High-Pressure Turbulent Flame Speeds and Chemical Kinetics of Syngas Blends With and Without Impurities

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Project Overview

3-Year Project Began in October, 2013

Project Highlights:

1. Duration: **Oct. 1, 2013 – Sept. 30, 2016**
2. DOE NETL Award **DE-FE0011778**
3. Budget: $498,382 DOE + $124,595 Cost Share
4. Principal Investigator: Dr. Eric L. Petersen

Project Overview

This Project Addresses Several Problems for HHC Fuels

1. Improve **NOx kinetics** for High-Hydrogen Fuels at Engine Conditions

2. Effect of **Contaminant Species** on Ignition and Flame Speed

3. Impact of **Diluents** on Ignition Kinetics and Flame Speeds

4. Data on **Turbulent Flame Speeds** at Engine Pressures

Project Overview

There are Five Main Work Tasks for the Project

Work Tasks:

Task 1 – Project Management and Program Planning

Task 2 – Turbulent Flame Speed Measurements at Atmospheric Pressure

Task 3 – Experiments and Kinetics of Syngas Blends with Impurities

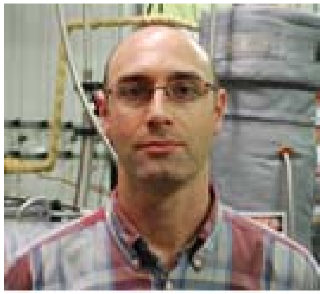
Task 4 – Design and Construction of a High-Pressure Turbulent Flame Speed Facility

Task 5 – High-Pressure Turbulent Flame Speed Measurements

Project Overview

TAMU Work is a Team Effort of Several People

Dr. Olivier Mathieu



Charles Keesee

Anibal Morones

Clayton Mulvihill

Dr. Sankar Ravi

Josh Hargis

Task 2 – Turbulent Flame Speed Measurements at Atmospheric Pressure

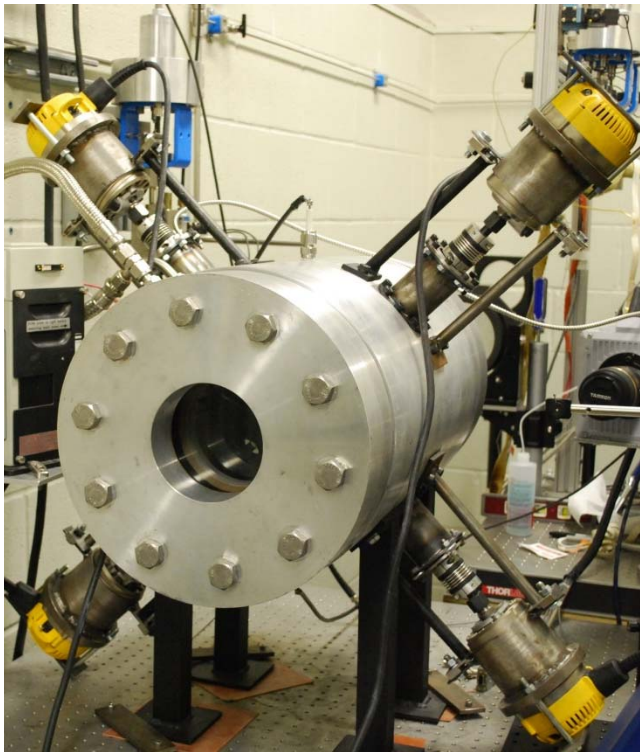
Task 2 – Turbulent Speeds

1-atm Turbulent Flame Speed Measurement will Build Upon Tests Done in Previous UTSR Project

- Utilize Existing Turbulent Flame Speed Hardware
- Extend Test Conditions to a Range of u' and Length Scale Values
- Design Test Matrices for Syngas Blends
- Perform Experiments for Syngas Blends at 1 atm Conditions

Task 2 – Turbulent Speeds

Existing Rig Characterized for One Main Condition



Features:

- 7075-T6 Heat-Treated Aluminum
- 4 radial impellers
- Diameter: 30.5 cm
- Length: 35.6 cm
- Window Port Diameter: 12.7 cm
- Maximum initial pressure: 1 atm
- Maximum initial temperature: 298 K

Turbulence:

