CFD Flare Modeling Update

SETPMTC Meeting

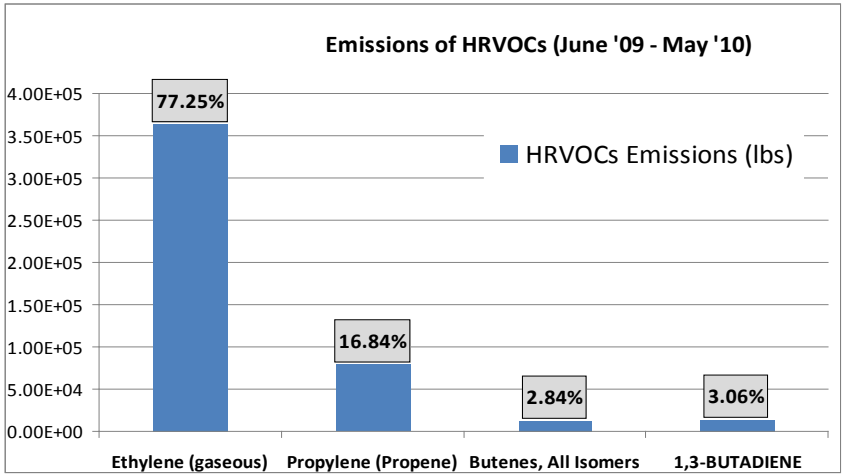
by
Daniel Chen, Helen Lou, Kuyen Li
D. F. Smith Chemical Engineering Dept.
Xianchang Li, Mechanical Engineering Dept.
Christopher Martin, Chemistry & Biochemistry Dept.
Lamar University, Beaumont, TX

Houston, TX, August 23, 2012

Contents

I. Introduction/Needs
II. Methodology
III. AQRP Project 11-022
IV. SEP Project 2009-009

Reasons for TCEQ to focus on Industrial Flares



- One **potential under-reported or non-reported source** is the flare operations
- Flare emissions: 60% of the **HRVOCs** (2007 HRVOC special inventory).
- Flare emissions depend heavily on **destruction & removal efficiency (DRE)**
  - Recent studies/gas imaging IR camera suggest that flares may not be as efficient as claimed (Environ, 2008;)
  - DRE may drop below 98% even when the flare operation is in compliance with 40 CFR § 60.18 (Allen, TCEQ 2010 Flare Study).
  - Complex issues such as **crosswind, high/low jet velocity, high air/steam assist, vent gas composition**, etc.
- Flare emissions also affected by **combustion efficiency (CE)** or the issue of **incomplete combustion products**
  - Current air emission inventory from flaring is simply a mass throughput with 98% (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 (Vent Gas Species/ Heating Value & Reaction Chemistry)
  - Refinery, Olefin, Polymer, Landfill, and Exploration fields (H2-C4)
- Operation Mode
  - Startup, Shutdown, Upset, Maintenance, and Standby (Turndown Ratio up to 15000:1)
- Flare Design/Control
  - Air assisted, Steam assisted, Non-assisted, Pressure-assisted
  - Elevated, Enclosed
  - Steaming, Aeration, Tip Diameter
- Meteorological condition
  - Crosswind, Humidity, etc.

Needs for Computational Fluid Dynamics (CFD) Flare Modeling

- Alternative to expensive flare tests
  - Grab sampling or remote sensing are costly
  - Impossible to test during start up, upset, and maintenance periods

- Validated flare model for parametric studies
  - Establish the data base for effect (trend) of crosswind, jet velocity, VOC species, heating value, air-assist, steam-assist, tip diameter
  - Investigate the interaction between crosswind, jet velocity, vent gas heating value, and assisted air/steam

- Easy-to-use correlations and NN models for DRE/CE/T_{max}

- Validated flare model for inferential control
  - Determine optimal set points for air/steam/makeup fuel flow given vent gas composition, heating value, jet velocity, and crosswind velocity

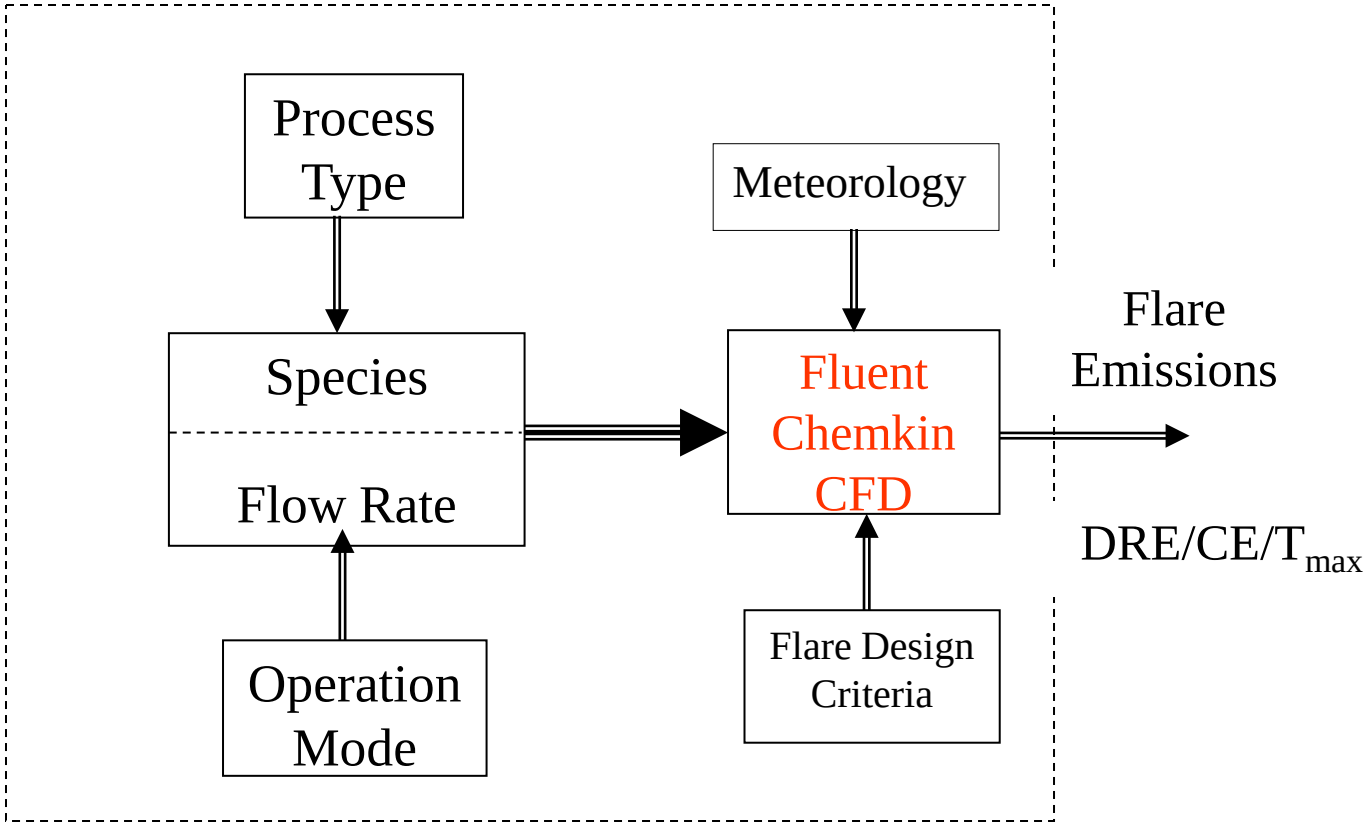
Objectives

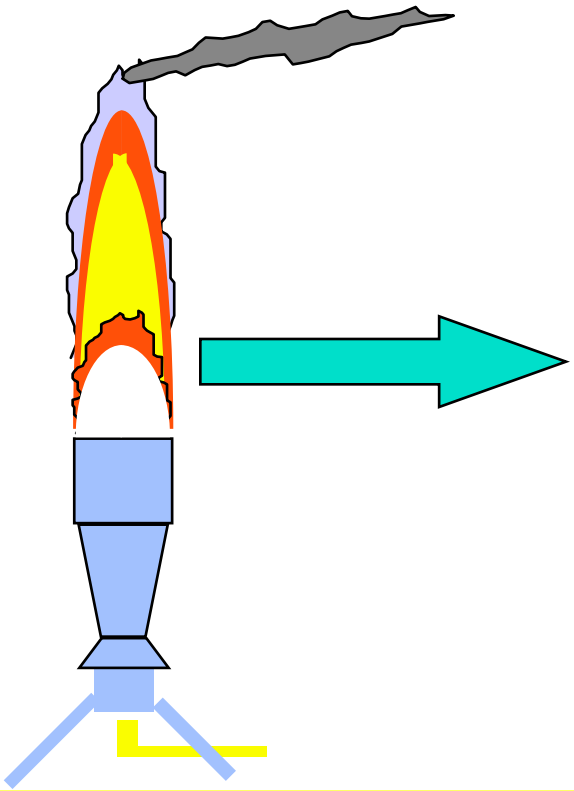
- Model laboratory flames (McKenna Burner and Sandia National Lab Flame D)
  - to validate the CFD with laboratory flames for which detailed, speciated composition profiles are available for incomplete combustion products (e.g., formaldehyde).
- Model controlled flares (TCEQ/UT 2010 Flare Study)
  - to validate the CFD with industrial flares for which DRE/CE, and certain speciated emission data are available under controlled conditions.
- Simulate industrial flares under various operating modes and meteorological conditions to investigate
  - the trend of crosswind, heating value, vent gas type, steam assist, air assist, jet velocity, and flare-tip diameter.
  - the interaction between crosswind, jet velocity, and heating value
- Develop easy-to–use correlations and neural network models
  - to identify the optimal operating regime for high DRE/CE/T_{max} and to facilitate inferential control
  - to estimate aldehydes/HO_x/NO_x emissions given crosswind, jet velocity, vent gas heating value, and other operating/ design conditions

Methodology

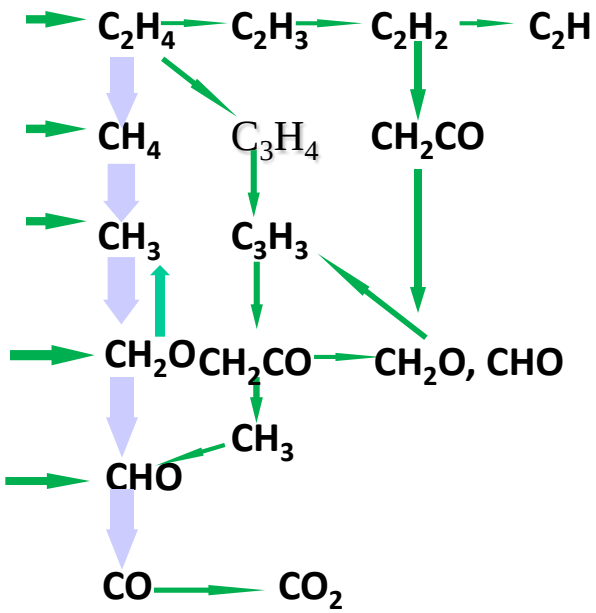
CFD modeling for Industrial Flares

- Model industrial flaring systems using Fluent /Chemkin CFD with a reduced (50 species) mechanism for ethylene/propylene combustion
- Validated with experimental flame/controlled flare performance data





Example: Ethylene Reaction Pathways



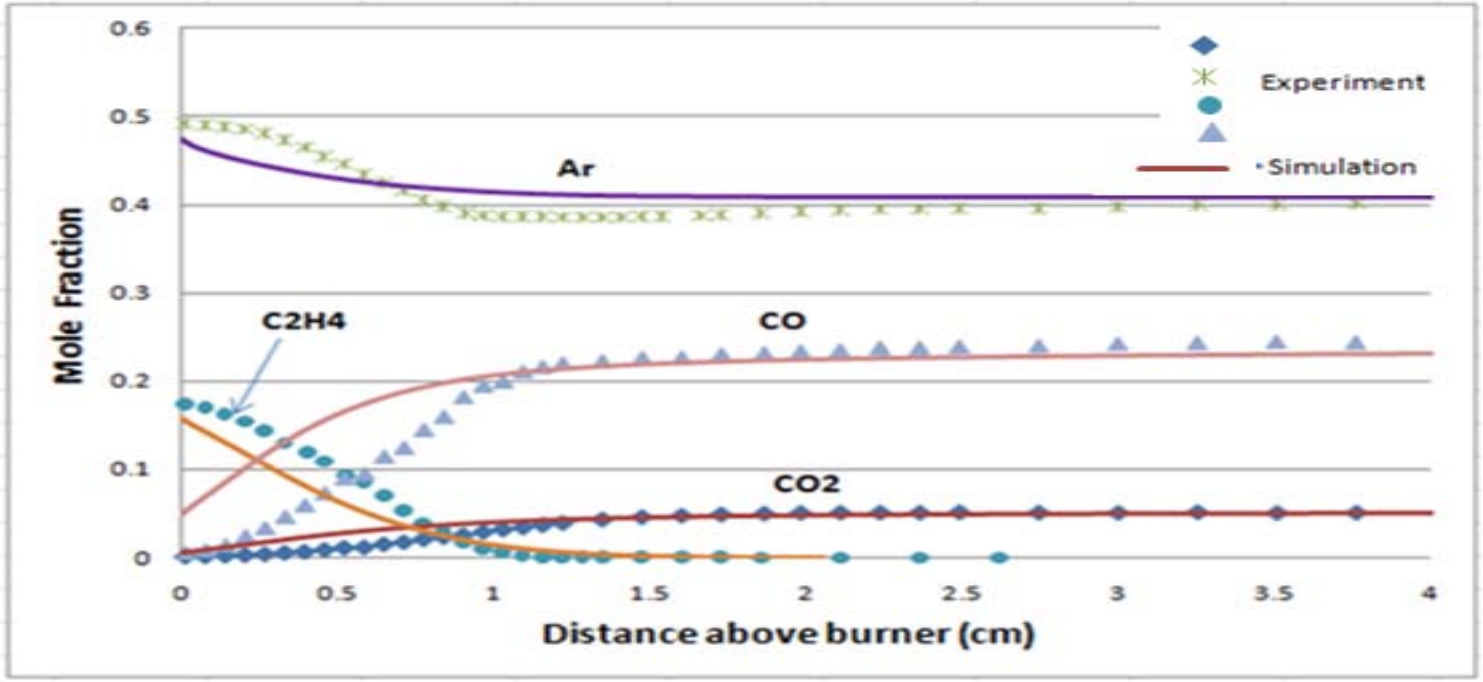
CHEMKIN Mechanisms

- We have combined the GRI-3.0 mechanism (optimized for methane) and the USC mechanism (optimized for ethylene but without the NO_x species) to obtain a mechanism containing 93-species and 600 reactions.
- A series of 50-species reduced mechanisms for the combustion of C_1-C_3 light hydrocarbons were developed. **LU1.0 & 1.1** were reduced based on analysis of rate constant, maximum mass fraction, and number of reactions involved in the reaction pathway. In LU 1.1, NO_2 replaces CN. **LU 2.0** has been developed based on minimizing the difference between the experimental data and mechanism predictions.
- All mechanisms were validated with experimental results like **laminar flame speeds, adiabatic flame temperature, ignition delay, and burner stabilized flame**.

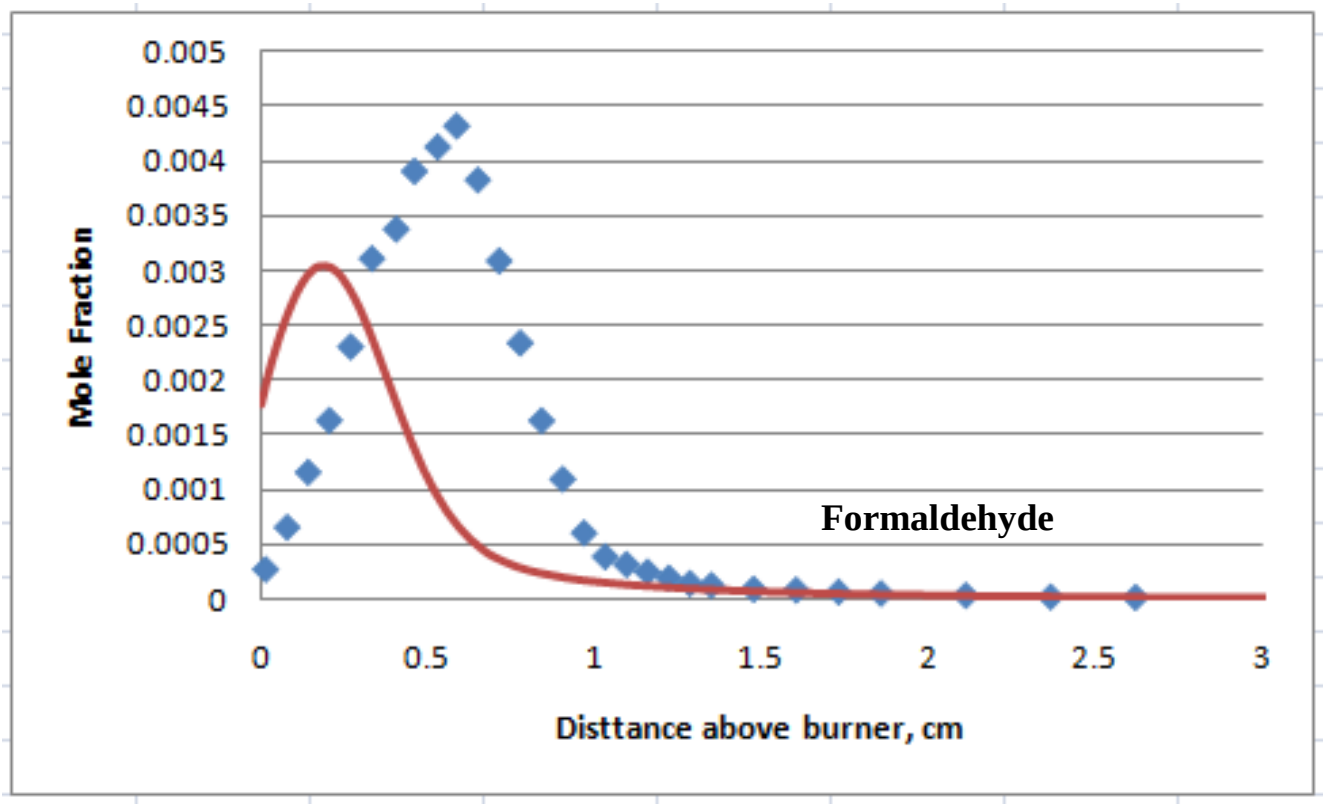
Journal Publications in Mechanism Development

"A reduced reaction mechanism for the simulation in ethylene flare combustion,“ *Clean Technologies and Environmental Policy*, June 16, 2011;
,"Validation of a Reduced Combustion Mechanism for Light Hydrocarbons," Clean Technologies and Environmental Policy, “ Clean Technologies and Environmental Policy, 14(1) 1-12, 2012.
"Optimal Reduction of the C1-C3 Combustion Mechanism for the Simulation of Flaring, " *Industrial & Engineering Chemistry Research*, February 13, 2012.

Validation of LU 1.0 Mechanism



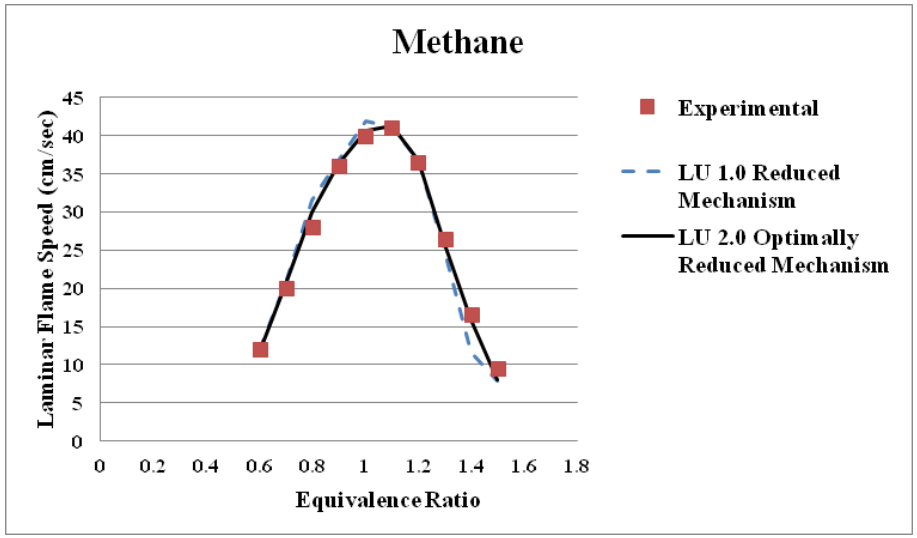
Comparison of the Molar Fraction of Major Species in Burner Stabilized Flame for $C_2H_4/O_2/Ar$ (phi = 1.9), LU 1.0



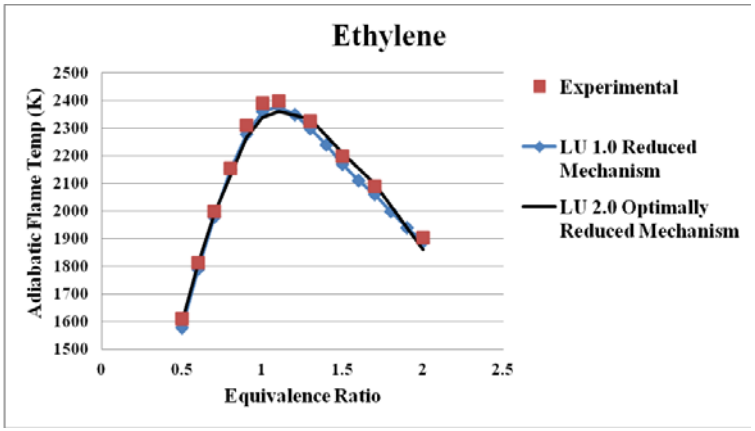
Comparison of Formaldehyde Mole Fraction Data for Burner Stabilized Flame, LU 1.0

Validation of **LU 2.0** Combustion Mechanism for C_1-C_3 Hydrocarbons

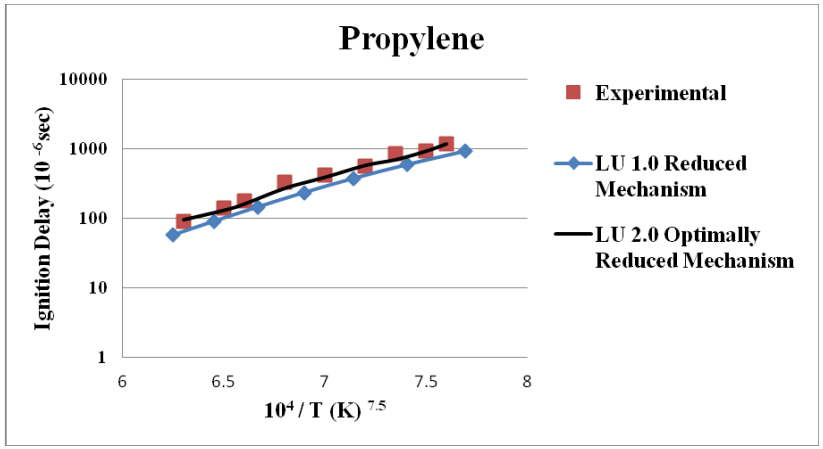
Laminar flame speed vs equivalence ratio for methane



Adiabatic flame temp vs. equivalence ratio for ethylene



Ignition delay vs. temperature for propylene



Indicators		% Error (Average)	
		LU1.0 vs. Experimental	LU2.0 vs. Experimental
Laminar Flame Speed	Methane	3.76	2.68
	Propylene	6.30	2.79
Adiabatic Flame Temperature	Methane	8.42	4.76
	Ethylene	2.07	1.08
Ignition Delay	Methane	2.09	1.41
	Ethylene	5.15	3.19
	Propylene	5.32	4.38
Overall		4.73	2.90

Data Base for Validation of CFD Modeling

- Laboratory Flames
  - Ethylene flames (MBMS, Bhargava 1998; Zhang 2006; Delfau, 2007)
  - Methane/Ethane/H_2/CO flames [TNF, 2012]

http://www.sandia.gov/TNF/DataArch/delft3.html

Image Source: 2010 TCEQ Flare Study Project, Final Report

- Controlled Flares
  - UT/John Zink (TCEQ 2010 Flare Study)
  - Propane flare with PFTIR (TCEQ/URS/UH, 2004)
  - Scaled-down flares in a large, closed-loop, wind tunnel facility (University of Alberta, 2004)
  - J.H. Pohl, *Evaluation of the Efficiency of Industrial Flares*, 1984/1985, EPA600-2-85-95 and 106
  - Propylene/Propane flare with Continuous Monitors/GC (EPA, 1983)

Validation of CFD with a CH_4 Sandia/ TU Darmstadt Flame

Fuel composition: CH_4 (25%), Air (75%) by volume.

