DEVELOPING A MODELLING APPROACH TO SIMULATE COMBUSTION OF AMMONIA/HYDROGEN MIXTURES

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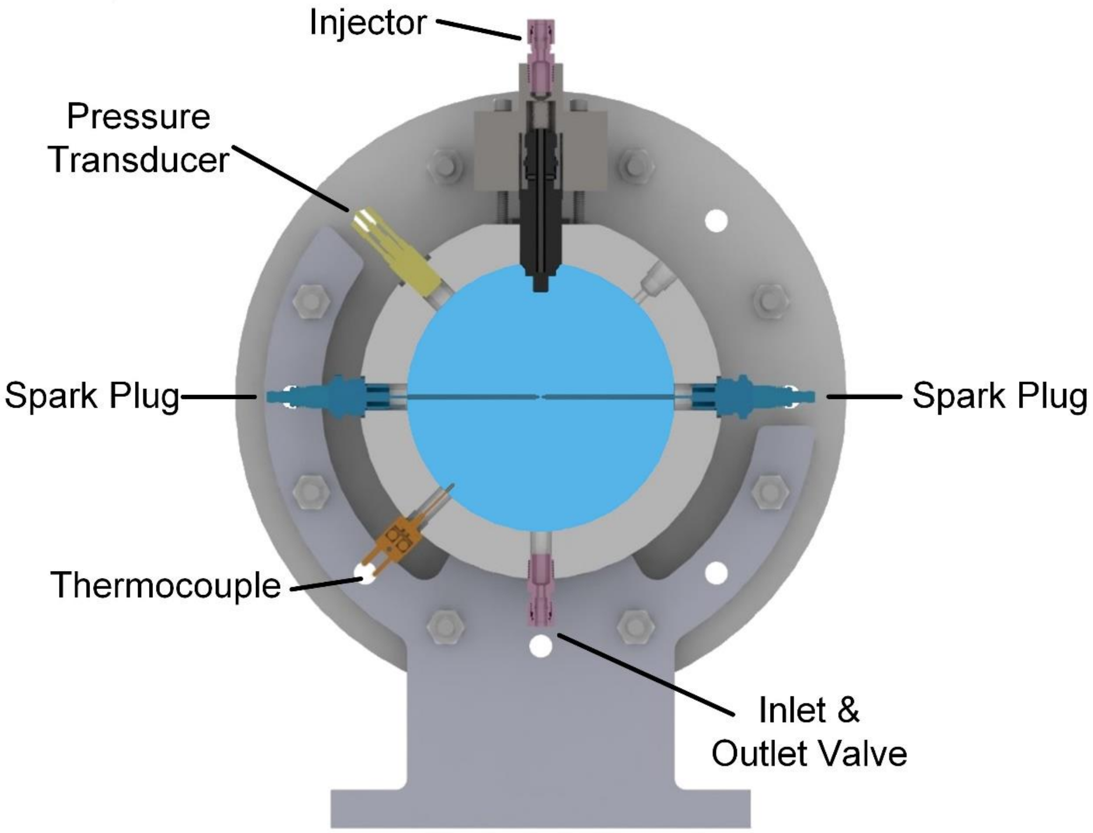
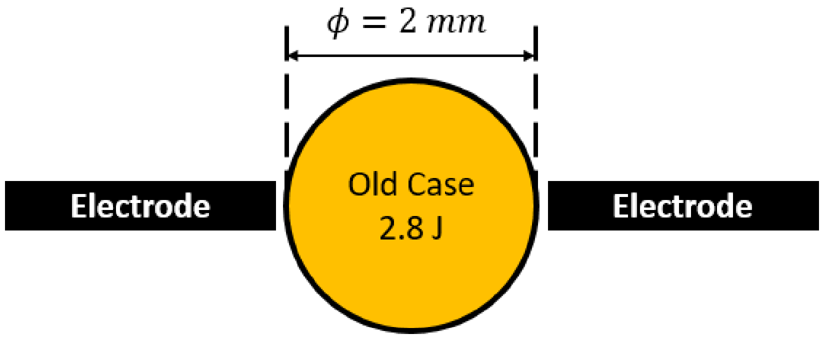
INTRODUCTION

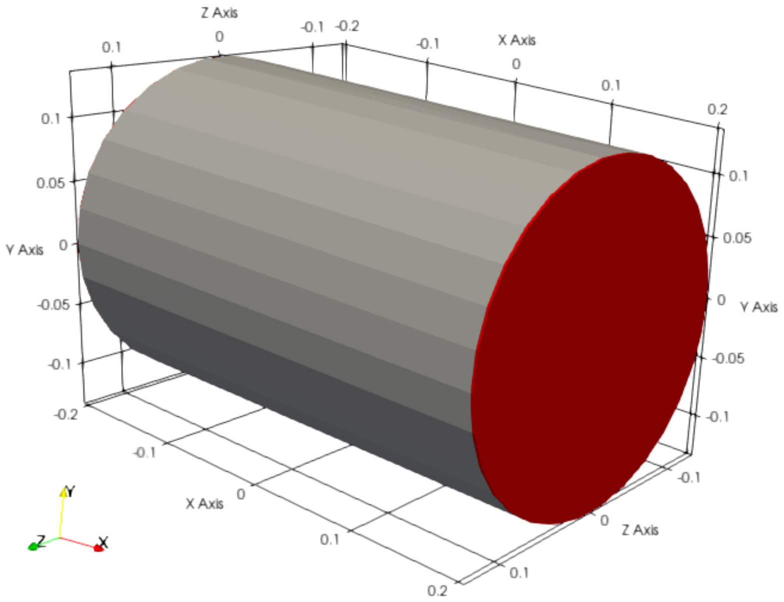
- Research on alternate fuels for IC engines for decarbonizing.
- Ammonia, a carbon free hydrogen carrier and an alternate fuel.
- Blended with hydrogen
- CONVERGE CFD 3.0 used to simulate the ammonia-hydrogen blend in a constant volume combustion chamber (CVCC).
- Simulation compared with Literature and companion CVCC experiments performed for the study.
- Selecting most promising mechanism.
- Investigating some of the assumptions of the flamespeed measurement.
- Different approaches for the ignition.



LITERATURE EXPERIMENT

- Akhirio Hayakawa et al. studied the unstretched laminar burning velocity and Markstein length of ammonia/air premixed flames.
- For the ammonia/hydrogen/air combustion Akinori Ichikawa et al. studied the same.
- The chamber in the study had an inner diameter of 270mm and height 410mm.
- Electrodes in the center spaced 2mm apart
- Chamber volume – 23L
- Electrostatic energy was set at 2.8J
- Energy source reduced to 0.2J for pure H2





A. Hayakawa, T. Goto, R. Mimoto, Y. Arakawa, T. Kudo, and H. Kobayashi, "Laminar burning velocity and Markstein length of ammonia/air premixed flames at various pressures," *Fuel*, vol. 159, pp. 98–106, Jul. 2015, doi: 10.1016/j.fuel.2015.06.070.

CHEMICAL KINETICS MECHANISMS

- Comparison of different mechanisms.
- Compared using 0-D and 1-D models in CHEMKIN-Pro.
- The four models were used for the calculation of laminar flame speed for ammonia/air combustion and five models for the hydrogen blend combustion
- Otomo et al was furthered used in the 3-D CFD analysis.

