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

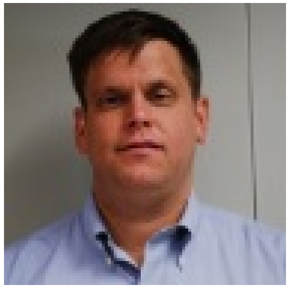
Task 5 – High-Pressure Turbulent Flame Speed Measurements

Project Overview

TAMU Work is a Team Effort of Several People

Dr. Olivier Mathieu

Charles Keesee



Anibal Morones

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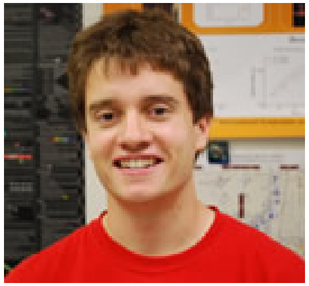


Task 2 – Turbulent Flame Speed Measurements at Atmospheric Pressure

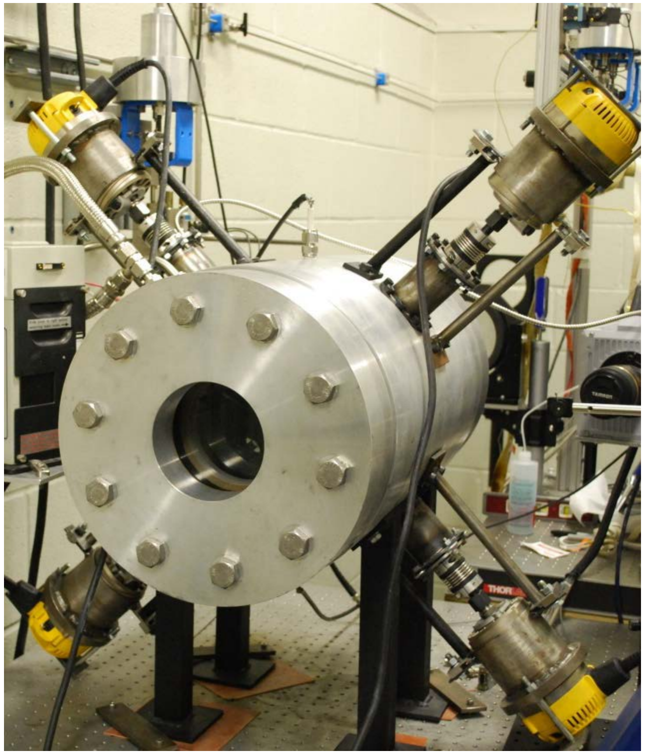
Task 2 – Turbulent Speeds

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
- Detailed Characterization of Existing Conditions with LDV
- Perform Experiments for Syngas Blends at 1 atm Conditions

Task 2 – Turbulent Speeds

Existing 1-atm Rig Characterized for 1 Main Condition



Features:

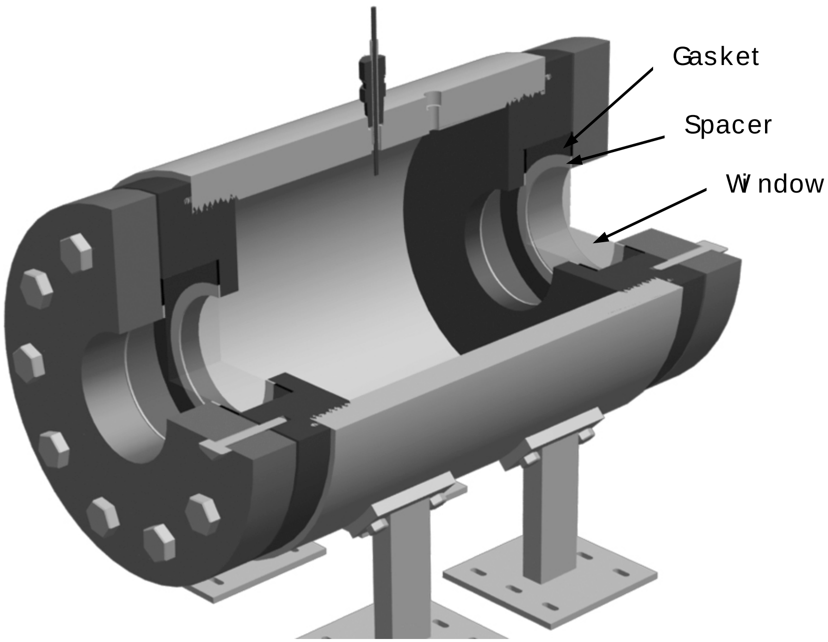
- 7075-T6 Heat-Treated Aluminum
- 4 radial impellers
- Diameter: 30.5 cm
- Length: 35.6 cm
- Window Port Diameter: 12.7 cm
- Maximum initial pressure: 1 atm
- Maximum initial temperature: 298 K

Turbulence:

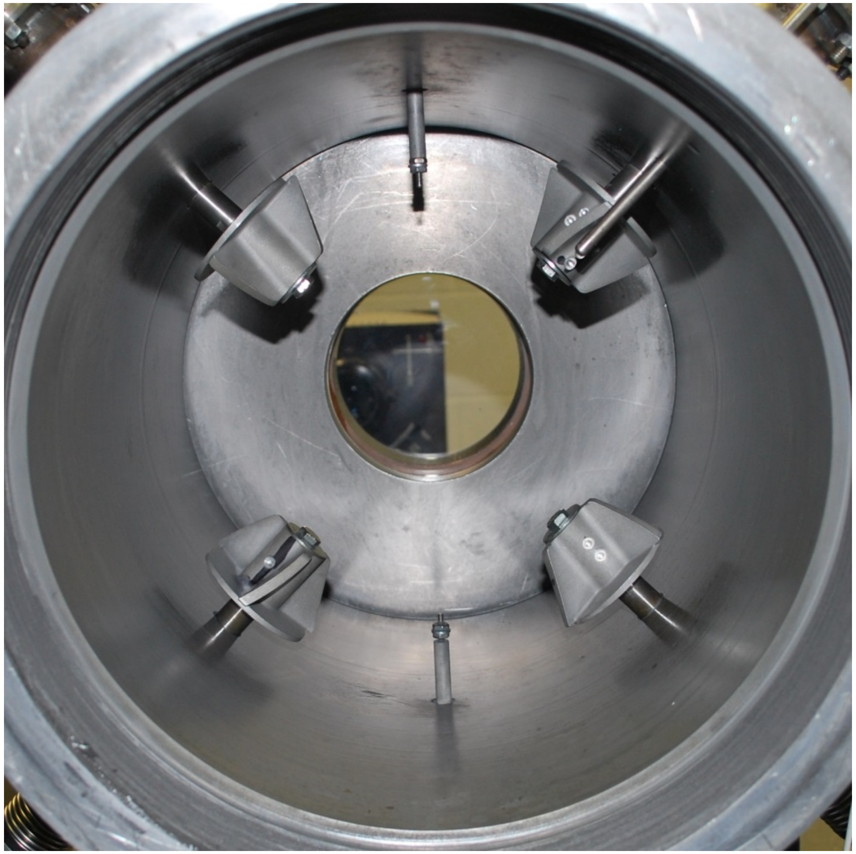
- Intensity: **1.5 m/s rms**
- Integral length scale: **27 mm**

Task 2 – Turbulent Speeds

Existing Rig Has 4 Fans Centrally Located, Added to Original Rig of de Vries (2009)



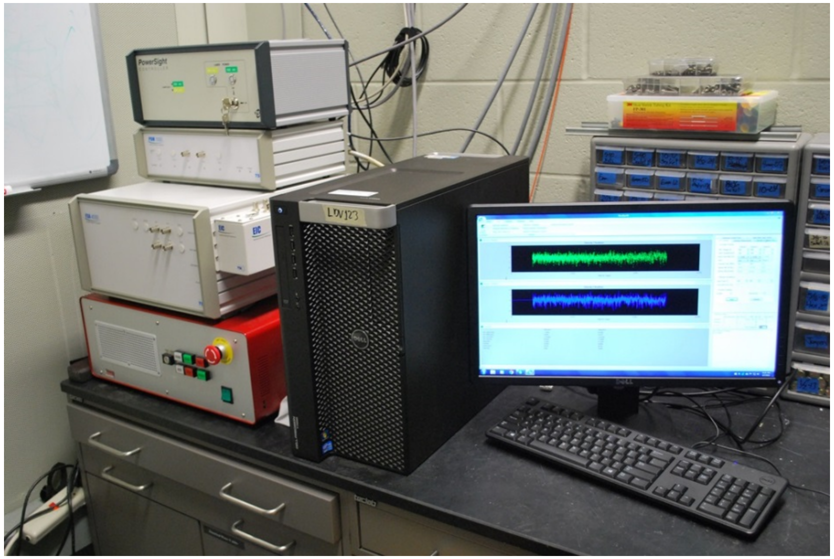
(De Vries 2009)



Task 2 – Turbulent Speeds

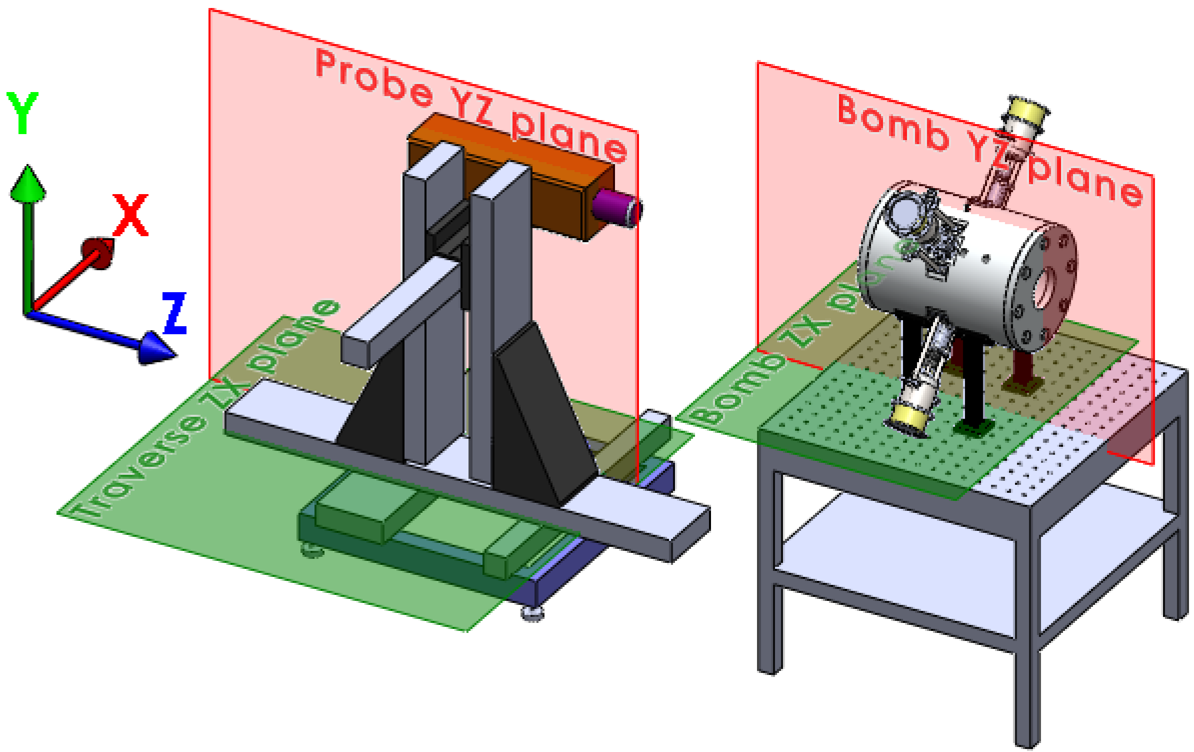
LDV Setup from TSI

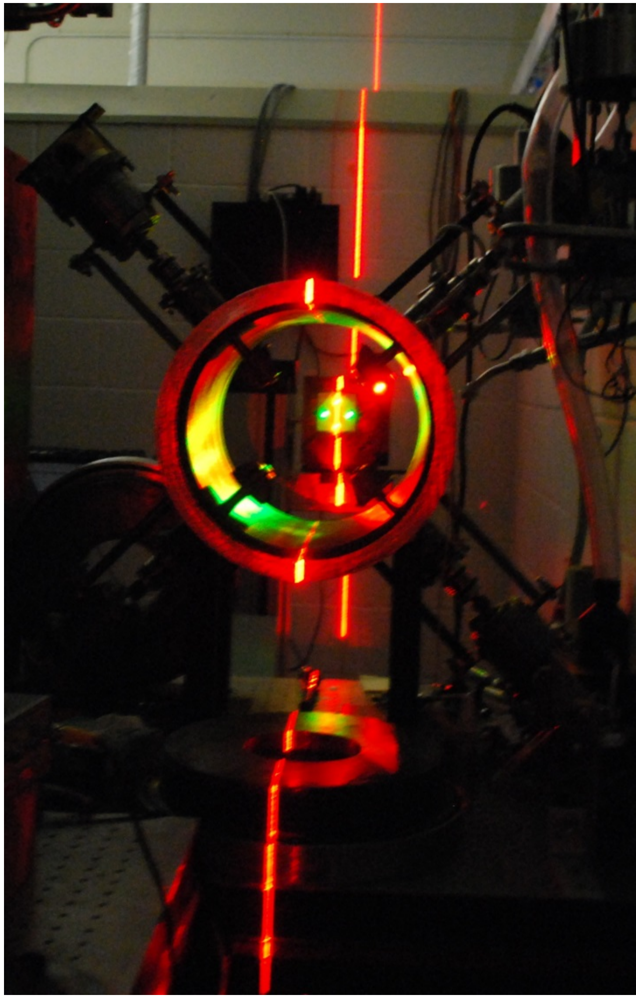
Device	Model
Transceiver	PowerSight TR-SS-2D
Signal processor	FSA4000-2
Traverse	Isel T3DH
Photomultiplier	PDM1000-2SS
Particle Generator	9306
Computer	Dell Precision T7600