Fuel exit velocity: 49.6 m/s

Nozzle diameter: 7.2 mm

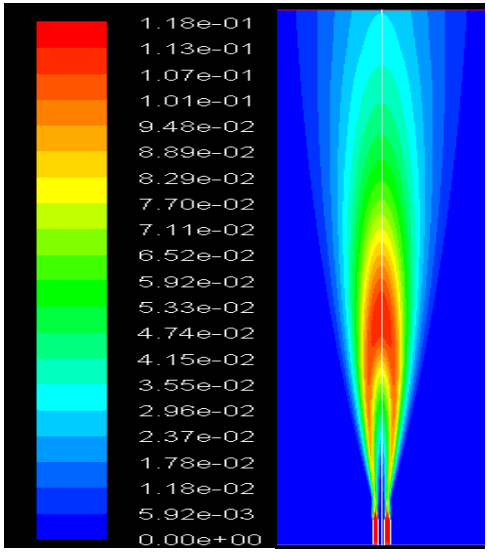
Pilot composition: CO (0.4%), CO_2(11%), H_2O(9.4%), O_2(5.4%), N_2(73.8%)

Pilot exit velocity: 11.4m/s

Pilot nozzle outer diameter:18.2 mm

Mechanism : GRI 3.0 (reduced to 35 species)

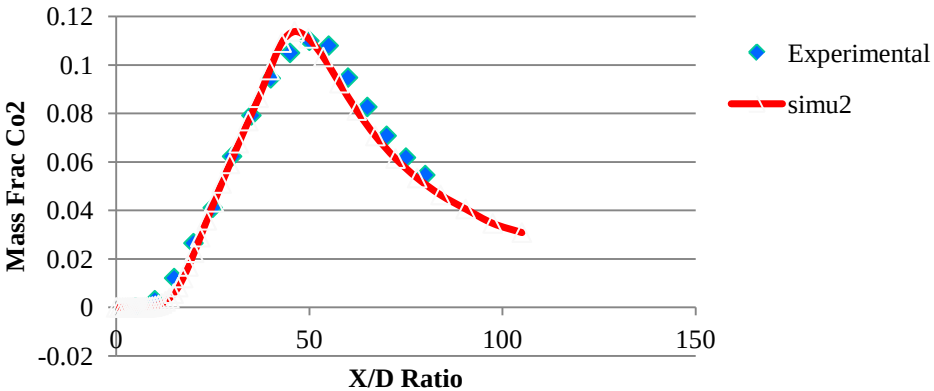
2-D simulation



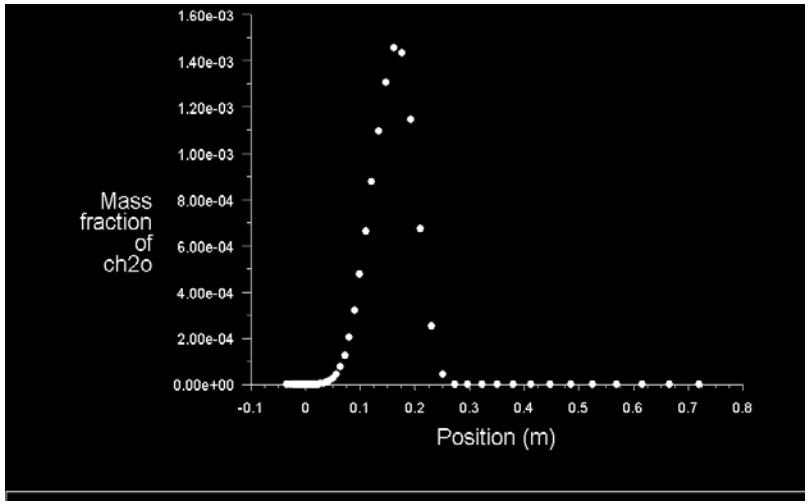
Sandia/TUD Piloted Flame

Temperature Profile

Mass Fraction of CO_2

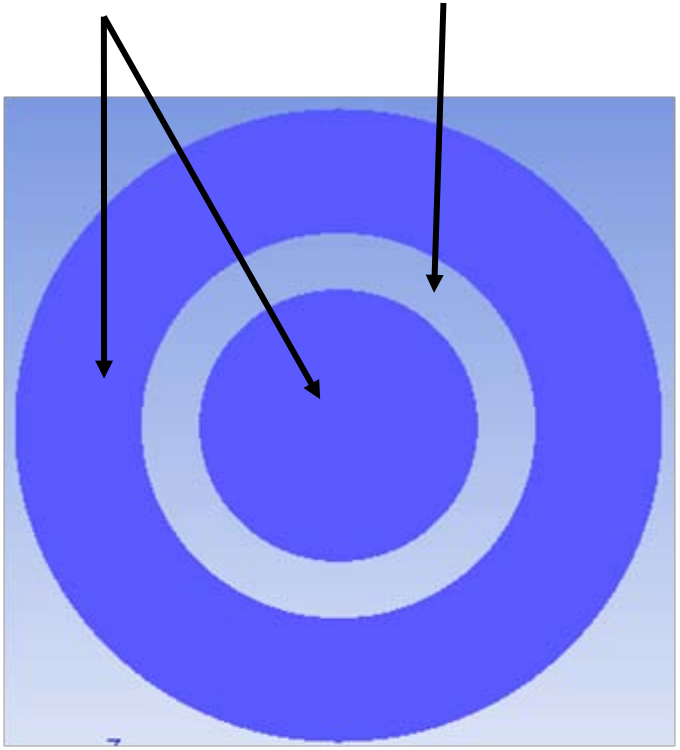


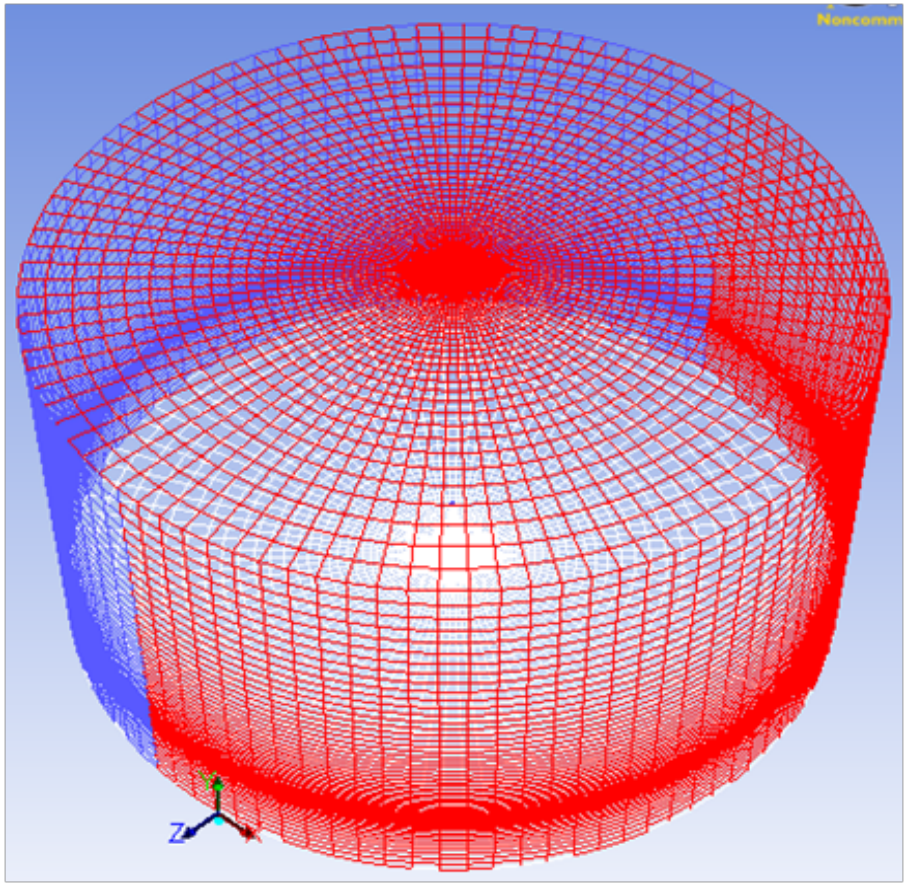
Formaldehyde Plot along Axis (Simulation)



Parametric Study of Industrial Flares

With Ring Shaped, Non-Premixed Geometry





Mass balance errors < 1%

Turbulence-Chemistry Interaction Models

Table 3: Comparison of EDC and PDF models

EDC (Eddy Dissipation Concept)	PDF (Probability Density Function)
Reactions taking place in the flame are governed by the Arrhenius rates	Reactions are governed by a conserved scalar quantity known as mixture fraction
Incorporates detailed chemical mechanisms	**Fast reactions are assumed (Valid for >2100 K).**
Molar concentrations are derived from Reaction rates, which are calculated using ISAT algorithm	Molar concentrations are derived from the predicted mixture fraction fields
Any number of inlet streams can be defined	Only two inlet streams are allowed i.e. Fuel and Oxidizer
Computationally very expensive; requires 5-6 days for convergence	Requires less time for convergence; only 2-3 days

Easy-to-Use Correlations

Polynomial Equations

$Y = a_0 + a_1*U + a_2*V_j + a_3*U*V_j + a_4*U^2 + a_5*V_j^2$

where a_i = *i* th weighting factor; U = crosswind; V = jet velocity

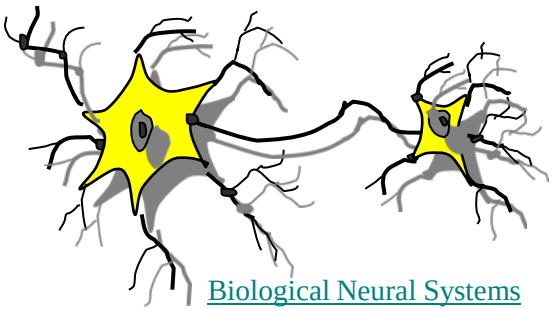
Exponential Equations

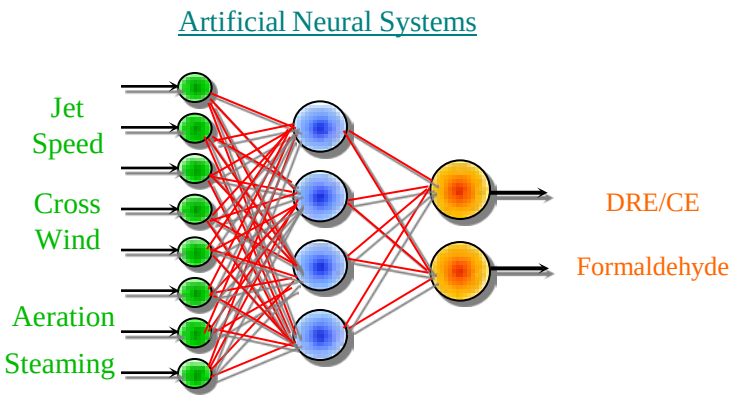
$Y=a*U^b*V_j^c$

where Y is DRE or CE, and a, b, & c are constants.

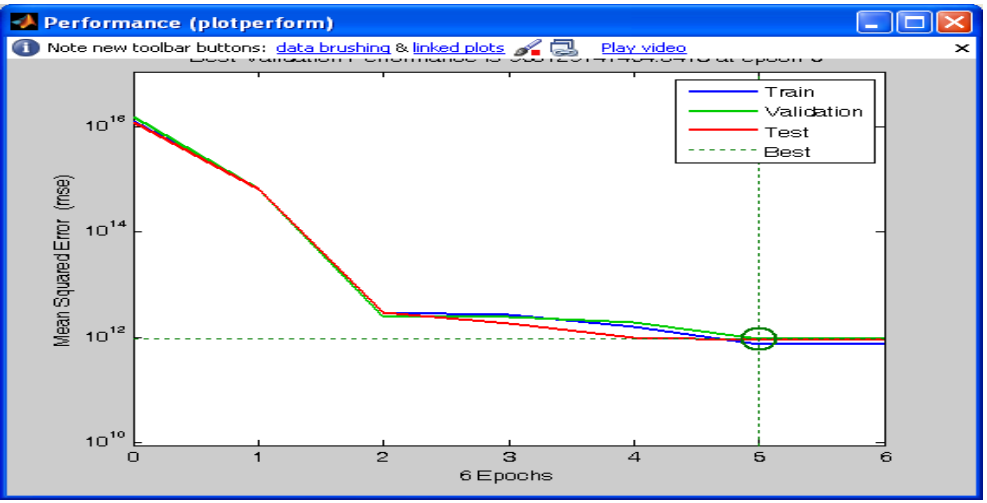
Neural Network Models

Biological vs. Artificial Neural Networks

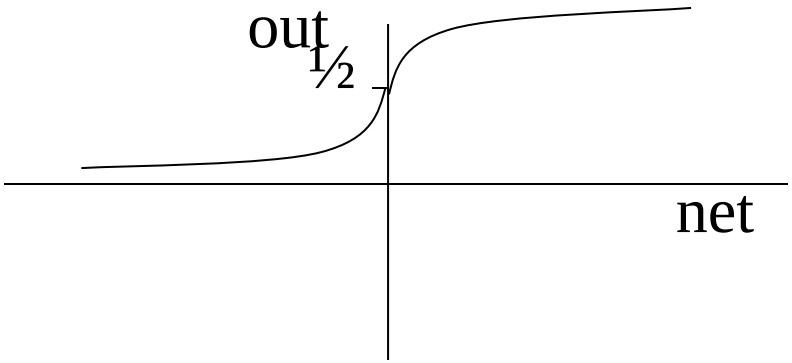




The weights and biases (similar to slope & intercept in a single input case) can be identified with **MATLAB Neural Network Toolbox**.



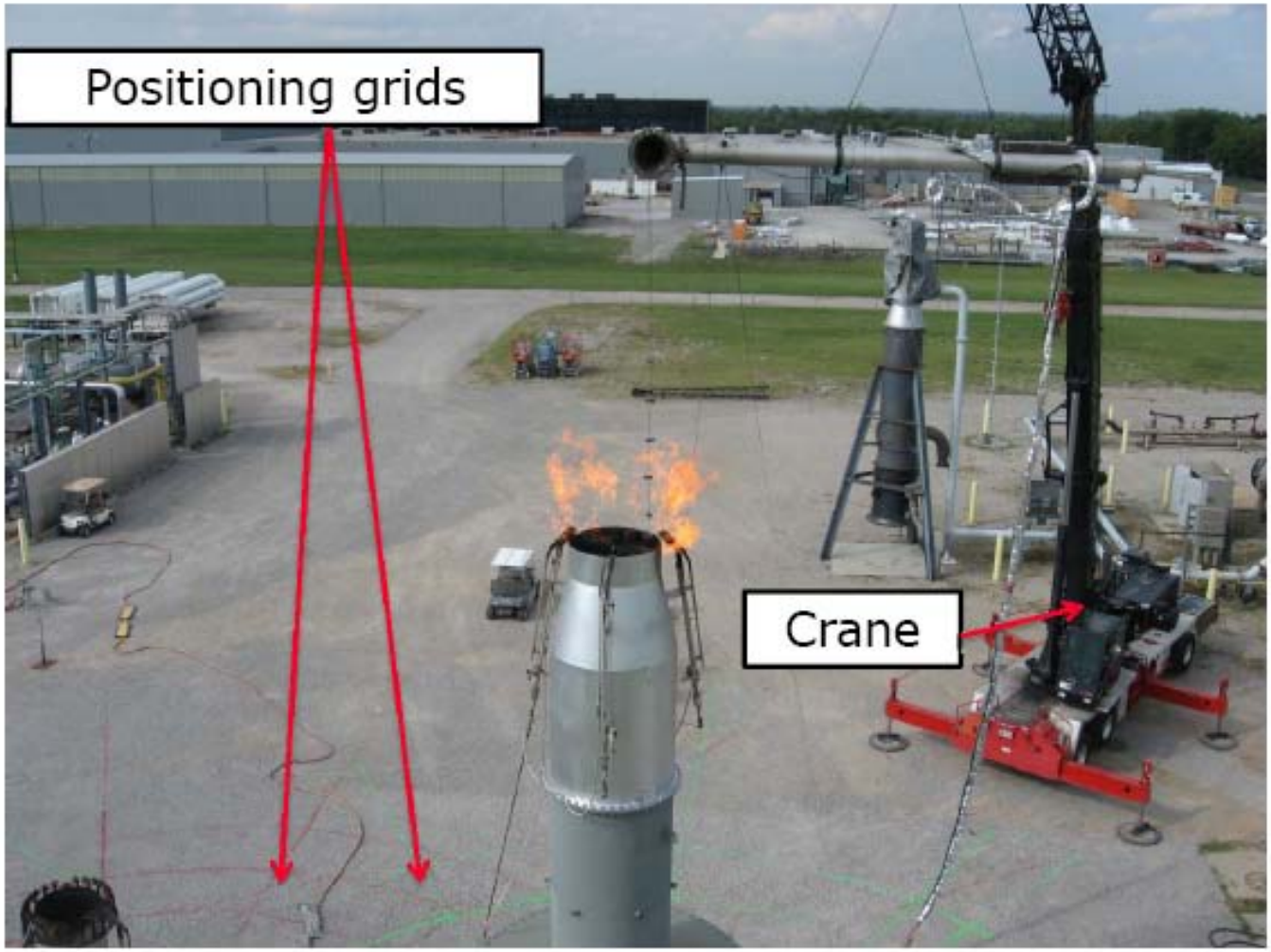
Neural network training to minimize the mean of square errors



Highly Nonlinear Sigmoid (Squashing) function:
out = 1/(1+e**(-λ*net*))

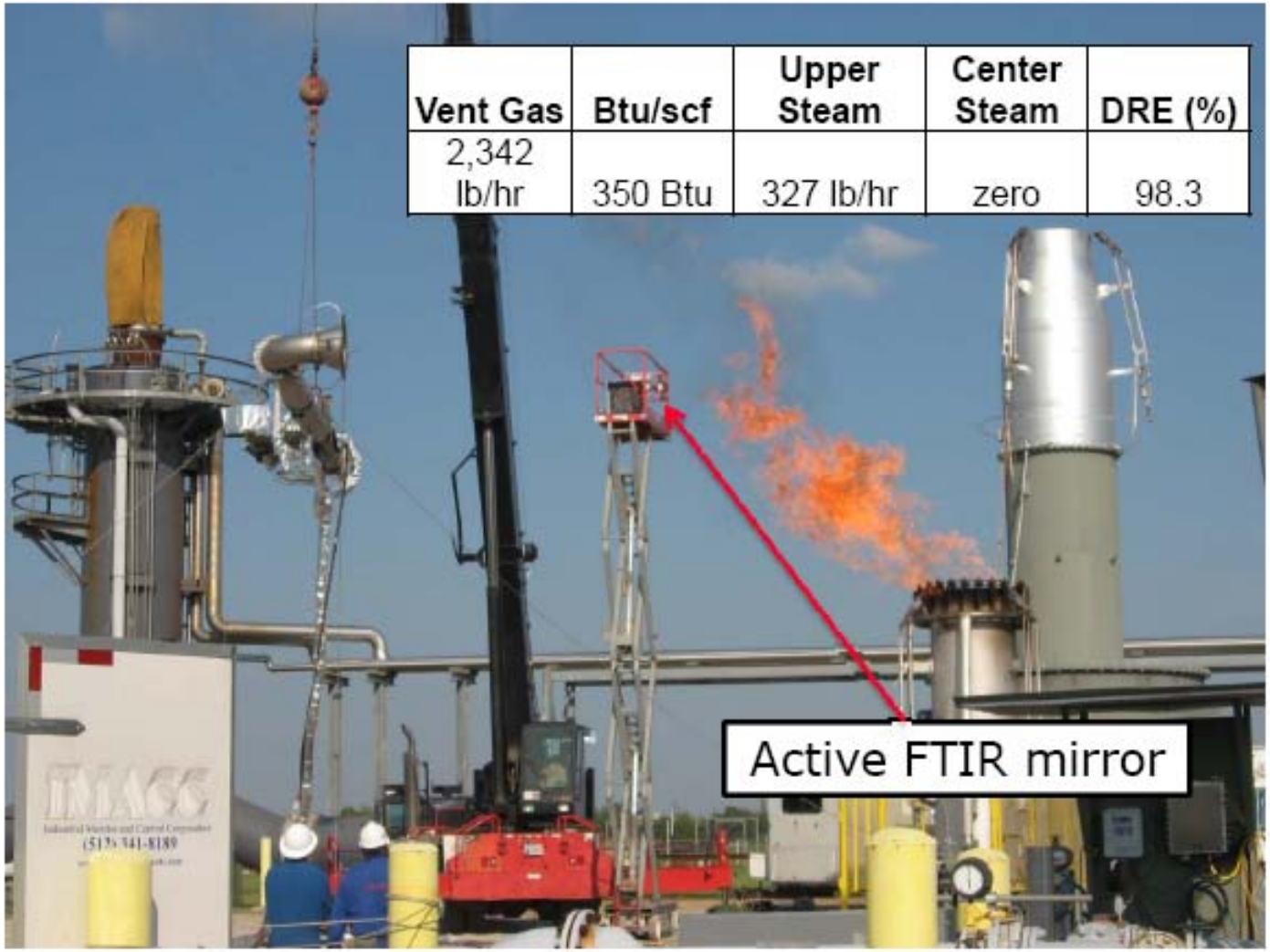
AQRP Project 11-022: Modeling John Zink Flare Tests, September 2010, Tulsa, Oklahoma

Elevated Position



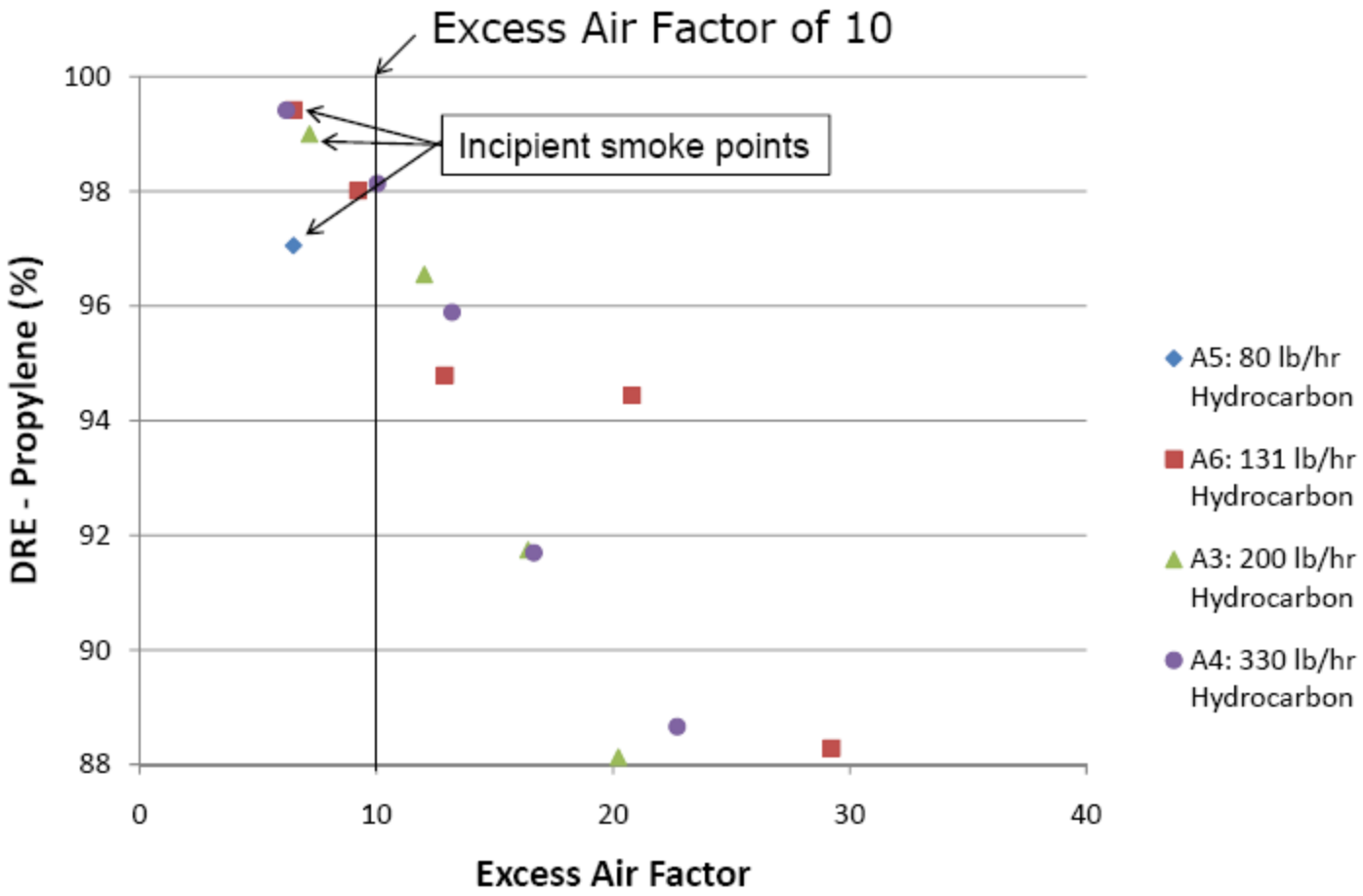
2010 TCEQ Flare Study Final Report, UT/CEER, TCEQ PGA No. 582-8-86245-FY09-04 and Task Order No. UTA10-000924-LOAT-RP9, Aug. 1, 2011.

