CFD Flare Modeling Update

SETPMTC Meeting

by
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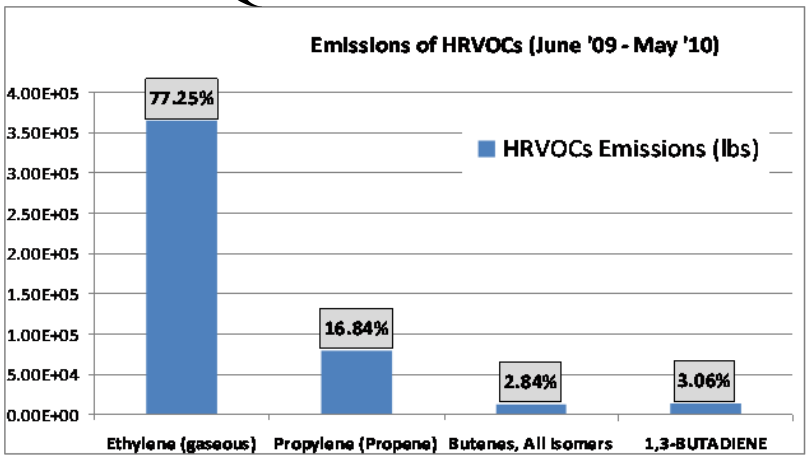
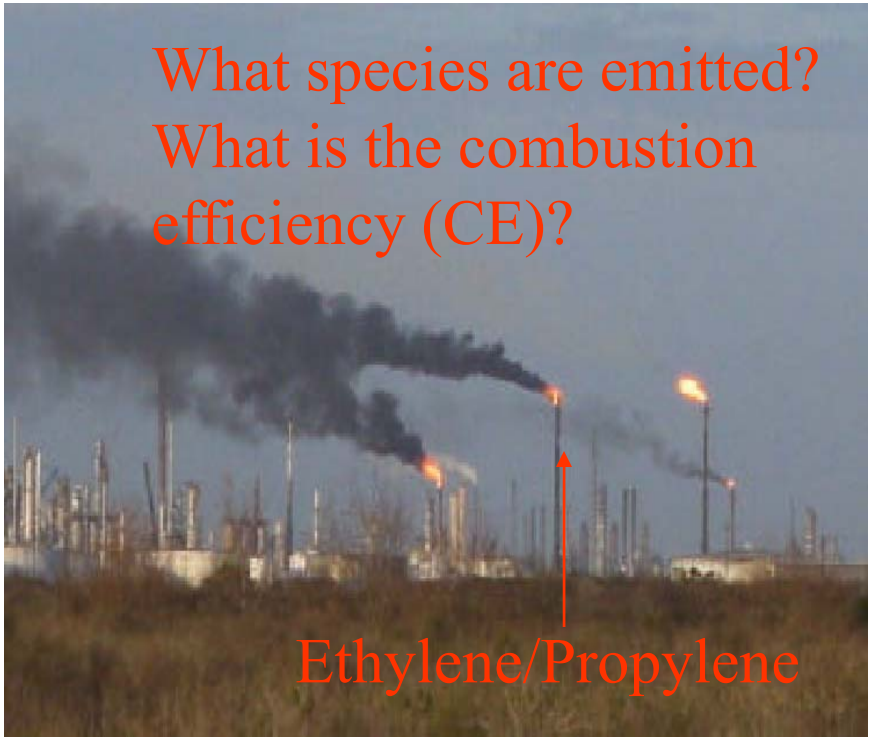
Reasons for TCEQ to focus on Industrial Flares



- Flare emissions account for 60% of the **HRVOCs** based on the 2007 HRVOC special inventory.
- Flare emissions depend heavily on a flare's **destruction & removal efficiency (DRE)**.
  - Recent studies/gas imaging IR camera suggest to the agency that flares may not be as efficient as claimed. (Susan Moore, TCC, 2009)
  - For propylene and propane tests, there were many conditions that did not achieve a 99% DRE even conducted in compliance with all criteria of 40 CFR § 60.18 (D. Allen, 2011, UT/JZ/TCEQ Comp. Flare Study) .
- Aside from DRE, there is an issue of incomplete combustion species
  - Current air emission inventory from flaring is simply a mass throughput with 98% reduction without any consideration of by-products or intermediates formation (TCEQ 2000)
- As a result, TCEQ is conducting an evaluation on flare operations that may serve as a basis for a future SIP revision (http://www11.tceq.state.tx.us/oce/eer/index.cfm)

Complexity in Flare Emissions

- Process Type (Relief gas)
  - Refinery, Olefin, Polymer, and Exploration fields (H2-C4)
- Operation mode
  - Startup, Shutdown, Upset, and Normal (Turndown ratio 20:1)
- Flare Design/Control
  - Steaming, Aeration, etc.
- Meteorological condition
  - Cross wind, humidity, etc.



How does rigorous flare modeling help SIP?

- Improve Emission Inventories
  - **Since the photochemical models indicated that the ozone formation in HGB is often radical-limited, the incomplete combustion products from flares may contain unreported radical and radical producing species.**
  - **Further, it is well known that the theoretical maximum amount of ozone that can be produced in the system is $[O_3] = [CH2O]_0 + [NO2]_0$, all photochemically important post-flared chemical species (HO_x, NO_2, CH_2O, C_2H_4O) will be considered in the EIs.**

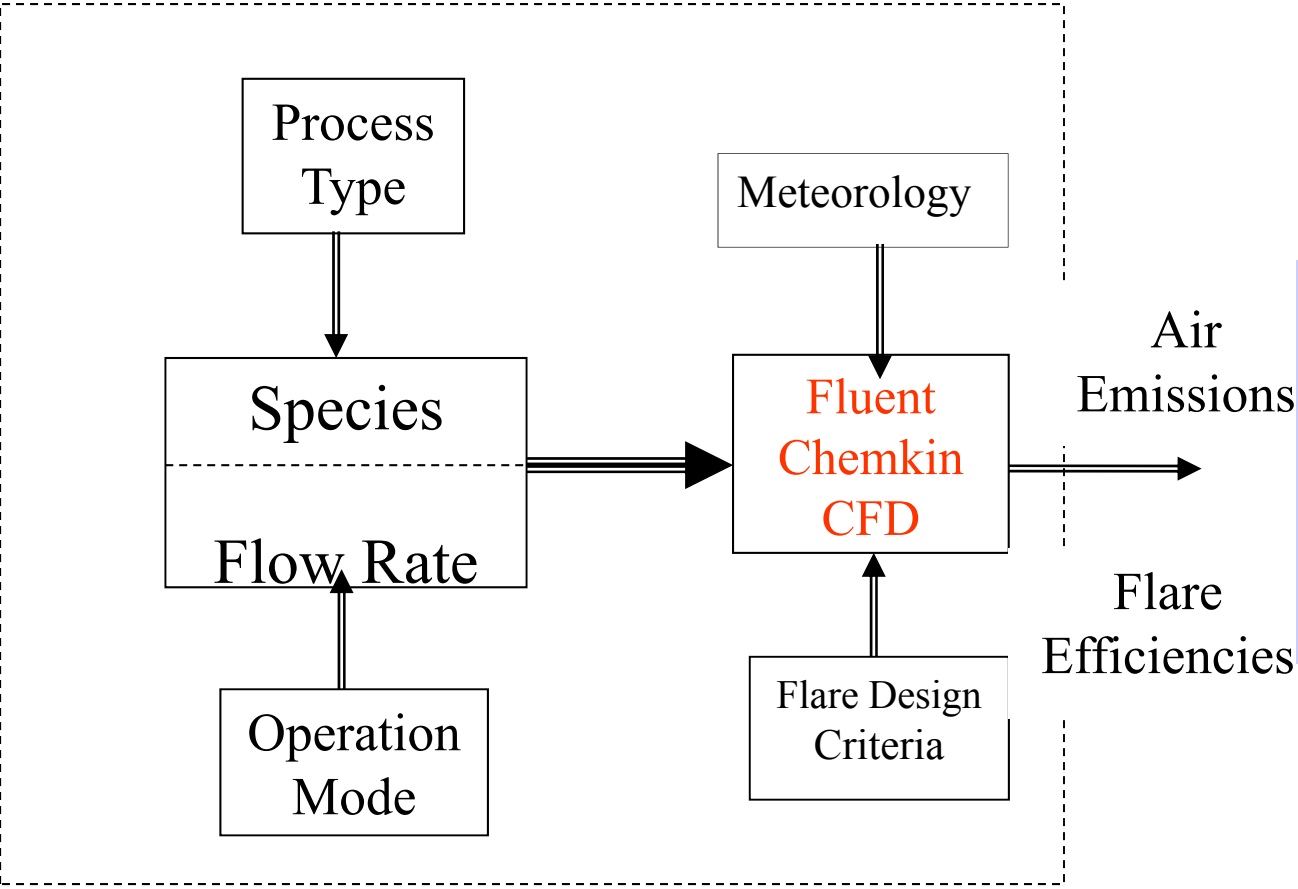
- To evaluate the impact of emission inventories on ozone formation using emission processors (EPS3 or SMOKE) and air quality models (CAMx or CMAQ)

- To organize the knowledge base & to help flare operations
  - to help industries and TCEQ identify the best practices in flare operations, especially during start up and upset periods
  - For example, **under a particular set of cross wind and mass flow rate conditions, what steaming and aeration should be used in an ethylene flare to increase flare efficiency and to reduce flare emissions?**

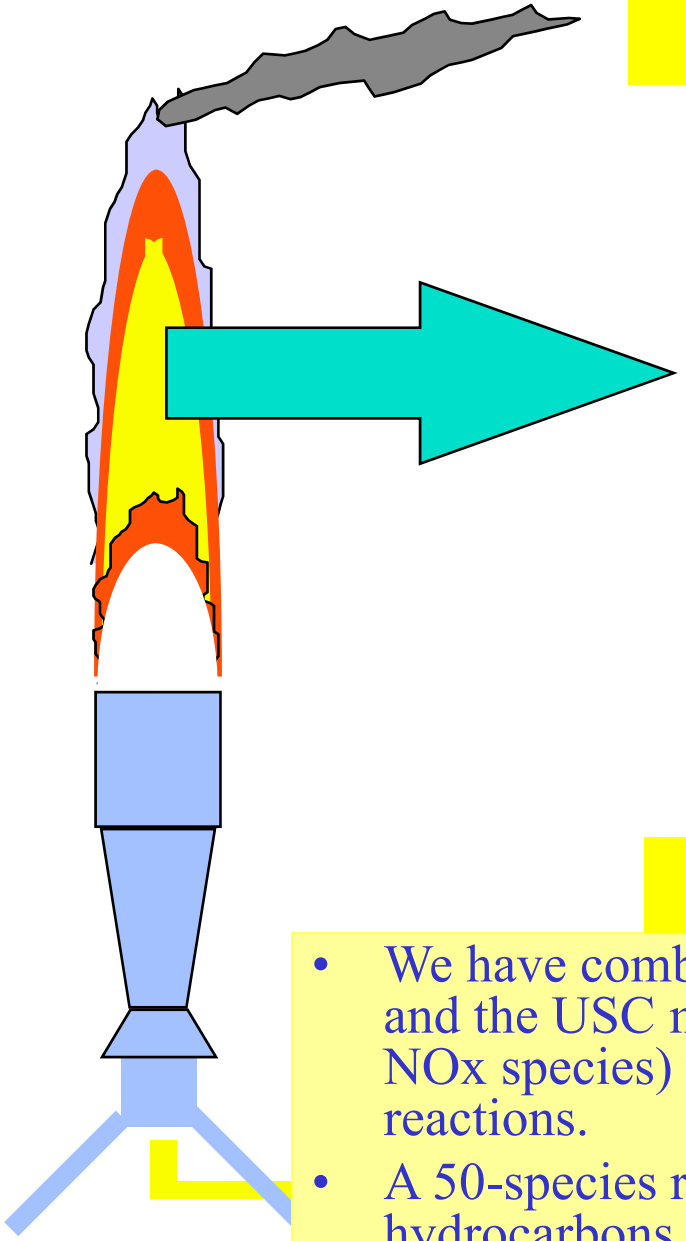
Methodology

Rigorous flare CFD simulations

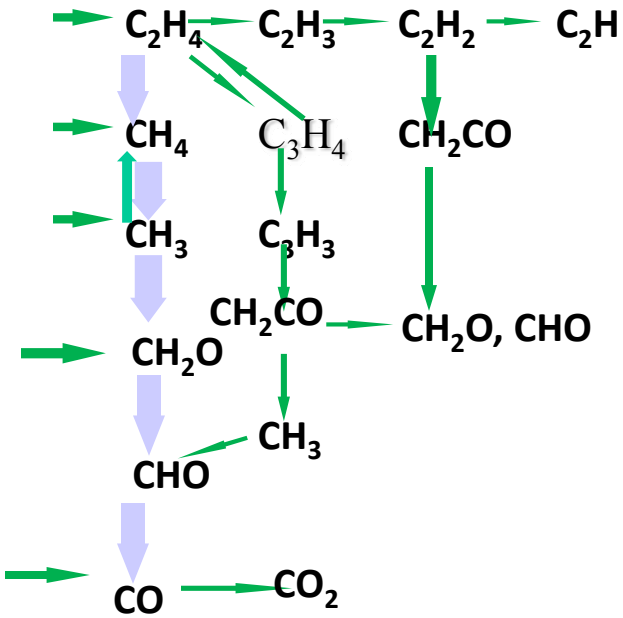
- Model industrial flaring systems using Fluent /Chemkin CFD for propylene/ethylene/methane combustion
- Mechanisms validated with experimental data (laminar flame speeds, adiabatic flame temperature, and ignition delay) for combustion of light hydrocarbons (C1-C3)



Infer the emission species and combustion efficiencies under various Crosswind/Flow rate/ Heating Value/ Aeration/ Steaming conditions.



Ethylene Reaction Pathways



Lou, H., Martin, C., Chen, D., Li, K., Li, X., Vaid, H., Vaid, H. Tula, A., Singh, K., "A Reduced Reaction Mechanism for the Simulation in Ethylene Flare Combustion," *Clean Technologies and Environmental Policy*, online edition, June 16, 2011.