Task 2 – Turbulent Speeds

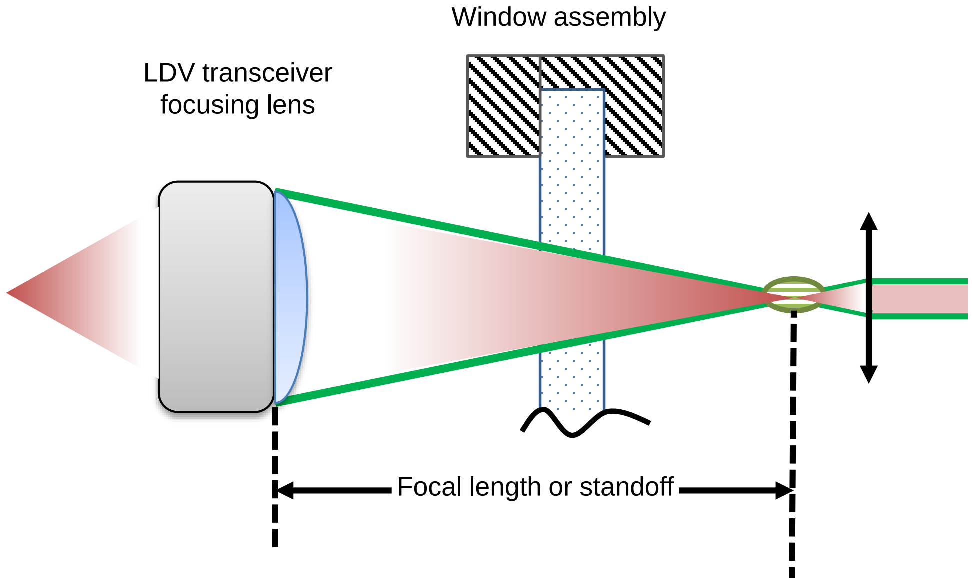
Optics Alignment

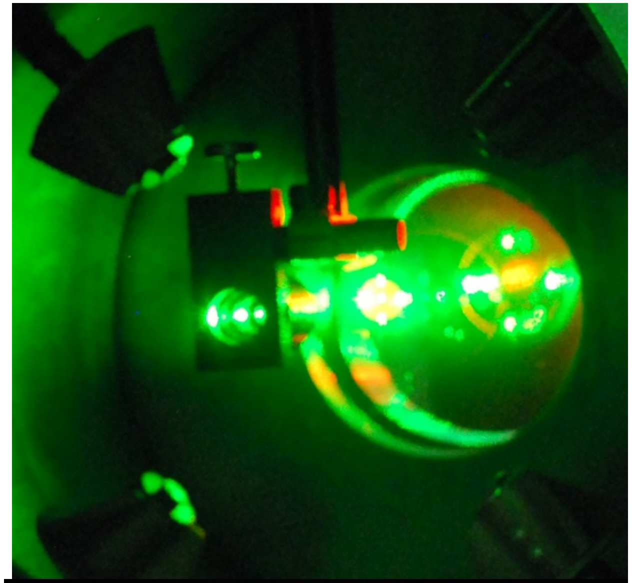


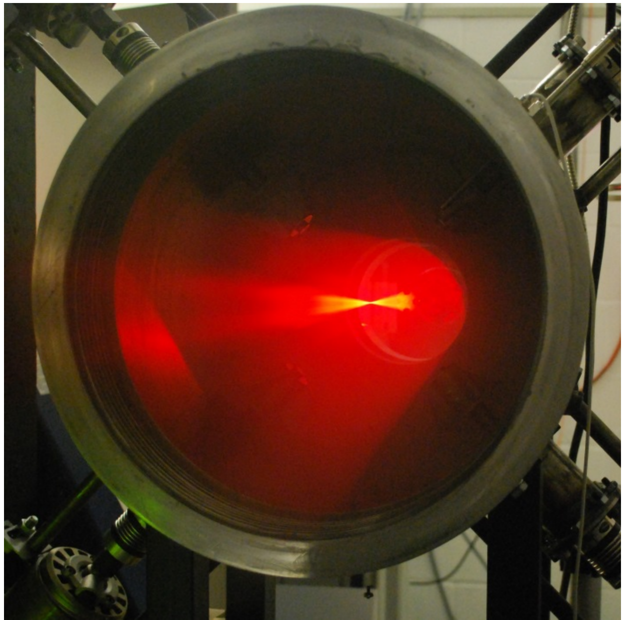


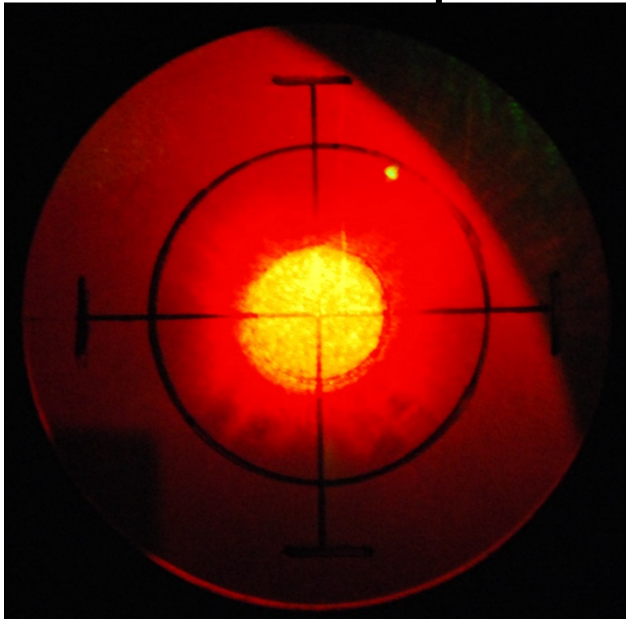
Task 2 – Turbulent Speeds

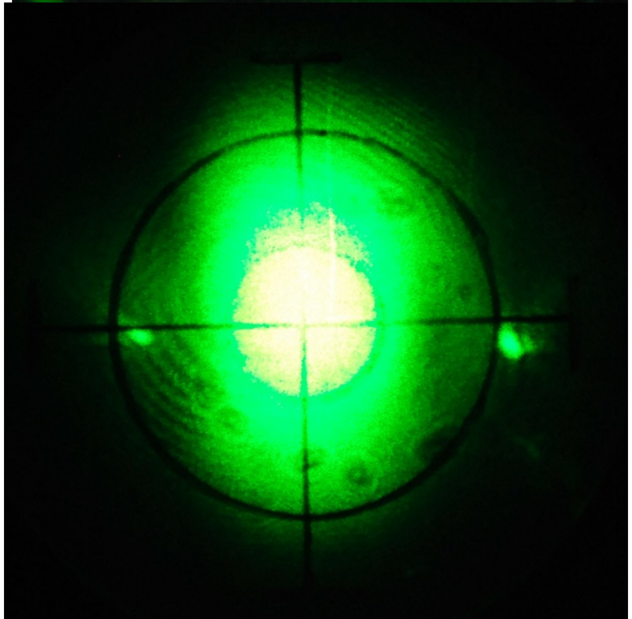
Collocating the probe volume and the receiving optics





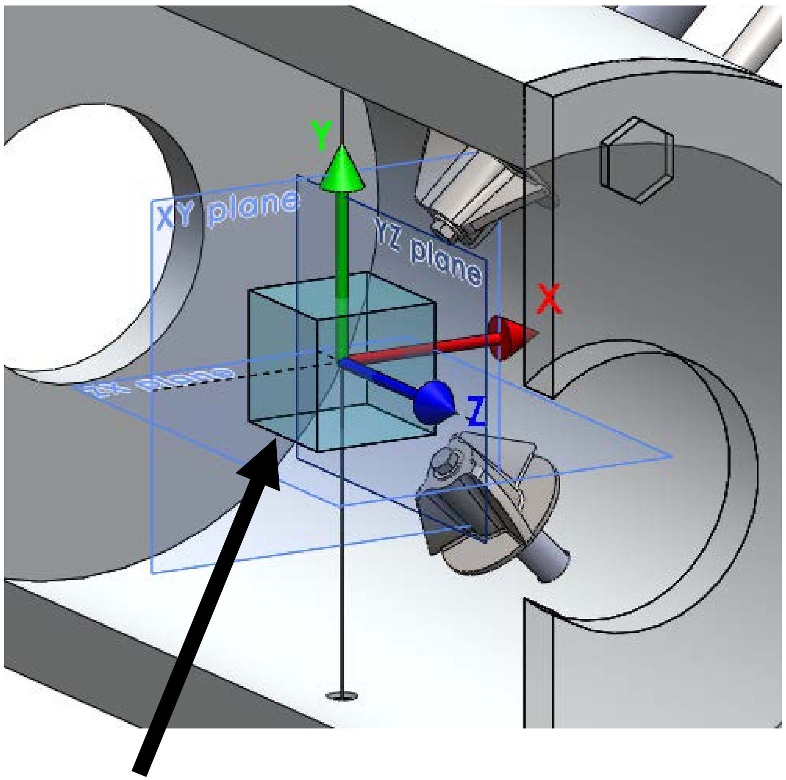




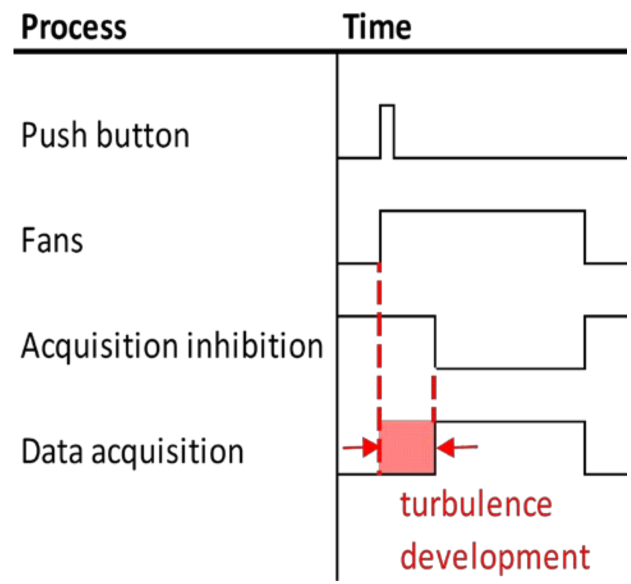


Task 2 – Turbulent Speeds

Timing Sequence Controlled to Capture Turbulence



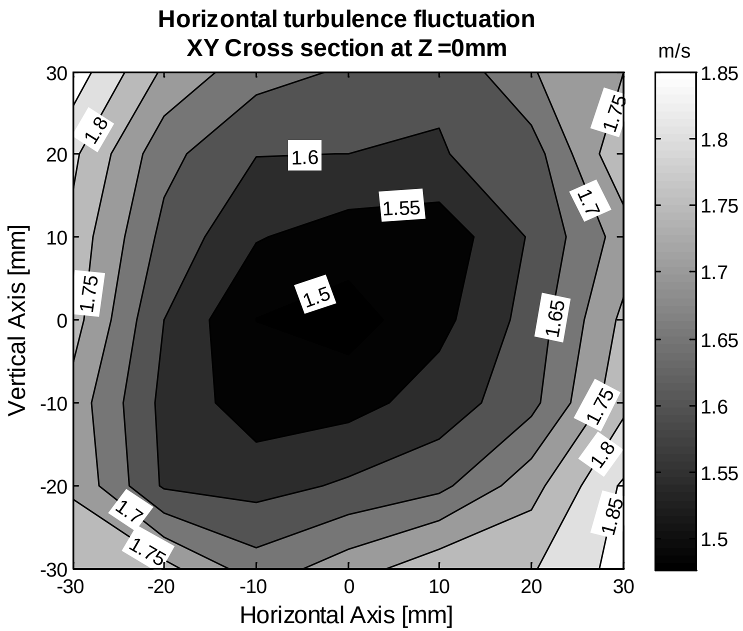
Test region
6×6×6 cm^3

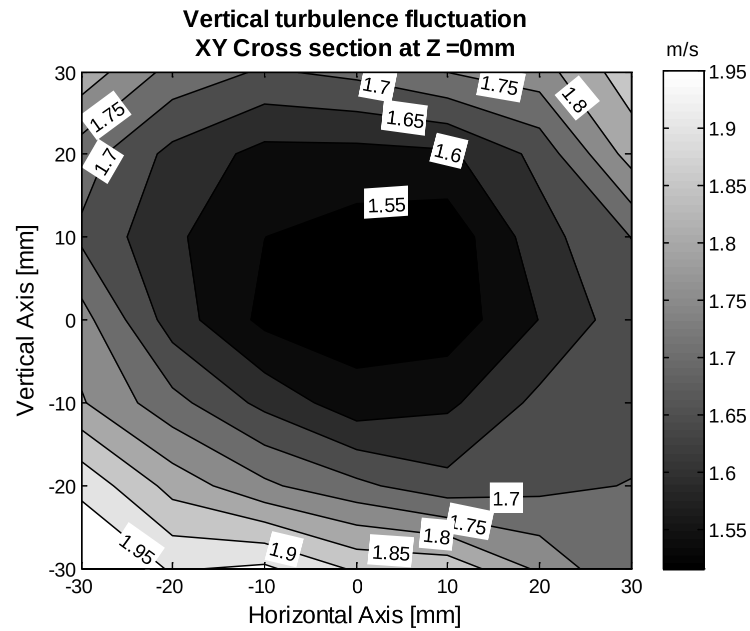


Task 2 – Turbulent Speeds

Turbulent Fluctuation rms Results

$$u_{i,rms}(\mathbf{x}) = \overline{u_i^2}^{1/2}(\mathbf{x}) = \sqrt{\frac{1}{N}\sum_{n=1}^{N}(u_i(t_n;\mathbf{x}))^2}$$

