Ammonia Combustion at Purdue

2nd September 2025

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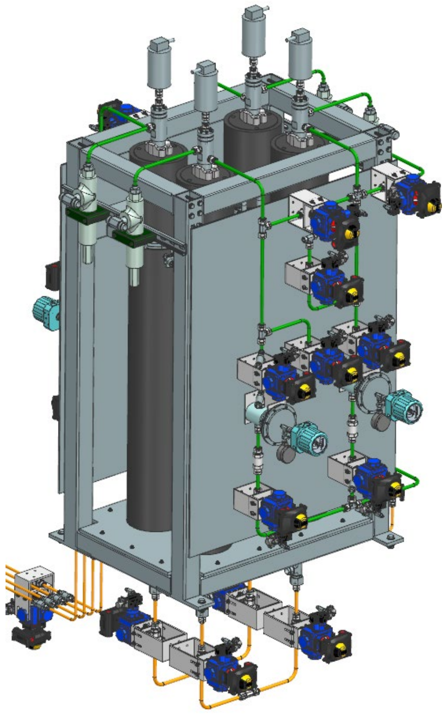
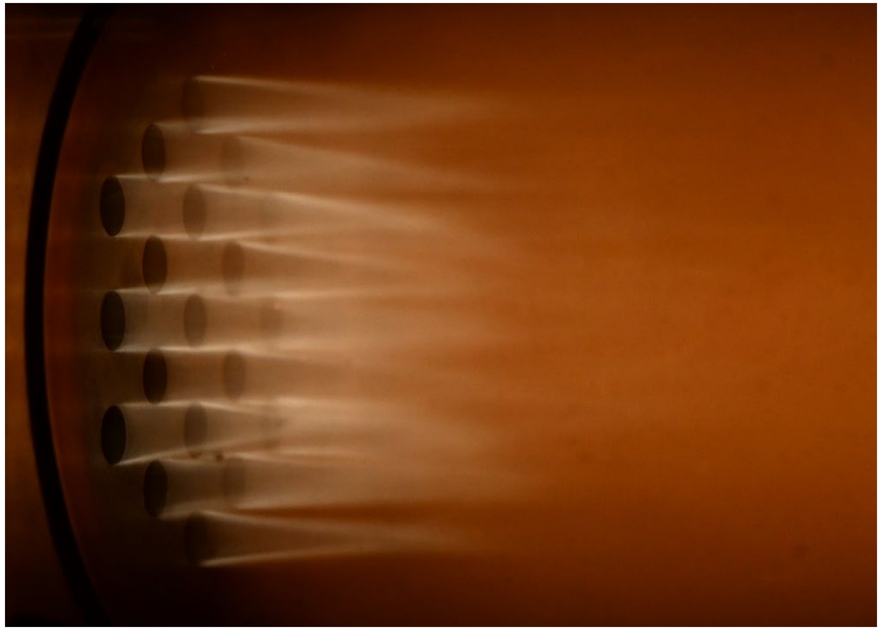




Ammonia Combustion at Purdue

Background

- Challenges with ammonia combustion (kinetics, emissions, etc.) motivates blending with other fuels like H_2 or CH_4
- Limited combustion investigations of these blended fuels at high pressure, Re, and $P_{thermal}$

Goals

- Develop a high-pressure ammonia storage system
  - Capable of liquid or gaseous injection
  - Large-scale storage capable of steady-state operation
- Conduct NH_3-blended combustion experiments at engine relevant conditions ($P_4 \geq 10$ bar, $T_3 \approx 750$ K)
  - Investigate impacts of fuel composition on combustion dynamics and emissions
  - Study flame structure and coupled behaviors under high turbulence

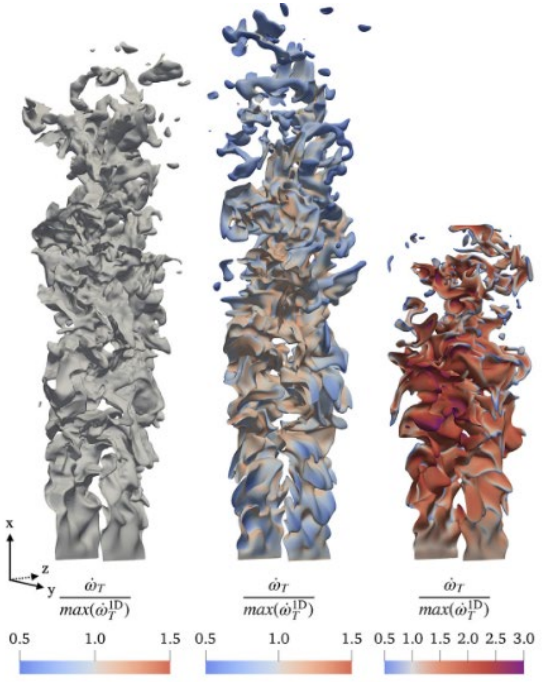


Fig. 3. Isosurfaces of $c = c^*$, retrieved at $t = 2\tau$ and colored by HRR normalized by the maximum value in the corresponding 1D unstretched laminar flame for all cases. CH_4 case at $c^*_{CH_4} = 0.72$ (left), NH_3–H_2 case at $c^*_{H_2O} = 0.78$ (center), H_2 case at $c^*_{H_2} = 0.85$ (right). (For interpretation of the references to color in this figure, the reader is referred to the web version of this article.)

Coulon et al. 2023

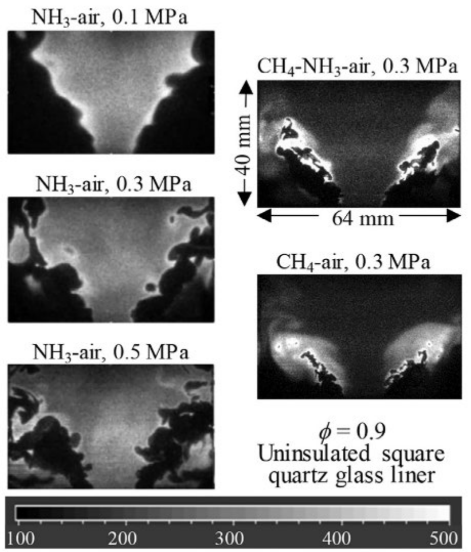
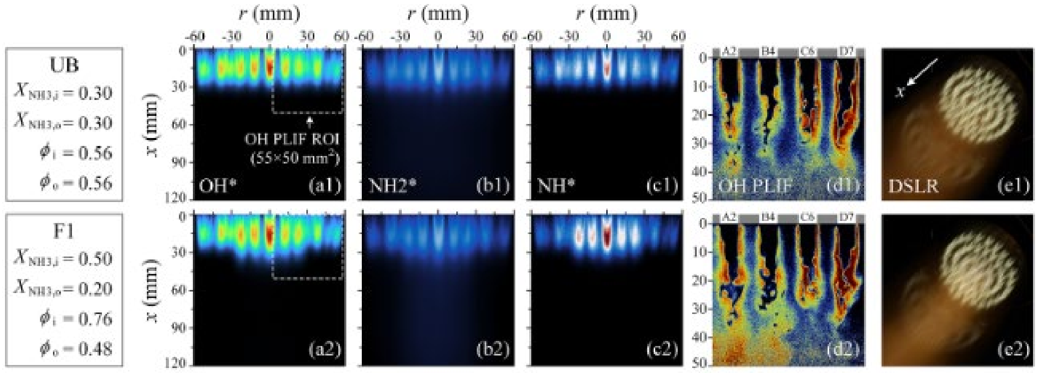


Fig. 2. OH-PLIF images of the swirl stabilized premixed flames in the uninsulated square-shaped liner.