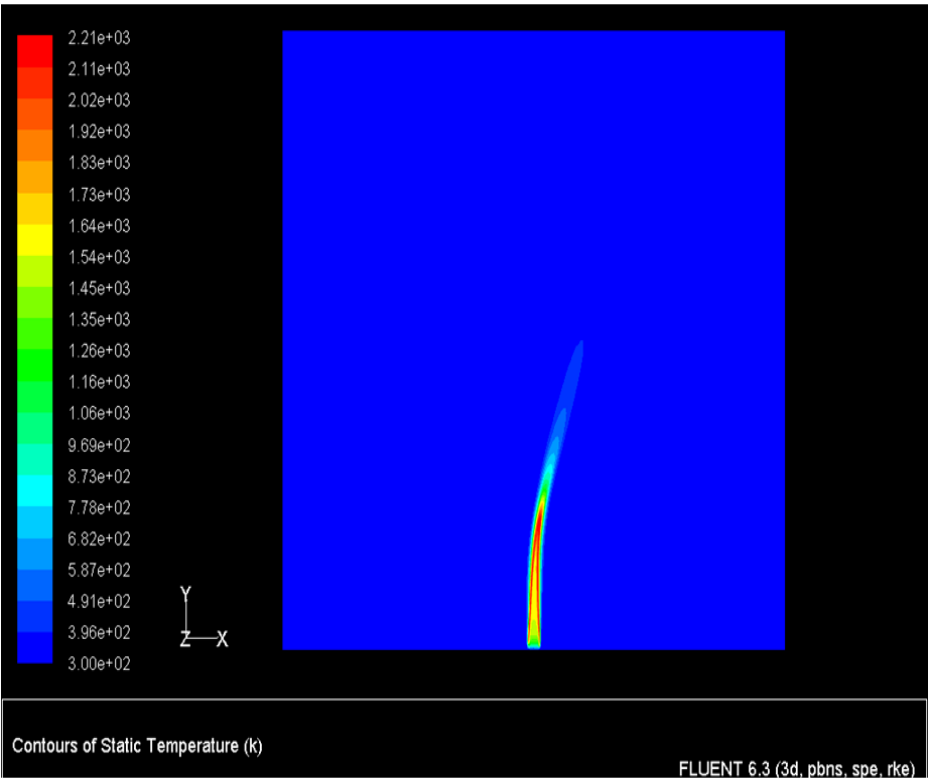
CHEMKIN Mechanisms

- We have combined the GRI-3.0 mechanism (optimized for methane) and the USC mechanism (optimized for ethylene but without the NOx species) to obtain a mechanism containing 93-species and 600 reactions.
- A 50-species reduced mechanism for the combustion of light hydrocarbons (C1-C3) was developed and validated with experimental results like laminar flame speeds, adiabatic flame temperature, and ignition delay, and burner stabilized flame.

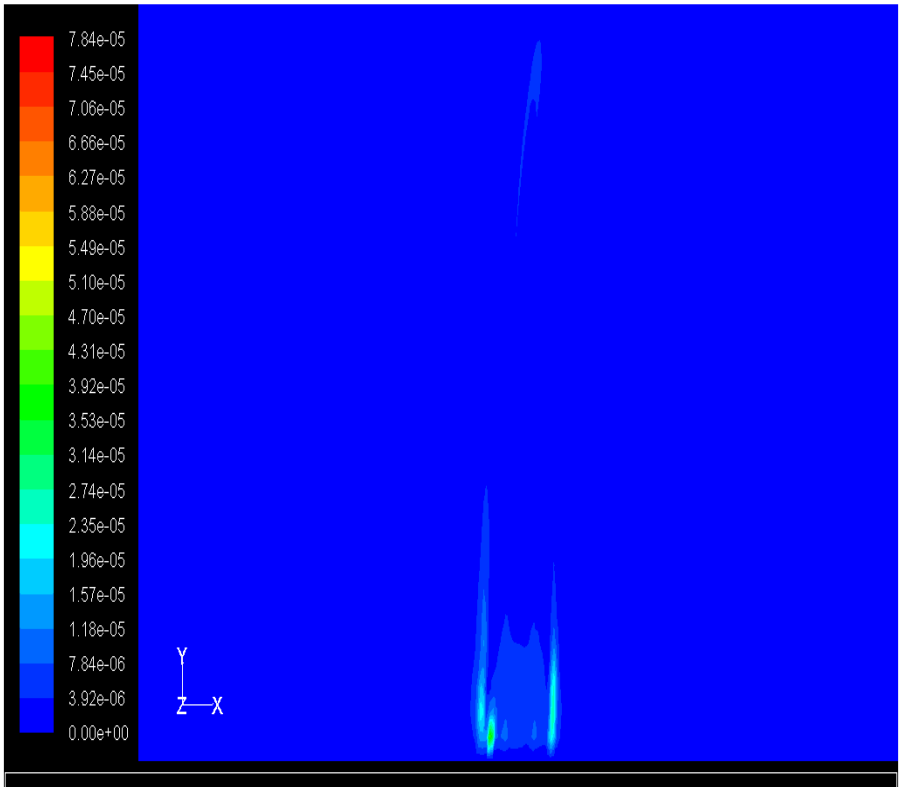
Prior Work: **TCEQ Project-2008-102 (Modeling Ethylene Flares) & HARC H-83 Project (Flare Speciation)**

Results from **TCEQ Project-2008-102 Modeling Ethylene Flares**

Contours of static temperature (K)



Contours of Mass fraction of CH2O (zoomed in near the jet stream)



Inlet temperature =400 K, Flare diameter = 0.762 m, Jet exit velocity = 2.5 m/s, Premixed Air =30% of stoichiometric air, crosswind velocity =2m/s

Lou, H. H., K. Y. Li, C. Martin, D. Chen, X. Li, H. Vaid, A. Tula, K. D. Singh and D. J. Bean, "**A Reduced Reaction Mechanism for the Simulation of Ethylene Flame**," the *2009 AIChE Annual meeting*, Nashville, TN.

Effect of Cross-Wind on Ethylene Flares

	U=10m/s	U=20m/s
Carbon Based Flare Efficiency	69.76%	68.57%
Destruction/Removal Efficiency	99.50%	97.69%

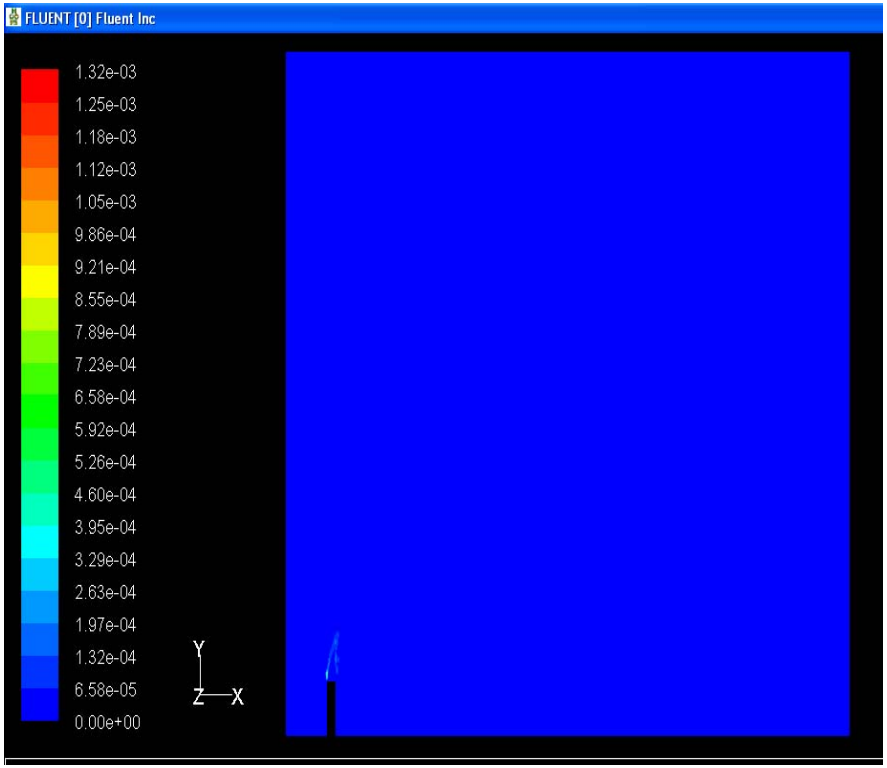
*30% pre-mixed air

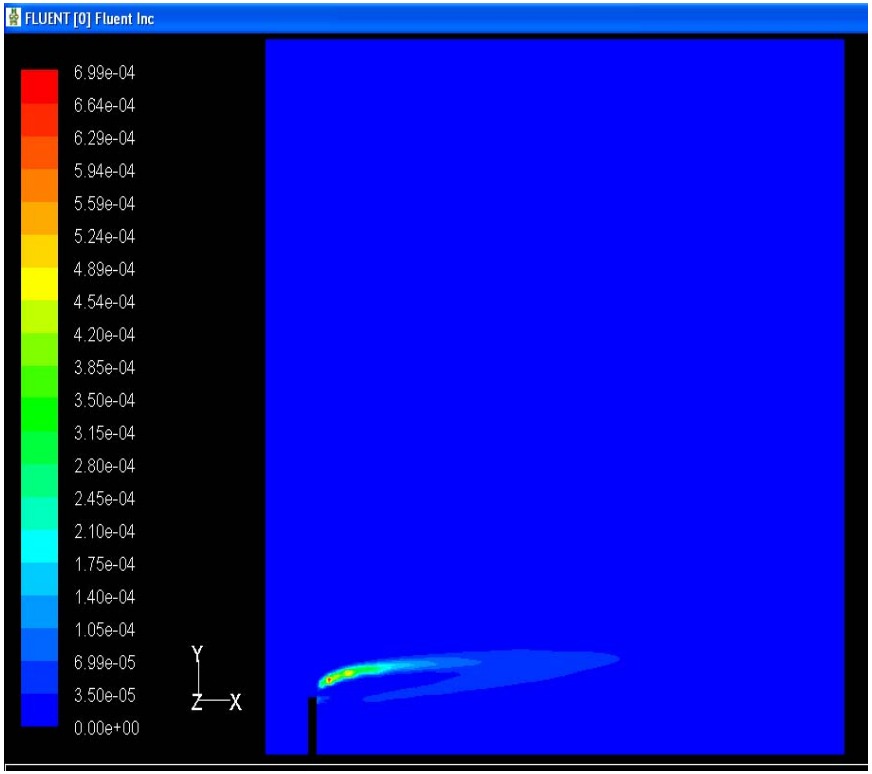
Increase in crosswind velocity clearly brings down the combustion efficiency (CE) even though the destruction & removal efficiency (DRE) does not change much.

Normalized emissions rate (kg/ kg of C2H4 feed)

	U=10m/s	U=20m/s
C2H4	5.05E-03	2.31E-02
OH	1.01E-03	1.10E-03
HO2	5.45E-03	8.97E-03
CH2O	2.00E-04	1.13E-03

Significant emissions of CH2O, OH, HO2, CO, and C2H2 that increase with cross wind

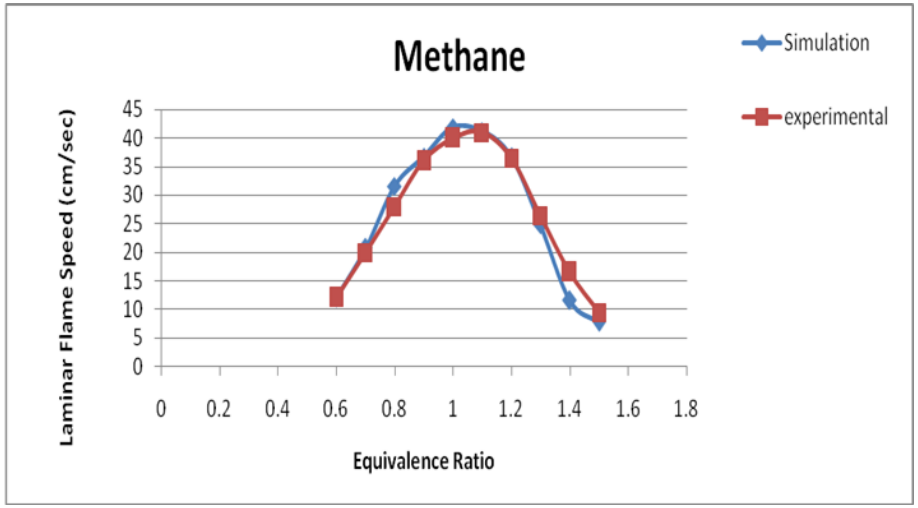




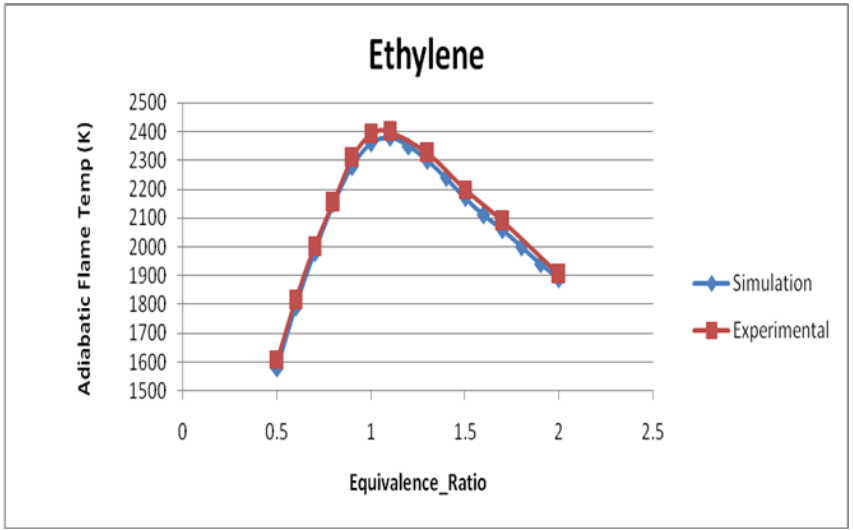
Mass fraction of Formaldehyde HCHO (U = 2m/s, L; U =20m/s, R)

Validation of Lamar's Combustion Mechanism for C1-C3 Hydrocarbons

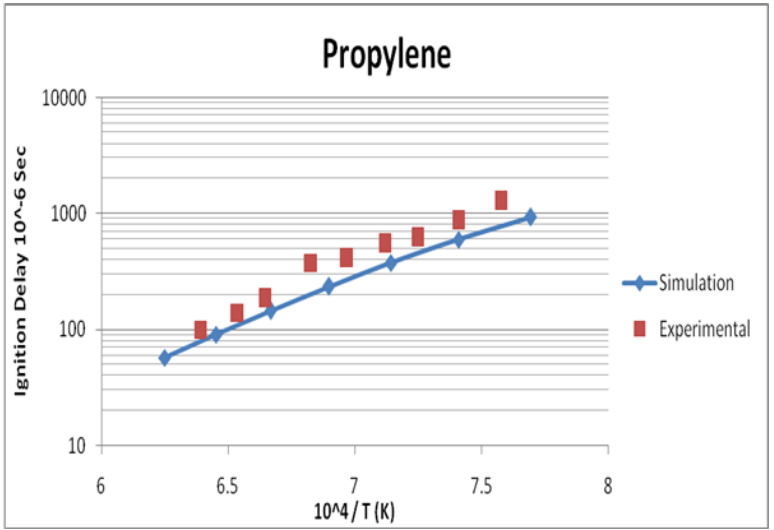
Laminar flame speed vs equivalence ratio for Methane



Adiabatic flame temp vs. equivalence ratio for ethylene



Ignition delay vs. temperature for Propene



Validation with a CH4 Sandia/ TU Darmstadt Flame

Fuel composition: CH4 (25%), Air (75%) by volume.

