Turbulent Flame Speeds and NOx Kinetics of HHC Fuels with Contaminants and High Dilution Levels

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Texas A&M University

2010 University Turbine Systems Research Workshop
Pennsylvania State University, State College, PA
19 October, 2010

Project Overview

New Three-Year Project Began this Month

Project Highlights:

1. Duration: **Oct. 1, 2010 – Sept. 30, 2013**
2. DOE NETL Award **DE-FE0004679**
3. Budget: $501,712 DOE + $125,500 Cost Share
4. Principal Investigator: Dr. Eric L. Petersen
5. Participating Organizations:
   - Rolls-Royce (Dr. Gilles Bourque)
   - The Aerospace Corporation (Dr. Mark Crofton)
   - Trinity College (Dr. John Mertens)

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

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

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

Project Overview

There are Six Main Work Tasks for the Project

Work Tasks:

Task 1 – Project Management and Program Planning

Task 2 – Turbulent Flame Speed Measurements

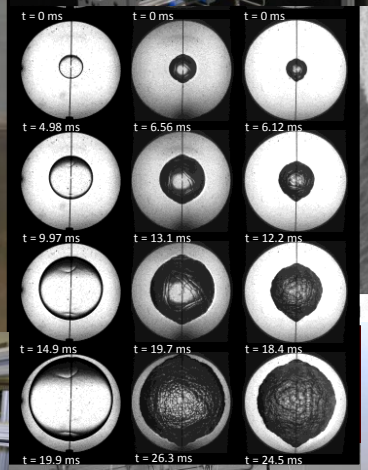
Task 3 – Laminar Flame Speeds with Diluents

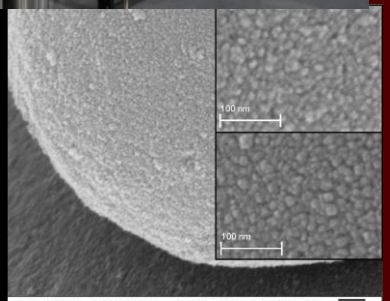
Task 4 – NOx Mechanism Validation Experiments

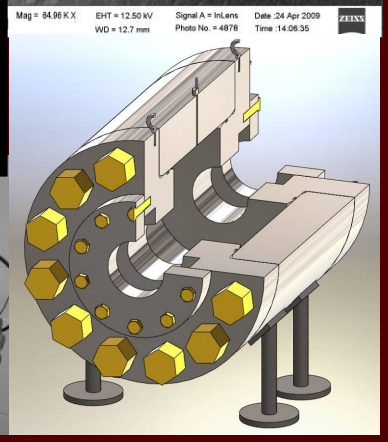
Task 5 – Fundamental NOx Kinetics

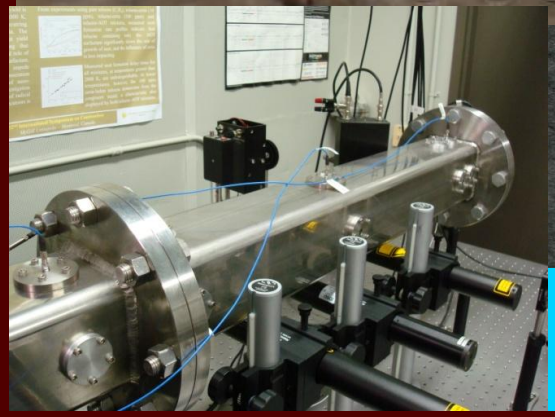
Task 6 – Effect of Impurities on Syngas Kinetics

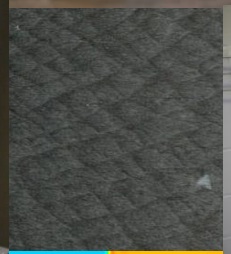
Petersen Group Research

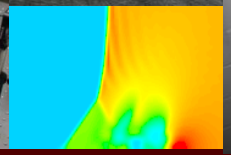


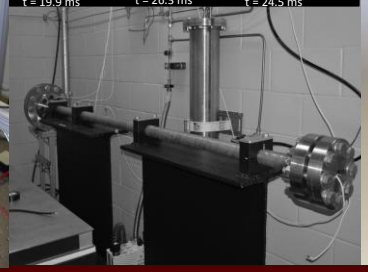










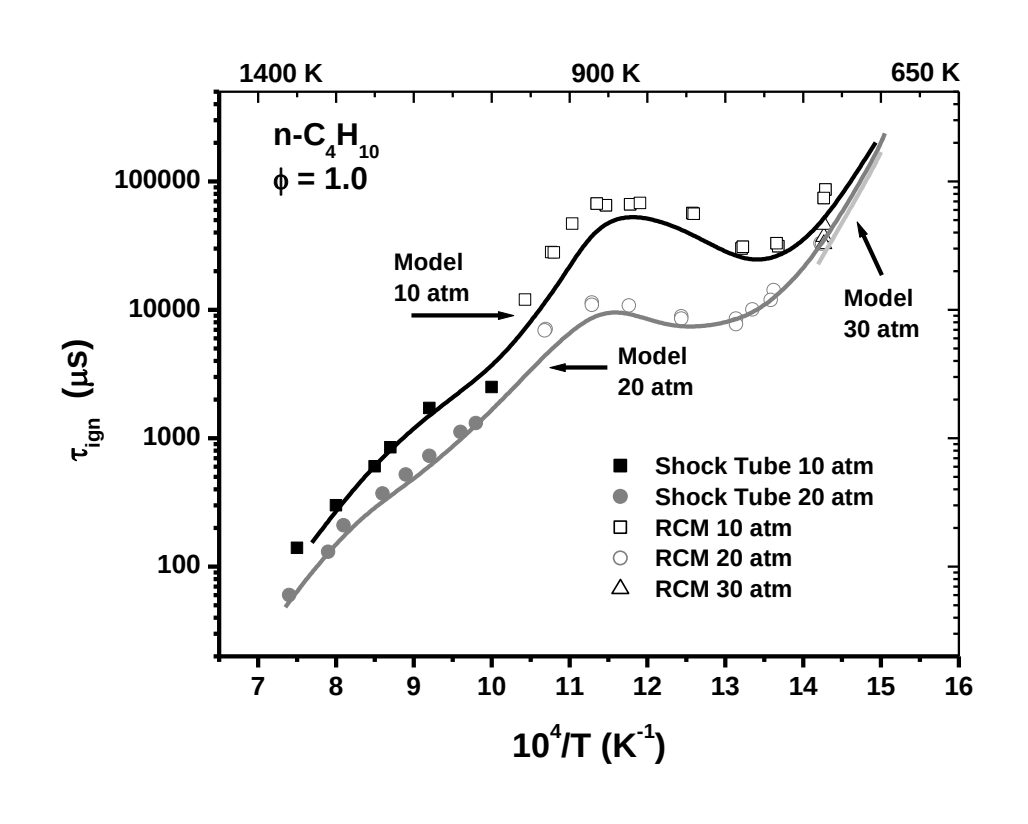


Recent Studies and Facilities

Chemical Kinetics Model

Current Model (Curran et al.):

- Verified with Real Fuel-Air Mixtures at High Pressures
- Considers Through C_5 Hydrocarbons
- 289-Species and 1580-Reactions



Validated with:

- CH_4, C_2H_6, C_3H_8
- CH_4/C_3H_8, CH_4/C_2H_6, CH_4/H_2, $CH_4/C_2H_6/C_3H_8$
- $CH_4/C_2H_6/C_3H_8/C_4H_{10}/C_5H_{12}$
- CH_4/DME, DME
- C_4H_{10}, iC_4H_{10}

Overview

***Finished** Ignition Time Studies of Hydrocarbon Blends*

- **CH_4/C_3H_8** in ratios ranging from 90/10% to 60/40%
  Shock Tube: 5 – 30 atm and 1000 – 1500 K
  31st Combustion Symposium (2007)

- **CH_4**, **CH_4/H_2**, **CH_4/C_2H_6**, and **CH_4/C_3H_8** from 90/10% to 60/40%
  Shock Tube: 0.5 – 30 atm and 1090 – 2000 K
  Journal of Engineering for Gas Turbines and Power (2007)

- **$CH_4/C_2H_6/C_3H_8$** from 90/6.6/3.3% to 70/20/10%
  Shock Tube & RCM: 1 – 50 atm and 770 – 1580 K
  Combustion and Flame (2008)

- **Natural Gas** Mixtures (**$CH_4/C_2H_6/C_3H_8/C_4H_{10}/C_5H_{12}$**)
  Shock Tube, RCM, & Flame Speed: 1 – 34 atm and 740 – 1660 K
  ASME Turbo Expo (2008) (Also: *J. Eng. Gas Turb. Power*, 2010)

- **n-C_4H_{10}/iso-C_4H_{10}**
  Shock Tube: 1 – 18 atm and 1050 – 1600 K
  ASME Turbo Expo (2009) (Also: *J. Eng. Gas Turb. Power*, 2010)

Overview

***Recent** Ignition Time Studies of Hydrocarbon Blends*

- **n-C_4H_{10}** (100%)
  Shock Tube & RCM: 1 – 45 atm and 690 – 1430 K; ϕ = 0.5, 1.0, 2.0
  Combustion and Flame (2010)

- **iso-C_4H_{10}** (100%)
  Shock Tube & RCM: 1 – 30 atm and 590 – 1570 K; ϕ = 0.3, 0.5, 1.0, 2.0
  Combustion and Flame (2010)

- **CH_4/n-C_4H_{10}** for 90/10 and 70/30
  RCM & Shock Tube: 10 – 30 atm and 660 – 1330 K; ϕ = 0.5, 1.0, 2.0
  Energy & Fuels (2010)

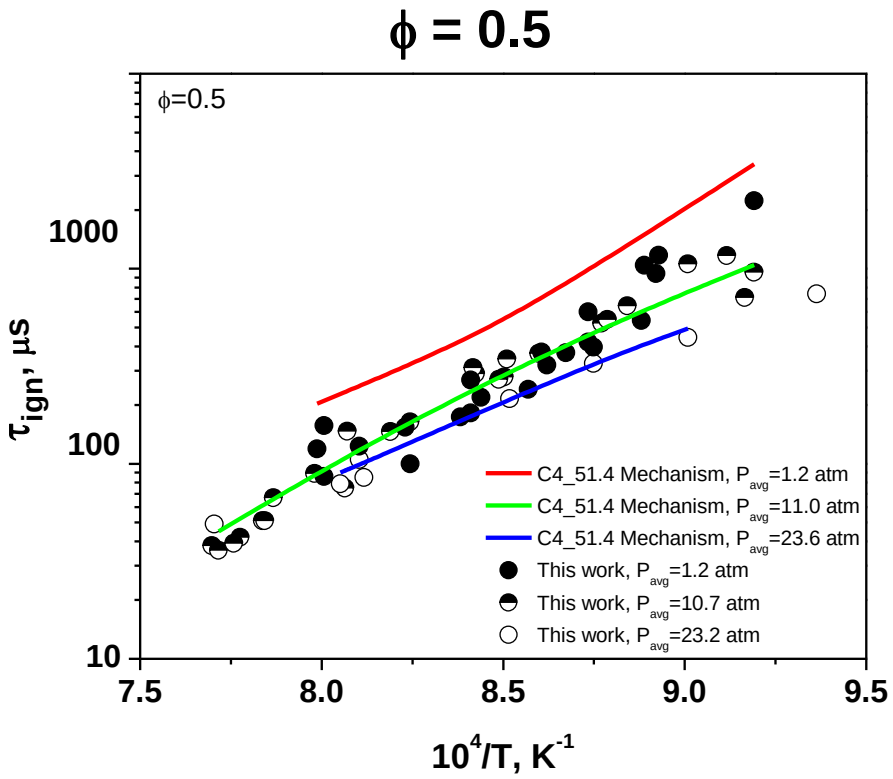
- **Quinternary** Mixtures (**CH_4/C_2H_6/C_3H_8/C_4H_{10}/C_5H_{12}**)
  RCM & Shock Tube: 8 – 30 atm and 630 – 1550 K; ϕ = 0.5, 1.0, 2.0
  Energy & Fuels (2010)

