Flame Speed Measurements of Ammonia-Hydrogen Mixtures

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Outline

☐ Motivation

☐ Experimental setup

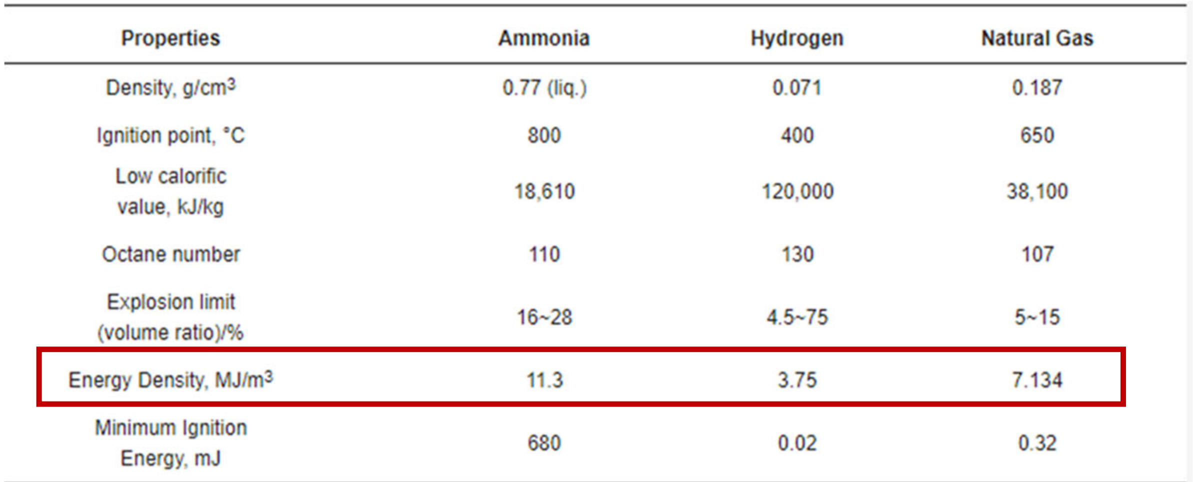
☐ Theoretical background

☐ Results and discussion

☐ Future works

Background – about NH_3

- CO_2 emission
  - Need to decrease
- Ammonia (NH_3)
  - NH_3 has higher volumetric energy density than H_2 and natural gas



Properties	Ammonia	Hydrogen	Natural Gas
Density, g/cm^3	0.77 (liq.)	0.071	0.187
Ignition point, °C	800	400	650
Low calorific value, kJ/kg	18,610	120,000	38,100
Octane number	110	130	107
Explosion limit (volume ratio)/%	16~28	4.5~75	5~15
Energy Density, MJ/m^3	11.3	3.75	7.134
Minimum Ignition Energy, mJ	680	0.02	0.32

Xu. et al. 2022

Background – about NH_3

- CO_2 emission
  - Need to decrease
- **Ammonia (NH_3)**
  - NH_3 has higher volumetric energy density than H_2 and natural gas
  - **Cheaper than H_2**

Background – about NH_3

- CO_2 emission
  - Need to decrease
- **Ammonia (NH_3)**
  - NH_3 has higher volumetric energy density than H_2 and natural gas
  - Cheaper than H_2
  - **Production, storage, transportation, and distribution**

https://www.dreamstime.com

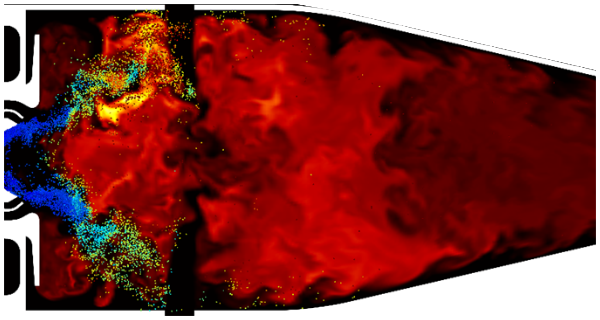
Background – about NH_3

- CO_2 emission
  - Need to decrease
- **Ammonia (NH_3)**
  - NH_3 has higher volumetric energy density than H_2 and natural gas
  - Cheaper than H_2
  - Production, storage, transportation, and distribution
  - **Toxic, but easy to detect by the distinctive smell**
  - **Strong fuel candidate for gas turbines, and engines**

Background

☐ Laminar burning speed

- Design internal combustion engine.
- Modeling turbulent combustion
- Validation of chemical kinetic mechanism

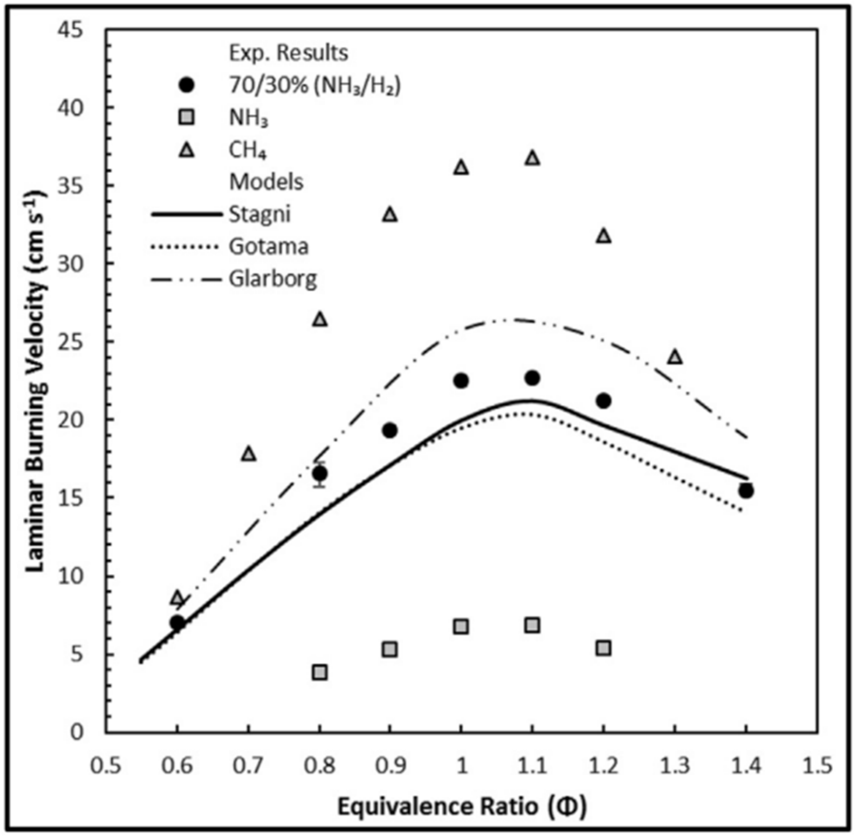


Challenges in Ammonia-Hydrogen Combustion

The current state of NH_3-H_2 combustion research is insufficient to accurately predict its explosion characteristics