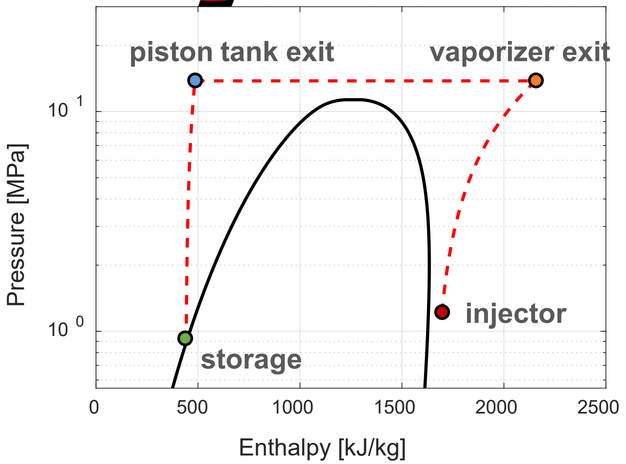
Okafor et al. 2021

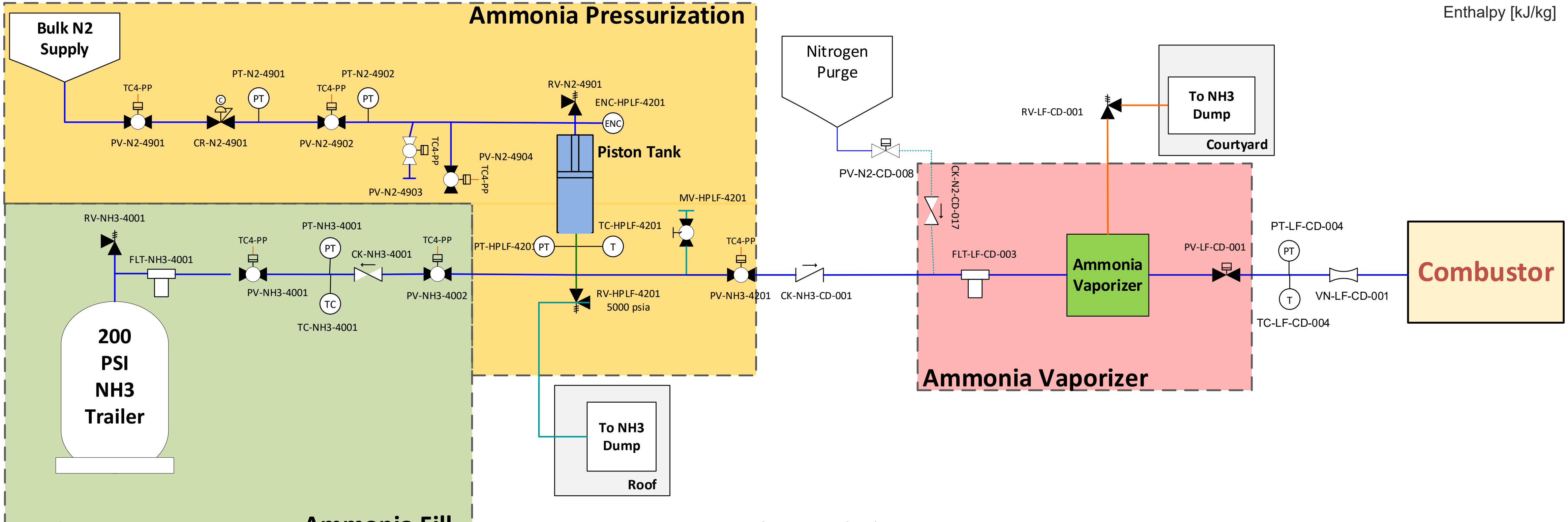


Jin and Kim 2024

Ammonia System Overview

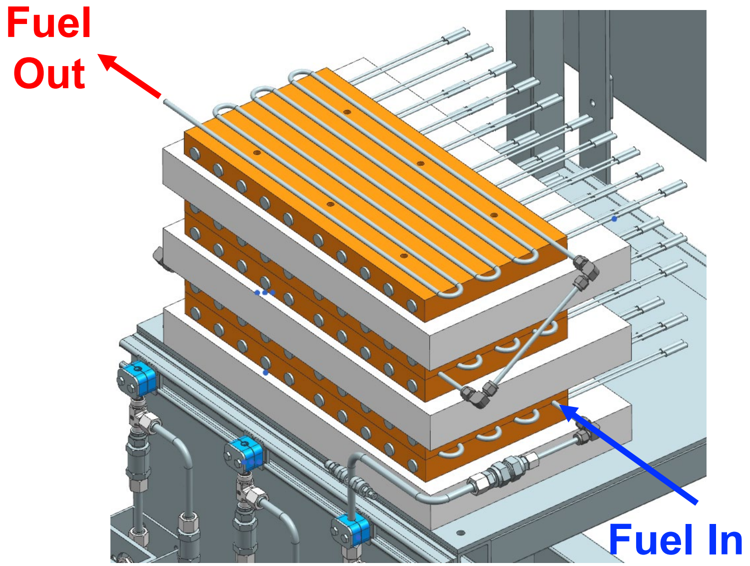
- Ammonia filled into piston tank as saturated liquid
- Liquid ammonia delivered from piston tank to vaporizer
  - Linear encoder provides position feedback from piston
- Gaseous ammonia flowrate metered using critical flow venturi nozzle