Fuel exit velocity: 49.6 m/s

Nozzle diameter: 7.2 mm

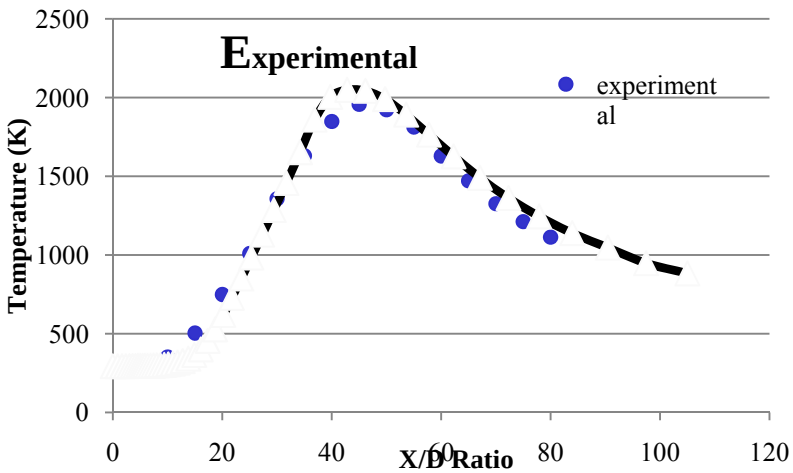
Pilot composition: CO (0.4%), CO2(11%), H2O(9.4%), O2(5.4%), N2(73.8%)

Pilot exit velocity: 11.4m/s

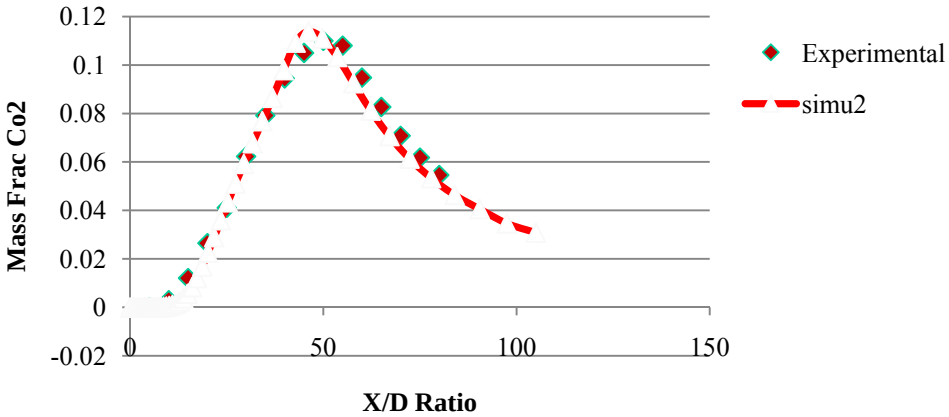
Pilot nozzle outer diameter:18.2 mm

Mechanism : Gri3.0 (reduced to 35 species)

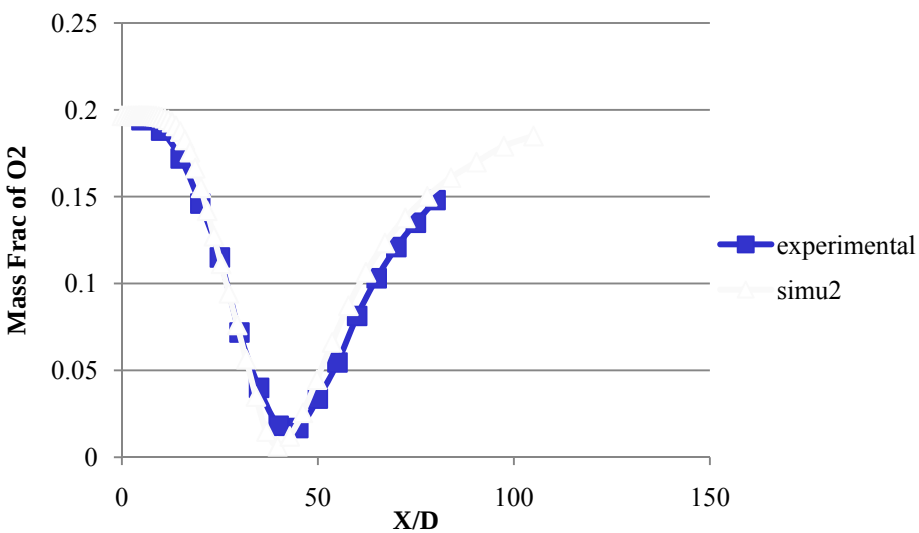
Temperature Profile



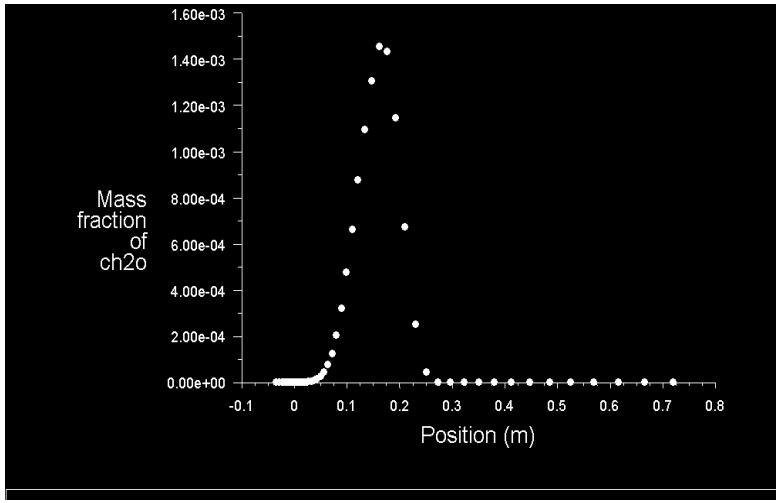
Mass Fraction of CO2



Mass Fraction of O2



Formaldehyde Plot along Axis (Simulation)



AQRP Project 22:
Modeling John Zink Flare Tests, September 2010, Tulsa, Oklahoma

Objectives of the UT/TCEQ/JZ Comprehensive Flare Study

- Assess the impact of high turndown (low flow) rate of vent gas on flare destruction and removal efficiency (DRE) and combustion efficiency (CE)
- Assess the effects of varying assist ratios, and vent gas heat content
- Identify and Quantify Hydrocarbon Emission Plumes Currently being Seen with Infrared (IR) Cameras

2010 TCEQ Flare Study Draft Final Report Summary, The University of Texas at Austin, TCEQ PGA No. 582-8-86245-FY09-04 & Task Order No. UTA10-000924-LOAT-RP9

Quality Assurance Project Plan, Texas Commission on Environmental Quality Comprehensive flare Study Project, PGA No. 582-8-862-45-FY09-04, Tracking No. 2008-81 UT/TCEQ/John Zink).

Texas Commission on Environmental Quality 2010 Flare Study Draft Report

Flare Task Force, Presented by Air Quality Division (AQD),May 18-19, 2011

Flare Tips Design & Operation

- Air-assisted flare (144,000 lbs/hr, 24 inch Diameter, Zink Model LHTS–24/60 Air Flare Tip)
  - LHV =350 and 600 Btu/scf
  - Vent gas flow rates =359 and 937 lbs/hr
  - Vary air assist from incipient smoke point (ISP) to < snuff
- Steam-assisted flare (937,000 lbs/hr, 36 inch diameter, Zink Model EEF-QSC-36" Steam Flare Tip)
  - LHV=350 and 600 Btu/scf
  - Vent gas flow rate = 937 and 2,342 lbs/hr
  - Vary steam assist from ISP to < snuff
- Vent gas composition: 1:4 natural gas to propylene ratio (volume basis) diluted to desired LHV with nitrogen

2010 TCEQ Flare Study Draft Final Report, The University of Texas at Austin, The Center for Energy and Environmental Resources, May 23, 2011

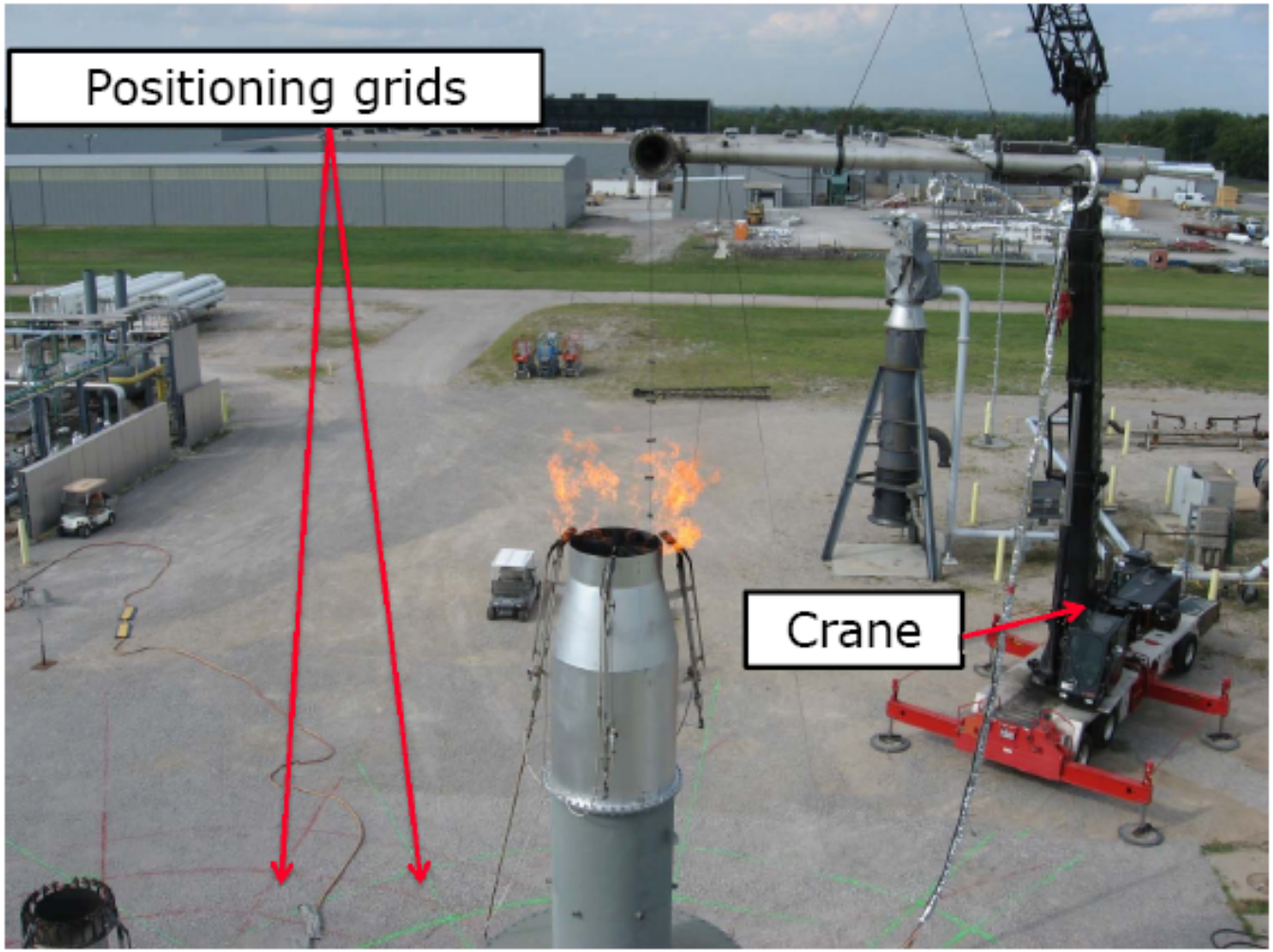
Flare Operating Conditions (I)

- Tip velocities are similar to those observed during field testing at Marathon facilities.
- Vent gas streams with heat content of 350, 600, and 2,149 (Btu/scf)
  - 40 CFR §60.18 minimum heating value for an assisted flare is 300 Btu/scf.
- Vent gas streams with low flow rate 0.1% & 0.25% of rated design capacity
  - Steam-assisted flare = 937 & 2,342 lb/hr
  - Air-assisted flare = 359 & 937 lb/hr