Inaccuracies exist in both the lean and rich regions for various mechanisms, necessitating reaction reduction for positively/negatively sensitive reactions

Greater knowledge of NH_3-H_2 combustion at higher pressures is needed to reach the design stage for turbine development



Source: S. Mashruk *et al*, 2022

Chemical Kinetic Modeling

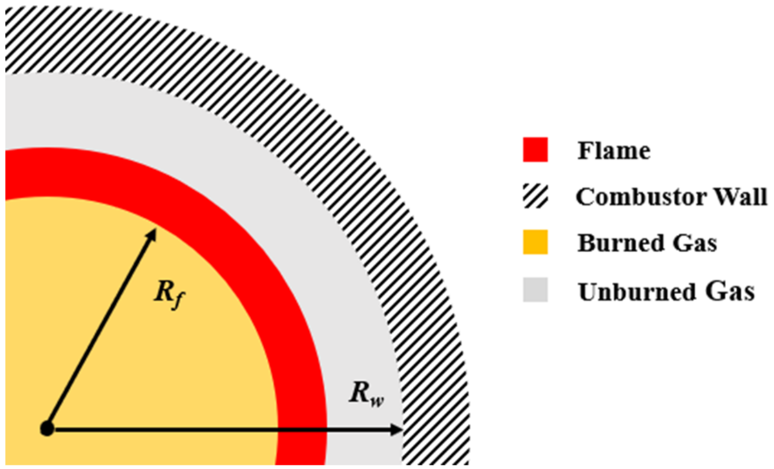
- The preliminarily model developed by UCF has been updated.
    - **256** Reactions *currently under development*

- Reactions for ammonia pyrolysis have been included from literature (Baker et al. and Alturaifi et al.)

- Reactions added for NH2, NH, NNH, N2H2, N2H3, N2H4 and H2NN relevant to pyrolysis.

Rxn.no	Reaction	A	n	Ea
1	NH2+M=NH+H+M	1.20E+15	0	75950
2	NH2+H=NH+H2	6.92E+13	0	3650
3	NH2+NH=NH3+N	9.57E+03	2.46	107
4	NH2+NH2=NH3+NH	5.64E+00	3.53	522
5	NH2+NH2=N2H2+H2	1.74E+08	1.02	11783
6	NH2+NH2=H2NN+H2	7.17E+04	1.88	8802
7	NH+M=H+N+M	1.80E+14	0	74760
8	NH+H=H2+N	1.00E+14	0	0
9	NH+N=N2+H	3.00E+13	0	0
10	NH+NH=N2+H+H	2.50E+13	0	0
11	NH+NH=NH2+N	5.66E-01	3.88	342
12	NNH+NH=N2+NH2	5.00E+13	0	0
13	NNH+NH2=N2+NH3	5.00E+13	0	0
14	N2H2=H2NN	9.20E+38	-9.01	67727
	PLOG / 0.1	9.20E+38	-9.01	67727
	PLOG / 1.0	2.00E+41	-9.38	68452
	PLOG / 10.0	1.30E+45	-10.13	70757
15	N2H3+H=N2H2+H2	2.40E+08	1.5	0
16	N2H3+NH2=N2H2+NH3	9.20E+05	1.94	-1152
17	N2H3+NH2=H2NN+NH3	3.00E+13	0	0
18	NH2+NH2(+M)=N2H4(+M)	5.60E+14	-0.414	66
	LOW / 1.60E+34 -5.49 1987/			
	TROE / 0.31 1E-30 1E30 1E30/			
19	N2H4=H2NN+H2	4.00E+44	-9.85	71353
	PLOG / 0.1	4.00E+44	-9.85	71353
	PLOG / 1.0	5.30E+39	-8.35	69307
	PLOG / 10.0	2.50E+39	-8.19	69664
21	N2H4+NH2=N2H3+NH3	3.90E+12	0	1500
22	H2NN=NNH+H	3.40E+26	-4.83	46228
	PLOG / 0.1	5.90E+32	-6.99	51791
	PLOG / 1.0	9.60E+35	-7.57	54841
	PLOG / 10.0	5.00E+36	-7.43	57295

Combustion model



Mutlizone Combustion Model

Definition of laminar burning speed

$$\rho_u S_u = \frac{1}{A_f}\frac{dm_b}{dt}$$

Bradley & O'Donovan et al. flame radius derivation

$$R_f = R_O\left(1 - (1 - X)\left(\frac{P_i}{P}\right)^{\frac{1}{\gamma}}\right)^{\frac{1}{3}}$$

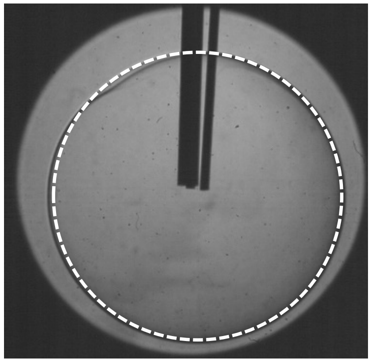
Generalized combustion model using flame radius and pressure data

$$S_u = \frac{R_O^3}{3R_f^2}\left(\frac{P_i}{P}\right)^{\frac{1}{\gamma}}\frac{dX}{dt}$$

Combustion model

$$S_u = \frac{R_O^3}{3R_f^2}\left(\frac{P_i}{P}\right)^{\frac{1}{\gamma}}\frac{d\color{red}{X}}{dt}$$

Single Layer



Linear model

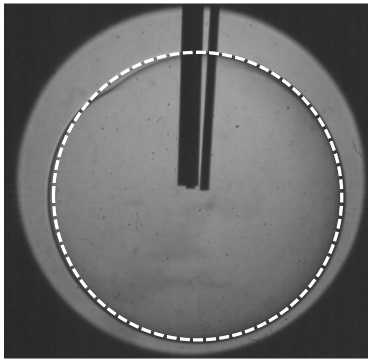
$$X = \frac{P - P_i}{P_e - P_i}$$

P_i: Initial pressure
P : Instantaneous pressure
P_e: Estimated peak pressure

Combustion model

$$S_u = \frac{R_0^3}{3R_f^2}\left(\frac{P_i}{P}\right)^{\frac{1}{\gamma}}\frac{d\mathbf{X}}{dt}$$