- Intensity: **1.5 m/s rms**
- Integral length scale: **27 mm**

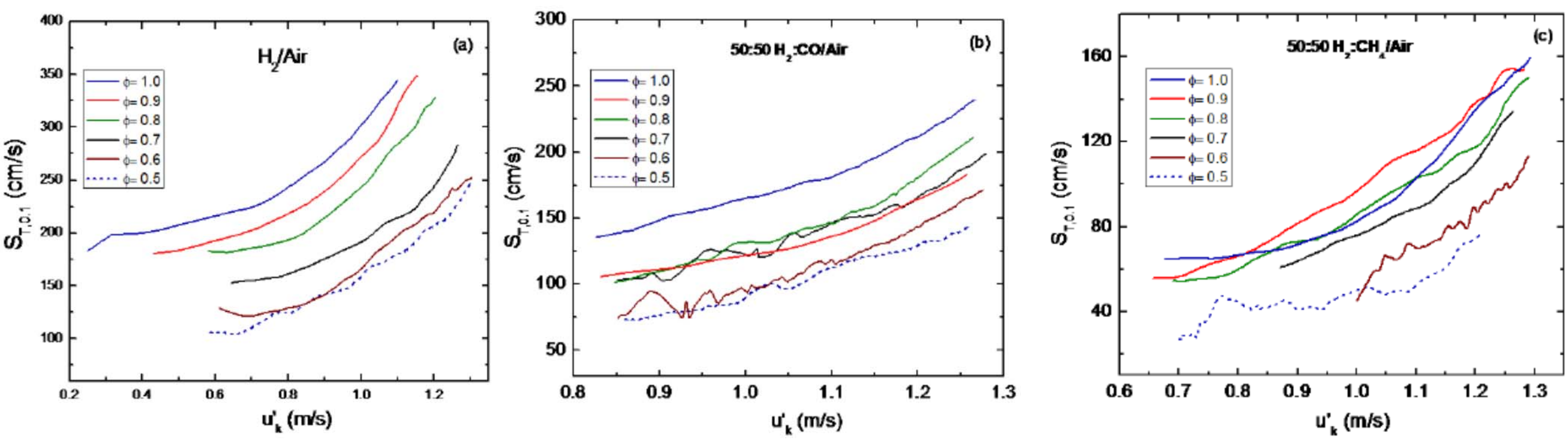
Task 2 – Turbulent Speeds

Recent Experiments Include Effect of Hydrocarbons on H_2-Based Mixtures

- Mixtures Studied: 100% H_2
  Syngas (50:50 H_2/CO)
  50:50 H_2/CH_4

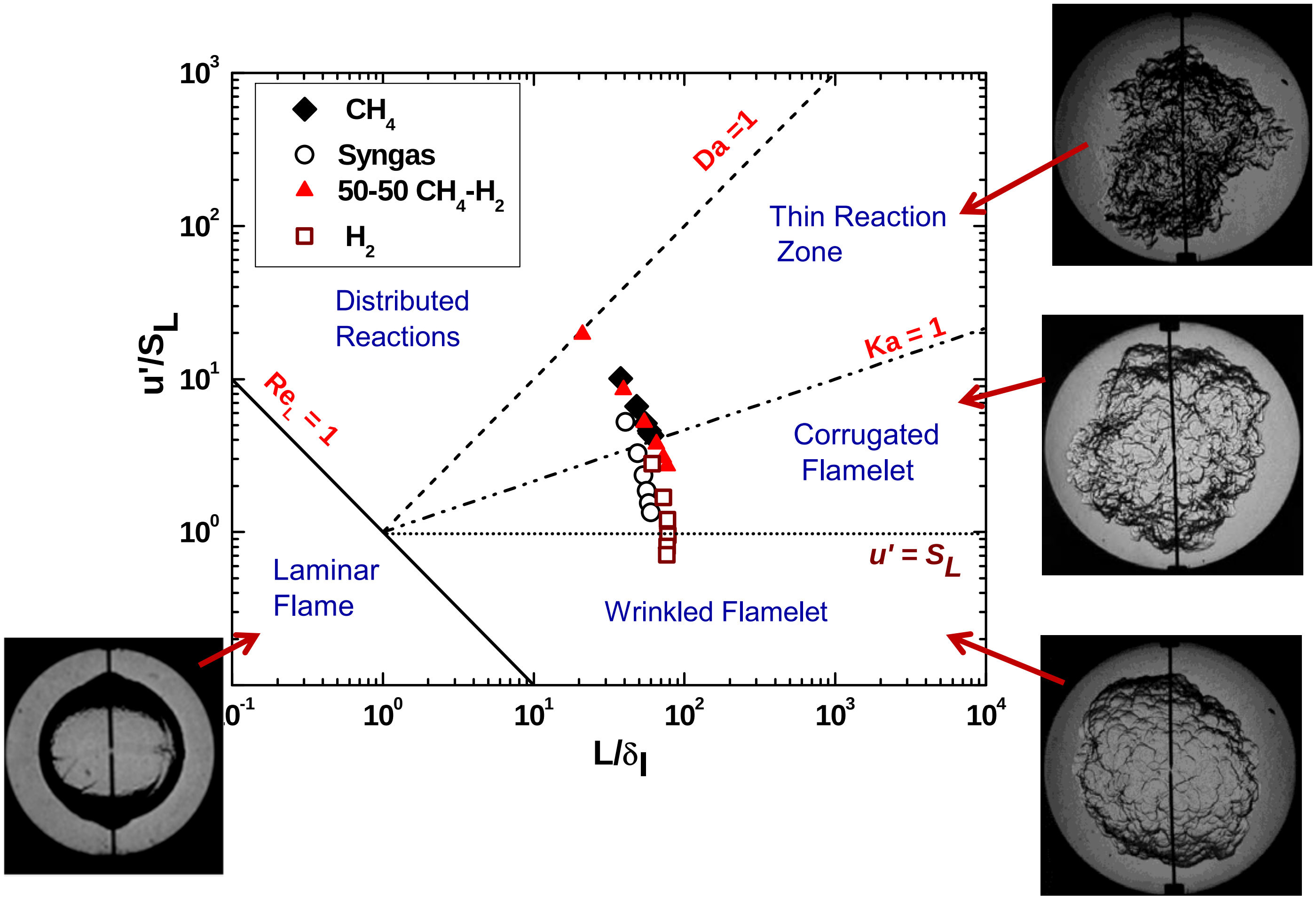
- 3 repeats per condition, typically

Global Displacement Speeds for Various ϕ



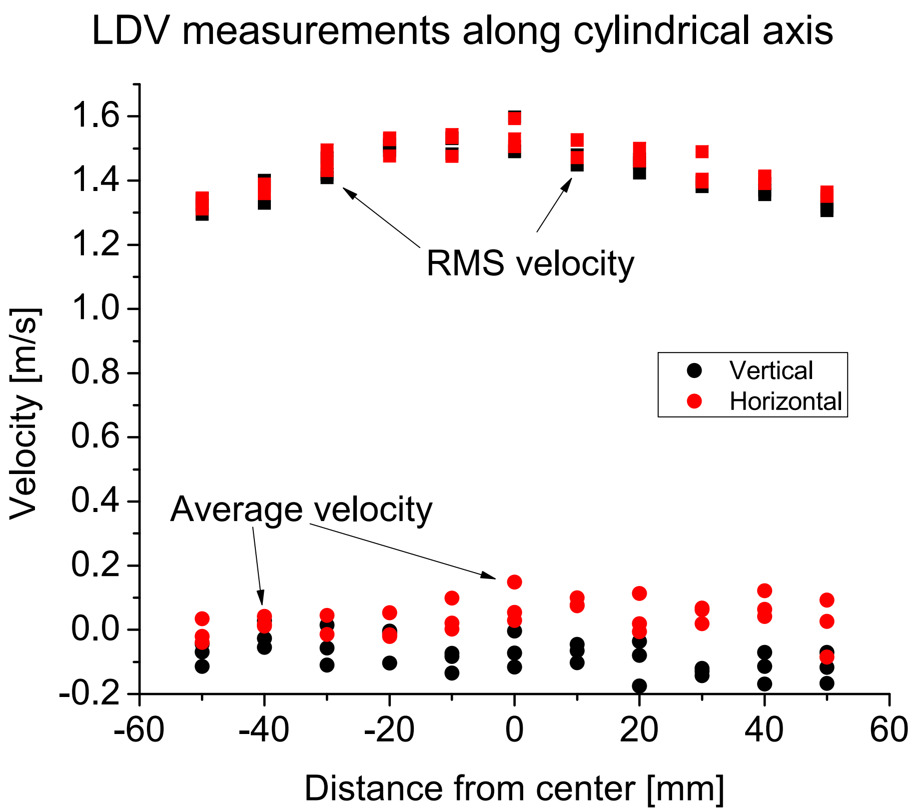
Task 2 – Turbulent Speeds

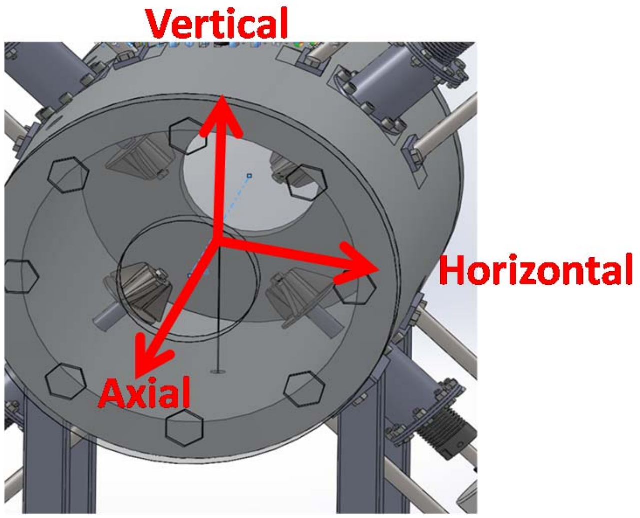
Recent Data Cover a Wide Range of Flamelet Regions

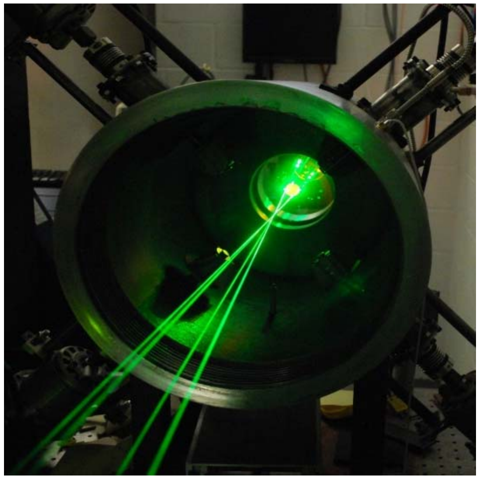


Task 2 – Turbulent Speeds

*Extensive Turbulence Field Characterization Underway Using **LDV System***







Task 3 – Experiments and Kinetics of Syngas Blends with Impurities

Task 3 – Impurity Effects

Overall Task Has 2 Main Goals

1. Study Impurity Composition Effect
   - Ignition delay time (τ_{ign}) measurements in a shock tube
   - Laminar flame speed measurements
   - Large range of P, T

2. Kinetics Modeling of Impurities

Task 3 – Impurity Effects

*Update Today Will Focus on **2 Main Projects***

1. Impurity Effect on Ignition {NH_3, H_2S, H_2O, CO_2, CH_4} for Coal Syngas

2. Hydrocarbon Effect on Laminar Flame Speeds

Mixture

Mixture derived from averaging 40 real coal syngas

- **Baseline (BS):** (60 CO / 40 H_2)/O_2 (Krecji, Petersen et al., 2013)

- **Baseline + others**
  - (98.47%)**BS** + (1.53%)$\mathbf{CH_4}$
  - (91.35%)**BS** + (8.65%)$\mathbf{CO_2}$
  - (99.50%)**BS** + (0.50%) $\mathbf{H_2S}$

- **Full Coal Syngas :** (60 CO / 40 H_2) + CH_4+ CO_2 + H_2O
  - (28.76%)$\mathbf{H_2}$+(39.73%)**CO**+(1.50%)$\mathbf{CH_4}$+(9.00%)$\mathbf{CO_2}$+(21.00%)$\mathbf{H_2O}$

- **Full Coal Syngas + impurities** ELP2
  - (97.87%)**Full Coal Syngas**+(1.70%)$\mathbf{NH_3}$ +(0.43%)$\mathbf{H_2S}$

Slide 15

ELP2 there is too much information on this one slide. It will be more effective to break it up into two slides, one on the mixture and one on the experimental conditions.

In fact, the mixture slide should be after the "Objectives" slide, before the shock tube details section.
Eric Petersen, 3/6/2014

Test Conditions

Investigated in dilute conditions at three pressures

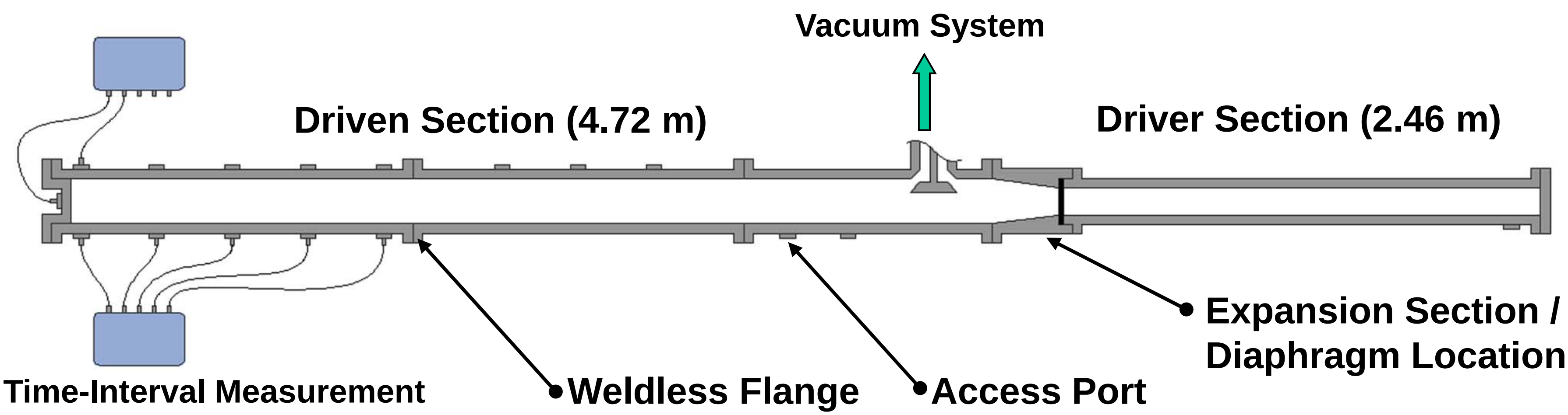
- Diluted conditions: **98 - 97.975% Ar**
- Equivalence ratio: **0.5**
- Pressure: **1.7, 13, and 32 atm**

Shock-Tube Apparatus

High pressure shock-tube facility at Texas A&M

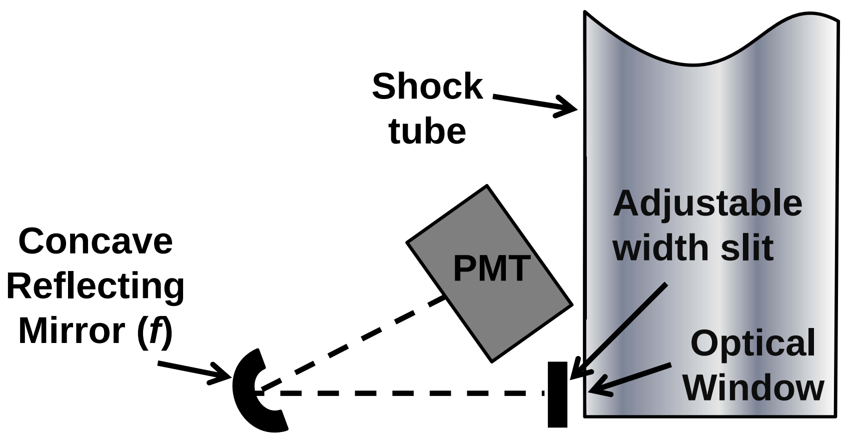
High-Pressure Shock-Tube Facility

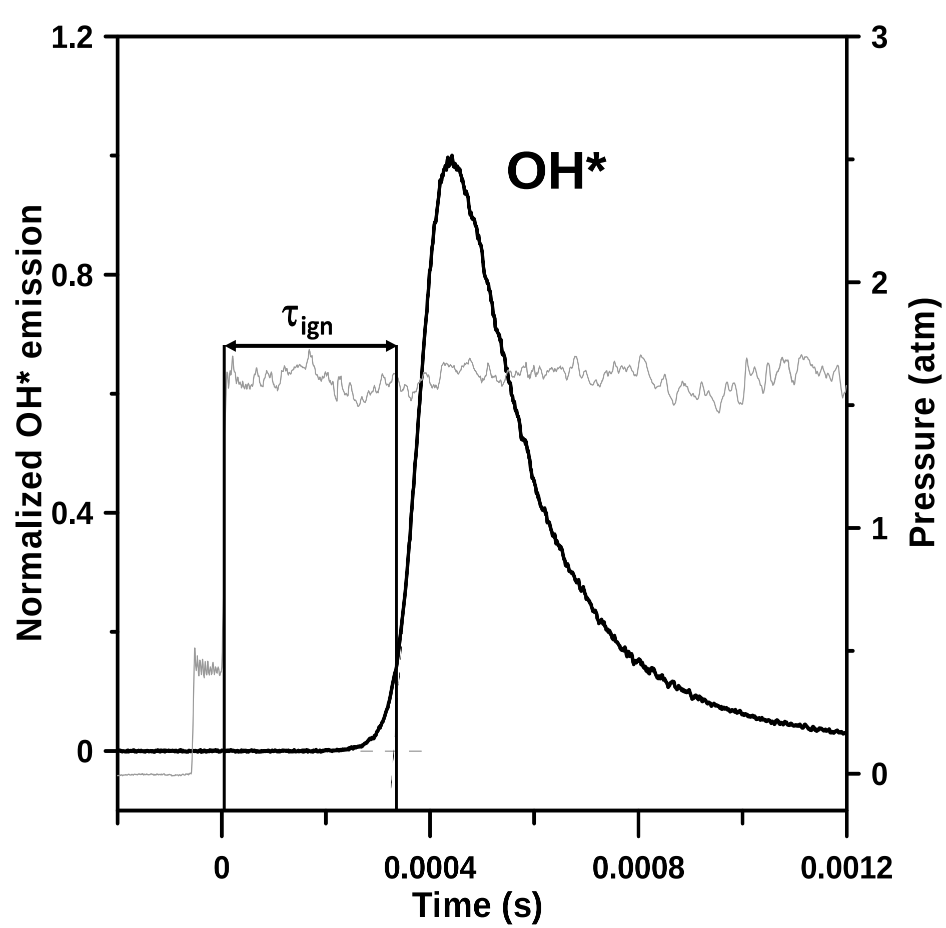
- 1 – 100 atm Capability
- 600 – 4000 K Test Temperature
- Up to 20 ms Test Time
- 2.46 m Driver and 4.72 m Driven
- 15.24 cm Driven Inner Diameter