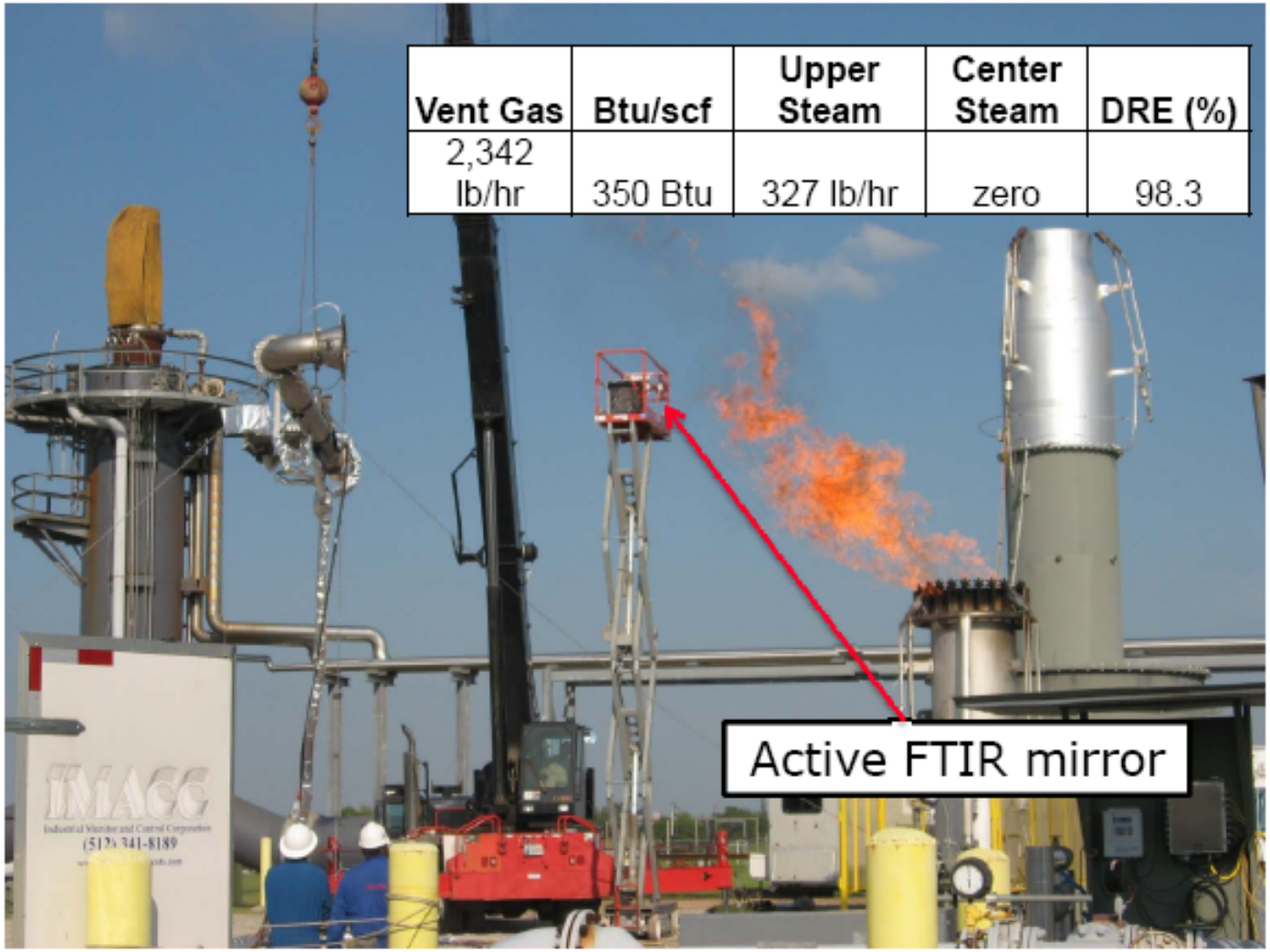
Flare Operating Conditions (II)

- Assist rates varied between zero assist to over assist near flameout (snuff point).
  - Measurements were taken at points between the incipient smoke point and near snuff point.
  - Four to six points per test series with up to three repetitions per point
  - Tip velocity of vent gas, including center steam, was between 0.6 and 2.0 feet per second (fps).

Elevated Position

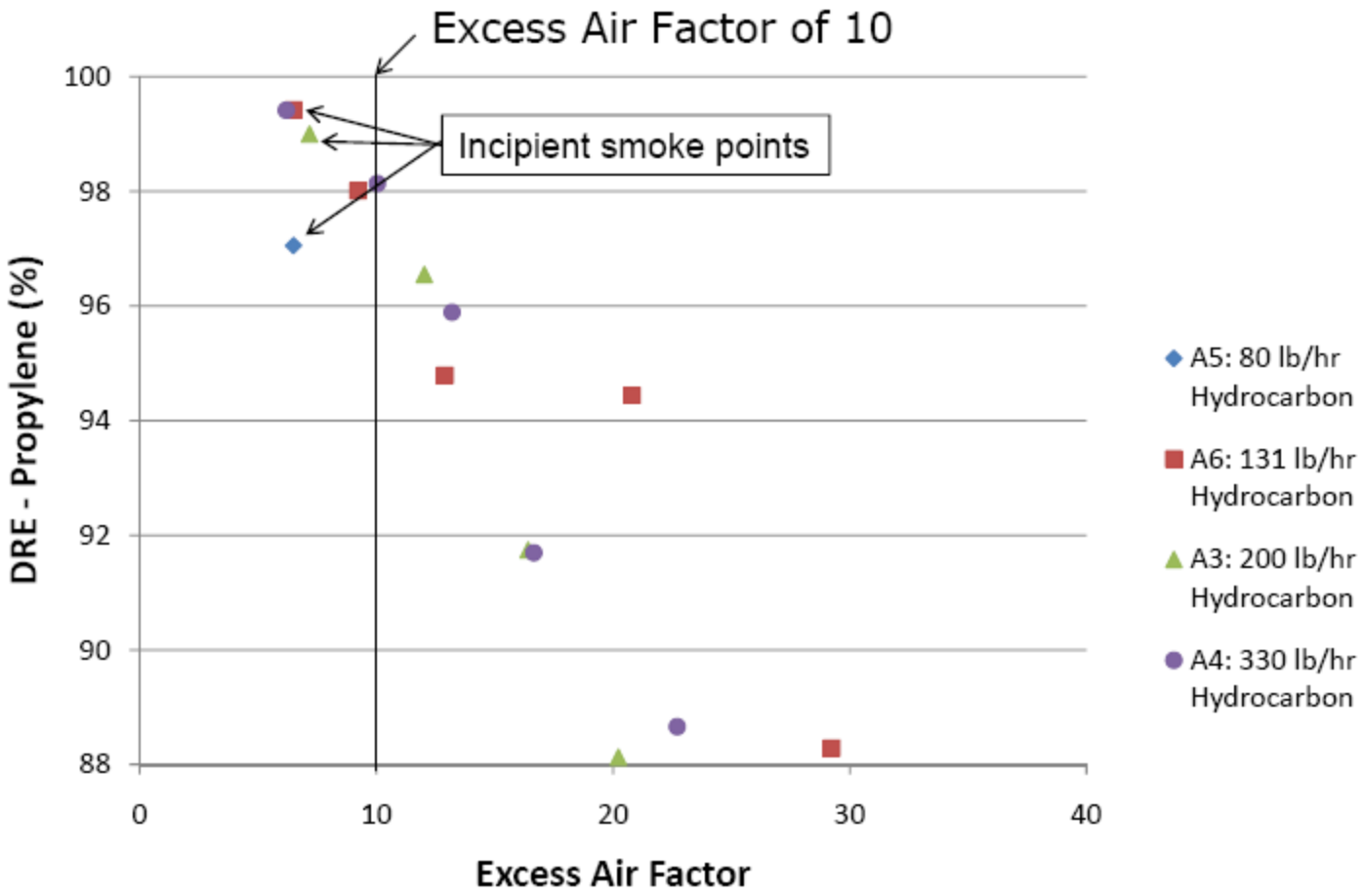


Test Point S4.4

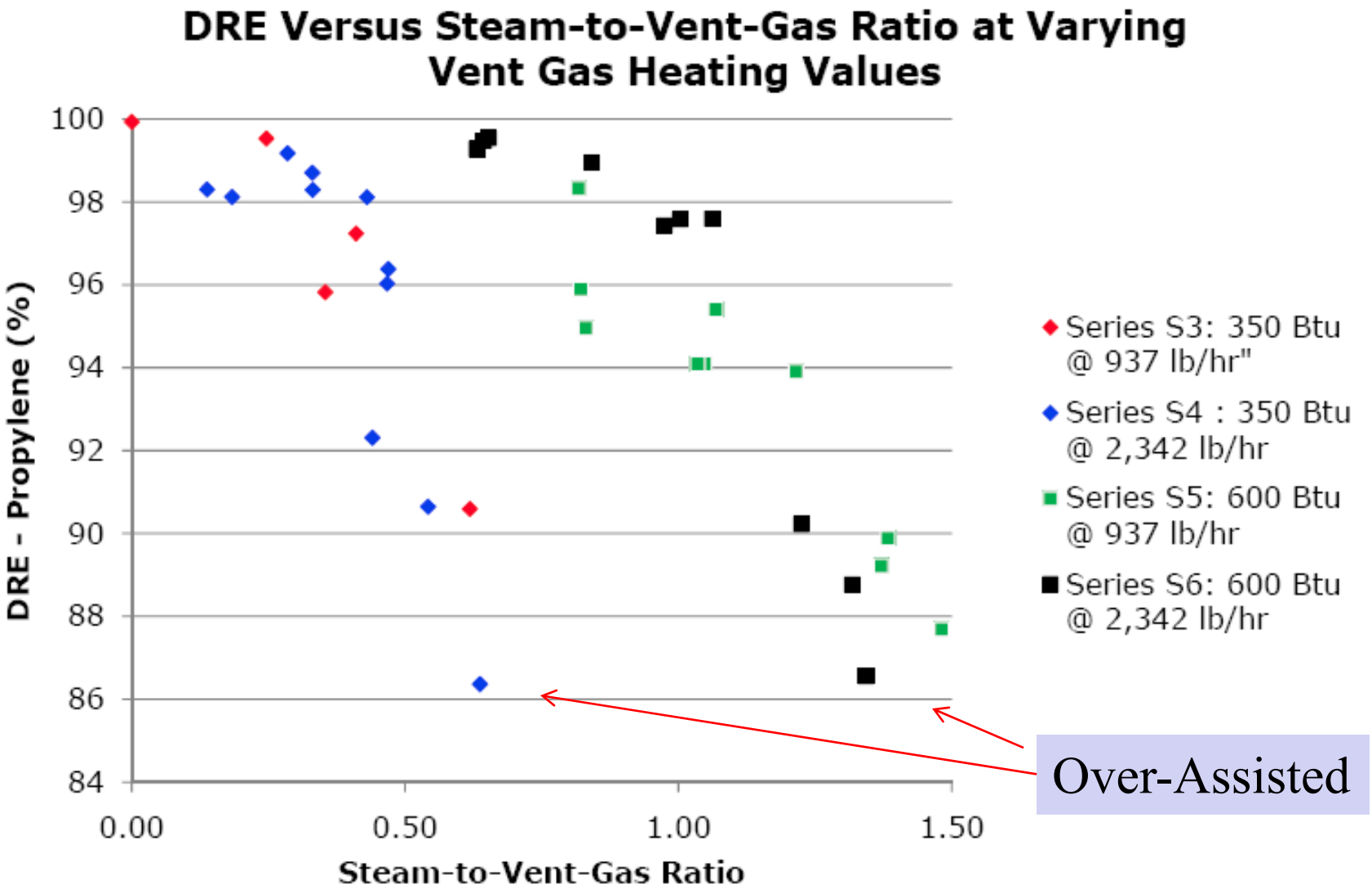


Vent Gas	Btu/scf	Upper Steam	Center Steam	DRE (%)
2,342 lb/hr	350 Btu	327 lb/hr	zero	98.3

DRE vs. Excess Air



2010 TCEQ Flare Study Draft Final Report, The University of Texas at Austin, The Center for Energy and Environmental Resources, May 23, 2011



2010 TCEQ Flare Study Draft Final Report, The University of Texas at Austin, The Center for Energy and Environmental Resources, May 23, 2011

Goals of AQRP Project 22

- Validate mechanisms used with laboratory data
- Model low-flow rate flares in the open-air conditions
- Predict effects of cross wind, mass flow rate, Btu, aeration, steaming, etc. for Propylene/Tulsa Natural Gas/N2 flares at the John Zink R&D Facility
- Tune models with available Literature and UT/John Zink data

New 50-Species Mechanism with NO2 Developed

- In 2010 John Zink flare tests, NO2 is a monitored species.
- The full 93 species mechanism was reduced based on mole fractions & their effect on other major species for use in the EDC model.
- Argon (inert gas, small mole fraction) was replaced with NO_2 in the existing 50-species mechanism.

The initial conditions for the mechanism simulation were:

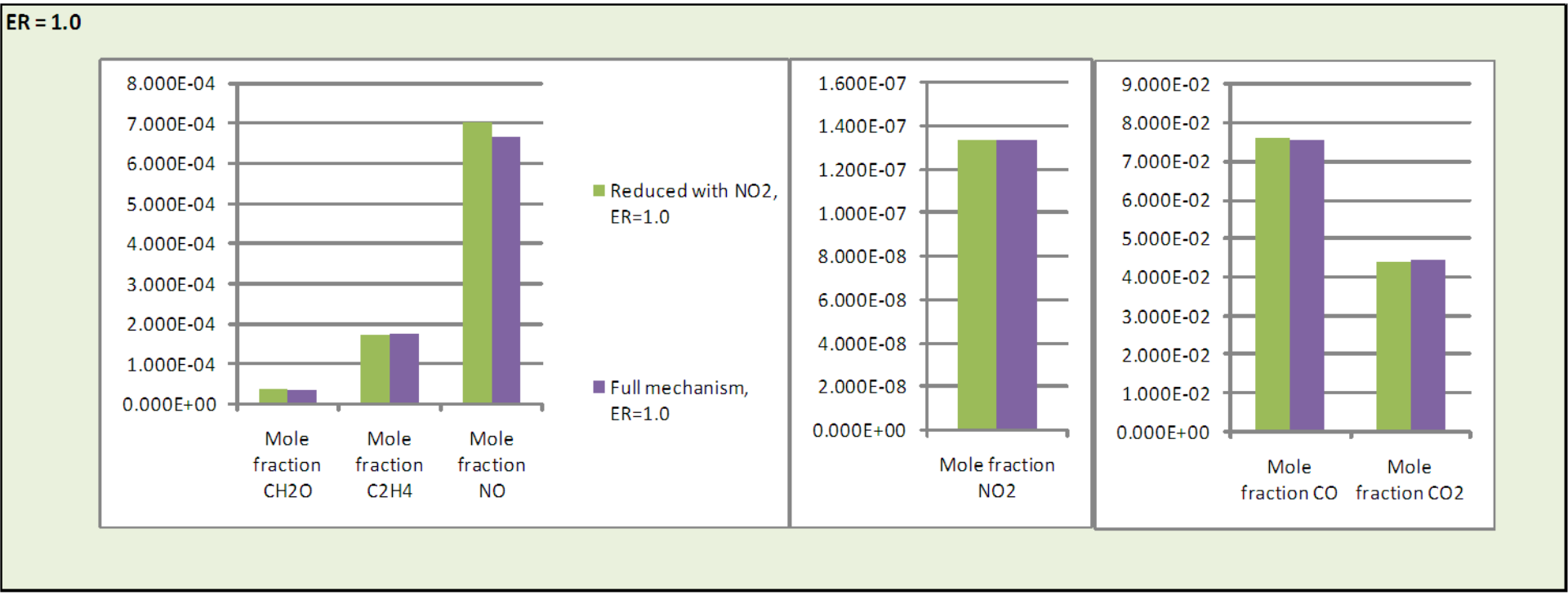
Evaluation Results

- The Reduced mechanism having 50 species with NO_2 was evaluated against the Full Mechanism (USC I + GRI) having 93 species

- The comparisons show very good agreement with the max. % error within ±3% for major species and ± 5% for minor species.