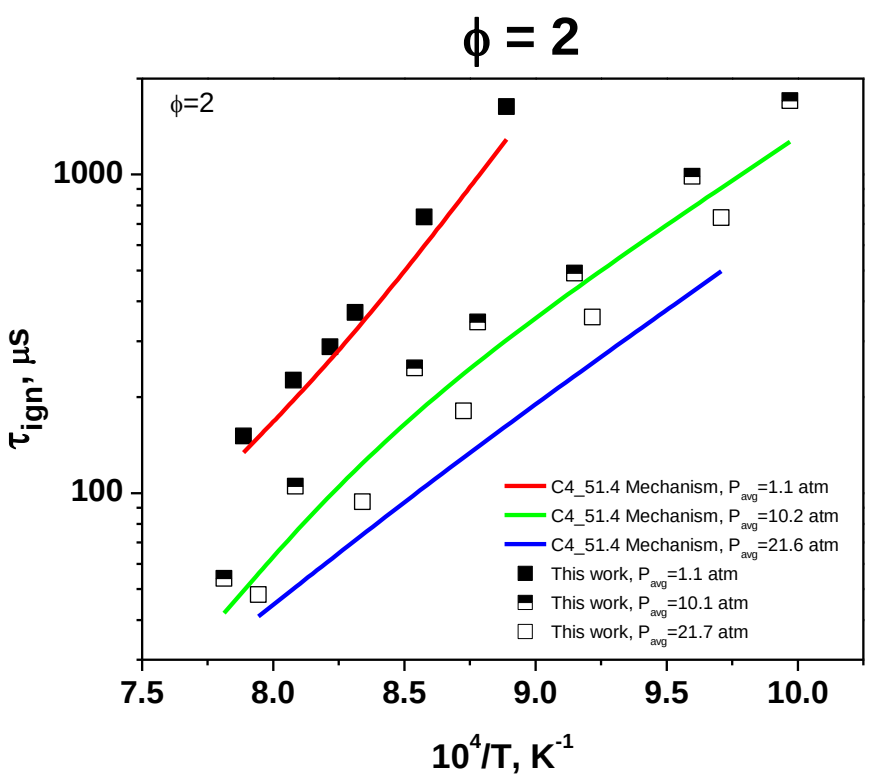
NUI Galway
OÉ Gaillimh

Rolls-Royce

Sample Results

C_2H_4-Air *Results Show Interesting Pressure-ϕ Behavior*

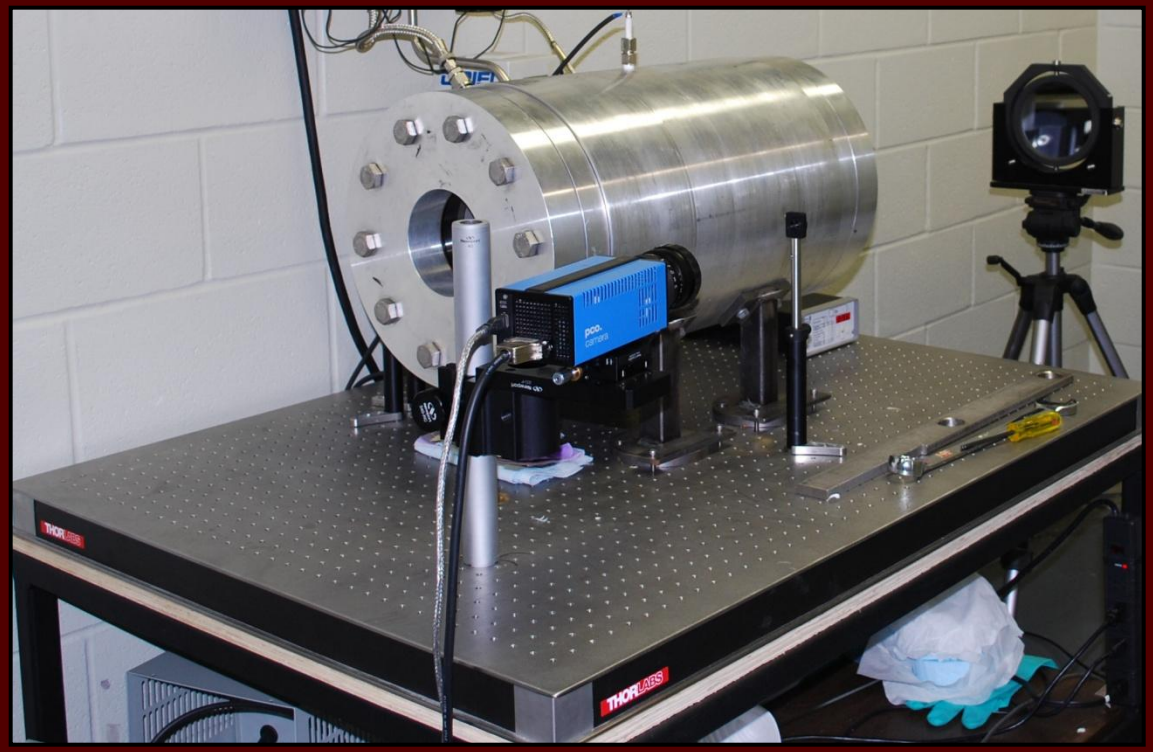




NUI Galway
OÉ Gaillimh

Flame Speed Facility

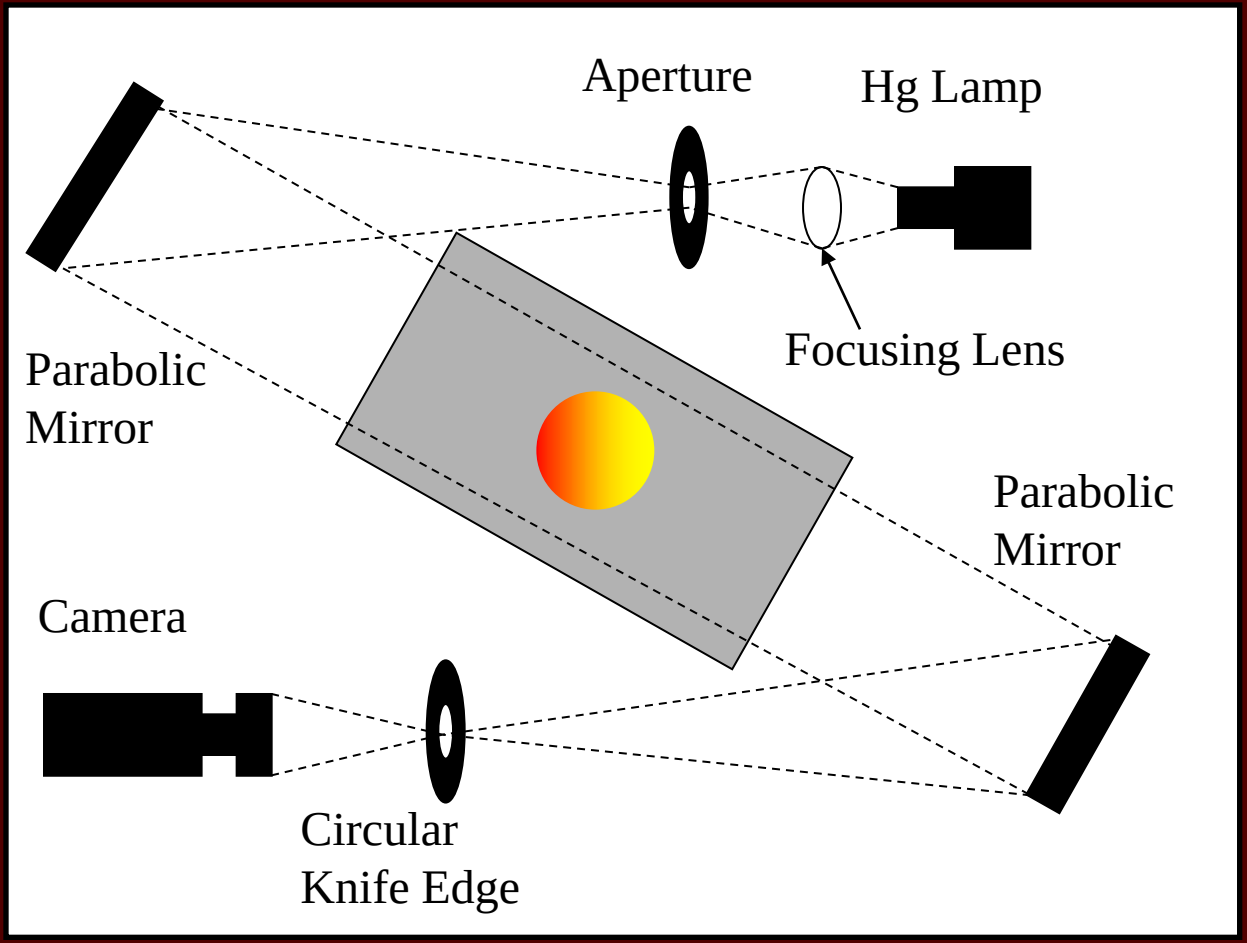
Vessel Capable of High-Pressure Tests



- **Vessel ID 31.74 cm**
- **Internal Length 35.6 cm**
- **6 cm Thick Fused Quartz Windows**
- **12.7 cm Diameter Windows**
- **Max Test Pressure ~ 20 atm**
- **Minimum Safety Factor of 4**

Flame Speed Facility

Z-Type Schlieren Setup



- f/8 Mirrors. (Dia. 6 in)
- Mercury Lamp
- Camera Cooke Corp. (PCO 1200-hs, 3000 fps)
- Circular knife edge

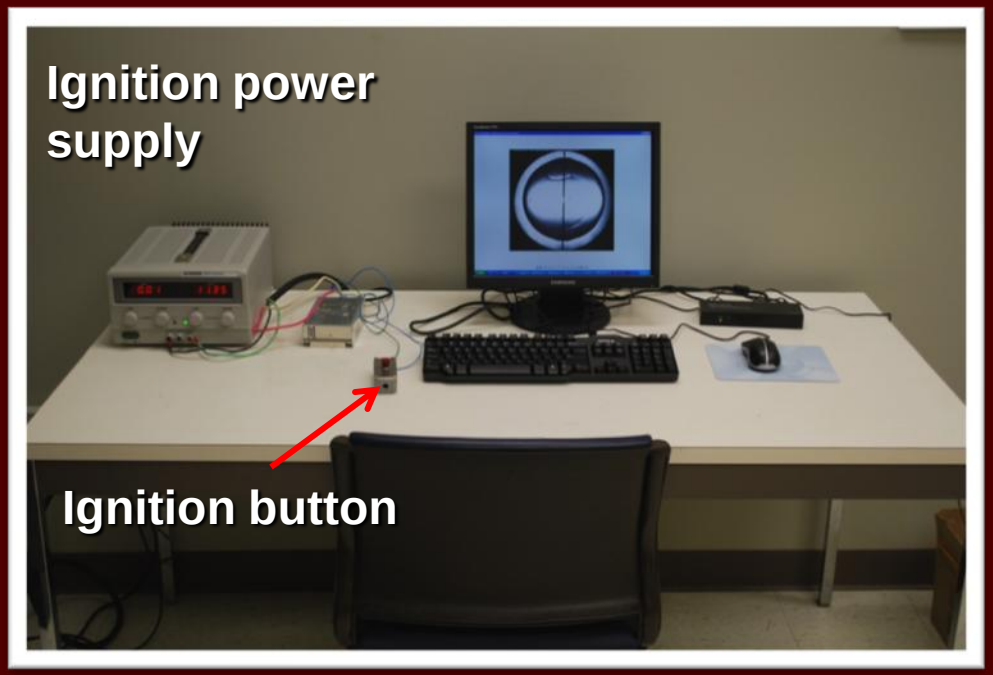
Flame Speed Facility

Mixing Manifold Protected by Blast Wall

- Mixtures Made Outside of Test Cell
- Separated by Concrete-Filled, Steel Reinforced Blast Wall

