Ignition, turbulent flame speeds, and emissions from high hydrogen blended fuels

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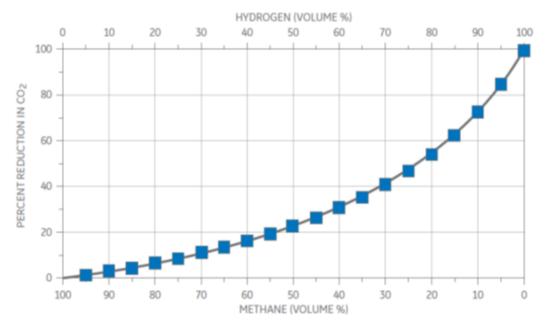
UTSR Workshop

Background and Motivation

- AOI 1: Hydrogen combustion fundamentals for gas turbines.
- Overarching goal: improve understanding of fundamental phenomena of hydrogen containing fuels.
- "A hydrogen economy is <u>again</u> gaining global attention for reducing carbon emissions."
- Again?
 - Tons of ignition delays and flame speeds data, am I going to measure them again?
 - How to define hydrogen containing fuels?
 - What is the knowledge gap?

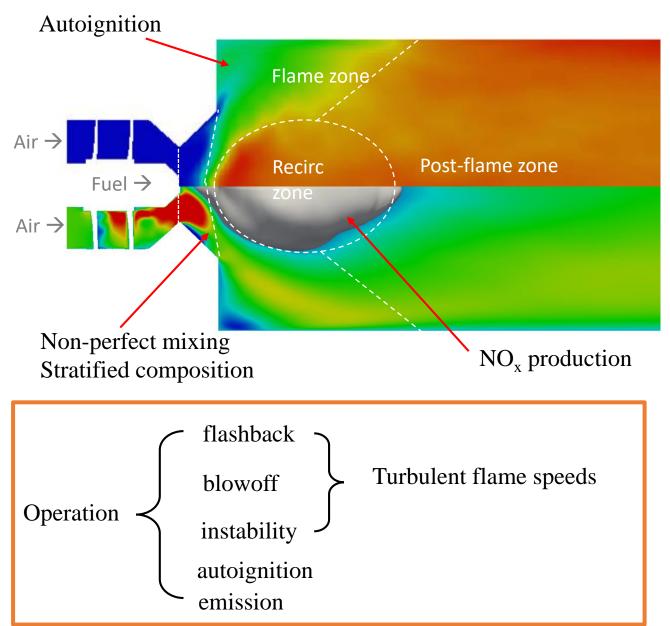
(High) Hydrogen Containing Fuels

- Pure hydrogen (H₂), carbon free hydrogen carrying fuels (such as ammonia, NH₃), mixtures of them and with natural gas
- Hydrogen fraction must be high enough (e.g., >50%) to achieve significant carbon reduction



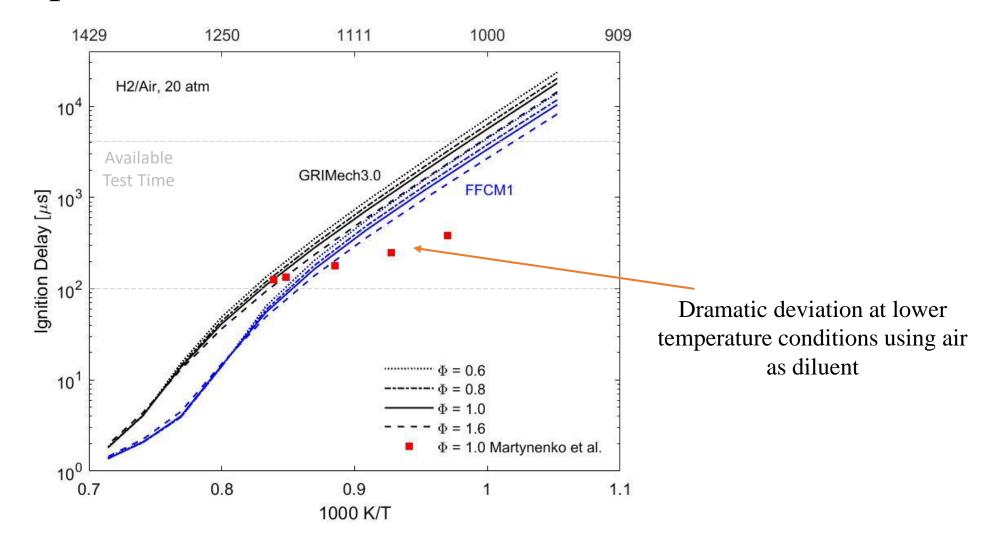
J. Goldmeer, "POWER TO GAS : HYDROGEN FOR POWER GENERATION Fuel Flexible Gas Turbines as Enablers for a Low or Reduced Carbon Energy Ecosystem," 2019

