

COMBUSTION CHARACTERIZATION AND MODELLING OF FUEL BLENDS FOR POWER GENERATION GAS TURBINES

University of Central Florida



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SCIES Project 04-01-SR114

DOE COOPERATIVE AGREEMENT DE-FC26-02NT41431

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Project Awarded (05/01/2004, 36-Month Duration)

\$556,937 Total Contract Value (\$405,990 DOE)

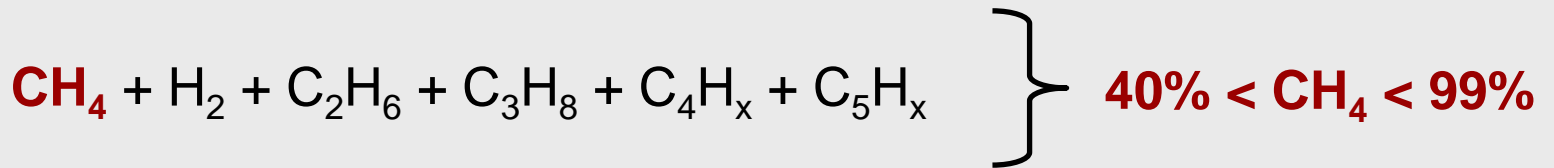
Gas Turbine Need

Fuel Composition Variation is a Concern

Natural Gas:



Exotic Fuel Blends:



Syngas:

H₂ : 9 – 45%
CO: 20 – 55%
H₂O: 0 – 40%

**Fuel Variation Impacts
Chemistry
&
Engine Performance !**

Project Objectives

There are Several Major Objectives...

1. Measure **Ignition Delay Times** of Fuel Blends at Engine Pressures
2. Develop Efficient **Test Matrices** to Cover Wide Range of Blends
3. Identify Appropriate Chemical **Kinetics Mechanisms**
4. Assemble **Reduced Kinetics** Mechanism(s) for CFD
5. Apply **Reacting-Flow CFD** Model to Explore Fuel Flex Issues
6. Measure **Flame Speeds** for Varying Fuel Blends
7. Acquire **Detailed Kinetics Data** for Model Improvement

Approach

Project is Divided into 7 Tasks

Task 1 – Test Matrix and Literature Search (Yr 1)

Task 2 – Autoignition Measurements (Yr 1, 2, 3)

Task 3 – Flame Speed Measurements (Yr 2, 3)

Task 4 – Chemical Kinetics Modeling (Yr 1, 2, 3)

Task 5 – CFD Modeling Effort (Yr 1, 2, 3)

Task 6 – NO_x Measurements (Yr 3)

Task 7 – Mechanism Validation Measurements (Yr 2, 3)

Results

We Have Had **Several Major Results** the 1st 17 Months

- Ignition Times for Several Binary **CH₄ Blends** ($\phi = 0.5$) Measured
 - H₂, C₂H₆, C₃H₈, C₄H₁₀, C₅H₁₂
 - 1100 – 1500 K, 1 – 25 atm
- Autoignition and Other **Test Matrices** Developed
- Ignition Delay Times of Several **CO/H₂ Blends** ($\phi = 0.5$) Measured
- Preburner **Autoignition Study** Completed
- Gas Turbine **CFD Model** Identified and Tested
- Flame Speed Rig Designed
- Detailed Kinetics Measurements for Syngas Mixtures Performed

Background and Experimental Setup

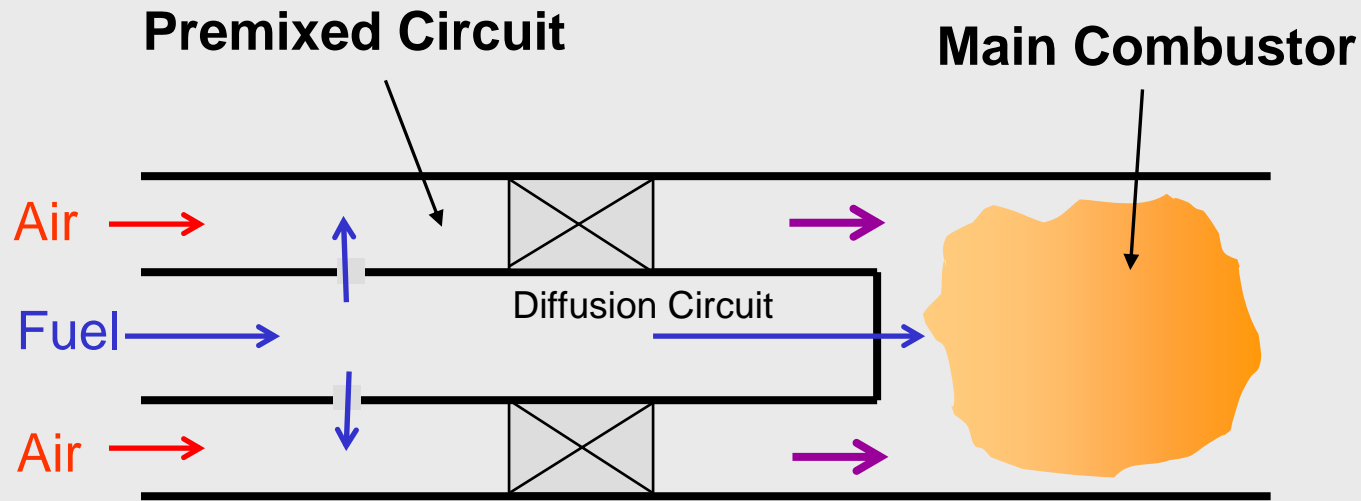
Background

Ignition Times Are Important for Two Reasons:

1. **Autoignition** of Premixed Fuel/Air Mixtures
2. **Characteristic Times** for Calibrating Chemical Kinetics

Background

Autoignition for Premixer and Characteristic Times for Burner



600 – 800 K
10 – 25 atm
~ 10 ms

Autoignition?