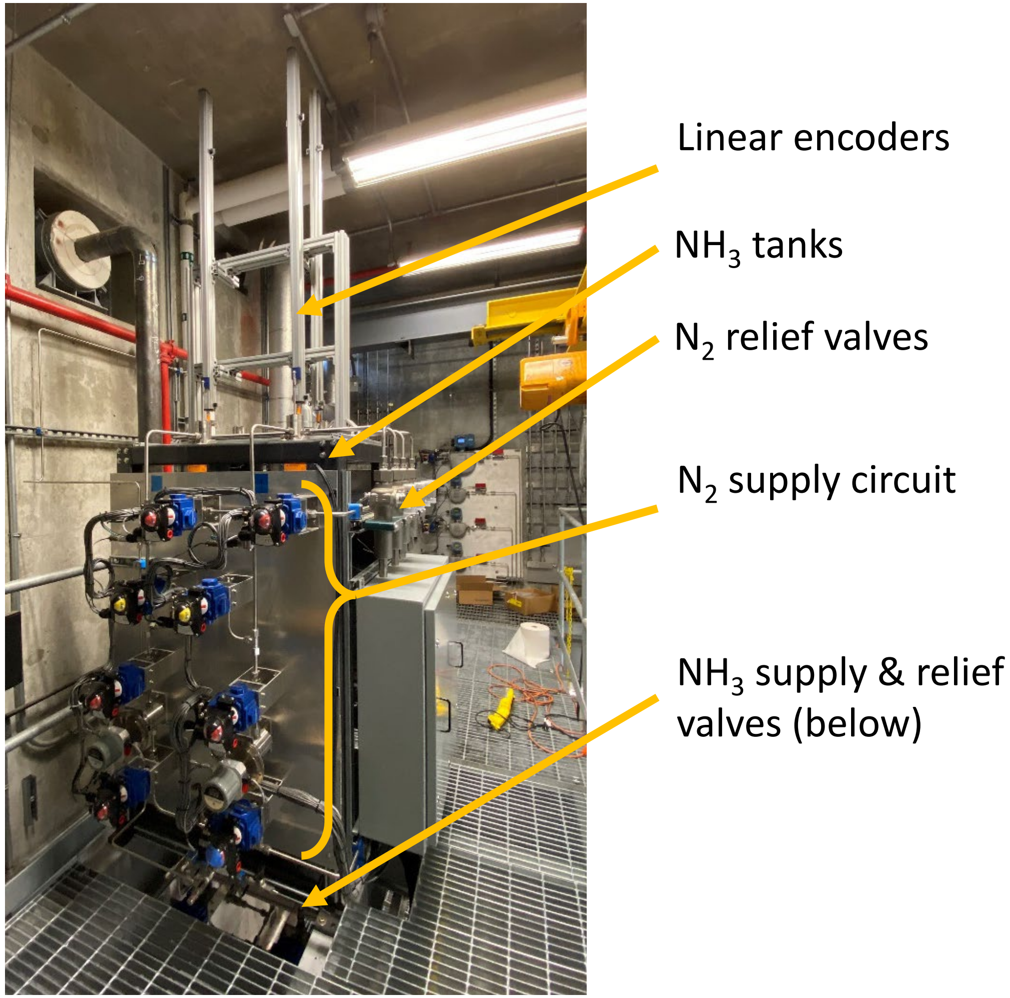




Ammonia System Specifications

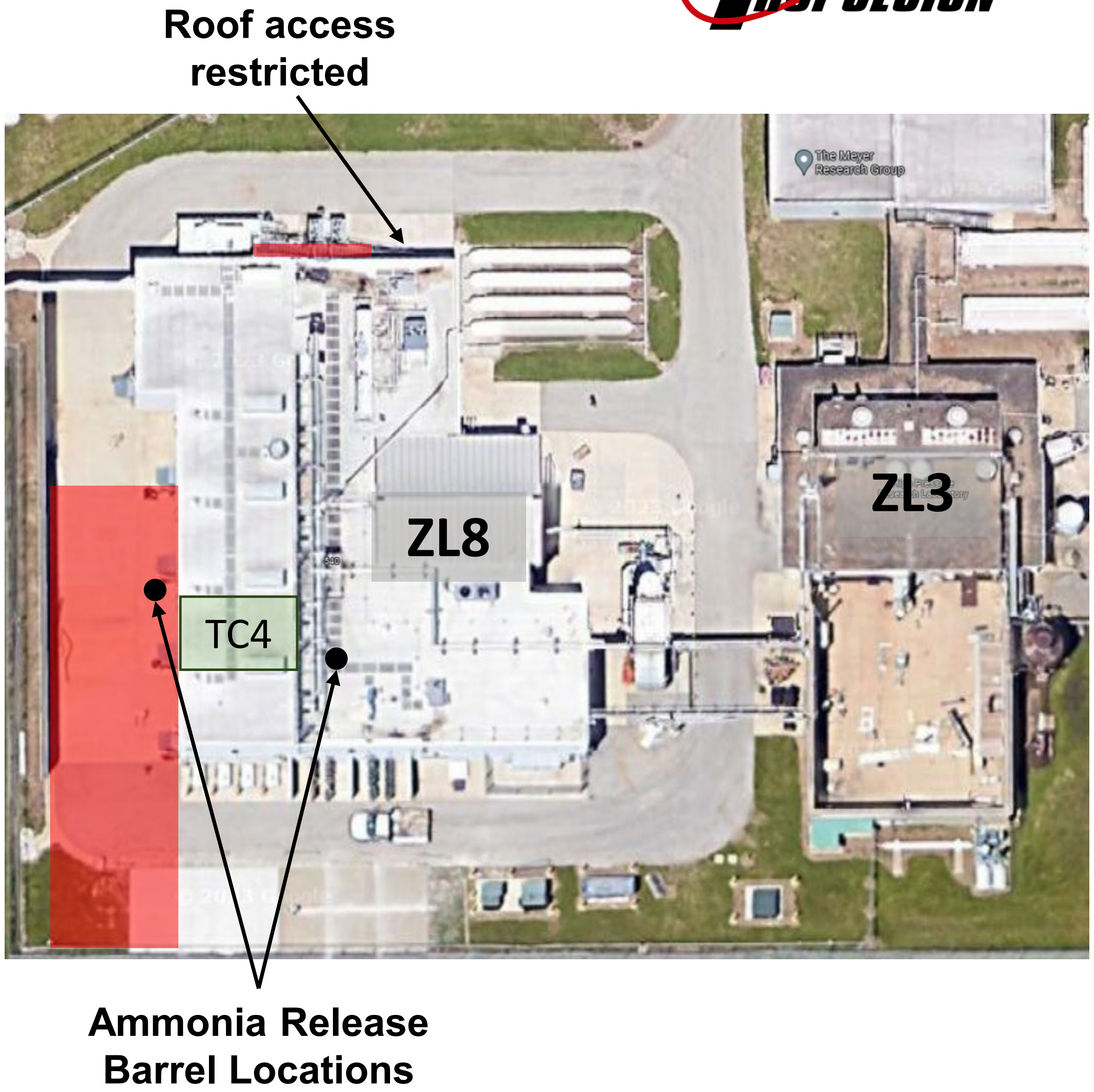
- 4 piston tanks, total of 115 liter storage up to 350 bar
- Accumulators capable of running individually or in parallel
- Ethylene propylene rubber (EDPM) or PTFE used for all elastomeric sealing
- Dump barrels filled with water + antifreeze
- 54 kW electrically heated ammonia vaporizer
- Lines from vaporizer outlet to experiment wrapped in heat tape





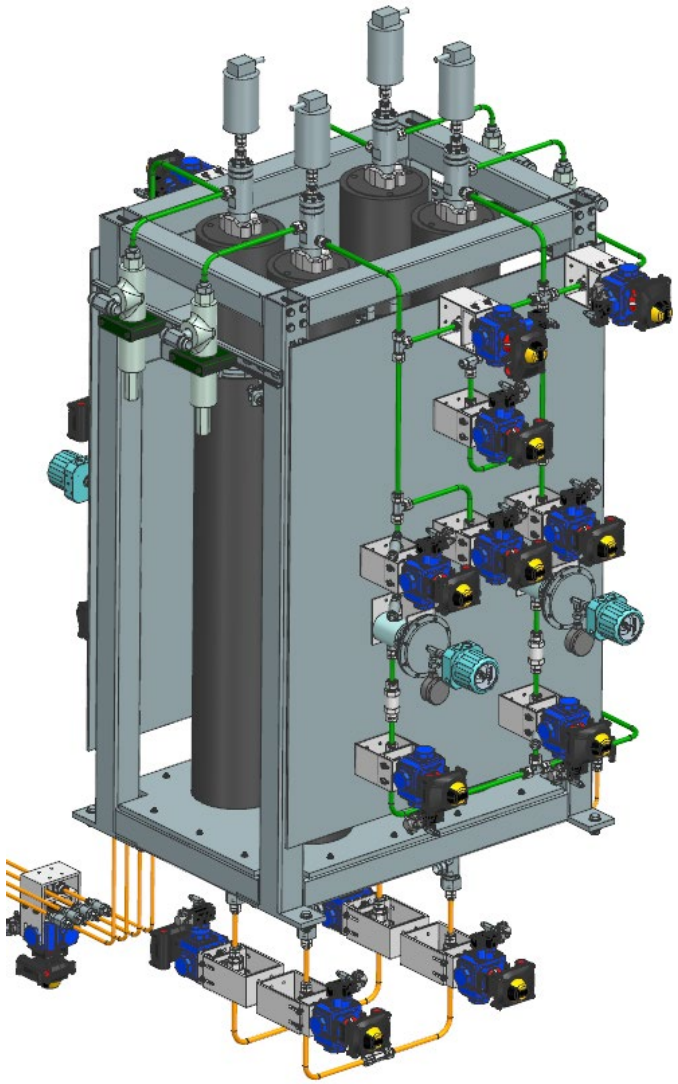
Safety and Detection

- All filling operations performed remotely
- 4 x ammonia gas sensors (0 – 75 PPM full-scale) located throughout test cell
- Restricted areas prevent access up to 20 ft minimum
- Full PPE required for all handling of ammonia



Ammonia System Lessons Learned

- Filling behavior dependent on ambient conditions
  - Lower temperature means less ΔP for filling
- Significant heating required to vaporize ammonia
  - High latent enthalpy of vaporization
  - Joule Thompson cooling during expansion
- Careful consideration of trapped liquid volumes
  - $\frac{dP_{vap}}{dT}$ is large near ambient conditions
  - Thermal expansion
- Lab goggles or full-mask respirators recommended for ammonia handling
- Human detection limit often lower than sensors
  - Easy to tell if concentration is rising well before it becomes dangerous