Test Point S4.4

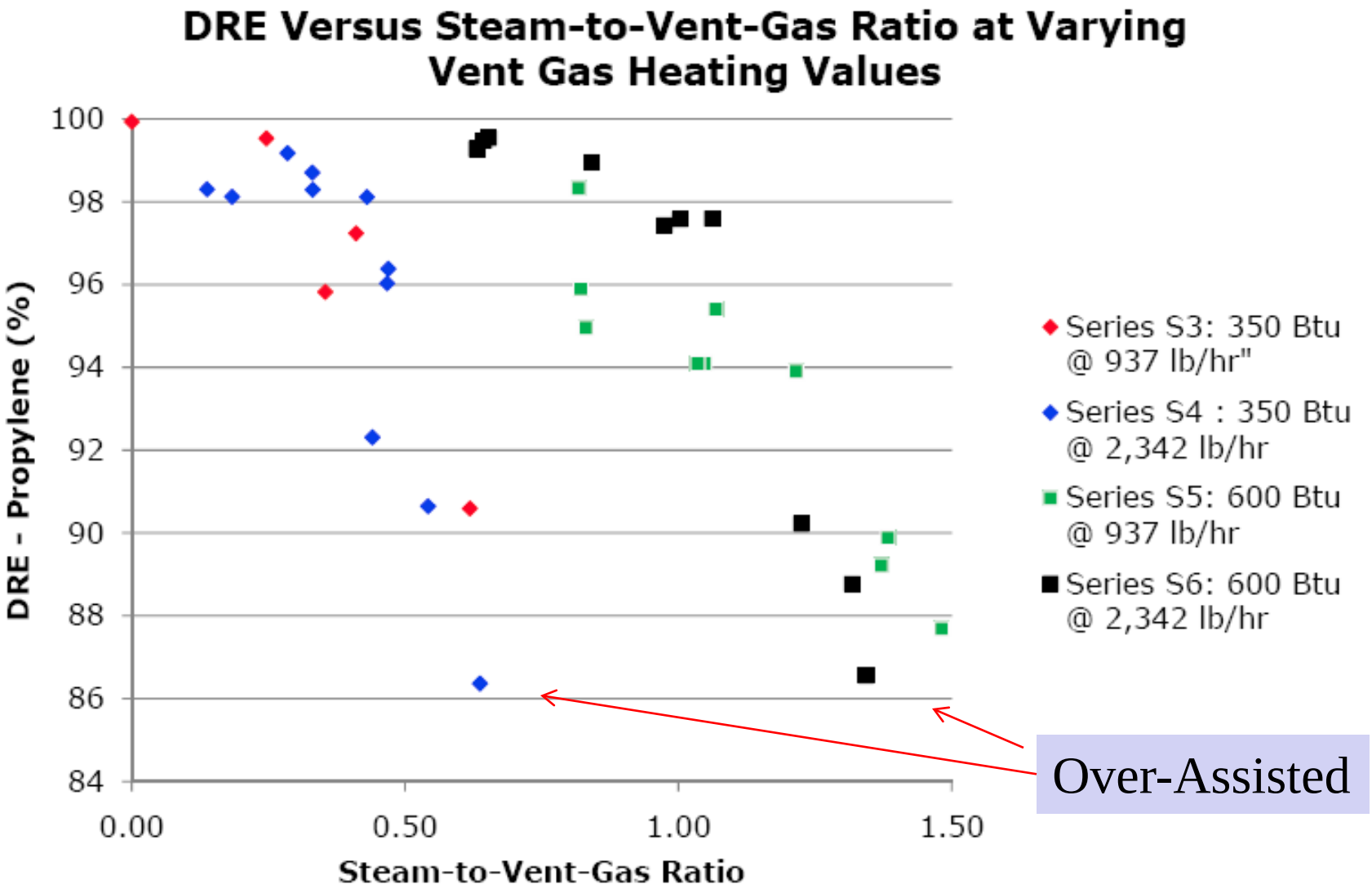


Vent Gas	Btu/scf	Upper Steam	Center Steam	DRE (%)
2,342 lb/hr	350 Btu	327 lb/hr	zero	98.3

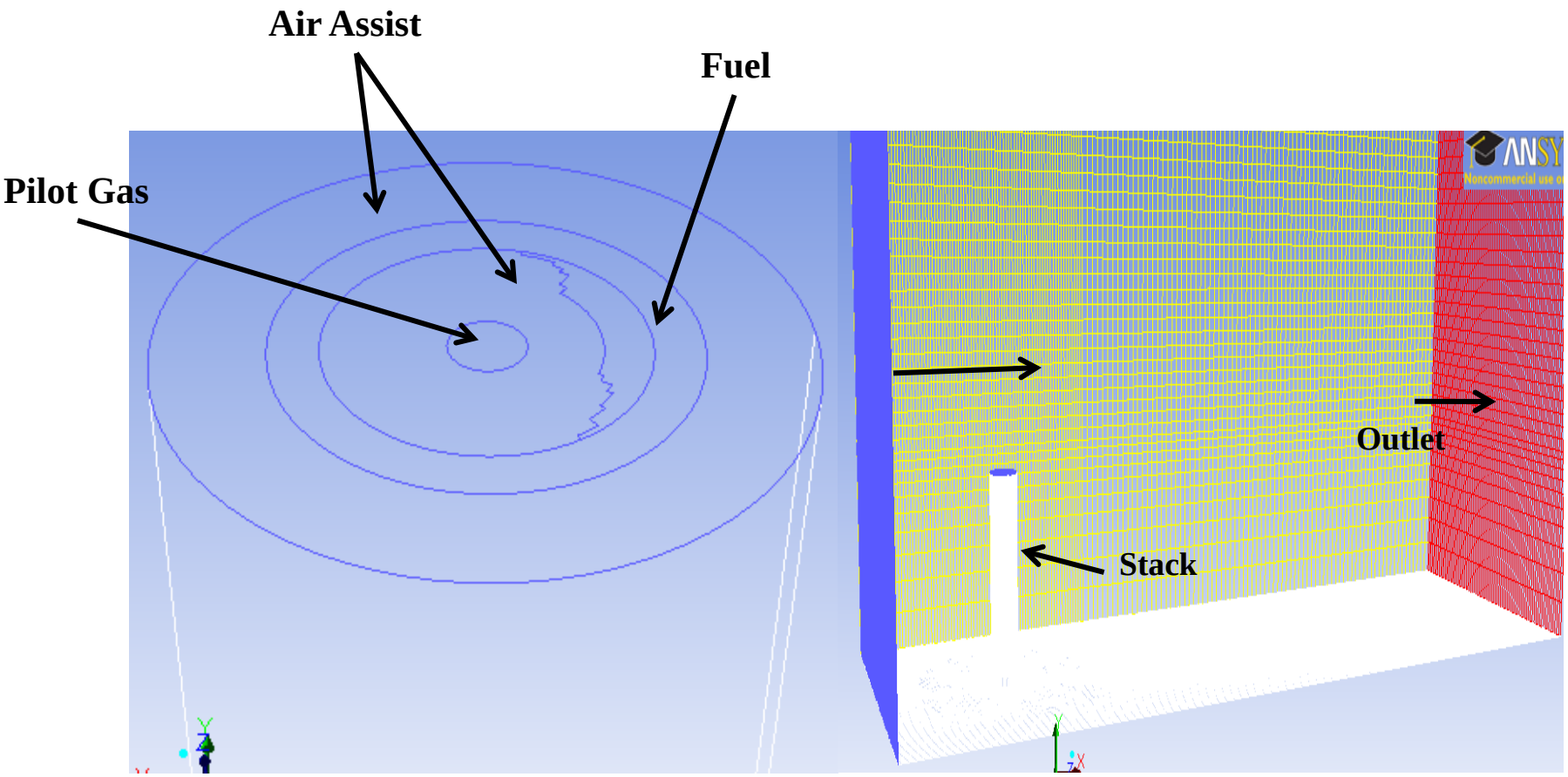
DRE vs. Excess Air

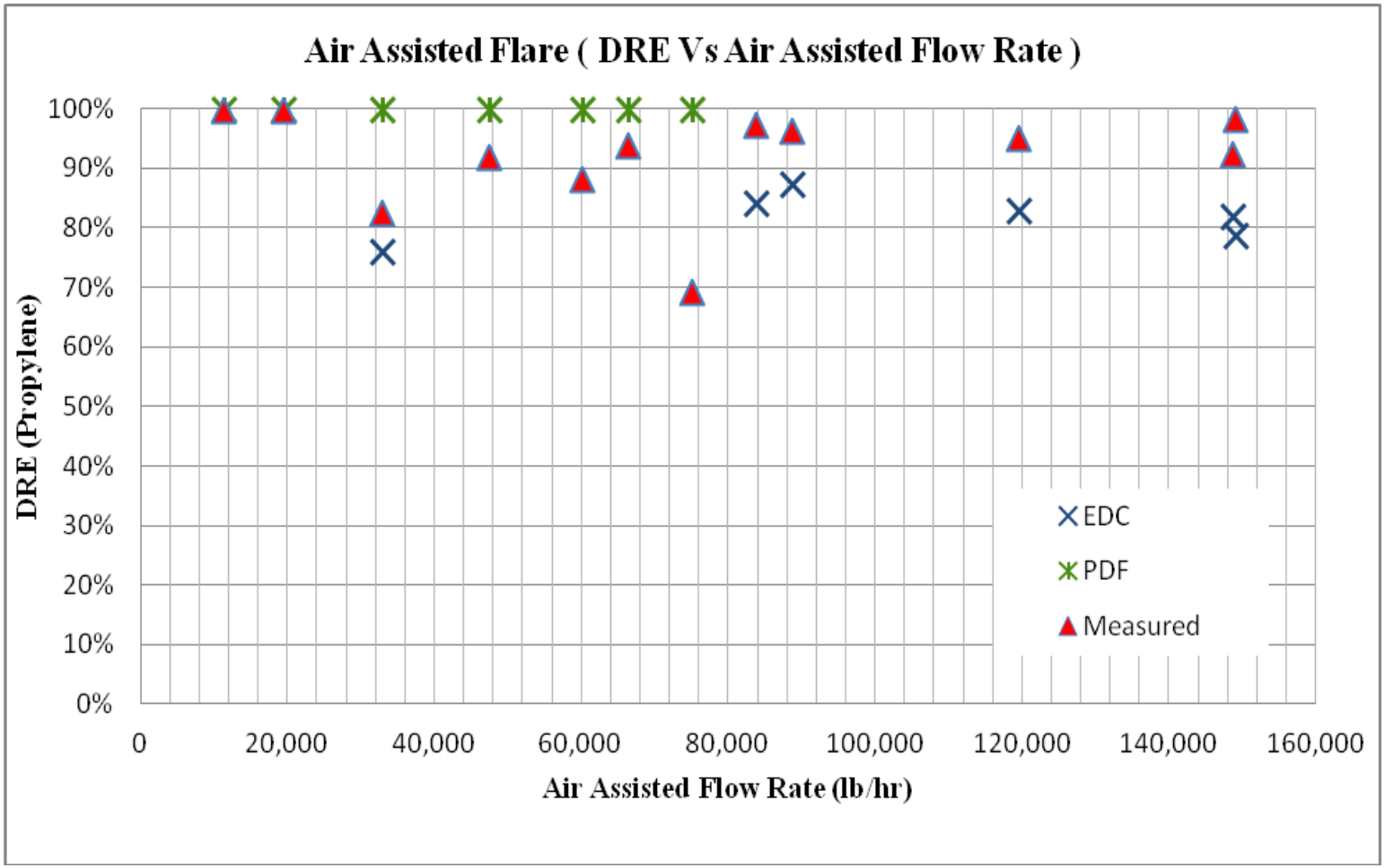


2010 TCEQ Flare Study Final Report, UT/CEER, TCEQ PGA No. 582-8-86245-FY09-04 and Task Order No. UTA10-000924-LOAT-RP9, Aug. 1, 2011.

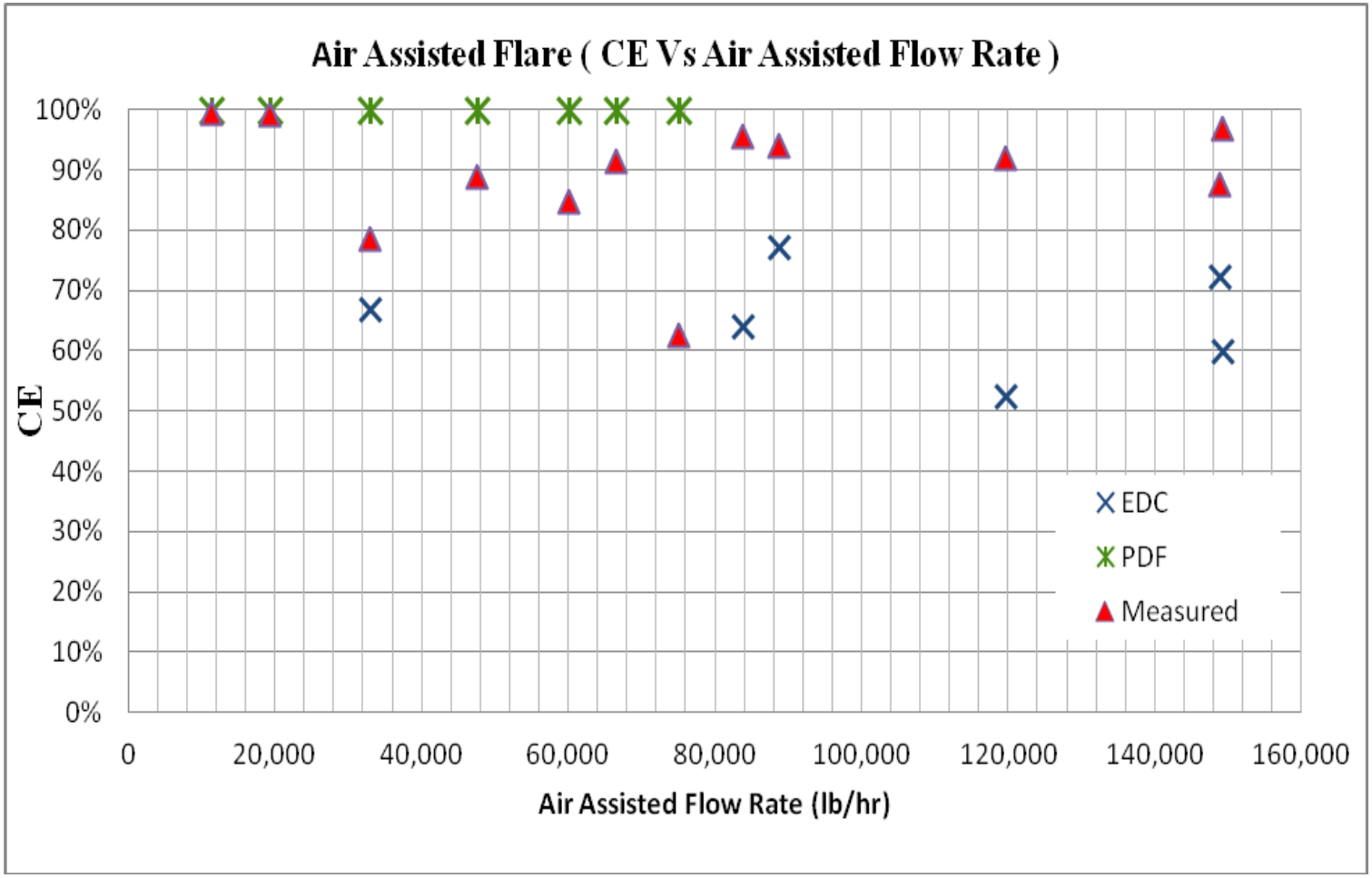

DRE Versus Steam-to-Vent-Gas Ratio at Varying Vent Gas Heating Values
DRE - Propylene (%)
100
98
96
94
92
90
88
86
84
0.00
0.50
1.00
1.50
Steam-to-Vent-Gas Ratio
Series S3: 350 Btu @ 937 lb/hr"
Series S4 : 350 Btu @ 2,342 lb/hr
Series S5: 600 Btu @ 937 lb/hr
Series S6: 600 Btu @ 2,342 lb/hr
Over-Assisted

Modeling Air-assisted flares *(using EDC approach)*



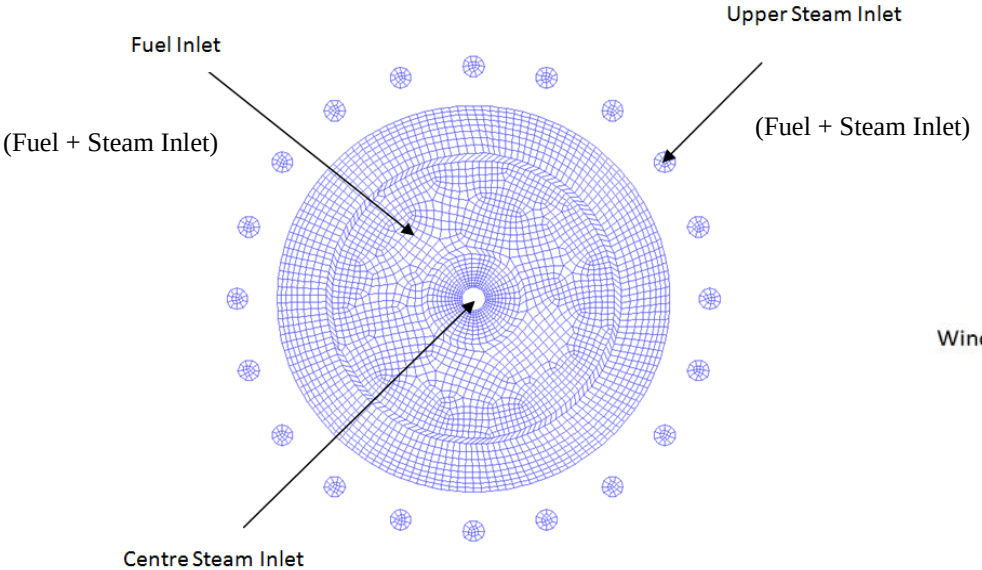


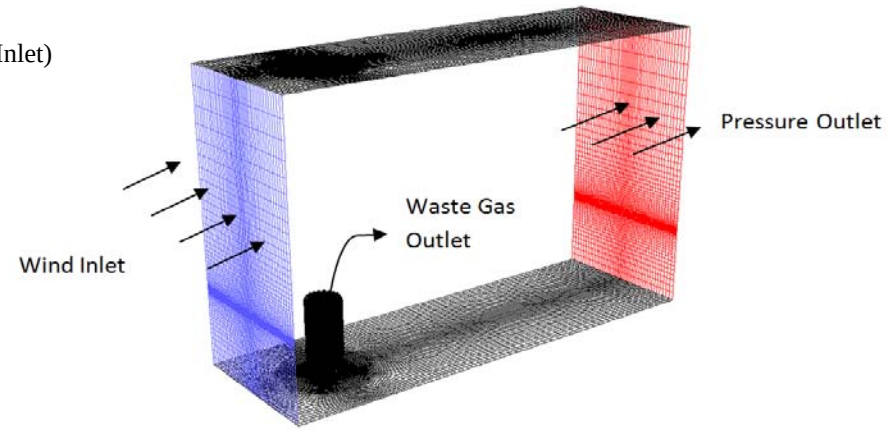
DRE as a function of assisted-air flow rate (measured vs. CFD, air-assisted cases)



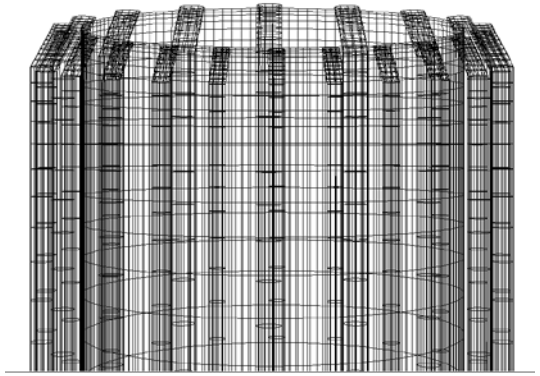
CE as a function of assisted-air flow rate (measured vs. CFD, air-assisted cases)

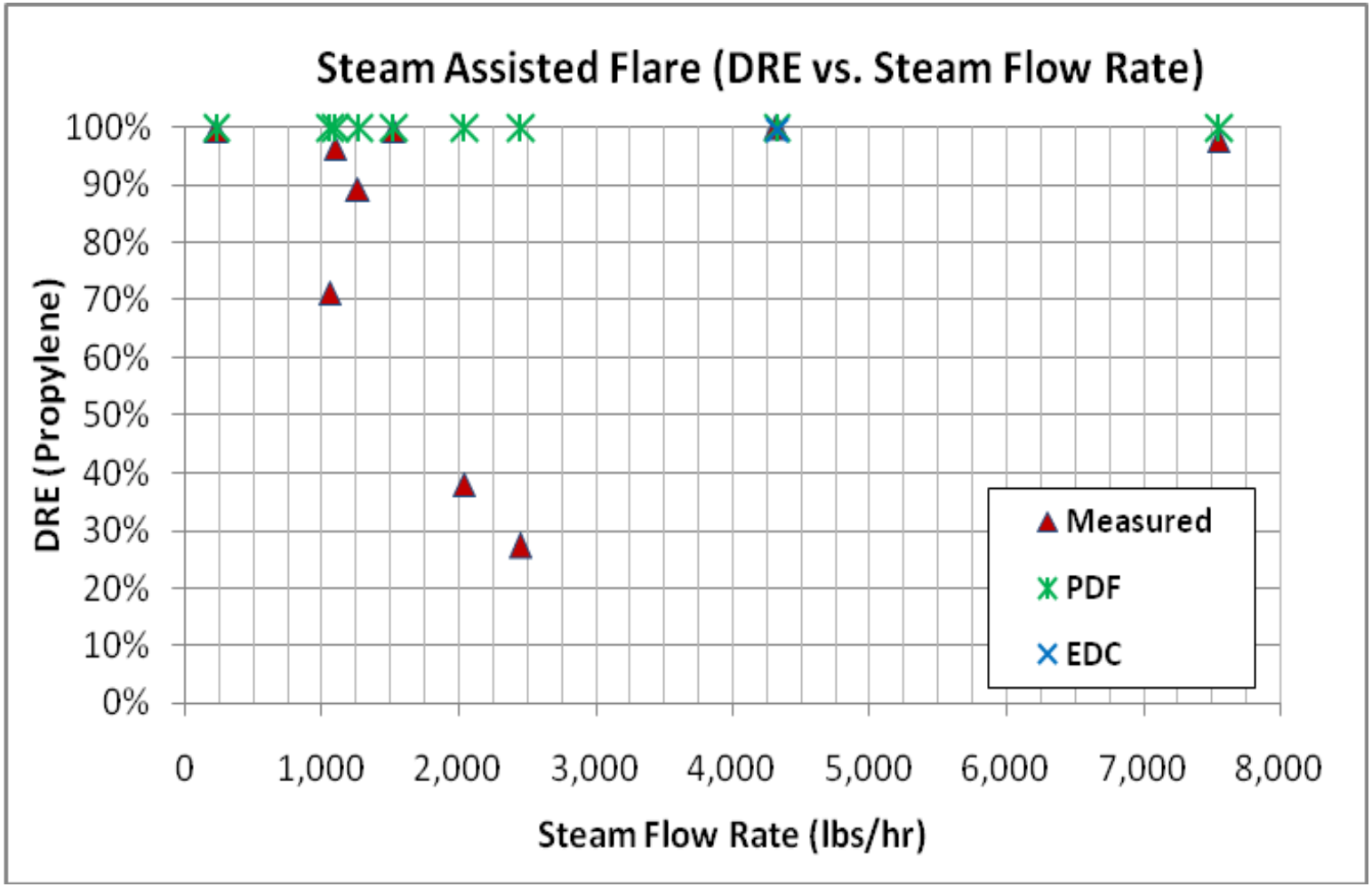
Steam-based test cases (PDF approach)



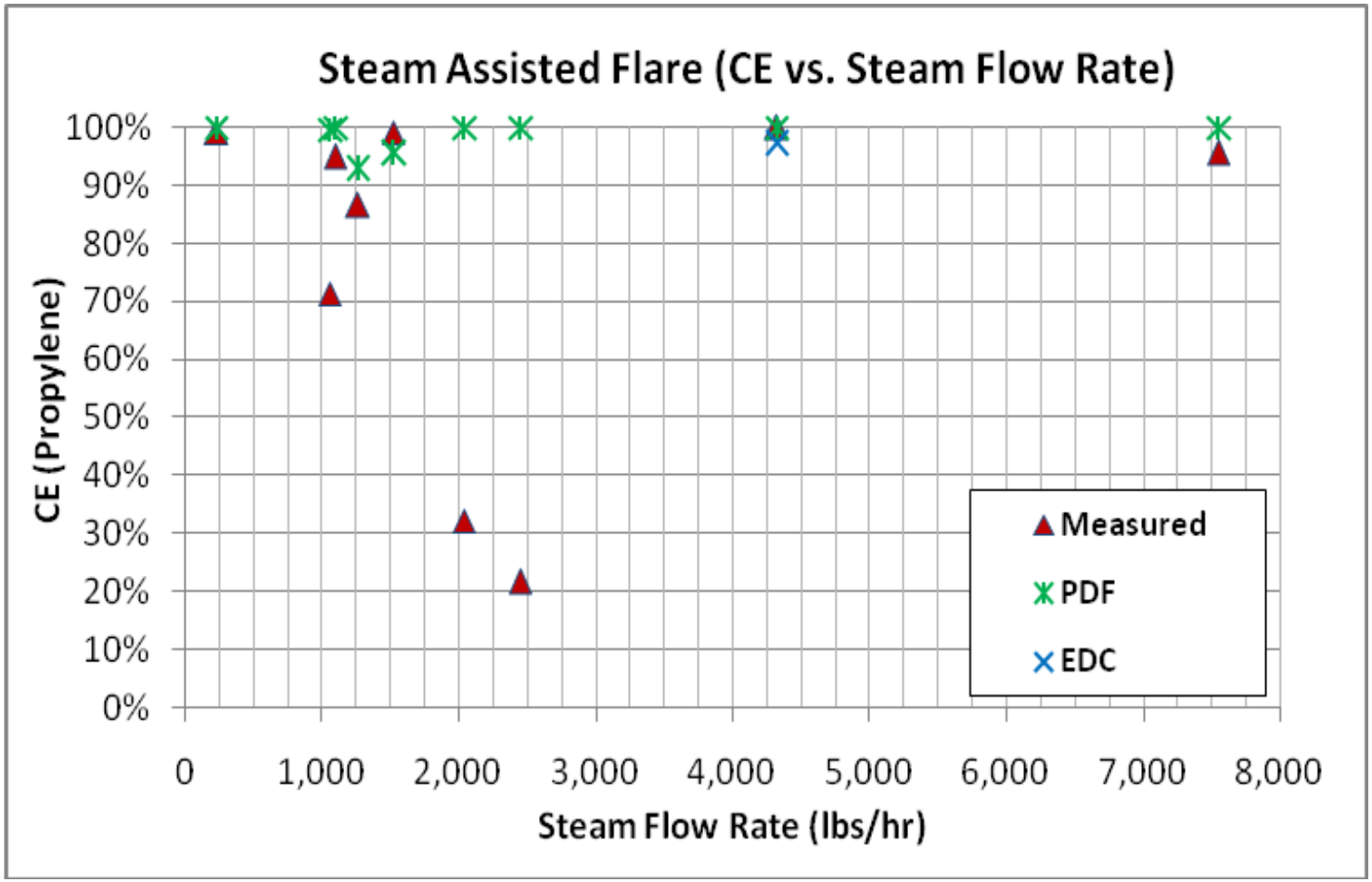


(Not Used)





DRE as a function of assisted-steam flow rate (measured vs. CFD, steam-assisted cases)



CE as a function of assisted-steam flow rate (measured vs. CFD, steam-assisted cases

Conclusions for AQRP-11-022 (1)

- The EDC model under- predicts DRE of air-assisted cases by 6% to 19% with an average of 12%. It under- predicts CE by 12% to 39% with an average of 25%. The potential causes for the large discrepancies may be
  - the low flow rates, low heating values, high air/steam assists,
  - large number of simulation cells coupled with complex chemistry/transport phenomena
  - the difference between local sampling and the full surface integration (CFD post processing).
- Even though the more rigorous EDC model under-predicts the experimental results (in all cases except steam case S 1.5) in low LHV/low jet velocity flares, the same EDC model has been used in numerous times for flare modeling that routinely gives >98% combustion efficiencies for high LHV/high jet velocity flares.