Knowledge Gaps



- H₂ is extremely reactive at low T
 - Potential autoignition inside combustor
- High H₂ fraction changes flow properties
 - High turbulence, high stretch
- Different conditions in realistic turbines and fundamental bench top studies
 - Diluents, fuel concentrations, T&P
- H_2 /natural gas $\neq H_2/CH_4$
 - H₂ interacts with higher hydrocarbons (C_3-C_5) at low T
- Catalytic effect of NO_x on H_2 ignition
- H₂ increases NO_x emissions
- H₂ ignites faster and its flame propagates faster at fuel rich conditions

Different conditions in realistic turbines and fundamental bench top studies



Martynenko, V. V., et al. "High-temperature ignition of hydrogen and air at high pressures downstream of the reflected shock wave." Journal of Engineering Physics and Thermophysics 77.4 (2004): 785-793.

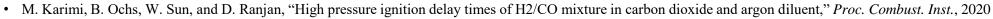
Objectives

- Objective 1: Development of comprehensive database on autoignition delays for hydrogen containing fuels, including pure hydrogen and ammonia, hydrogen/natural gas blends, and ammonia/hydrogen blends at realistic gas turbine conditions.
- Objective 2: Measurement of turbulent flame speeds and emissions of hydrogen containing fuels at different turbulence levels.
- Objective 3: Measurement of laminar flame speeds of hydrogen containing fuels at high preheating conditions in shock tube.
- Objective 4: Validation and optimization of existing kinetic models using data obtained from experiments and development of reduced kinetic model specific for hydrogen containing fuels.

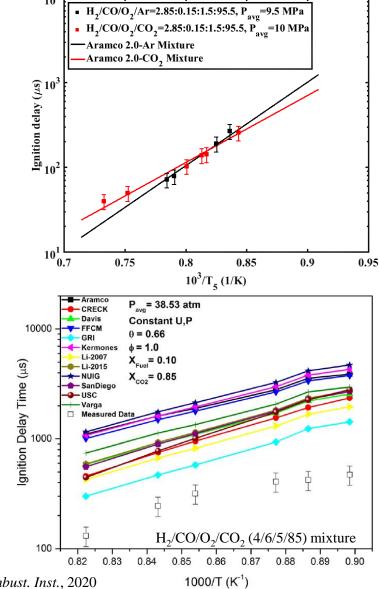
Task 1: Project Management and Planning

- We will manage and direct the project in accordance with a Project Management Plan to meet all technical, schedule and budget objectives and requirements.
- We will coordinate activities in order to effectively accomplish the work.
- We will update the Project Management Plan 30 days after award and as necessary throughout the project to accurately reflect the current status of the project.
- We will submit quarterly report, attend program review meetings, and arrange regular meetings with program manager.

- Data still inconsistent
- Autoignition delay times (IDTs) will be measured at practical gas turbine conditions at a broad range of conditions to create a comprehensive database.
- Fuels: H_2 /natural gas mixture and NH_3/H_2 mixture
- Temperature range: 600 K to 1400 K
- Equivalence ratio: 0.6 to 1.6
- Pressure: ~20 atm
- Facility: high pressure shock tube
- Q1 to Q8



• S. Barak, E. Ninnemann, F. Barnes, J. Kapat, and S. Vasu, "High-Pressure Oxy-Syngas Ignition Delay Times With CO2 Dilution : Shock Tube Measurements and Comparison of the Performance of Kinetic Mechanisms," *J. Eng. Gas Turbines Power*, vol. 141, p. 021011, 2019



- Fuel testing Matrix for IDTs
- NG: $CH_4/C_2H_6/C_3H_8/n-C_4H_{10}/n-C_5H_{12}=81.25/10/5/2.5/1.25$ proposed by Donohoe et al.