Flame Speed Facility

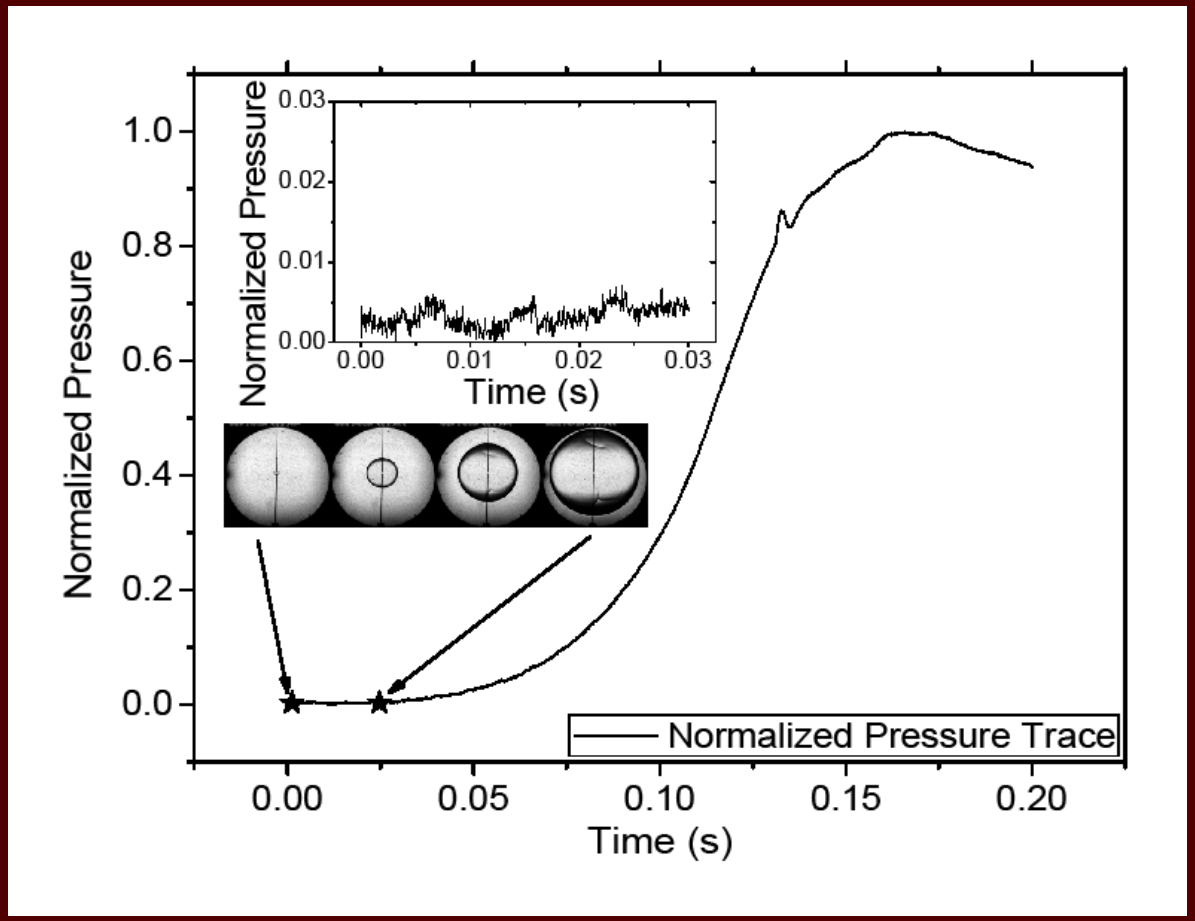
Separate Control Room



- **All Tests are Controlled Remotely from a Separate Control Room**

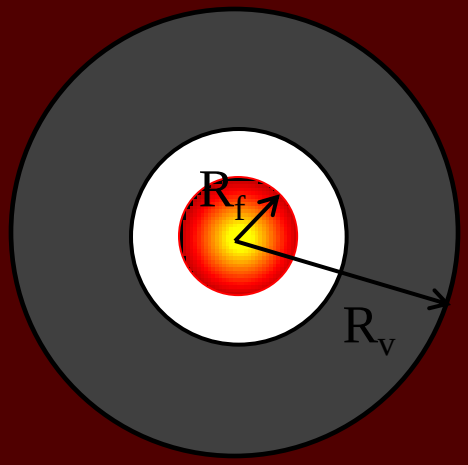
Data Analysis

Pressure remains constant during the experiment



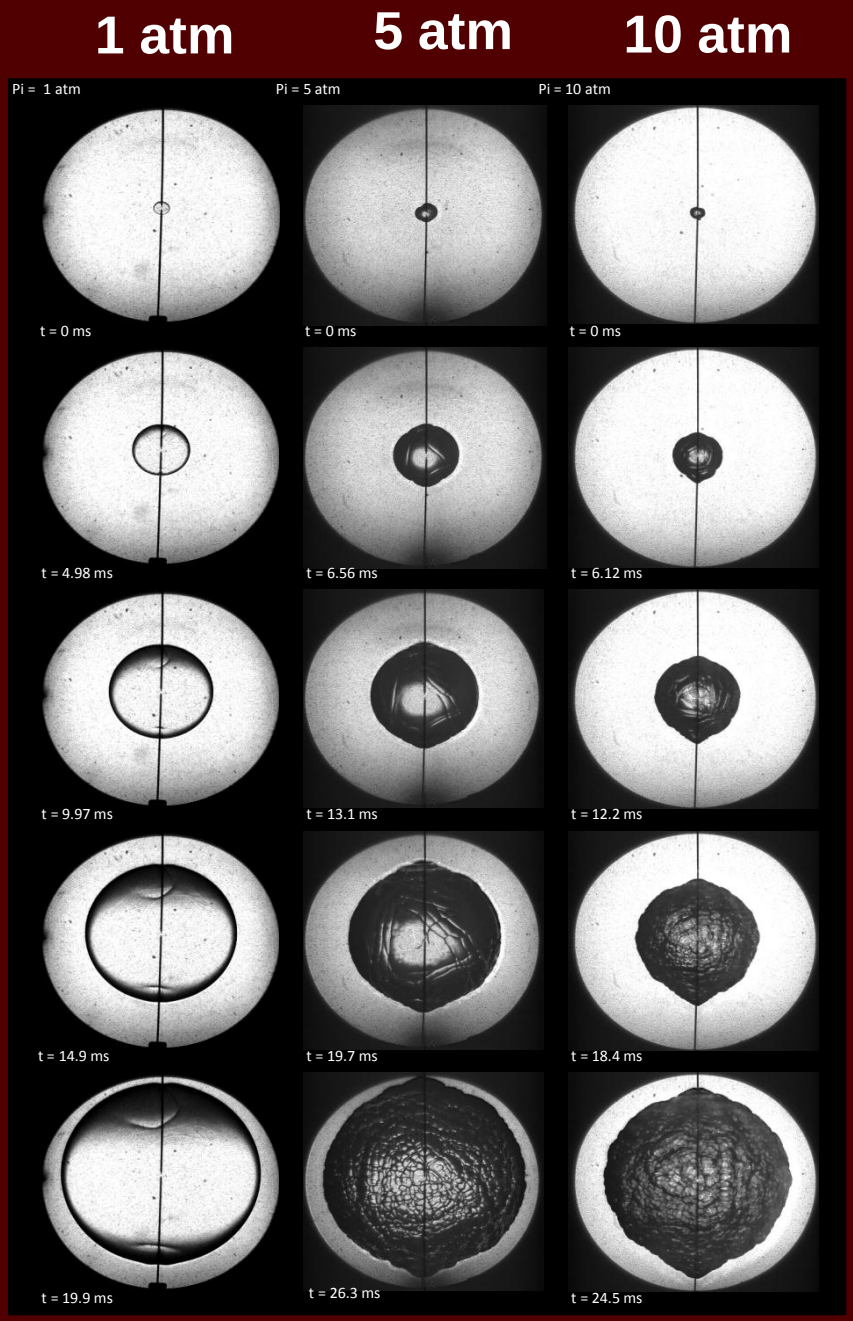
- **R_f/R_v = 0.4 - Error < 5%**
  - Chen and Ju (AIAA 2007)
- **R_f/R_v < 0.3**
  - Burke et al. (Comb. Flame 2009)

R_f allowable is 4.7cm.