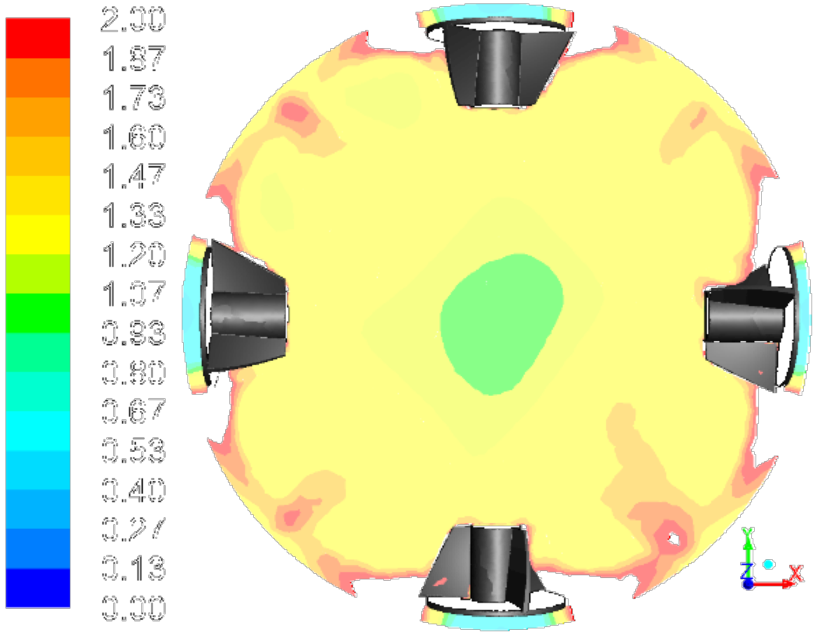


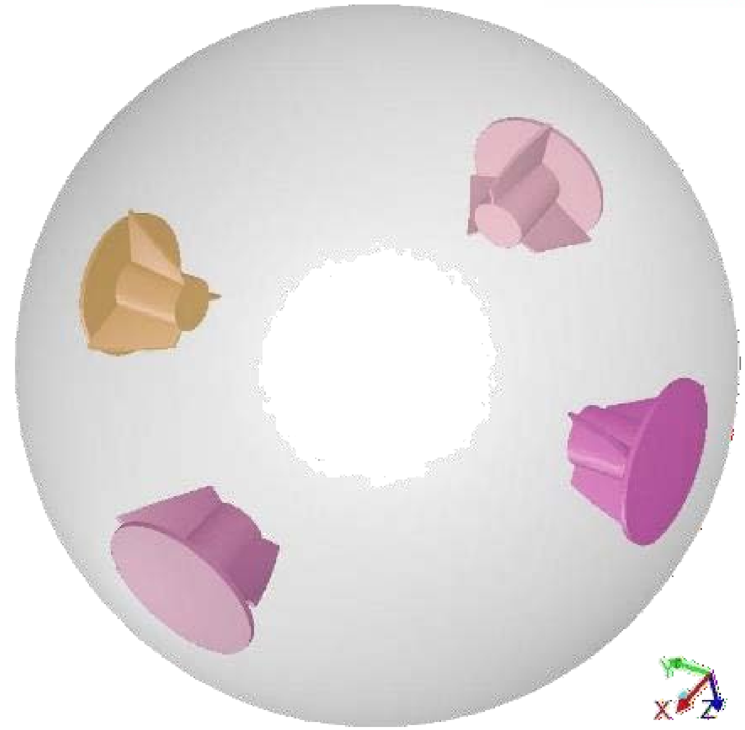


Test region average: horizontal 1.60 m/s; vertical 1.63 m/s

USC simulations

Agreement with numerical model





Reference	Technique	Turbulence fluctuation	Average velocity
(Ravi, Peltier et al. 2013)	PIV	1.48	0.03
(Davani and Ronney 2015)	Simulation	1.63	0.12
This work	LDV	1.62	0.40*

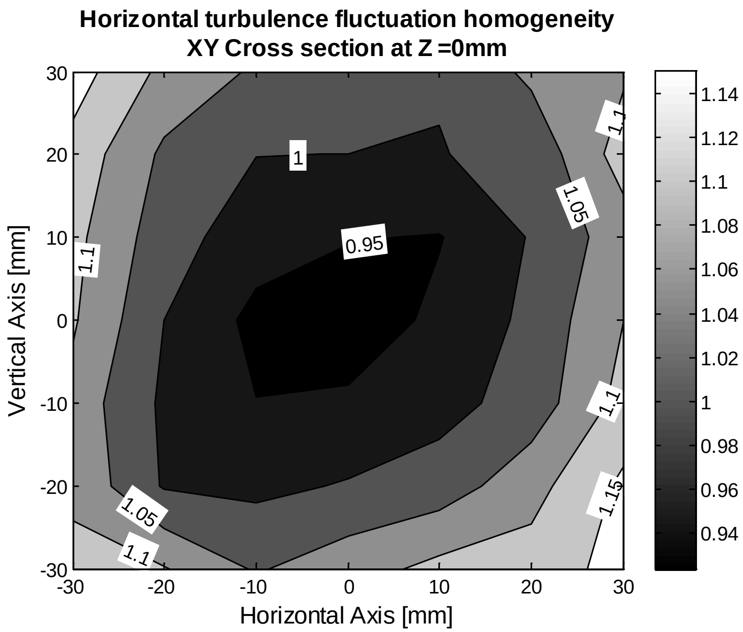
*axial

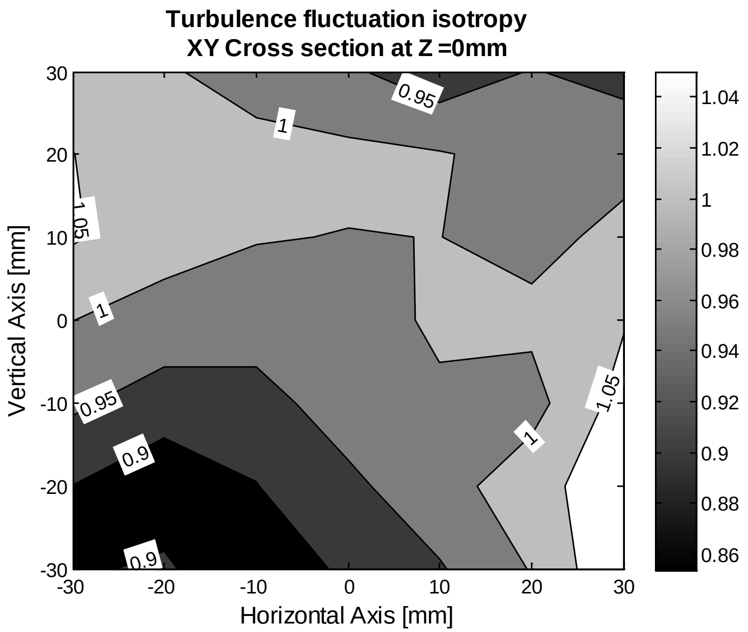
Task 2 – Turbulent Speeds

Turbulence Homogeneity and Isotropy

$$H_i(\mathbf{x}) = \frac{u_{i,rms}(\mathbf{x})}{\overline{u_{i,rms}}}$$

$$I_{xy}(\mathbf{x}) = \frac{u_{x,rms}(\mathbf{x})}{u_{y,rms}(\mathbf{x})}$$





$$\overline{u_{i,rms}} = \frac{1}{M}\sum_{1}^{M} u_{i,rms}(\mathbf{x}_m)$$

Isotropy test region average 0.98

Task 2 – Turbulent Speeds

Integral time scale comparable to flame experiment duration

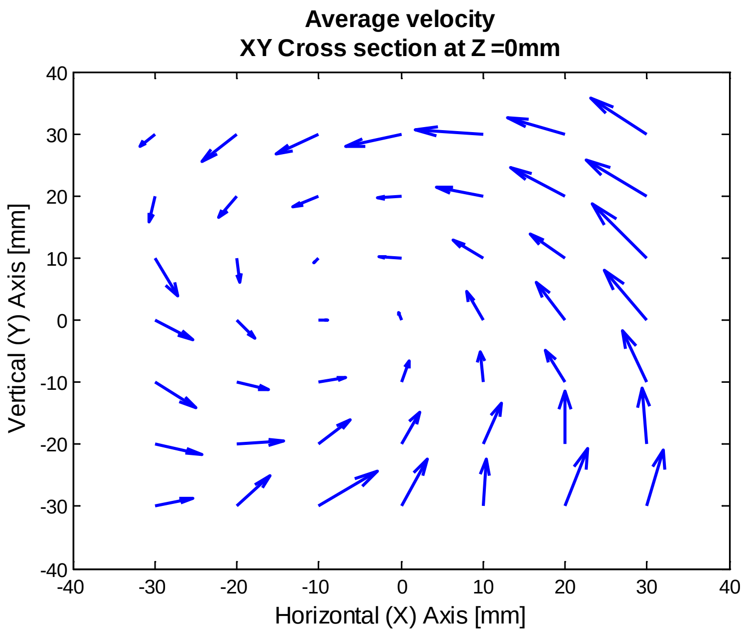
Run #	Location	Integral time scale [ms]		Taylor microscale [ms]	
		Horizontal	Vertical	Horizontal	Vertical
285	0, 0, 0	13.5	12.5	0.60	0.45
1112	30, 0, 0	10.2	8.5	0.53	0.38
943	-30, 0, 0	10.5	8.8	1.66	0.46
1015	0, 30, 0	11.3	11.6	1.36	2.09
1040	0, -30, 0	13.2	15.9	1.9	1.95
436	0, 0, 30	12.4	11.4	1.85	1.95
1592	0, 0, -30	10.1	9.9	1.43	1.43

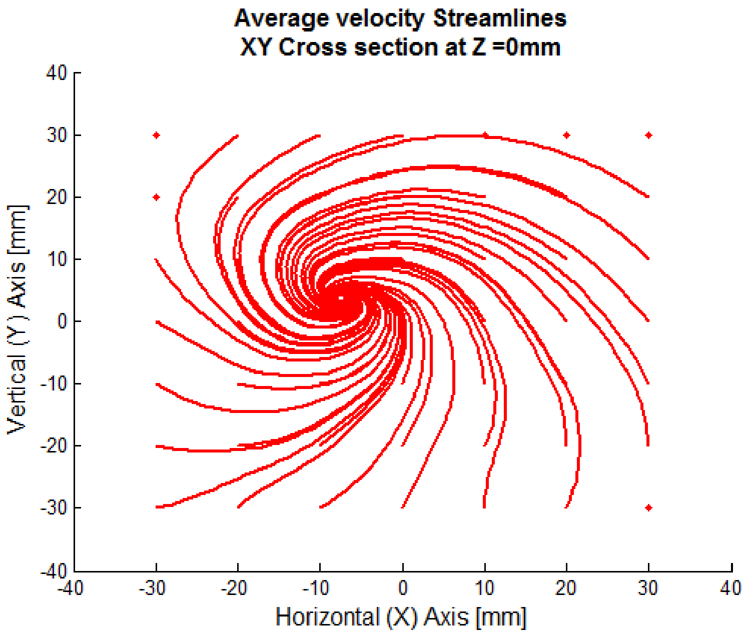
$$\Lambda_t \equiv \int_0^\infty r(\tau)\, d\tau$$

$$\lambda_t^2 \equiv -2 \Big/ \left.\frac{\partial^2 r}{\partial \tau^2}\right|_{\tau=0}$$