1300 – 1900 K
10 – 25 atm

- Chemical Kinetics
- Flame Speed
- Stability

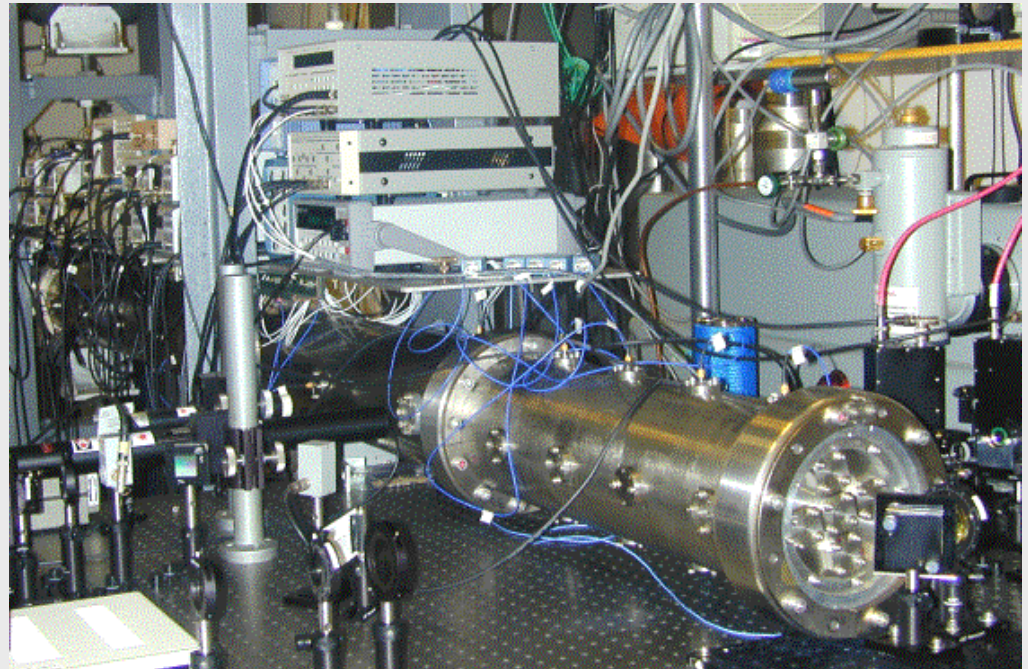
Experiment

*Shock-Tube Facility is Capable of **Elevated Pressures***

Specifications

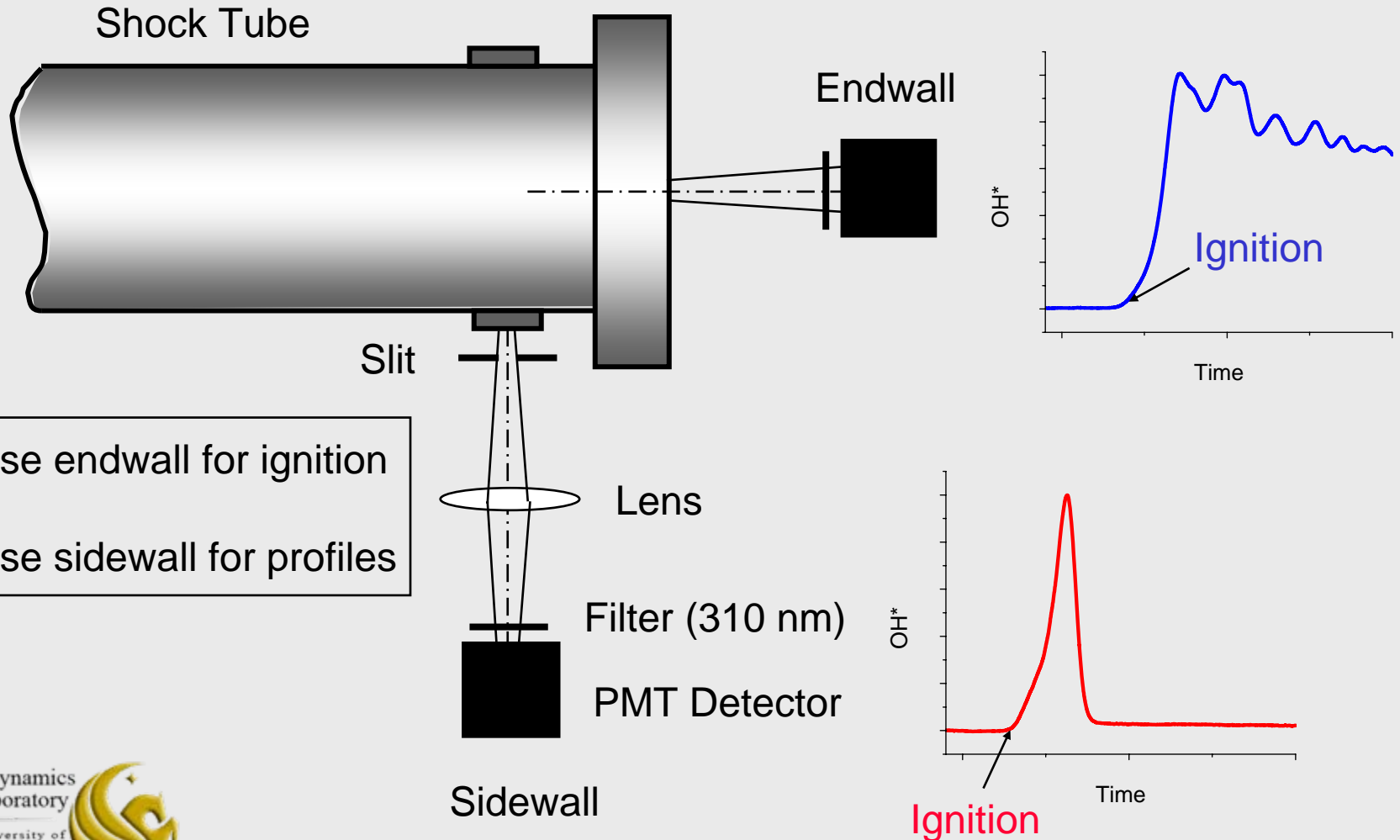
- Driver: 7.6 cm Dia, 3.5 m
- Driven: 16.2 cm Dia, 10.7 m
- Digital DAQ (5 MHz, 12 bit)
- Optical Diagnostics
- Pressure (1 – 100 atm)

Aerospace Shock Tube Facility



Experiments

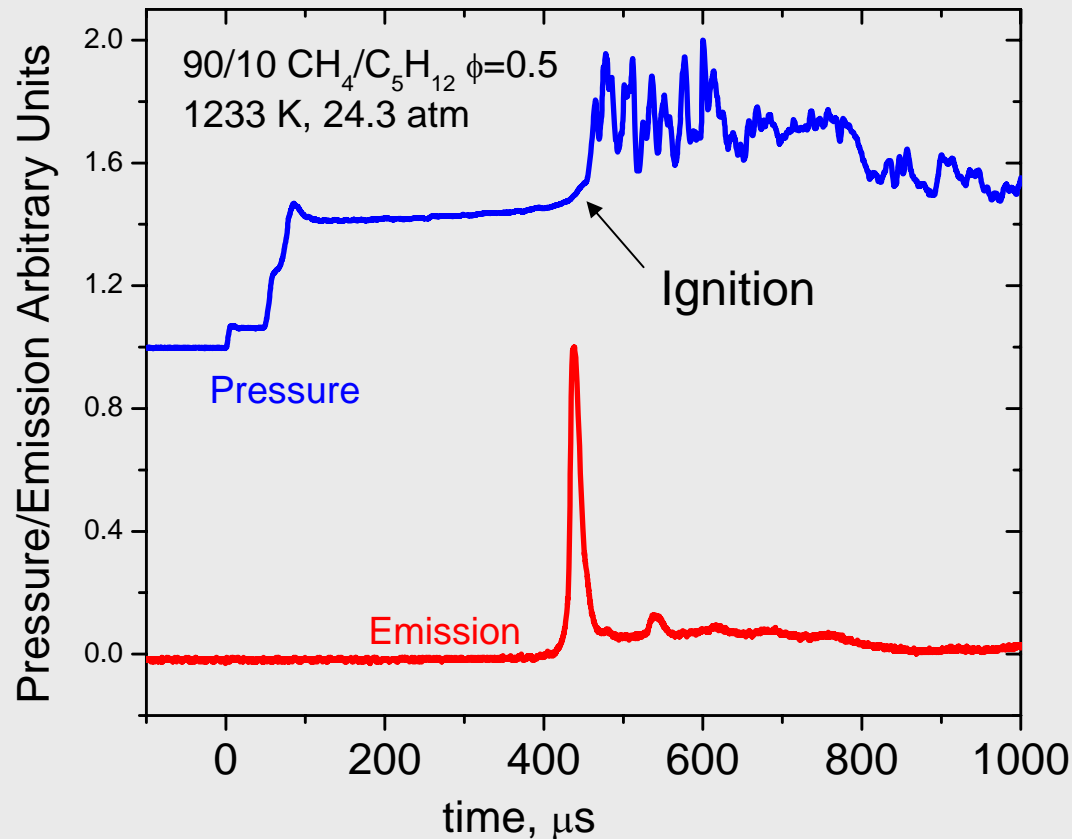
Chemiluminescence (OH^ or CH^*) Detected at Endwall and Sidewall*



Experiment

Sample **Sidewall Emission and Pressure** Show Highly Exothermic Reaction

Sidewall Data Traces



Technical Results

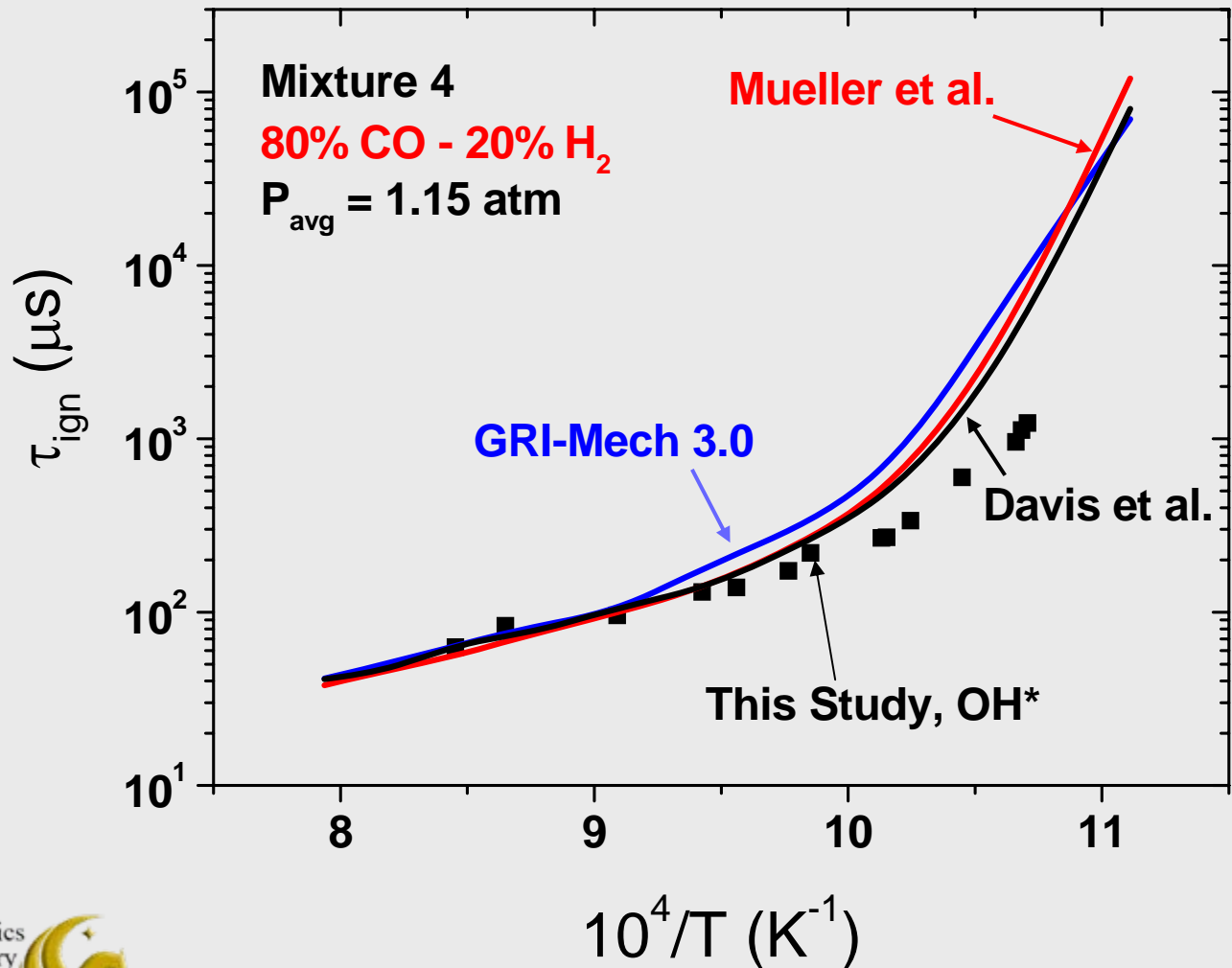
Task 2 – Ignition (CO/H₂)