H ₂ /NG (volume ratio) in air	50%/50%	70%/30%	90%/10%	100%/0
H ₂ /NG/NO (volume ratio) in air	50%/50%/(10 ppm)	70%/30%/(10 ppm)	90%/10%/(10 ppm)	100%/0/(10 ppm)
NH ₃ /H ₂ (volume ratio) in air	30%/70%	50%/50%	80%/20%	100%/0
NH ₃ /H ₂ /NO (volume ratio) in air	30%/70%/(10 ppm)	50%/50%/(10 ppm)	80%/20%/(10 ppm)	90%/10/(10 ppm)

N. Donohoe *et al.*, "Ignition delay times, laminar flame speeds, and mechanism validation for natural gas/hydrogen blends at elevated pressures," *Combust. Flame*, vol. 161, no. 6, pp. 1432–1443, 2014.

• GT high pressure shock tube (funded by NETL UTSR Program)

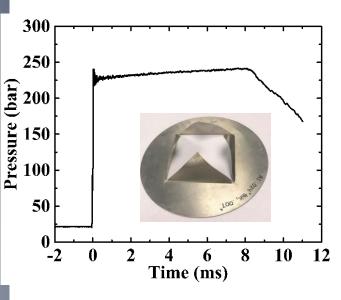
Key features:

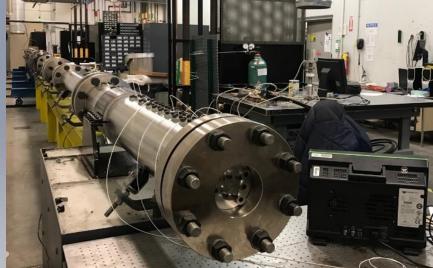
- Large internal bore (6 inch or 15.24 cm)
- 69 ft long (~50 ms test time)
- Certified at 376 atm
- 0.2 μm surface finish (electropolishing)
- Optical access

Optical windows

Diaphragm section (single or double)

Contoured valve for vacuum



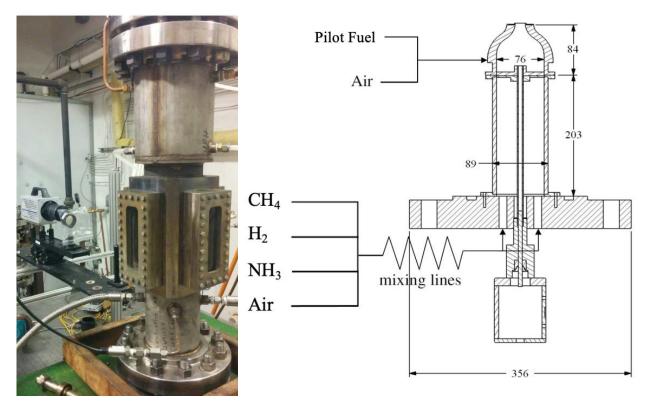


Task 3: Investigation of turbulent flame speeds of high hydrogen fuels at high turbulence levels

- Unknown effect from pressure, preheat conditions and fuel sensitivity
- Study to be performed at high preheat temperatures (~800K) and pressures (~20 bar)
- Proposed study:
 - 1. Constant laminar flame speeds measurements of turbulent flame speed
 - 2. Constant Reynolds number studies for turbulent flame speed
 - 3. Constant equivalence ratio measurements of turbulent flame speed

Task 4: Measurement of emissions from turbulent flames of high hydrogen fuels

- H₂ increase emissions
- NO_x emission from ammonia is huge
- For emissions:
 - From premixed H₂/NG turbulent flames
 - From premixed H₂/NH₃ turbulent flames
 - From non premixed H₂/NH₃ turbulent flames