Measurement

Ignition Delay Time Obtained from OH Time History*



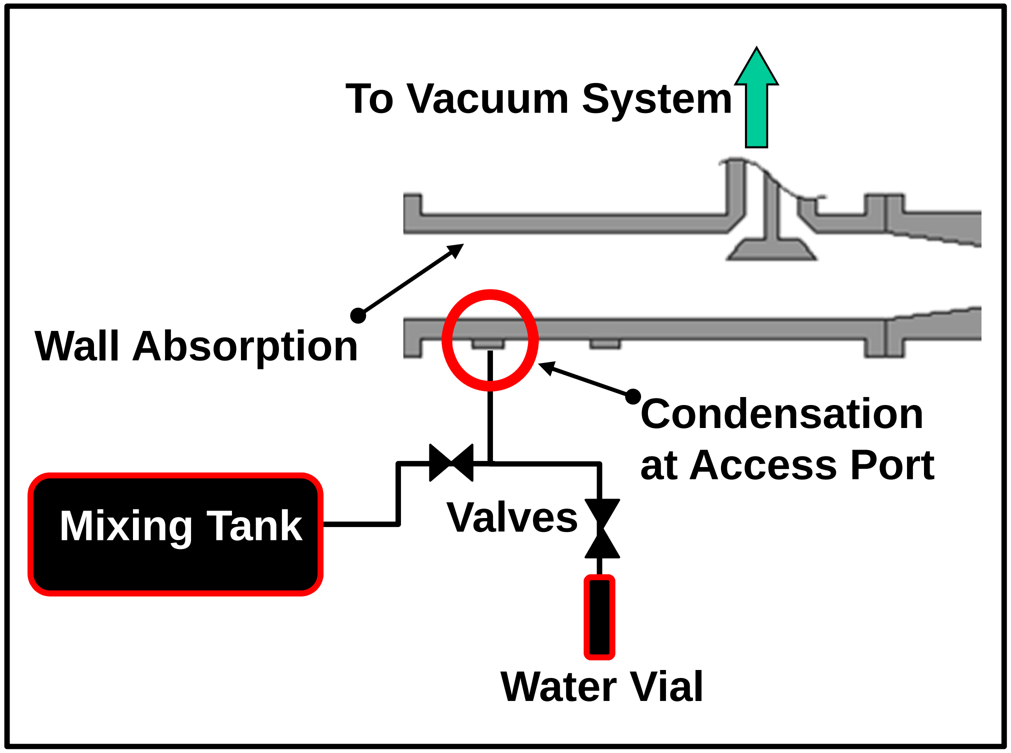


- $A^2 \Sigma^+$ (OH*) light at 307 nm
- Highly Diluted Mixtures (98% Ar)

Condensation Problem

Water can condense and change mixture composition

- Condensation of H_2O during filling process
- Absorption onto shock tube walls
- Uncertainties in H_2O concentration in tank mixture

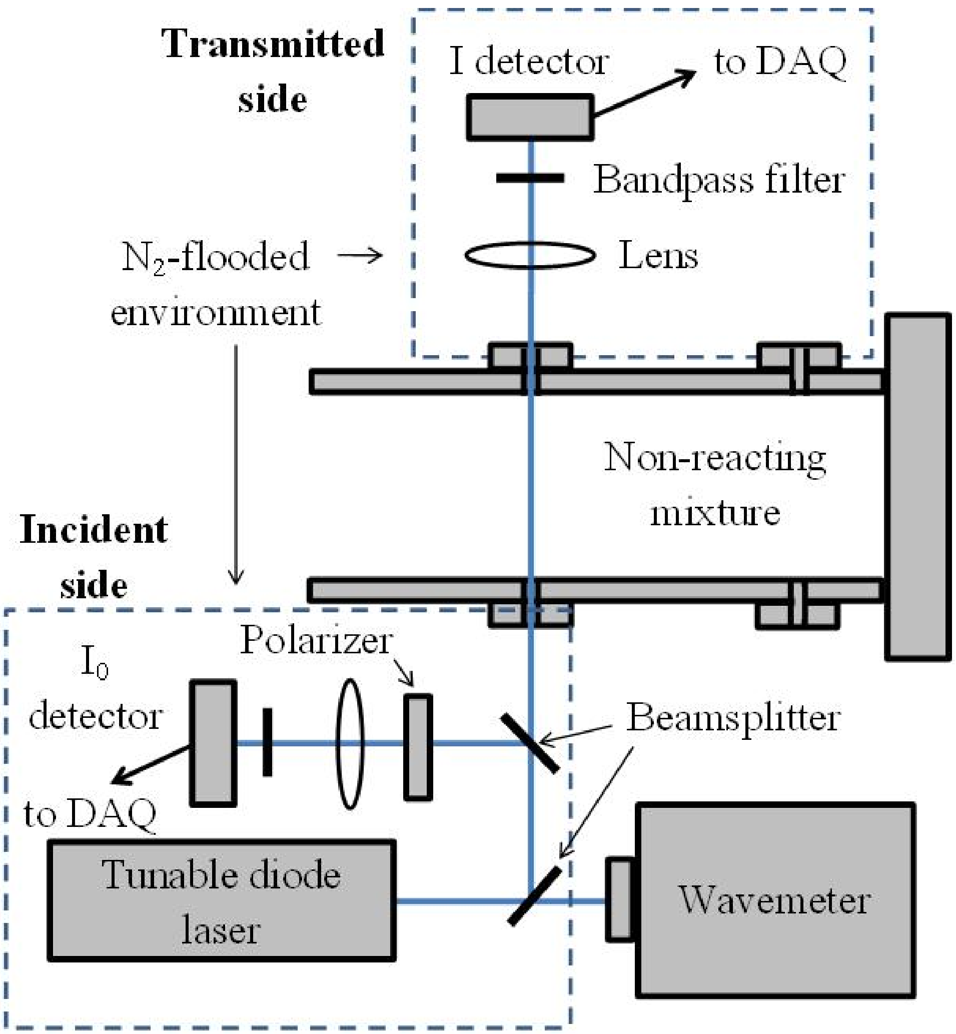


Full Coal Syngas Fuel Mixture:

(28.76%)$\mathbf{H_2}$+(39.73%)**CO**+
(1.50%)$\mathbf{CH_4}$+(9.00%)$\mathbf{CO_2}$+
(21.00%)$\mathbf{H_2O}$

Measurement

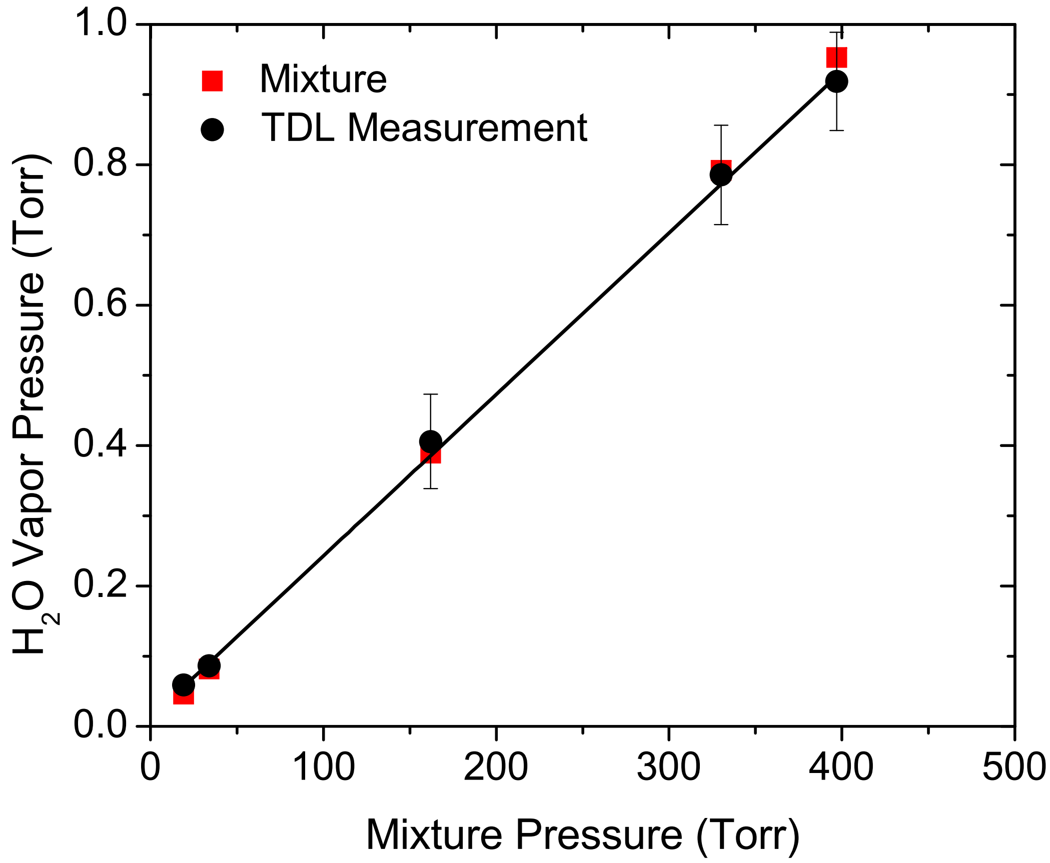
Water concentration measured by laser light absorption



- ν1+ν3 transition band absorption
- Near 1387.877 nm
- Highly Diluted Mixtures (98% Ar)