Reactor Conditions	
Equivalence ratio of fuel to oxidizer	0.5, 1.0, 1.5
Reactor temperature	1700 K

Evaluation of the New 50-Species Mechanism with NO2



	CH2O	C2H4	NO					NO2			CO	CO2
% Error	4.89	-2.92	5.29					0			0.57	-1.47

Air-Assisted Flare: Case A2.1

- FUEL: Pure Propylene, 0.17 m/s , 355 lb/hr
- LHV= 2125 BTU/SCF
- Assist Air = 13 m/s, 83,818 lb/hr
- Excess Air Factor = 16
- Cross wind = 5.7 m/s (12.8 mile/hr)

Model Selection

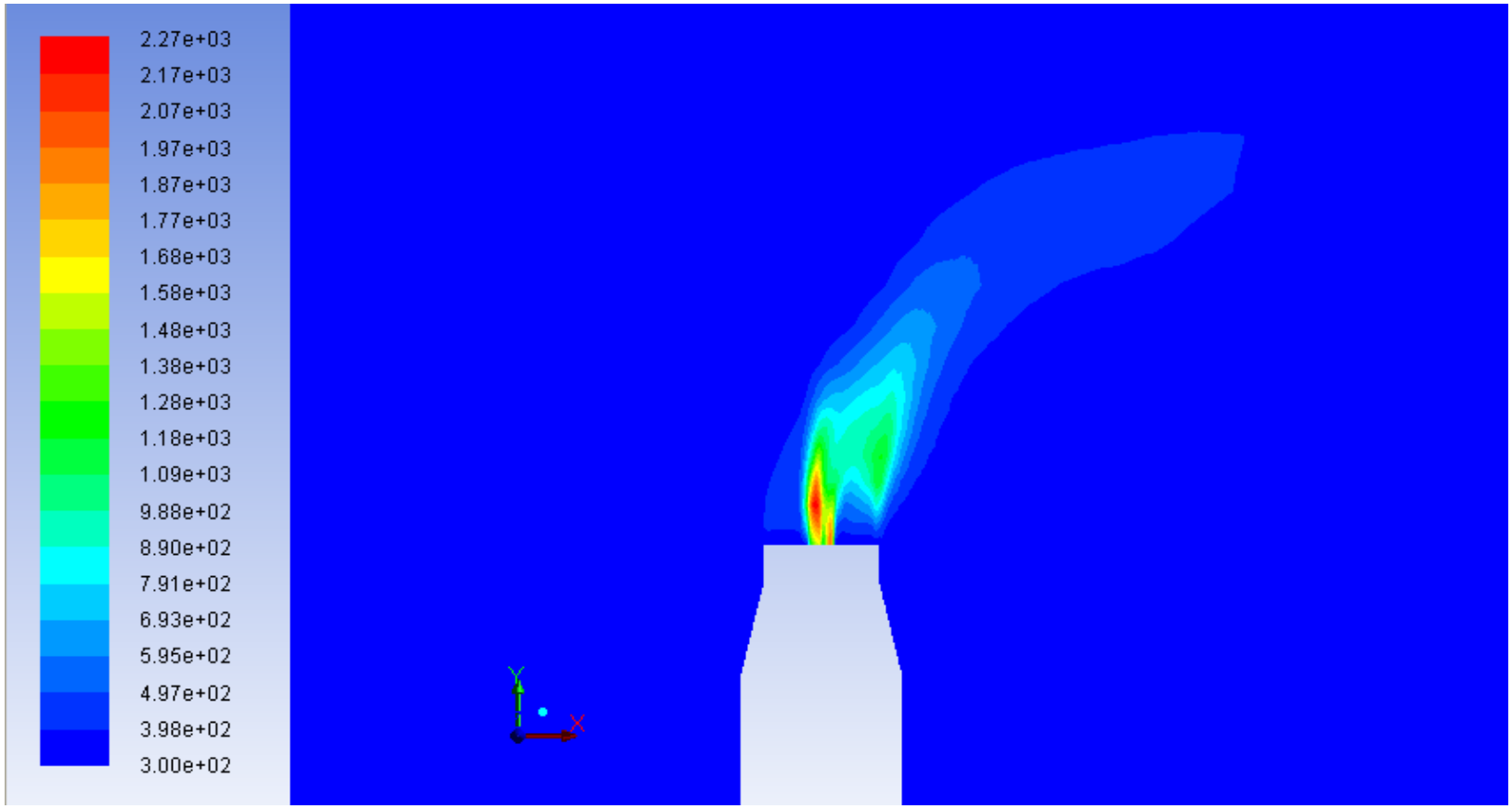
- Solver - Pressure based solver
- Solution Methods: Green-Gauss Cell based
- k-ε realizable turbulence model
    - Turbulence Intensity = 15%
    - Turbulence Viscosity Ratio = 10
- Eddy Dissipation Concept Model (turbulence-chemistry interaction).
- Reduced 50-species mechanism derived from a full 93-species GRI 3.0 + USC Mechanism.

Case A2.1 Results

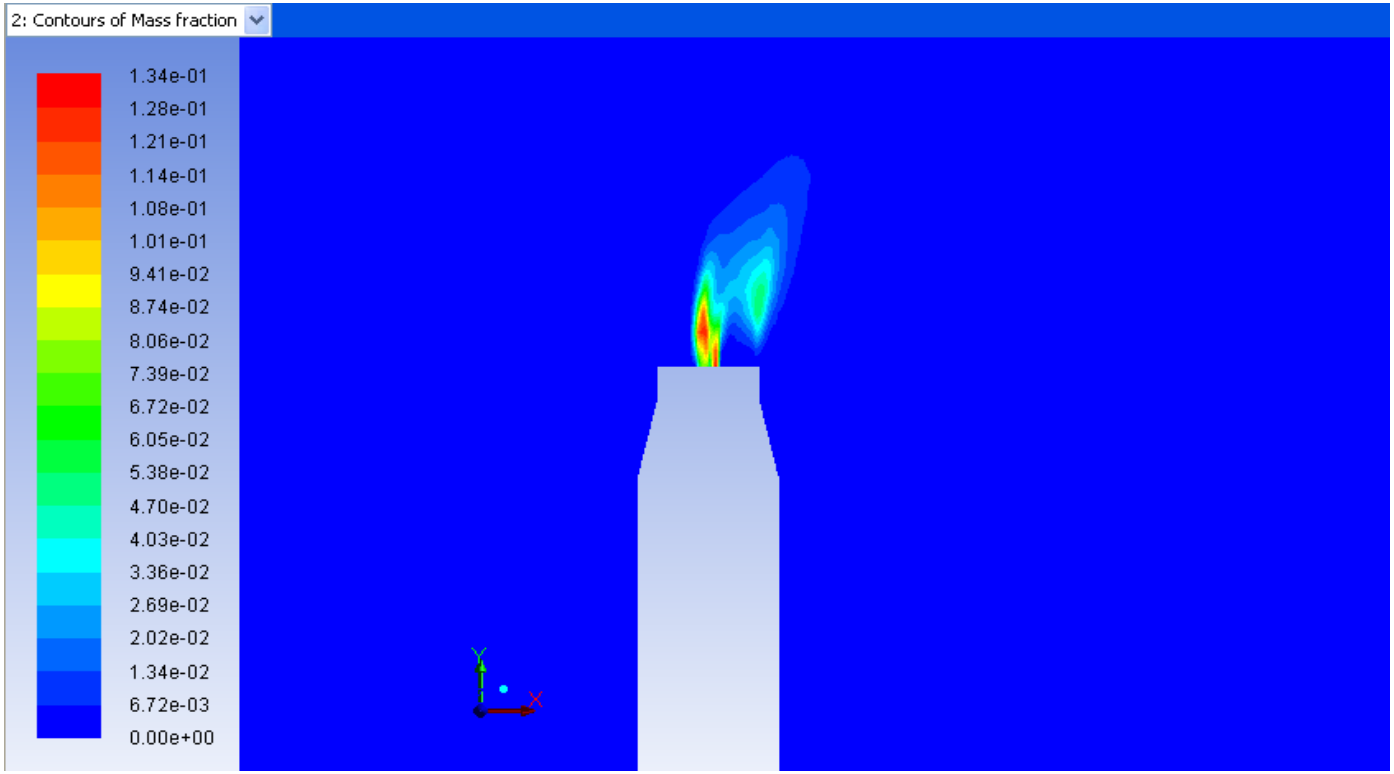
Emissions		
Fuel(C3H6) in	360.17	lb/hr
C3H6 out	3.05	lb/hr
CO2 out	1055.12	lb/hr
C in (as C3H6)	308.72	lb/hr
C out (as CO2)	287.76	lb/hr

	CFD Simulations	Tests
DRE	99.15%	97.15%
CE	93.21%	95.54%

Contours of Static Temperature (K)



Contours of Mass fraction of CO_2



Mechanism Validation

TCEQ SEP 2009-009 Project: Task 2-A Flare Speciation Study Using Advanced Computational Methods

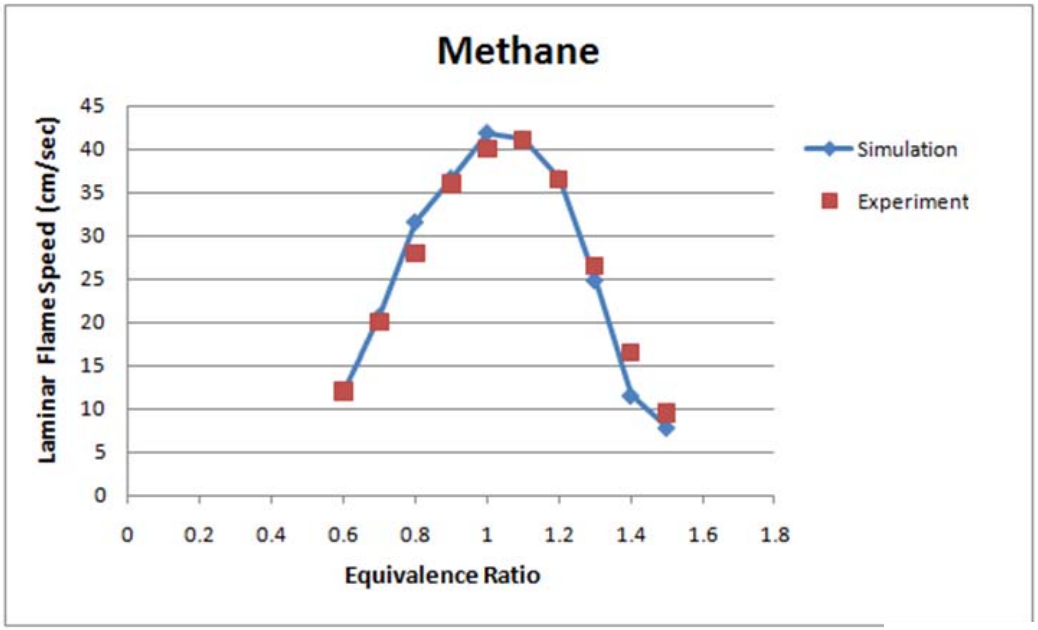
Lab data used for Validation

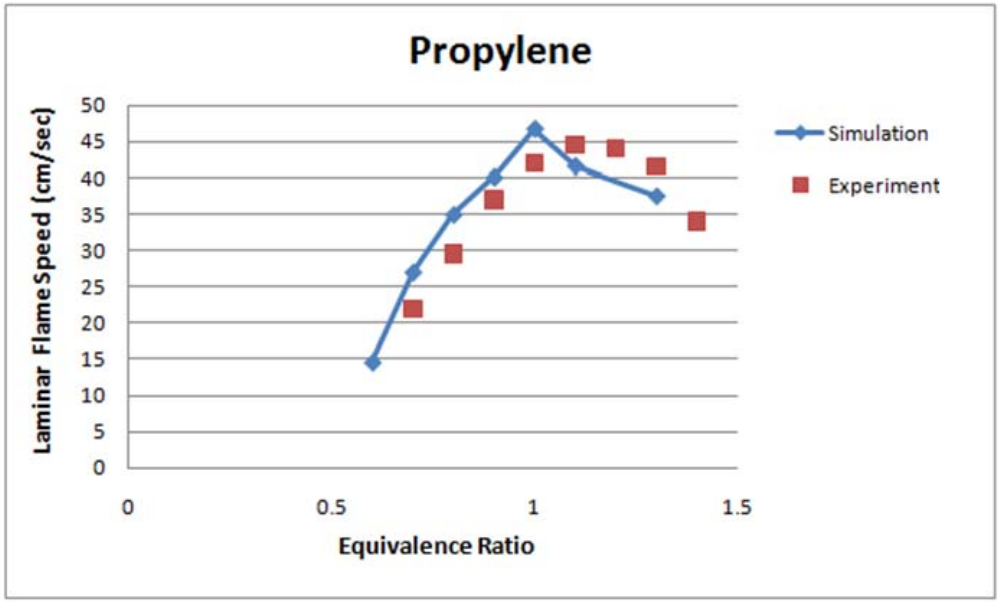
- Laminar Flame Speed
- Burner Stabilized Flame
- Adiabatic Flame Temperature
- Ignition delay
- CFD Simulation of Experimental Flames