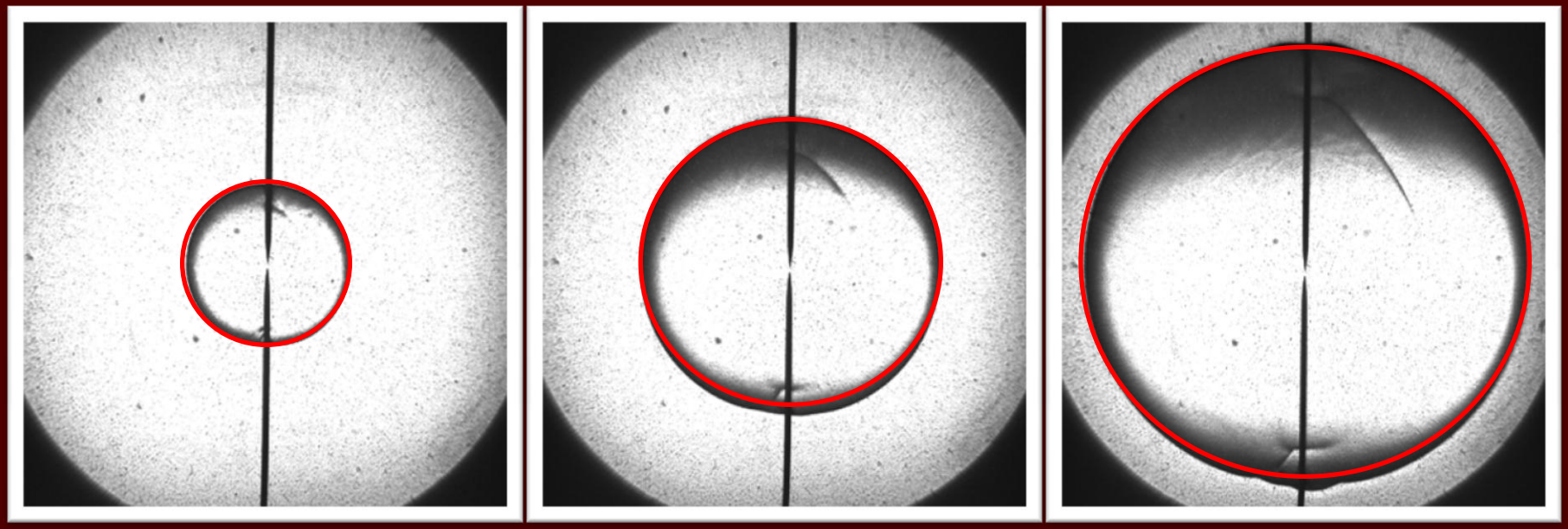
CH_4/C_2H_6
60/40

Instabilities are seen at Higher Pressure



Data Analysis

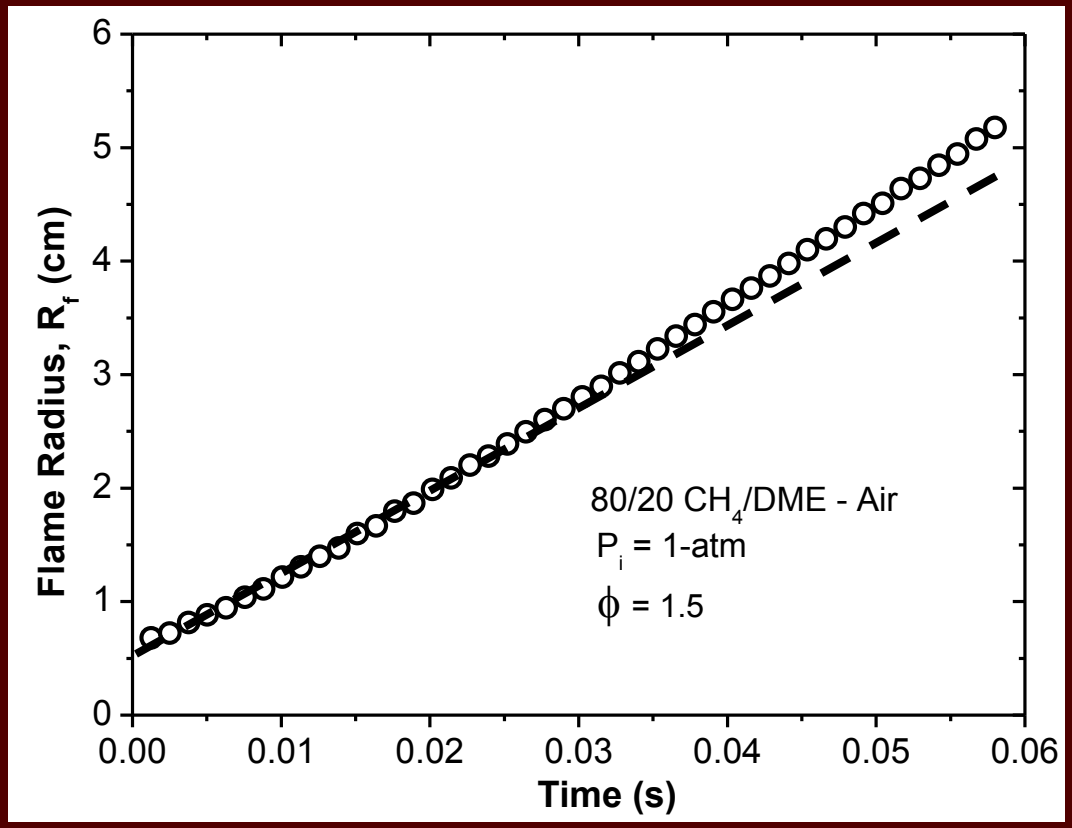
Data reduction obtained by fitting a best circle



Best fit using the Levenberg-Marquardt method (Least Square)
L. Maisonobe (2007)

Data Analysis

Radius versus time is used to find S_L and L_m



$$S_{L,b} = \frac{dR_f}{dt}$$

dR_f/dt is <u>NOT</u> constant!
flame speed depends on flame stretch α

$$\alpha = \frac{2}{R}\frac{dR_f}{dt}$$

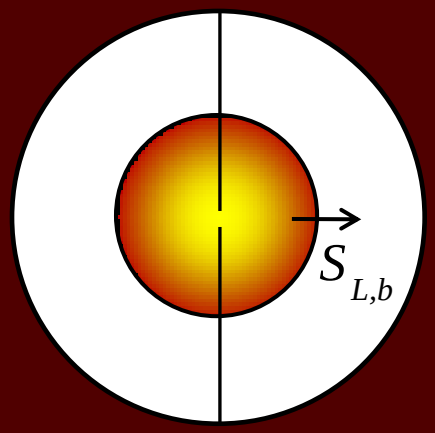
Markstein (1964)

$$S_{L,b}^{o} = S_{L,b} + L_m \alpha$$

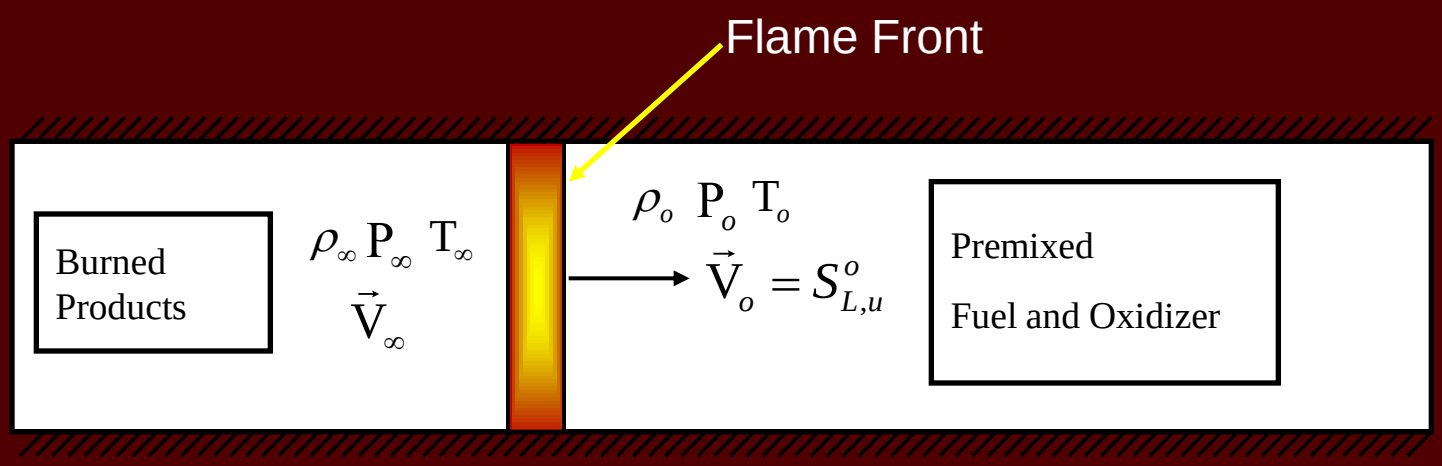
Data Analysis

Experimentally determined flame speed must be corrected

- Spherically expanding flames undergo stretch



- We are interested in the unburned, unstretched flame speed



Flame Speed Overview

Laminar Flame Speed Studies of Hydrocarbon Blends

- **Pure Alkanes (CH_4, C_2H_6, and C_3H_8)**
  Pressures: 1 – 15 atm
  ASME Turbo Expo (2010)

- **Binary Blends (CH_4/C_2H_6 and CH_4/C_3H_8)**
  Pressures: 1 –15 atm
  ASME Turbo Expo (2010)

- **Pure DME**
  Pressures: 1 – 15 atm
  Fuel (in press)

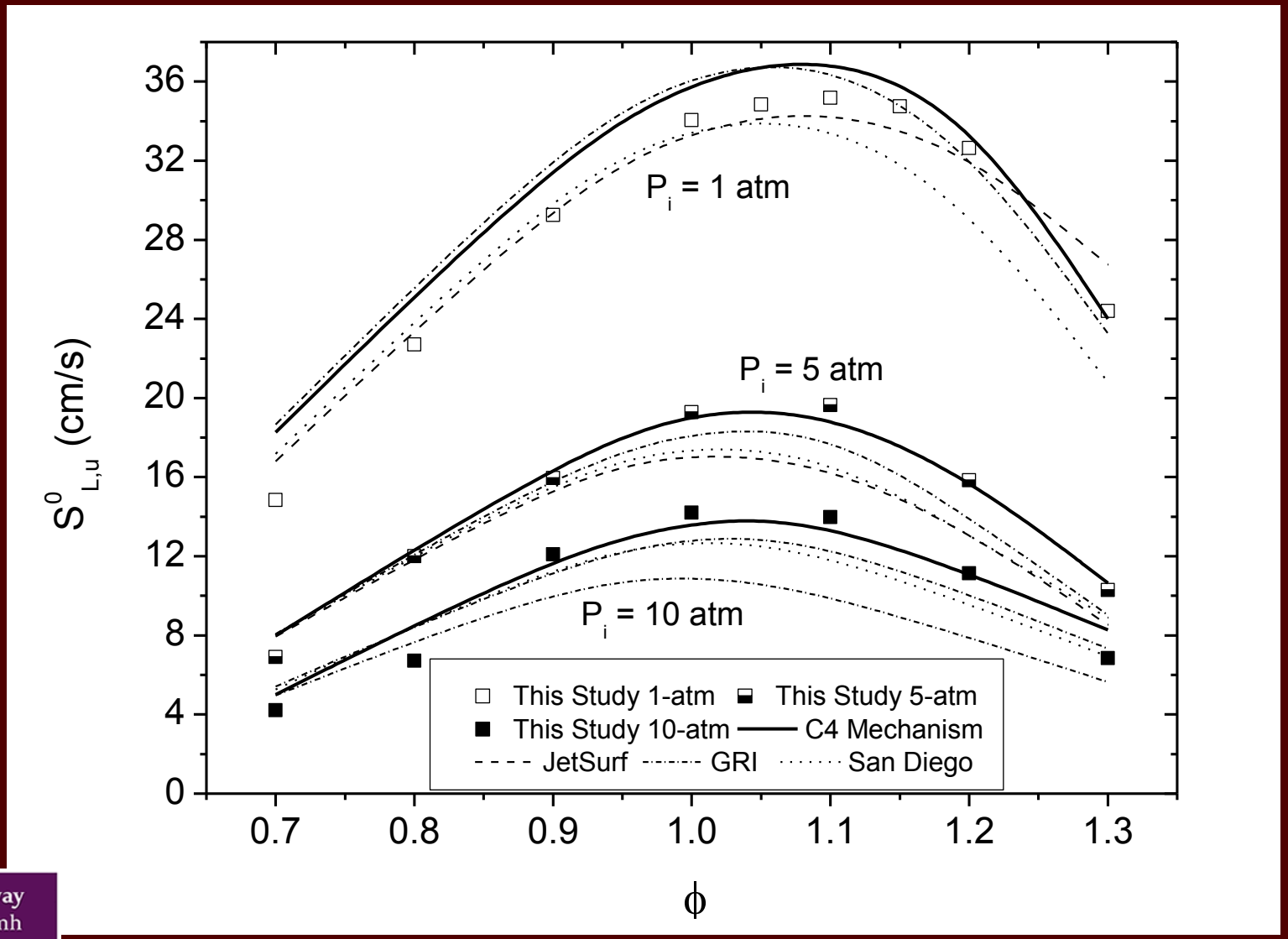
- **CH_4/DME Blends**
  Pressures: 1 – 15 atm
  Proc. Comb. Inst. (in press)