*Many **Syngas Blends** Have been Studied Over a Wide Range of Temperature and Pressure*

1. CO/H₂ Blends: from **95% CO** to **5% CO**
2. T = **890 – 1300 K**
3. P = **1 - 15 atm**
4. Fuel-Lean: **$\phi = 0.5$**
5. Comparison with Kinetics Models

Task 2 – Ignition (CO/H_2)

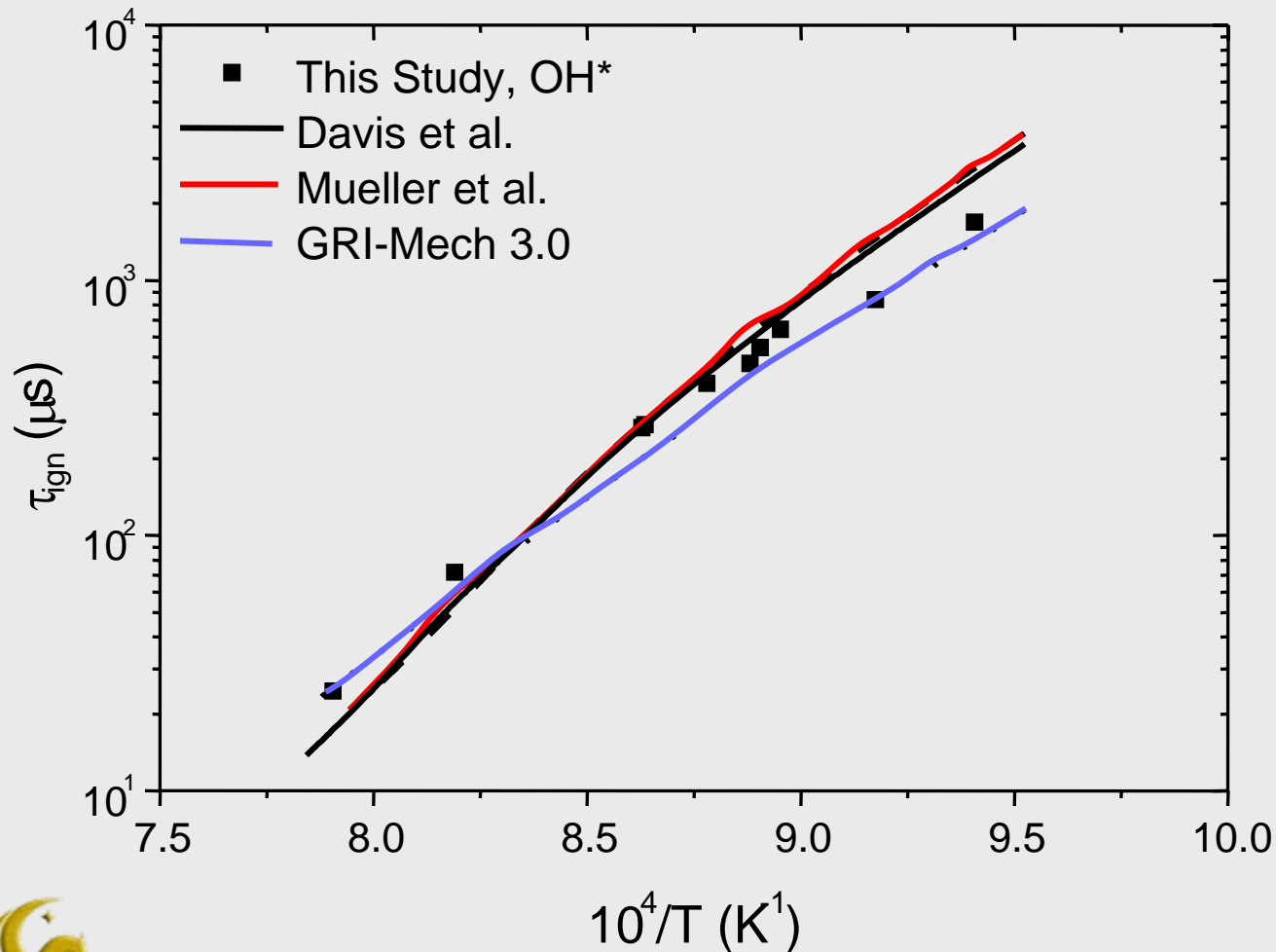
Kinetics Models Capture Basic Trends, Particularly at High T



- 80/20 CO/H_2
- $\phi = 0.5$

Task 2 – Ignition (CO/H_2)

Models Show Good Agreement at Highest Pressures



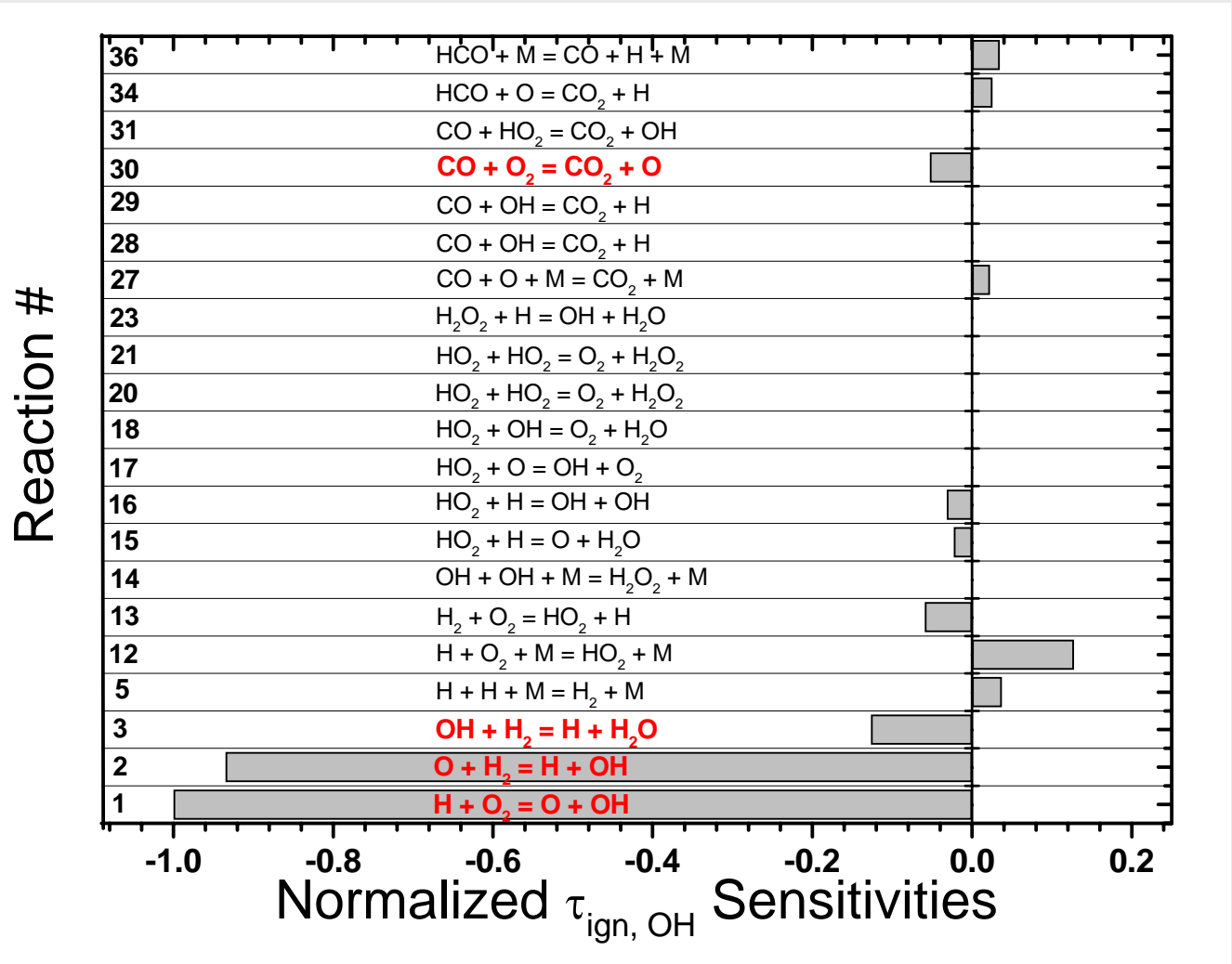
- 90/10 CO/H_2
- 14.3 atm

Task 2 – Ignition (CO/H₂)