Task 2 – Turbulent Speeds

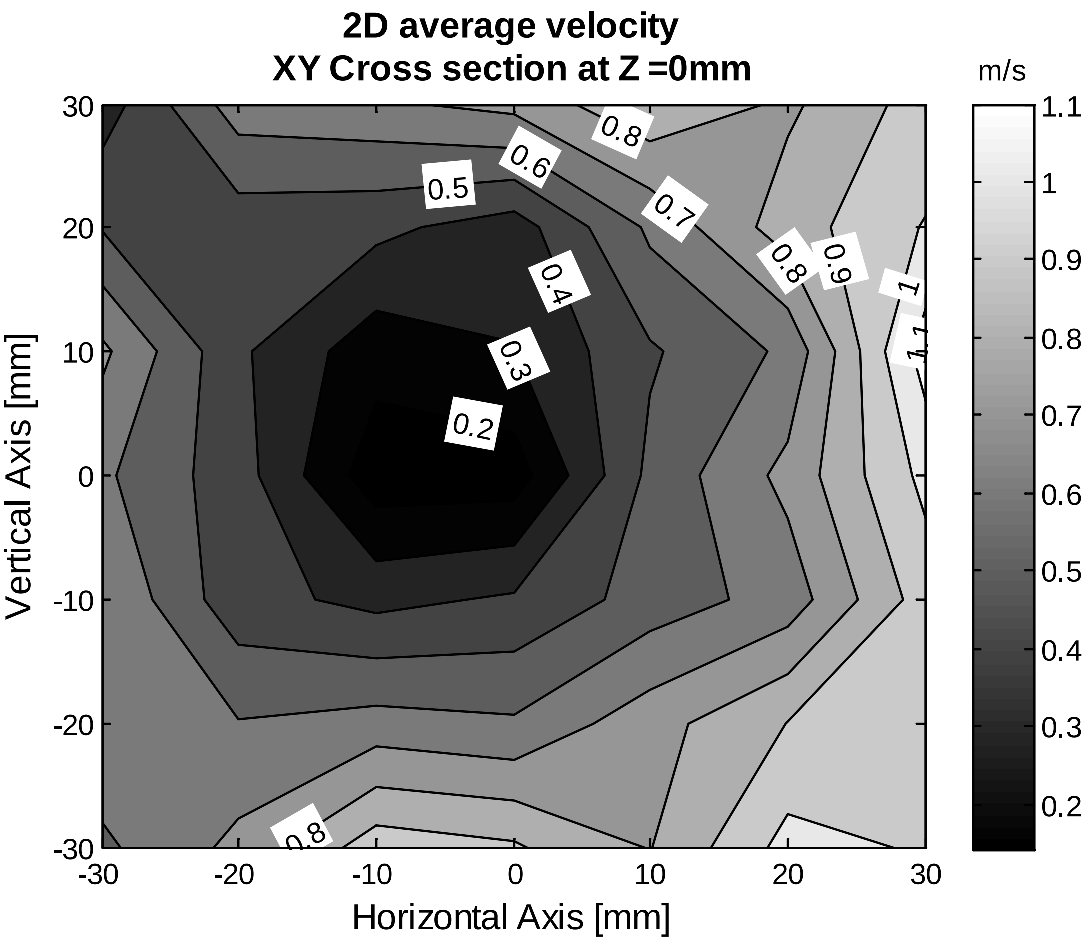
Results Indicate a (Slow) Overall Vortex Pattern





Task 2 – Turbulent Speeds

2-D Average Velocity Results



- Radial pattern
- Test region average 0.58 m/s

Task 2 – Turbulent Speeds

1. Results agree qualitatively with the previous work of Ravi (2013).
2. HIT turbulence confirmed
3. Extension of measurements to a 3-D region revealed unfavorable characteristics previously missed.
4. The axial component found to have a resultant mean flow of 0.4 m/s.
5. A regular polyhedron fan distribution is advised

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

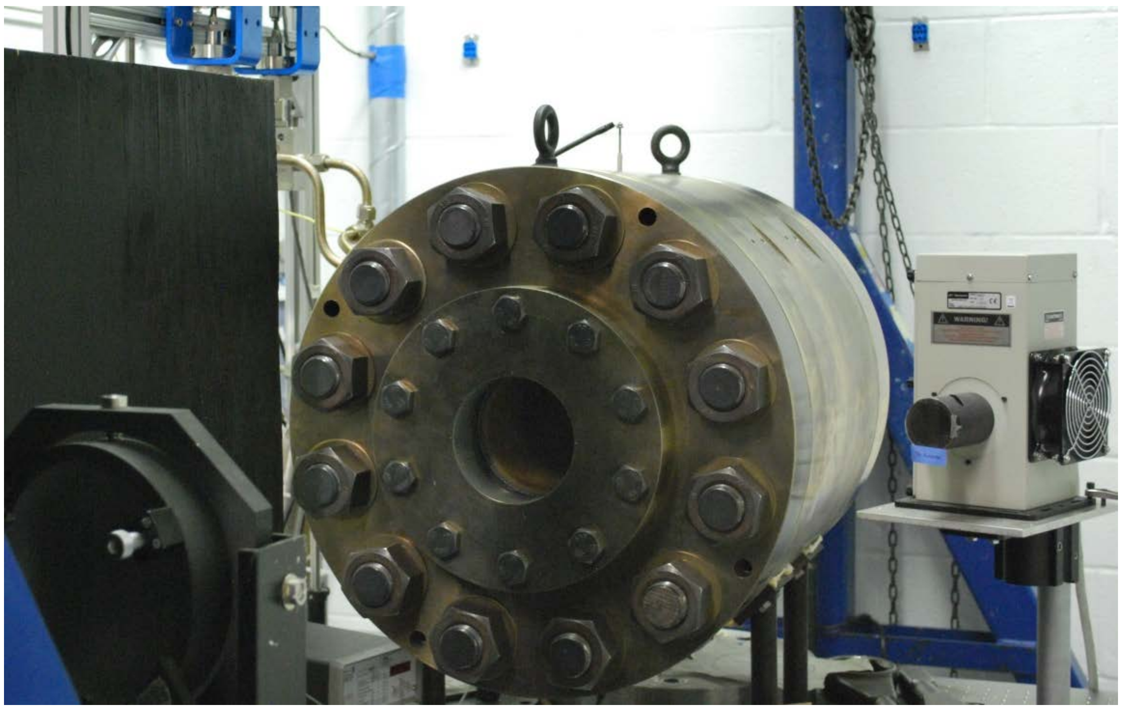
Update Today Will Focus on ***2 Main Projects***

1. **H_2S Impurity** Effect on Laminar Flame Speeds for Coal Syngas

2. **H_2S Oxidation Kinetics** and Shock-Tube Measurements

Task 3 – Impurity Effects

High-Temperature, High-Pressure Vessel Used for Laminar Flame Experiments



Vessel Internal Dimensions:

31.8 cm	Diameter
28 cm	Length
12.7 cm	Window Diameter

Task 3 – Impurity Effects

***Laminar Flame Speed** Measurements Performed With H_2S Impurity*

- Baseline "coal" syngas: **60% CO / 40% H_2**
- Equivalence ratio Sweep
- Pressure: **1 atm**
- H_2S: 1% by Volume
- **Argon** instead of N_2

Task 3 – Impurity Effects

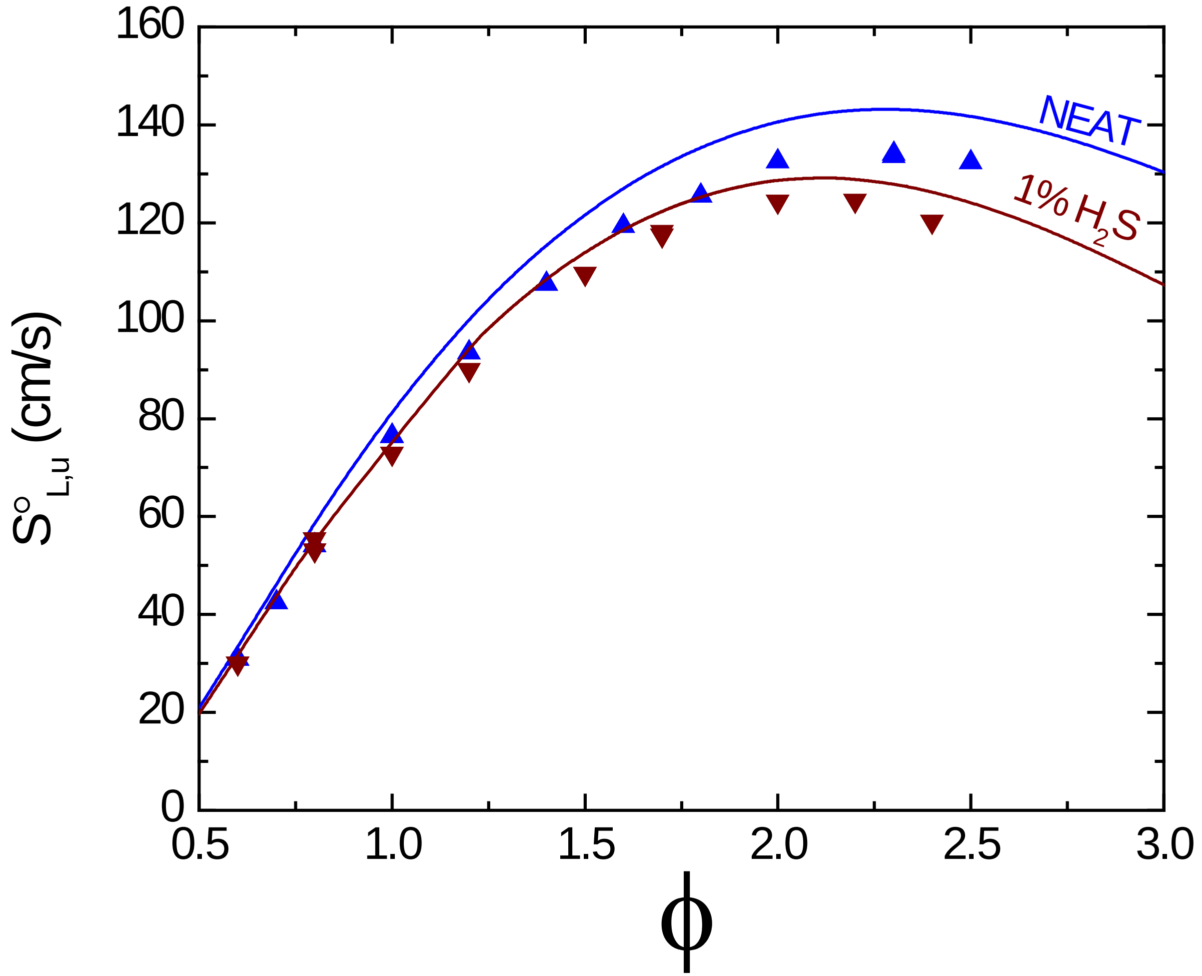
Mixtures Investigated for Flame Speed Study

Mixtures Investigated (Mole Fraction)						
Mixture	Fuel			Oxidizer		
	CO	H_2	H_2S	O_2	N_2	Ar
Coal - Neat, Air	0.6	0.4	-	0.21	0.79	-
Coal - Neat, Argon	0.6	0.4	-	0.145	-	0.855
Coal - 1% H_2S, Argon	**0.594**	**0.396**	**0.01**	**0.145**	**-**	**0.855**

O_2/Ar ratio chosen to match Flame Temp with air over same ϕ range

Task 3 – Impurity Effects

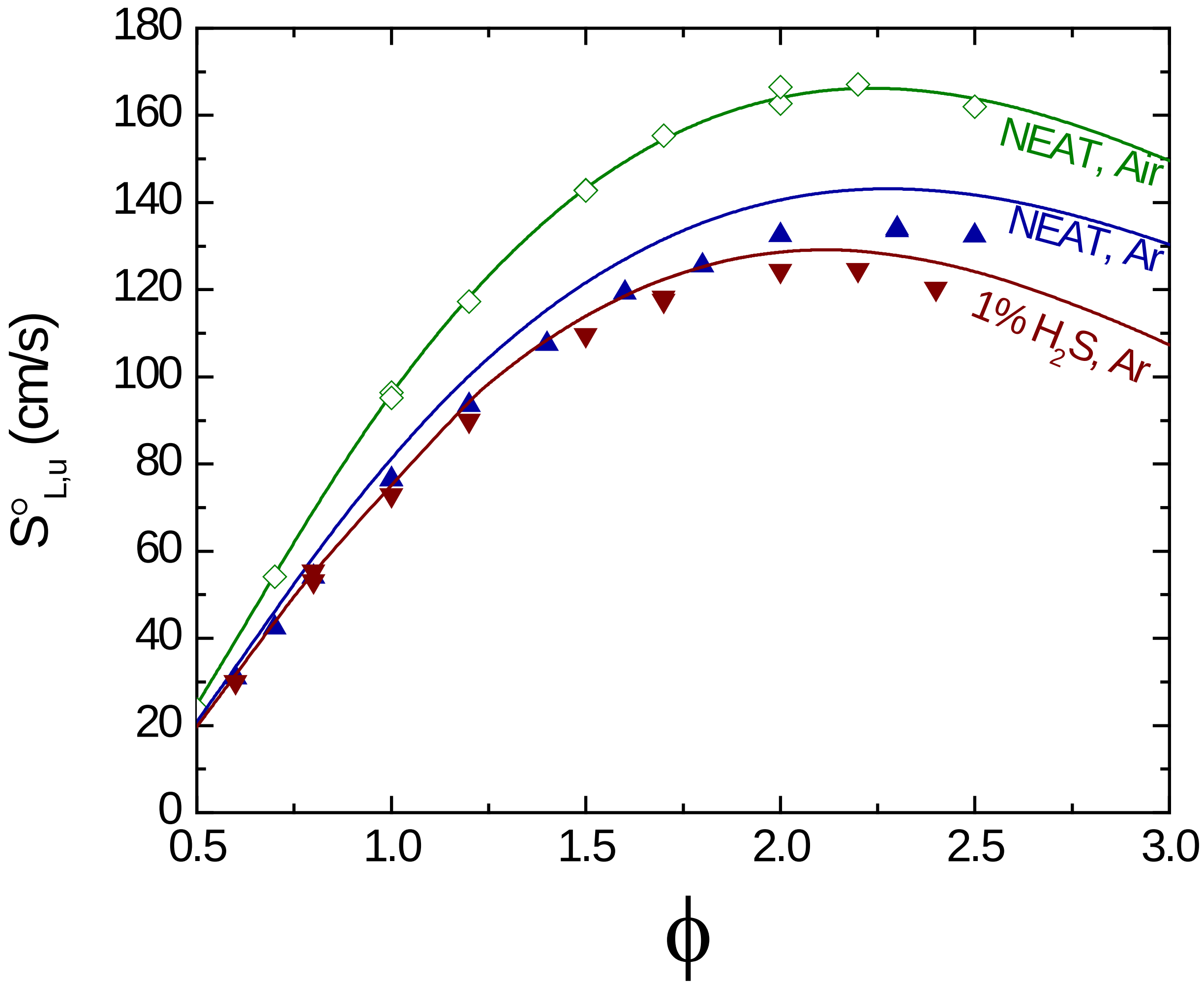
H_2S Has Small Effect and Only for Rich Mixtures