NUI Galway
OÉ Gaillimh

Rolls-Royce

Sample Results

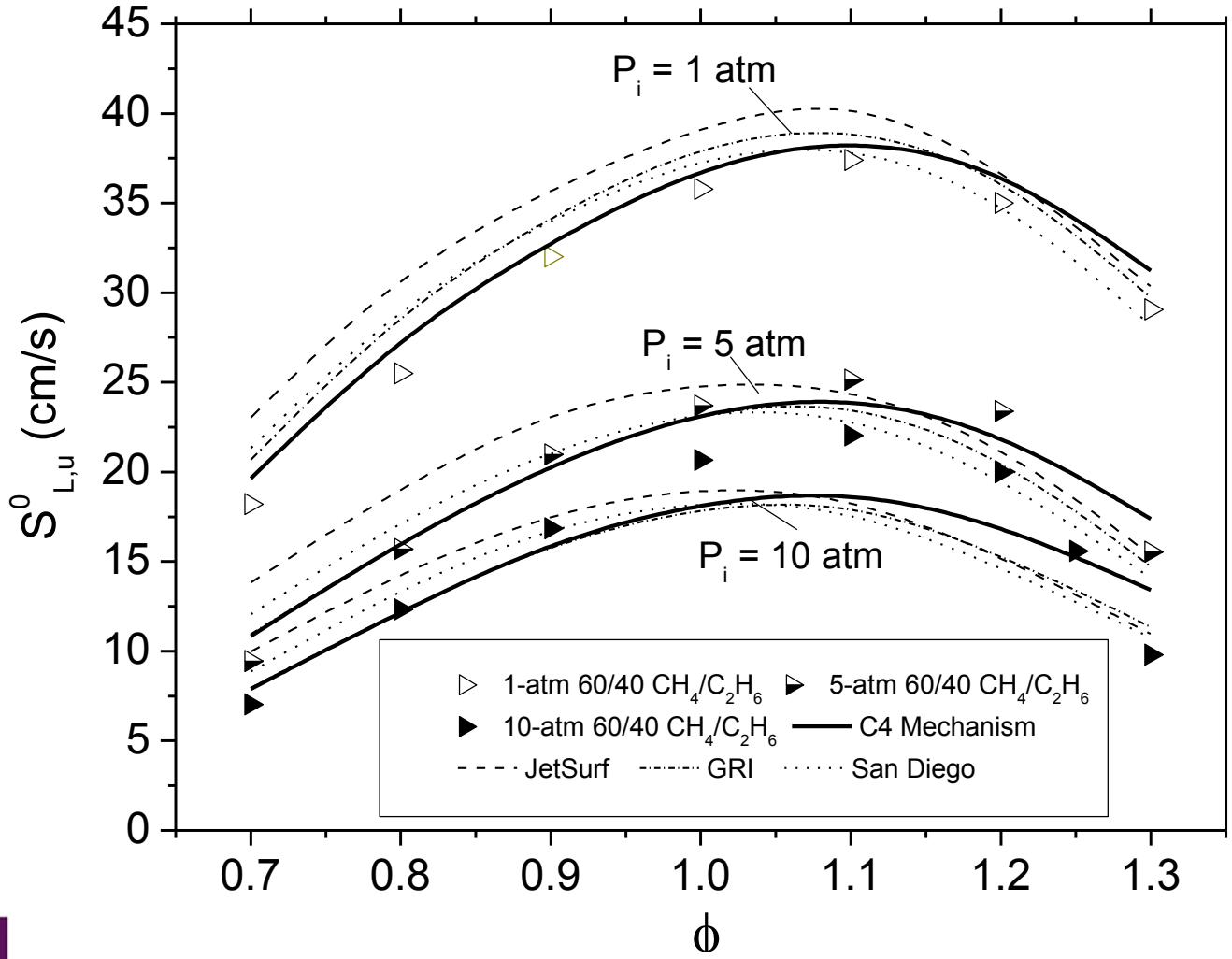
Methane/air for 3 Different Pressures



NUI Galway
OÉ Gaillimh

Sample Results

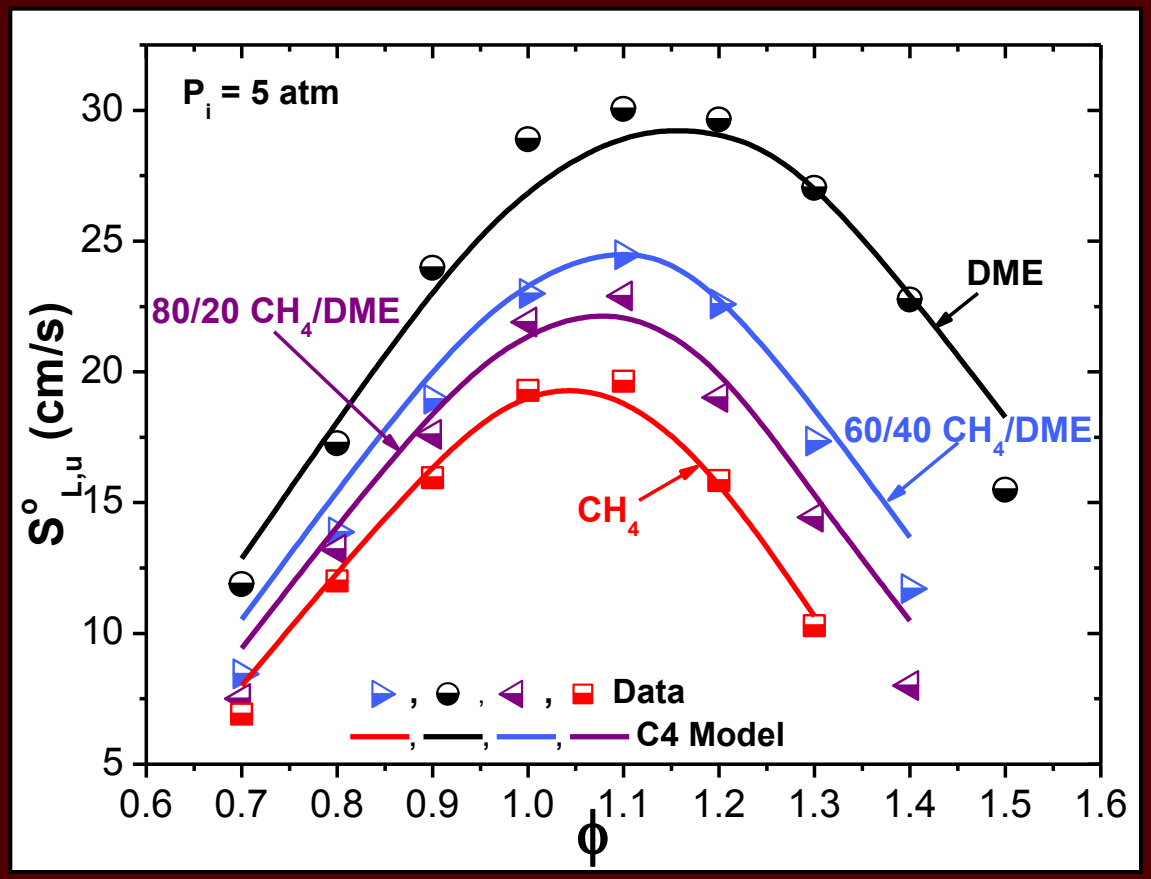
CH_4/C_2H_6 Blend (60/40) *for 3 Different Pressures*



NUI Galway
OÉ Gaillimh

Sample Results

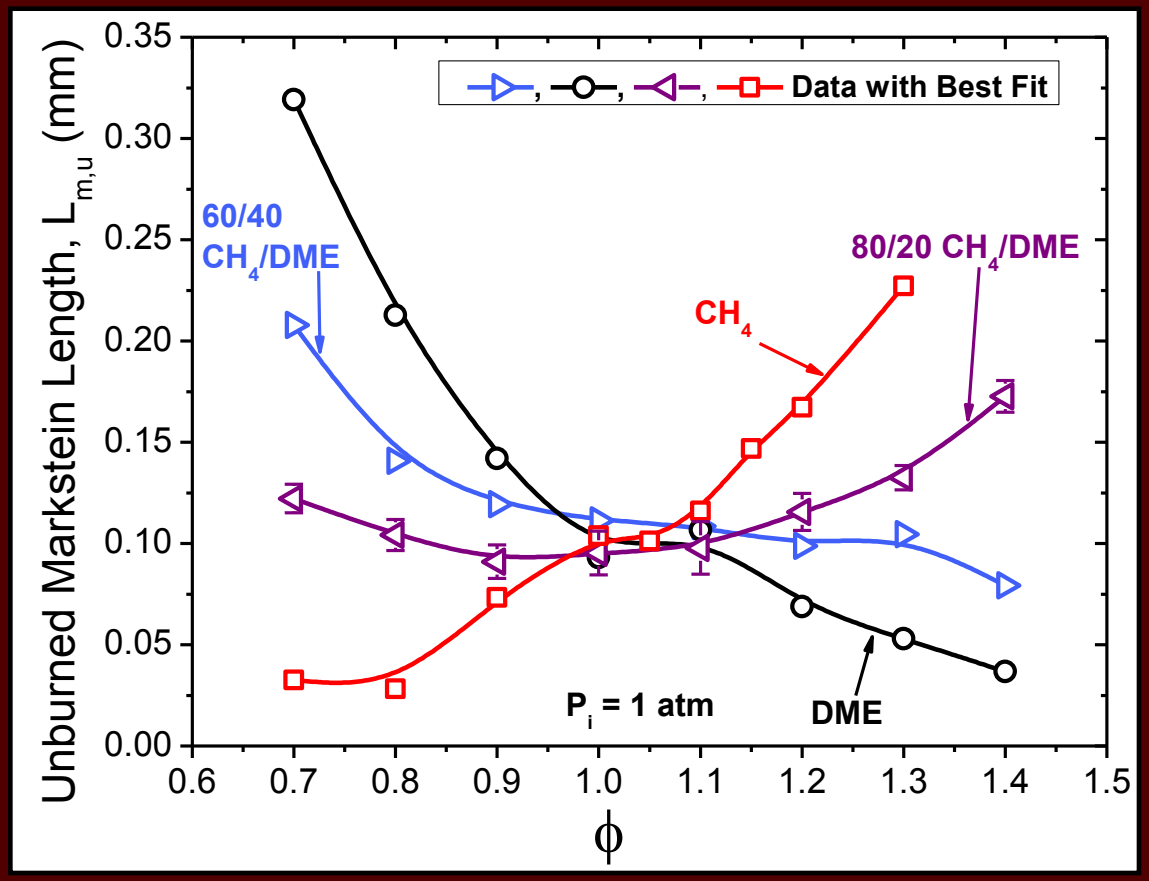
Flame speed for DME/CH_4 blends falls between pure fuel values at 5 atm



Model captures chemistry and accurately predicts flame speed for pure fuels and blends

Sample Results

Markstein length for DME/CH_4 blends falls between pure fuel values at 1 atm



Small amount of DME addition alters Methane Markstein length greatly

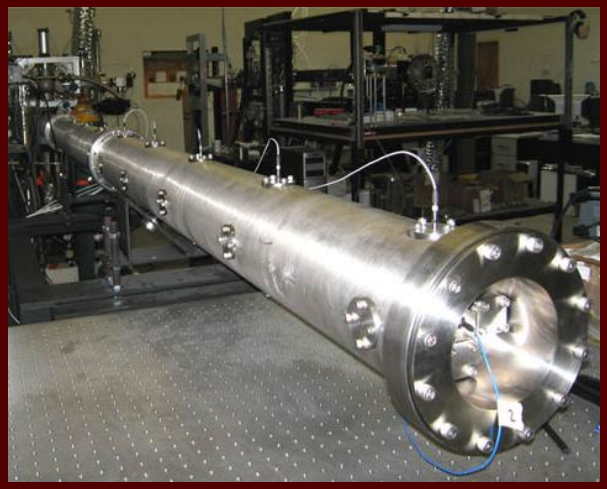
Shock Tube Experiments

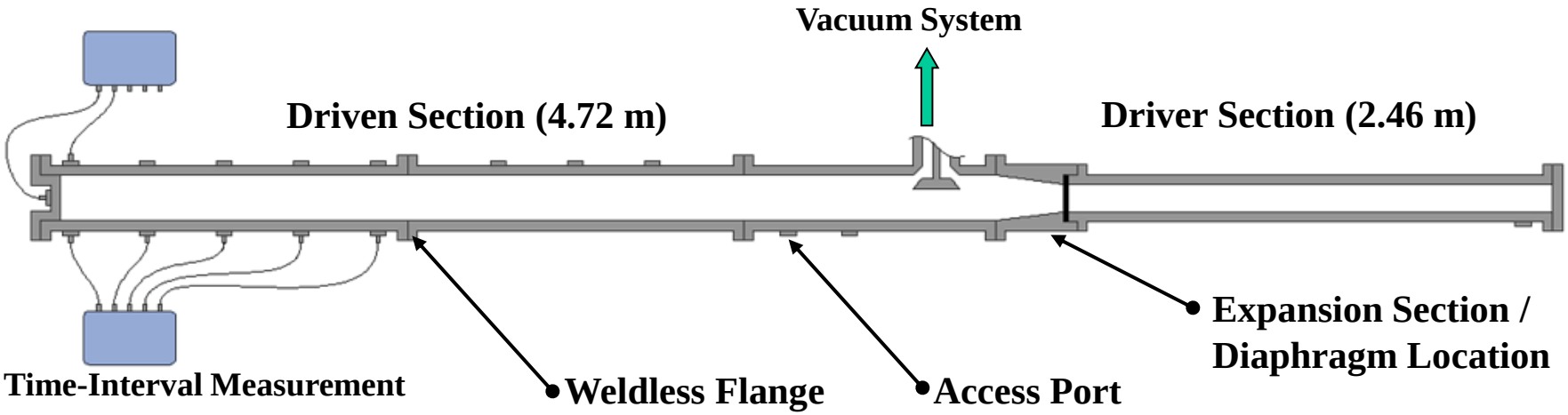
Texas A&M High-Pressure Shock Tube

Shock Tube Experiments

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 Sections
- 15.24 cm Driven Inner Diameter