Hydrogen Oxidation Kinetics Dominate Ignition at **Higher Temp.**

95% CO – 5% H₂

T= 1250 K

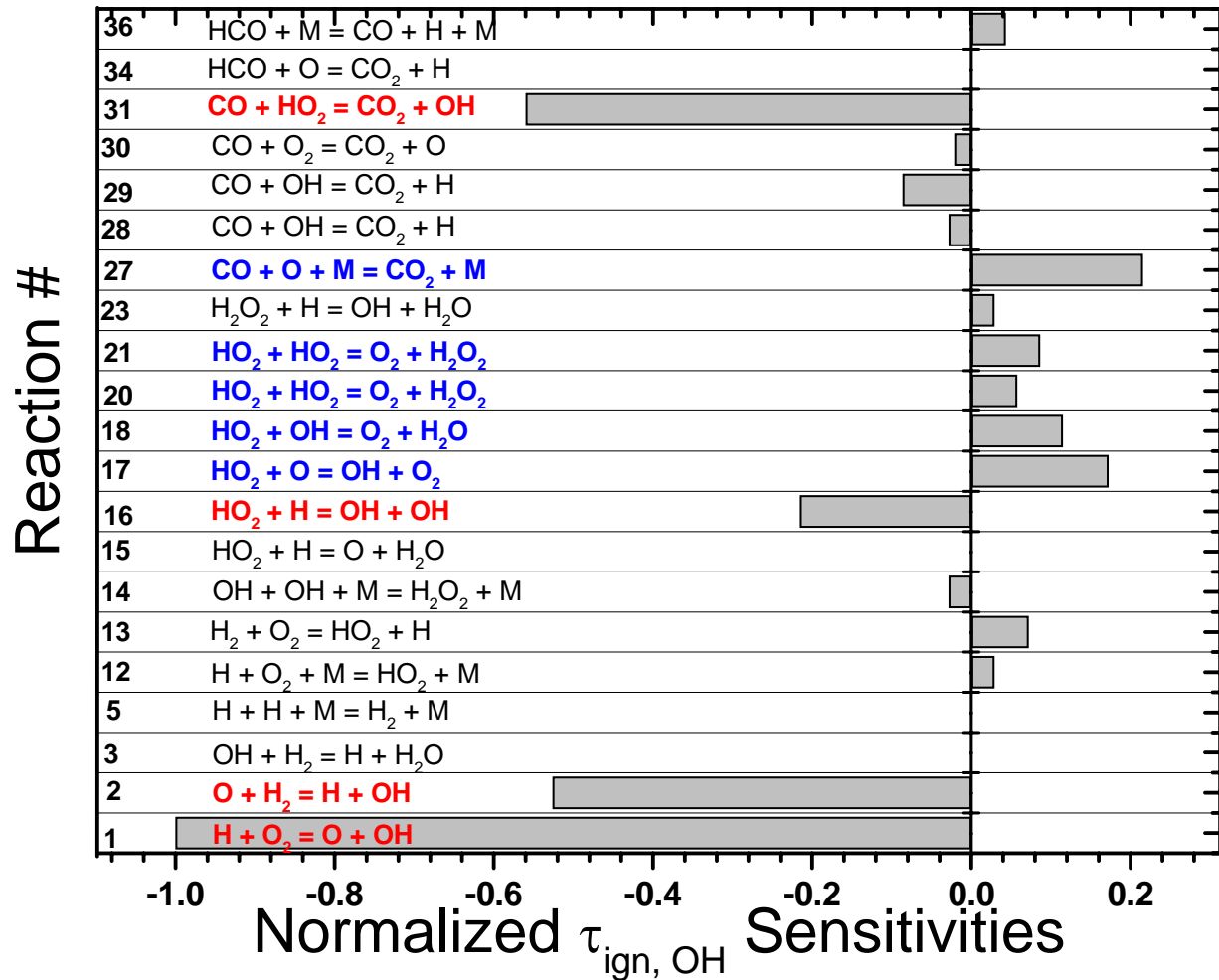


Task 2 – Ignition (CO/H₂)

Peroxide and CO Reactions Also Contribute at **Lower Temp.**

95% CO – 5% H₂

T= 900 K



Task 2 – Ignition (CH_4 /Other)

Several **CH_4 -Based Blends** Were Explored at Lean Conditions

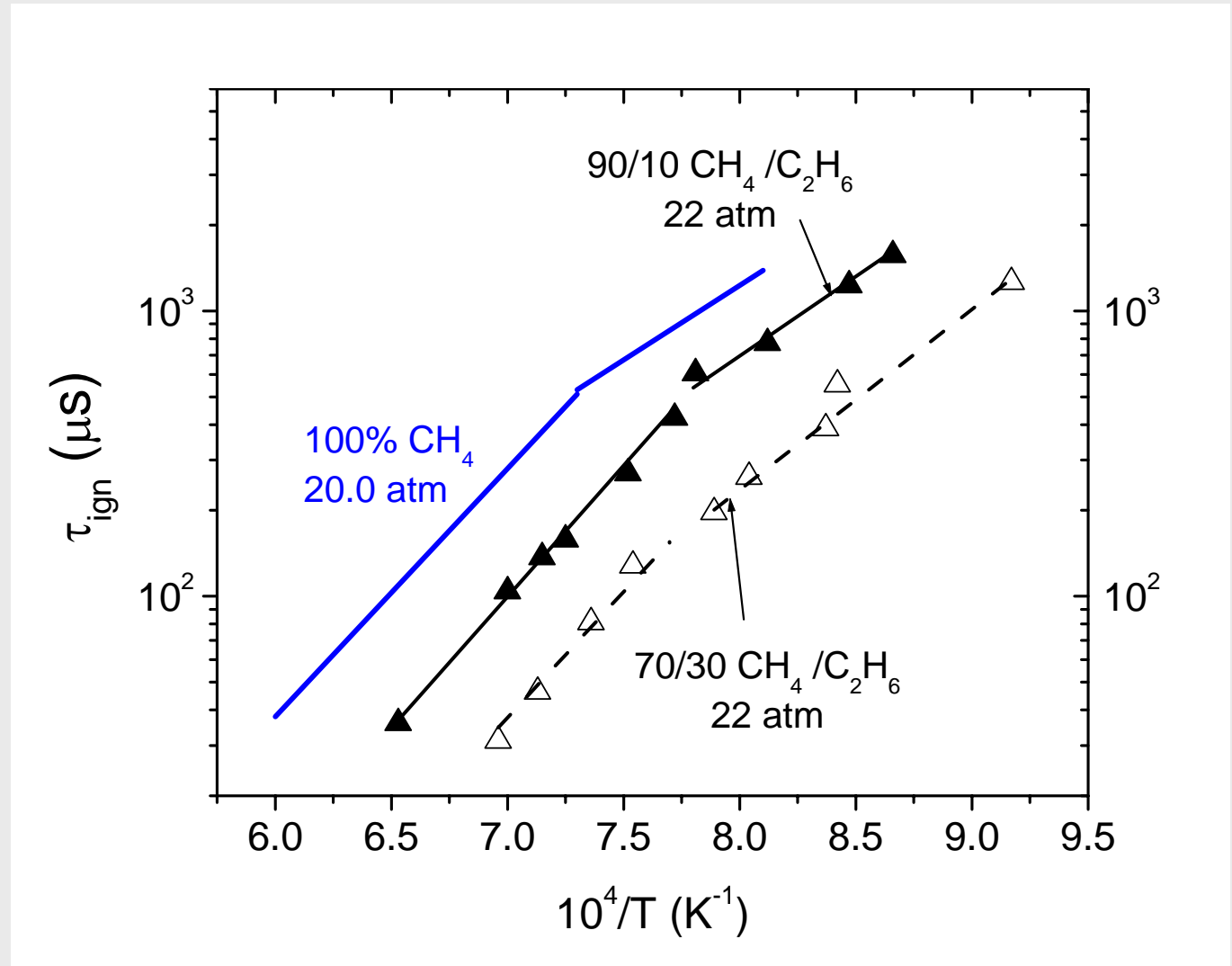
1. CH_4 /Other Binary Blends
 - H_2 (80/20, 60/40)
 - C_2H_6 (90/10, 70/30)
 - C_3H_8 (80/20, 60/40)
 - C_4H_{10} (90/10, 70/30)
 - C_5H_{12} (90/10, 70/30)
2. $T = 1100 - 1500 \text{ K}$
3. $P = 1 - 25 \text{ atm}$
4. Fuel-Lean: $\phi = 0.5$

Task 2 – Ignition (CH_4/Other)