Single Layer



Linear model

$$X = \frac{P - P_i}{P_e - P_i}$$

P_i: Initial pressure
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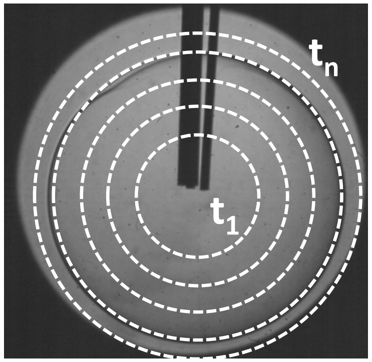
Multiple zones



Multizone model

$$X = \sum_{i=1}^{n} x_i$$

- Cantera

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Experimental conditions

- **Experimental conditions**

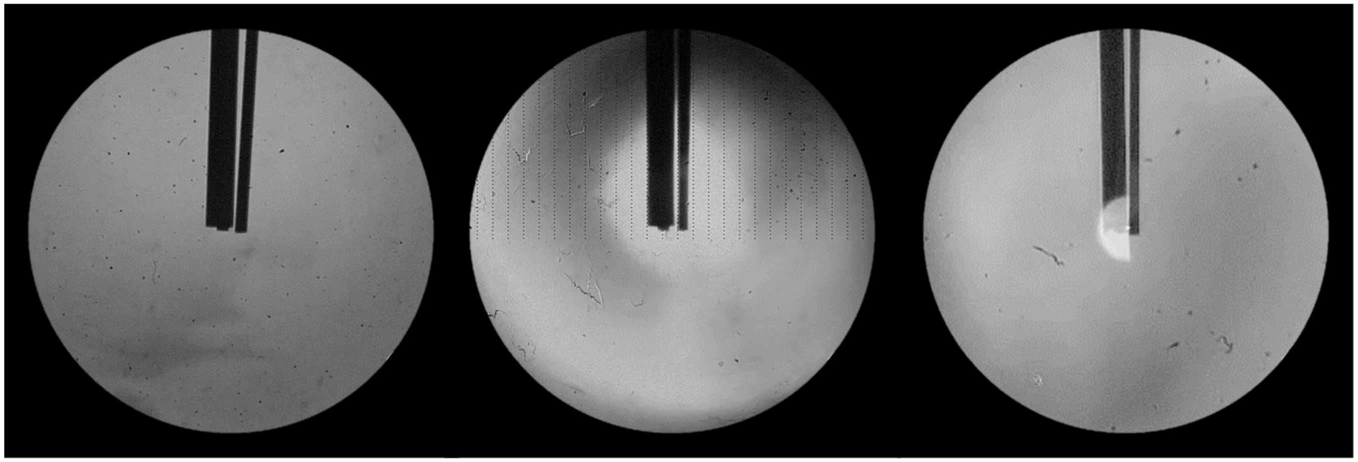
Synthetic air		Initial conditions		Fuel
Oxidizer	Diluent	Temperature	Pressure	
O_2	He/Ar/N_2	296 K	5 atm	NH_3/H_2
1	variety			

- **Synthetic air details**

		Fuel		
Ratio of NH_3/H_2		1/0	0.5/0.5	0.7/0.3
Ratio of	O_2	1.0		
	N_2	1.0		
	Ar	1.5	0	0
	He	0	1.5	3