Shock Tube Experiments

Low-Pressure Shock-Tube Facility is also Utilized

TAMU Low Pressure Shock-Tube Facility

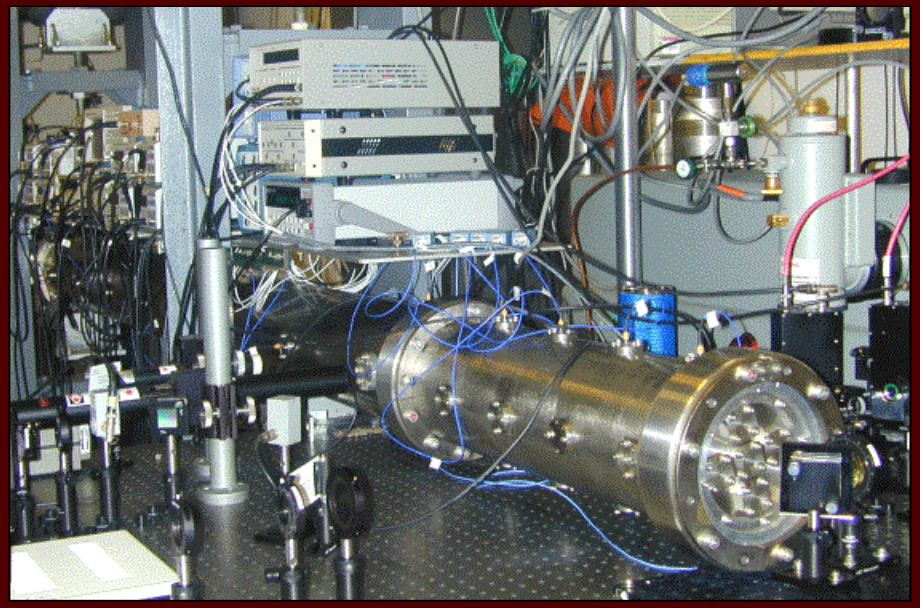
- 4 x 4 in Cross Sectional Driven Area
- 1 – 10 atm Capability
- 1-2 ms Test Time
- 6.1 m Length

Shock Tube Experiments

Second High-Pressure Shock Tube Located at Aerospace Corp.

Aerospace High Pressure Shock-Tube Facility

- 1 – 100 atm Capability
- 600 – 4000 K Test Temperature
- 3 ms Test Time
- 3.5 m Driver and 10.7 m Driven Sections
- 16.2 cm Driven Inner Diameter



THE AEROSPACE CORPORATION

Task 1 – Project Management and Program Planning

Task 1 - Management

Work to be Performed Primarily at and by TAMU

Dr. Eric Petersen (PI)

Flame Speed Team

Flame Speed Grad Student 1

Flame Speed Grad Student 2

Flame Speed UG Student

Shock Tube Team

Postdoctoral Researcher

Shock Tube Grad Student 1

Shock Tube UG Student

Dr. Mark Crofton (Aerospace)

Dr. John Mertens (Trinity)

Task 1 - Management

Interaction and Feedback from Industry Will be Important

Industrial Advisory Panel

Rolls-Royce Canada:
Dr. Gilles Bourque

Siemens:
Dr. Scott Martin
Dr. Ray Laster

General Electric:
Dr. Hasan Karim
Mr. Joel Hall

Power Systems Mfg.:
Dr. Peter Stuttaford
Mr. Khalid Oumejjoud

- Mixture Compositions and Test Conditions

- Possible Contaminant Species

- Important, Related Aspects and Ultimate Usage of Models

Task 2 – Turbulent Flame Speed Measurements

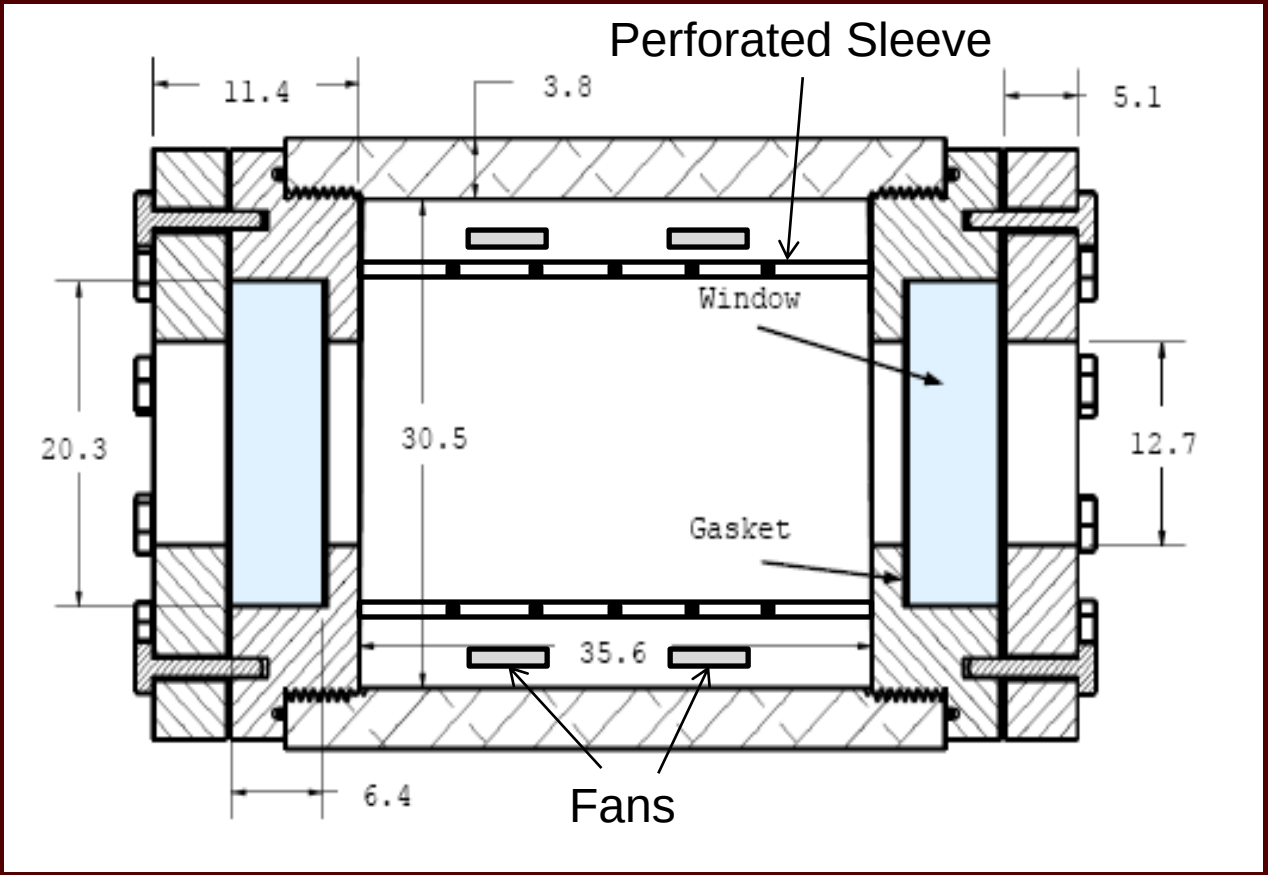
Task 2 – Turbulent Speeds

Turbulent Flame Speed Measurement will Require Development of Techniques

- Utilize Existing Flame Speed Hardware
- Induce Turbulence Using Fans
- Similar to Bomb Experiments of Kido and Coworkers
- Coordinate with Ongoing UTSR Projects Using Other Methods

Task 2 – Turbulent Speeds

Experiment will Use Modified Version of Existing Bomb Facility



Task 3 – Laminar Flame Speeds with Diluents

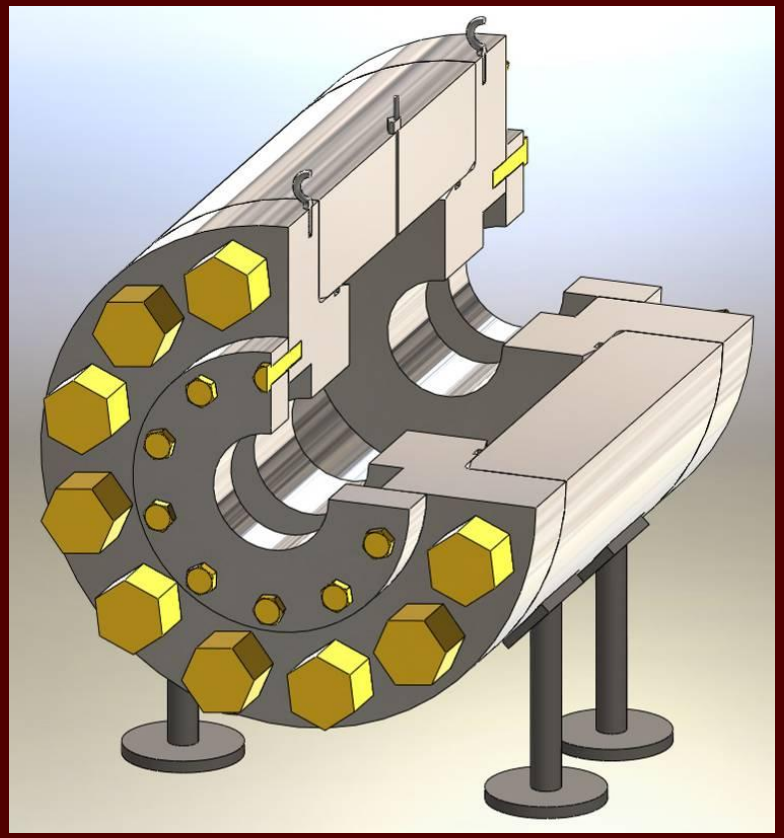
Task 3 – S_L with Diluents

HHC with High Levels of Dilution Will be Studied

- Water, CO_2, N_2, other?
- Laminar Flame Speeds Using Established Methods
- Utilize New Heated Vessel for Water Mixtures
- Pertinent Mixtures of Interest to Industry

Task 3 – S_L with Diluents

New Vessel for High Pressures and High Temps Coming on Line Now



Design Parameters:

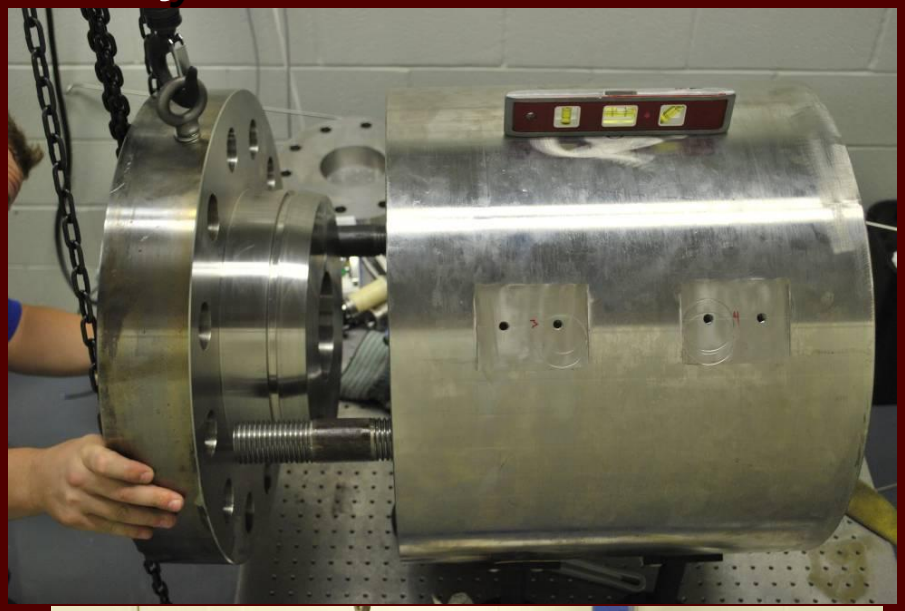
- *Maximum initial pressure:* ***30 atm***
- *Maximum initial temperature:* ***600 K***

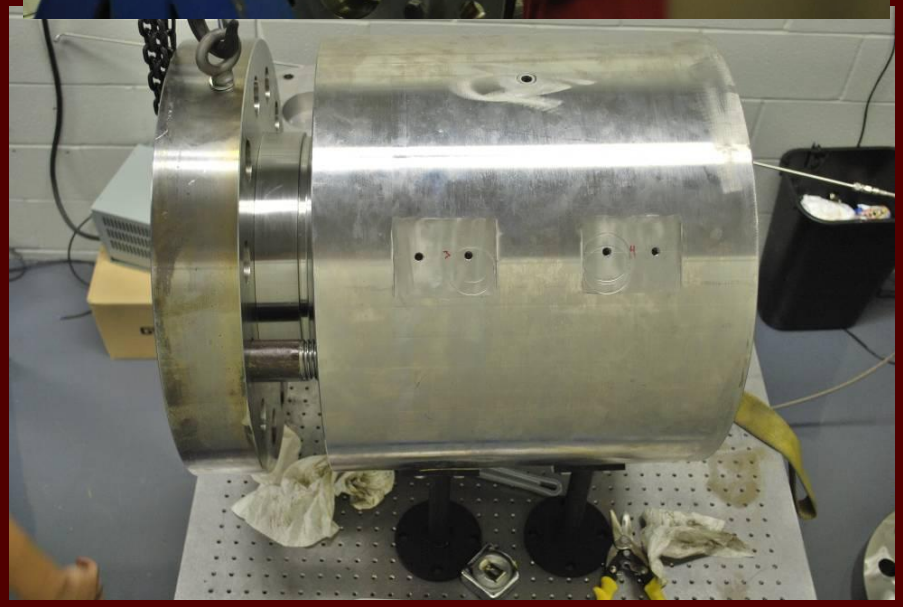
Vessel Dimensions:

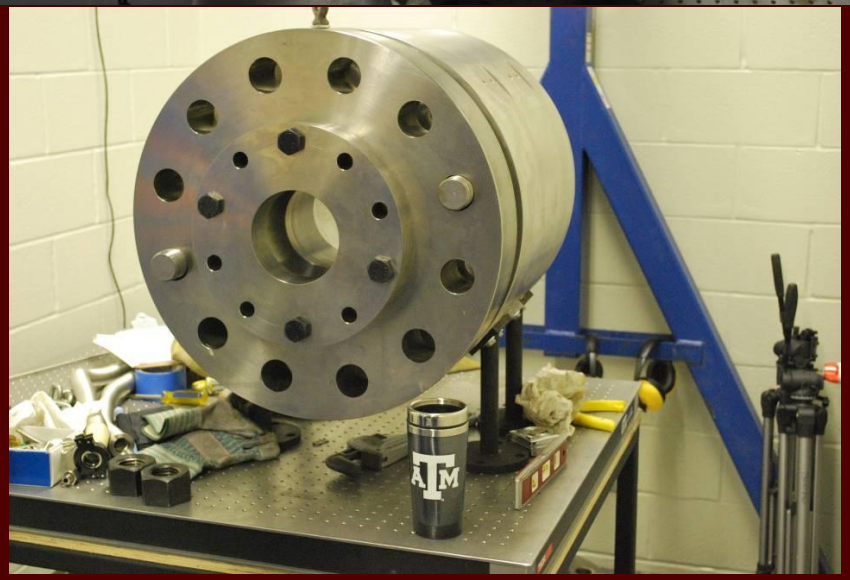
- *Outer Diameter: 54.6 cm*
- *Inner Diameter:* ***31.8 cm***
- *External Length: 63.5 cm*
- *Internal Length:* ***27.9 cm***
- *Window Port Diameter: 12.7 cm*
- *Approximate Weight: 1800 lbs*