All Blends **Accelerated Methane Ignition** over Range Studied

$\text{CH}_4 - \text{C}_2\text{H}_6$

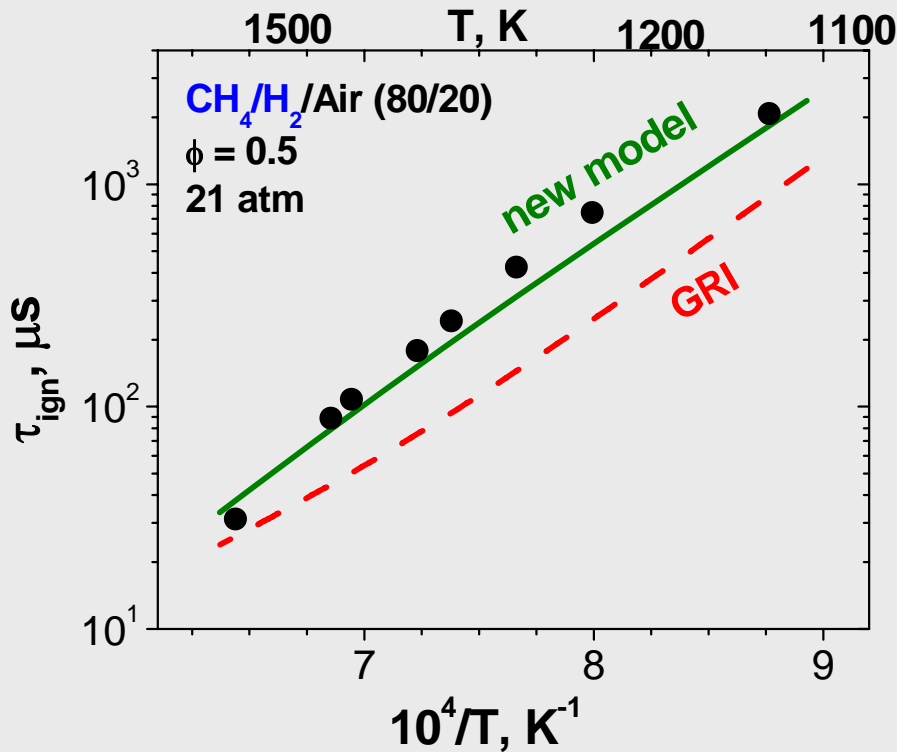
$\phi = 0.5$



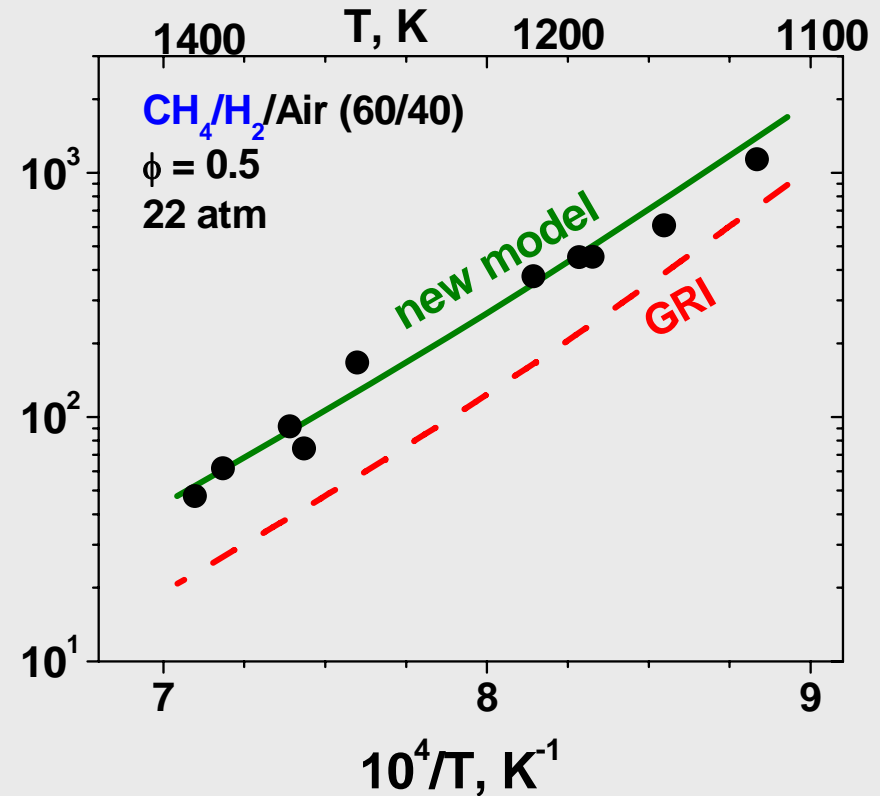
Task 2 – Ignition (CH_4/Other)

Improved Mechanism for CH_4+H_2 at Elevated P Developed

80/20



60/40



Task 2 – Autoignition

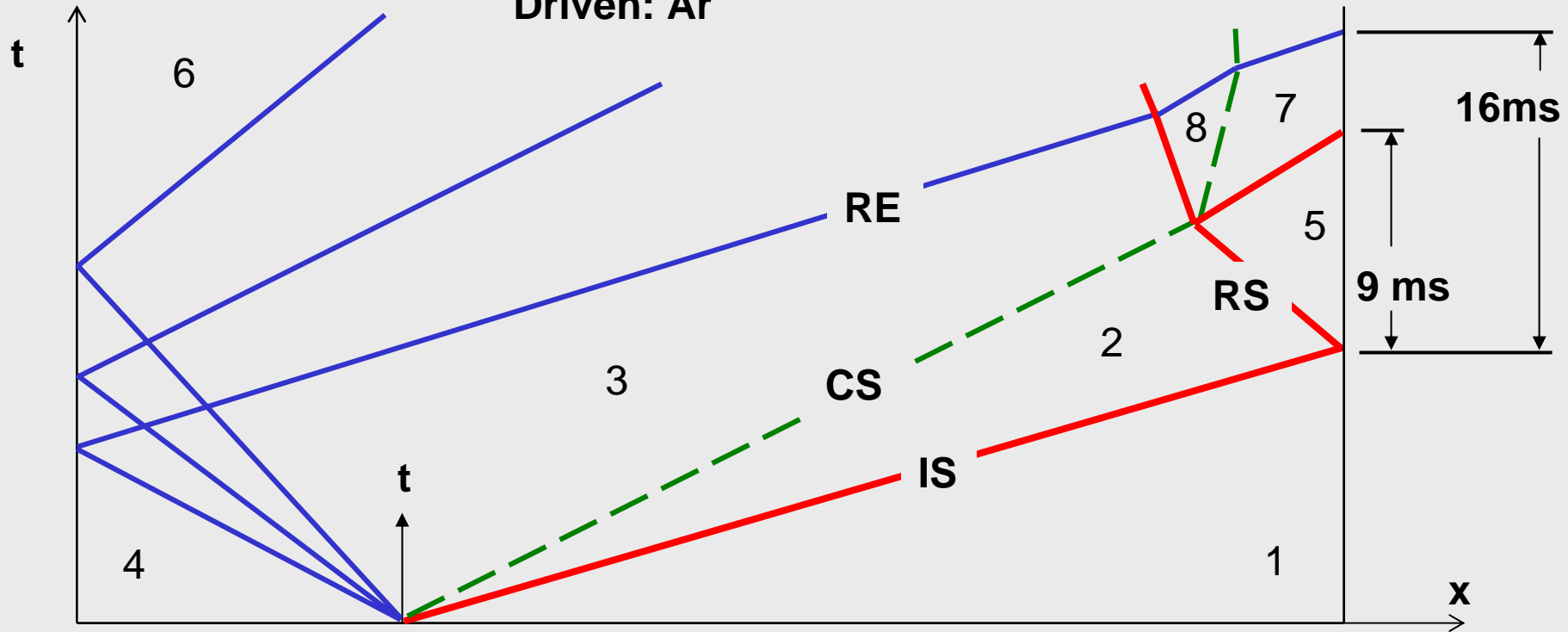
*A Separate Study was Conducted to Gauge **Autoignition Tendency** of a Wide Range of CH₄-HC Blends*

1. Fuel-Lean Mixtures: $\phi = 0.5$
2. T = **800 K** (Upper Limit of Burner Inlet)
3. P = **18 atm**
4. CH₄ + C₂H₆, C₃H₈, C₄H₁₀, C₅H₁₂, H₂
5. Will the Mixture Ignite within **10 ms**?