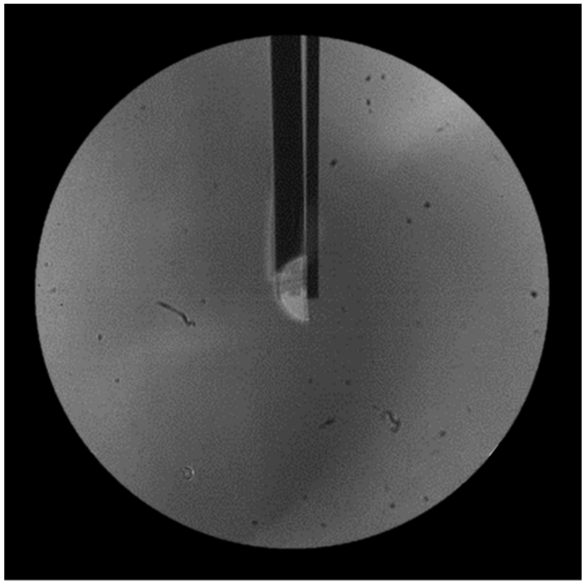
High pressure experiment - challenges

428K and Equivalence ratio of 1.3

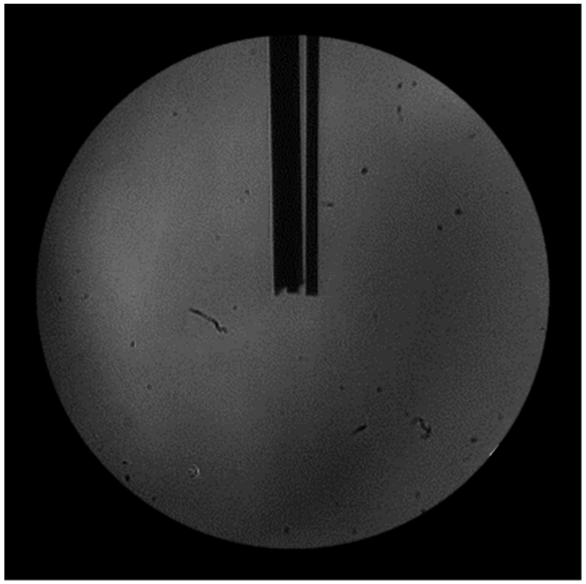


1 atm　　2 atm　　10 atm

High pressure experiment - challenges

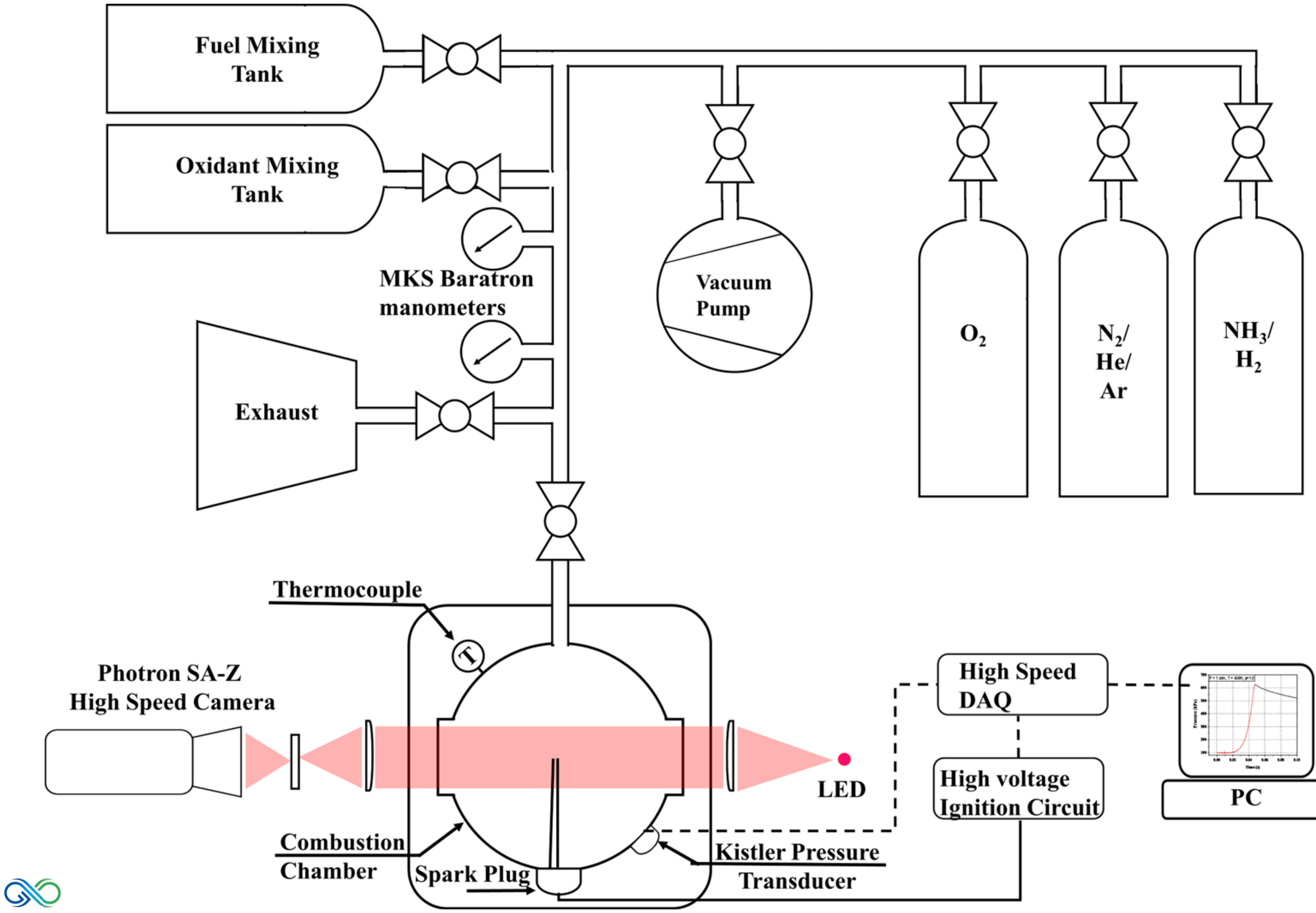


$\phi = 1.3$ with N_2 and He



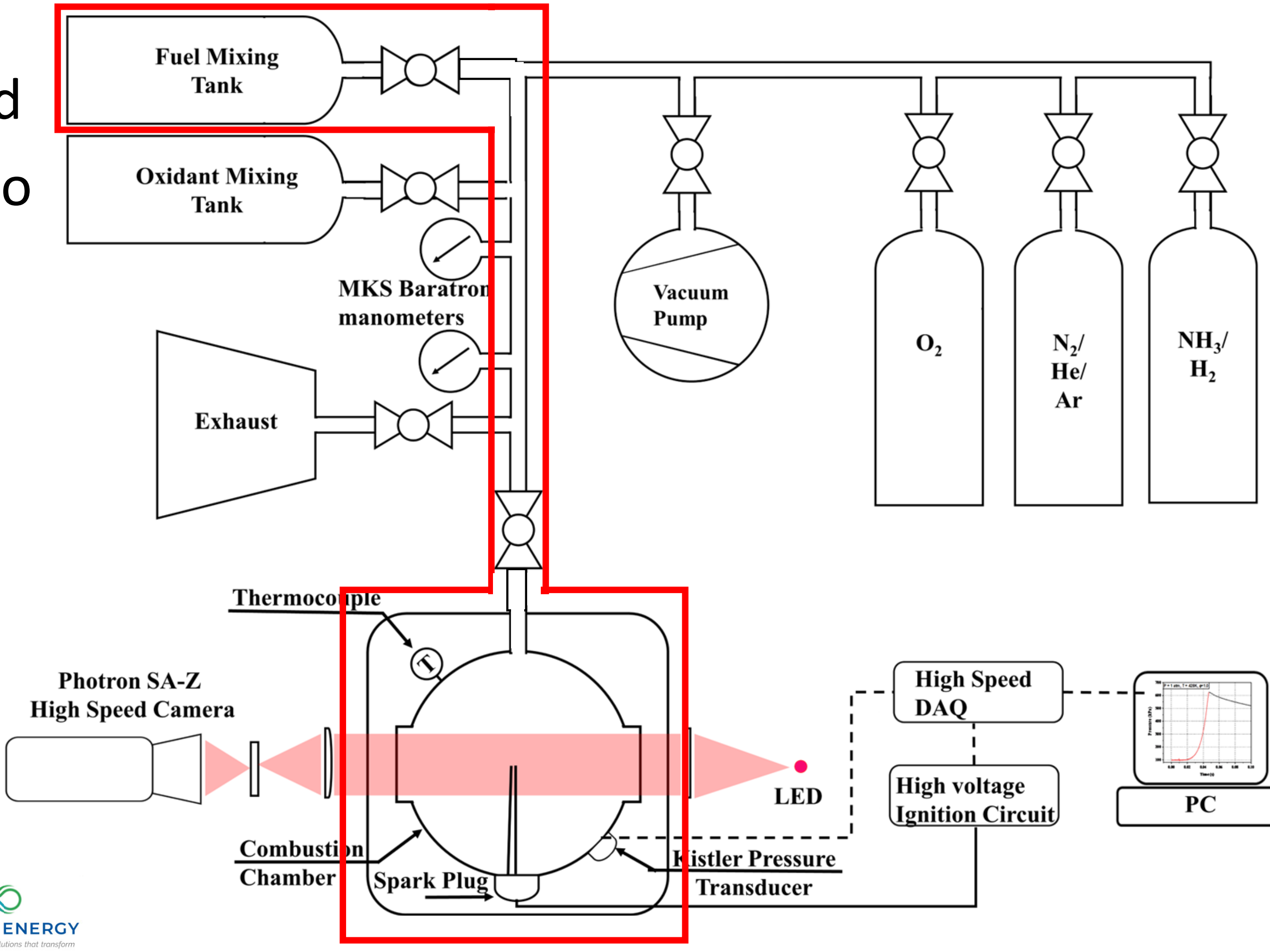
$\phi = 1.3$ with N_2

Experimental setup



Experimental setup

- Setup are in the fume hood
- Exhaust line is connected to exhaust valve of building
- Schlieren image setup also is in the fume hood
- High speed camera is at outside the fume hood.