Task 3 – S_L with Diluents

Photographs of New Facility Assembly

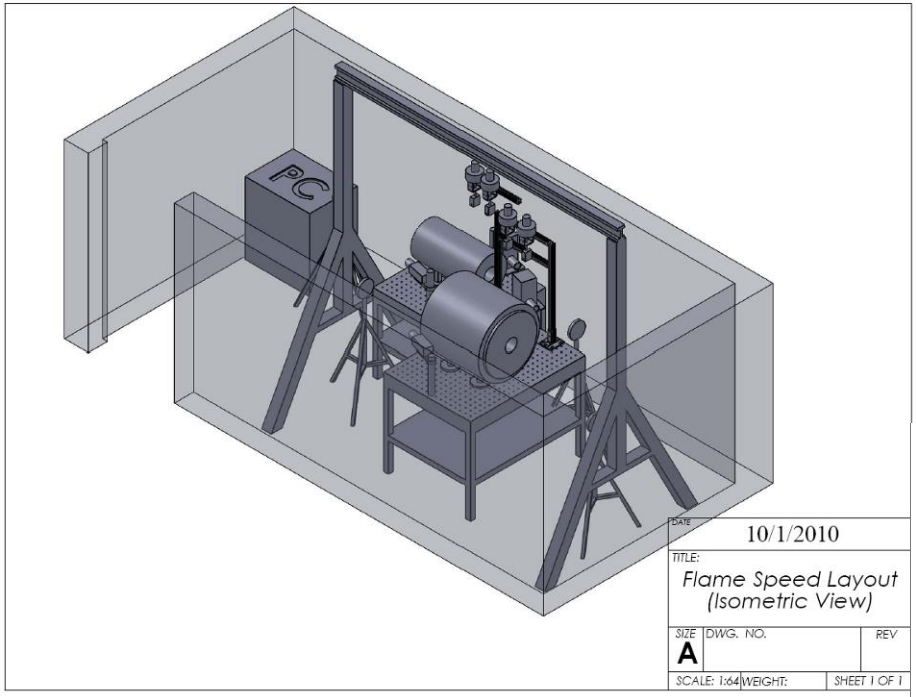


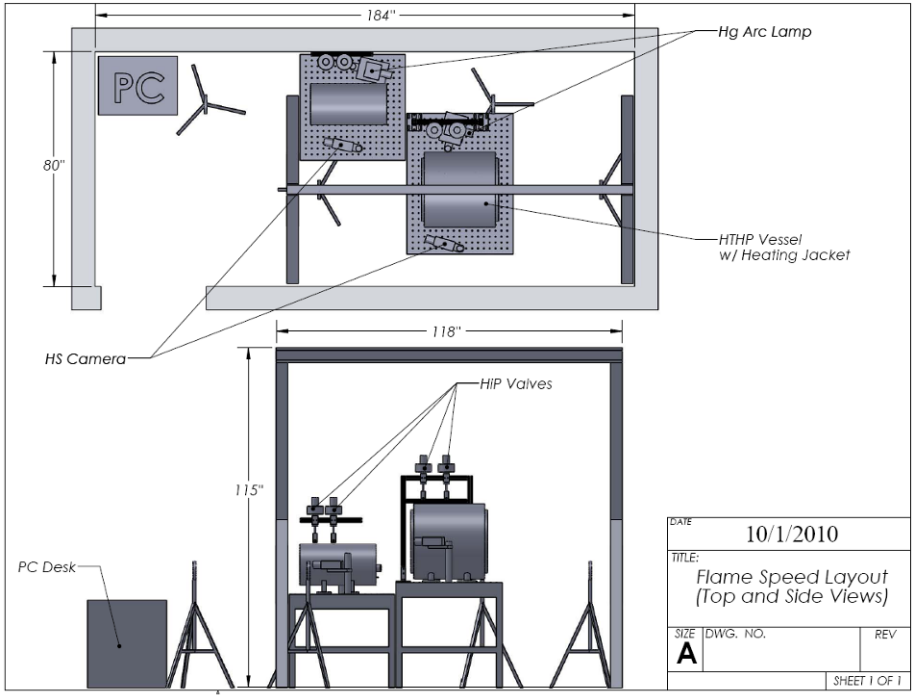




Task 3 – S_L with Diluents

Both Flame Speed Facilities will be in Operation Together





Task 4 – NOx Mechanism Validation Experiments

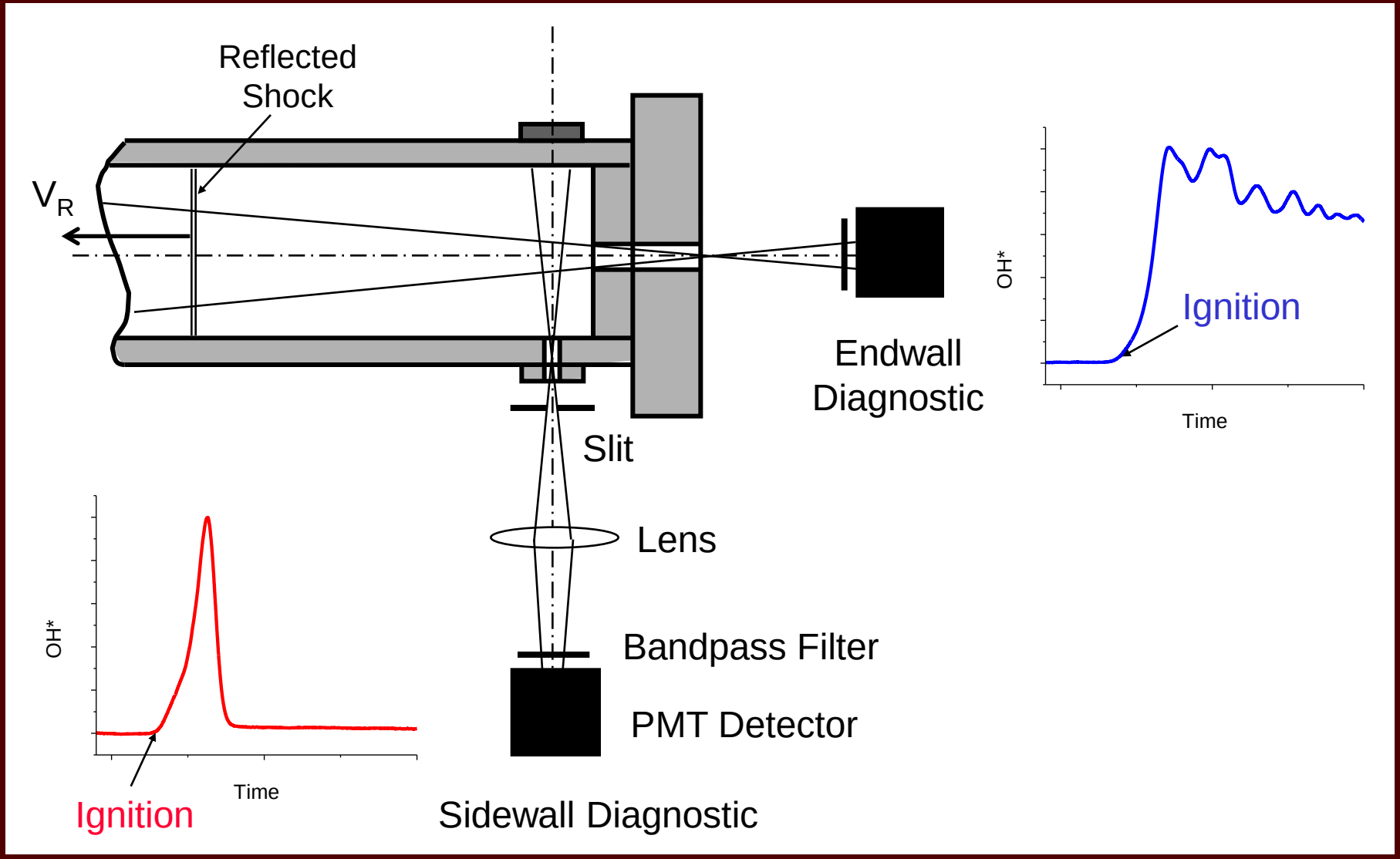
Task 4 – NOx Mechanism

Kinetics Mechanism Validation with NOx at Engine Conditions will be Performed

- Mechanism Based on Galway C5 Mechanism
- Initial NOx Mechanism from Recent Dagaut and Brezinsky Work
- Ignition Times with NOx Precursors for Validation (and EGR-Related)
- Species Time Histories at Dilute Conditions
- Suggest Calibrated Mechanism at End

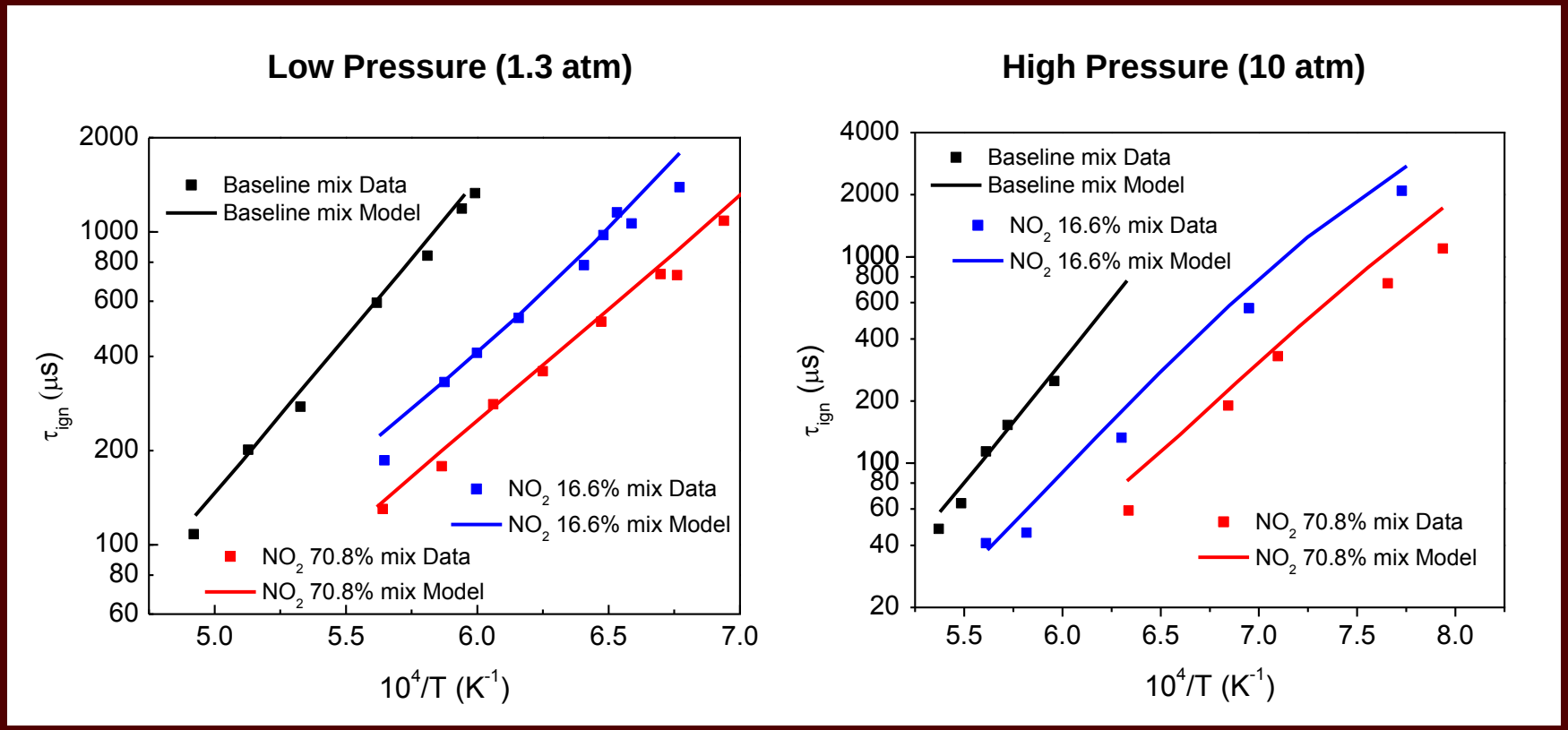
Experimental Apparatus

***Emission** and **Pressure** Measured from Endwall and Sidewall*



Task 4 – NOx Mechanism

Recent Ignition Experiments Using CH_4-Based Mixtures Demonstrate the Concept



Base Mixture: $CH_4 + O_2$ in Argon (97.5%), $\phi = 0.5$

Task 5 – Fundamental NOx Kinetics

Task 5 – NOx Kinetics

Rate Coefficients Will be Measured Directly for Key Reactions in HHC System

- Identify Specific Reaction(s) for Study
- Utilize Laser Absorption of NH (336 nm)
- Requires Very Dilute Mixtures
- Explore NNH Pathways for Prompt NOx

Task 5 – NOx Kinetics

NNH Pathway Will be the Focus of the Detailed Kinetics Experiments

- NNH Mechanism:

$$N_2 + H_2 \rightarrow NNH + H$$

$$N_2 + H + M \rightarrow NNH + M$$

$$NNH + O \rightarrow NO + NH$$

$$NNH + O_2 \rightarrow N_2O + OH$$

- Few Direct Measurements

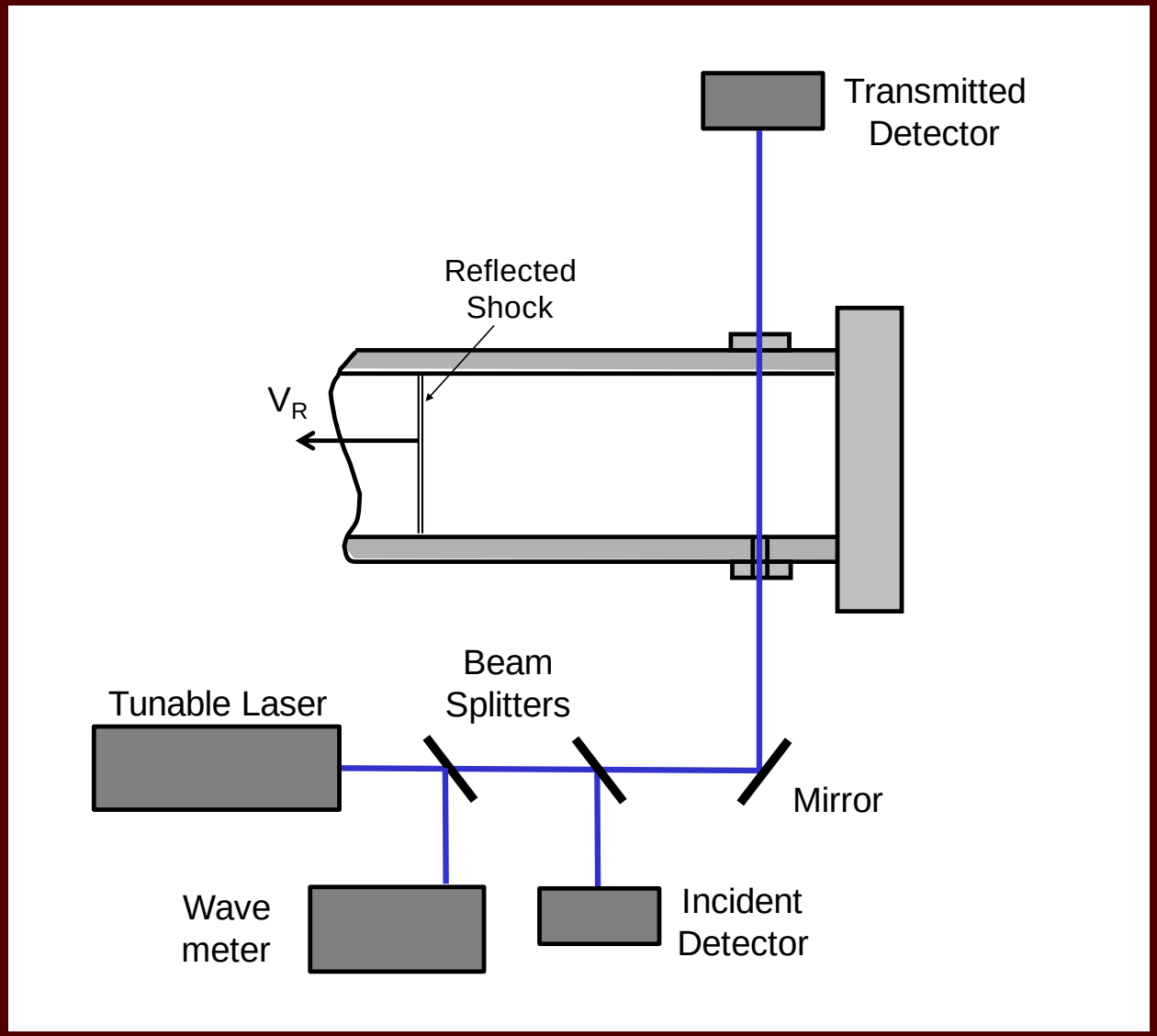
- Study will Focus on

$$N_2 + H + M \rightarrow NNH + M$$

$$\mathbf{NNH + O \rightarrow NO + NH}$$

Task 5 – NOx Kinetics

Laser Absorption of NH at 336 nm Will be Targeted



Task 6 – Effect of Impurities on Syngas Kinetics

Task 6 – Impurities

Trace Impurities Will be Studied Using Both Methods

- Trace Species (H_2S, NH_3, HCN, NOx, HC fuel, other?)
- Laminar Flame Speeds Using Established Methods
- Dilute Shock-Tube Experiments (Ignition and Time Histories)
- Pertinent Mixtures of Interest to Industry

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