Measurement

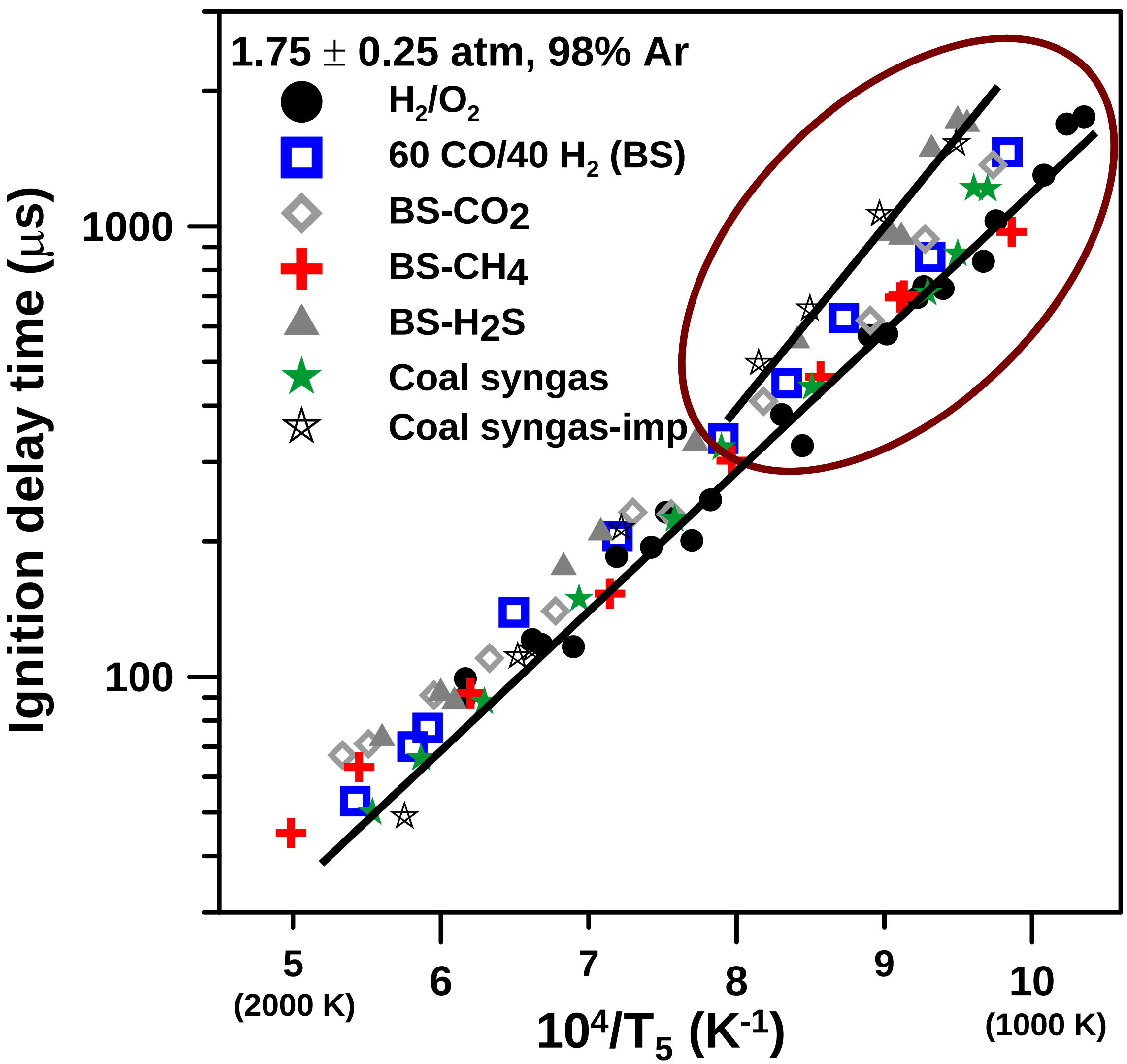
Water concentration measured by laser light absorption