Task 2 – Autoignition

Model Predicts **16-ms Test Time** at 1000 K for He-C₃H₈ Driver

$T_5 = 1000 \text{ K}$
Driver: **55% He + 45% C₃H₈**
Driven: Ar



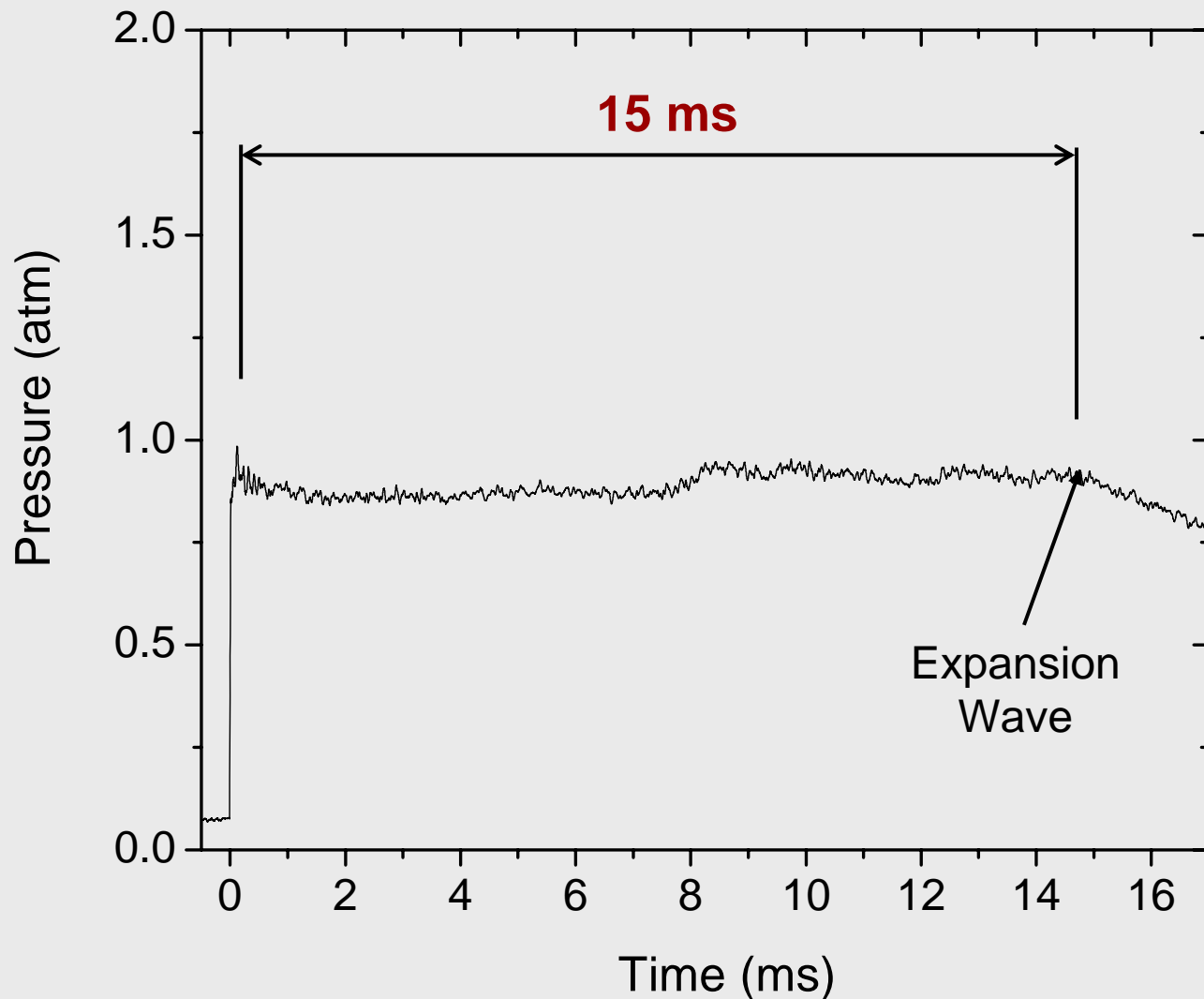
Task 2 – Autoignition

Experiments with **Extended Test Time Demonstrated**

$T_5 = 891 \text{ K}$
 $P_5 = 0.87 \text{ atm}$

Driver: **45% C_3H_8**
+ 55% He

Driven: Ar



Task 1 – Matrix Development

Experiment Parameter Space Constrained by GT Application

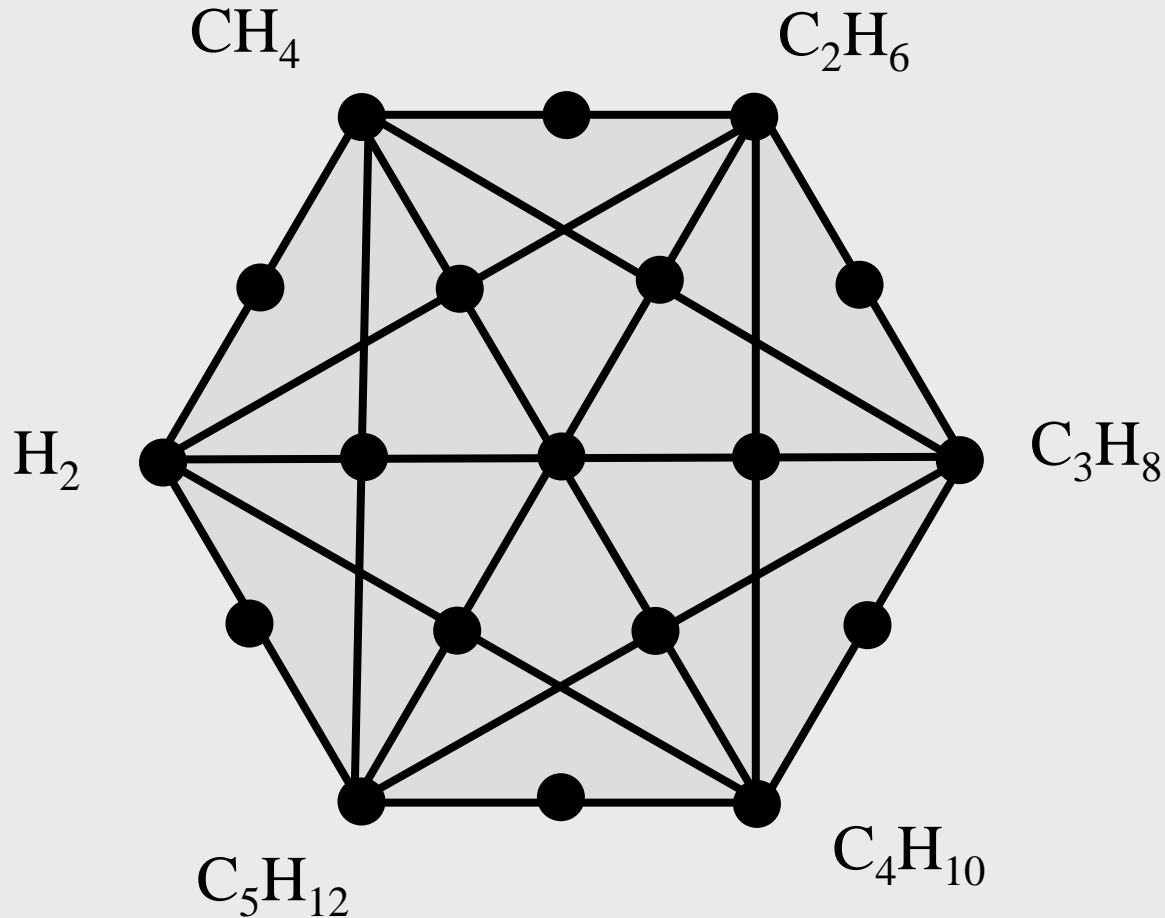
Fuel Blends:

- C_2H_6 0, 20, 40 %
- C_3H_8 0, 15, 30 %
- C_4H_x 0, 10, 20 %
- C_5H_x 0, 5, 10 %
- H_2 0, 10, 20 %
- Balance CH_4

5 factors, 3 levels
⇒ **243 blends!**

Task 1 – Matrix Development

*Statistical Mixture Theory Used To Develop **DOE Matrix***



Task 1 – Matrix Development

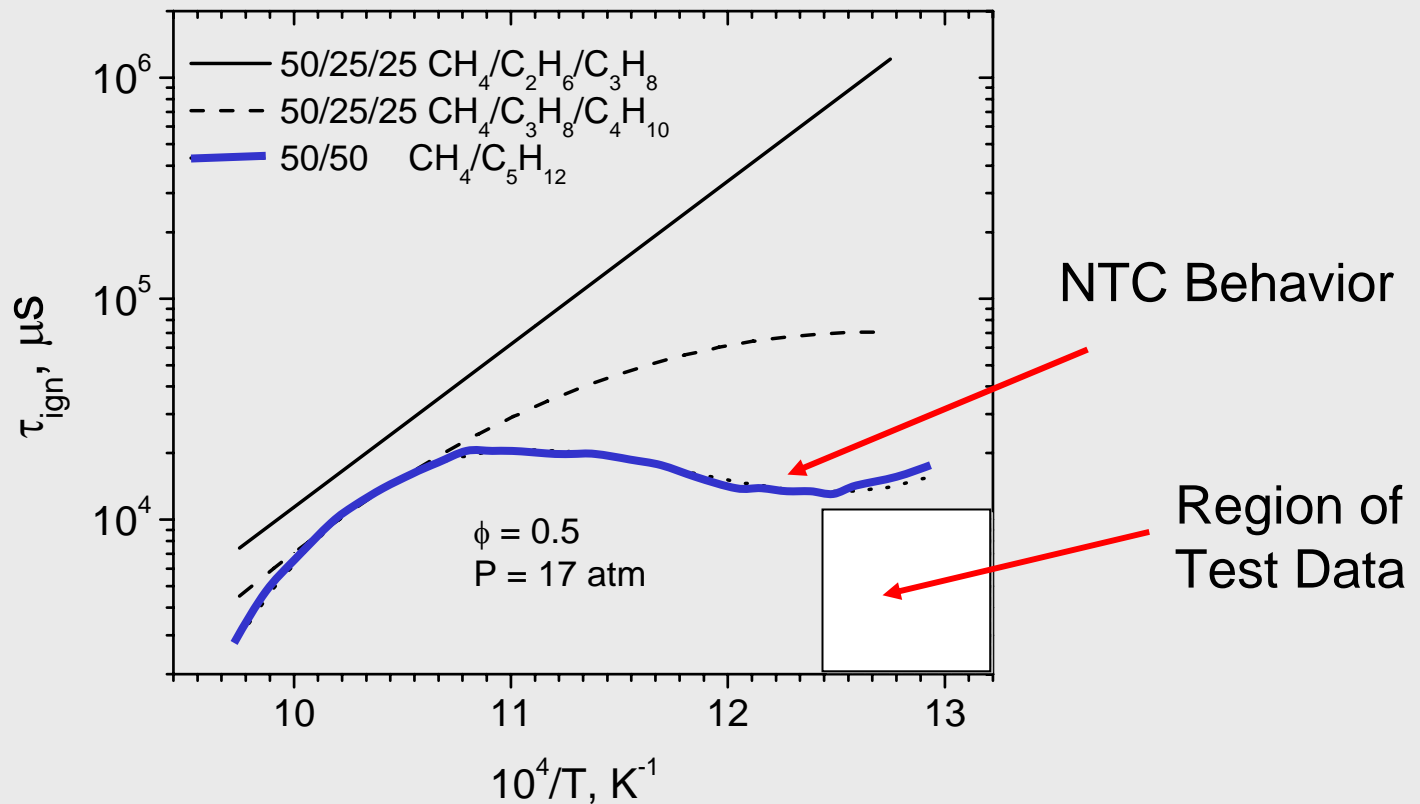
21-Test Matrix of Fuel Blends Designed for Autoignition Tests

mix #	X_{CH_4}	$X_{C_2H_6}$	$X_{C_3H_8}$	$X_{C_4H_{10}}$	$X_{C_5H_{12}}$	X_{H_2}
1	100	0	0	0	0	0
2	75	25	0	0	0	0
3	75	0	25	0	0	0
4	75	0	0	25	0	0
5	75	0	0	0	25	0
6	75	0	0	0	0	25
7	50	50	0	0	0	0
8	50	25	25	0	0	0
9	50	25	0	25	0	0
10	50	25	0	0	25	0
11	50	25	0	0	0	25
12	50	0	50	0	0	0
13	50	0	25	25	0	0
14	50	0	25	0	25	0
15	50	0	25	0	0	25
16	50	0	0	50	0	0
17	50	0	0	25	25	0
18	50	0	0	25	0	25
19	50	0	0	0	50	0
20	50	0	0	0	25	25
21	50	0	0	0	0	50

