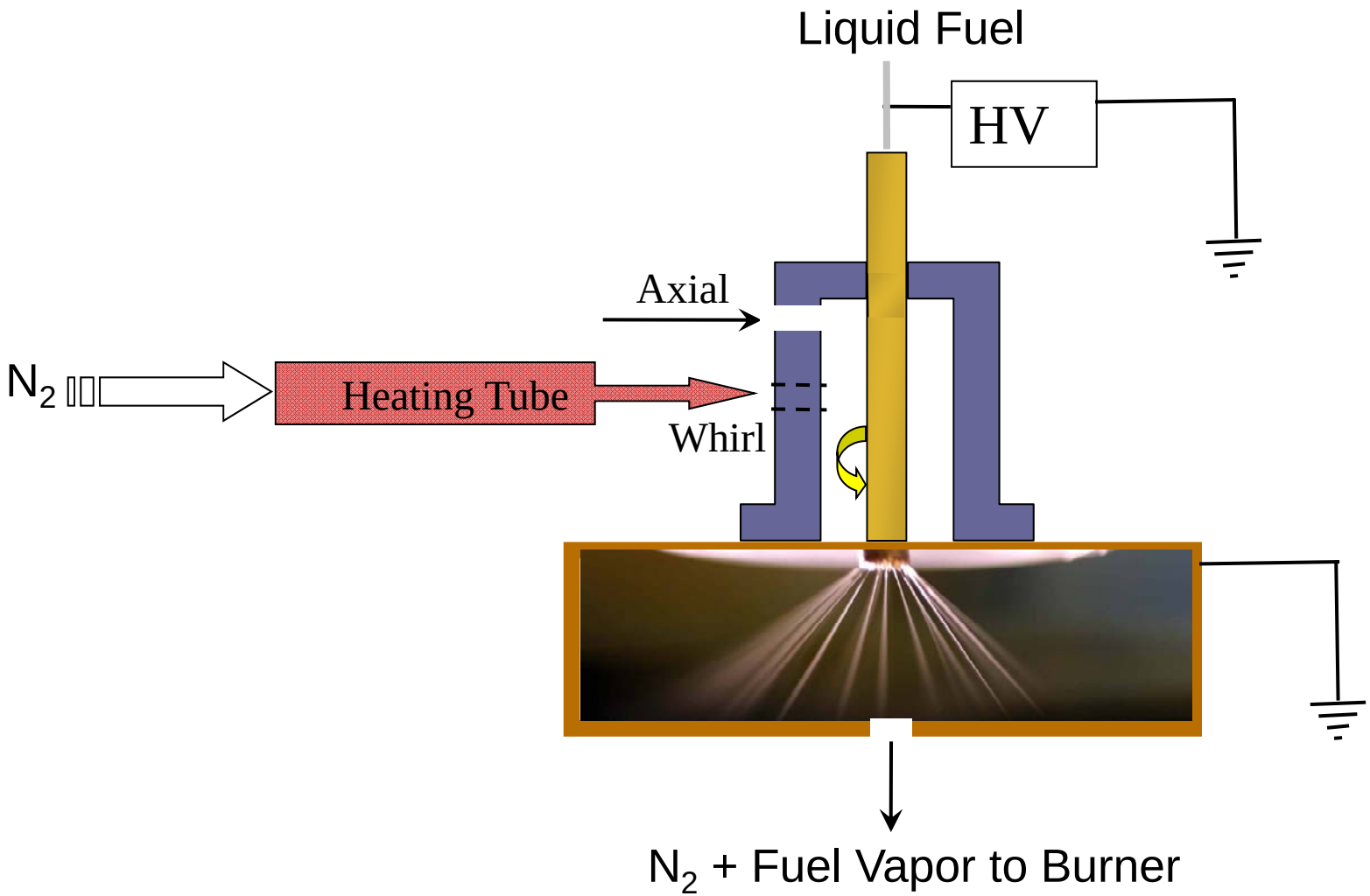
Efficient parallelization is possible also for small mechanisms if the ratio of halo-points to internal points is smaller than 30%