Measured concentration within 5% of target value

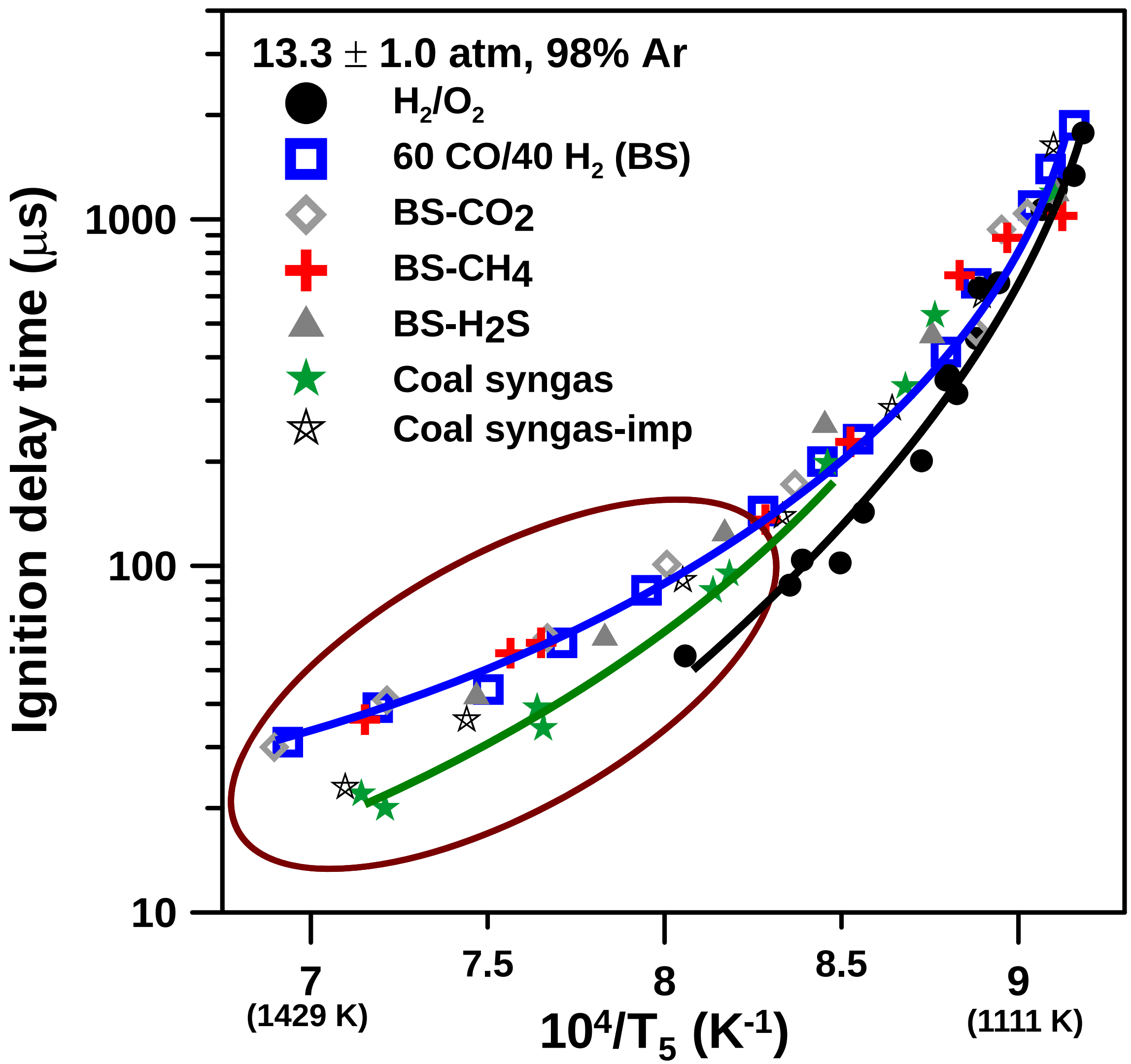
Results – 1.7 atm

Only ***H_2S*** *addition has a noticeable effect at low temperatures*



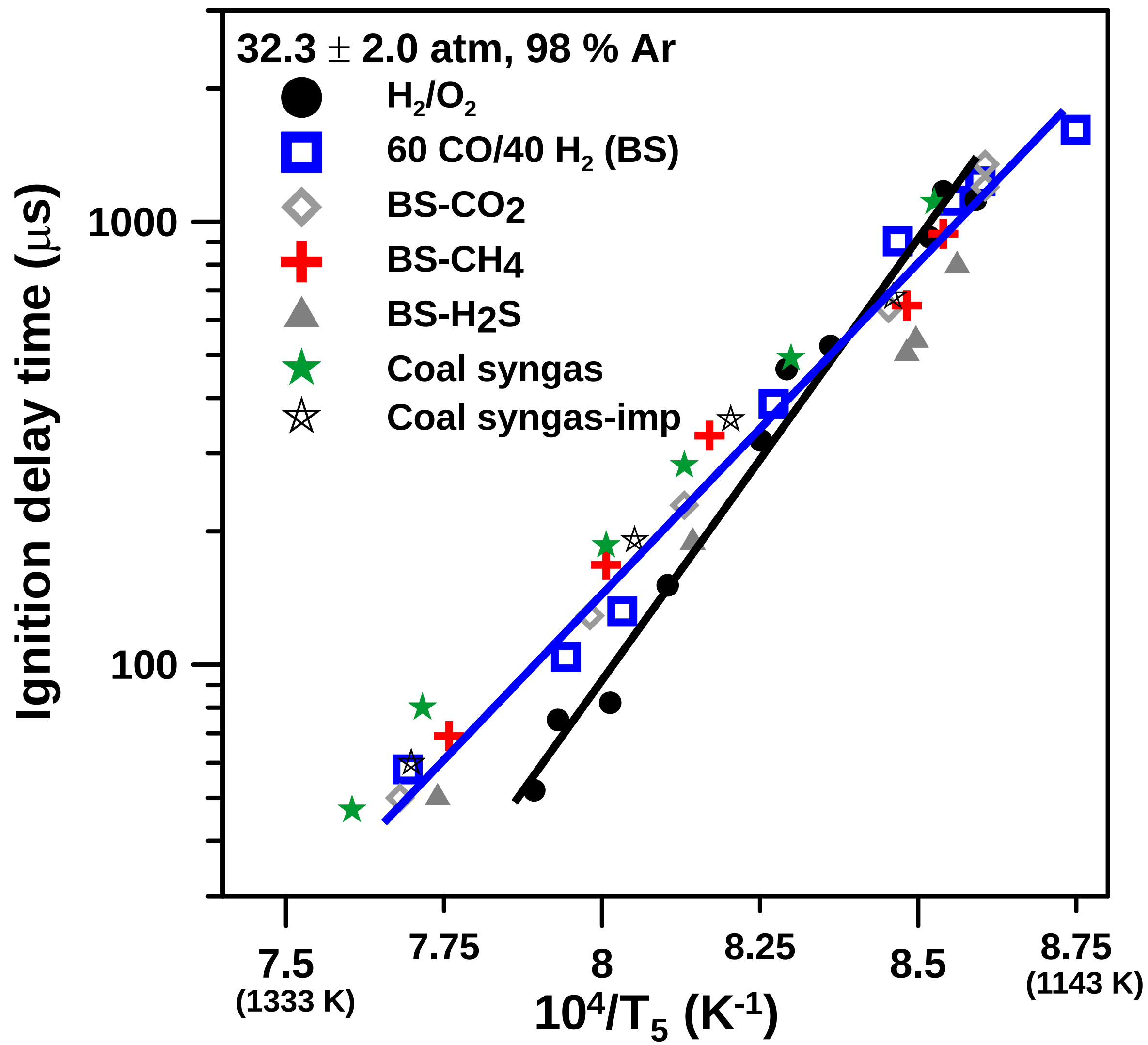
Results – 13 atm

τ_{ign} shorter for the full mixture at high temperatures



Results – 32 atm

All mixtures have similar behavior at 32 atm



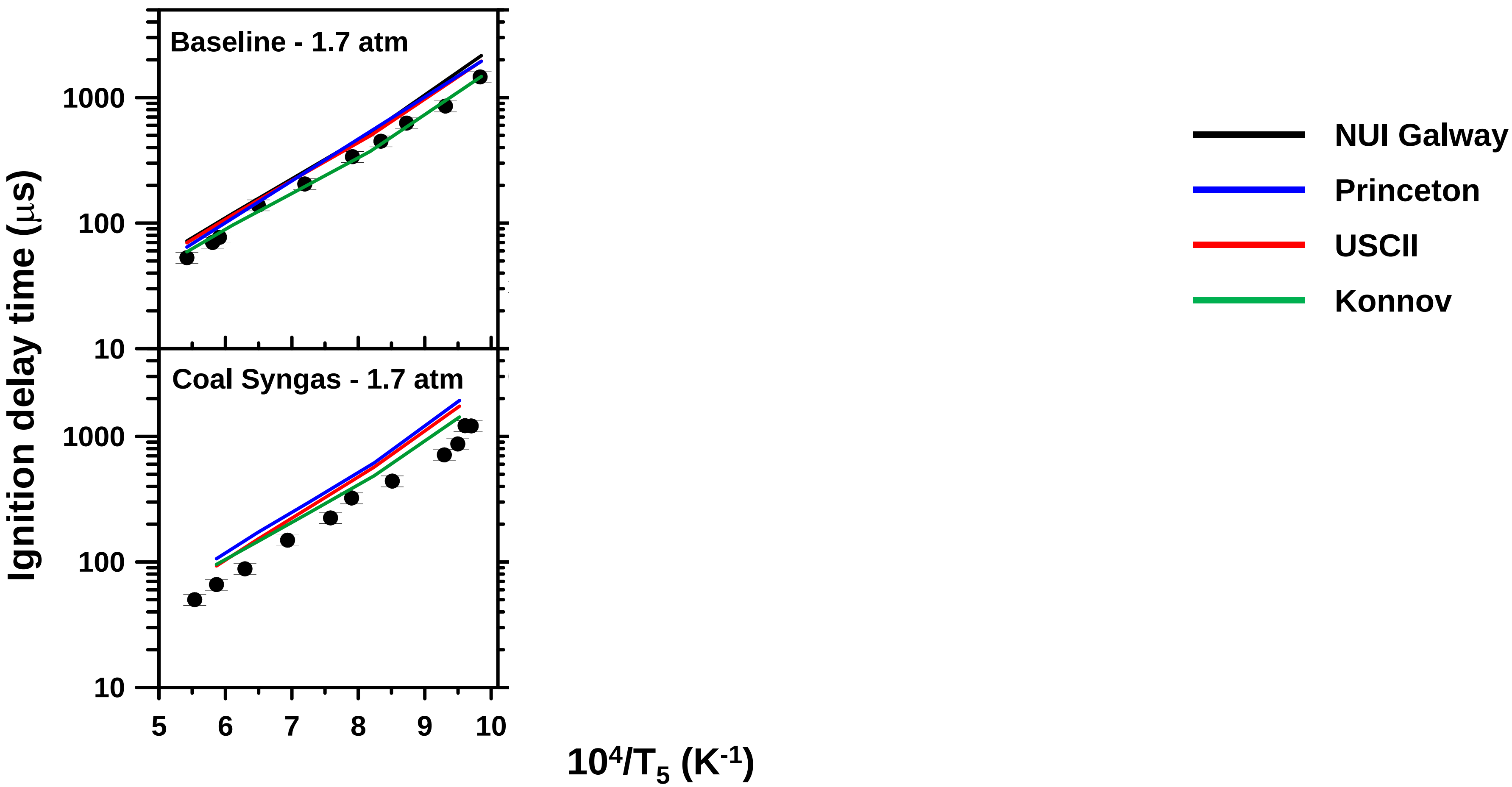
Model

Comparison of the data with literature mechanisms

- C0-C4 from Wang et al., 2007 (**USCII**)
- C0-C1 from Li et al., 2007 (**Princeton**)
- Small HC mechanisms from **Konnov**, 2009
- C0-C3 from Metcalfe et al., 2013 (**NUI Galway**)
- Addition of the OH* sub-mechanism from Hall and Petersen, 2006 (if needed)

Model - Results

NUIG and PRCT Models Agree Best with Data at Higher Pressures



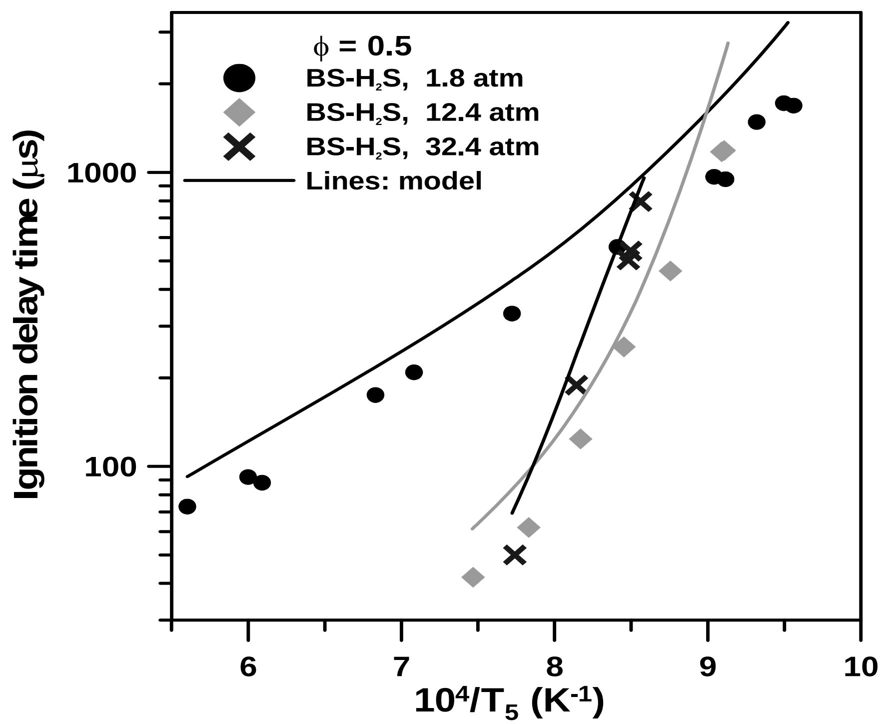
Disagreement at 13 atm and high temp. for the Coal syngas

Model - Results

Mixtures with H_2S Impurity Were Also Modeled

- CO/H_2 Chemistry from Metcalfe, Curran et al. (2013)
- H_2S Chemistry from Mathieu, Petersen et al. (2014)
- OCS from Glarborg and Marshall (2013)

BS CO/H_2 mixture with H_2S



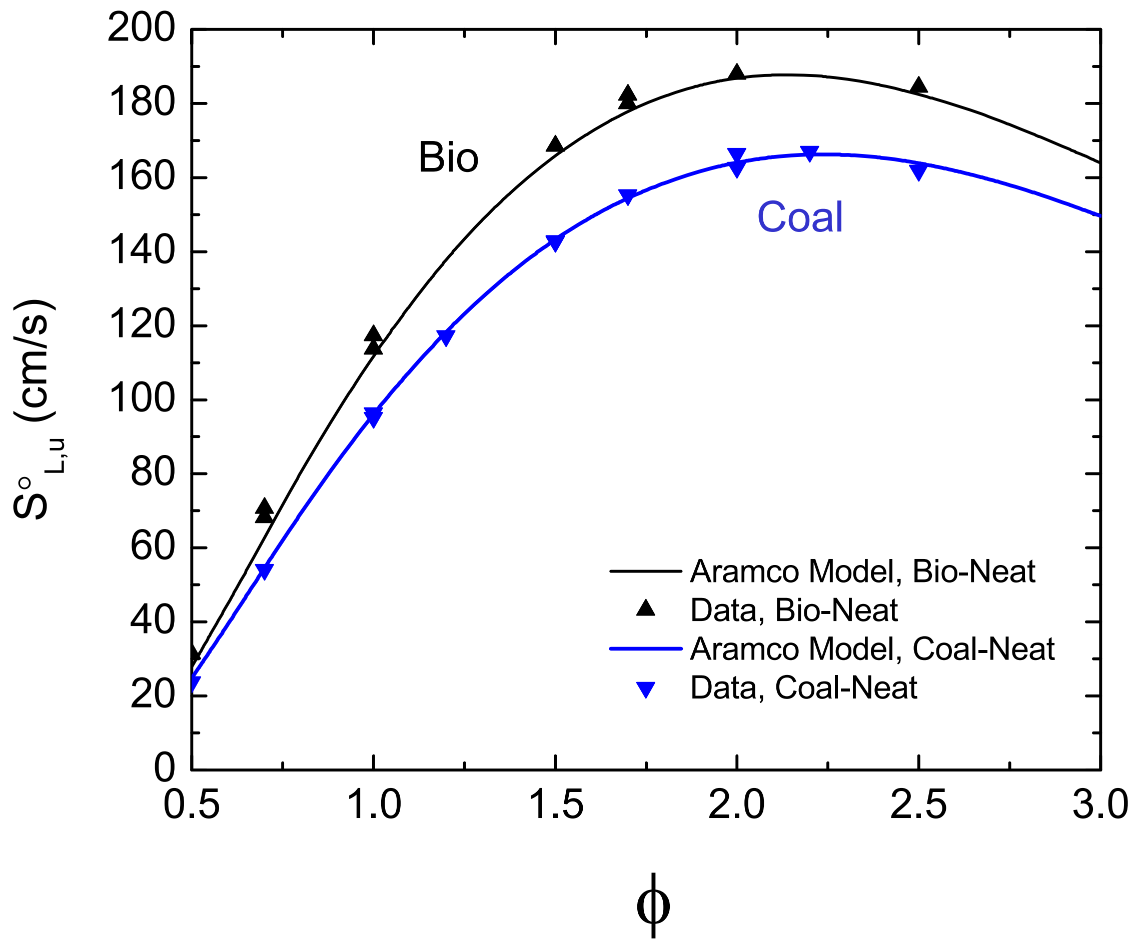
Task 3 – Impurity Effects

Laminar Flame Speed Study Focused on Hydrocarbons

1. Coal-Syngas and Bio-Syngas Blend Baselines
   - Coal: 40/60 H_2/CO
   - Bio: 50/50 H_2/CO
2. Coal Syngas with 1.6%, 7.4% CH_4
3. Coal Syngas with 1.7% C_2H_6
4. Bio Syngas with 5%, 15% CH_4
5. Bio Syngas with 1.6% C_2H_6