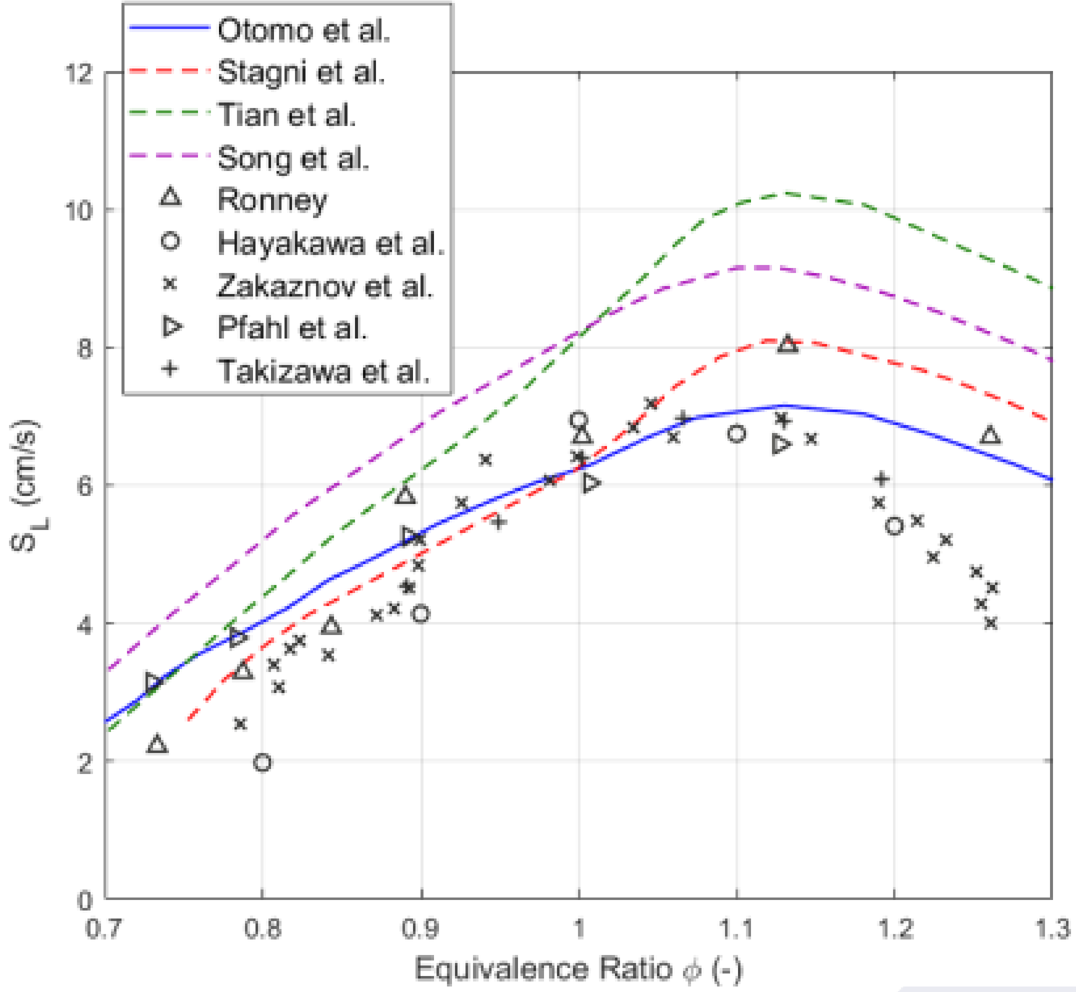
Ammonia/ air combustion			
Model	Species	Reactions	Year
Tian et al.	84	703	2009
Song et al.	34	204	2016
Otomo et al.	32	211	2017
Stagni et al.	31	203	2020

Ammonia/hydrogen/air combustion			
Model	Species	Reactions	Year
Tian et al.	84	703	2009
Otomo et al.	32	211	2017
Stagni et al.	31	203	2020
Konnov et al.	127	1207	2001
GRI-Mech 3.0	53	325	-

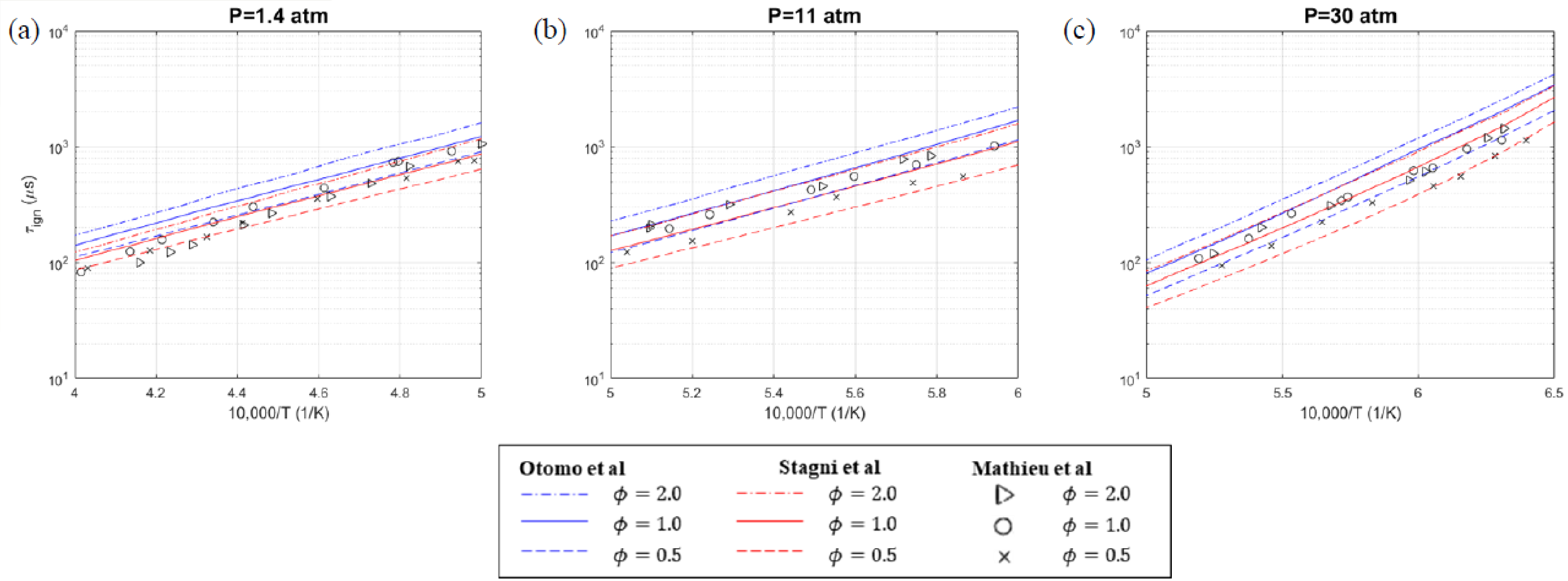
0-D, 1-D AMMONIA COMBUSTION RESULTS

1-D Flame Speed Model

- Calculations done in 1-D domain with AMR, length adjusted for each ammonia case.
- The initial temperature and pressure were at 298K and 0.1 MPa
- Laminar flame speed for ammonia case is lower than conventional fuels.
- At $\varphi = 1.1$ peak laminar flame for ammonia (7 cm/s)
- Chemical Kinetics method overpredicted the laminar flame speed