Conclusions: Parallel Coflow Flame Studies

Scaling of the Parallel Coflow Flame Model

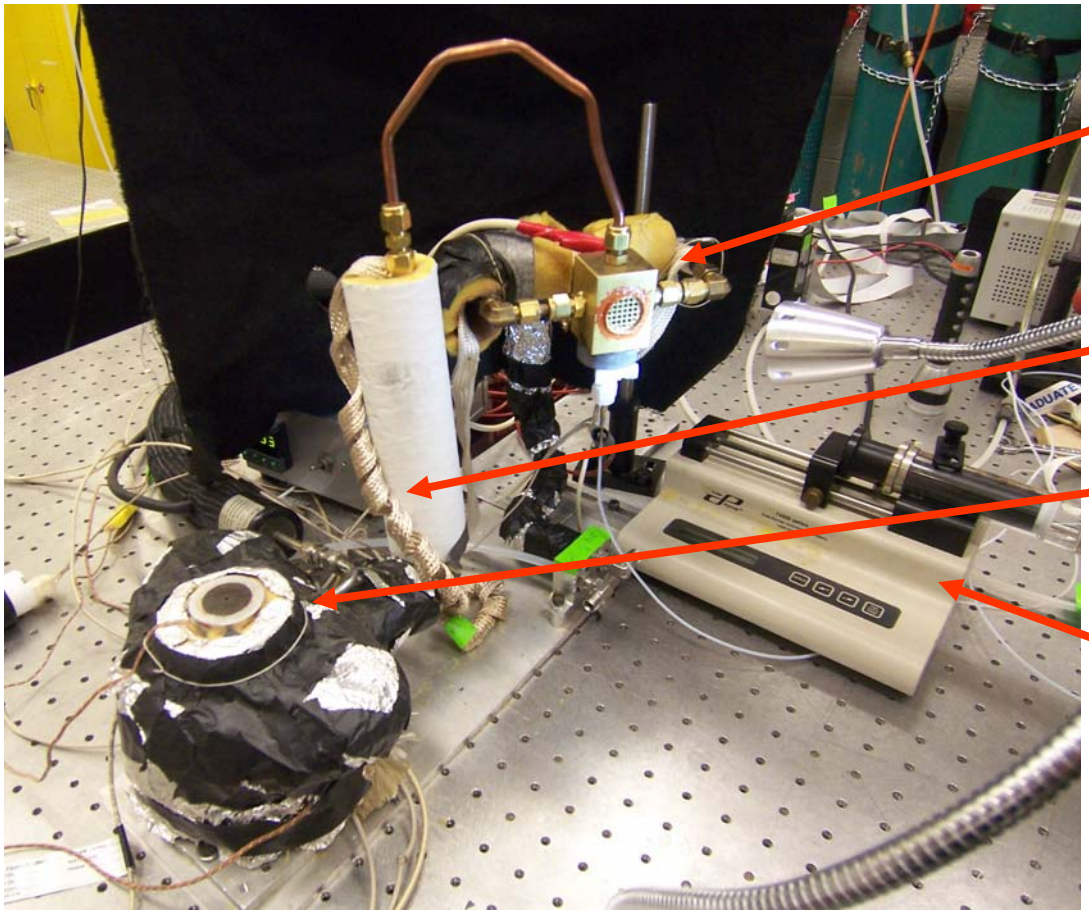
- ⇒ Reduces total computational time from 183378 seconds on a single processor to 1735 seconds across 128 processors (80% efficiency)
- ⇒ Efficiency indicates that further scaling above 128 processors is possible
- ⇒ Preliminary tests show that the developed parallel-implicit algorithm could also be viable for problems with small chemical mechanisms but a large number of grid points

Experimental Coflow Flame Electrospray Evaporator



Experimental Coflow Flame
Coflow Burner

Jet-fuel coflow burner under development



Future Work

- Analyze additional flames doped with critical surrogate components including: dodecane and n-propylbenzene or others that may emerge from the work of the surrogate teams.
- Increase the dopant concentration, to see if it affects the agreement, and compare also with other, more extensive kinetic mechanisms, when available
- Continue high pressure soot models for additional fuels
- Obtain soot size (distribution) information using automated software
- Correlate High Resolution TEM with spatial location
- Perform surface enhanced Raman scattering (SERS) on collected samples to sort out aliphatic from aromatic components
- Comparison of coflow experiments and model

Acknowledgements

- Luca Tosatto, Hugo Bufferand and Saeed Jahangirian performed the bulk of the experiments; Luca Tosatto developed the implicit parallel solver and the on-the-fly reduction methodology; Lorenzo Figura designed and tested the high-pressure chamber; and Bruno Coriton helped with OH LIF experiments
- Dr. Med Colket and Bob Hall provided collaboration on the high pressure soot model
- Dr. James (Tim) Edwards (WPAFB) supplied the JP-8.