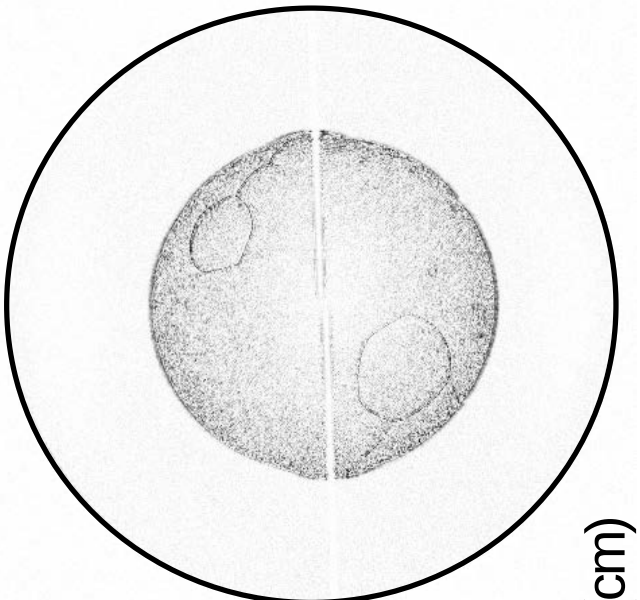
Model: NUIG mechanism with TAMU H_2S kinetics

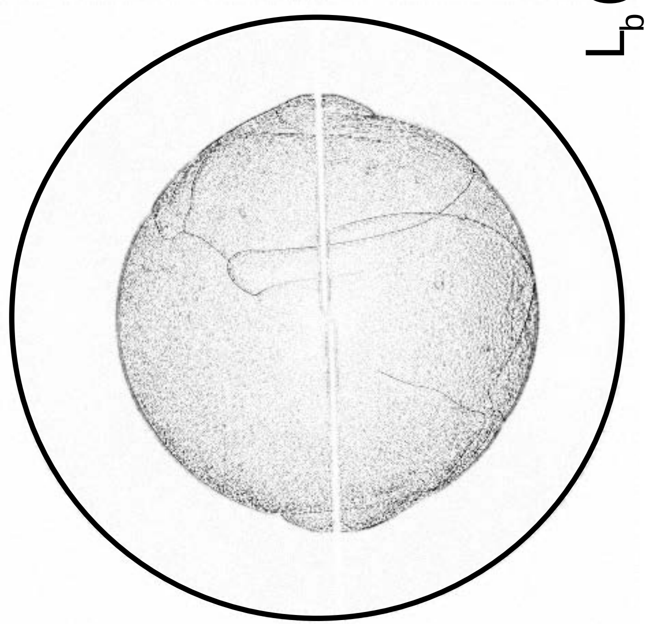
Task 3 – Impurity Effects

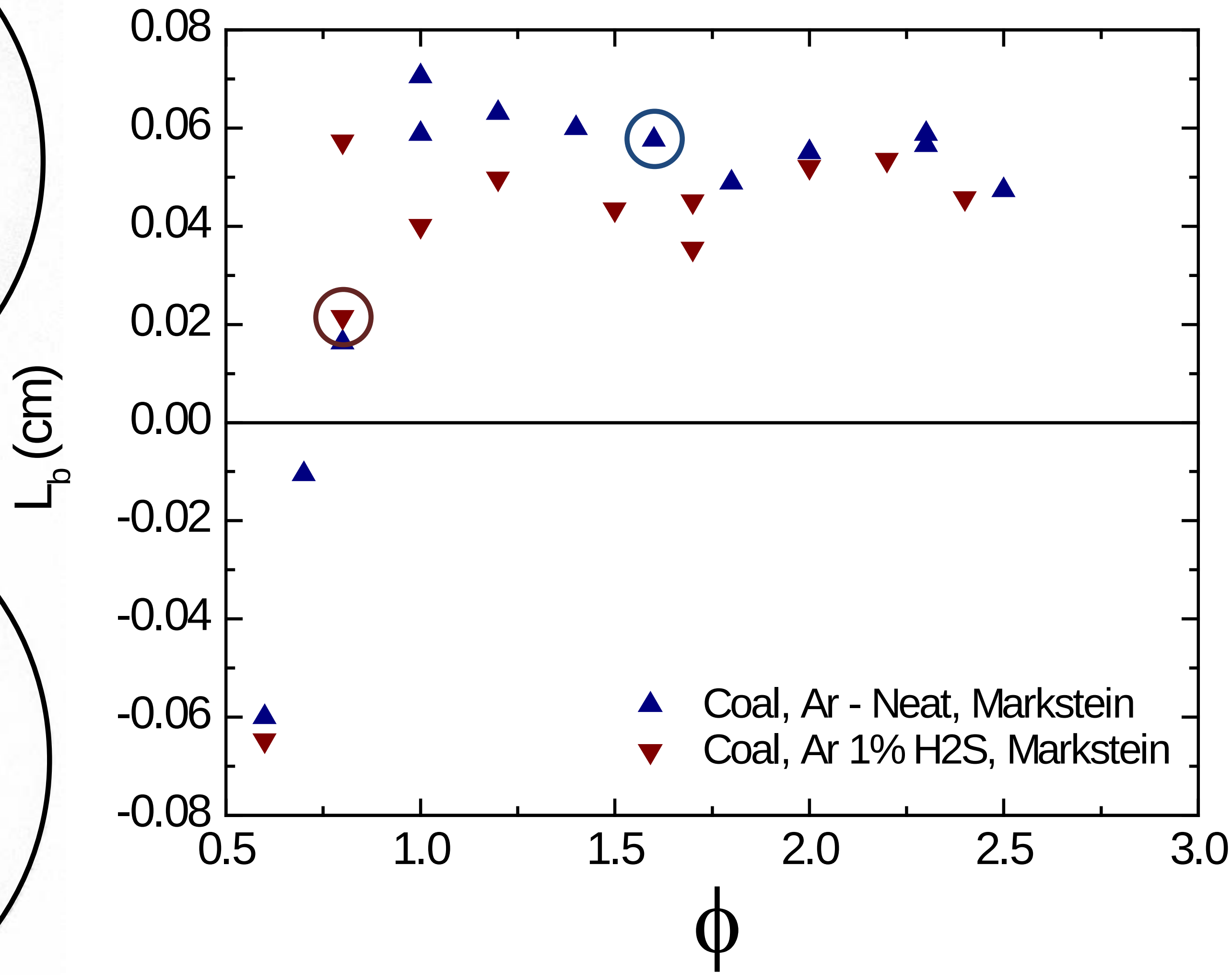
Argon-Based Flame Speeds Noticeably Lower than N_2-Based Ones



Argon-Diluted Mixture Markstein Lengths

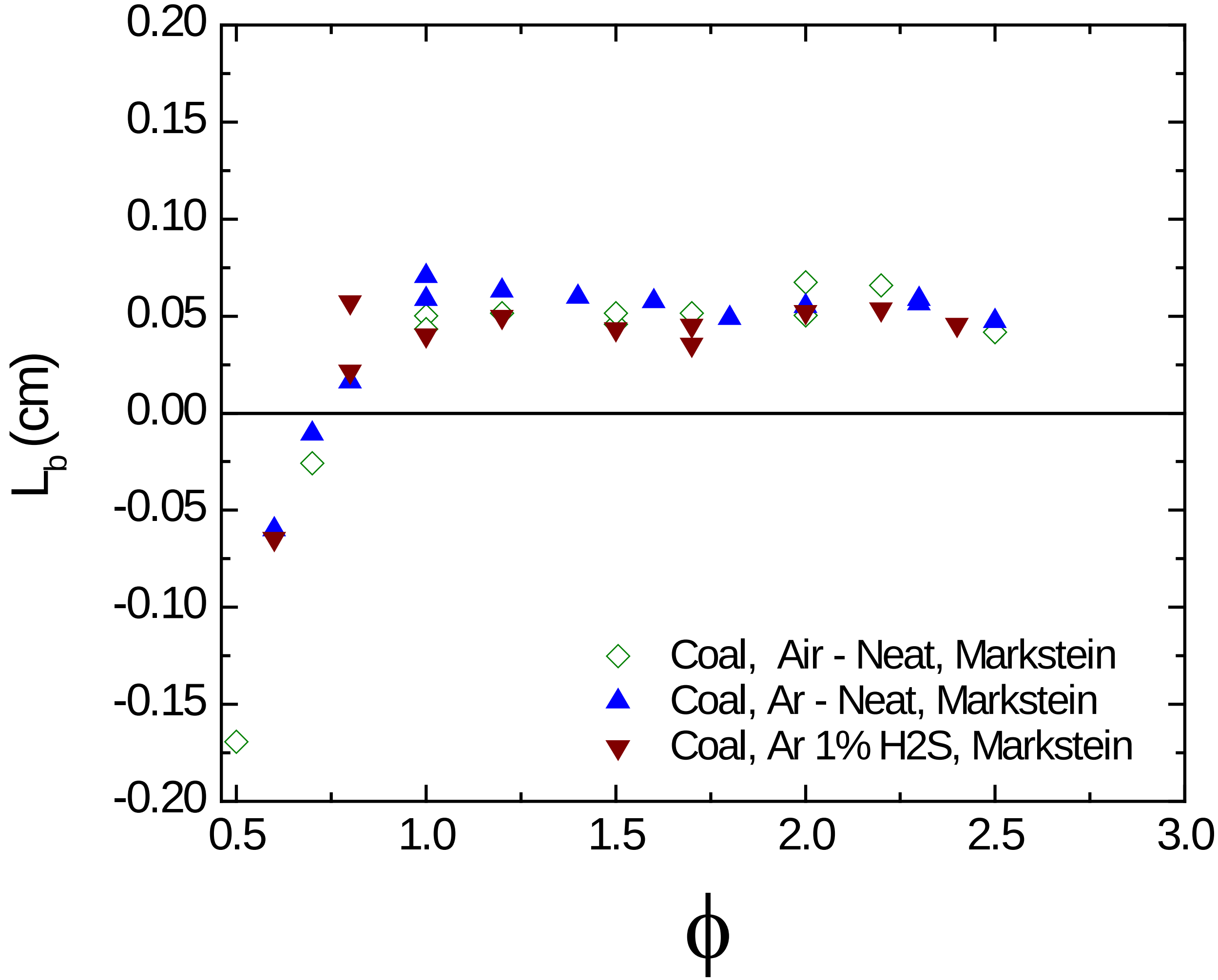






Task 3 – Impurity Effects

Air and Argon/O_2-Based Markstein Lengths are Similar



Shock-Tube *Experiments Focused on H_2S Oxidation*

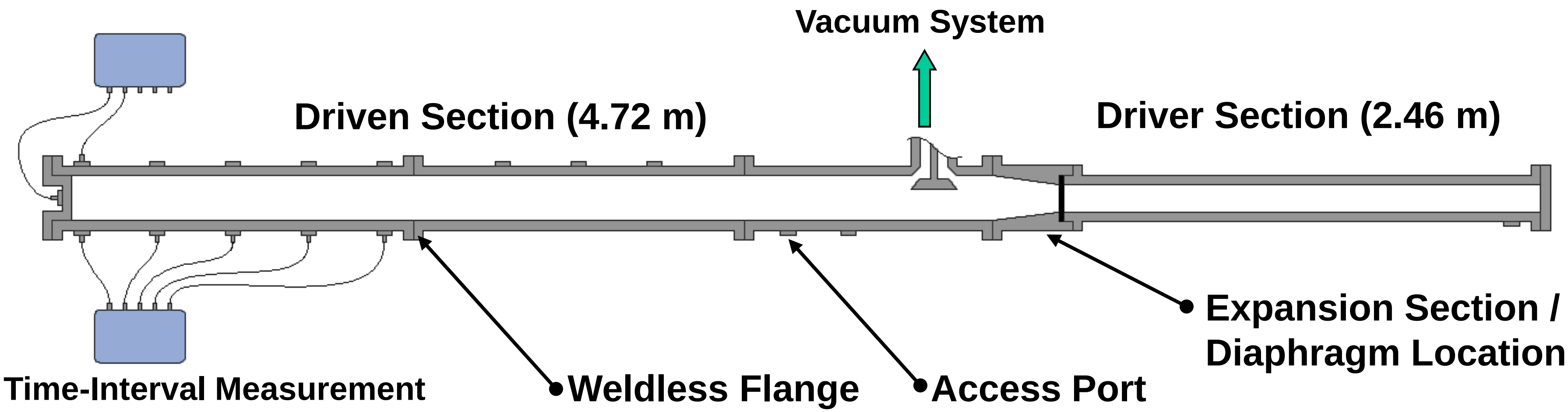
- H_2S – O_2 – Argon mixtures (98% Ar dilution)
- Equivalence ratios: **0.5, 1.0, 1.5**
- Pressure: **1.7 atm**
- Ignition delay times
- Water concentration time histories