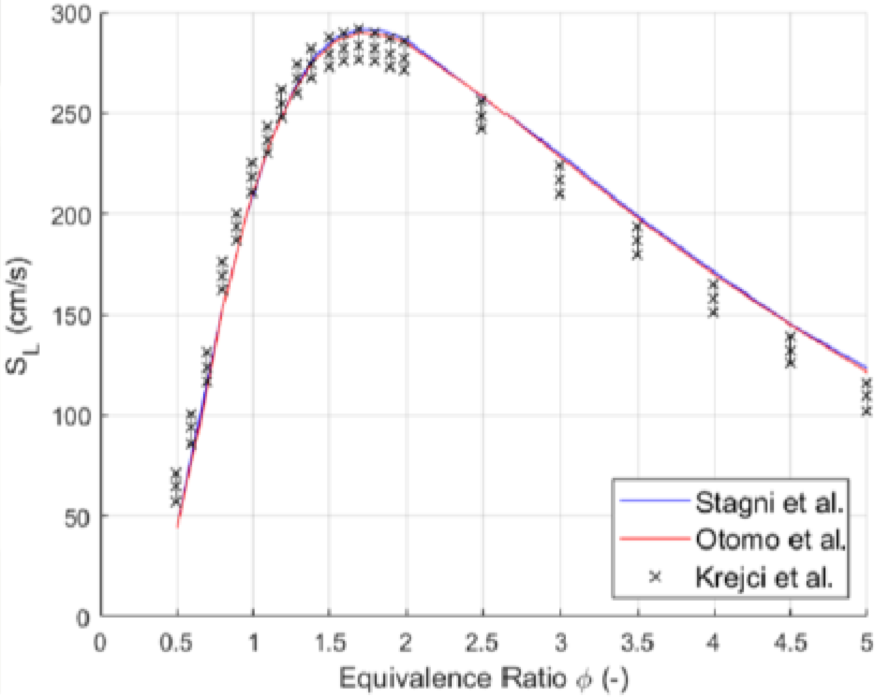
0-D, 1-D AMMONIA COMBUSTION RESULTS



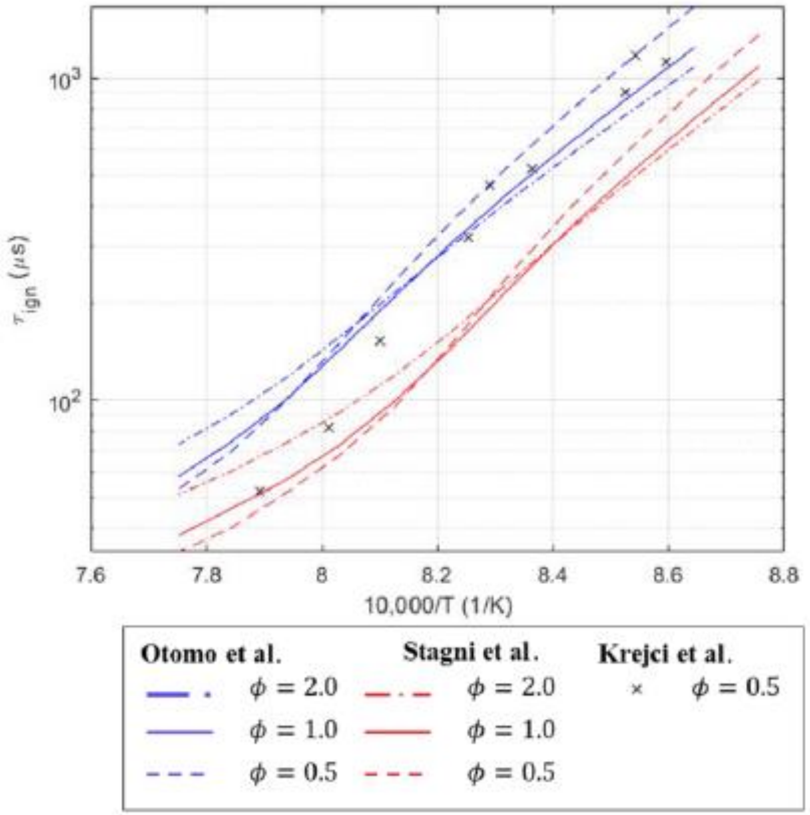
0-D Ignition delay

- Ignition delay measured on time of chemiluminescence emission of excited state hydroxyl radical.
- In simulations temperature was analyzed and peak rate of change of the temperature was determined to be ignition delay.
- Stagni et al gives closer results to the experiments done by Mathieu et al.
- Shortest ignition delay in lean mixtures and longest in rich mixtures

RESULTS OF NH3/H2/AIR

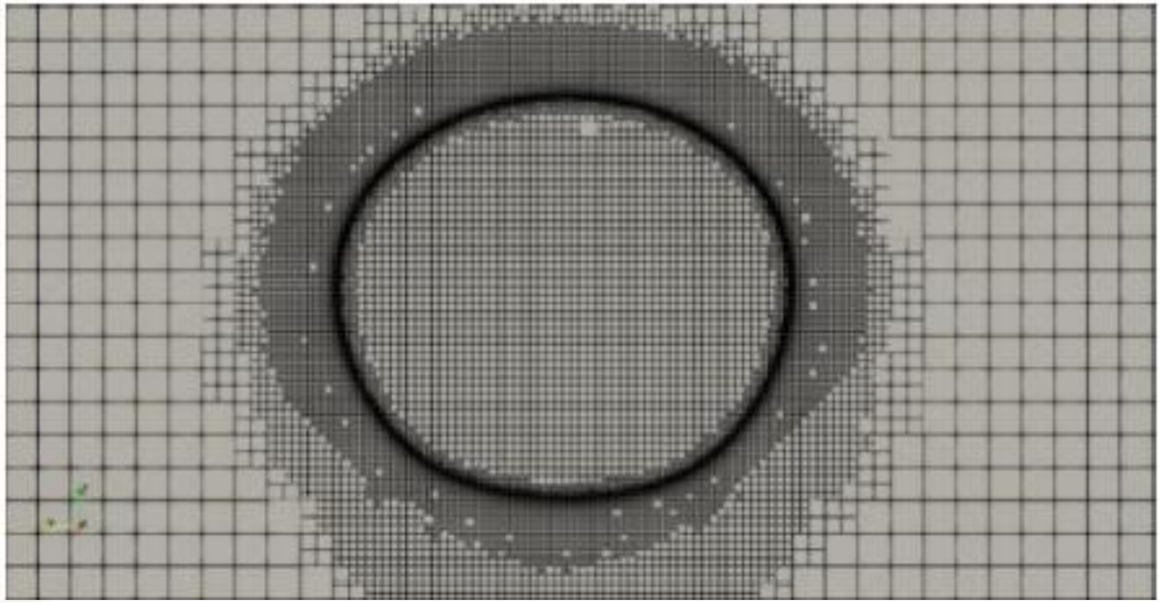


- Simulations in agreement with the experiment data by Krejci et al.
- Higher laminar flame speed than ammonia case.
- Maximum flame speed under richer conditions.



- Higher temperature Stagni et al. predicted better autoignition.
- Lower temperature Otomo et al. was more accurate.
- Leanest predicts the fastest ignition at higher temperature and richest at lower temperatures.