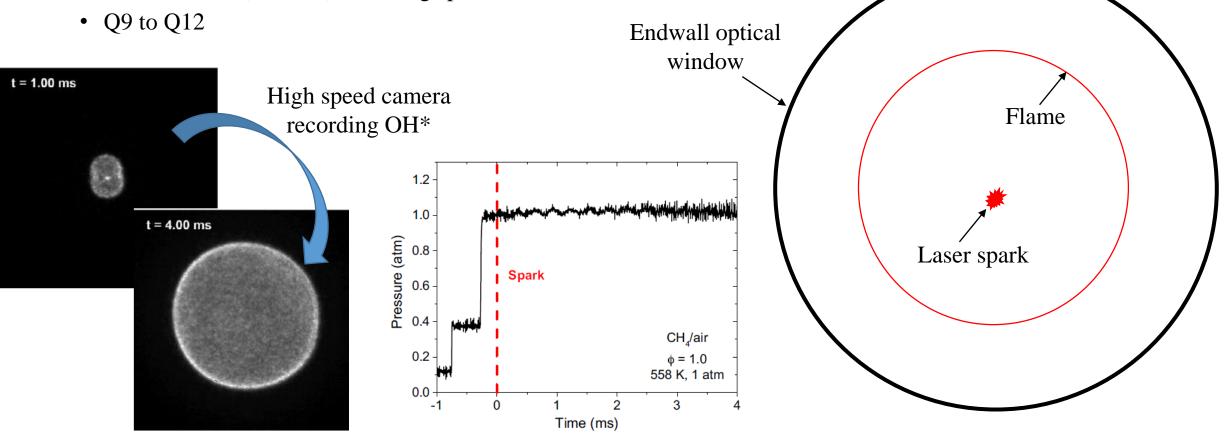


Fuel composition matrix for turbulent flame speeds and emissions

H ₂ /NG (volume ratio) in air with 5% H ₂ O in mixture	50%/50%	70%/30%	90%/10%	100%/0
NH ₃ /H ₂ (volume ratio) in air with 5% H ₂ O in mixture	30%/70%	50%/50%	80%/20%	100%/0

Task 5: Investigation of laminar flame speeds at high preheating conditions

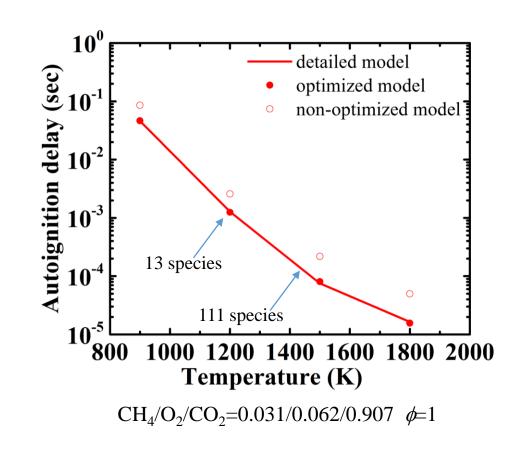
- Laminar flame speeds with high preheating temperatures (600 K to 800 K)
- Shock tube naturally is a high pressure vessel
- Replace endwall to a large optical window
- in house code (ASURF) modeling spherical flame



A. M. Ferris, A. J. Susa, D. F. Davidson, and R. K. Hanson, "High-temperature laminar flame speed measurements in a shock tube," Combust. Flame, vol. 205, pp. 241–252, 2019

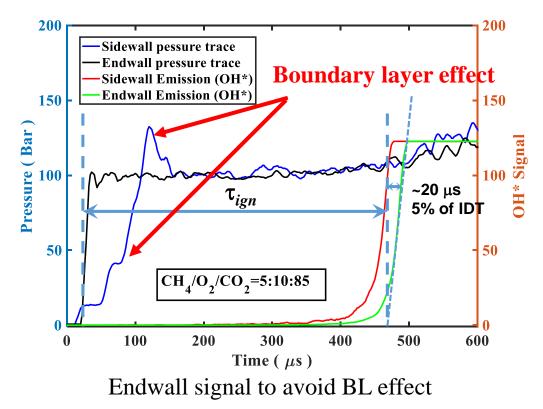
Task 6: Development of reduced and optimized chemical kinetic models for hydrogen containing fuel

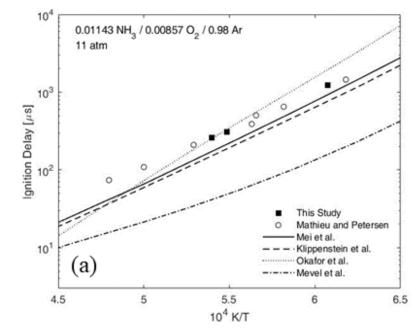
- A comprehensive kinetic model is needed including H₂, CH₄, C₂-C₅, NH₃, and NO_x modules.
- We will develop a kinetic model based on existing kinetic models; evaluate its performance, optimize and reduce the model.
- Global Pathway Selection (GPS) method for model reduction and optimization



Thank you & Questions?

- (Potential) challenges on IDTs measurements at proposed conditions
- Thick boundary layer induced by air
- Sensitivity to impurity (H_2) and wall passivation (NH_3)
- Solution: experimental protocol established in previous UTSR project





Validated with existing data, passivation is negligible in large shock tube

O. Mathieu and E. L. Petersen, "Experimental and modeling study on the high-temperature oxidation of ammonia and related NOx chemistry," Combust. Flame, vol. 162, no. 3, pp. 554–570, 2015