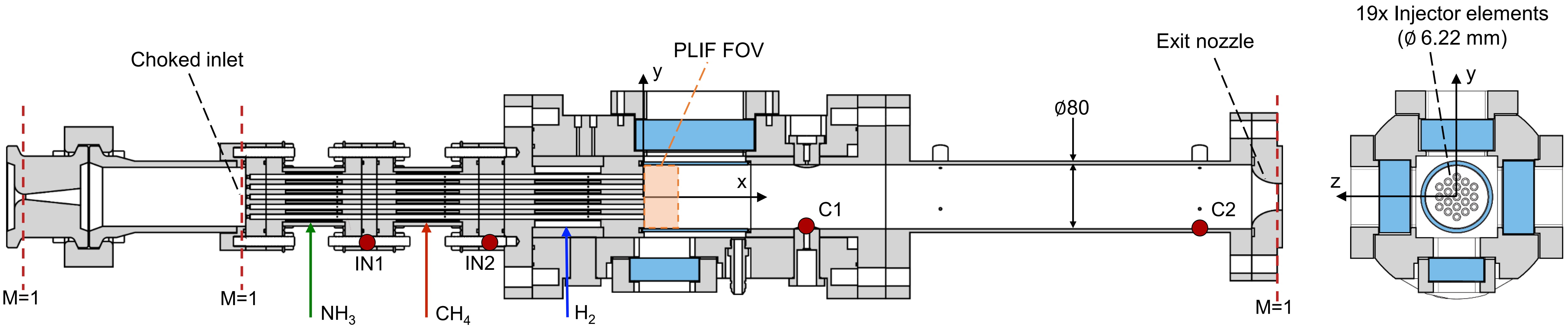
Experiment Methodology

- 0.7 MW high pressure (~10 bar) optically accessible combustion chamber
- Canonical combustor configuration with well defined acoustic boundaries suitable for model validation
- Explore flame structure and dynamics with hydrogen, ammonia, and mixtures of these fuels with methane
- Premixed multi-stage, multi-tube, micromix (M^3) injector
  - $Re_{inj} \approx 150000$

Fuel Composition

$$\chi\left[\eta\left(\frac{3}{2}H_2+\frac{1}{2}N_2\right)+(1-\eta)NH_3\right]+(1-\chi)CH_4$$

χ = hydrogen fraction
η = ammonia decomposition efficiency



Micromixer Flame Structure

- 100 kHz planar laser-induced fluorescence of OH performed using burst mode laser
  - Time-resolved flame structure imaging
  - Time-average shows prominent features
- Multi-plane imaging reveals 3D flame structure
  - Reactions occur through entire injector circumference on average

Fuel Composition

$$\chi\left[\eta\left(\frac{3}{2}H_2+\frac{1}{2}N_2\right)+(1-\eta)NH_3\right]+(1-\chi)CH_4$$

χ = hydrogen fraction
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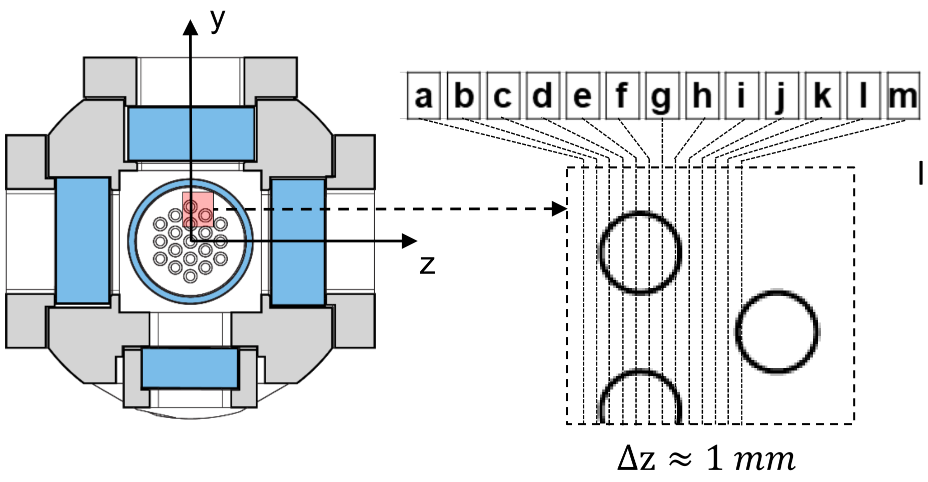
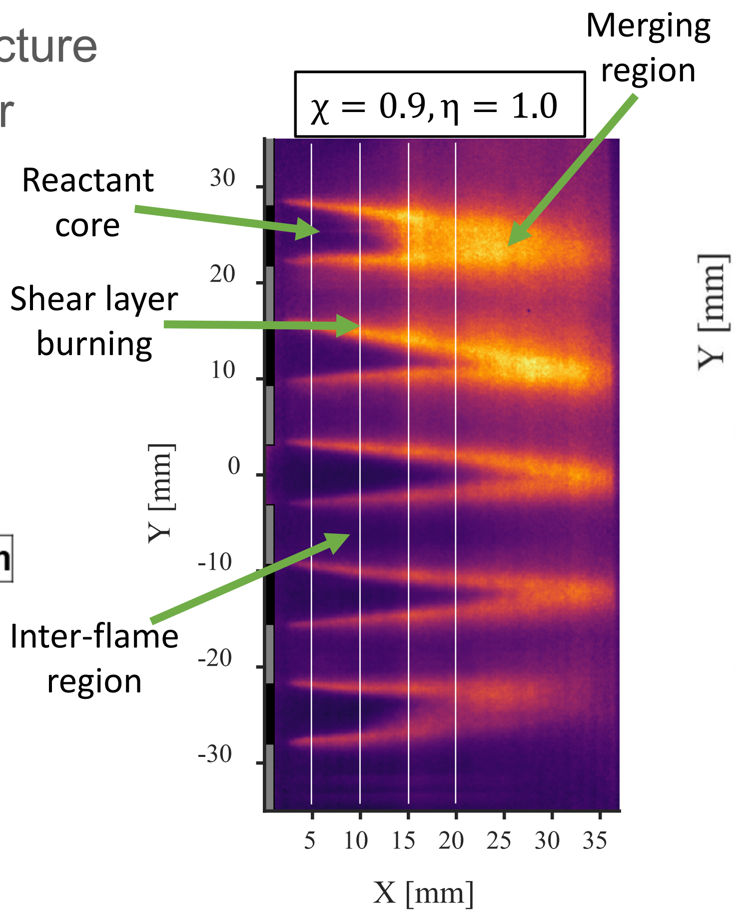
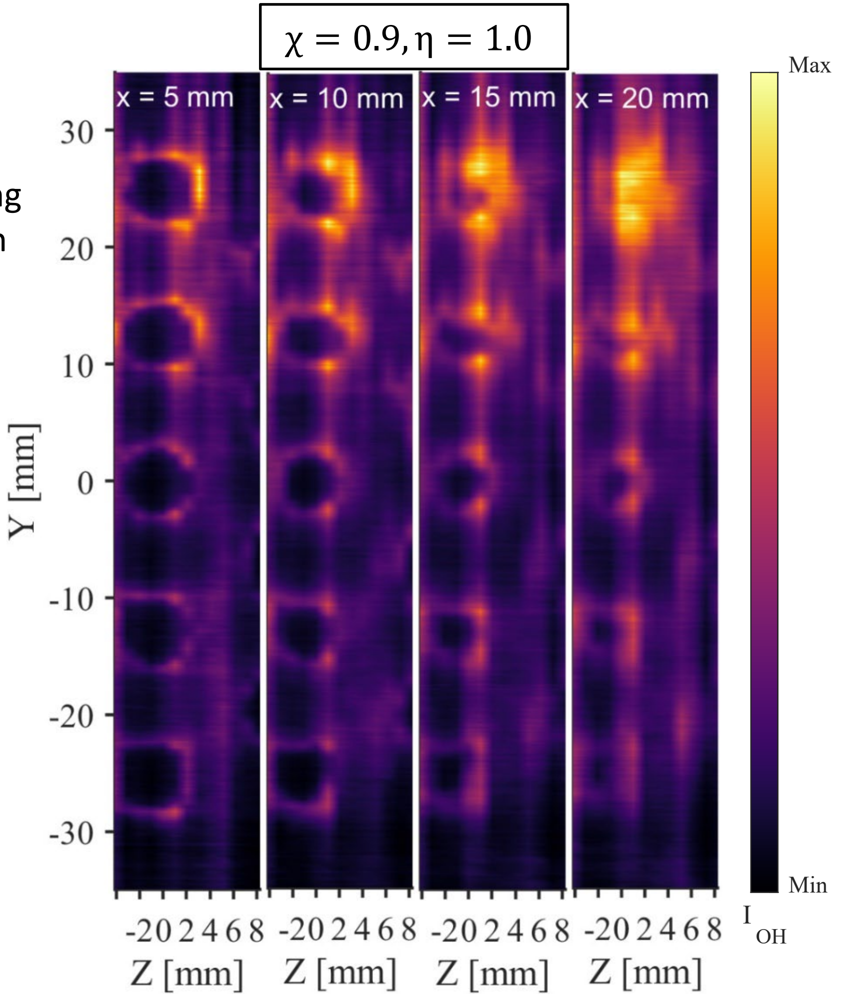