CONVERGE SETUP



Turbulence model	None
Combustion model	SAGE
Max CFL number	1
Outlet boundary conditions	Pressure: 101325 Pa
Maximum timestep	1×10^{-4} s
Minimum timestep	1×10^{-8} s

Embedding Level	6
Cell size	0.078125 mm
Radius	0.005mm
Embedding level	5
Cell size	0.3125 mm
Radius	0.01 mm
Embedding level	3
Cell size	3.75 mm
Radius	0.03 mm

	Pure Ammonia	Ammonia/H2
Initial cell count	4×10^5	20×10^6
Embedding scale	6	7
Minimum cell size	0.15625 mm	0.078125 mm
Base Grid	10mm	
Fixed cell embedding shape	Sphere	
AMR variables	Temperature and density	
Temperature value	1K	
Density value	0.1kg/m^3	

FLAME SPEED CALCULATIONS

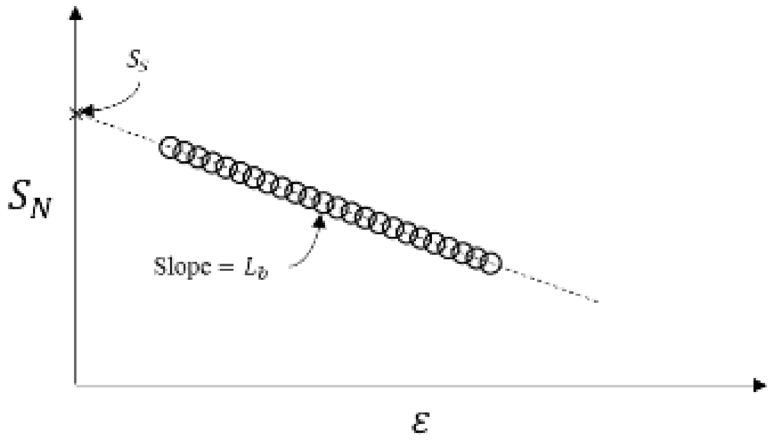
- Stretched flame speed and stretch rate used to determine the laminar flame speed and Markstein length.
- Key is to accurately calculate the radius of the flame to determine laminar flame speed.
- Three methods used to calculate the rate of change of the flame radius.
- Method 1: equivalent area method
- Method 2: moving center method
- Method 3: image processing method

$$S_N = \frac{dr_{flame}}{dt}$$

$$\varepsilon = \frac{1}{A} \cdot \frac{dA}{dt}$$

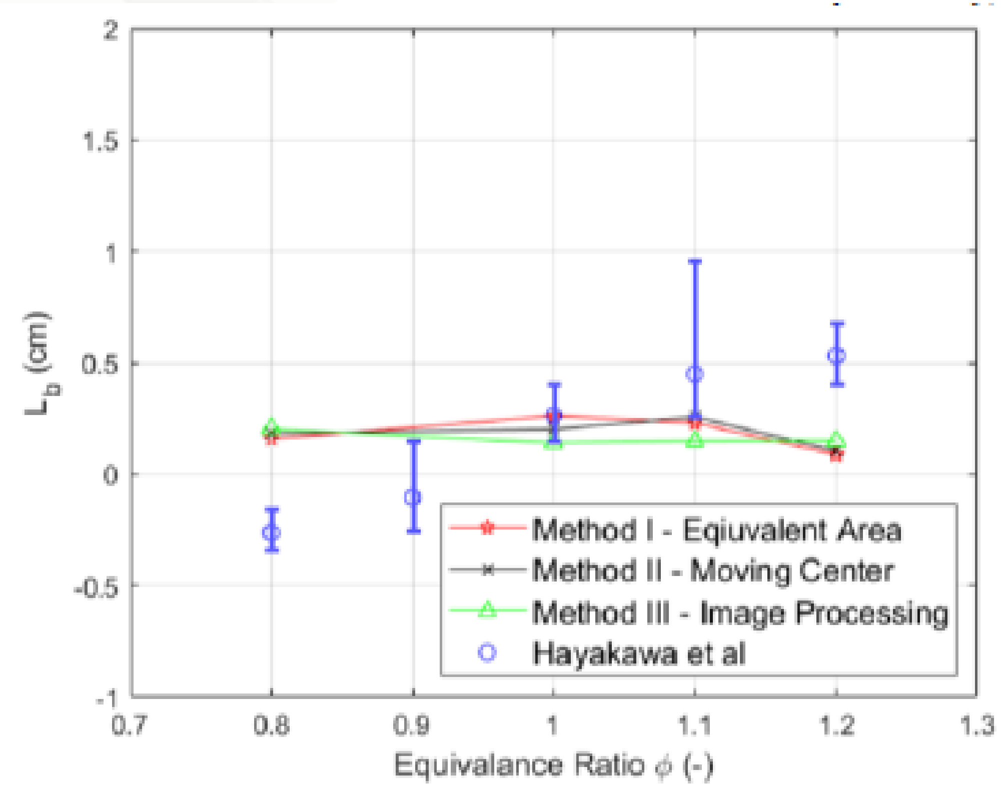
$$S_N = S_S - L_b \cdot \varepsilon$$

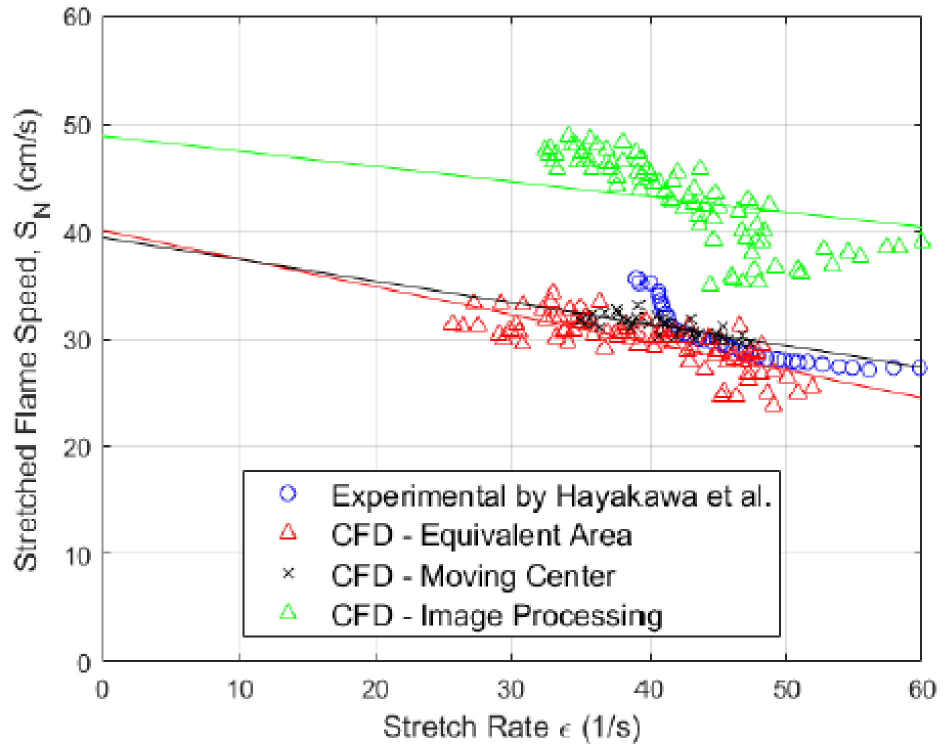
$$S_L = \frac{\rho_b}{\rho_u} \cdot S_s$$



3-D CFD AMMONIA COMBUSTION RESULTS

- Difference between equivalent area and moving center is method 1 has more scattered data than method 2.
- Method 3 gives higher unstretched flame speeds