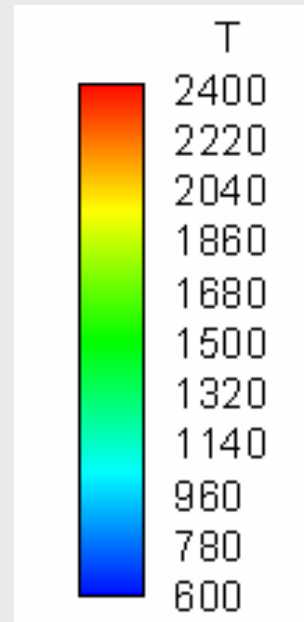
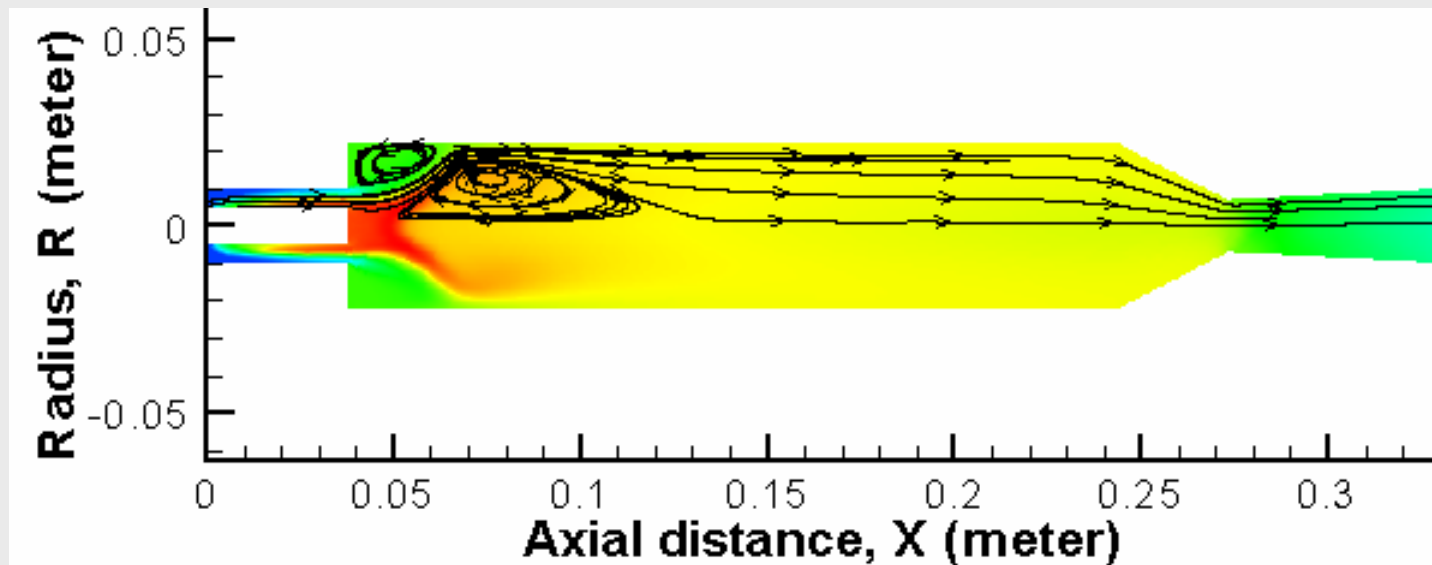
Task 2 – Autoignition

Data Seem to Exhibit **NTC Behavior** Seen in Higher HC

Calculated Results and Region of Test Results



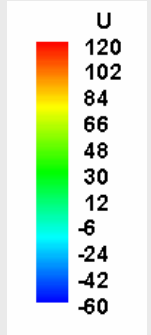
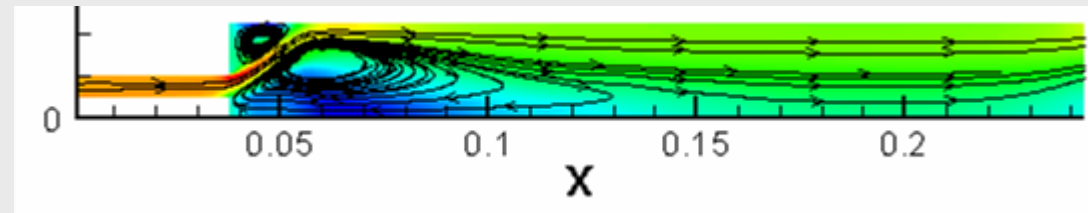
Penn State Burner Chosen as Model Geometry



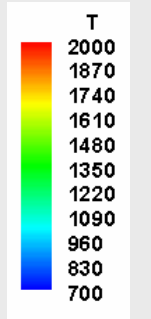
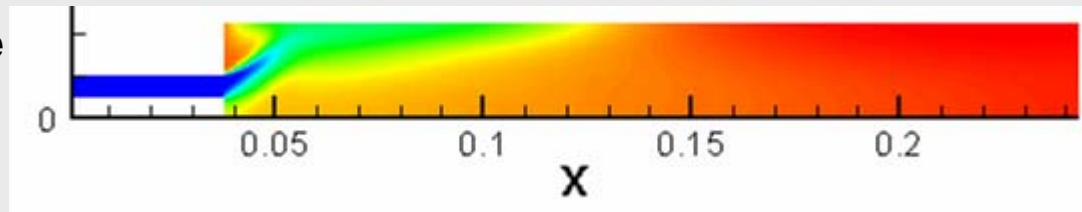
- **Lean Premixed, Swirl Stabilized**
- **Methane, $\phi = 0.6$**
- **Inlet: 0.46 MPa, 660 K**

Finite-Rate CH_4 Chemistry, $\phi = 0.6$

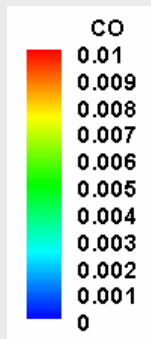
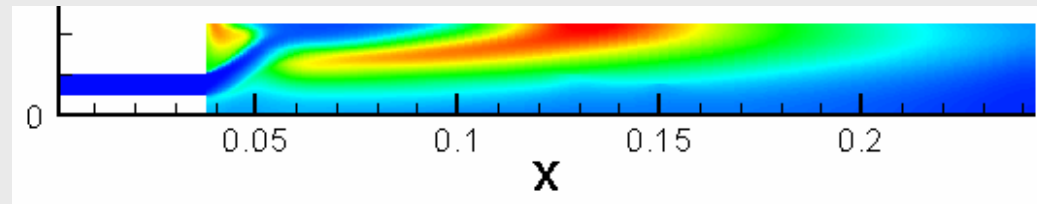
Axial velocity
w/ streamlines



Static temperature



CO mass fraction

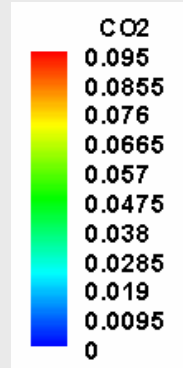
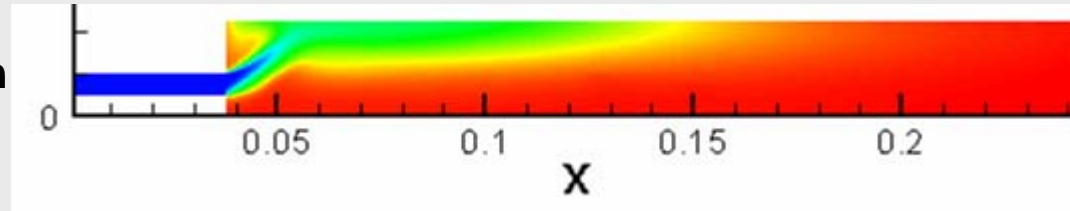


Task 5 – CFD Model

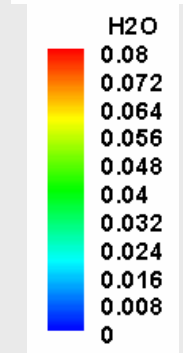
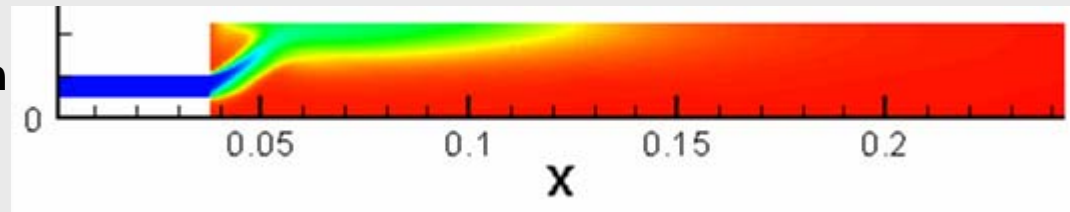
Flow Parametrics

Finite-Rate CH₄ Chemistry, $\phi = 0.6$

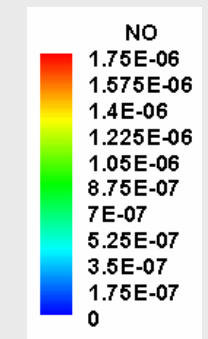
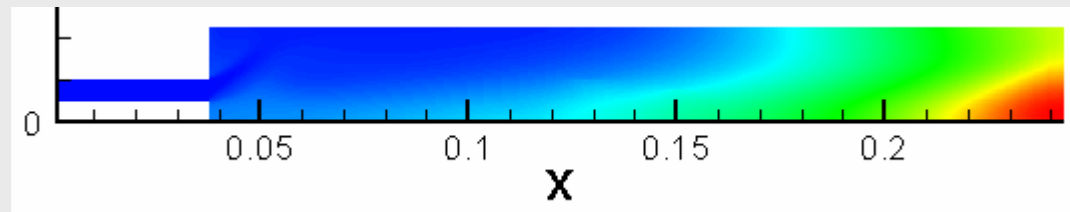
CO₂ mass fraction