Task 3 – Impurity Effects

High pressure shock-tube facility at Texas A&M

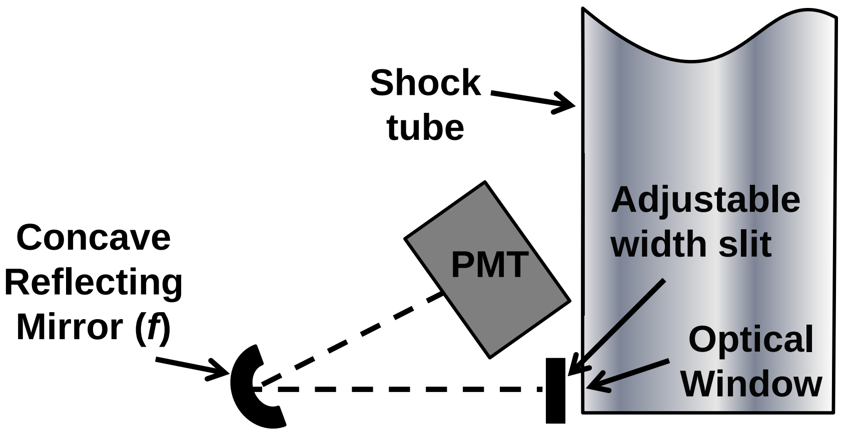
High-Pressure Shock-Tube Facility

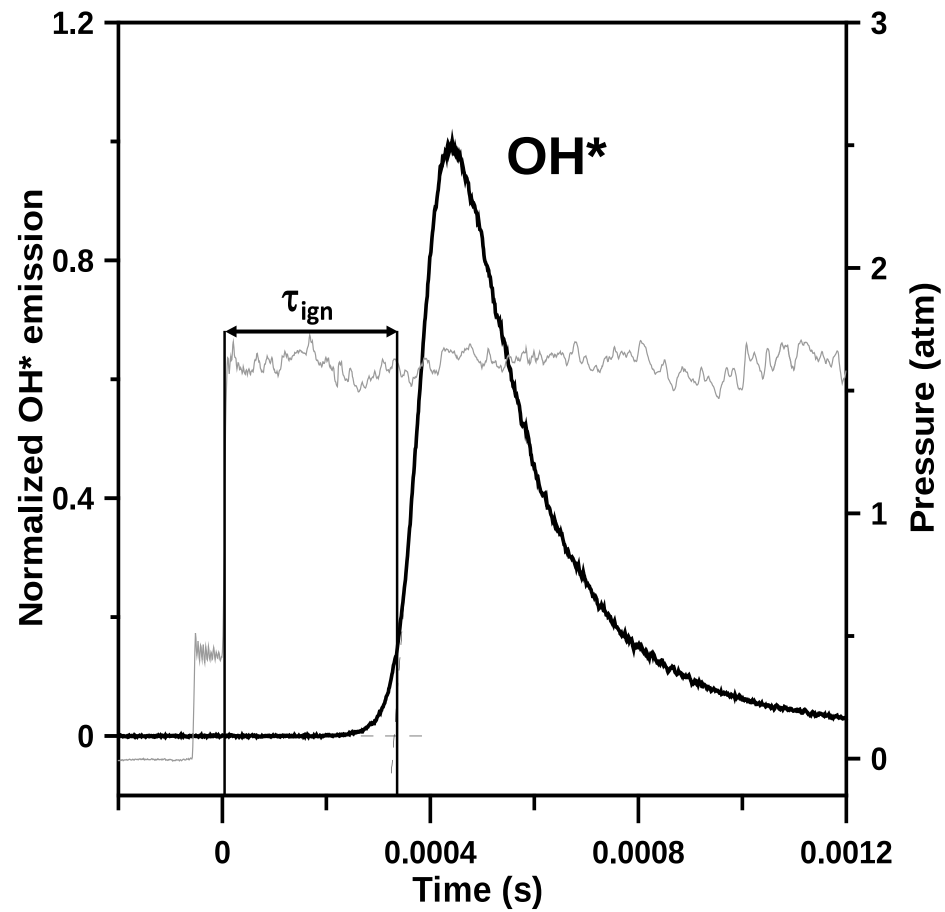
- 1 – 100 atm Capability
- 600 – 4000 K Test Temperature
- Up to 20 ms Test Time
- 2.46 m Driver and 4.72 m Driven
- 15.24 cm Driven Inner Diameter



Task 3 – Impurity Effects

Ignition Delay Time Obtained from OH Time History*



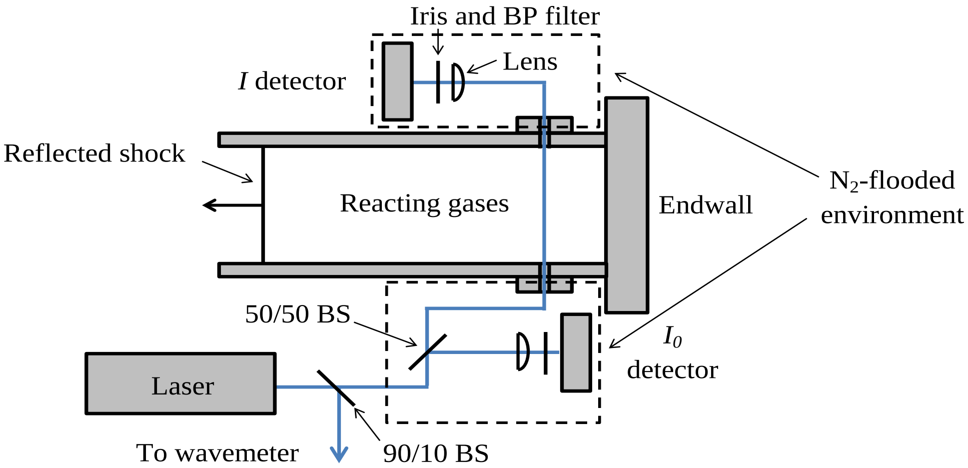


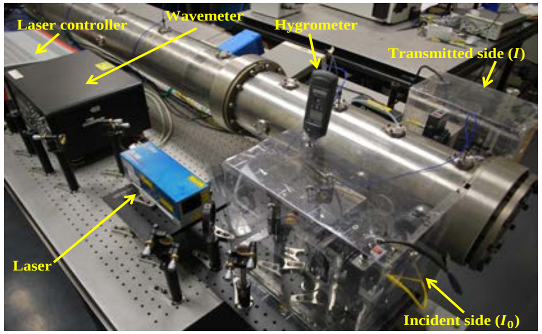
- $A^2\Sigma^+$ (OH*) light at 307 nm
- Highly Diluted Mixtures (98% Ar)

Task 3 – Impurity Effects

Tunable laser diagnostic used for transient H_2O concentrations

- Control and monitoring of laser
  - Toptica Photonics DL 100: CW, narrow width laser
  - Toptica Photonics DC 110: current and temperature control
  - Burleigh WA-1000: monitoring of laser wavelength
- Common mode rejection
- Lexan enclosures
  - Purged by N_2
  - Monitored by hygrometer
  - < 0.1% RH for all experiments

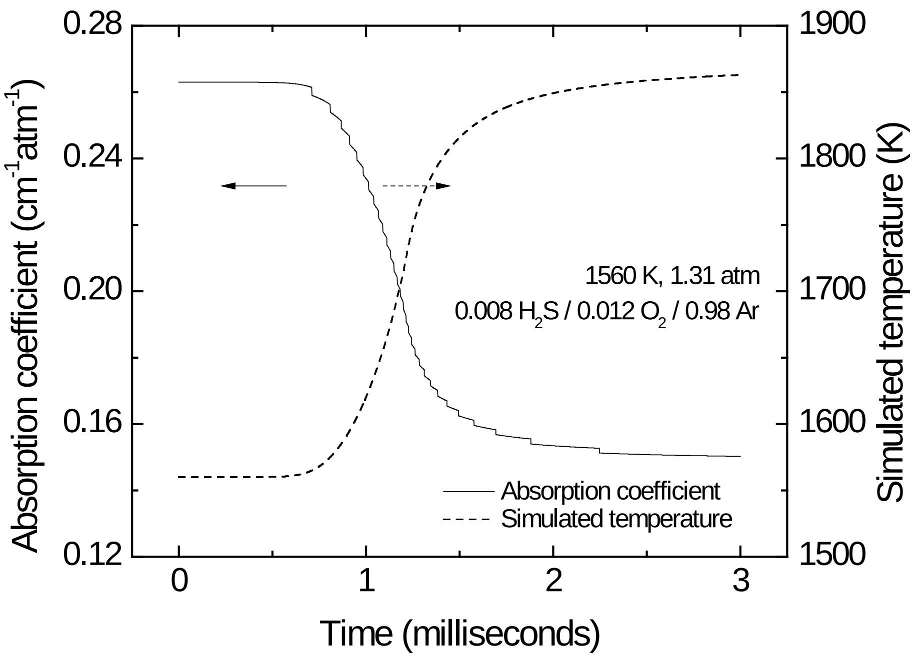




Task 3 – Impurity Effects

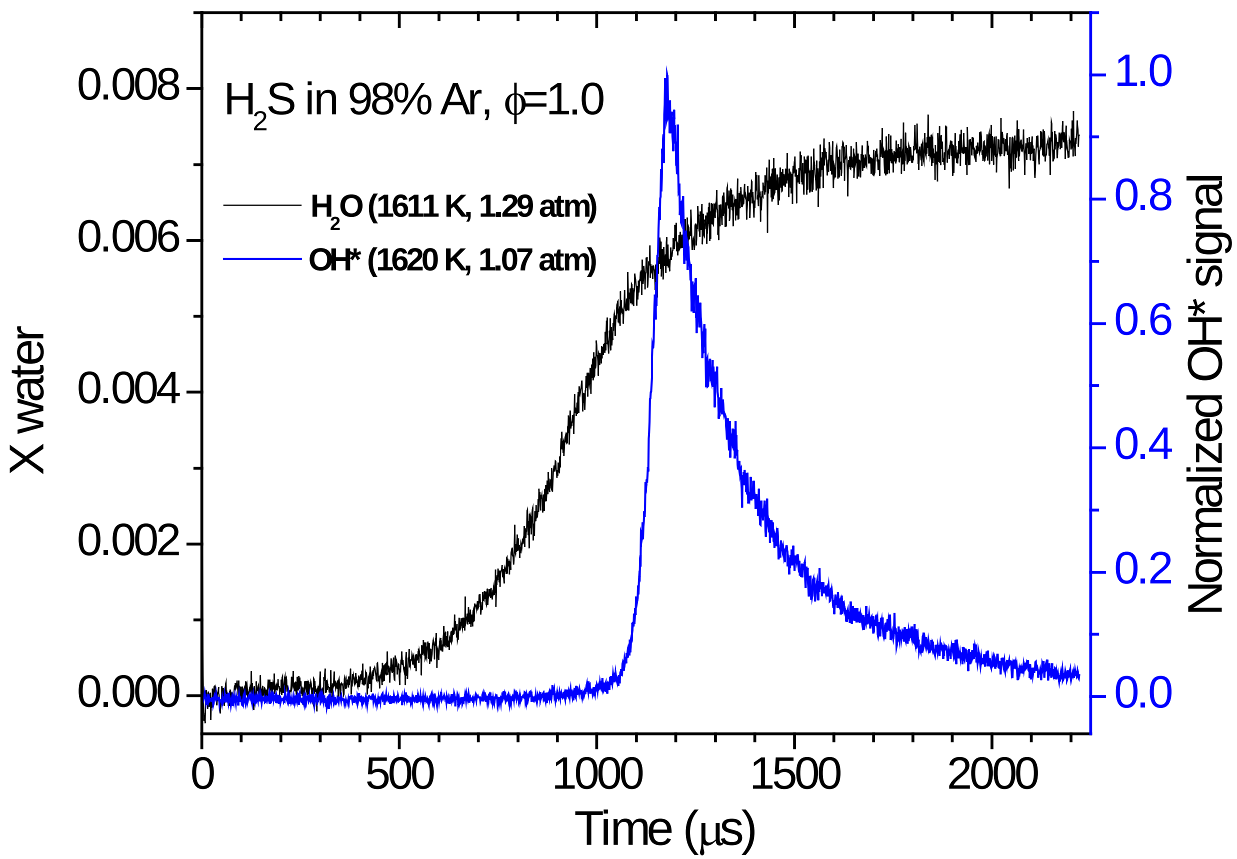
The temperature rise due to combustion causes a significant change in the absorption coefficient

- Temperature rise simulated by CHEMKIN (typically 200-300 K)
- In-house routine created to correct raw data with simulated temperature rise
- Modified mechanisms used to iterate on accurate solution