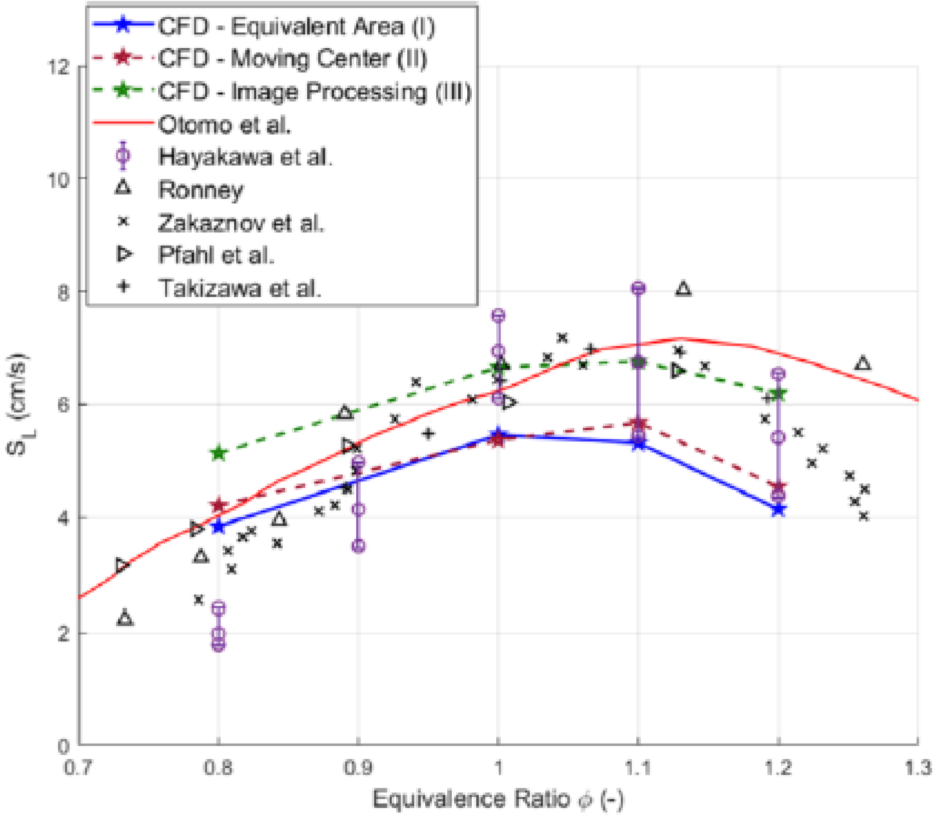




- There is no variation in the Markstein length in either of the three methods used.
- More curvature and different shapes in actual flames is difficult to predict.

3-D CFD AMMONIA COMBUSTION RESULTS

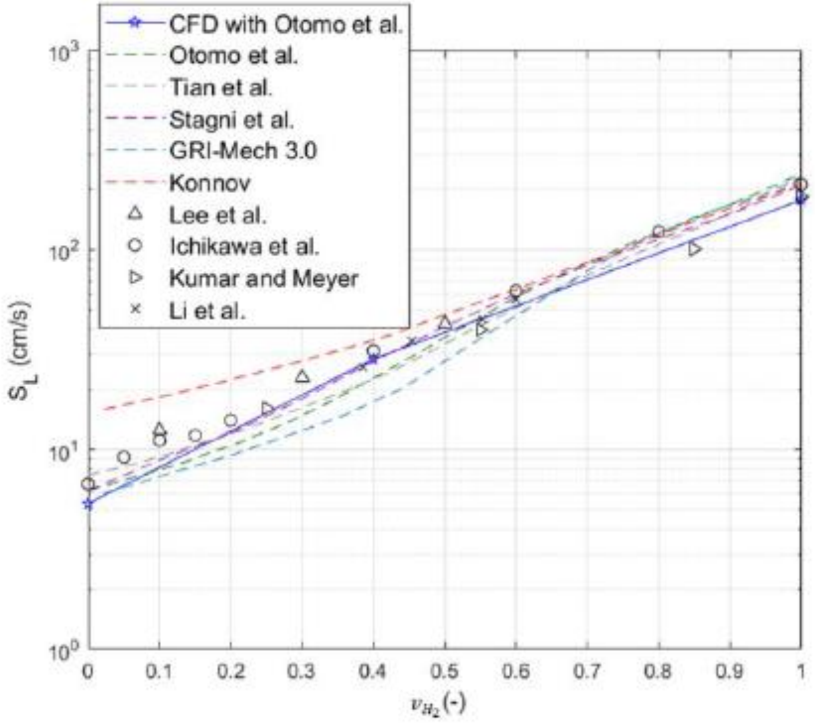
- The 3-D model predictions is close to the 1-D simulations for lean and stochiometric cases.
- Underpredicted the flame speed for rich cases.
- Overall, the CFD simulation is in good agreement with the experimental data.
- Methods 1 & 2 similar and in accordance with the experimental data.
- Higher flame speed recorded by method 3.

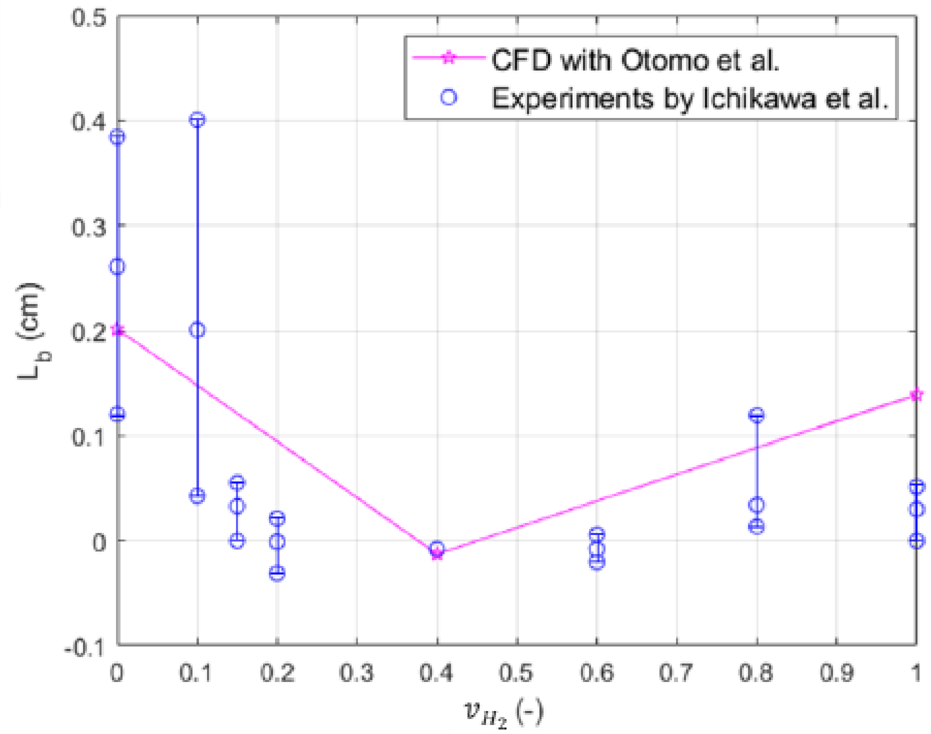


UMASS LOWELL

3-D AMMONIA/HYDROGEN/AIR RESULTS

- Hydrogen to ammonia at different volumetric fuel fraction at constant $\varphi = 1$.
- GRI-Mech 3.0 is lagging in this as it is developed for natural gas.
- More accurate than ammonia combustion.
- Moving center method used to determine laminar flame speed.