Conclusions for AQRP-11-022 (2)

- The Probability Density Function model is not suitable for modeling low flow rate low heating value flares because the underlying assumption of infinitely fast combustion, while valid for high temperatures (>2100 K), is not appropriate at the modeled temperature range (1600-1950K)
  - Contrary to the EDC model, the PDF model over- predicts DRE by 0.1% to 72% with an average of 16%. It over- predicts CE by 0% to 78% with an average of 18%.
- Further studies are warranted
  - a cylindrical domain with more efficient, structured meshes need to be explored
  - the Large Eddy Simulation turbulence model, a transient formulation method, has the potential to give better results
  - combining the two models, PDF and EDC for simulating a low jet and low LHV flare is a viable option. An initial flame developed by the PDF model can be put into more rigorous chemistry-turbulence interaction by using the EDC model.

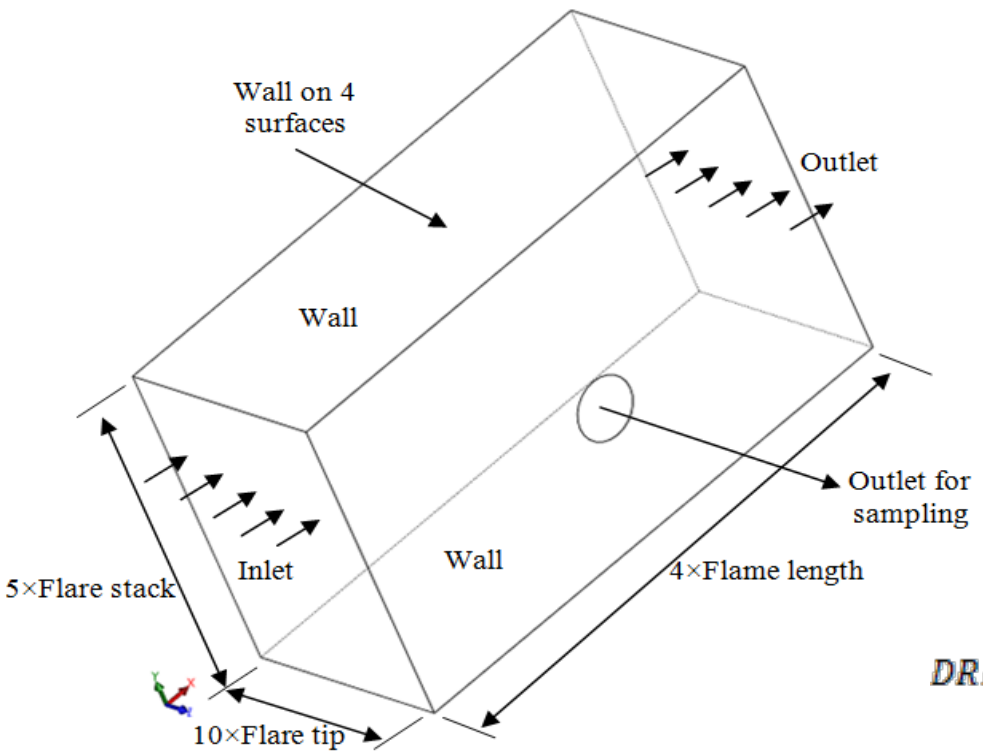


Fig. 3 Grab sampling described with a CFD simulation domain

The plume measurements were carried out approximately in the center of the flare plume at a distance of two flame lengths downwind from the flare tip and with the inlet face perpendicular to the plume travel, Fig. 3.

$$DRE\,(\%) = \frac{(C_3H_6)_{in} - (C_3H_6)_{plume}}{(C_3H_6)_{in}} * 100 \qquad (1)$$

$$CE\,(\%) = \frac{(CO_2)_{plume}}{(CO_2)_{plume} + (CO)_{plume} + \sum \text{hydrocarbons}_{\text{plume}}} * 100 \qquad (2)$$

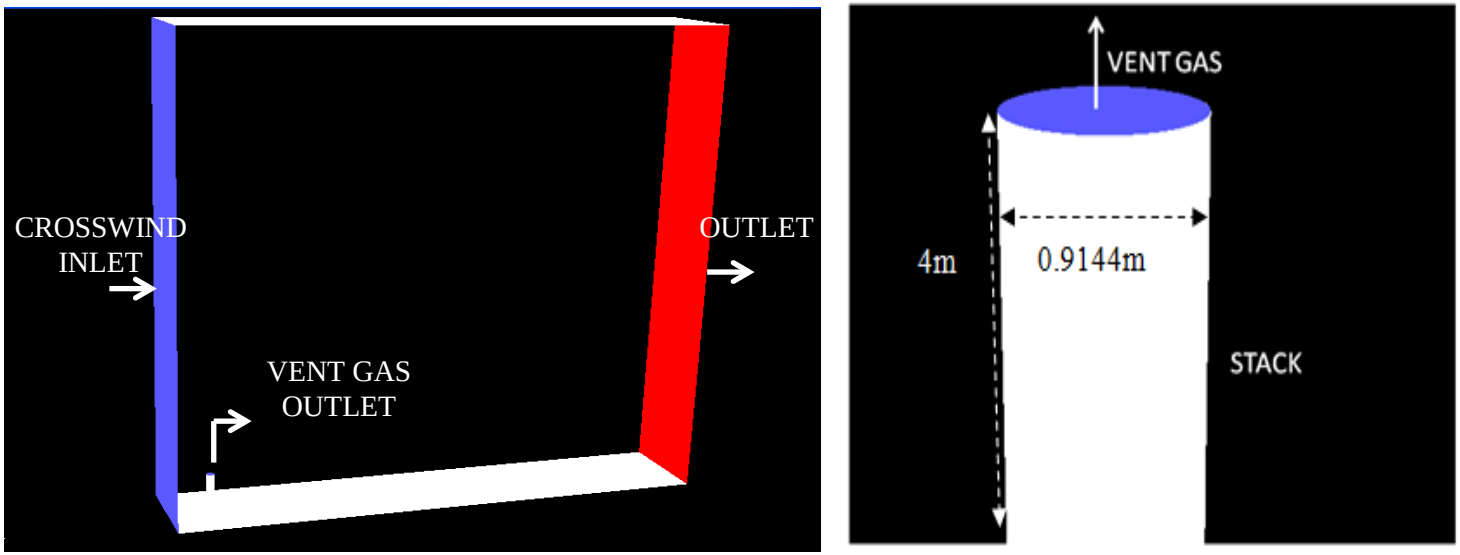
CFD predicted DRE and CE values using Eqns. (3) and (4)

$$DRE\,(CxHy) = \frac{\text{Amount of } C_xH_y \text{ fed} - \text{Amount of } C_xH_y \text{ in flue gas}}{Amount\ of\ C_xH_y\ fed\ to\ the\ flare} \quad (3)$$

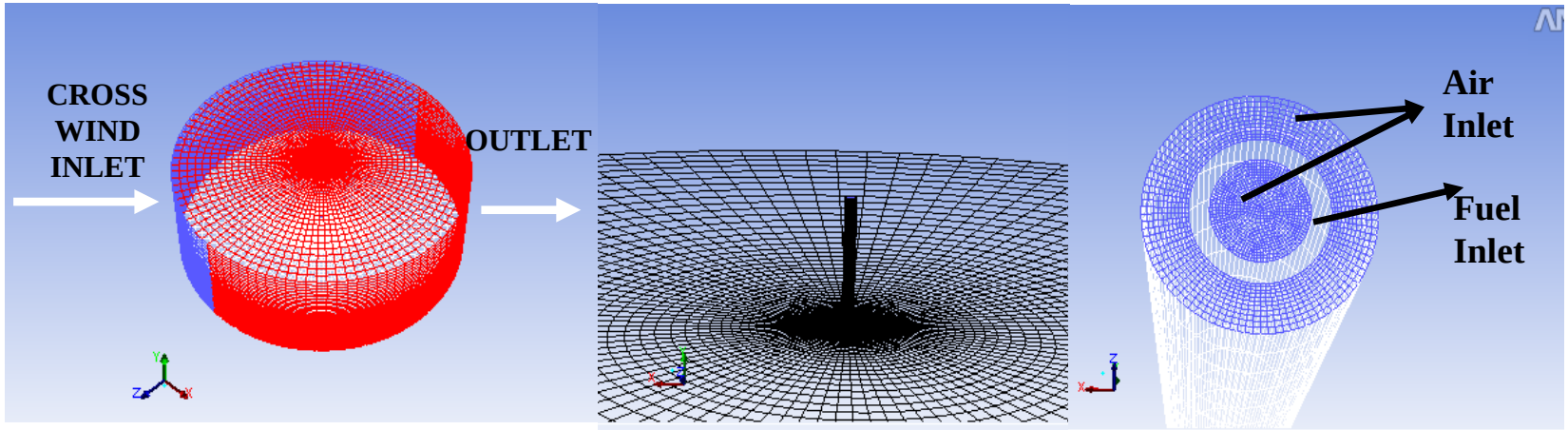
$$CE = \frac{\text{Amount of fuel converted to } CO_2}{Amount\ of\ fuel\ fed\ to\ the\ flare} \quad (4)$$

based on emission mass flow rates using rigorous integration over certain outlet surfaces. Future studies based on CFD simulation to explore the differences between local sampling at various selected locations and the full pressure outlet surfaces integration are thus warranted.

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



Rectangular premixed geometry: (a) Geometry showing inlet and outlets, and (b) Flare stack dimensions

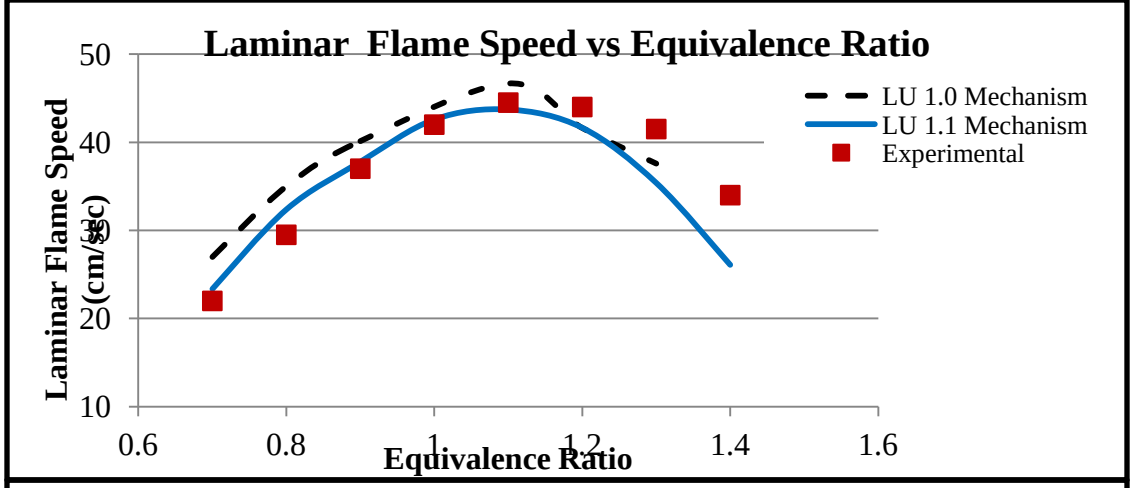


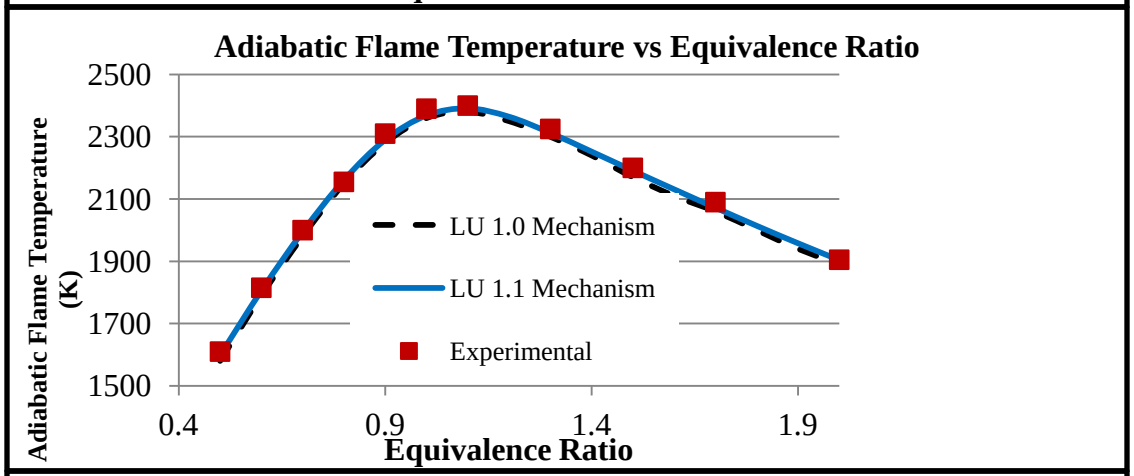
Cylindrical ring-shaped geometry: (a) Meshed geometry showing inlet and outlet, (b) Flare stack at the center of the cylinder, and (c) Details of flare tip (ring-shaped geometry)

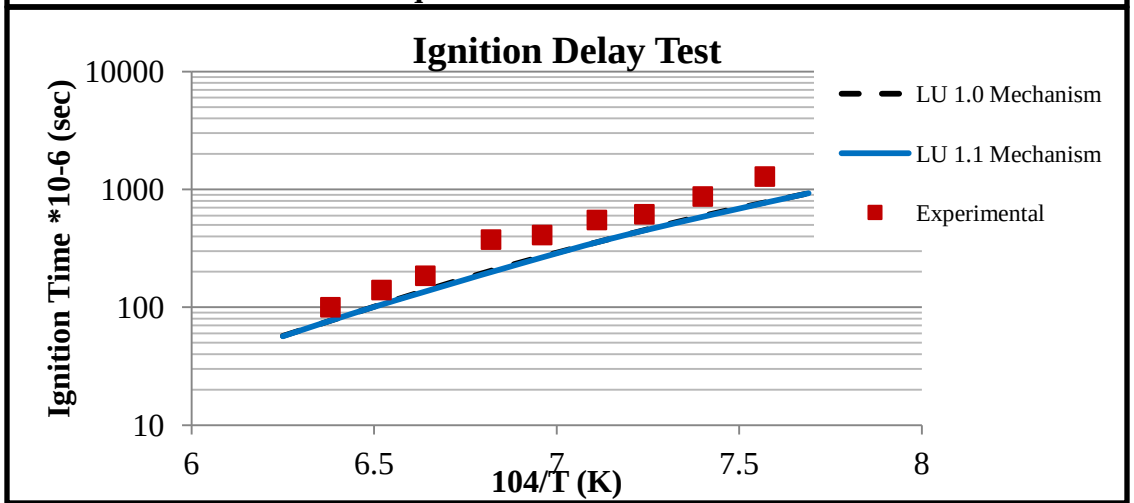
New 50-Species Mechanism with NO_2 (LU 1.1)

- In 2010 John Zink flare tests, NO_2 is a monitored species.
- The full 93 species mechanism was reduced based on mole fractions, rate constants, & their effect on other major species for use in the EDC model.
- CN was replaced with NO_2 in LU 1.1.

LU 1.1


Laminar Flame Speed vs Equivalence Ratio
Laminar Flame Speed (cm/sec)
50
40
30
20
10
0.6
0.8
1
1.2
1.4
1.6
Equivalence Ratio
LU 1.0 Mechanism
LU 1.1 Mechanism
Experimental

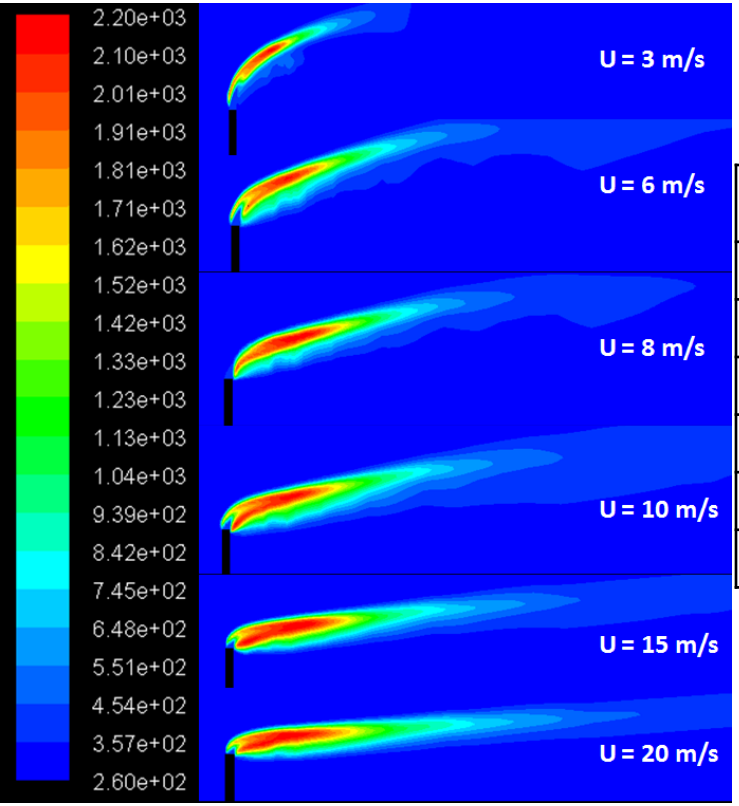

Adiabatic Flame Temperature vs Equivalence Ratio
Adiabatic Flame Temperature (K)
2500
2300
2100
1900
1700
1500
0.4
0.9
1.4
1.9
Equivalence Ratio
LU 1.0 Mechanism
LU 1.1 Mechanism
Experimental


Ignition Delay Test
Ignition Time *10-6 (sec)
10000
1000
100
10
6
6.5
7
7.5
8
104/T (K)
LU 1.0 Mechanism
LU 1.1 Mechanism
Experimental

Parametric Studies

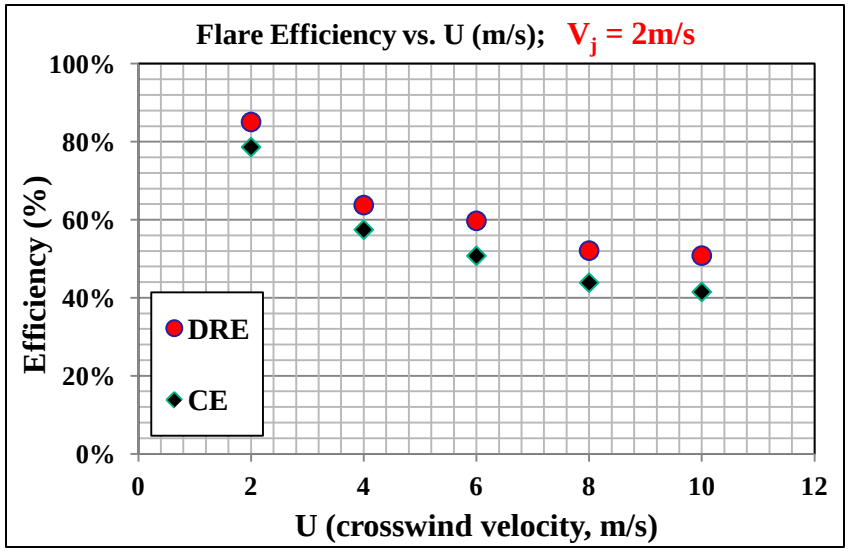
I. Effect of Crosswind
II. Effect of Jet velocity
III. Effect of Assisted Air

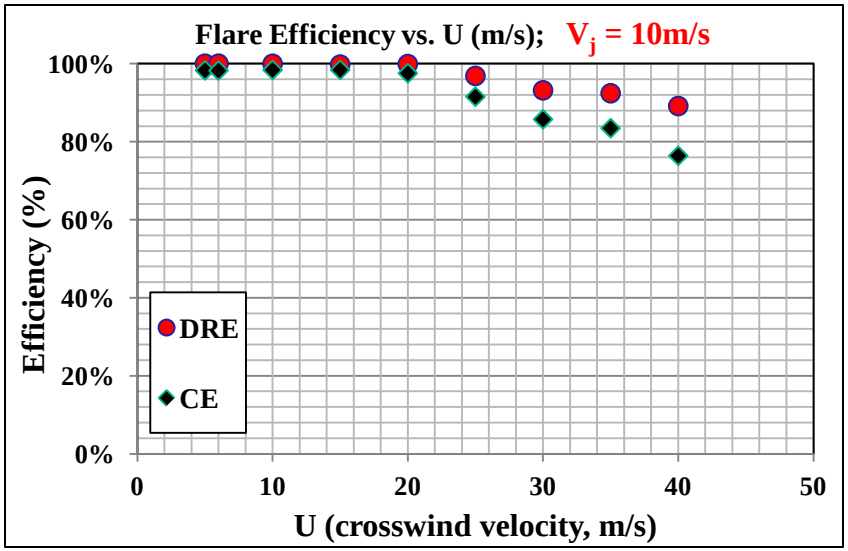
Effect of Crosswind: Air-Assisted Flares