Hodge et al., "Time-Resolved Structure of H 2 –NH 3 and H 2 –CH 4 Flames in a High-Pressure Micromix Combustor," International Journal of Hydrogen Energy, Vol. 163, 2025, p. 150596. https://doi.org/10.1016/j.ijhydene.2025.150596

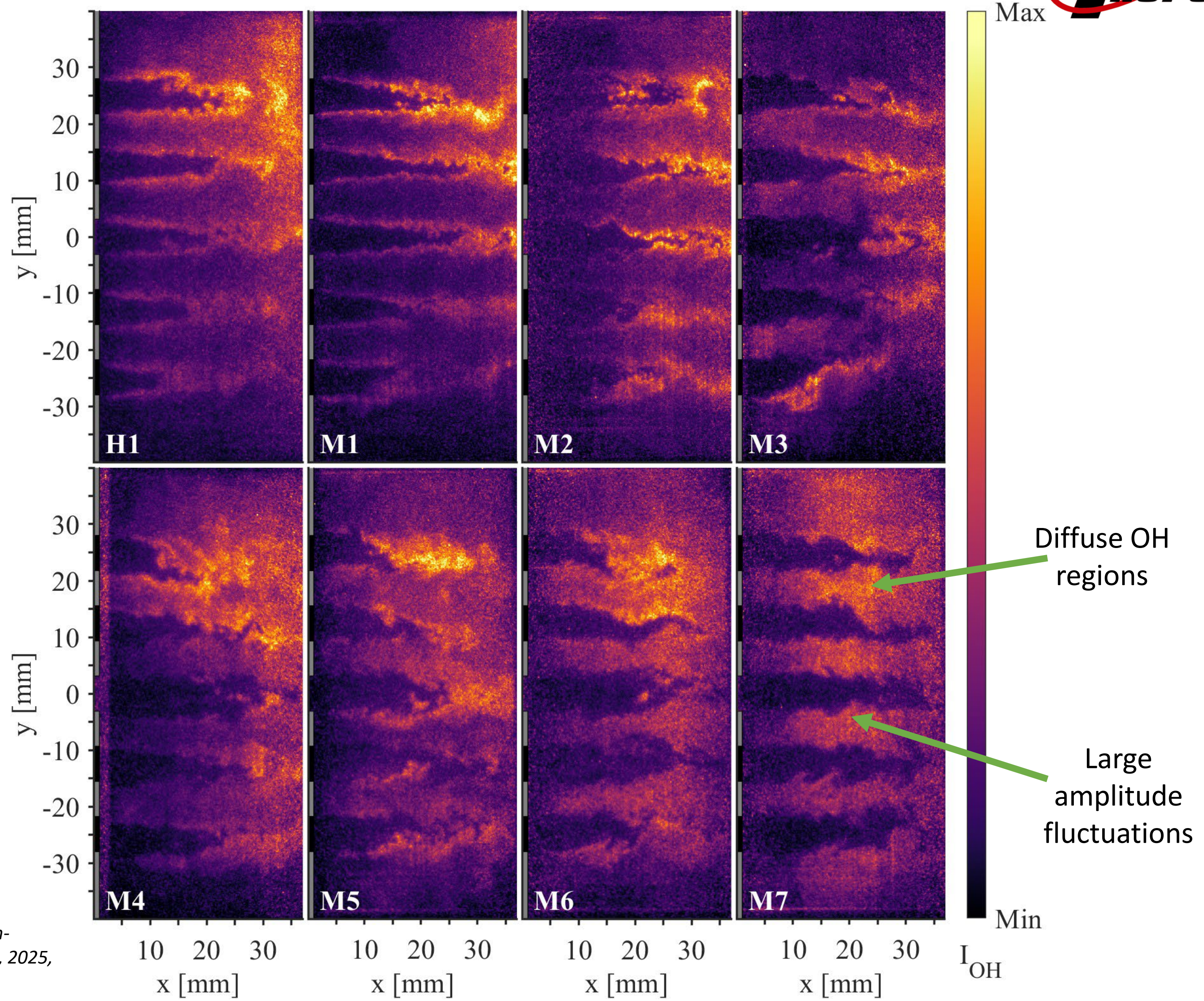
Effect of CH_4 Addition

- H_2 flame has a compact, highly curved flame front
- Reactivity and flame speed decreases with CH_4
- Distribution of OH is more diffuse
- Reactant core angle increases
- Flame wrinkling length scale increases
- OH broadens out to inter-flame region

Fuel Composition

$$\chi\left[\eta\left(\frac{3}{2}H_2 + \frac{1}{2}N_2\right) + (1-\eta)NH_3\right] + (1-\chi)CH_4$$

χ = hydrogen fraction
η = ammonia decomposition efficiency



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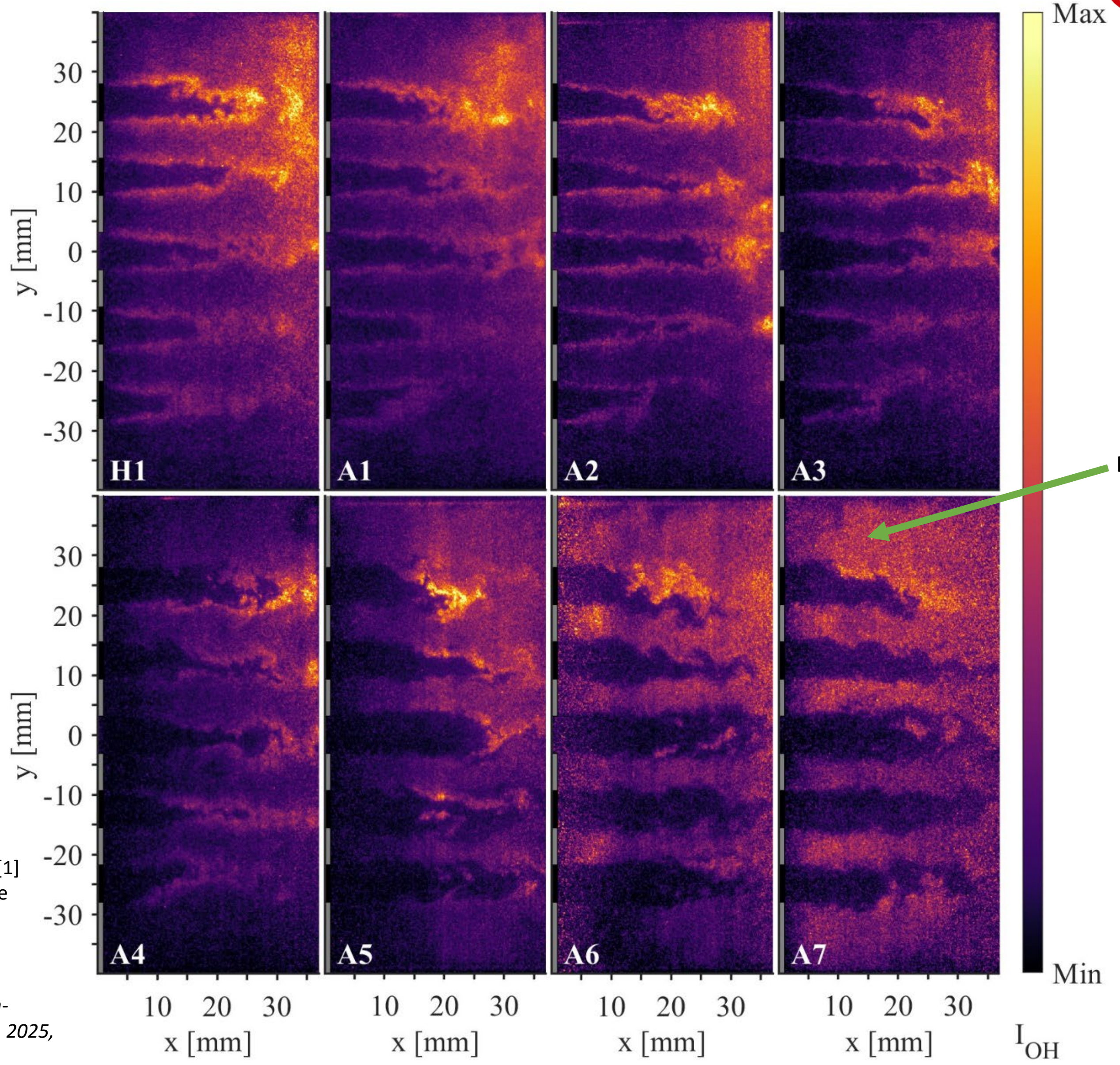
Effect of NH_3 Addition