Fuel Used: C1-C3

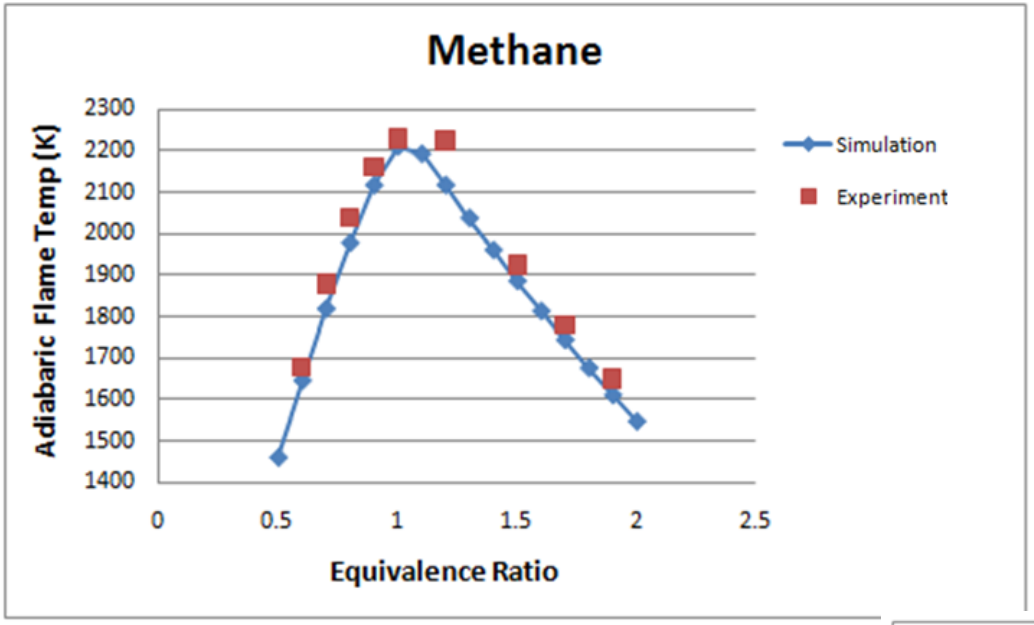
Test	Fuels used
Laminar Flame Speed	Methane and Propylene
Burner Stabilized Flame	Ethylene
Adiabatic Flame Temperature	Methane and Ethylene
Ignition delay	Methane, Ethylene and Propylene
CFD Simulation of Experimental Flames	Methane

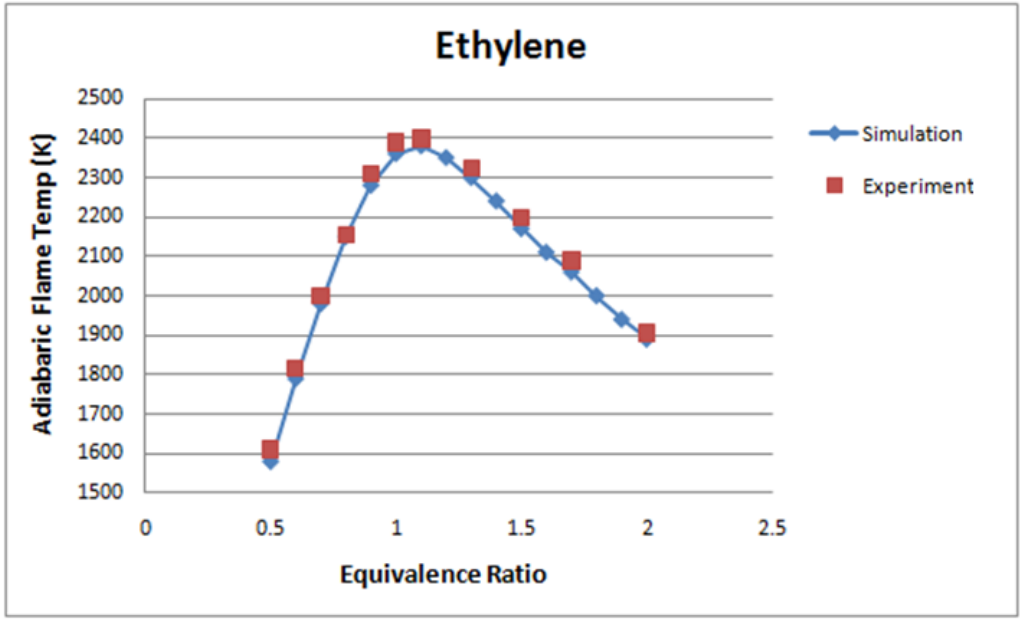
Laminar Flame Speed



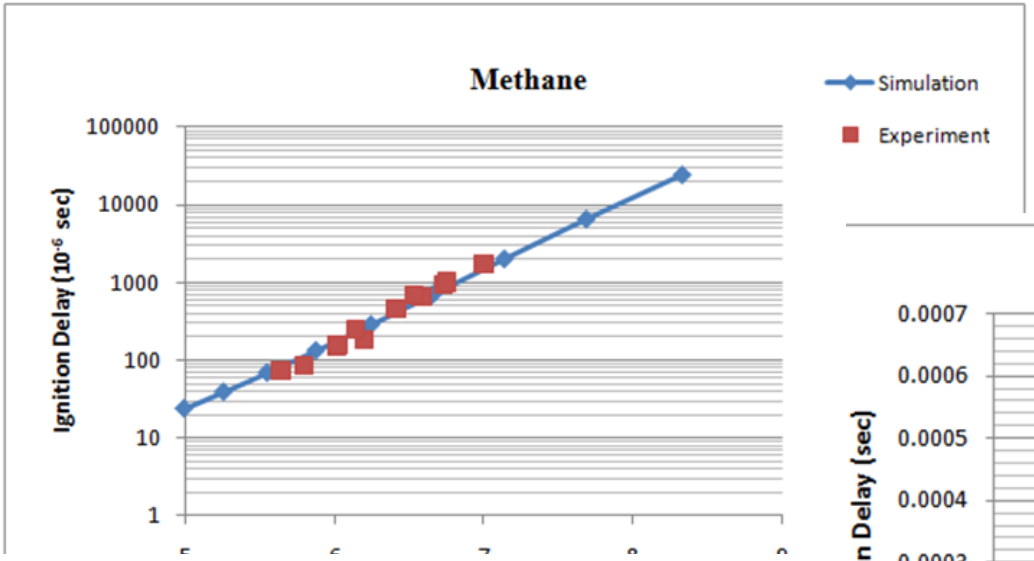


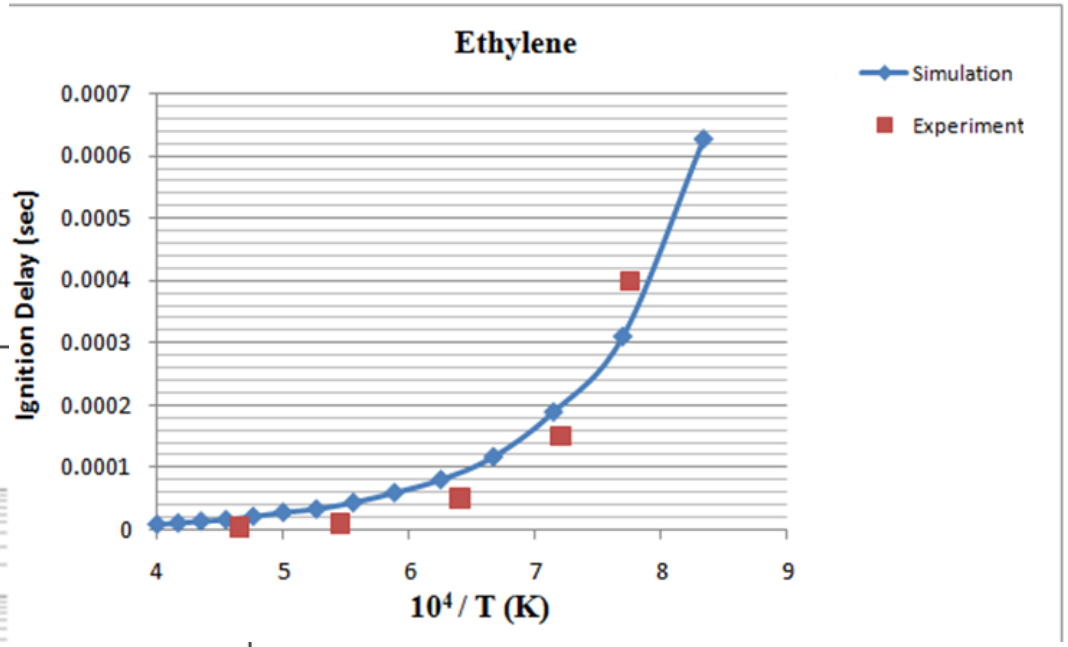
Adiabatic Flame Temperature

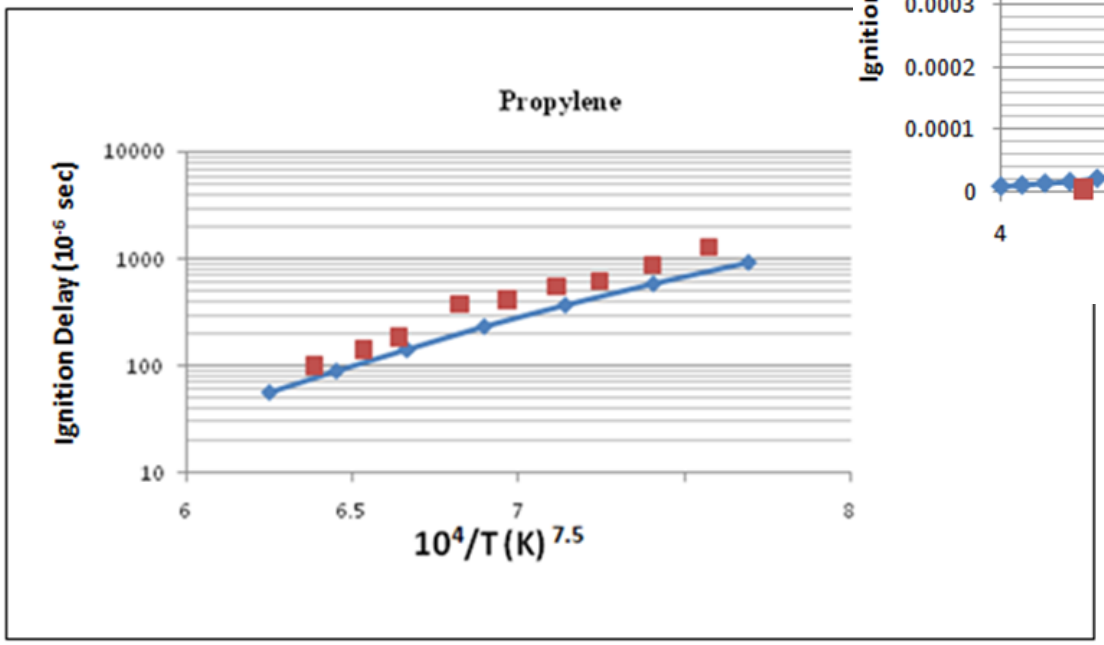




Ignition delay







Burner Stabilized Flame

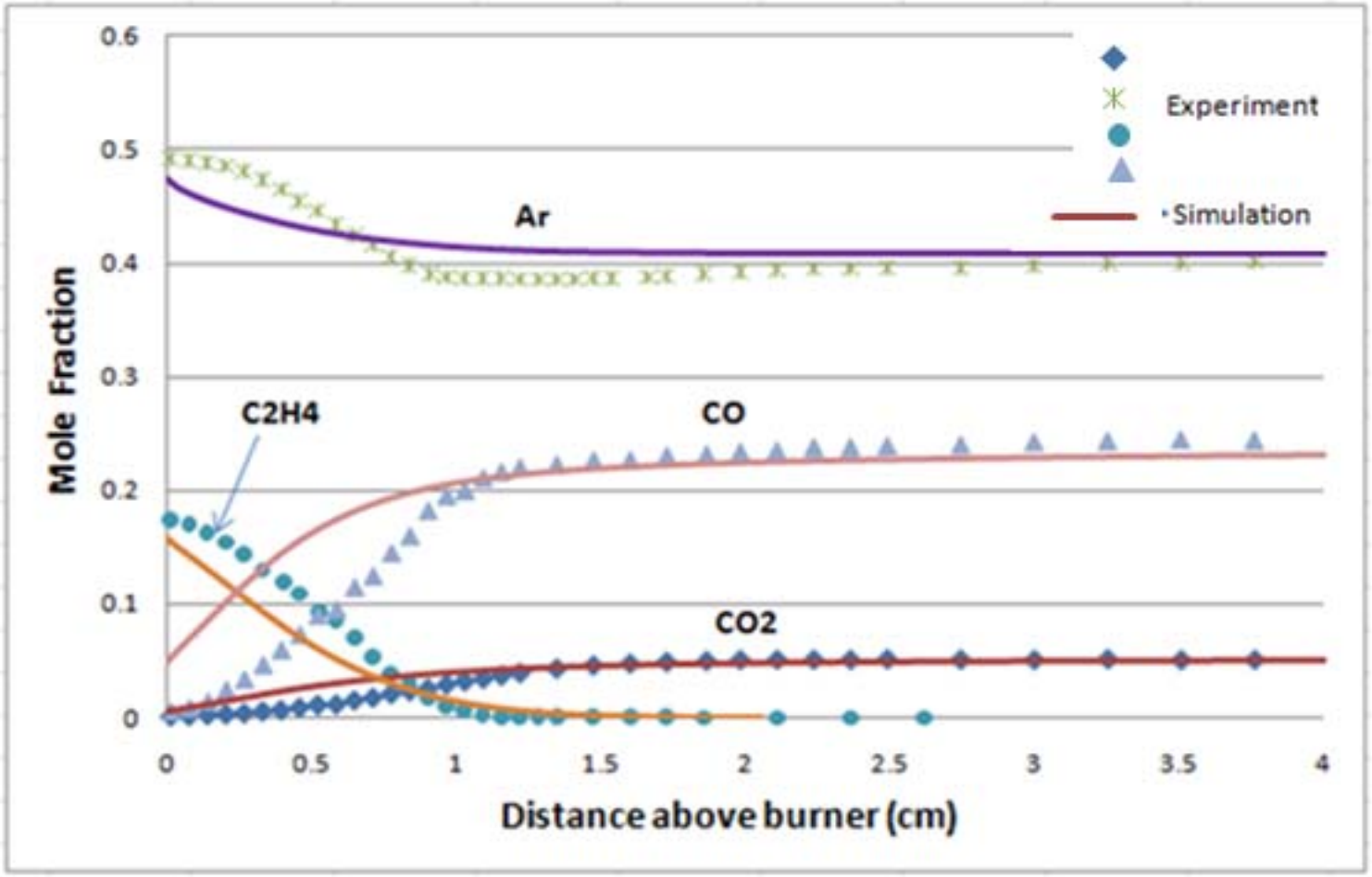


Figure B.1: Comparison of the Molar Fraction of Major Species in Burner Stabilized Flame for $C_2H_4/O_2/Ar$ (phi = 1.9)