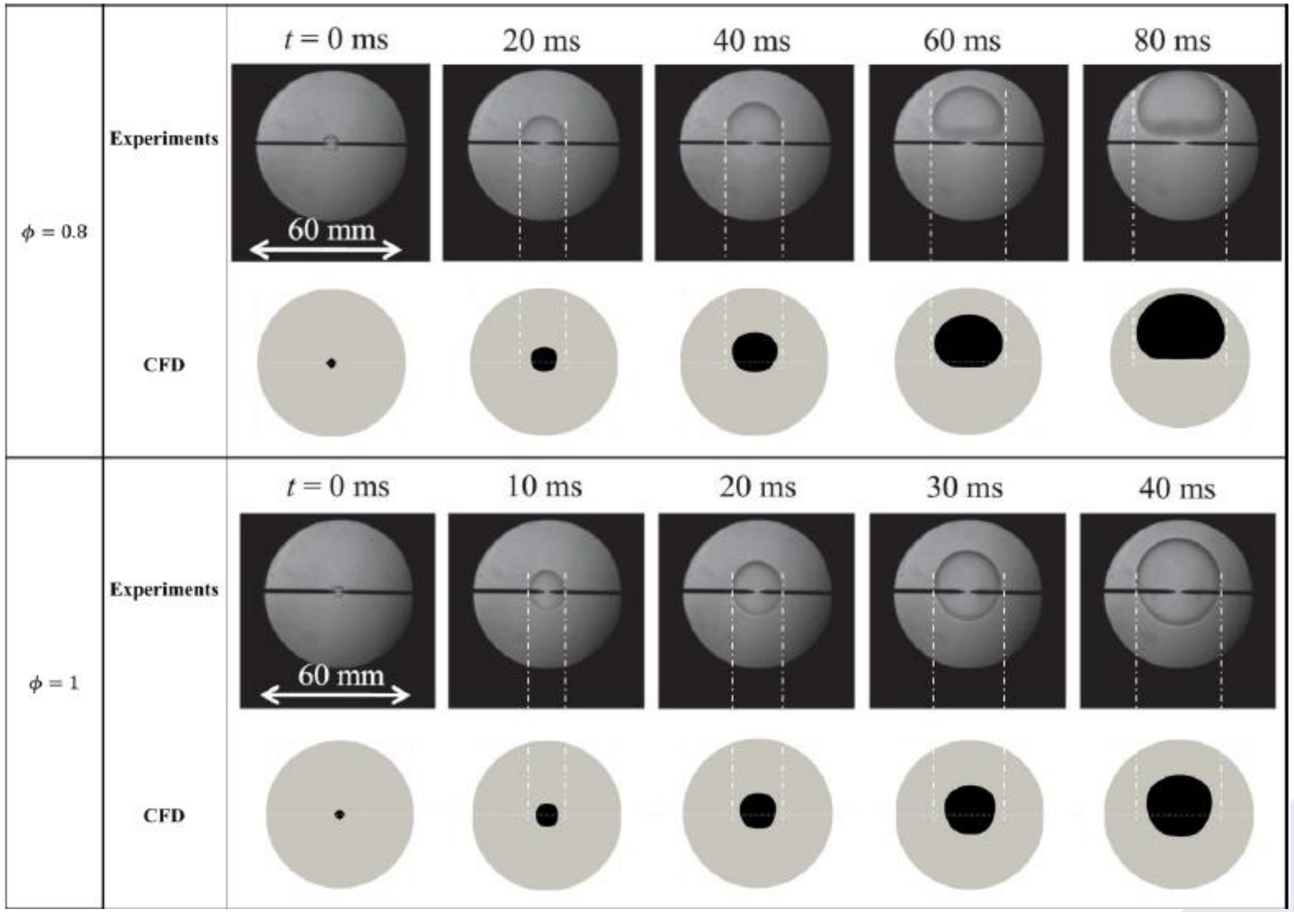




- CFD with Otomo et al. model predicted better Markstien length than the ammonia models.
- For pure hydrogen overpredictions of the flame speed can be seen due to overprediction of Markstien length.

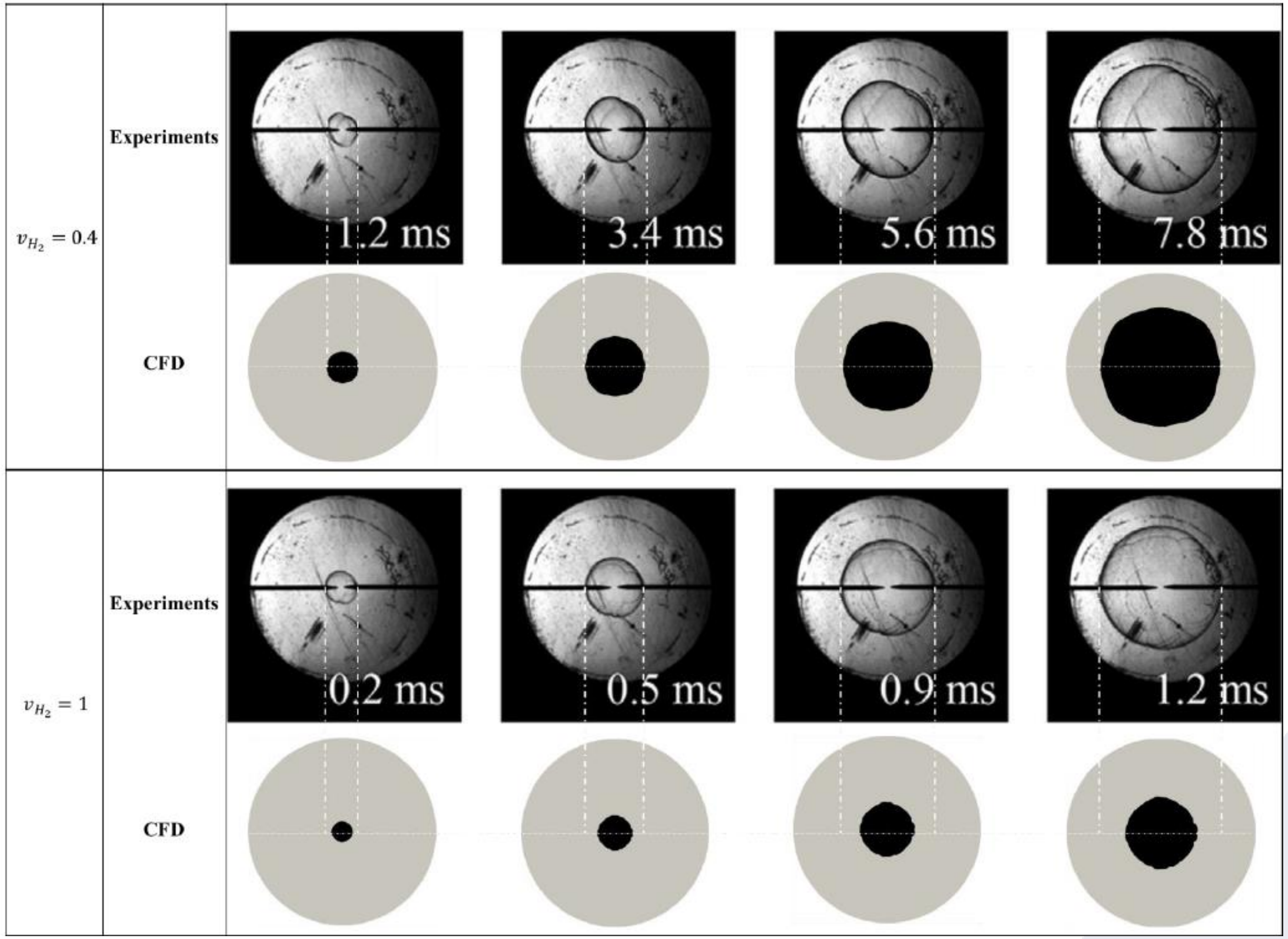
FLAME IMAGES NH3/AIR

- Buoyancy effects can be seen in lean case.
- At t = 10ms the laminar flame speed is closest to the experimental value.
- Flame growth visually seems to be giving the same speed as the experiment, but the flame radius isn’t the same at a given time.