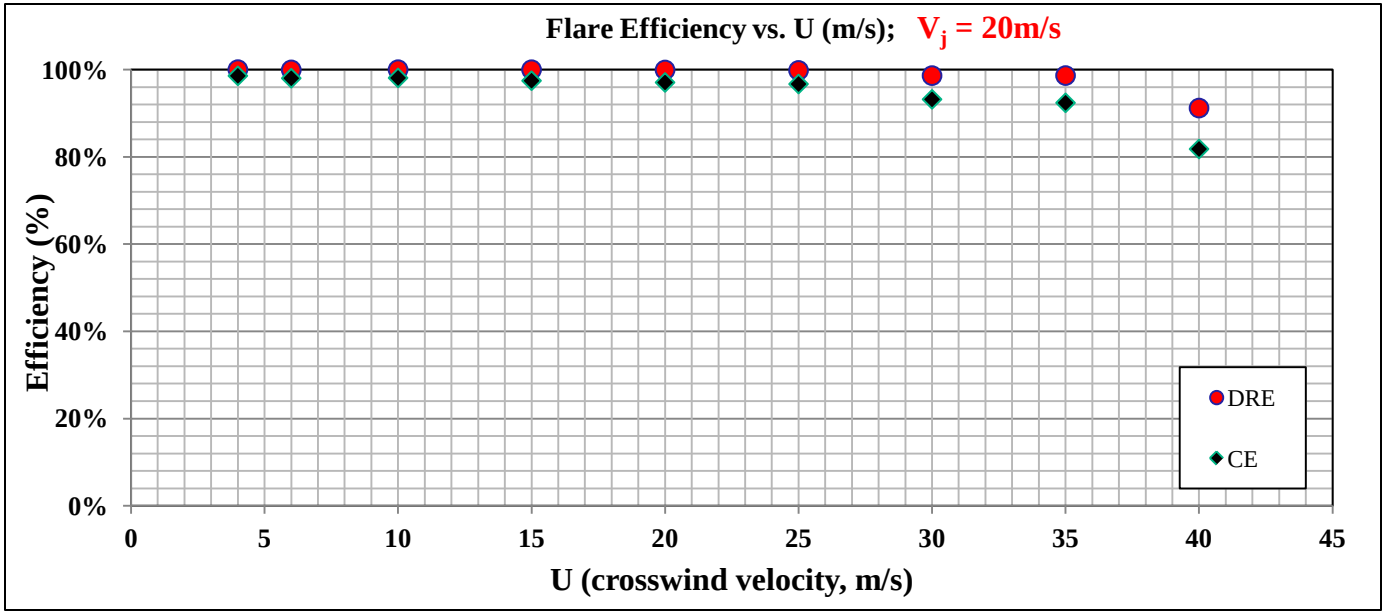


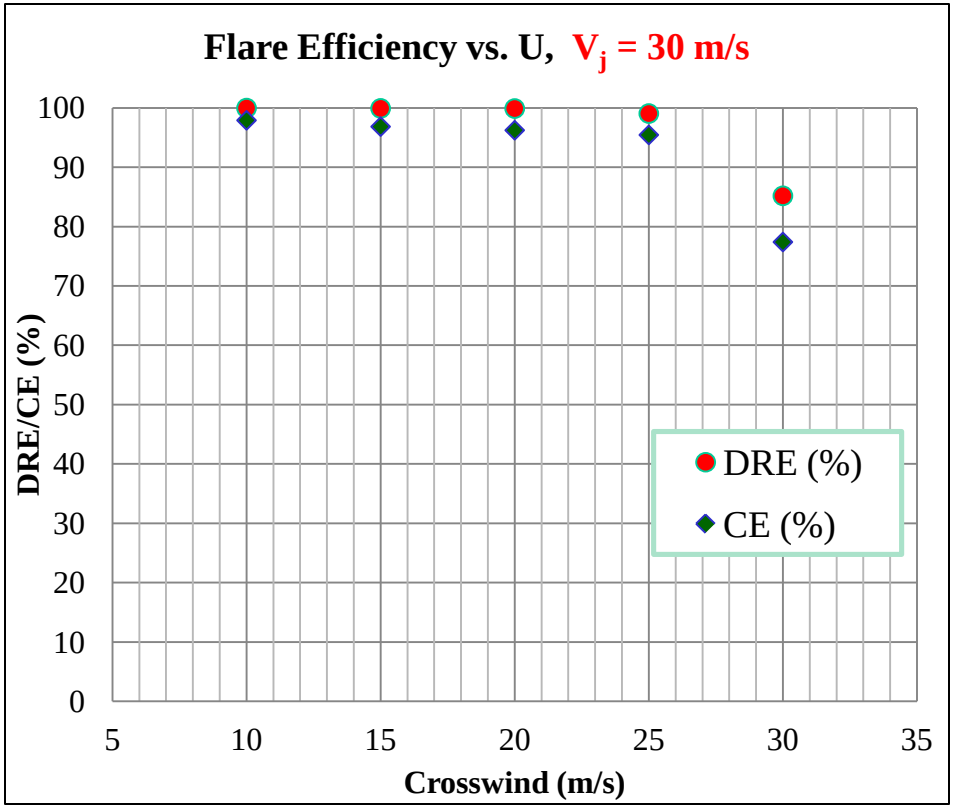
Base Case	
Fuel	C_2H_4
Jet Velocity (m/s)	20.00
Fuel Inlet Temperature (K)	400.00
Premixed Air (% of stoichiometric Air)	30%
Tip Diameter (m)	0.6096
CFD Model	EDC

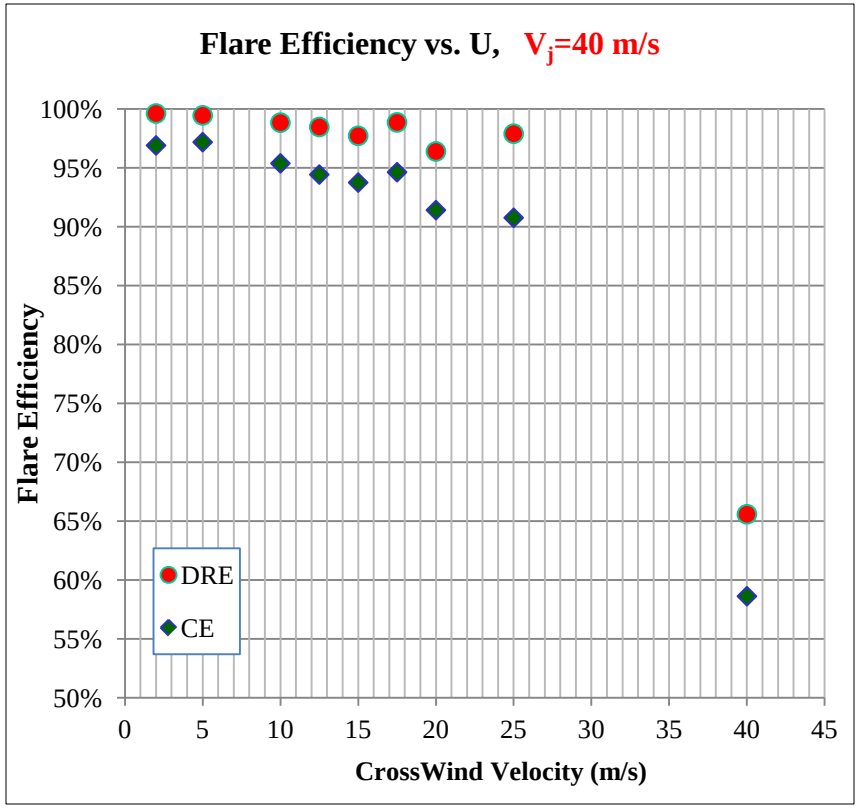
Effect of Crosswind on DRE/CE @various Jet Velocities







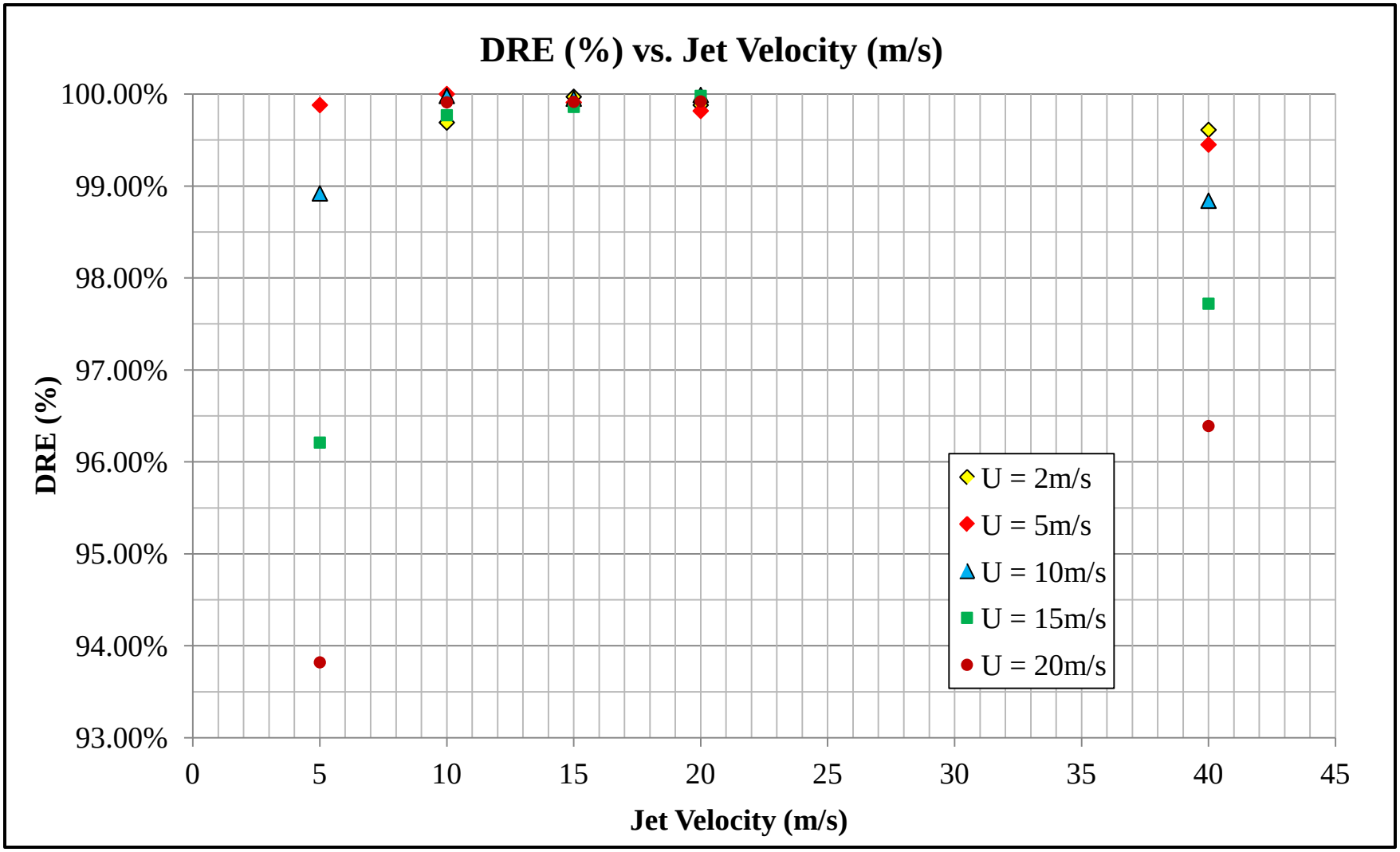




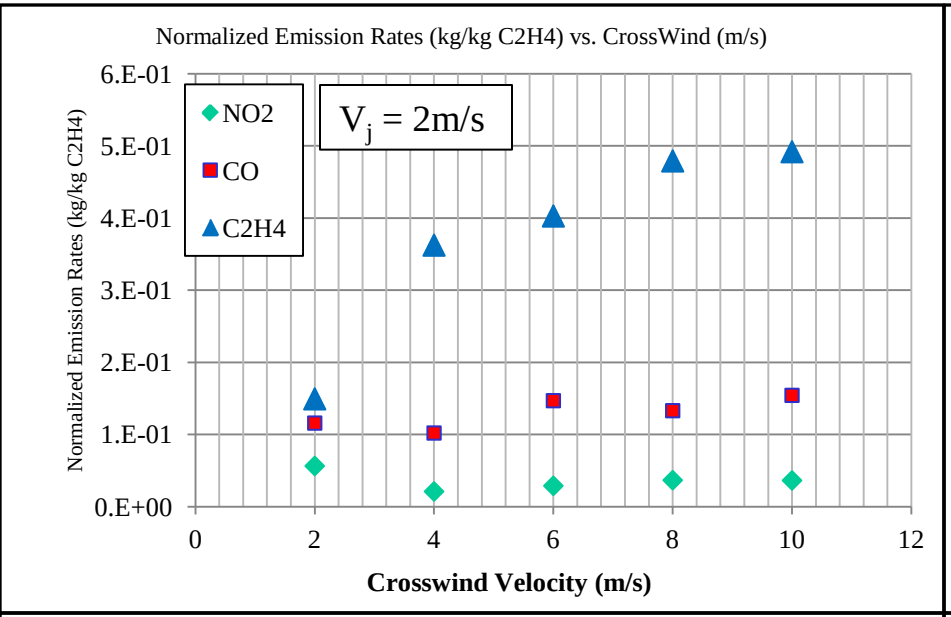
For **$10 \le V_j \le 30$ m/s & $5 \le U \le 20$ m/s $\Rightarrow$DRE>98%**

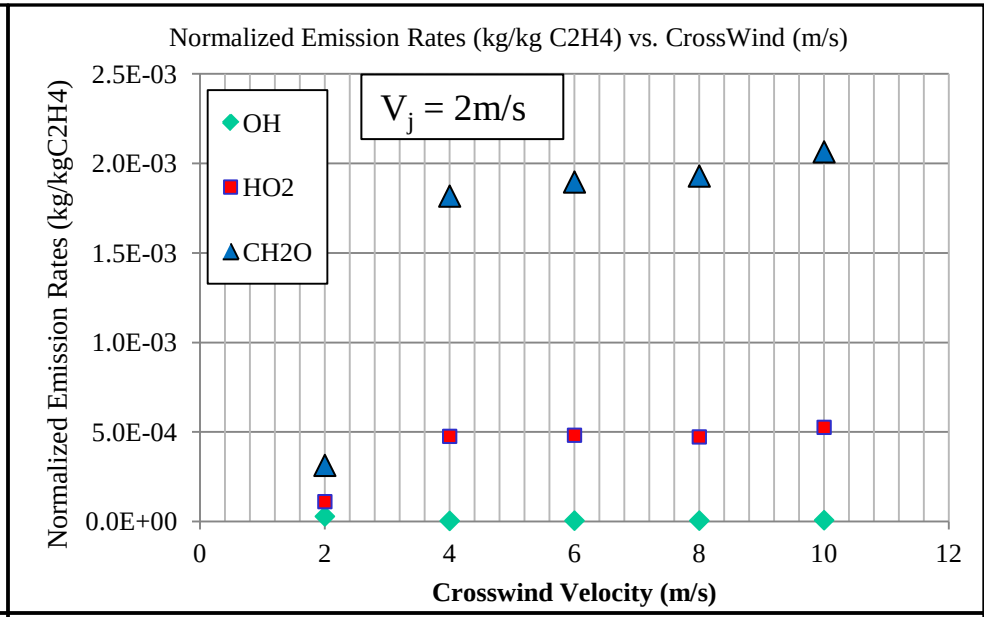
$V_{j,\,max}$ =48.80 m/s for ethylene (LHV=1512 BTU/scf), Non-premixed , LU 1.1 mechanism

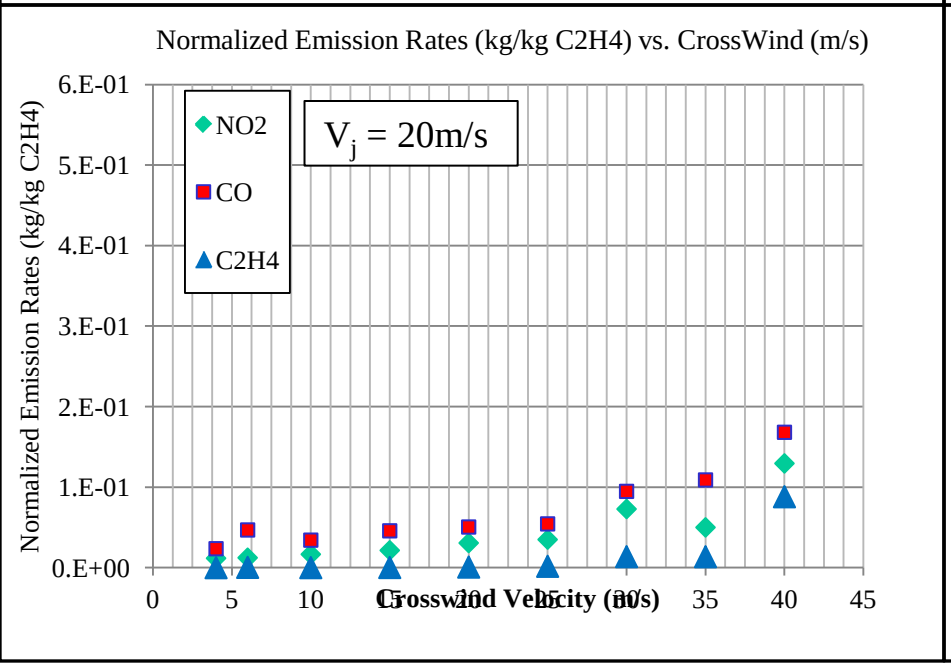
Effect of Jet Velocity on DRE

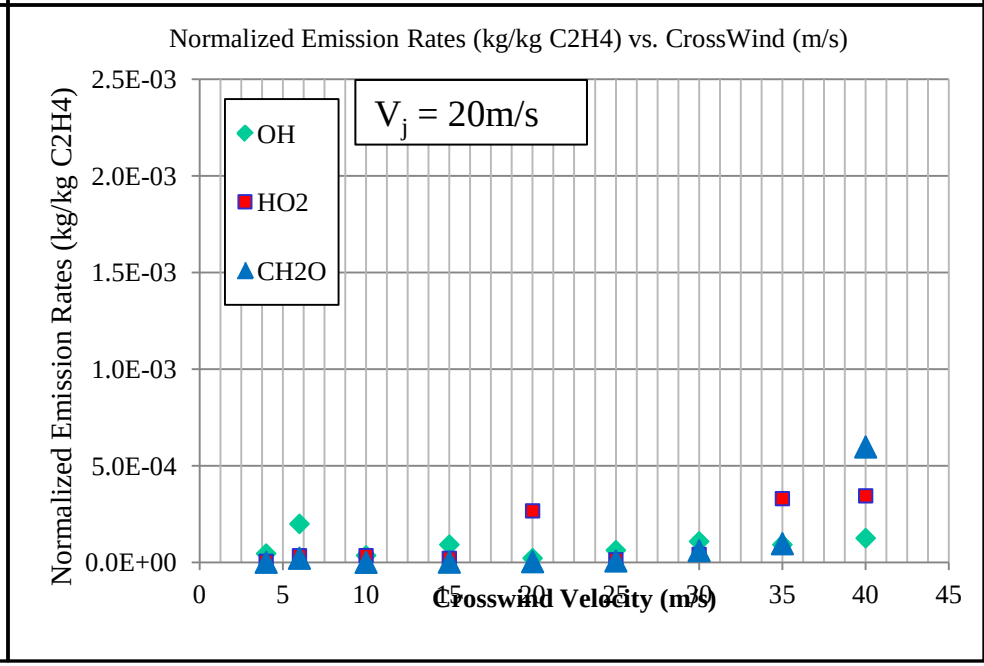


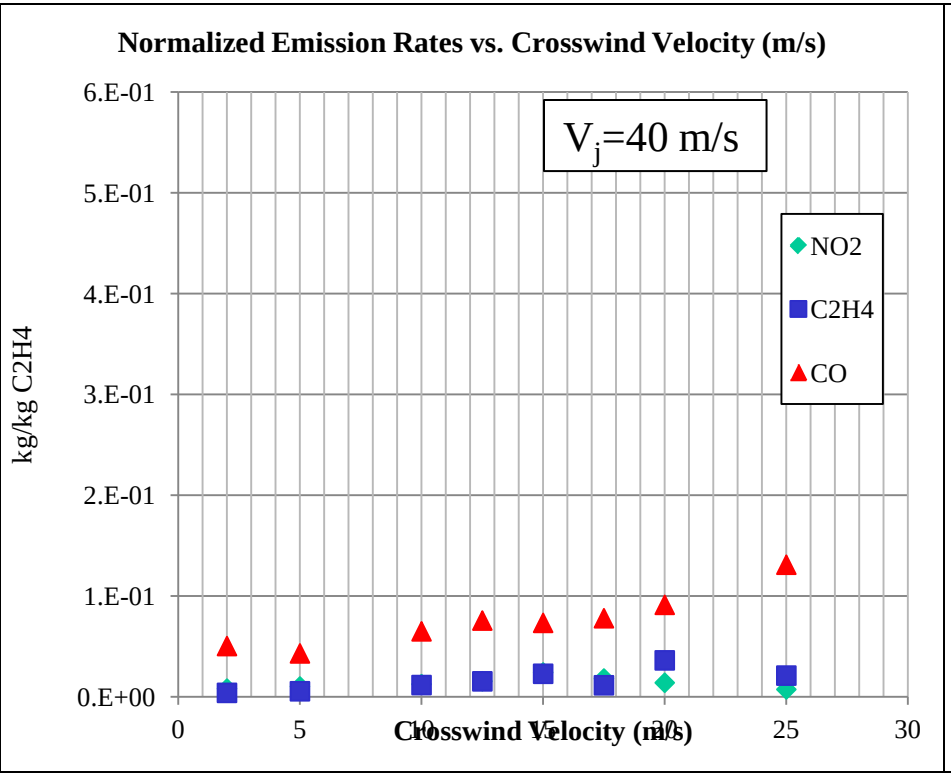
Effect of Crosswind on Emissions @Various Jet Velocities

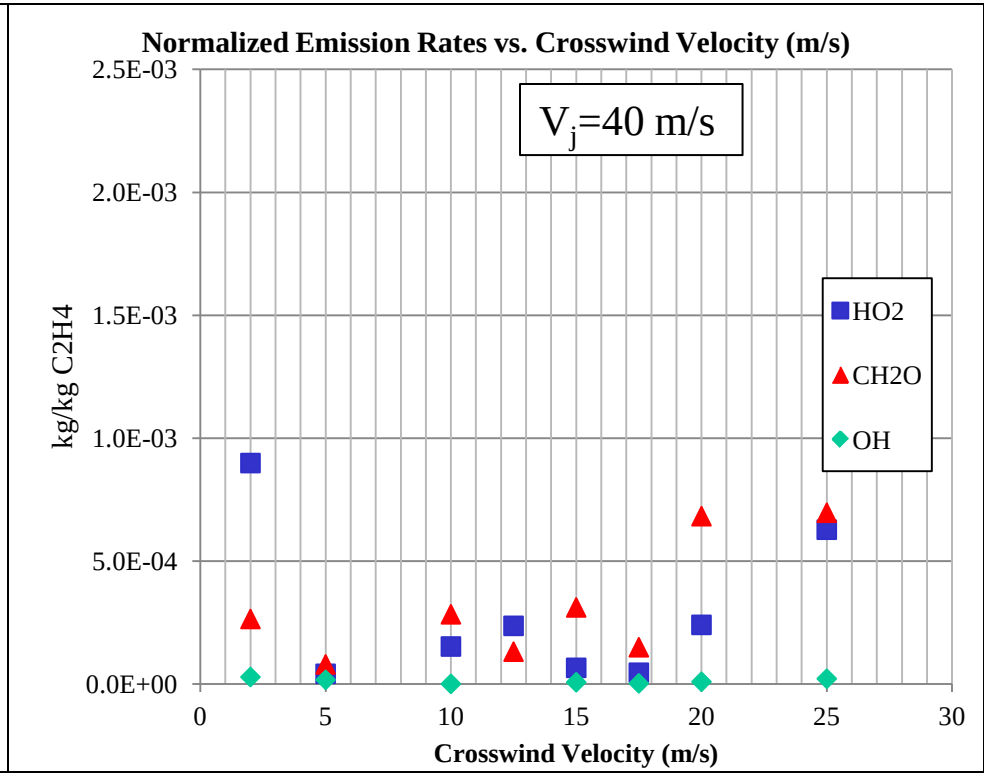




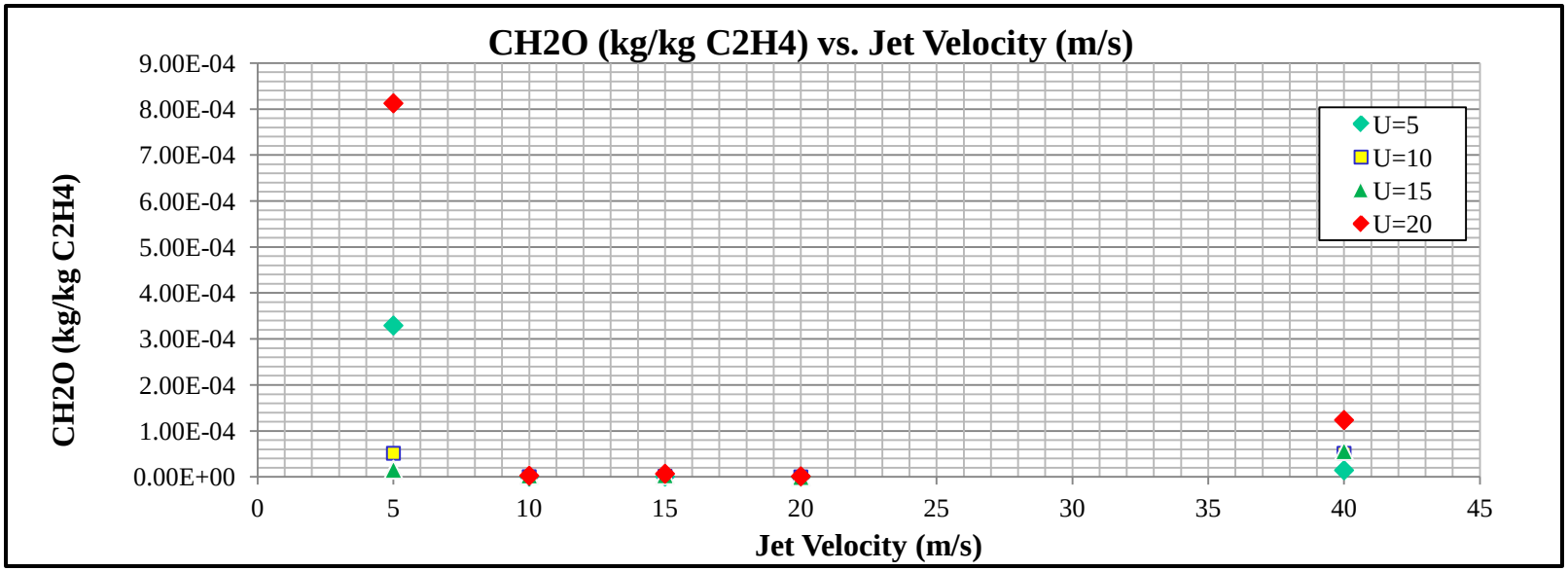


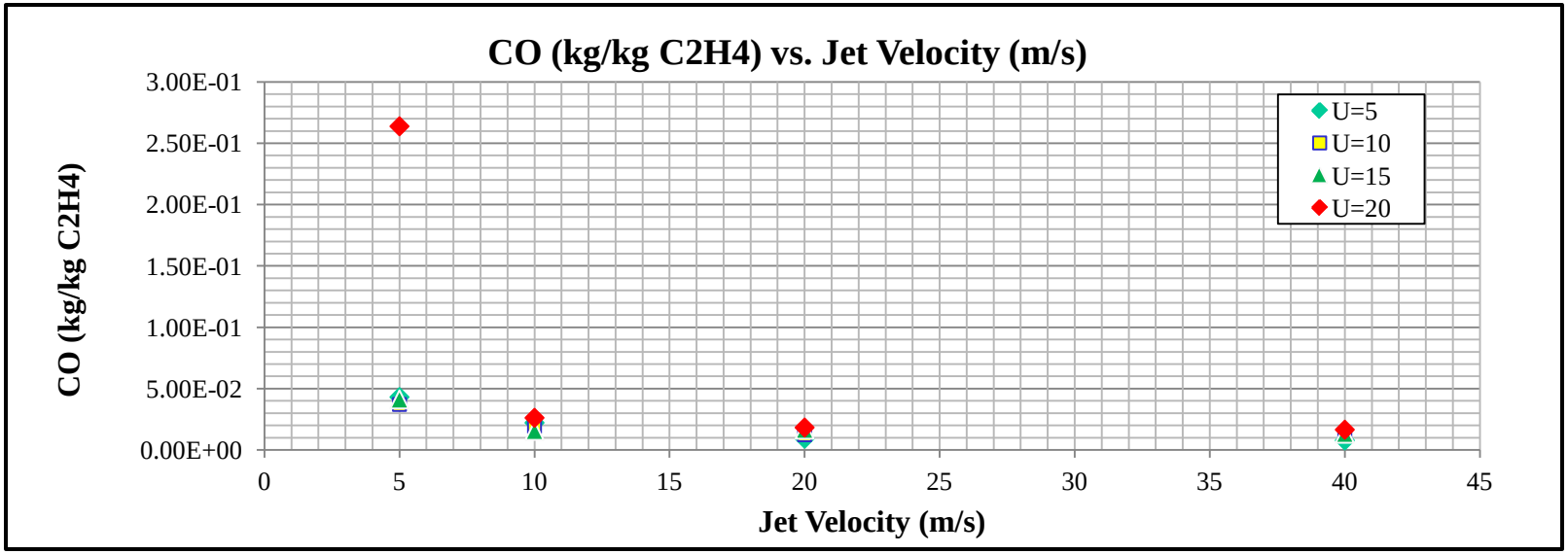



Normalized Emission Rates vs. Crosswind Velocity (m/s)
V_j=40 m/s
NO2
C2H4
CO
kg/kg C2H4
6.E-01
5.E-01
4.E-01
3.E-01
2.E-01
1.E-01
0.E+00
0
5
10
15
20
25
30
Crosswind Velocity (m/s)