- OH regions are more diffuse compared to CH_4 addition
- Reactant core length increases significantly
- Global decrease in OH
- Significant disparity in reactant core length
  - Highlights presence of near-wall recirculation zones[1]



Near-wall recirculation zones

[1]

Fuel Composition

$$\chi\left[\eta\left(\frac{3}{2}H_2+\frac{1}{2}N_2\right)+(1-\eta)NH_3\right]+(1-\chi)CH_4$$

χ = hydrogen fraction
η = ammonia decomposition efficiency

[1] Zhang et al., "Three-Dimensional Analysis of Hydrogen Fuel Effects in Multi-Tube Combustor," *Proceedings of the Combustion Institute*, Vol. 41, 2025, p. 105790. https://doi.org/10.1016/j.proci.2025.105790

Hodge et al., "Time-Resolved Structure of H 2 –NH 3 and H 2 –CH 4 Flames in a High-Pressure Micromix Combustor," International Journal of Hydrogen Energy, Vol. 163, 2025, p. 150596. https://doi.org/10.1016/j.ijhydene.2025.150596

Parametric Survey of Dynamics

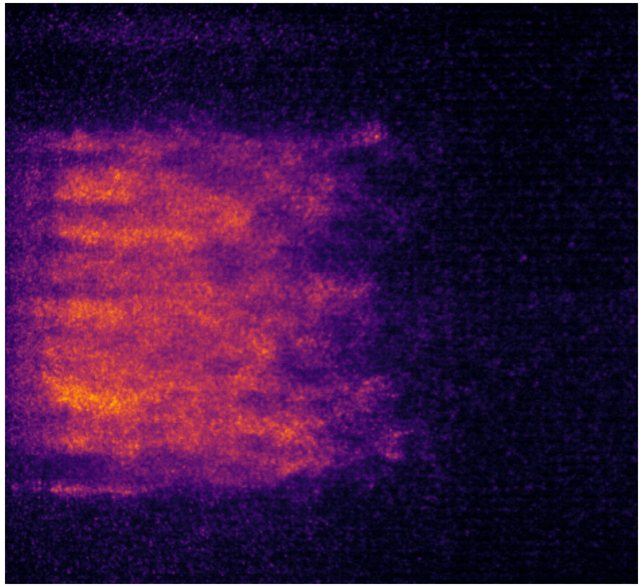
- High amplitude pressure fluctuations (p') observed
  - Methane addition observed to promote combustion instabilities
  - Combustion instability amplitude is largely invariant to the addition of ammonia in absence of methane
  - As hydrogen content is decreased, ammonia addition increases combustion instability amplitudes

Fuel Composition

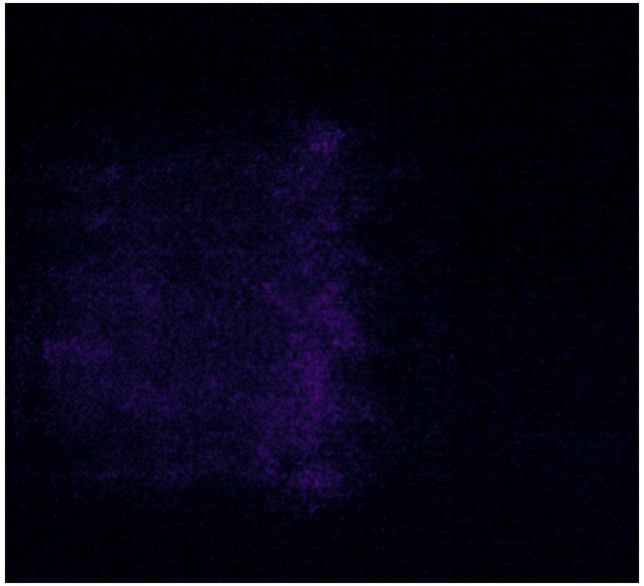
$$\chi\left[\eta\left(\frac{3}{2}H_2 + \frac{1}{2}N_2\right) + (1-\eta)NH_3\right] + (1-\chi)CH_4$$

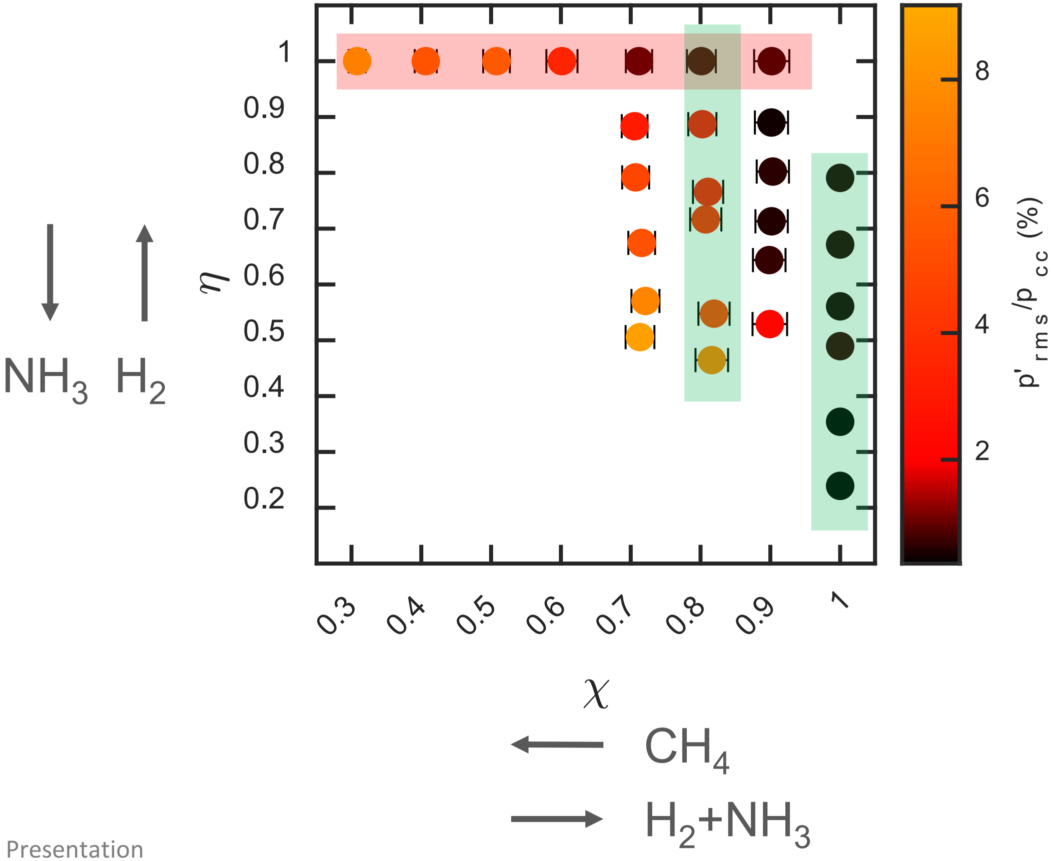
χ = hydrogen fraction
η = ammonia decomposition efficiency