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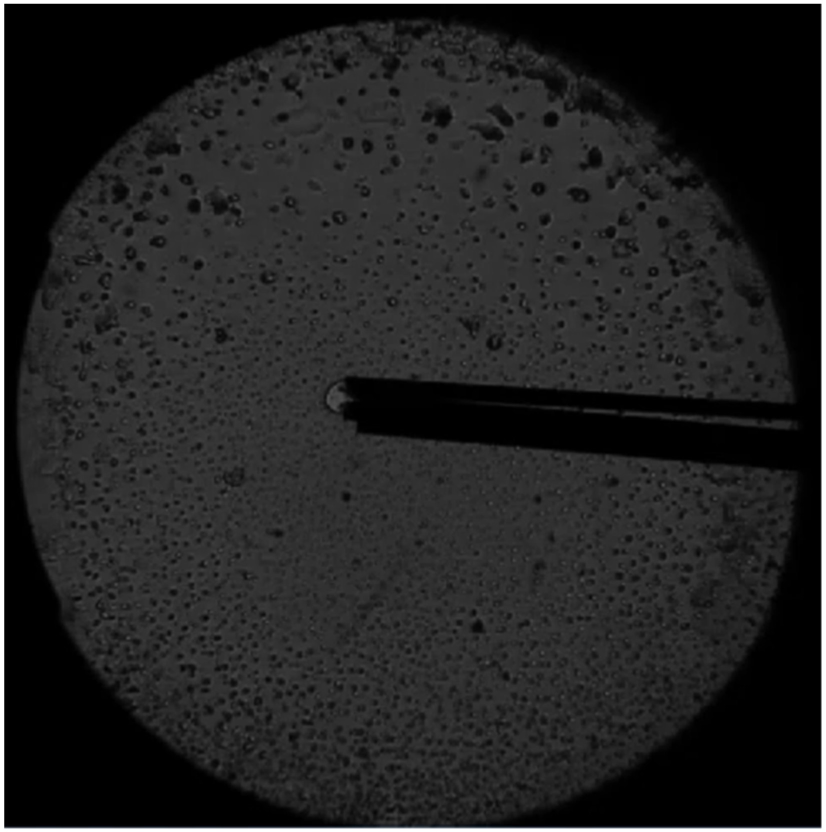
Laminar Burning Speed of Ammonia-Hydrogen Mixtures

Experimental Validation:

Schlieren imaging was used to visualize the flame surface during kernel development and validate optimum oxidant conditions

The Schlieren images validate the following assumptions in our combustion model:

- Flame is smooth and thin
- No buoyancy forces present
- The flame is spherical in nature



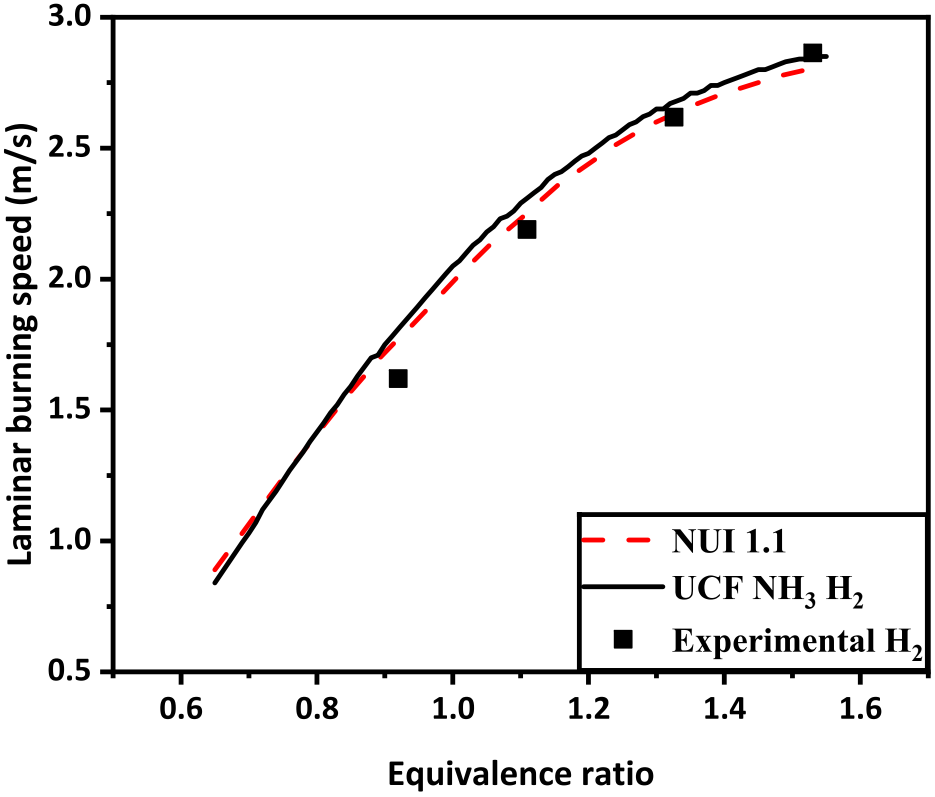
FLAME PROPAGATION VIDEO FOR H_2-ENHANCED NH_3 USING CUSTOMIZED OXIDANT MIXTURE

Laminar Burning Speed of Ammonia-Hydrogen Mixtures

Experimental Validation:

Pure H_2 was ignited in air at room temperature and 1 atm to validate the experimental setup and combustion model

- The UCF NH_3-H_2 mechanism accurately predicted experimental LBS values for pure H_2 ignition



LBS OF H_2 IN SYNTHETIC AIR AT ROOM TEMPERATURE AND 1 ATM

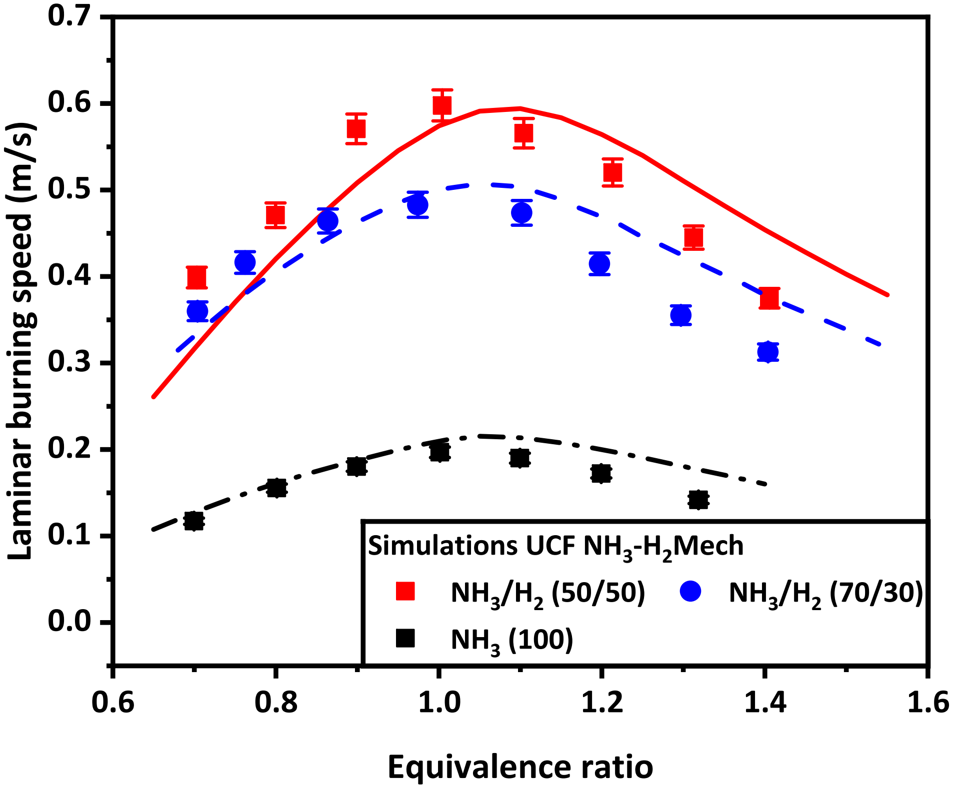
Laminar Burning Speed of Ammonia-Hydrogen Mixtures

Effect of H_2 Addition to NH_3:

The flame speed was increased significantly with H_2 addition. Laminar flames were achieved using the customized oxidant prepared prior to experimentation

Chemical-Kinetic Mechanism:

The UCF NH_3-H_2 mechanism shows increased underprediction of the LBS in the lean region with increased H_2 concentration



LBS OF ALL NH_3 IGNITIONS AT 296 K AND 5 ATM

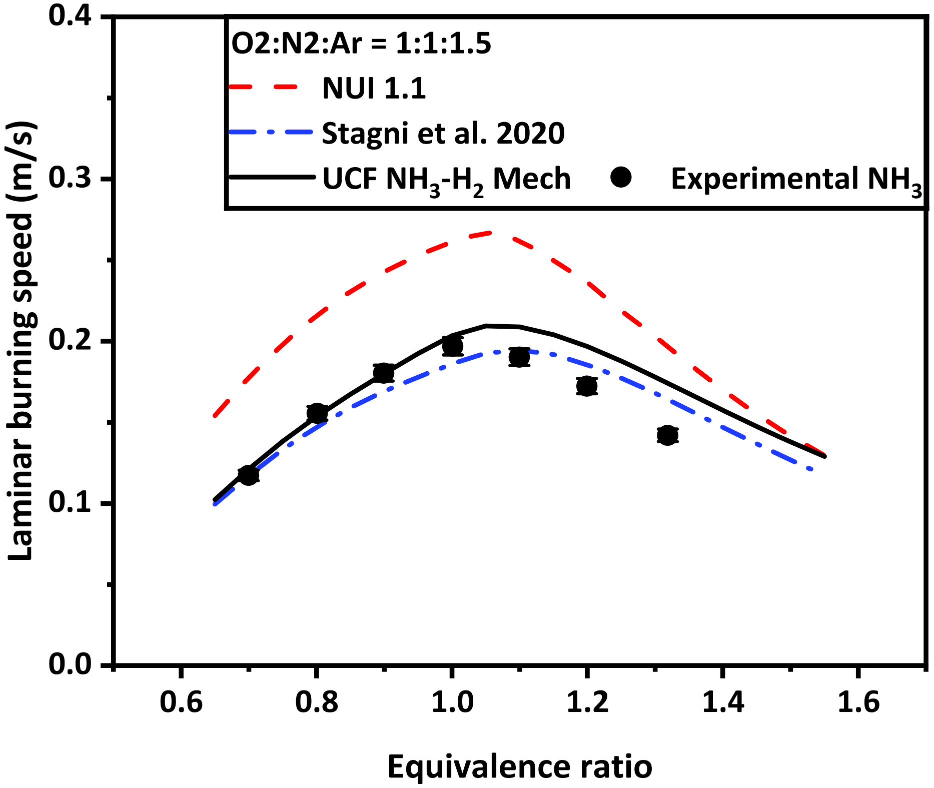
Laminar Burning Speed of Ammonia-Hydrogen Mixtures

Pure NH_3 Flames:

The maximum laminar burning speed (LBS) for pure NH_3 ignitions was determined to be 0.2 m/s at stoichiometric conditions (ϕ = 1.0)

Chemical-Kinetic Mechanism:

The UCF NH_3-H_2 mechanism accurately predicted LBS values for pure NH_3 flames. The model overestimates the LBS values in the fuel-rich region



LBS OF PURE NH_3 IN SYNTHETIC AIR AT 296 K AND 5 ATM

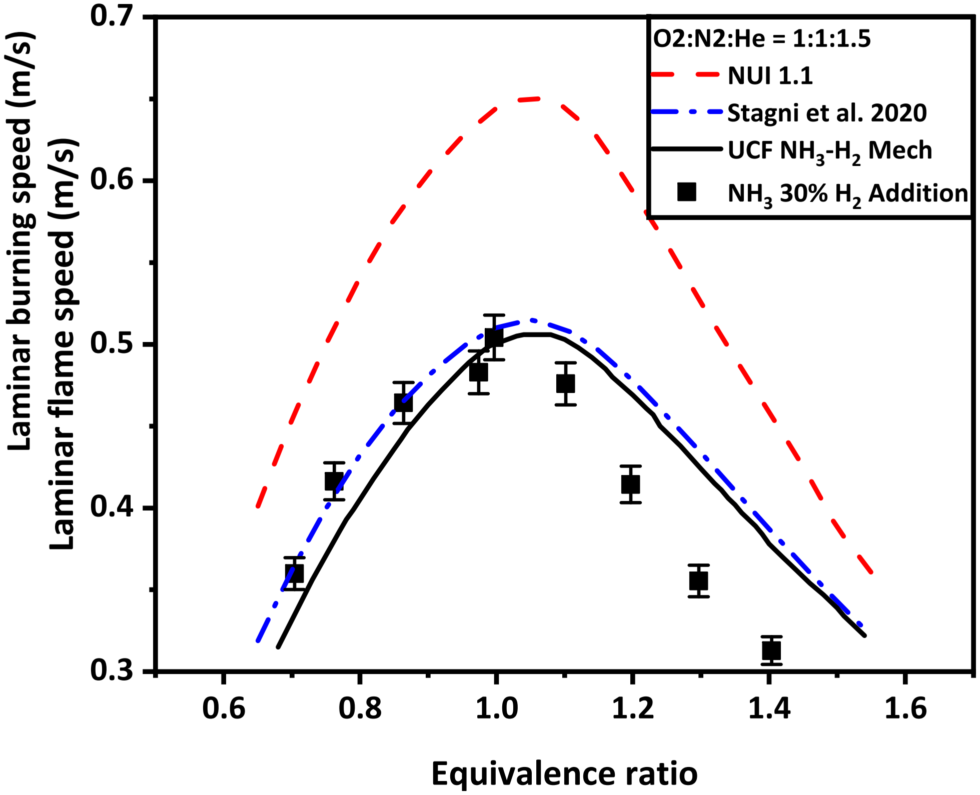
Laminar Burning Speed of Ammonia-Hydrogen Mixtures

H_2-Enhanced NH_3 Flames (70/30):

The maximum laminar burning speed (LBS) for 70% NH_3 + 30% H_2 ignitions was found to be 0.5 m/s at stoichiometric conditions (ϕ = 1.0)

Chemical-Kinetic Mechanism:

The UCF mechanism developed for this investigation accurately predicted experimental LBS values for those in the fuel-lean region



LBS OF 70% NH_3 + 30% H_2 IN SYNTHETIC AIR AT 296 K AND 5 ATM

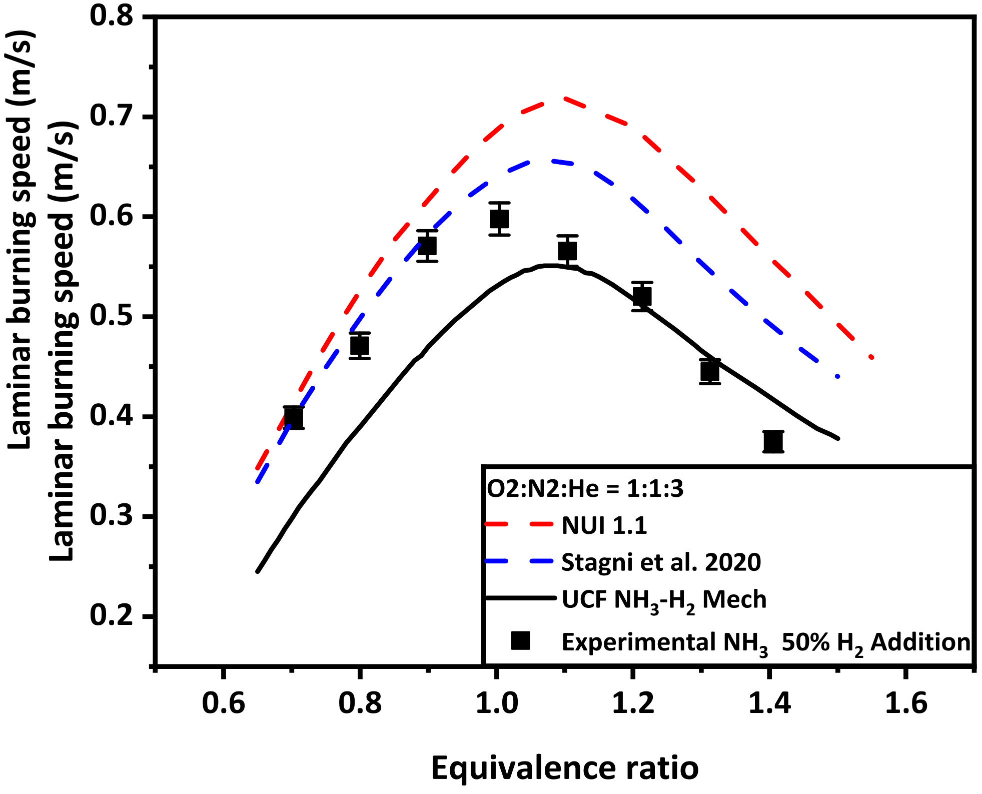
Laminar Burning Speed of Ammonia-Hydrogen Mixtures

H_2-Enhanced NH_3 Flames (50/50):

The maximum laminar burning speed (LBS) for 50% NH_3 + 50% H_2 ignitions was found to be 0.6 m/s at stoichiometric conditions (ϕ = 1.0)

Chemical-Kinetic Mechanism:

The NH_3-H_2 mechanism developed for this study underestimated LBS values for the fuel-lean region.