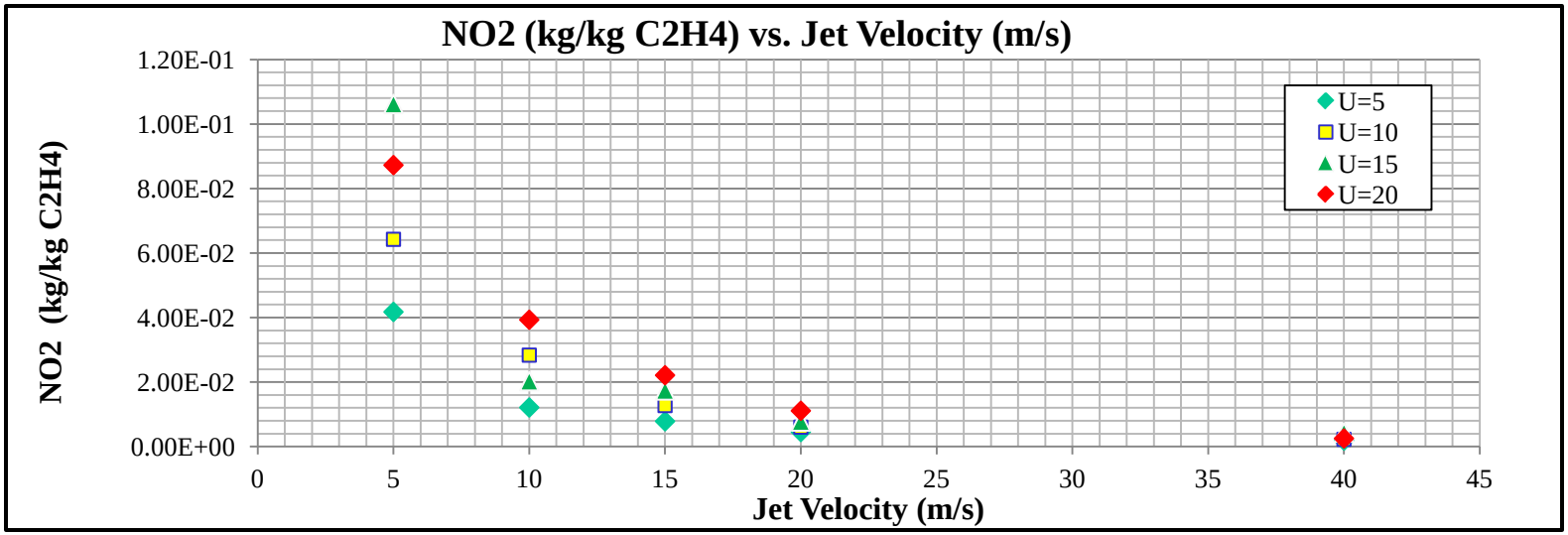

Normalized Emission Rates vs. Crosswind Velocity (m/s)
V_j=40 m/s
HO2
CH2O
OH
kg/kg C2H4
2.5E-03
2.0E-03
1.5E-03
1.0E-03
5.0E-04
0.0E+00
0
5
10
15
20
25
30
Crosswind Velocity (m/s)

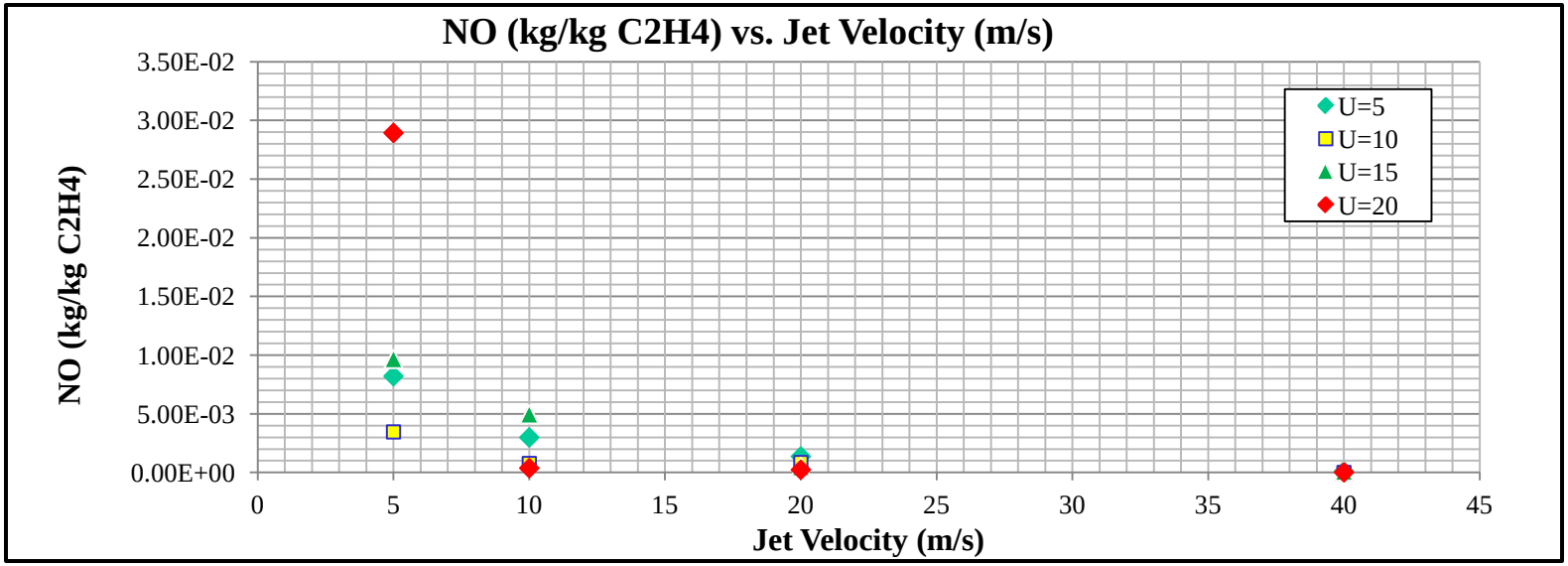
Effect of Jet Velocity on Emission Rates



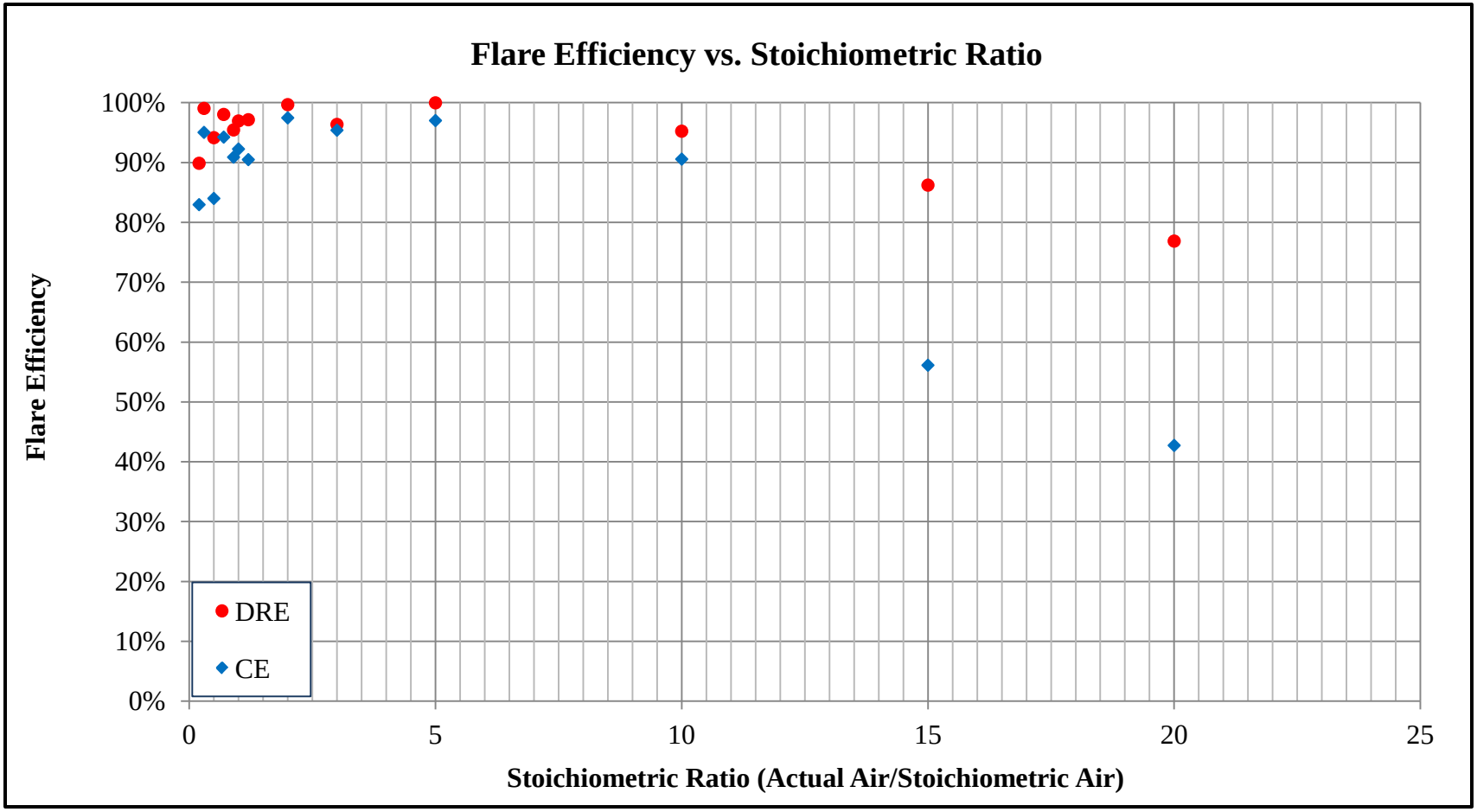


Effect of Jet Velocity on Emission Rates





Effect of Assisted-Air (in terms of Stoichiometric Ratio SR) on DRE/CE

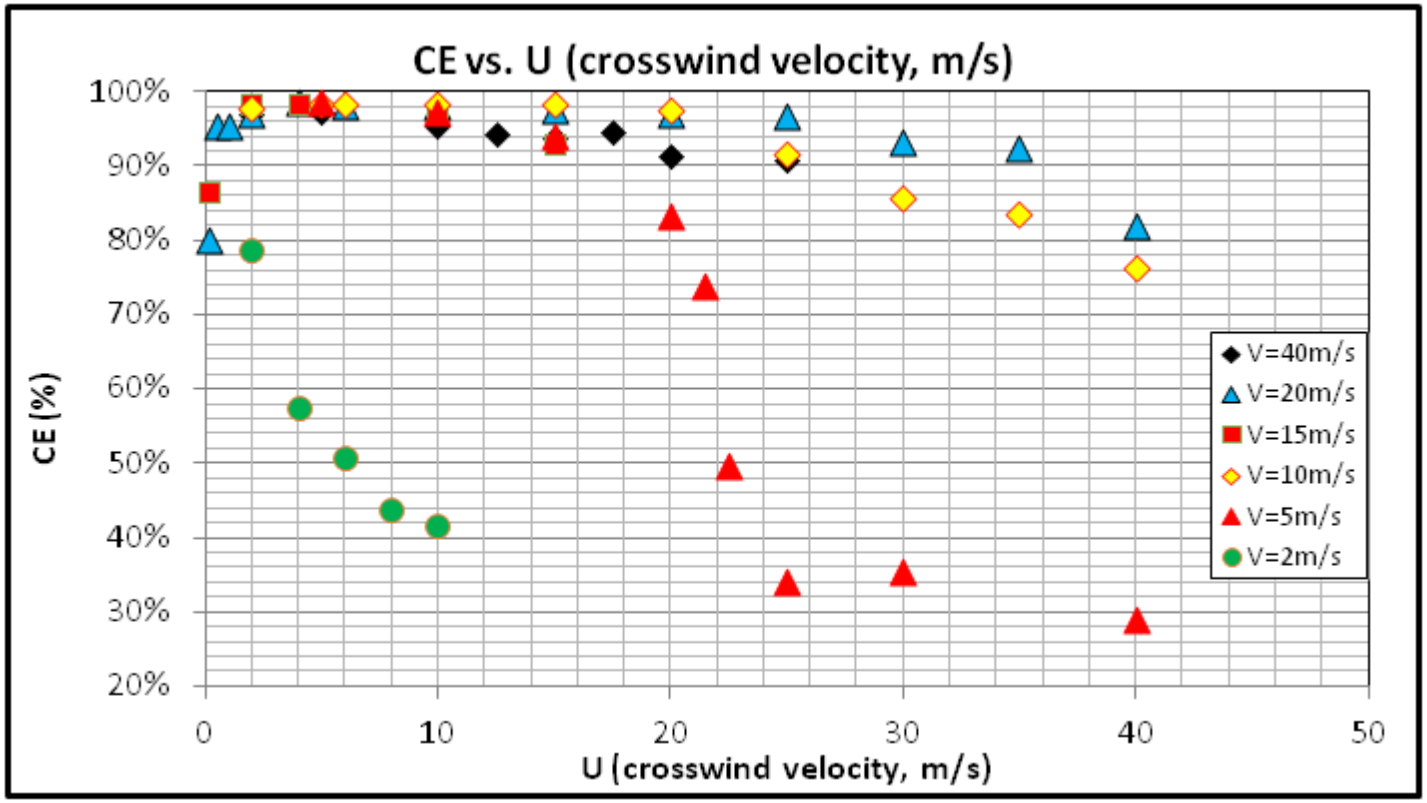


$$SR = \frac{Actual\ air\ (lb/hr)}{Stoichiometric\ air\ (lb/hr)}$$

Correlation Development

I. DRE/CE vs. U & V

II. Emissions vs. CE



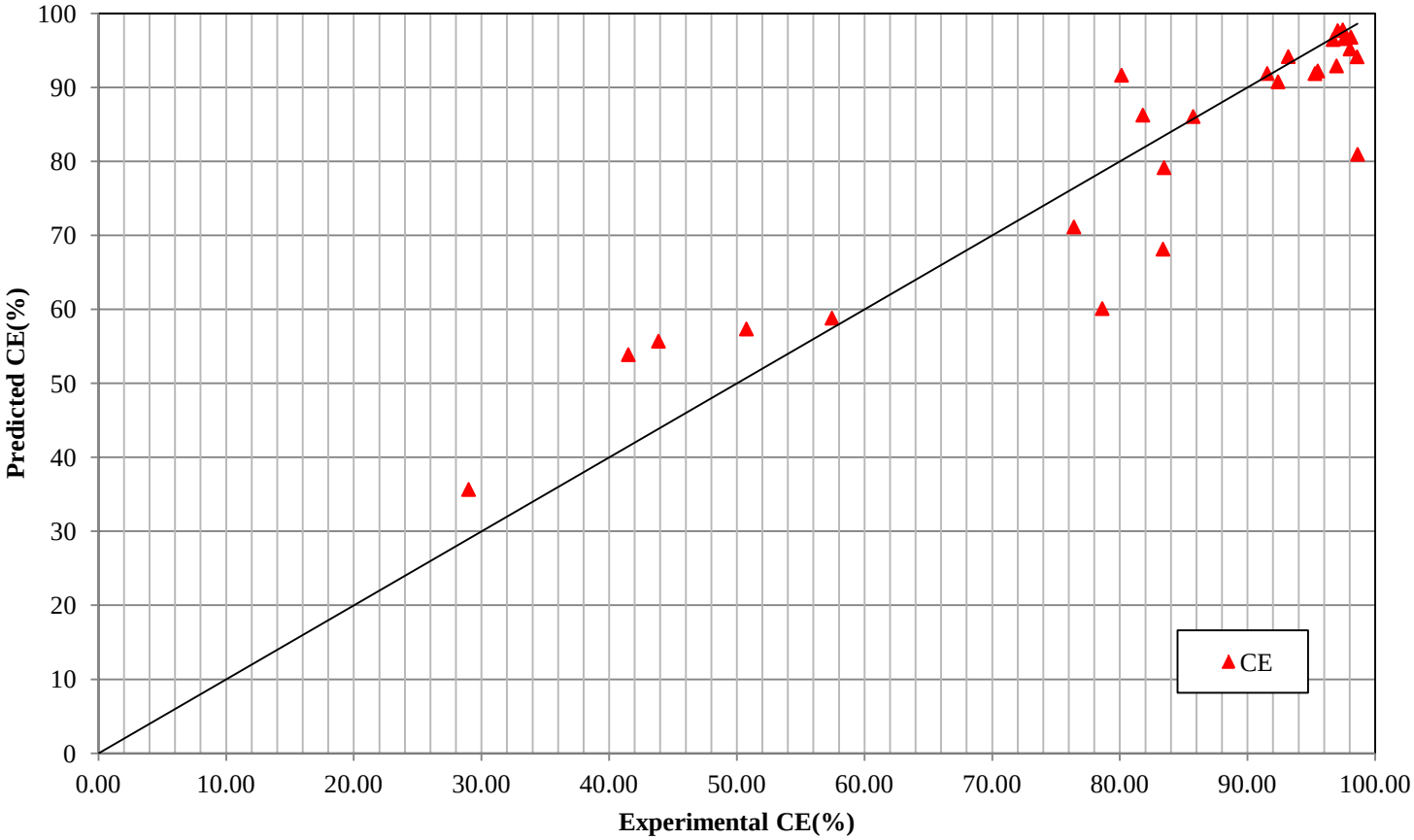
CE vs. Crosswind for all jet velocity cases

Quadratic Correlation for CE

- 31 data points
- $2m/s \leq V_j \leq 20m/s$
- $\mathbf{R^2 = 0.86}$

Experimental vs. Predicted CE(%)

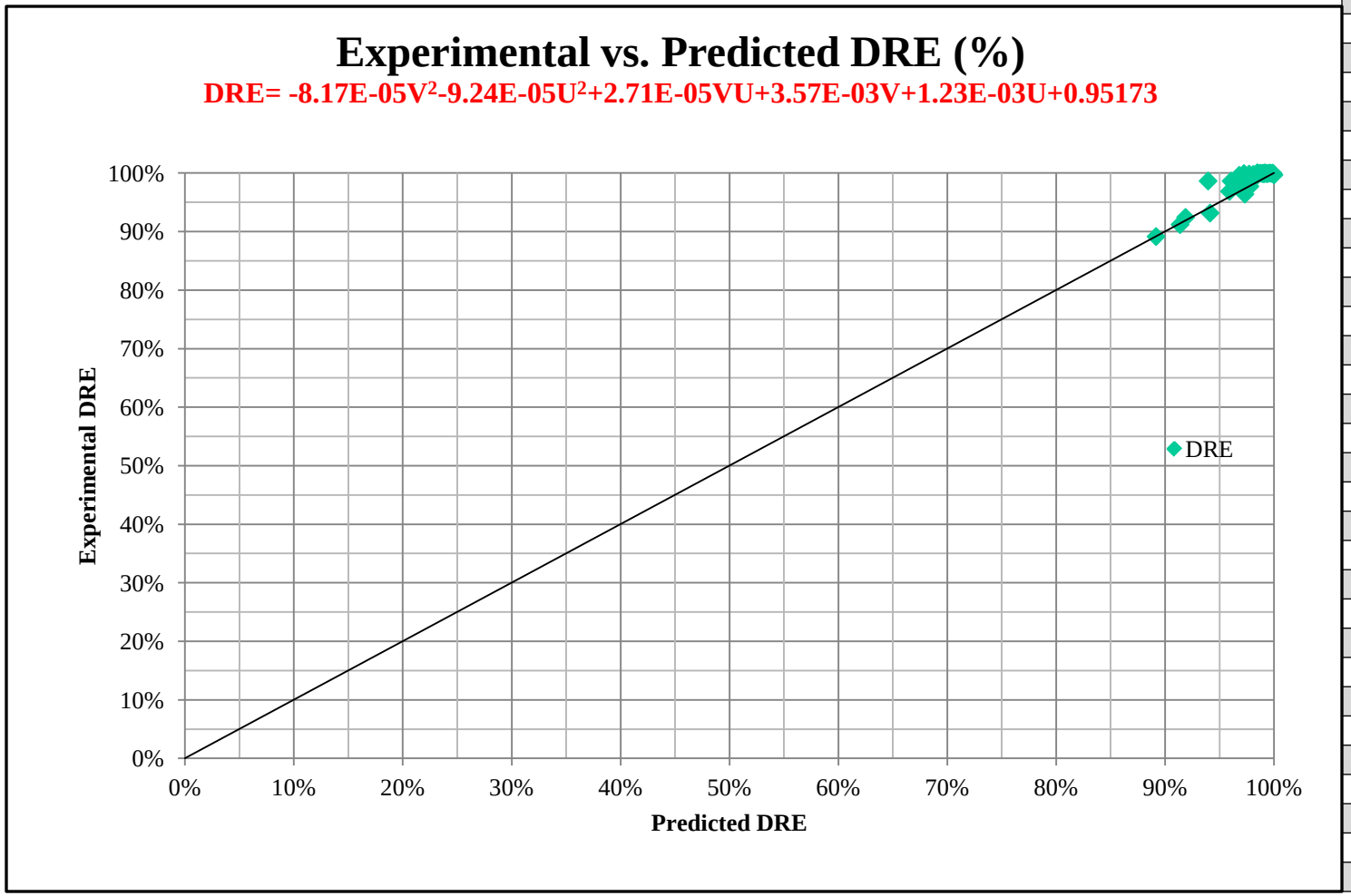
$$CE = -0.028U^2-0.372V^2+0.07U*V-0.655U+9.87V+42.97$$



Vj (m/s)	U (m/s)	CE (%)
2	2	78.62
2	4	57.45
2	6	50.75
2	8	43.86
2	10	41.50
5	5	98.62
5	20	83.38
5	40	28.99
10	2	97.69
10	5	98.29
10	6	98.24
10	10	98.41
10	15	98.41
10	20	97.56
10	25	91.54
10	30	85.74
10	35	83.46
10	40	76.40
20	0.2	80.13
20	0.5	95.28
20	1	95.50
20	2	96.97
20	4	98.58
20	6	98.03
20	10	98.10
20	15	97.46
20	20	97.06
20	25	96.70
20	30	93.19
20	35	92.39
20	40	81.80

Quadratic Correlation for DRE

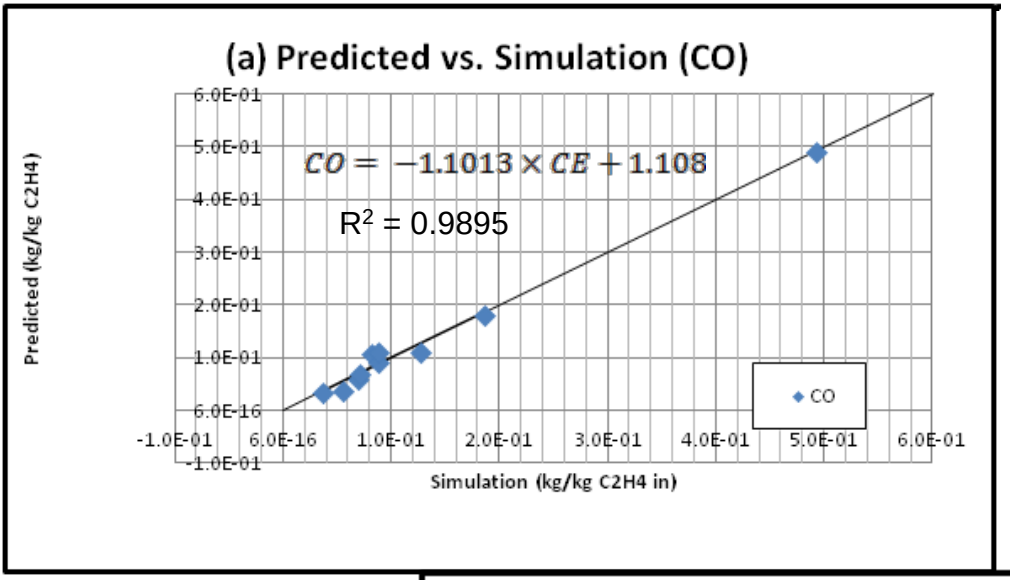
- 36 data points
- $10\text{m/s} \leq V_j \leq 40\text{m/s}$
- $\mathbf{R^2 = 0.84}$, RMS Error = 0.0018