H₂O mass fraction

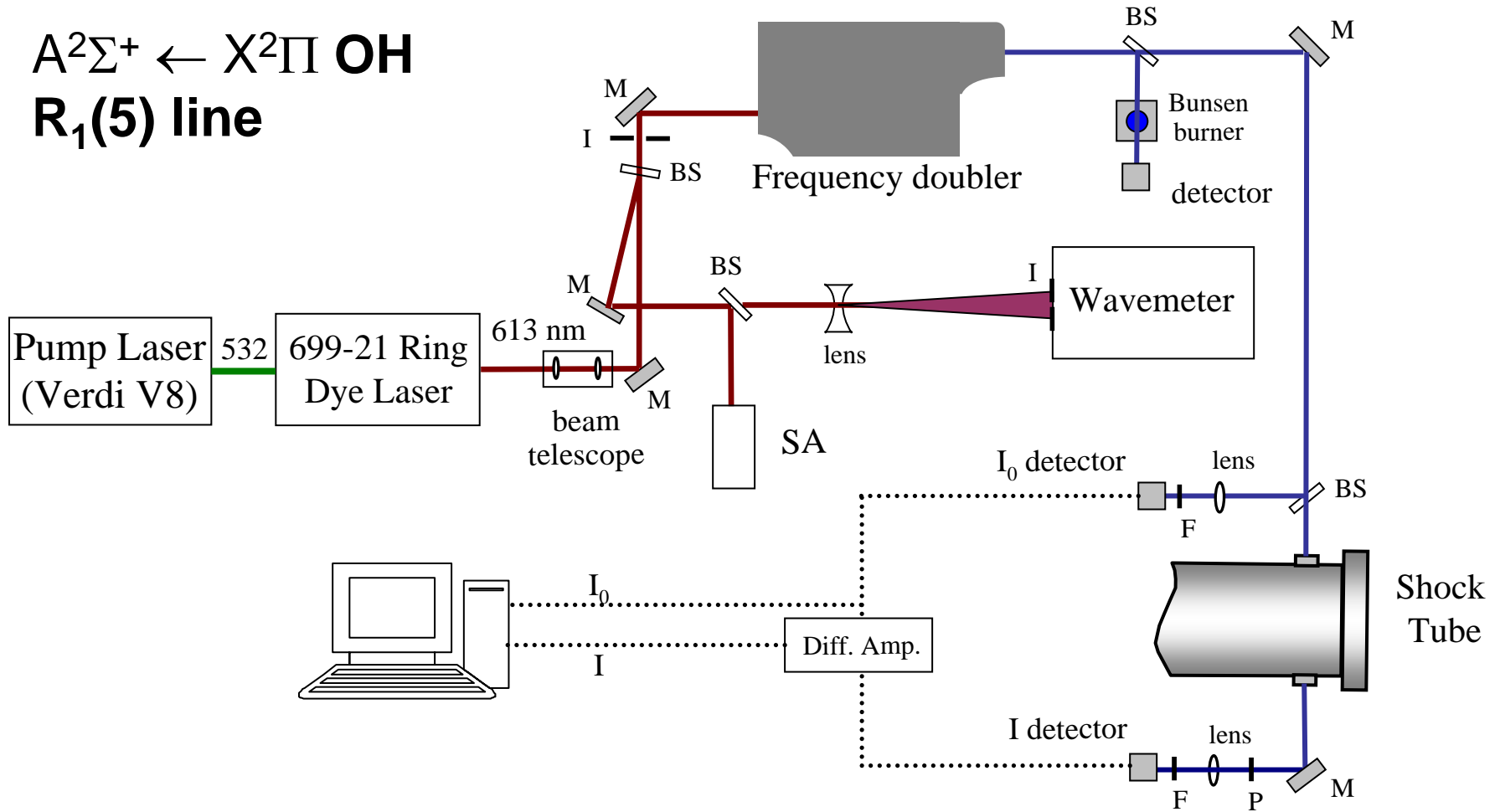
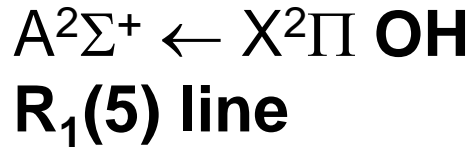


NO mass fraction



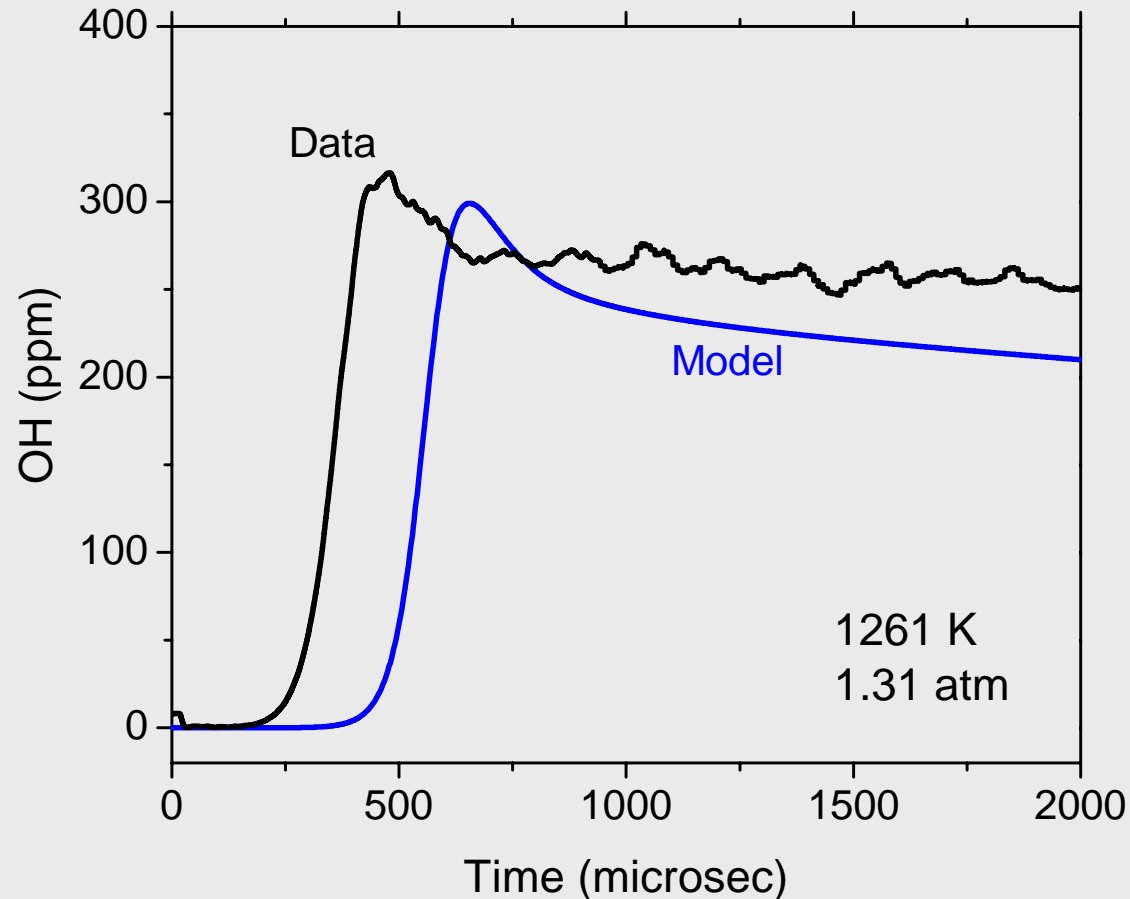
Task 7 – Mechanism Validation

OH Conc. Time Histories can be Obtained by **Laser Absorption**



Task 7 – Mechanism Validation

Comparison between Model and OH ppm for Dilute Mixtures

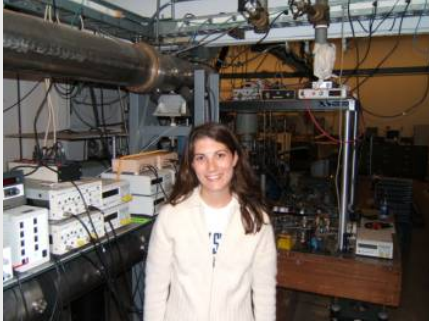


- 0.4% H₂ + 0.6% CO + 1% O₂
- 98.0% Ar
- R₁(5) line
- $V_C = 32617.46 \text{ cm}^{-1}$

Summary

1. Lean Syngas Ignition Times Obtained.
2. Lean Methane Fuel Blend Ignition Times Measured.
3. Kinetics Models for Syngas and CH₄ Identified.
4. Autoignition Matrix Completed.
5. CFD Model and Geometry Established.
6. Mechanism Validation Tests Underway.

Questions?



Danielle Kalitan



Joel Hall



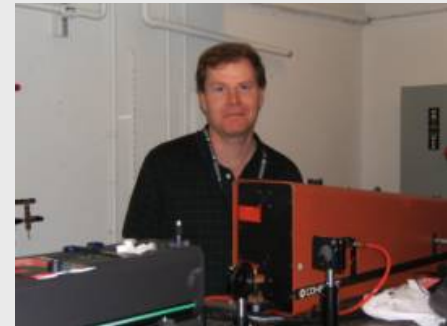
Jaap de Vries



Tony Amadio



Stefanie Simmons



Dr. Mark Crofton (Aerospace)