Burner Stabilized Flame

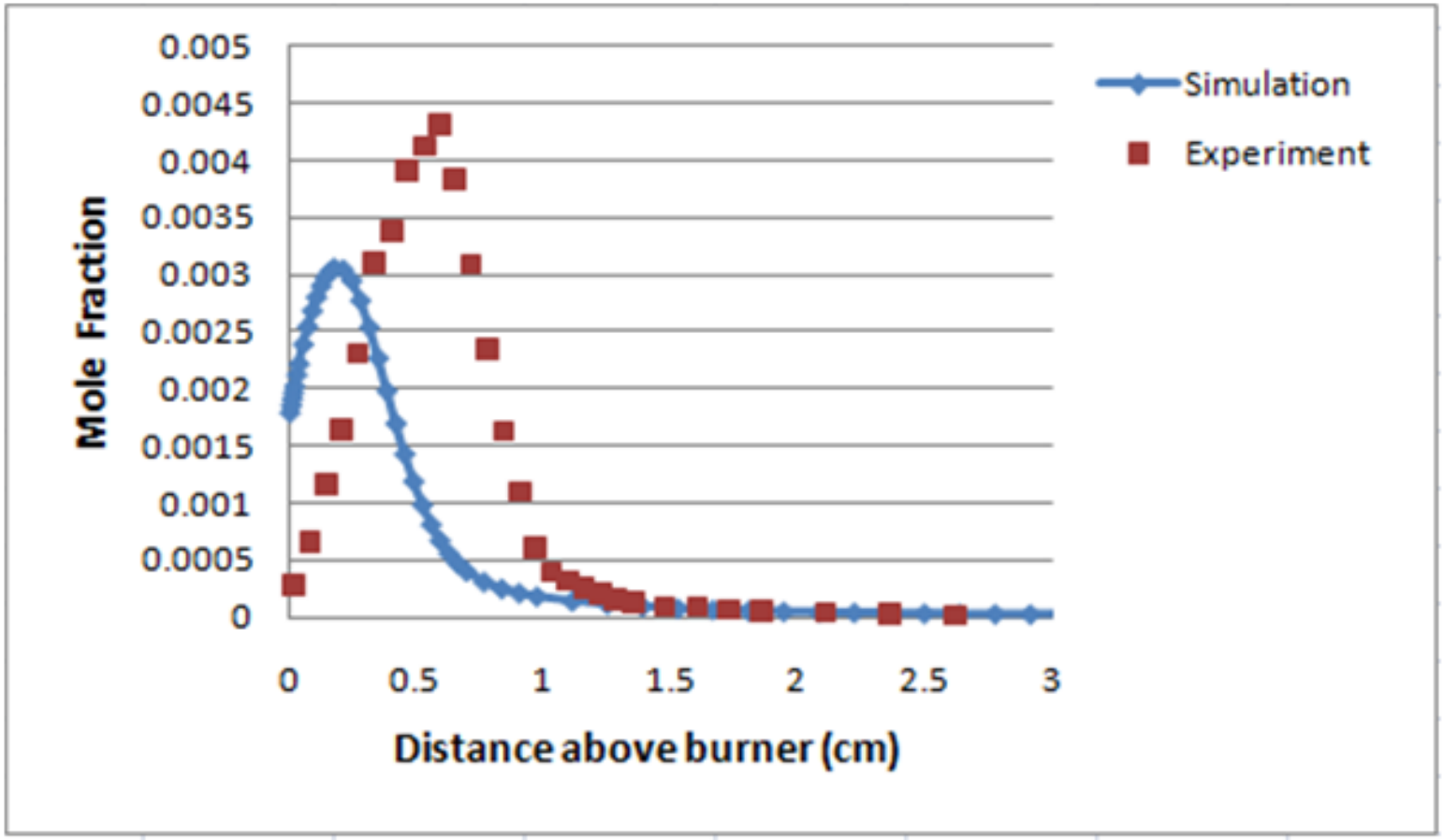


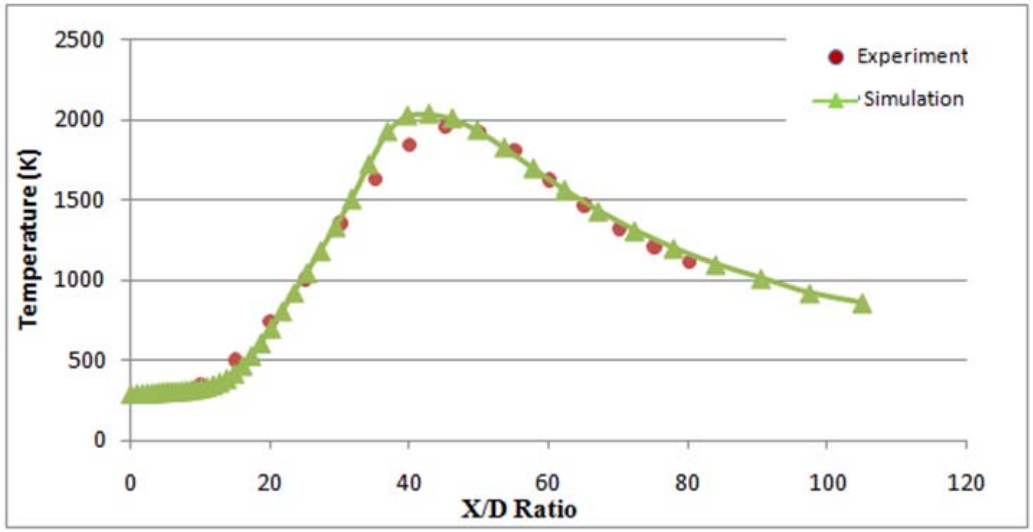
Fig. A.1.2: Comparison of Formaldehyde Mole Fraction Data for Burner Stabilized Flame

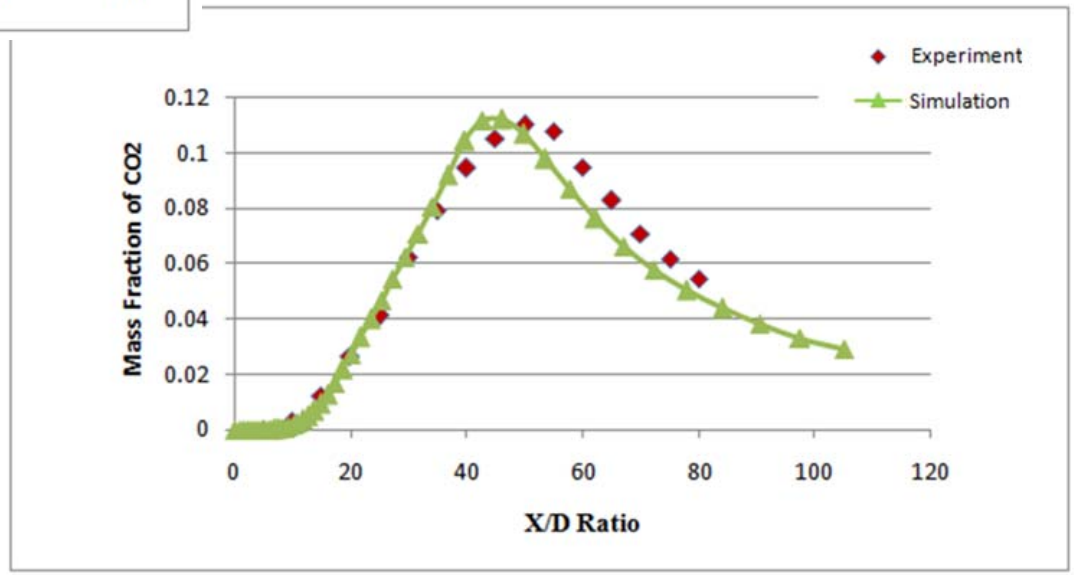
CFD Simulation of the Sandia/TUD Pilot Methane Flame

CH_4/Air Jet Flame (Sandia/ TU Darmstadt, 2006)

- Fuel composition: CH_4 (25%), Air (75%) by volume.
- Fuel exit velocity: 49.6 m/s (Re=22400)
- Nozzle diameter: 7.2 mm
- Pilot composition: CO (0.4%), CO_2 (11%), H_2O (9.4%), O_2 (5.4%), N_2 (73.8%) by volume.
- Pilot exit velocity: 11.4 m/s
- Pilot nozzle outer diameter:18.2 mm

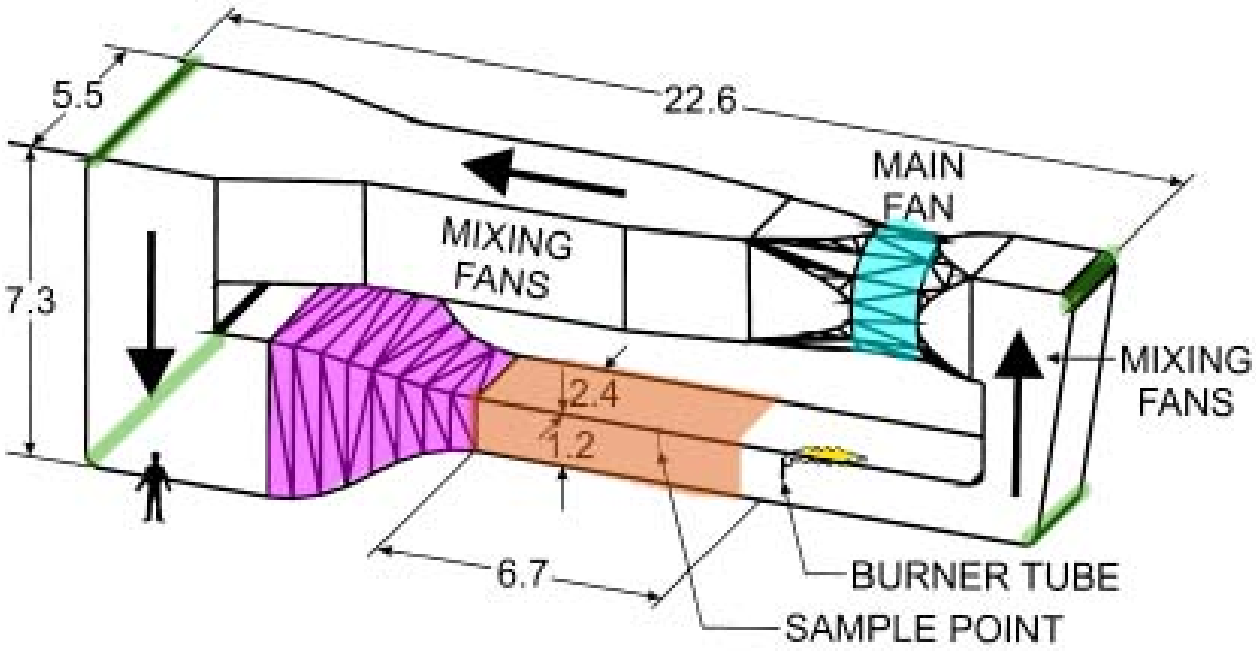
CFD Simulation Results: Sandia/TUD Pilot Methane Flame