V(m/s)	U(m/s)	DRE %
23.5354	10.1356	0.9969
10.0000	5.0000	1.0000
10.0000	6.0000	1.0000
10.0000	10.0000	0.9998
10.0000	15.0000	0.9977
10.0000	20.0000	0.9991
10.0000	25.0000	0.9687
10.0000	30.0000	0.9317
10.0000	35.0000	0.9242
10.0000	40.0000	0.8915
15.0000	0.2000	0.9997
15.0000	2.0000	0.9997
15.0000	4.0000	0.9999
15.0000	10.0000	0.9995
15.0000	15.0000	0.9986
20.0000	0.2000	0.9997
20.0000	0.5000	0.9998
20.0000	1.0000	0.9999
20.0000	2.0000	0.9988
20.0000	4.0000	1.0000
20.0000	6.0000	0.9994
20.0000	10.0000	0.9999
20.0000	15.0000	0.9998
20.0000	20.0000	0.9992
20.0000	25.0000	0.9982
20.0000	30.0000	0.9863
20.0000	35.0000	0.9864
20.0000	40.0000	0.9119
40.0000	2.0000	0.9961
40.0000	5.0000	0.9945
40.0000	10.0000	0.9884
40.0000	12.5000	0.9847
40.0000	15.0000	0.9772
40.0000	17.5000	0.9886
40.0000	20.0000	0.9639
40.0000	25.0000	0.9790

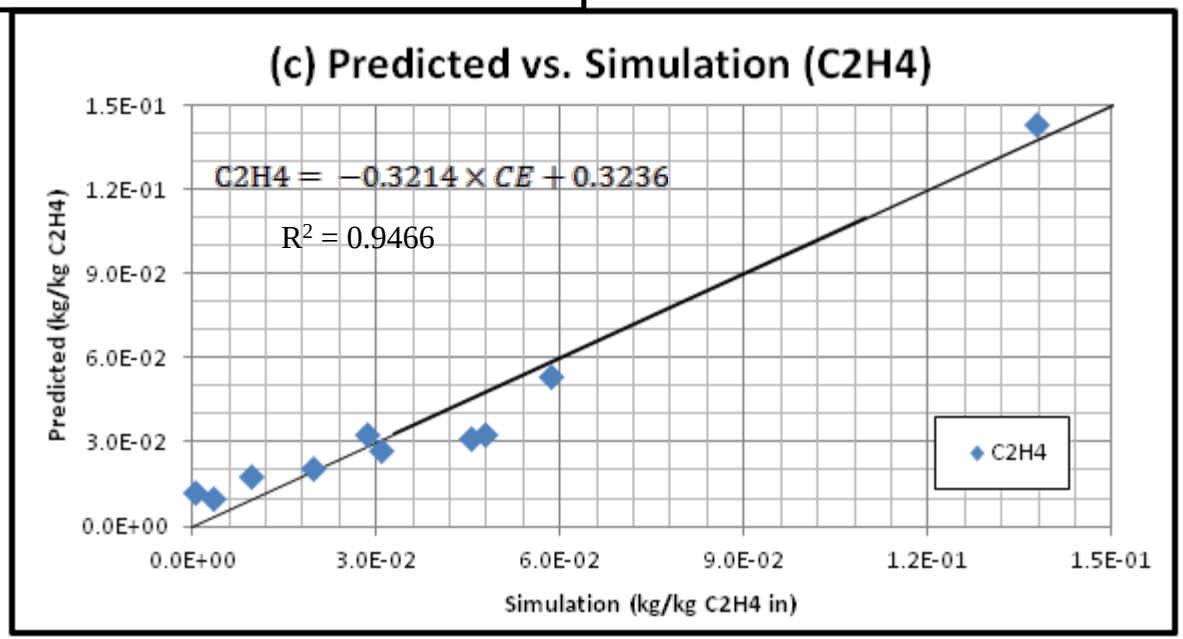
Speciated emission rates vs. combustion efficiency

Correlations between Emission Rates and Combustion Efficiency



$$CH2O = -0.0414 \times CE + 0.0394$$

$R^2 = 0.9461$



PATHLINES COLORED BY TEMPERATURE

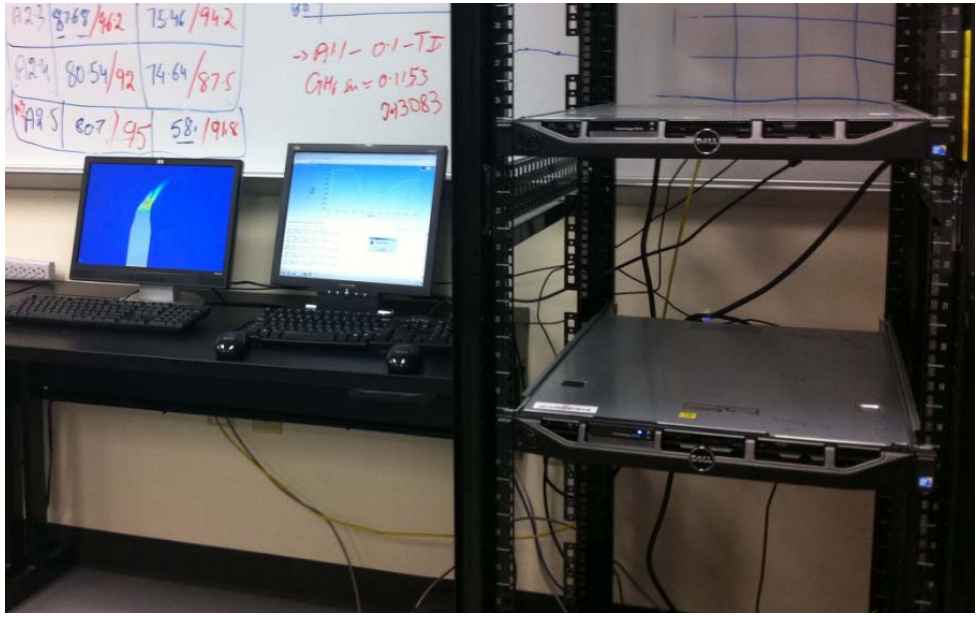
Case: Jet = 10 m/s and Crosswind = 10 m/s

PATHLINES COLORED BY MASS FRACTION OF C_2H_4

Case: Jet = 10 m/s and Crosswind = 10 m/s

Lamar University CFD Lab

- Cutting Edge High Performance Computing (HPC) Cluster
  - 3 X 12 core servers; Intel Xeon X5670 @2.93GHz
  - More than 50 high speed processors
  - Up to 10GBs/second of data transfer speed for faster parallel computing



Thank You

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.

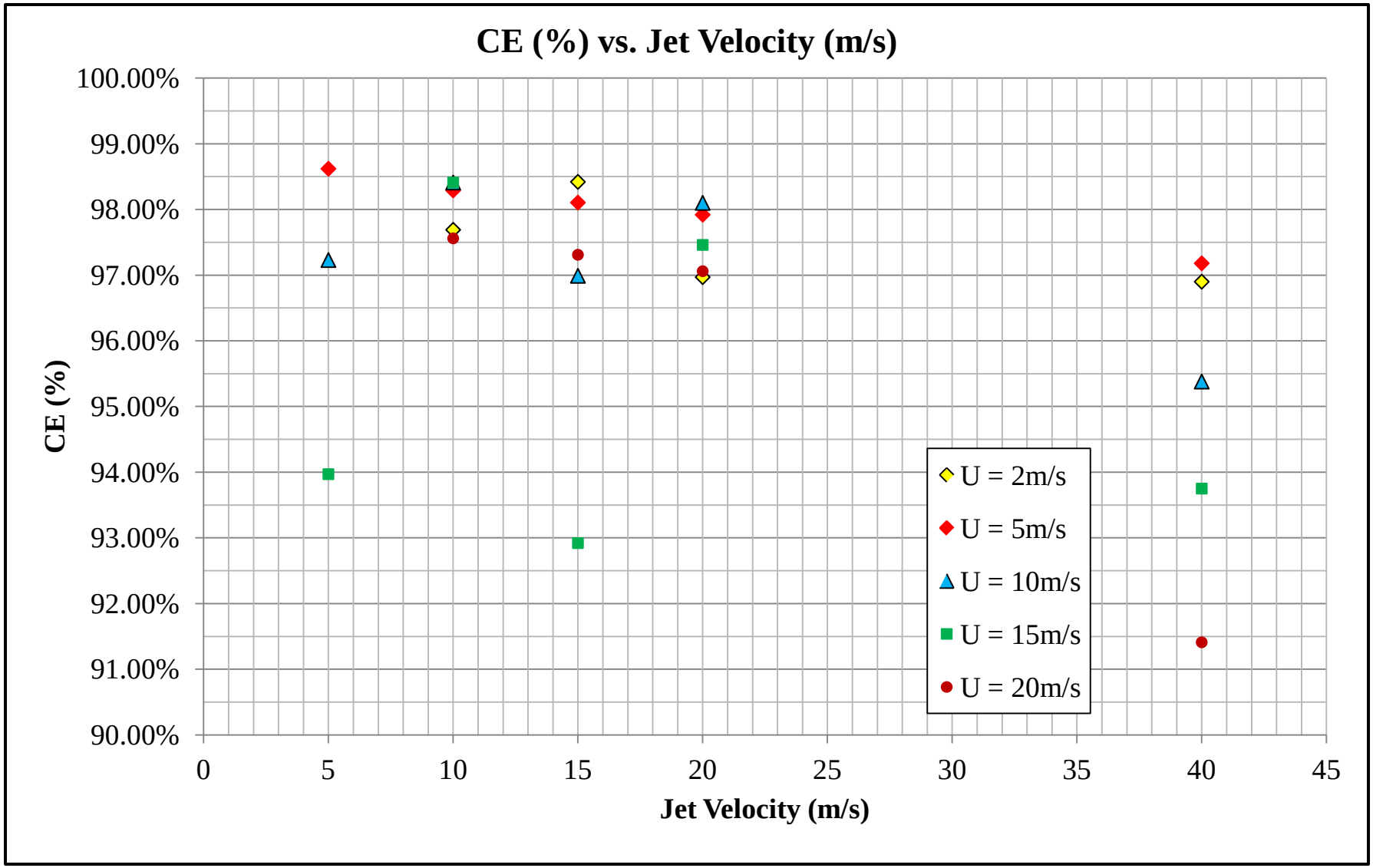
Preliminary Results of Correlations

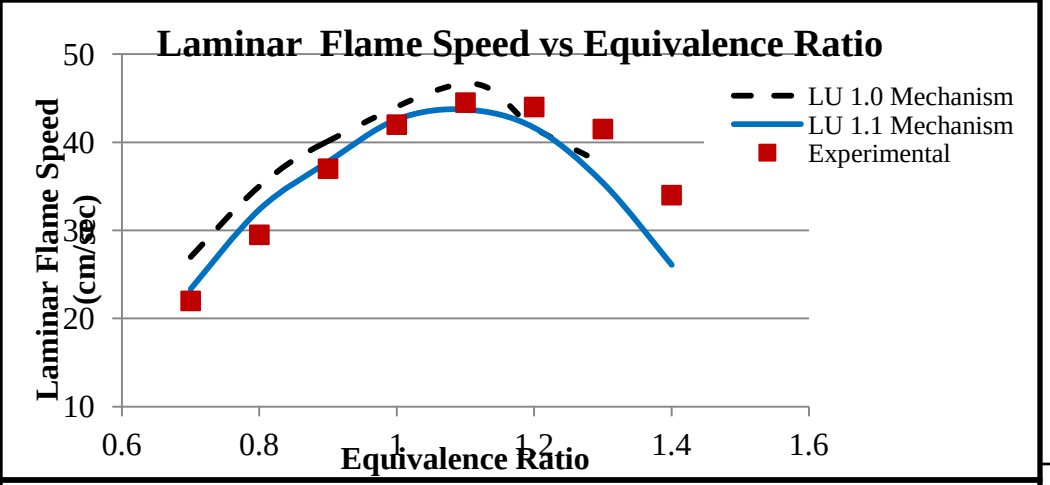
An exponential equation for CE (%):

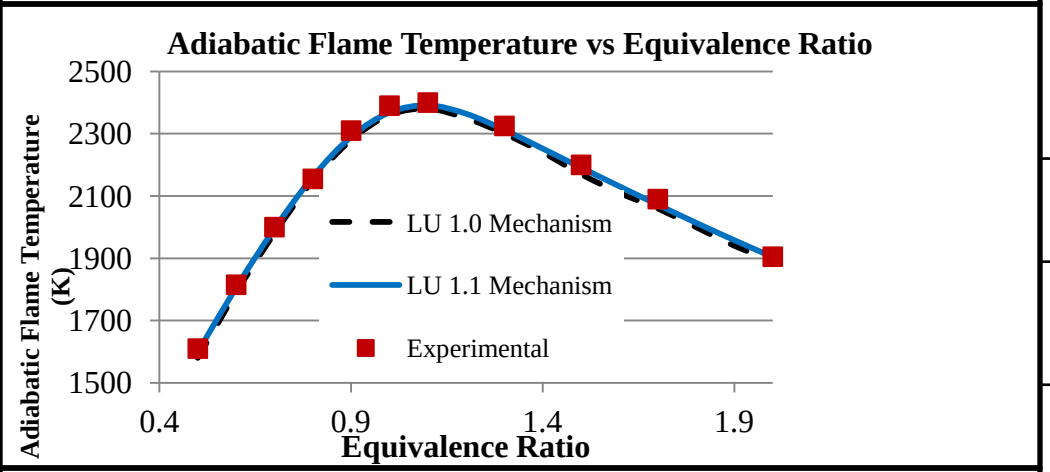
$$CE = 52.67 * U^{0.0022} * V_j^{0.2043} \qquad R^2 = 0.65$$

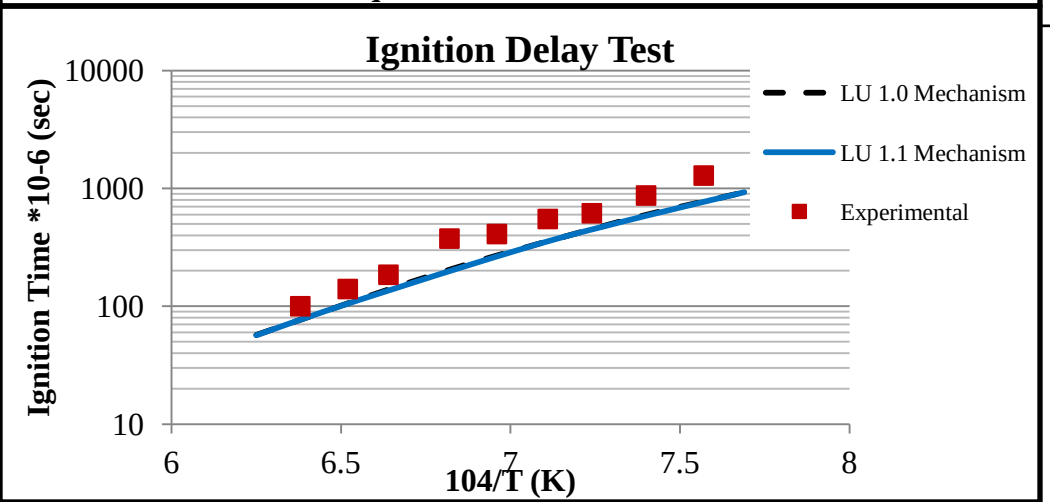
- Ethylene flames
- Use crosswind U and jet velocity V_j as input variables

Effect of Jet Velocity on CE

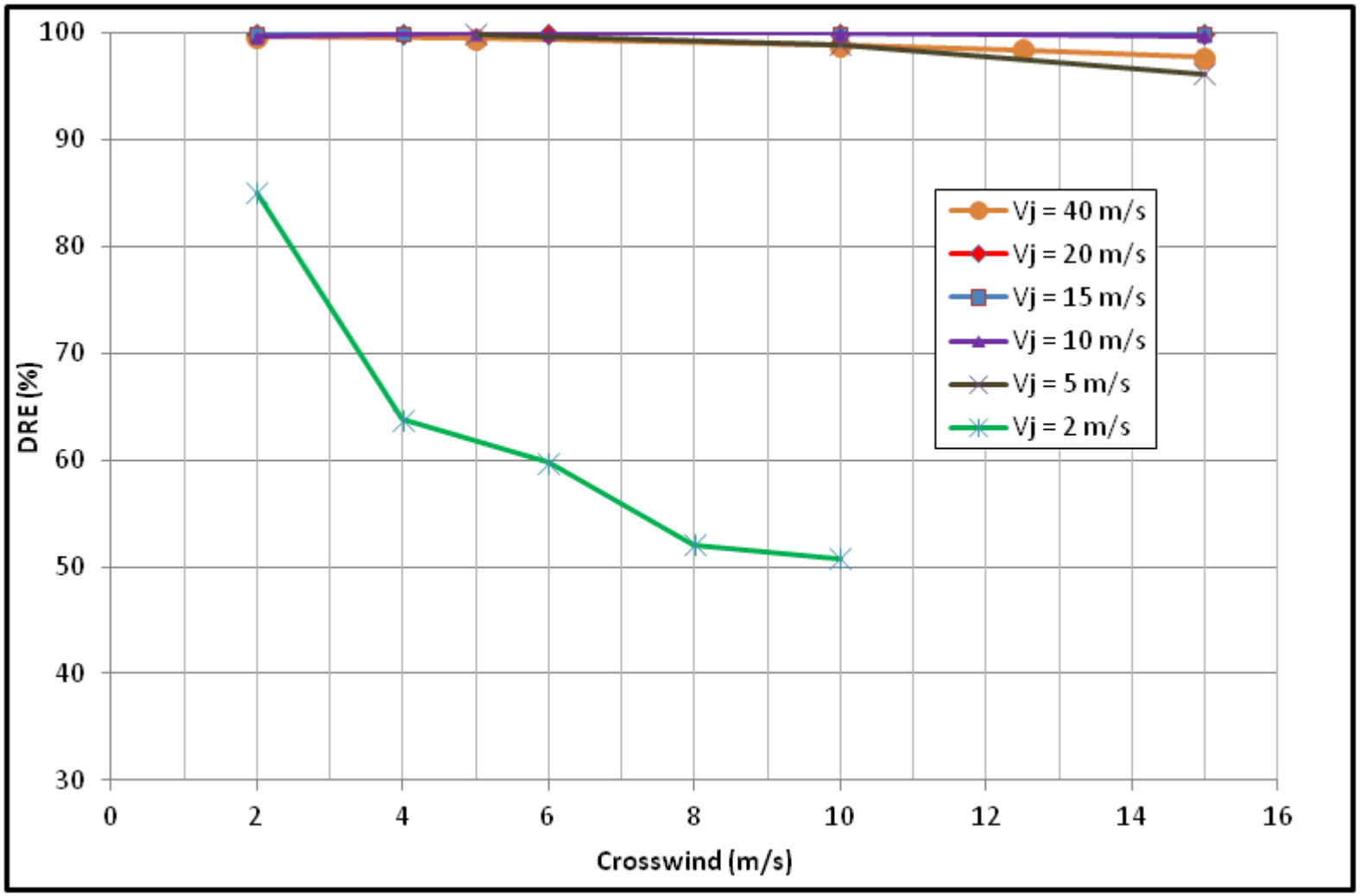




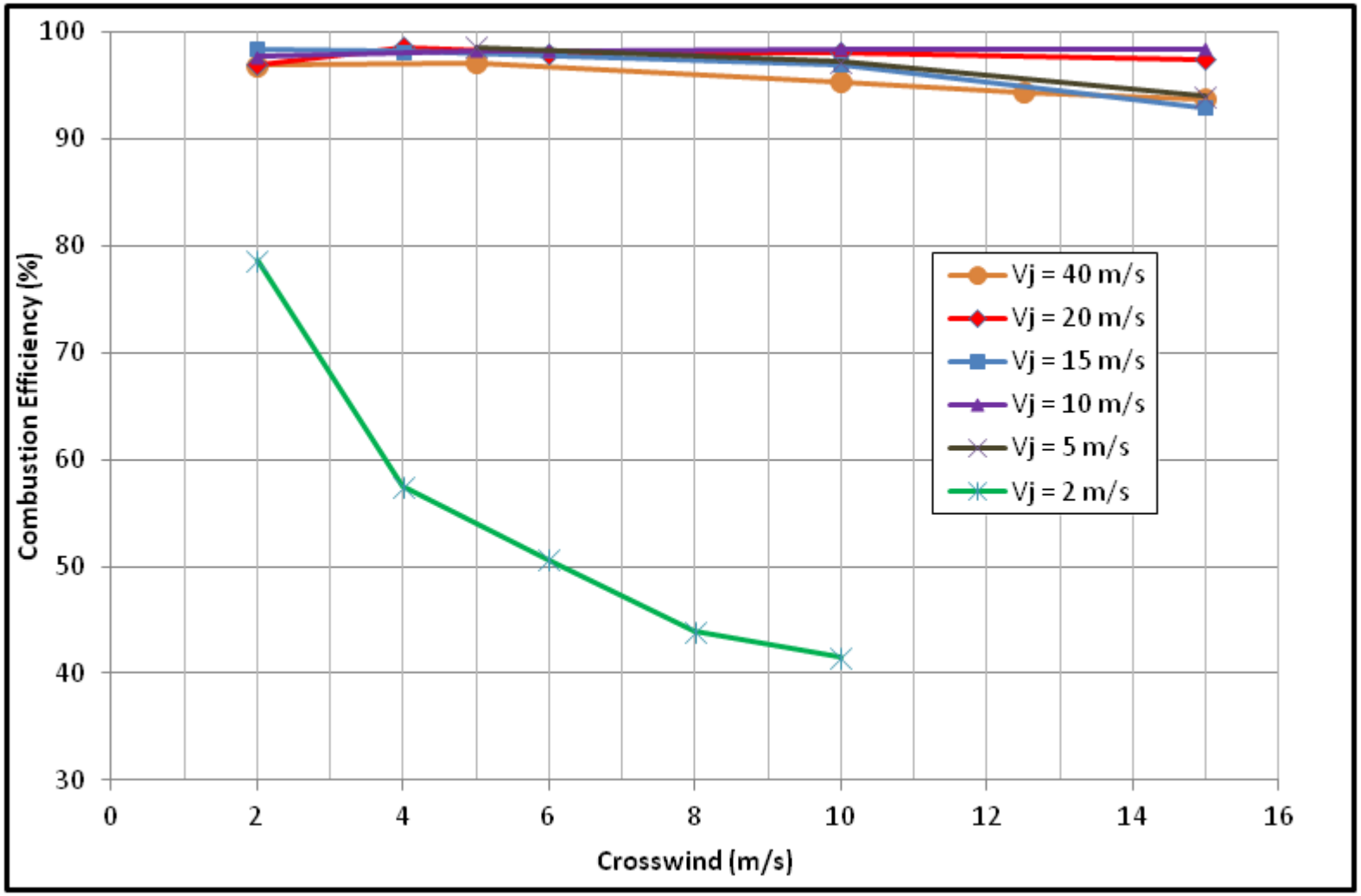




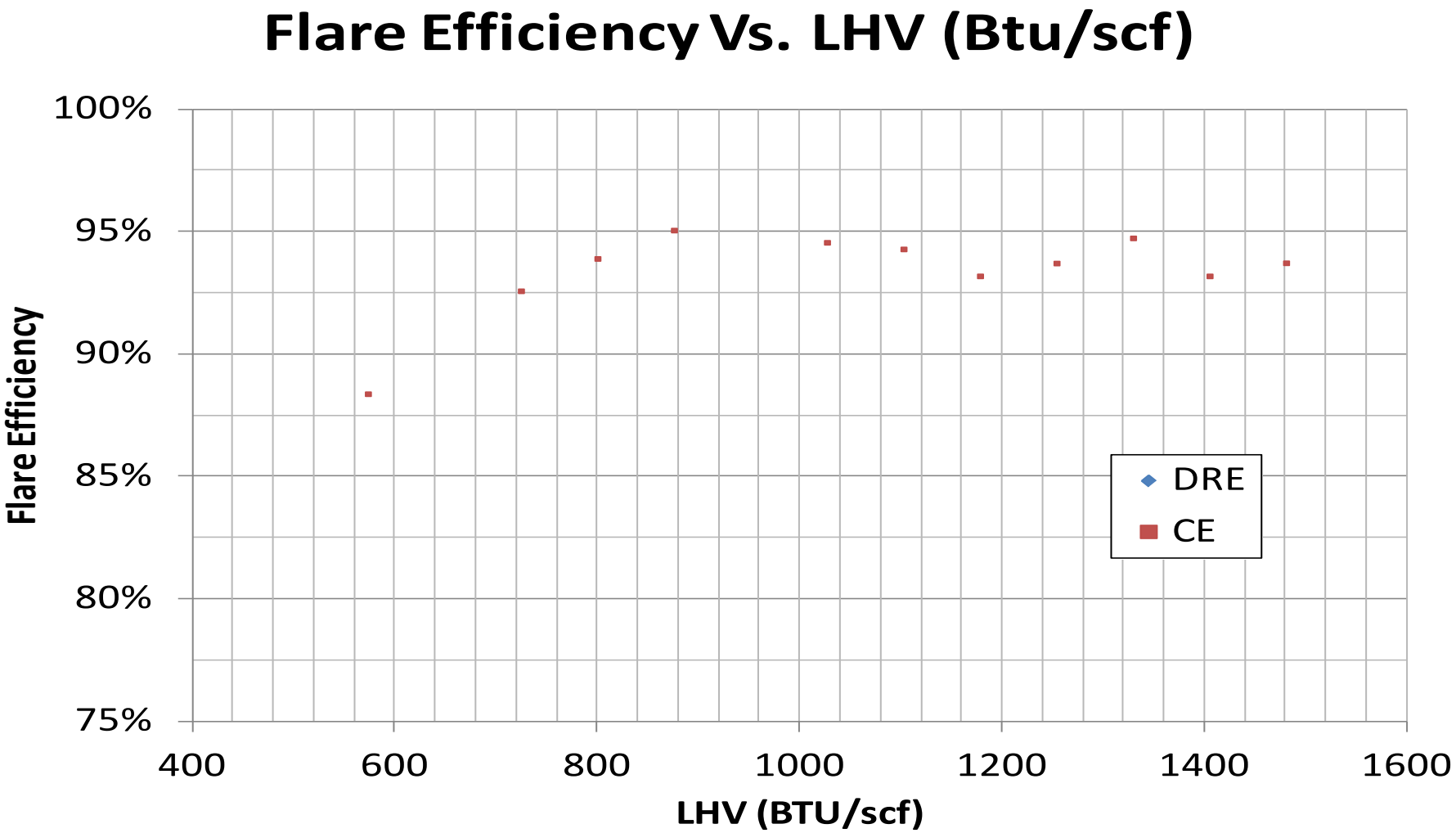
Indicators		Average Percentage Error	
		Without NO_2 (LU 1.0)	With NO_2 (LU 1.1)
Laminar Flame Speed	Propylene	11.605	8.058
Adiabatic Flame Temperature	Ethylene	1.138	0.527
Ignition Delay	Propylene	30.68	31.25