$\chi = 0.7, \eta = 1.0$



$\chi = 0.7, \eta = 0.7$



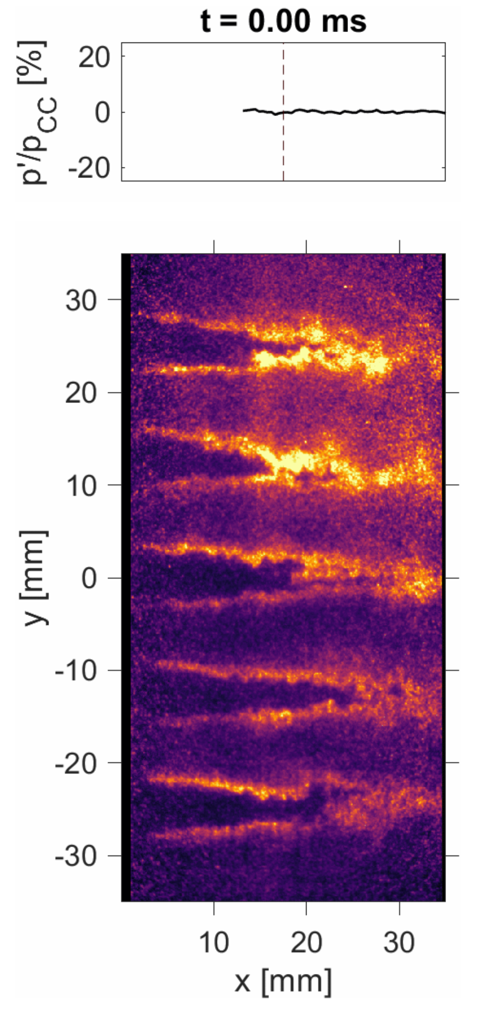


Shahin et al., "Dynamics of Hydrogen–Ammonia–Natural Gas Lean-Premixed High-Pressure Flames," Fuel, Vol. 385, 2025, p. 134016. https://doi.org/10.1016/j.fuel.2024.134016

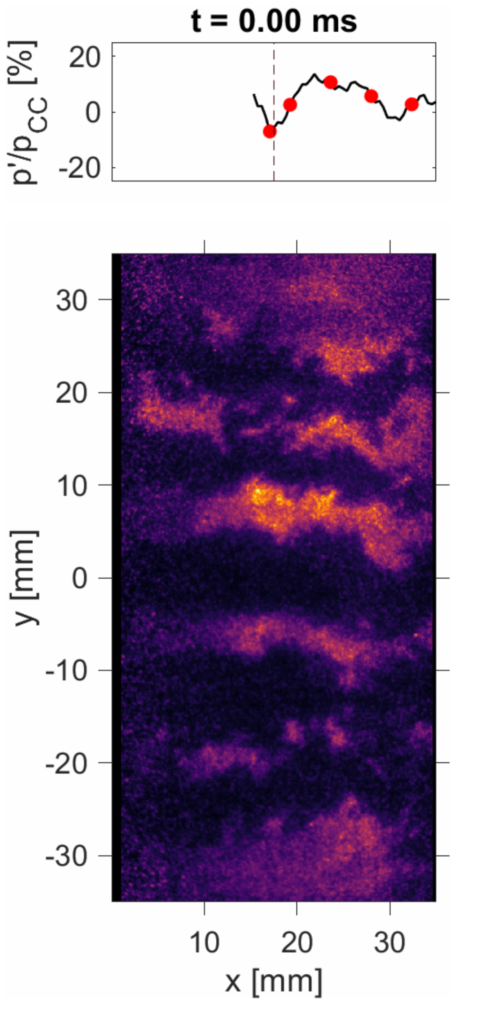
Dynamics Sensitivity to Methane Addition

- Time-resolved OH PLIF shows flame response during instability cycle

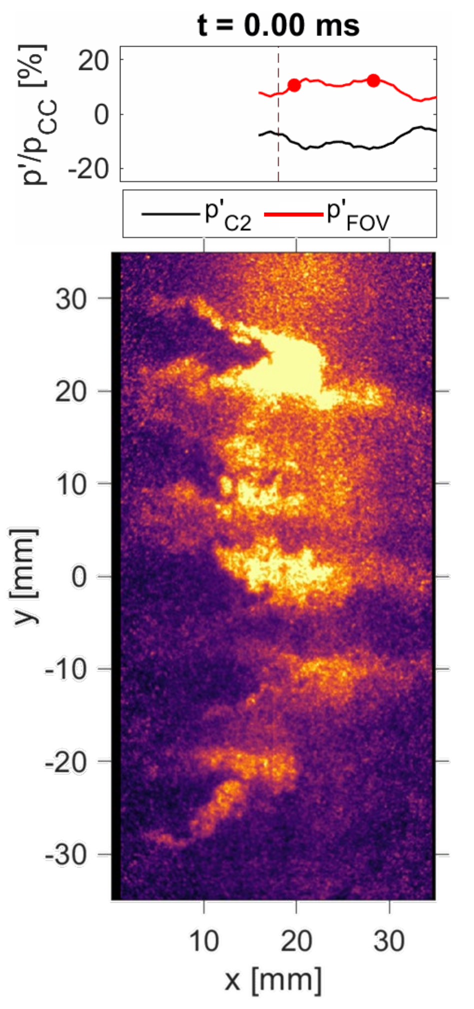
$\chi = 0.90, \eta = 1.00$



$\chi = 0.41, \eta = 1.00$



$\chi = 0.31, \eta = 1.00$

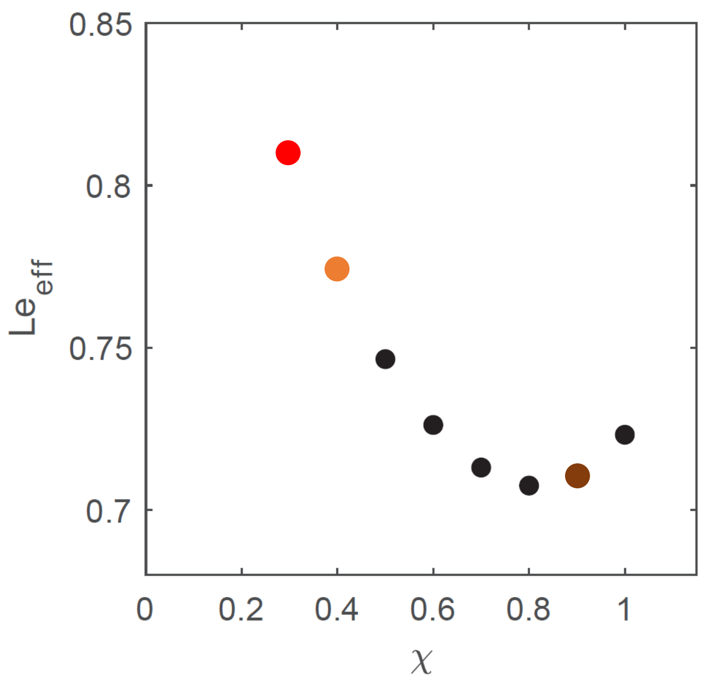


Fuel Composition

$$\chi\left[\eta\left(\frac{3}{2}H_2 + \frac{1}{2}N_2\right) + (1-\eta)NH_3\right] + (1-\chi)CH_4$$