Modeling and Simulation of Wind Tunnel Data

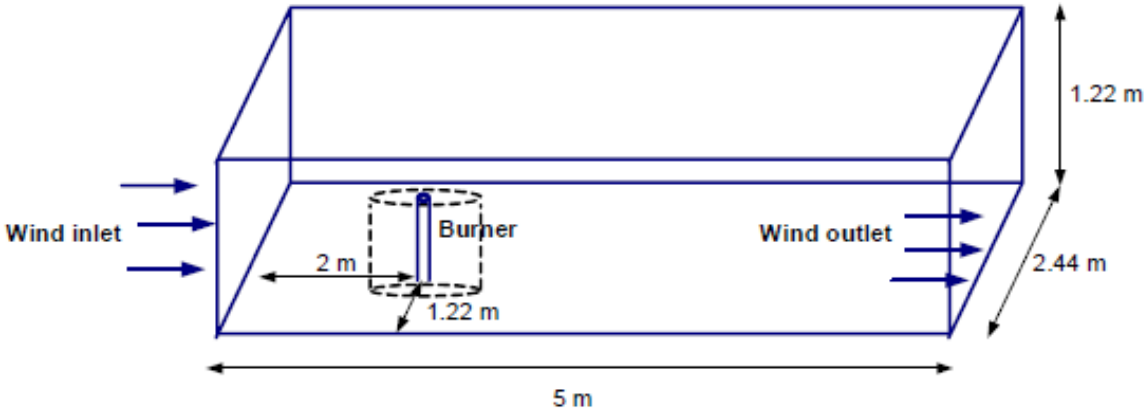
TCEQ SEP 2009-009 Project

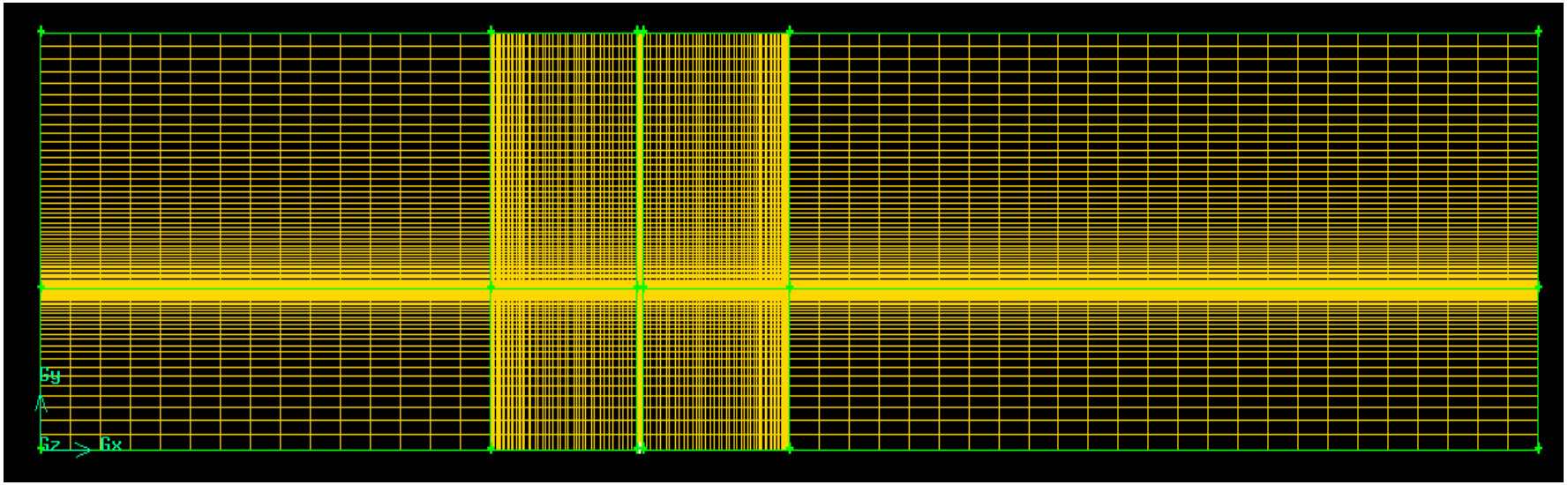


Schematic of a closed-loop wind tunnel facility (all dimension in meters) at the University of Alberta.

Kostiuk, L, Johnson, M. and Thomas, G., University of Alberta Flare Research Project Final Report (2004).

Geometry



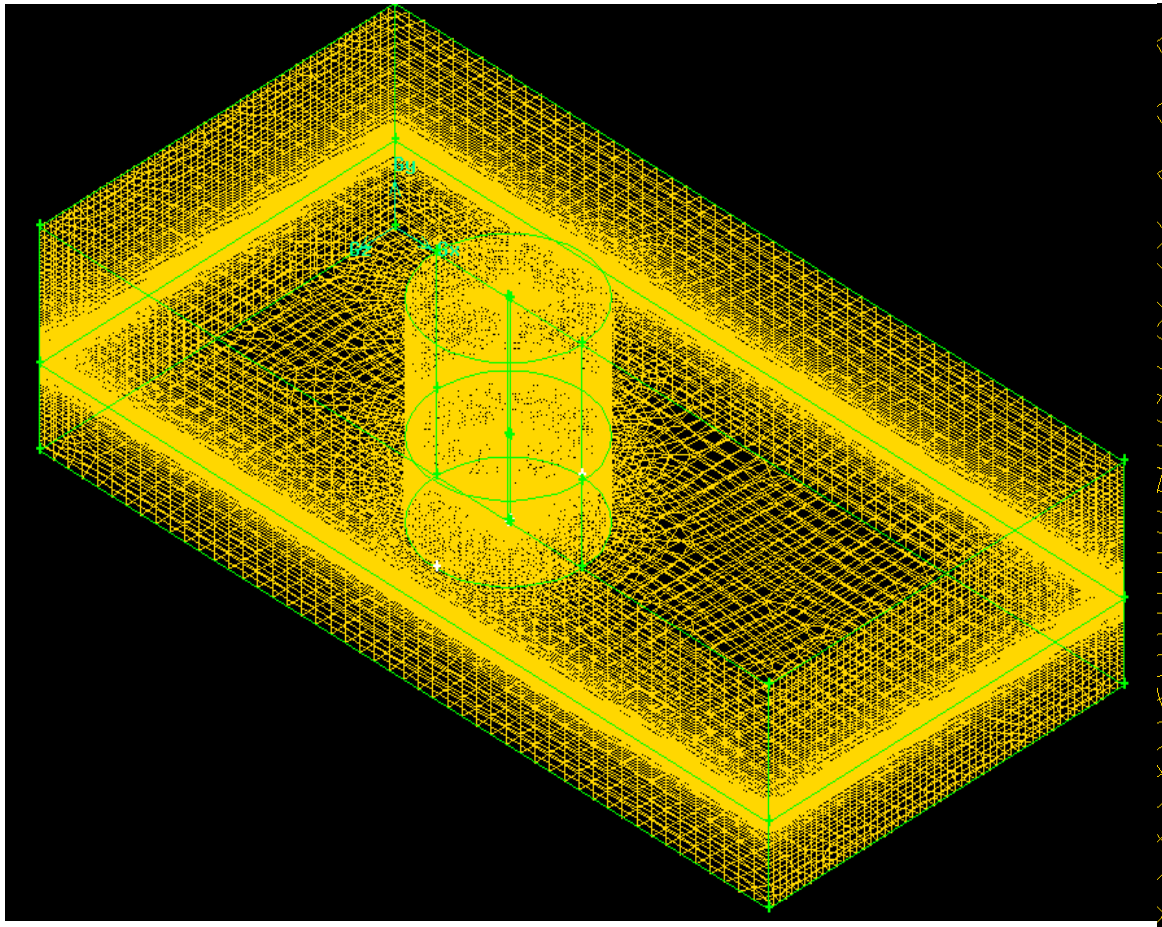


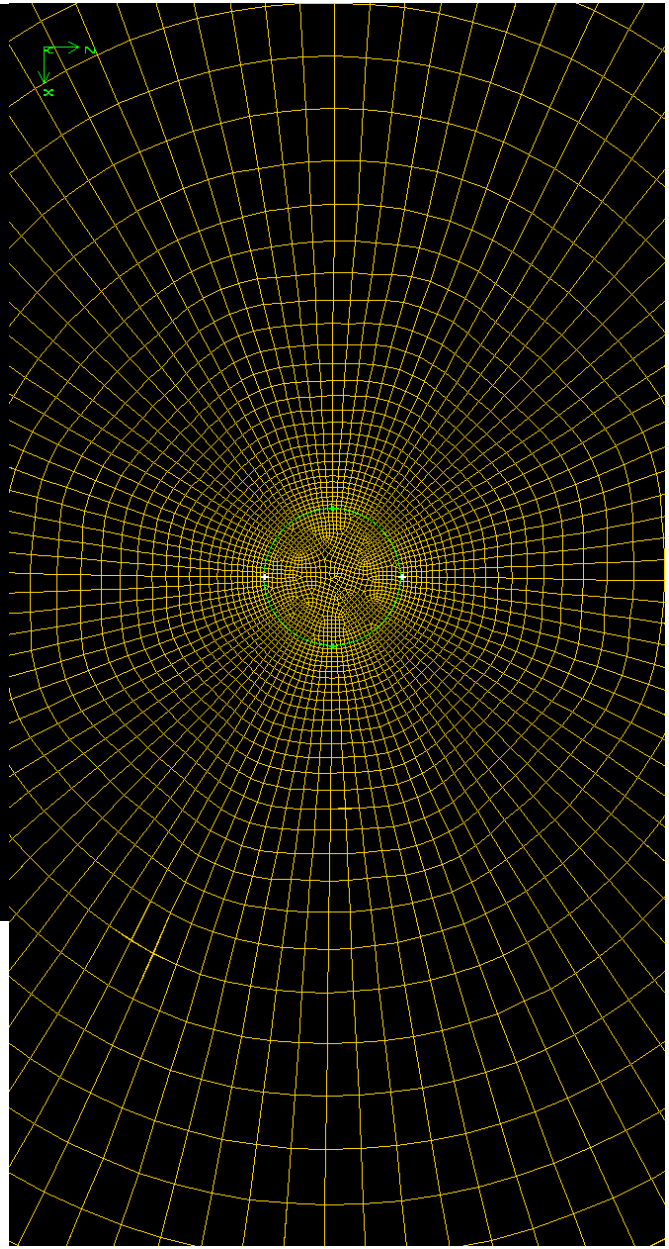
Grid Size

Cells: 636640

Faces: 1929038 Nodes: 655841

Structured Mesh were generated Using Size Functions.





Meshed Geometry

Boundary Conditions

	Jet	Cross Wind
Velocity (m/s)	2.011	8.27
Hydraulic Diameter(m)	0.0221	1.94
Turbulence Intensity (%)	15	0.2

Fuel	Mass Fraction
CH4	0.9129
CO2	0.0202
C2H4	0.0035
C2H6	0.0364
N2	0.0271

Model Selection

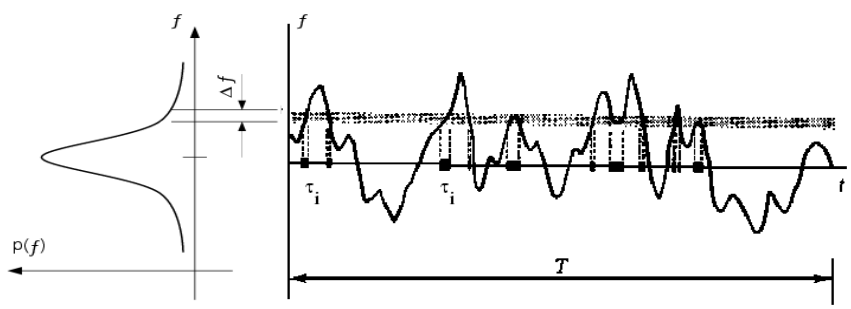
- Pressure based solver
- k-ε realizable turbulence model
- Non-premixed (PDF + Mixture Fraction) combustion model.
- GRI 3.0 Mechanism (54 species).

Non-Premixed Model

- The mixture fraction concept plays a vital role in Non-premixed combustion model.
- The probability density function can be thought of as the fraction of time that the fluid spends in the vicinity of the state *f*.

$$p(f)\Delta f = \lim_{T\to\infty}\frac{1}{T}\sum_{n}\tau_n$$

Where,

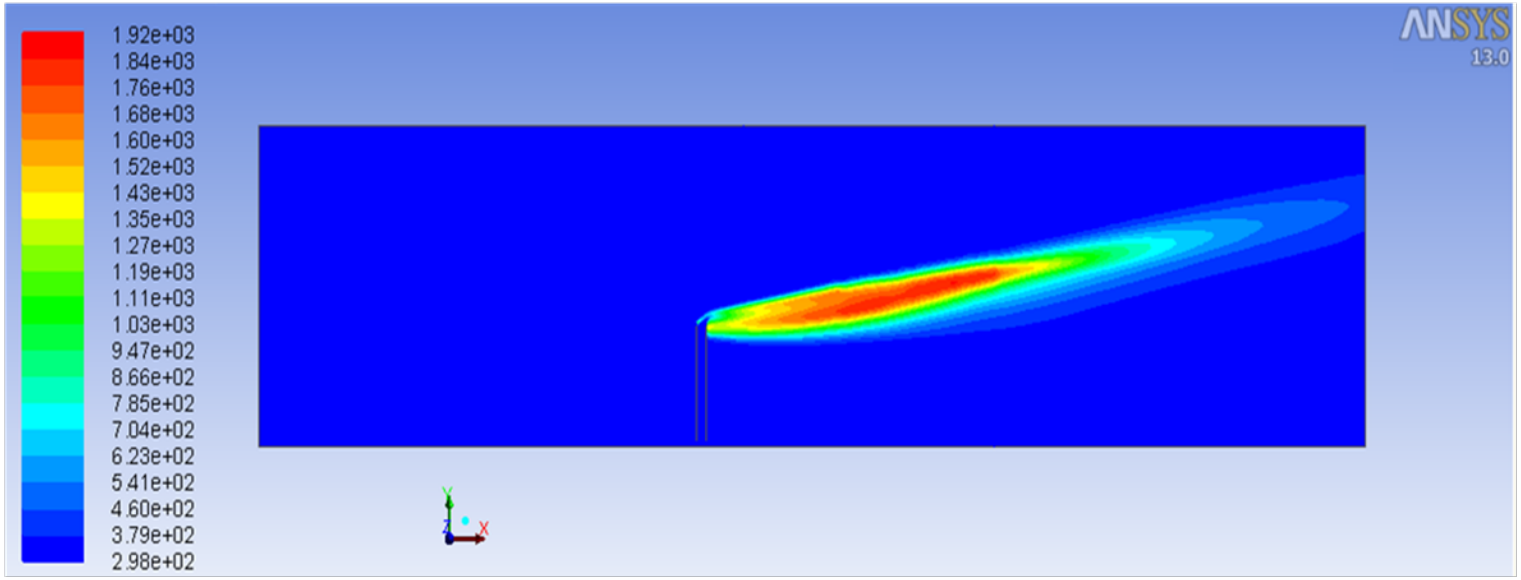


T is the time scale

τ_n is the amount of time that *f* spends in the band.

ANSYS FLUENT 6.3 User's Guide, Fluent Inc (2006)

Temperature Contours (Enhanced Wall Treatment)



Color image of the natural gas flame in a crosswond (Experimental)

Carbon Flow Rate, Efficiency, and Mass Balance

Species Mass Flows (10^{-5} Kg/s)

	IN (10^{-5} Kg/s)				Out (10^{-5} Kg/s)		
	CH4	CO2	C2H4	C2H6	CH4	CO2	CO
	48.21	1.067	0.1848	1.922	0.142	128.18	7.95
Carbon	36.158	0.291	0.158	1.5376	0.107	34.958	3.407

Total Carbon In (10^{-5} Kg/s)	38.14
Total Carbon Out (10^{-5} Kg/s)	38.47
Combustion Efficiency	91.65%
Mass Balance Error	-0.858%

Experimental CE ≈ 94%

Flare research project, final report, University of Alberta, September 2004

Thank You