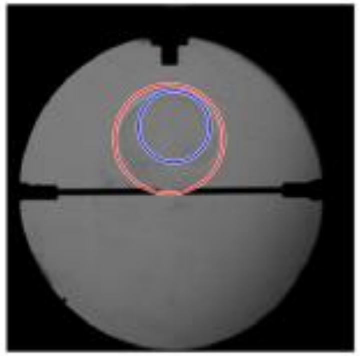
FLAME IMAGES NH3/H2/AIR

- Accurate flame development, structure and radius at 40% hydrogen.
- Slow ignition for pure hydrogen case.
- Estimating flame speed shape is pivotal to determine the laminar flame speed.
- Lower stretched flame speed resulted in slower laminar flame speed.

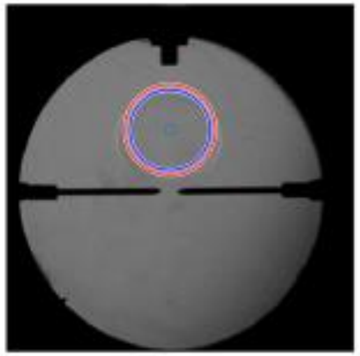


CIRCULARITY METRICS

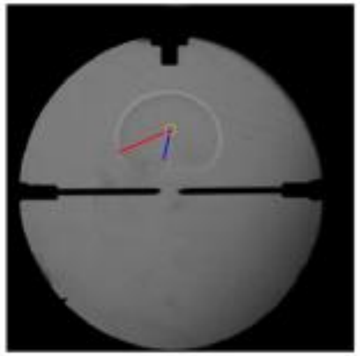
$$\text{Circularity} = \frac{4\pi \times \text{Area}}{\text{Perimeter}^2}$$



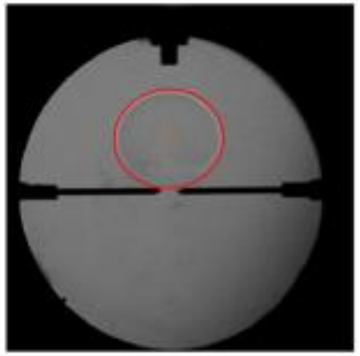
$$\text{Roundness} = \frac{R_{in.}}{R_{circum.}}$$



$$\text{Avg. Radius} = \frac{R_{avg.}}{\sqrt{\text{Area}/\pi}}$$



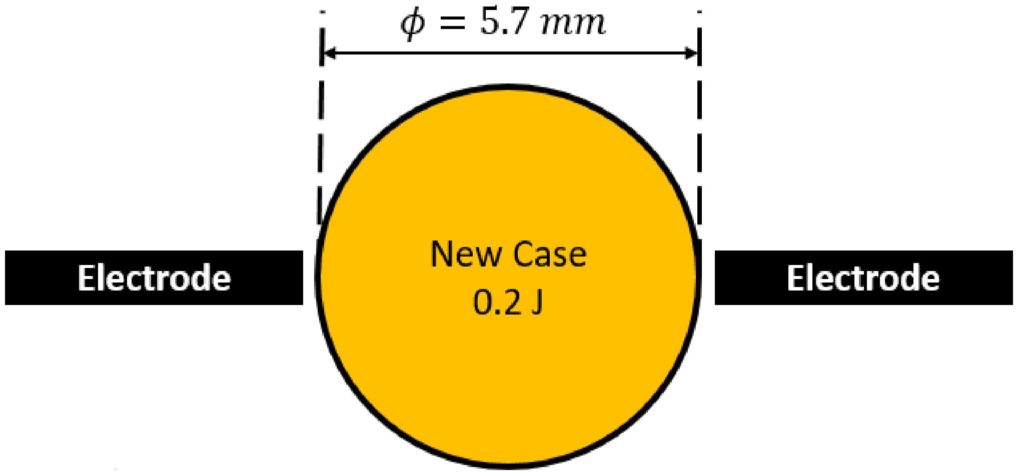
$$\text{Min. Max. Radius} = \frac{R_{min}}{R_{max}}$$

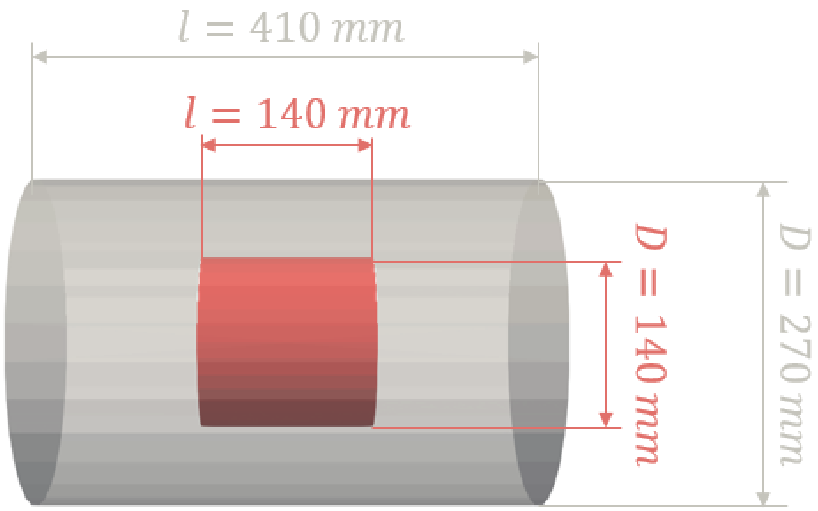


$$\text{Eccentricity} = \sqrt{1 - \frac{b^2}{a^2}}$$

UML CVCC

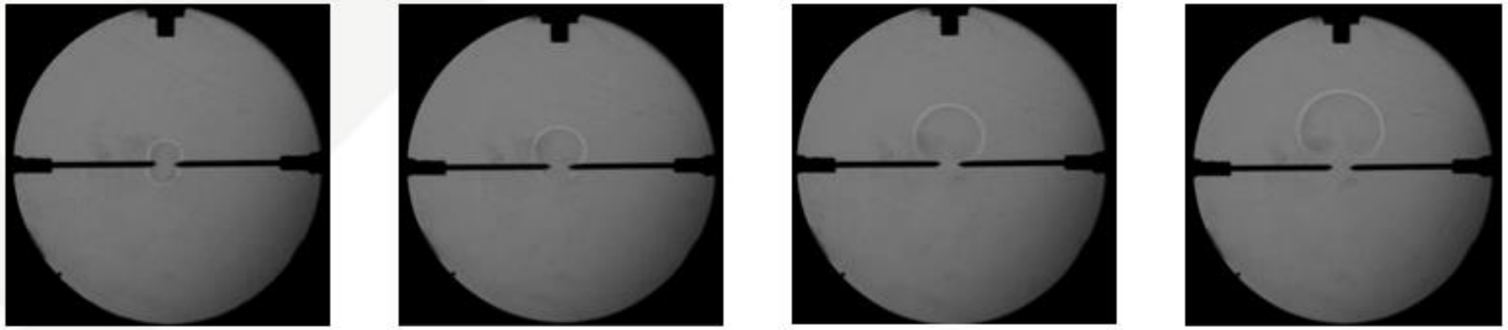
- The UML chamber was a bit different for real time results
- The UML experimental setup used a wider electrode gap and utilized less ignition energy to achieve successful ignition.
- Not achieved in Converge with the same ignition modelling as the Hayakawa et al. case.
- Tiny timesteps for the large energy provided.