DRE at Different Jet Velocities



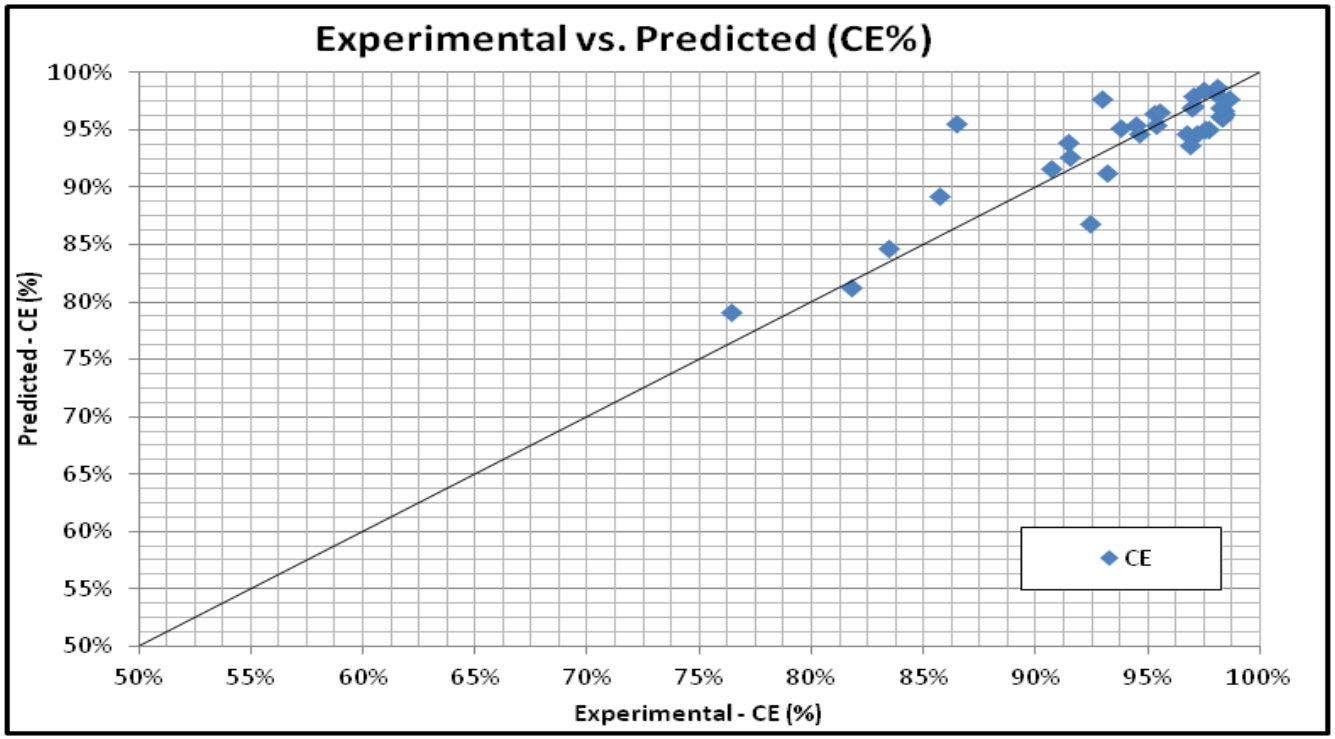
Comparison of CE at Different Jet Velocities



C_2H_4/N2 Mixture, C_2H_4 from 100% (1512 Btu/scf) to 40% (605 Btu/scf)
U = 10 m/s, V = 10 m/s

Preliminary Results of Correlations

$$CE = aU^2 + bV^2 + cUV + dU + eV + f$$



where:
a = -2.09E-04
b = -1.19E-04
c = 5.57E-04
d = 4.53E-03
e = 5.49E-03
f = 9.00E-01

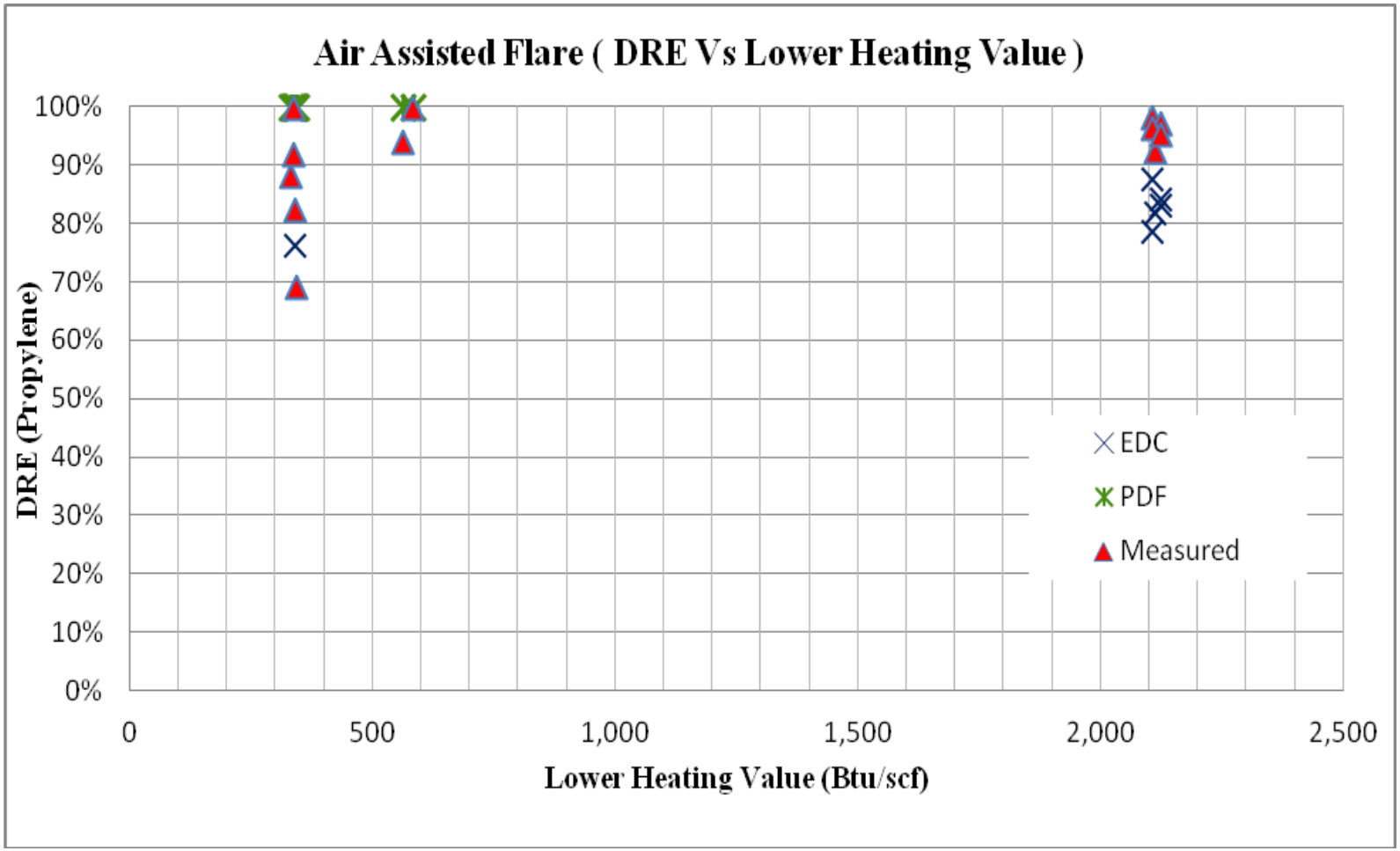
$R^2 = 0.76$
RMS=2.63%

- Ethylene flames
- Valid for:
  - Crosswind (U) : 0.2 m/s to 40 m/s
  - Jet Velocity (V_j) : 10m/s to 40 m/s

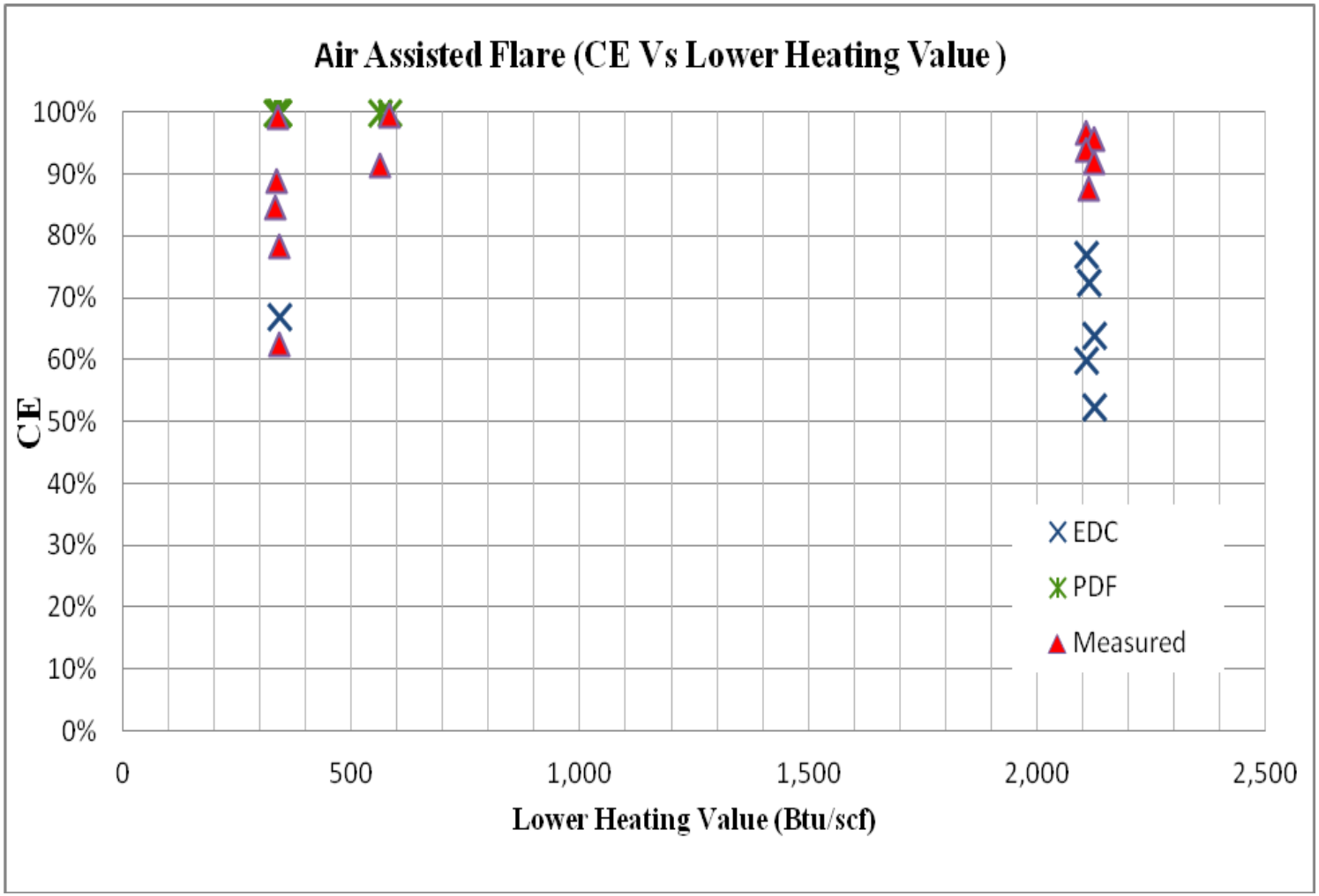
Air-assisted flare test cases

	Test Point	Actual Vent Gas (VG) Flow Rates				Vent Gas Vel	Air Assist Vel	Cross Wind Vel	EDC	PDF
		Propylene	TNG	Nitrogen	LHV					
		lb/hr	lb/hr	lb/hr	Btu/scf	m/s	m/s	m/s		
High LHV	A1.1	918.88	0.00	0.00	2107.71	0.43	23.12	5.69	✓	×
	A2.1	355.02	0.00	0.00	2125.45	0.17	12.99	5.74	✓	×
	A2.3	352.14	0.00	0.00	2108.22	0.17	13.76	4.51	✓	×
	A2.4	352.87	0.00	0.00	2112.57	0.17	23.06	4.49	✓	×
	A2.5	354.71	0.00	0.00	2123.55	0.17	18.53	5.94	✓	×
Low LHV	A3.1	181.23	18.77	702.55	338.67	0.59	3.00	4.61	×	✓
	A3.3	181.23	18.37	700.60	333.86	0.59	9.32	4.96	×	✓
	A3.6	181.23	18.76	704.18	337.55	0.59	7.36	5.31	×	✓
	A5.2	72.29	7.69	274.41	342.86	0.23	11.65	0.96	×	✓
	A5.3	71.26	7.55	271.37	341.87	0.23	5.10	1.12	✓	✓
Medium LHV	A4.3	298.74	30.30	591.10	562.91	0.58	10.30	4.79	×	✓
	A6.1	117.80	11.86	221.21	583.73	0.22	1.77	7.12	×	✓
	A6.4	118.06	12.08	221.25	584.89	0.22	6.29	6.31	×	×
	A6.5	117.85	12.08	221.11	584.44	0.22	8.77	6.92	×	×
	A6.6	118.55	12.44	220.68	588.07	0.22	22.67	6.69	×	×

- ✓ : Cases Simulated × : Cases Not Simulated



DRE as a function of LHV (measured vs. CFD, air-assisted cases)

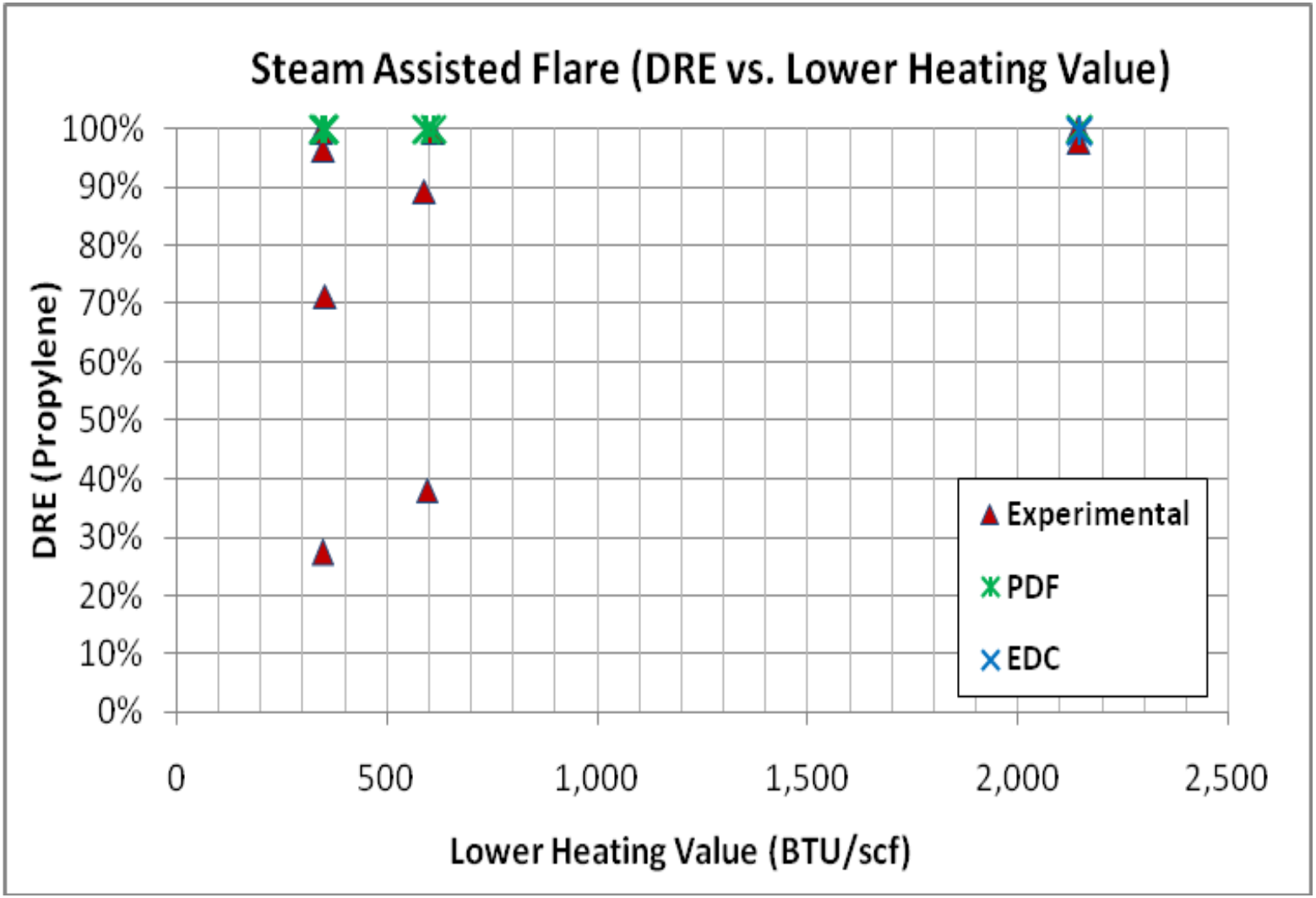


CE as a function of LHV (measured vs. CFD, air-assisted cases)

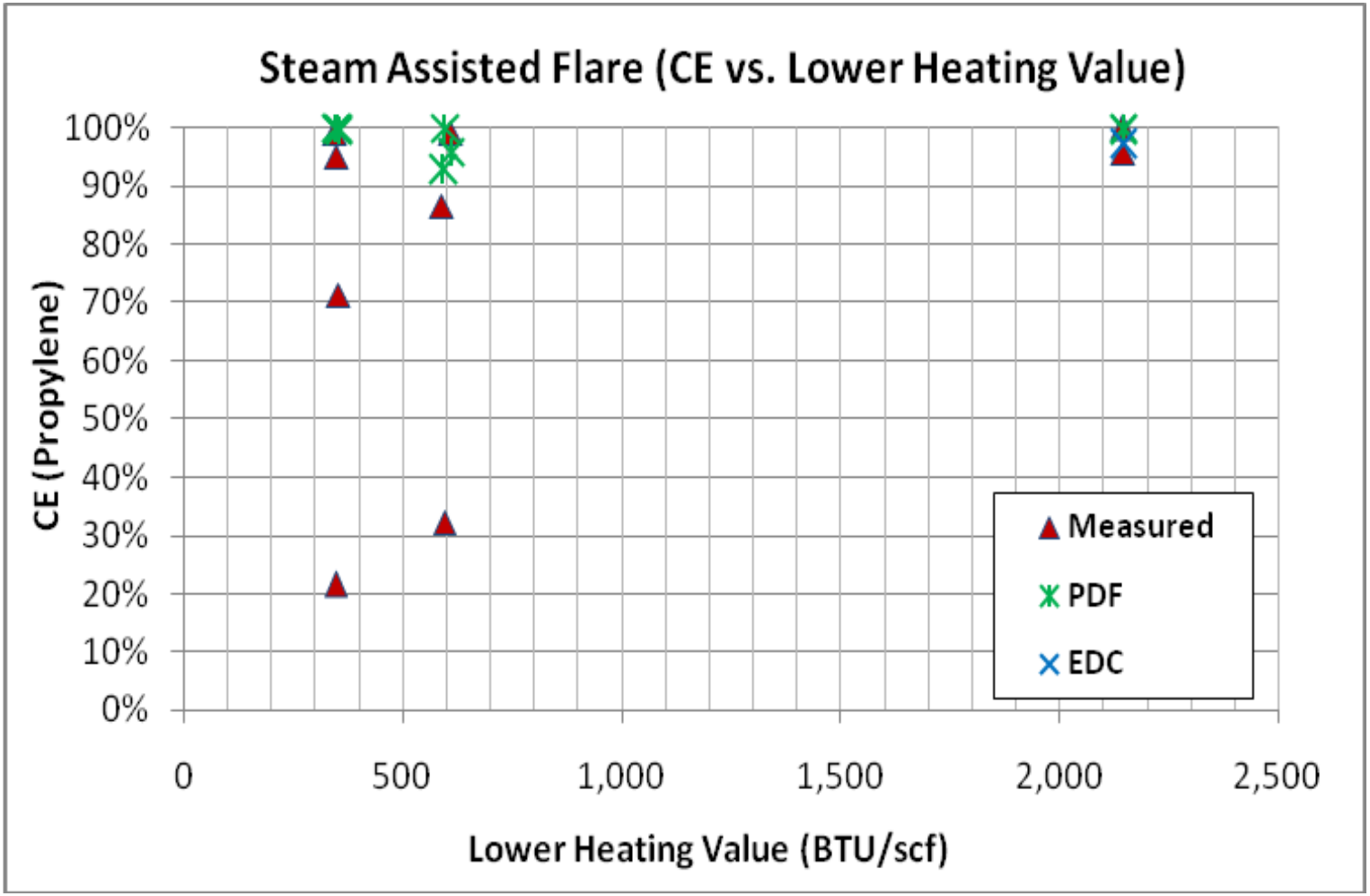
Steam-assisted flare test cases

	Test Point	Vent Gas Flow Rates C_3H_6 lb/hr	TNG lb/hr	N_2 lb/hr	Actual Vent Gas LHV Btu/scf	Actual Vent Gas Velocity m/s	Steam Flow Rates Center lb/hr	Steam Flow Rates Upper lb/hr	Steam to Gas Ratio	Wind Speed m/s	EDC	PDF
High	S1.5	2337.5	0.0	0.0	2145.1	0.5	525.9	3794.0	1.8	3.5	×	✓
	S1.8	2338.4	0.0	0.0	2146.0	0.5	505.9	7044.1	3.2	3.8	×	✓
	S1.9	2336.6	0.0	0.0	2144.3	0.5	504.9	7939.3	3.6	3.9	×	×
	S2.2	937.0	0.0	0.0	2103.1	0.3	541.6	7769.5	8.9	4.8	×	×
	S2.3	937.0	0.0	0.0	2122.5	0.3	539.3	4761.3	5.7	3.4	×	×
Low	S3.7	191.3	18.9	715.5	345.5	0.2	0.0	227.8	0.2	3.2	×	✓
	S4.1	490.5	45.0	1799.7	349.6	0.6	559.9	536.3	0.5	2.5	×	✓
	S4.3	485.2	45.0	1801.6	346.4	0.6	567.3	1879.5	1.0	2.3	×	✓
	S4.3	500.4	46.6	1802.1	355.2	0.6	627.8	2447.4	1.3	3.0	×	×
Medium	S5.2	319.8	33.8	584.7	595.4	0.3	454.5	1580.4	2.2	4.5	×	✓
	S5.3	312.3	31.7	578.0	589.6	0.3	481.5	782.5	1.4	4.1	×	✓
	S5.4	317.6	32.2	579.4	595.4	0.3	483.7	1220.8	1.8	4.8	×	×
	S5.6	312.2	31.8	577.2	590.1	0.3	490.6	462.9	1.0	4.3	×	×
	S6.1	826.4	79.1	1455.6	608.9	0.6	517.8	1002.9	0.6	3.9	×	✓
	S7.3	296.8	29.9	1083.6	352.8	0.4	515.6	537.9	0.7	3.5	×	✓

- ✓ : Cases Simulated × : Cases Not Simulated



DRE as a function of LHV (measured vs. CFD, steam-assisted cases



CE as a function of LHV (measured vs. CFD, steam-assisted cases)