Task 3 – Impurity Effects

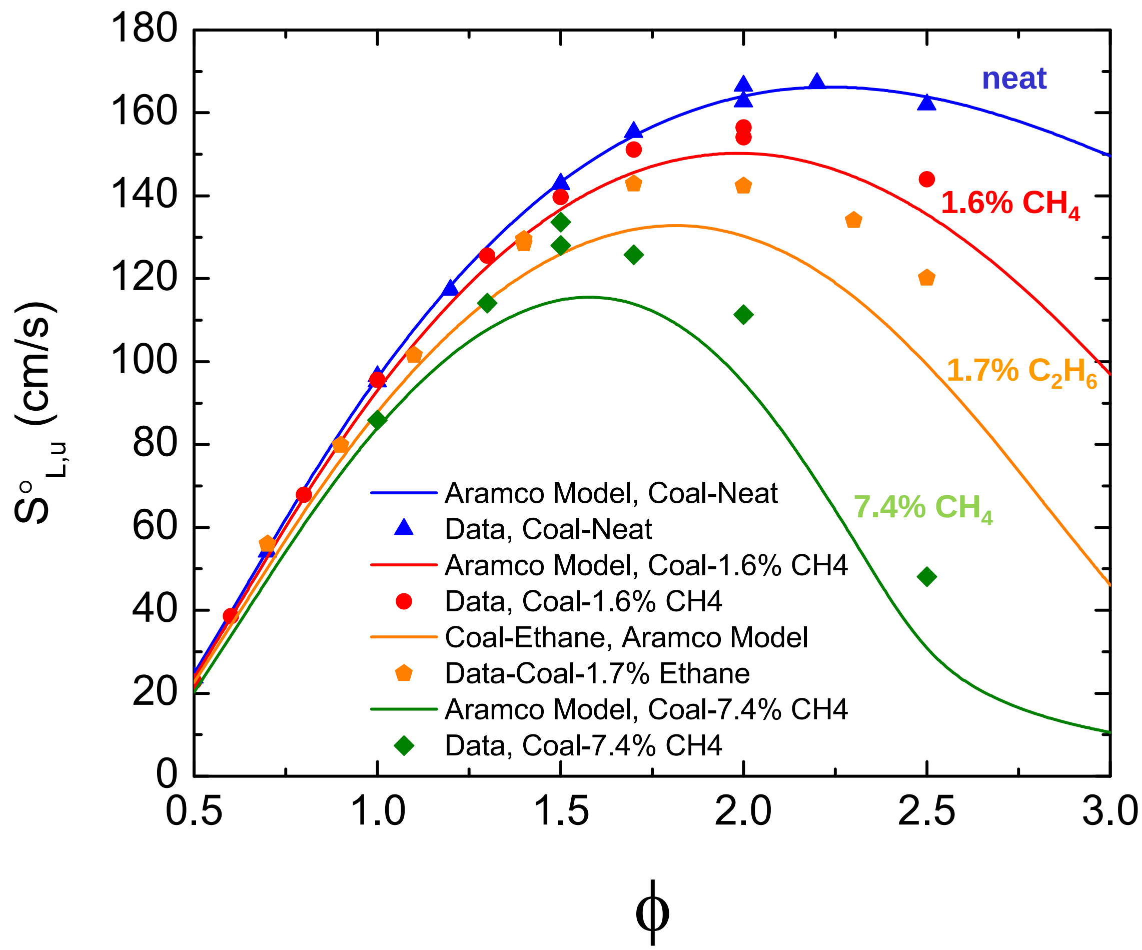
Baseline Mixtures and Model Show Good Agreement



Model: AramcoMech 1.3

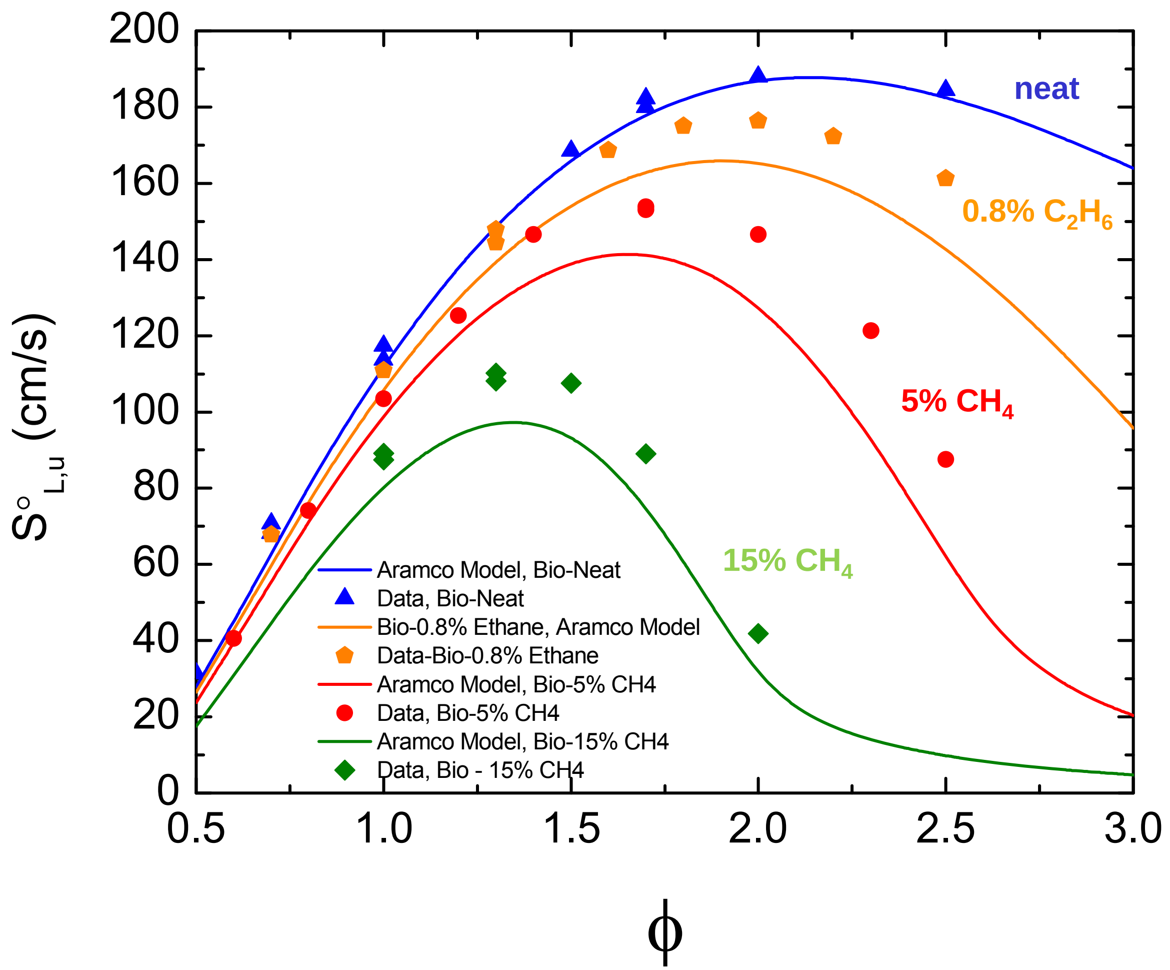
Task 3 – Impurity Effects

Coal-Derived *Syngas Results*



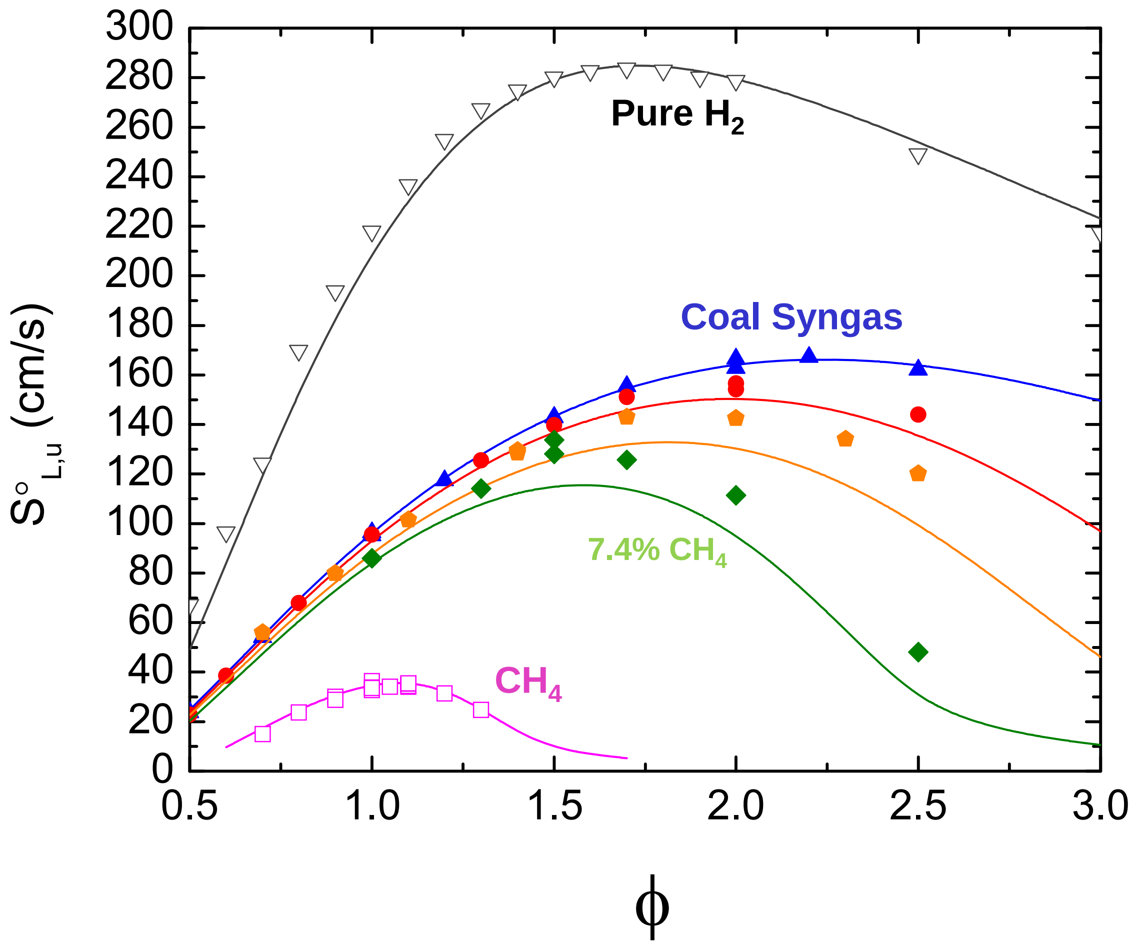
Task 3 – Impurity Effects

Bio-Derived *Syngas Results*



Task 3 – Impurity Effects

Model Good at Extremes but Improvements Needed For Blends



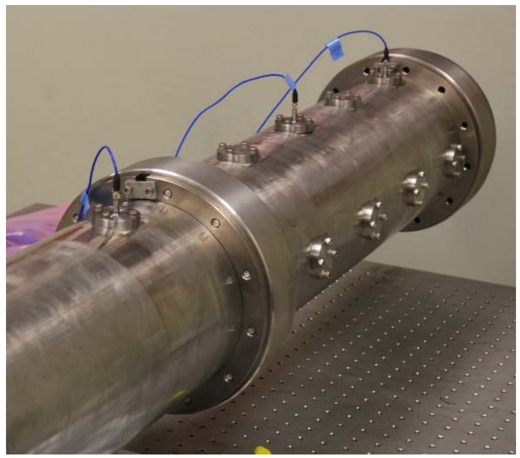
Task 3 – Impurity Effects

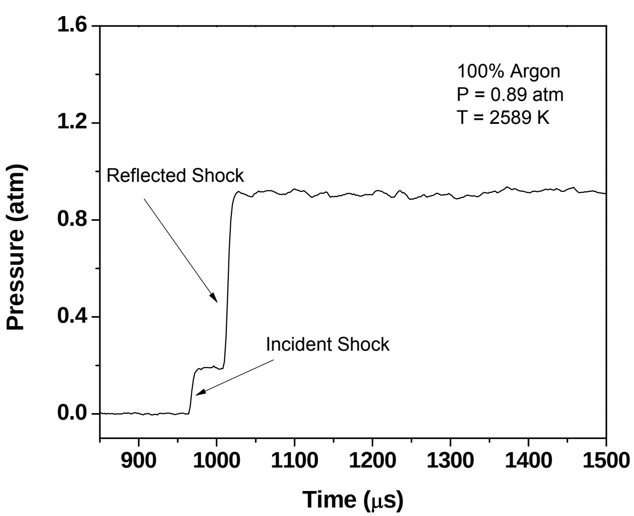
Several Other Tasks Have been Completed or are Underway