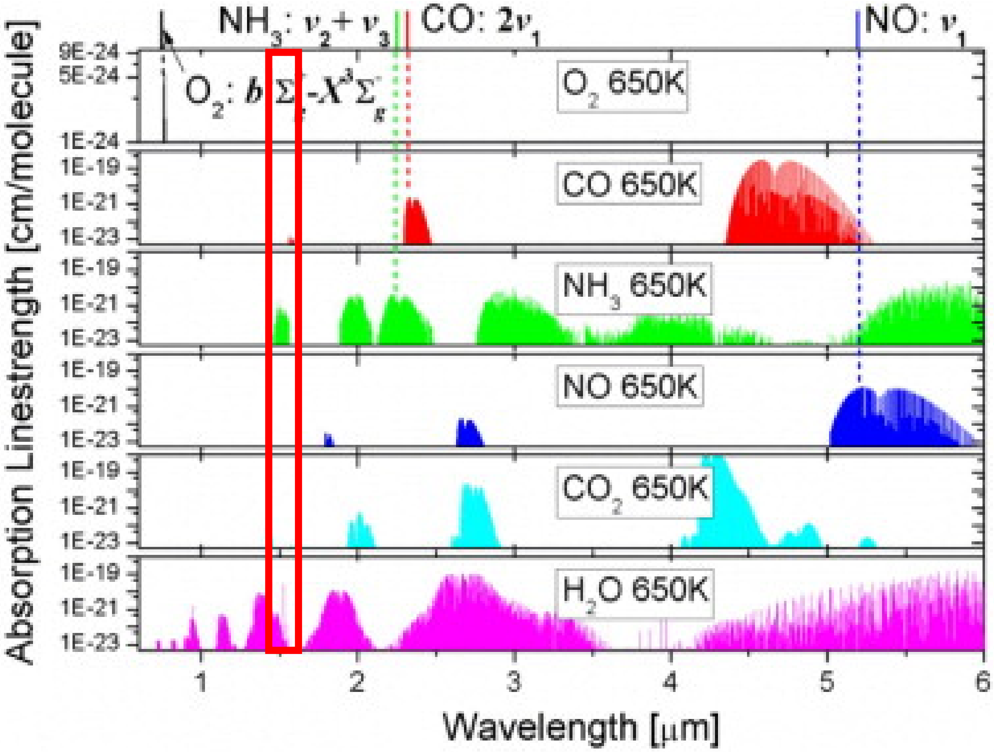


LBS OF 50% NH_3 + 50% H_2 IN SYNTHETIC AIR AT 296 K AND 5 ATM

Ongoing work – 10 atm experiment strategy

Need to check condensation of NH_3

- NH_3 wavelength w/o interference
- 1.55 µm

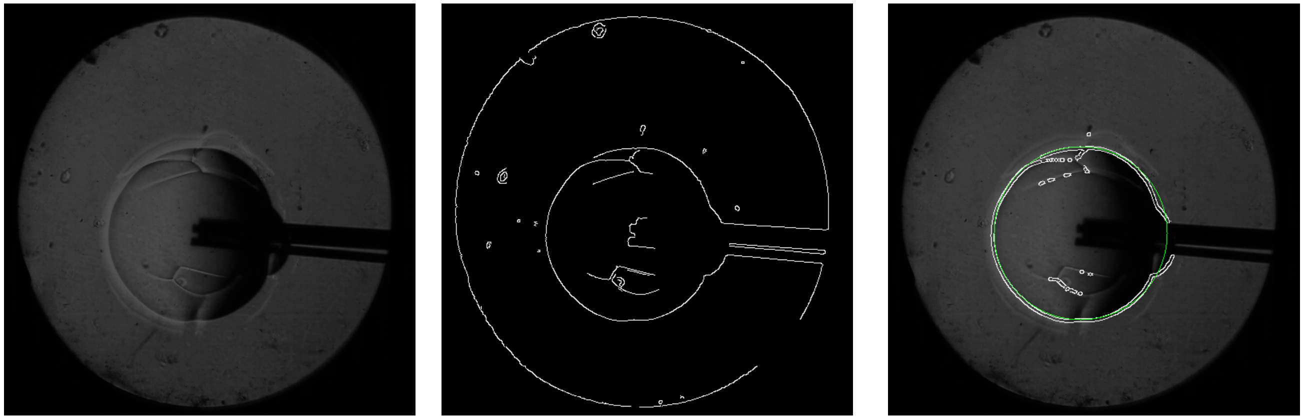


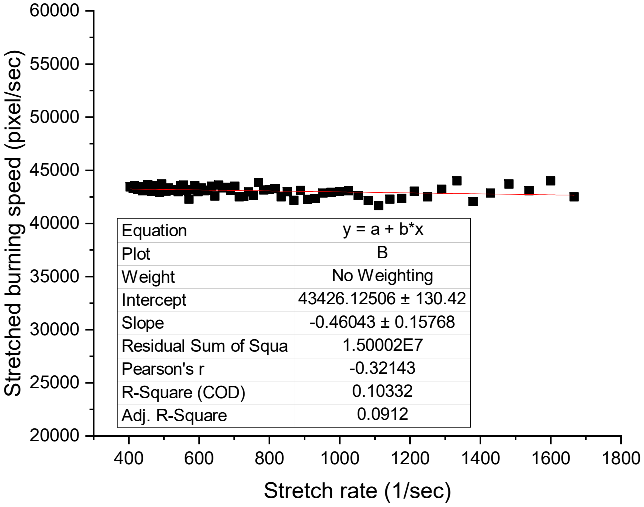
UCF

Ongoing work – 10 atm experiment strategy

- Constant Pressure method
  - Extraction image from video
  - Find edges with Edge Detector
  - Find flame and calculate radius
  - Calculate unstretched burning speed with radius
  - Convert to Laminar burning speed ($S_u = \rho_b / \rho_u \cdot S_0$)

phi	CVM (m/s)	CPM (m/s)	Difference (%)
0.70	0.350	0.345	1.61
0.91	0.576	0.563	2.29





Equation	y = a + b*x
Plot	B
Weight	No Weighting
Intercept	43426.12506 ± 130.42
Slope	-0.46043 ± 0.15768
Residual Sum of Squa	1.50002E7
Pearson's r	-0.32143
R-Square (COD)	0.10332
Adj. R-Square	0.0912

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