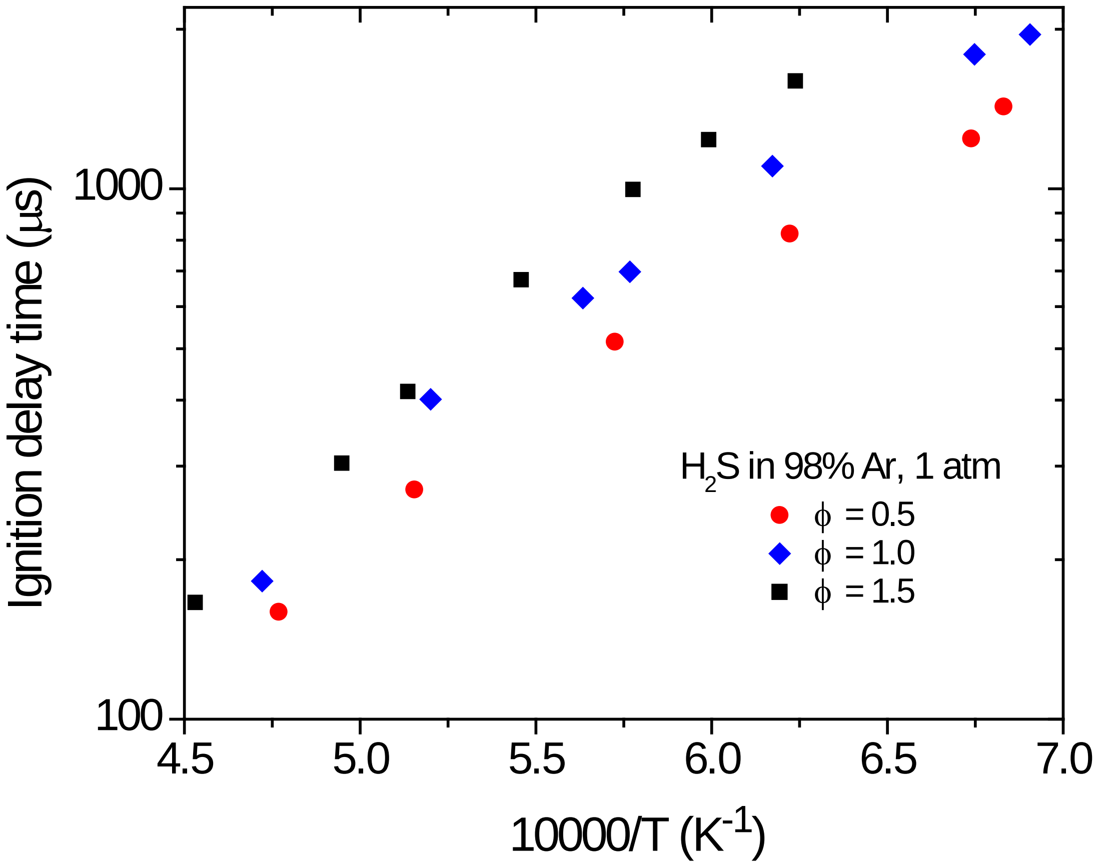
Task 3 – Impurity Effects

Typical OH and H_2S Time Histories Show Main Ignition During Middle of Water Formation*



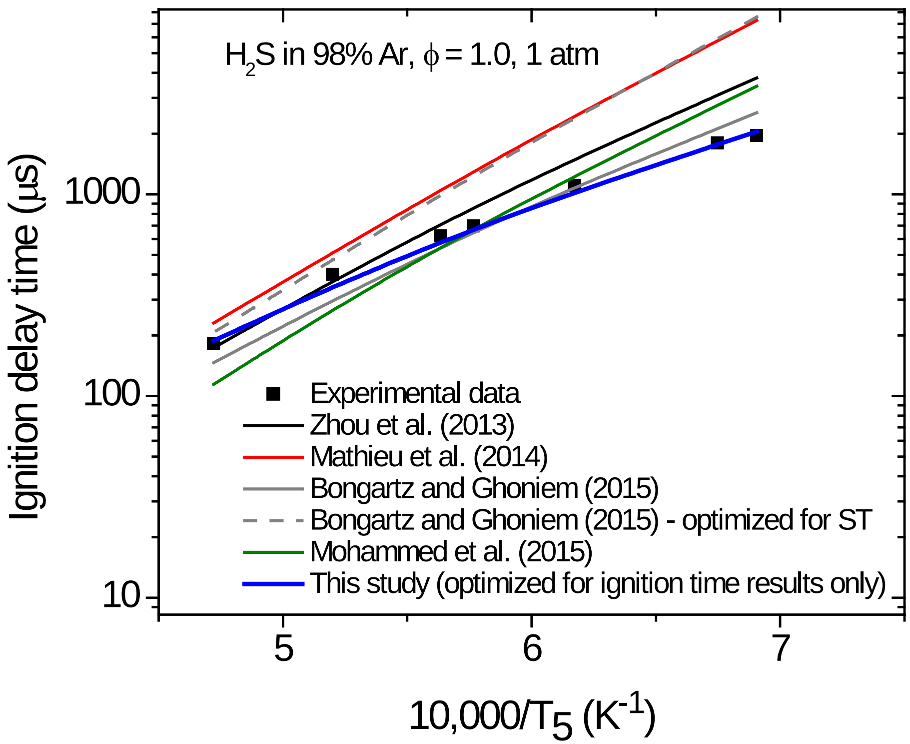
Task 3 – Impurity Effects

*First **Ignition Delay Time** Results Obtained for H_2S Oxidation*



Task 3 – Impurity Effects

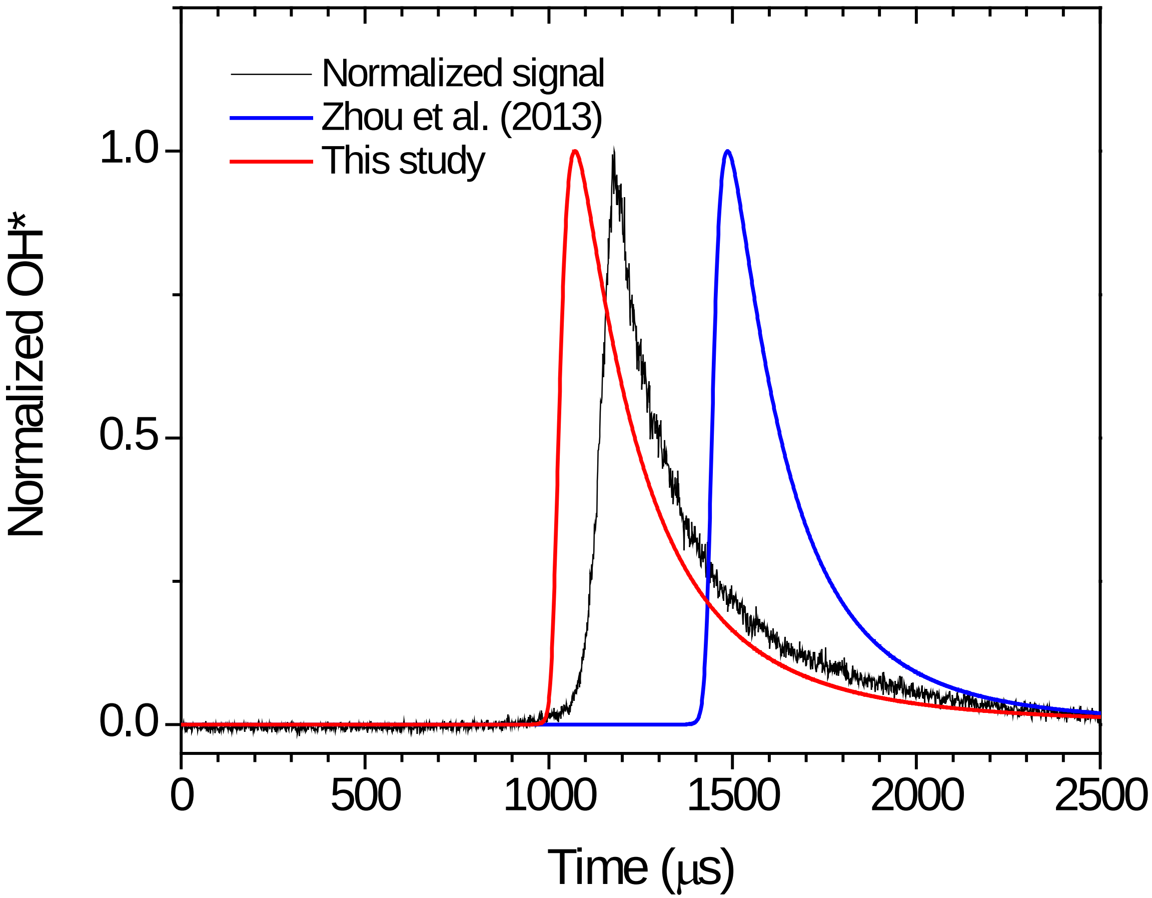
Kinetics Modeling of Ignition is Ongoing…



- All recent literature based on model from Zhou, Haynes, et al., 2013
- Original model from Zhou et al. not in good agreement with the new set of data.
- Model from Mathieu, Petersen et al. (2014) not working well here.
- This study: fair agreement with new data and w/ former literature ST data => new meas. helpful
- Not possible to reconcile both shock tube and flow reactor data w/ current models.

Task 3 – Impurity Effects

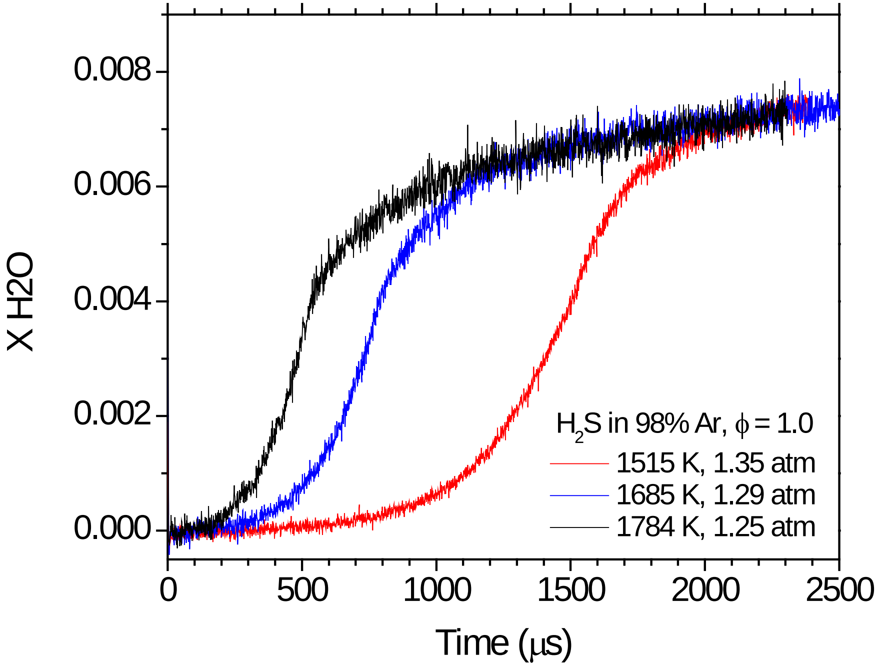
Kinetics Model Predicts Shape of ***OH* Time History*** *Rather Well*



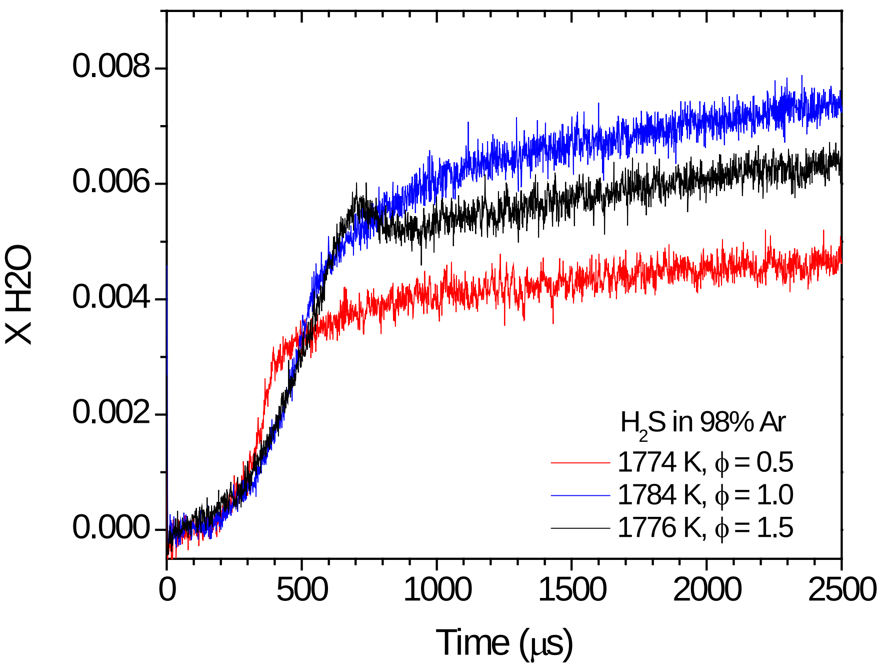
Task 3 – Impurity Effects

Water Time Histories Provide Valuable Information for Improving H_2S Kinetics Mechanism