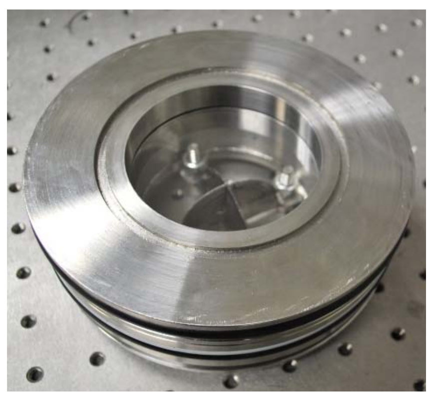
- Completed Numerical Study of Effect of Impurities (NOx, H_2S) on Syngas Blend Kinetics at Real Engine Conditions
- Applying **OH Laser Absorption Diagnostic** in Collaboration with Aerospace Corporation (Los Angeles, CA)
- **Set up “New” Shock Tube** at TAMU (inherited from Aerospace Corporation)
- Finished **Kinetics Mechanism for NOx and Ammonia** Chemistry with H_2/CO

Task 3 – Impurity Effects

Aerospace Shock Tube *Has Been Installed at TAMU*



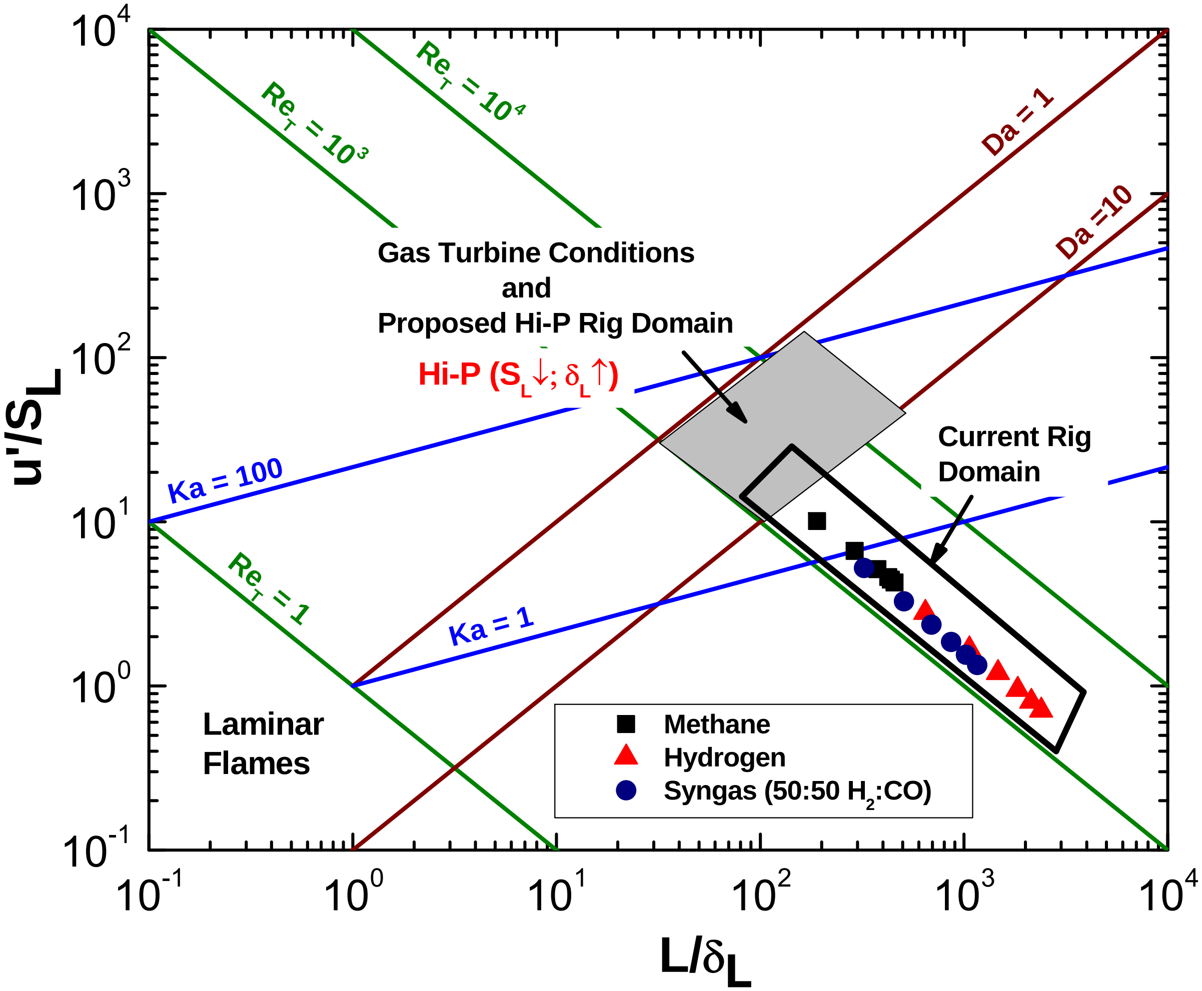




Task 4 – Design and Construction of a Turbulent Flame Speed Facility

Task 4 – New Facility

Borghi Diagram shows Current and Desired Regions for Turbulent Flame Speeds



Task 4 – New Facility

New Facility Will be Designed and Built at TAMU

1. Detailed Design and Structural Analysis
2. Fabrication of Vessel Components
3. Installation of Vessel
4. Characterization of Flow Conditions

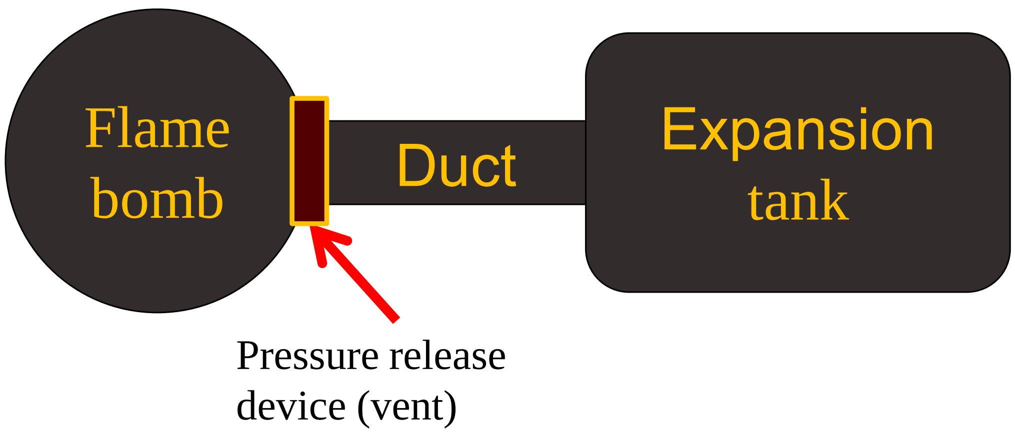
Task 4 – New Facility

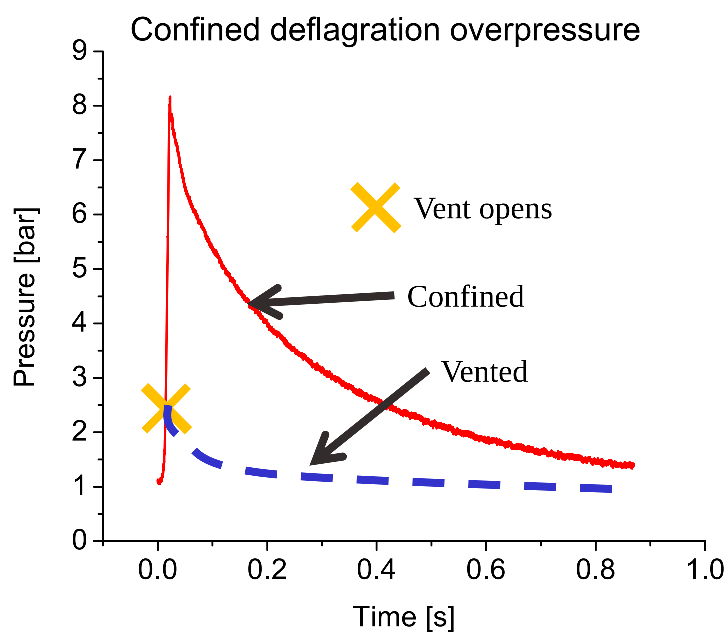
Task 4 Design Effort is Underway

- Survey of Existing Turbulent Flame Speed Facilities Completed
- Trade-off Study for Final Design Finished
- Critical Aspect is how to Handle or Reduce the Overpressure
- **Will Move Toward a Design that Involves a Blowout Disk and Reservoir for Overpressure**
- Detail Design is Underway