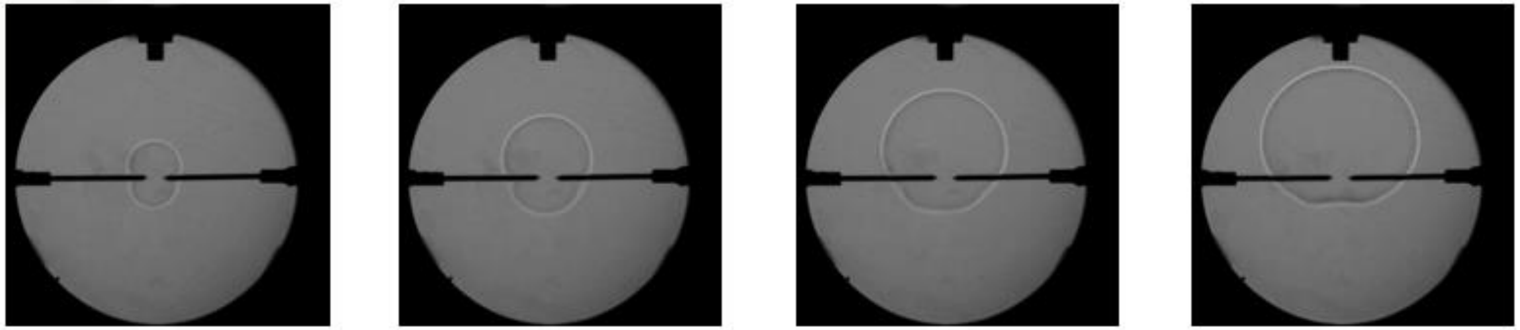


EXPERIMENT IMAGES

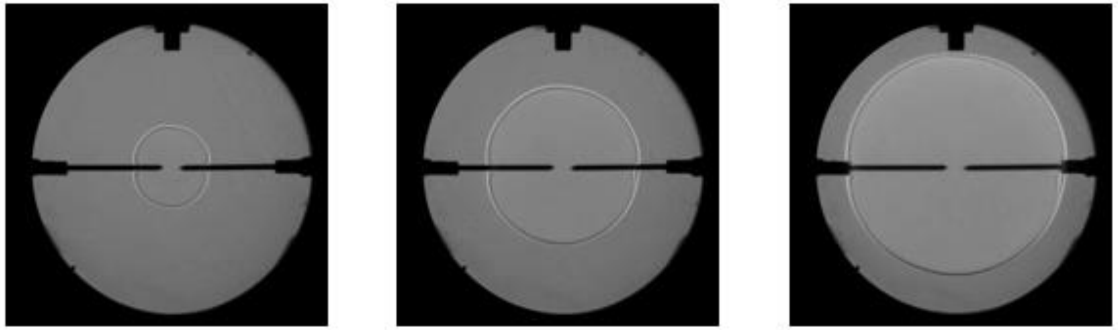
0% hydrogen at 1 bar $\varphi = 0.7$



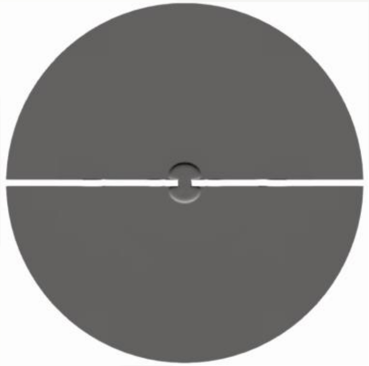
10% hydrogen at 1 bar $\varphi = 0.7$



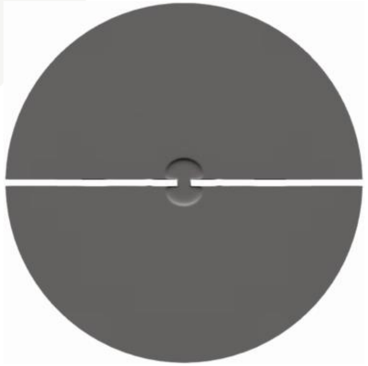
40% hydrogen at 1 bar $\varphi = 1.3$



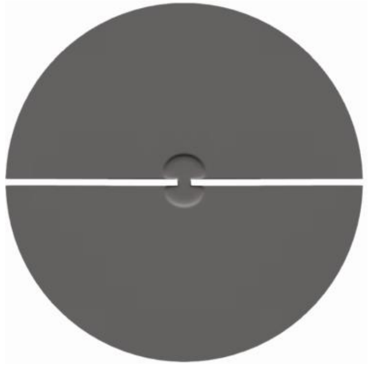
SIMULATION IMAGES



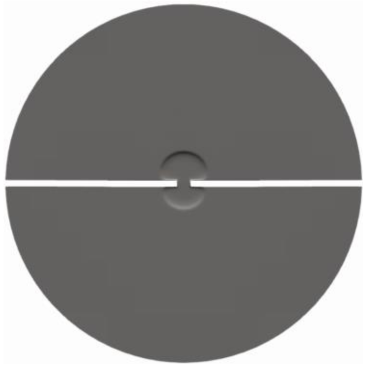
5ms



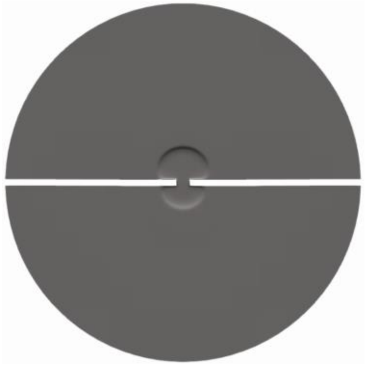
10ms



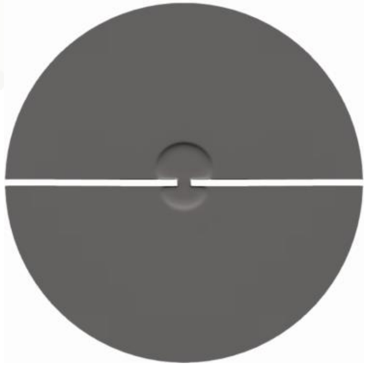
15ms



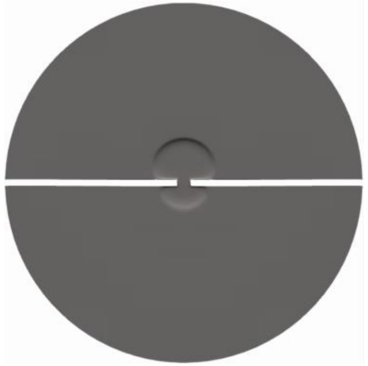
20ms



25ms



30ms



35ms

40ms

45ms

50ms

FUTURE WORK

- To run different setups to enhance the accuracy of the simulation.
- To what impact does the electrode do to the flame.
- Using different kinetics models.
- Use different shapes for the flame in the simulation.
- Calculate accurate laminar flame speed for the UML CVCC.

REFERENCES

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- Noah Van Dam, Behlol Nawaz, Md Nayer Nasim, Amr Shaalan, Dimitris Assanis, Hunter Mack, “Non-spherical NH3-H2-air flames and laminar burning velocity measurements”.
- Noah Van Dam, Behlol Nawaz, Md Nayer Nasim, Amr Shaalan, Dimitris Assanis, Hunter Mack, “Understanding ammonia/hydrogen fuel combustion modeling in A quiescent environment”

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