Effect of Temperature

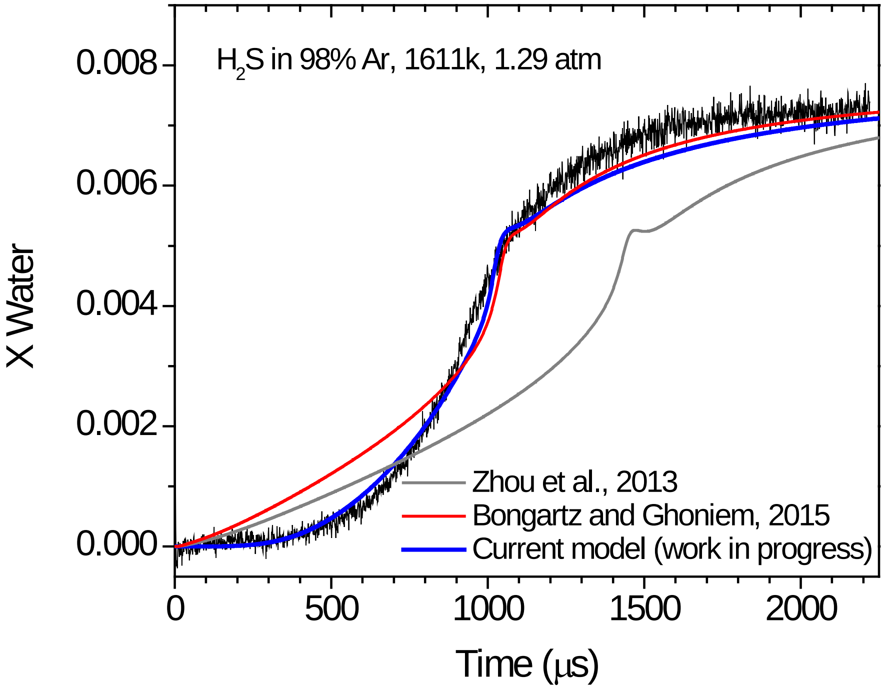


Effect of ϕ



Task 3 – Impurity Effects

H_2O Profiles Uncovered Large Deficiencies in Previous Mechanisms…

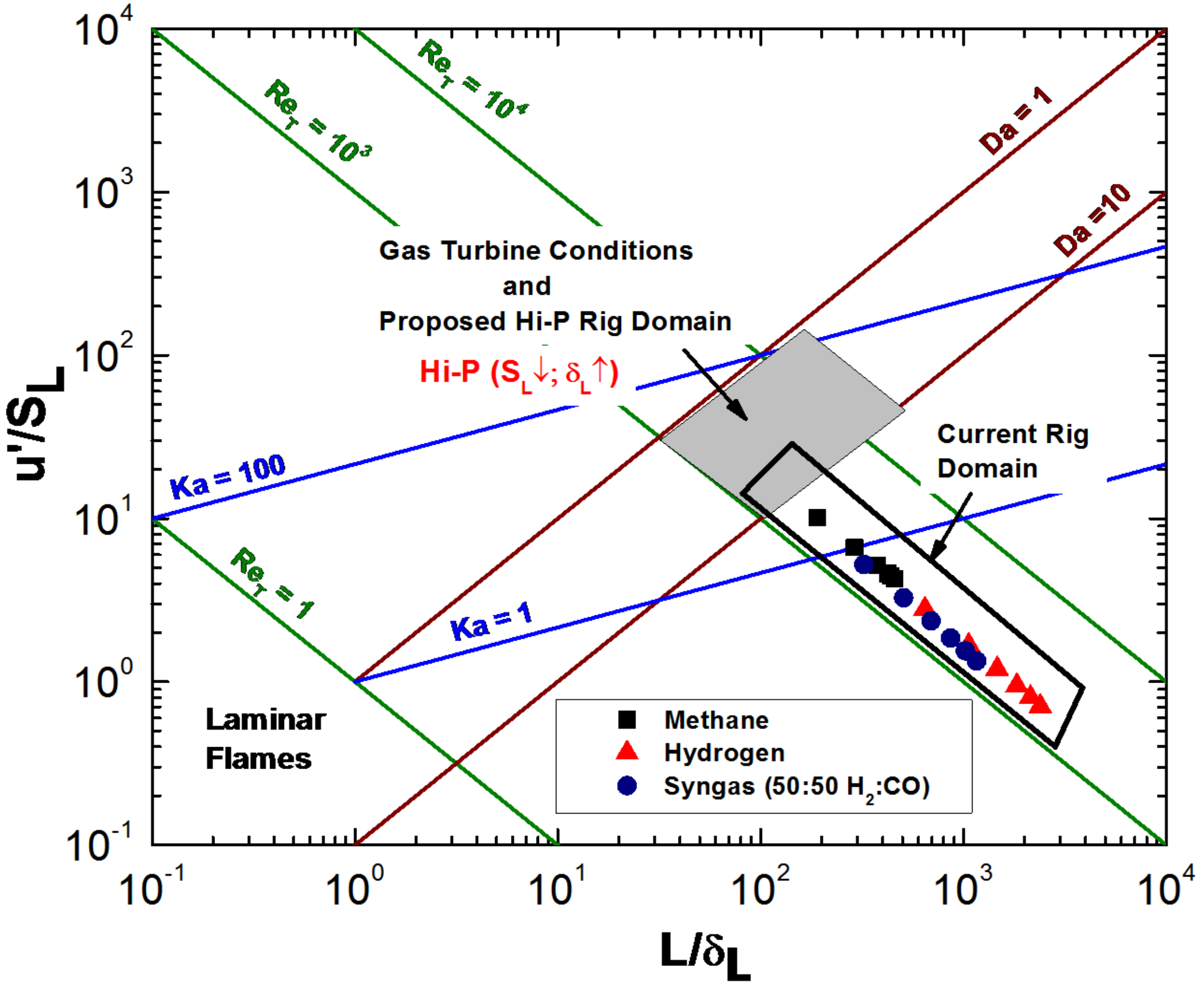


- All recent models predict H_2O starting too early
- Mainly due to **$H_2S + O_2 = SH + HO_2$ (R1)**
- R1 rate needs to be modified
- Rate of SH + O_2 = HSO + O changed w/rate meas. in lit.
- Other rxns. suspicious (SH + SH + M = HSSH + M)
- **More data at different conditions and rate measurements sorely needed!**

<u>Task 4</u> – 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

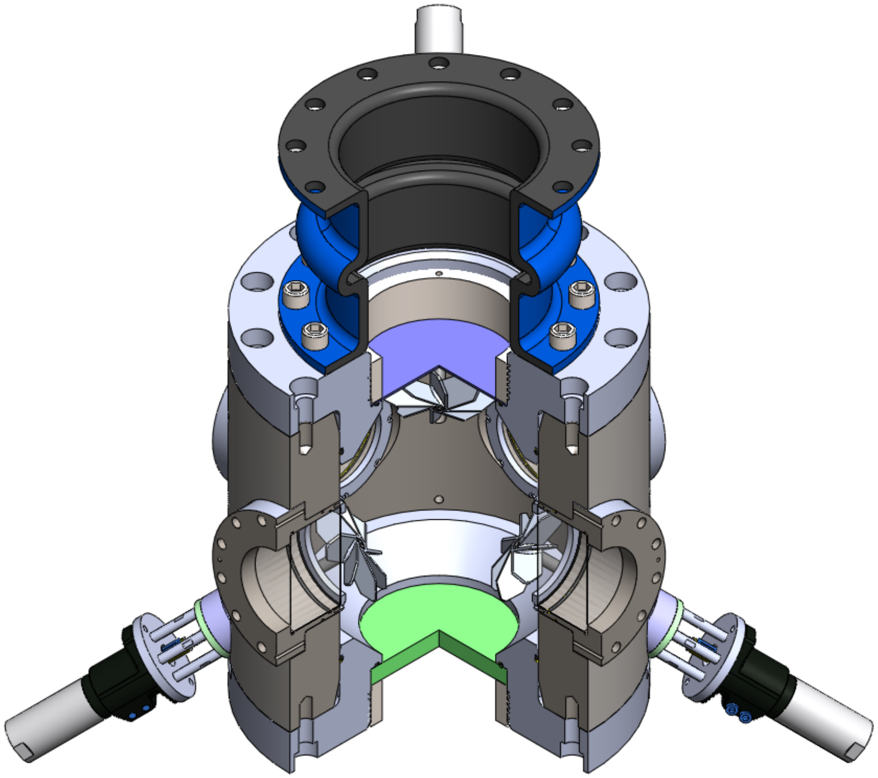
Task 4 Design and Installation is Underway

- 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 Complete
- Fabrication is Underway

Task 4 – New Facility

New Design is Complete

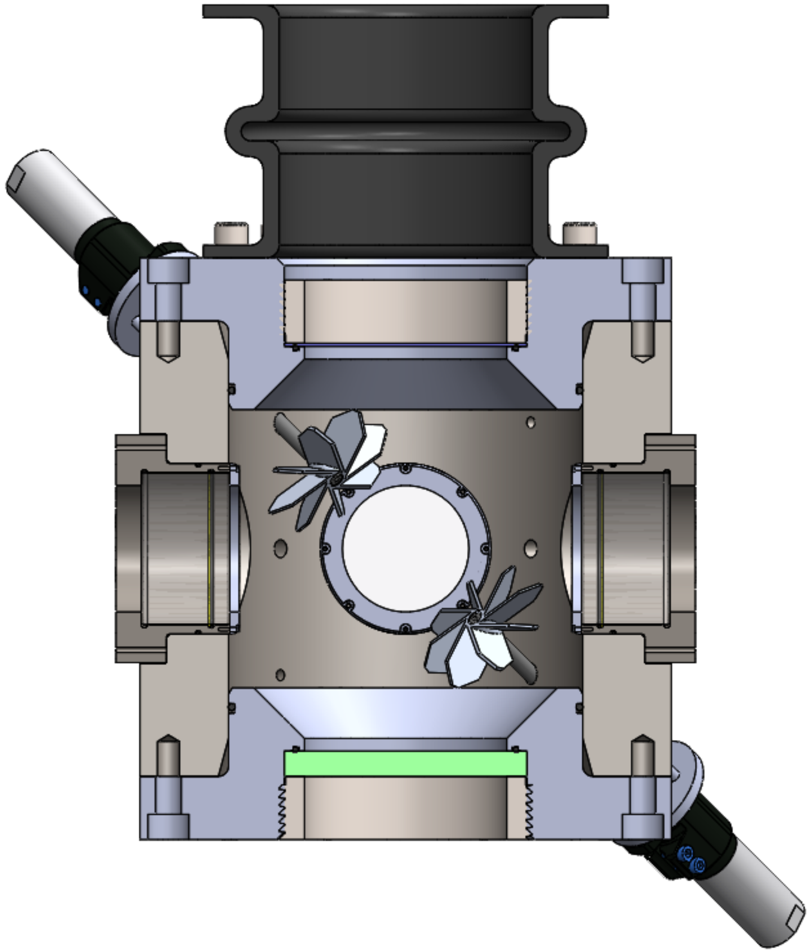
- Built in forged SS
- ID 14”; height 18”
- 4 windows; ∅5” aperture
- 4 stirring fans; ∅5.75”
- Max. allowable pressure: 200 atm



Task 4 – New Facility

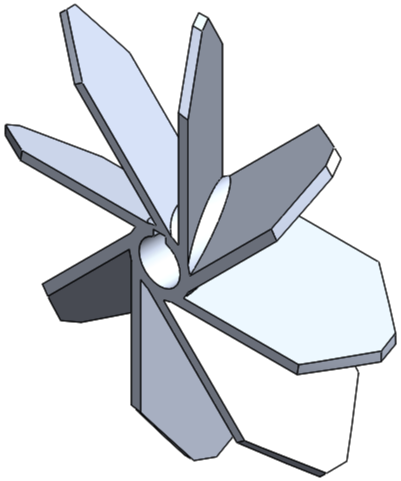
Breach and Diaphragm Method Selected for Venting

- Breach ∅8”
- Vented deflagration through diaphragm (top)
- Bottom breach is reconfigurable:
  - Heater
  - Injection port
  - Spark plug gland



Task 4 – New Facility

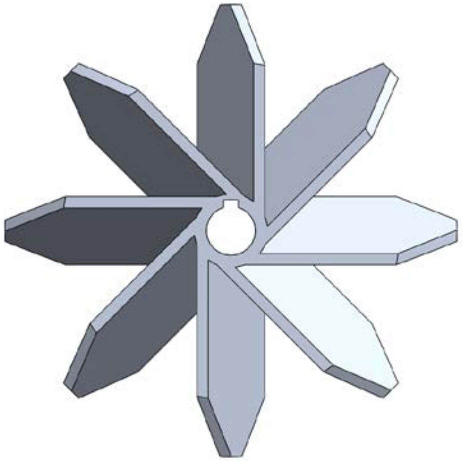
New Fan Design was Implemented, Based on LDV Results from Existing Rig



- Arranged in tetrahedral configuration

- Max. speed: 10,000 rpm

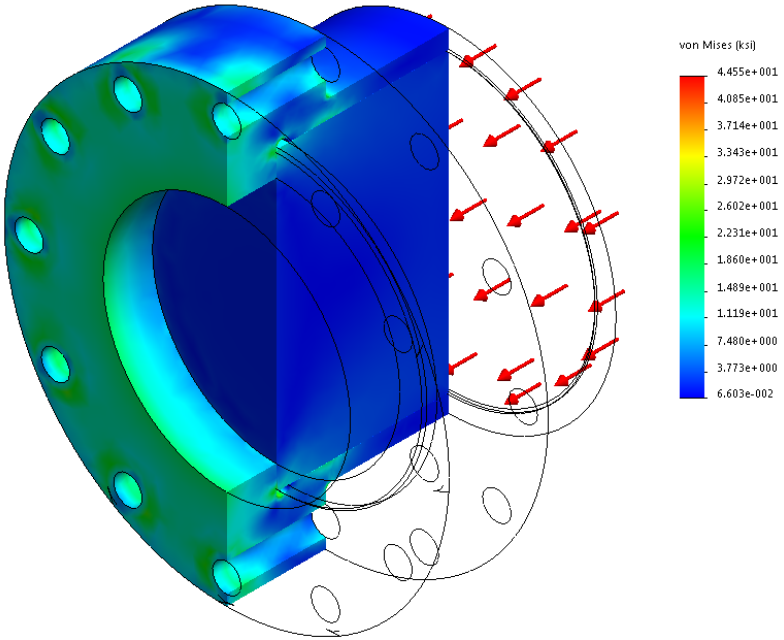
- 8-bladed radial impeller with 30° pitch and 1.25” axial depth.



Task 4 – New Facility

Optical Access Allows 2 Lines of Sight and Based on Prior Experience

- Fused quartz substrate
- Two orthogonal lines of sight
- Size and proportions of window and vessel have been proven to produce data free of ignition and confinement effects.



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

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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Task 2 – Turbulent Speeds

Recent Data Cover a Wide Range of Flamelet Regions