Task 4 – New Facility

New Design Will Utilize a Pressure Relief System

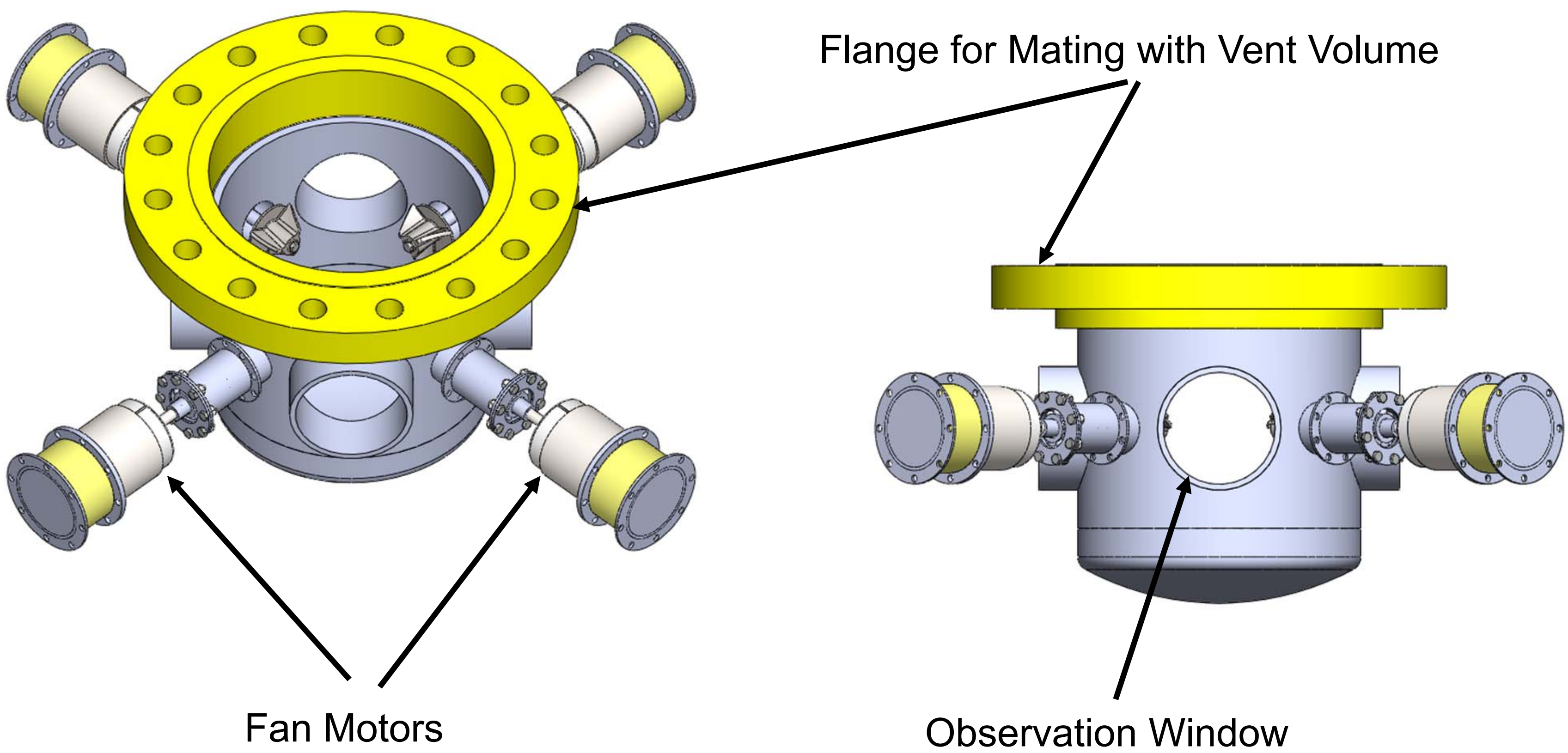




- Max Initial Pressure: **30 atm**
- Vessel Size: ~ **30.5 cm Dia (12 in)**
- Motor and Fans similar to existing rig

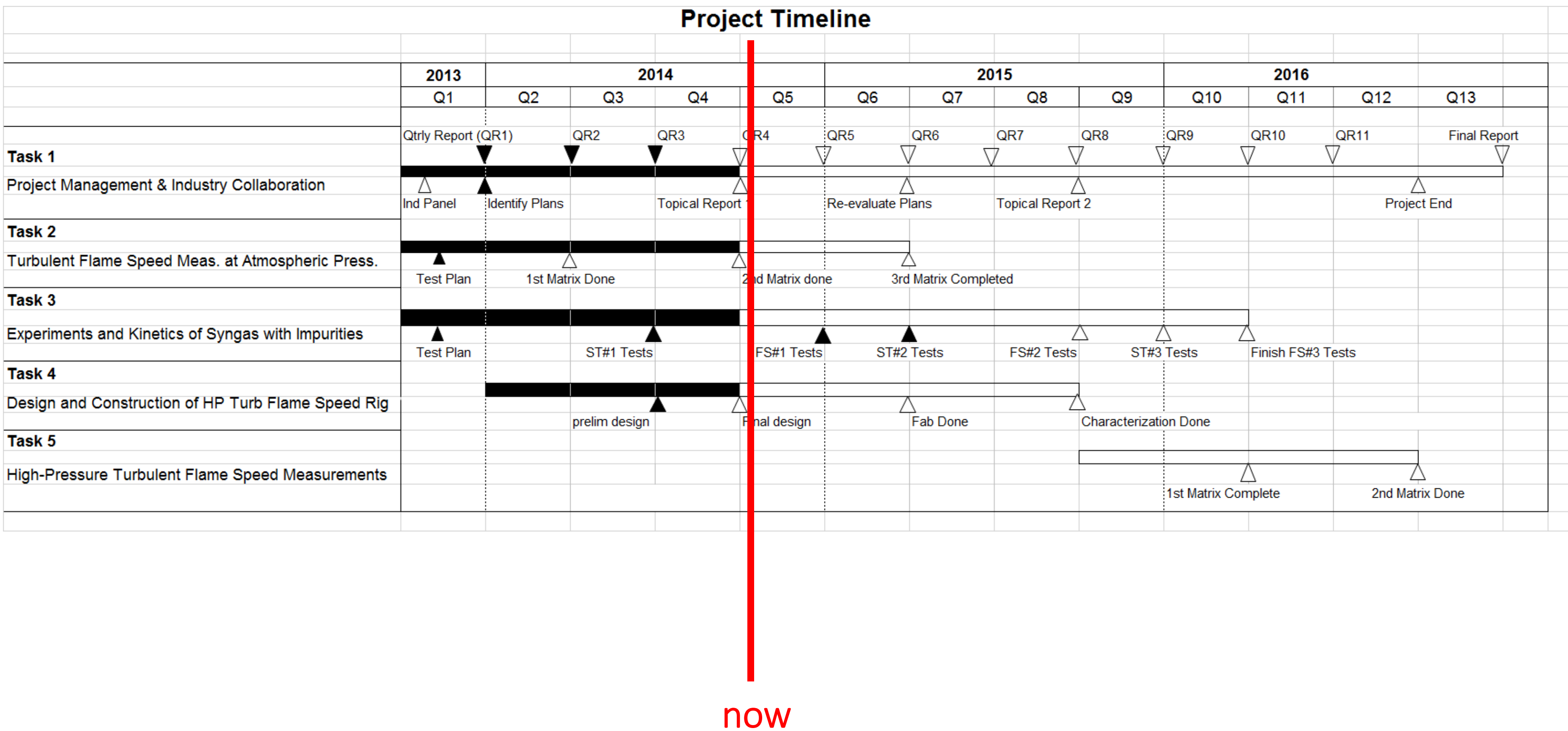
Task 4 – New Facility

Conceptual Design is Complete



Task 4 – New Facility

Timeline Showing Task 4



Task 5 – High-Pressure Turbulent Flame Speed Measurements

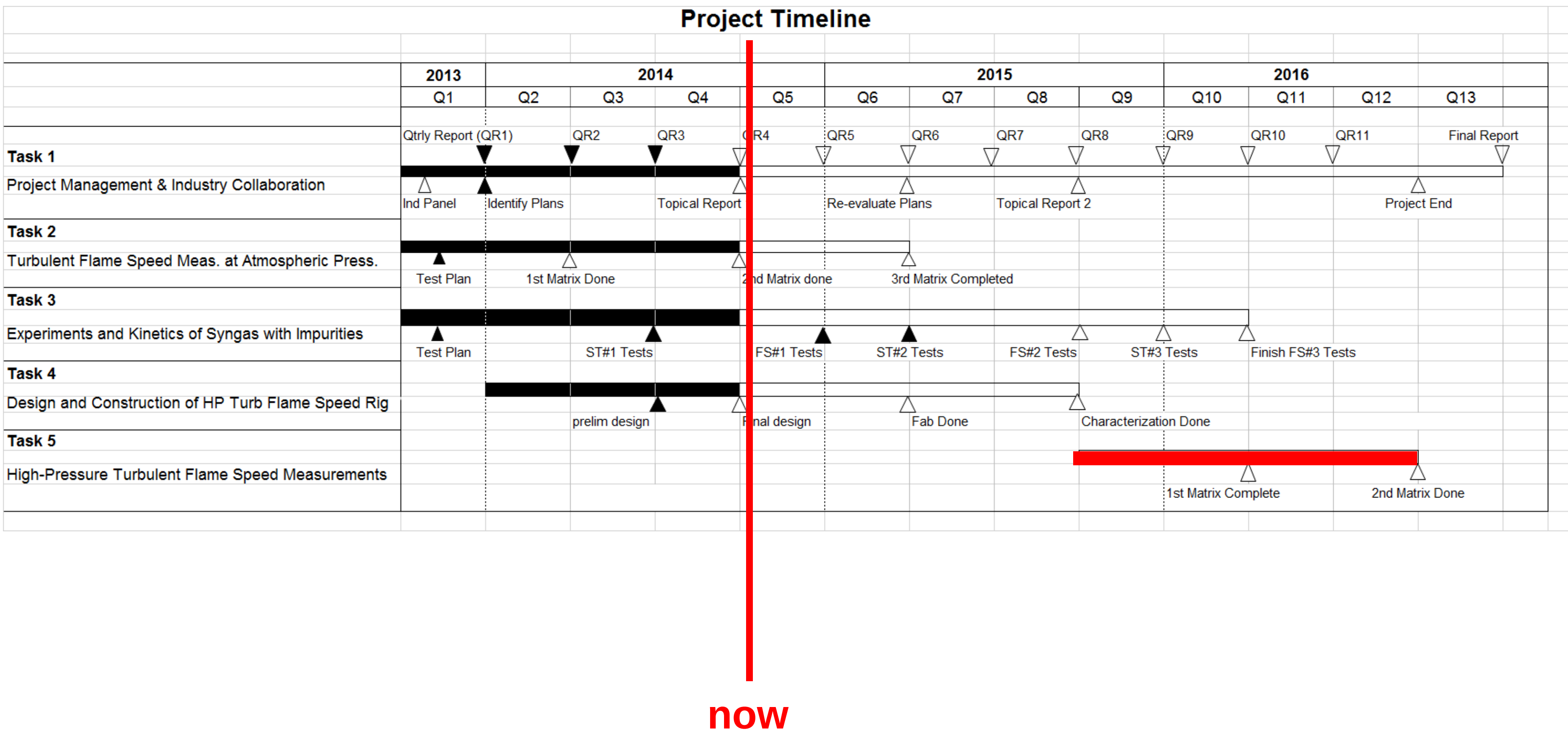
Task 5 – High-Pressure Turbulence

High-Pressure Experiments Will be Performed for Selected Syngas Blends

- Identify Two Test Matrices (Fuel Blends) for Study
- Utilize Results from Tasks 2 and 3 for Guidance
- Perform Experiments at Elevated Pressures
- Parallel High-Pressure Laminar Tests Should also be Done

Task 5 – High-Pressure Turbulence

Timeline Showing Task 5



Summary

Progress on the Five Main Work Tasks for the Project Was Presented

Task 1 – Project Management and Program Planning

Task 2 – Turbulent Flame Speed Measurements at Atmospheric Pressure

Task 3 – Experiments and Kinetics of Syngas Blends with Impurities

Task 4 – Design and Construction of a High-Pressure Turbulent Flame Speed Facility

Task 5 – High-Pressure Turbulent Flame Speed Measurements

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