χ = hydrogen fraction

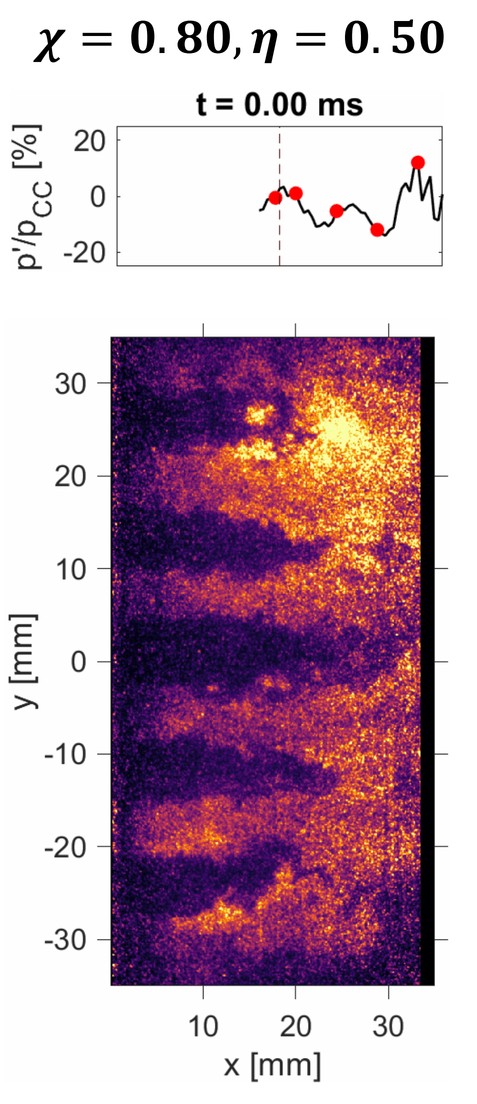
η = ammonia decomposition efficiency

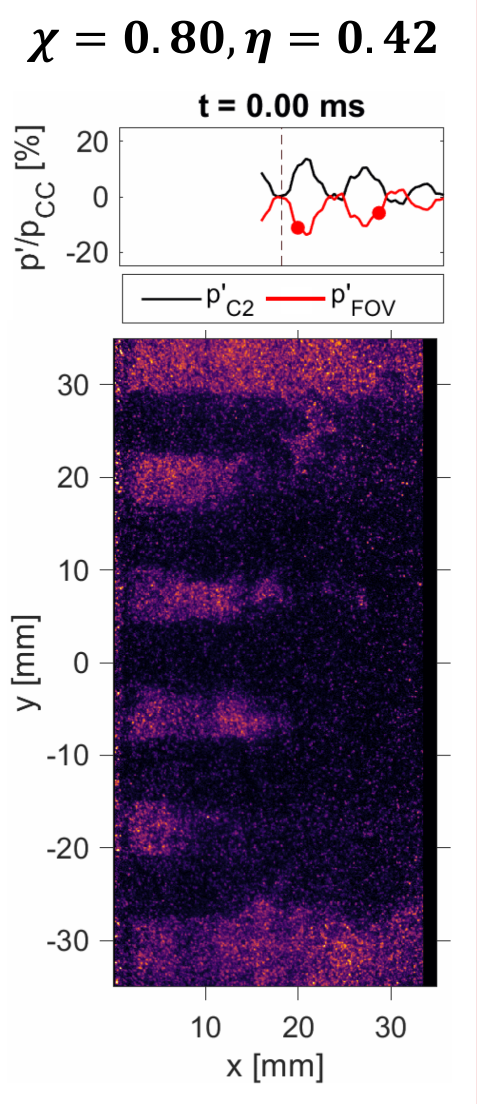


Shahin et al., "Structure of High-Pressure Premixed Ammonia, Hydrogen, and Methane Flames with 100 kHz OH-PLIF Measurements," Journal of Engineering for Gas Turbines and Power, 2025, pp. 1–14. https://doi.org/10.1115/1.4069450

Dynamics Sensitivity to Ammonia Addition

- Time-resolved OH PLIF shows flame response during instability cycle





Fuel Composition

$$\chi\left[\eta\left(\frac{3}{2}H_2 + \frac{1}{2}N_2\right) + (1-\eta)NH_3\right] + (1-\chi)CH_4$$

χ = methane fuel fraction
η = hydrogen decomposition efficiency

Shahin et al., "Structure of High-Pressure Premixed Ammonia, Hydrogen, and Methane Flames with 100 kHz OH-PLIF Measurements," Journal of Engineering for Gas Turbines and Power, 2025, pp. 1–14. https://doi.org/10.1115/1.4069450

Dynamics Sensitivity to Ammonia Addition

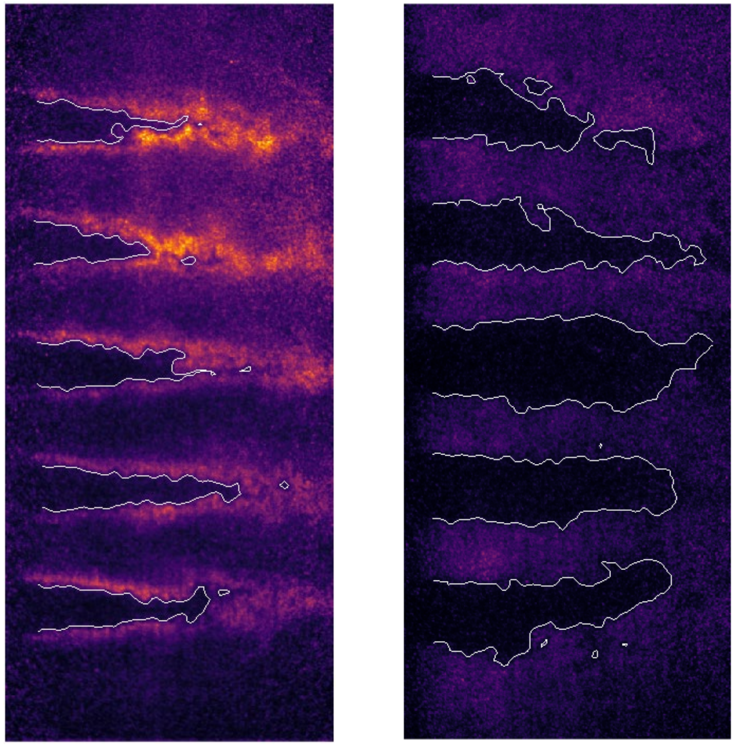
- Image binarization achieved using semantic segmentation
  - Employs convolutional neural network
  - Model identifies the reactant jet
- Noticeable improvement over gradient-based edge tracking
- Allows for time-resolved tracking of reactant area and flame front
- Instability mode switch can be tied to the duration of reactant area consumption
  - 27 frames (270 μs) to consume reactants in 2L case (longer than 2L methane case)
  - 60 frames (600 μs) to consume reactants in 1L case

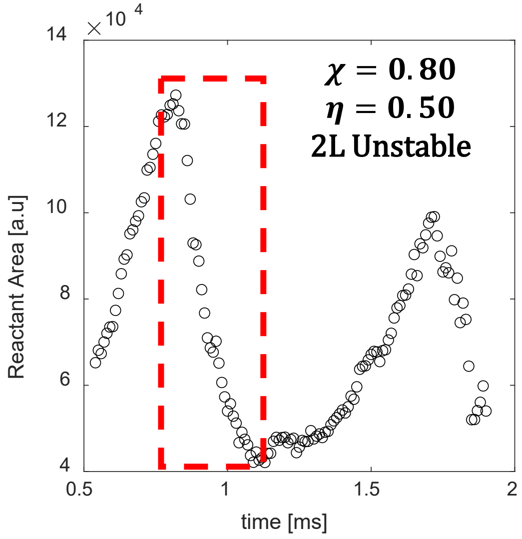
Fuel Composition

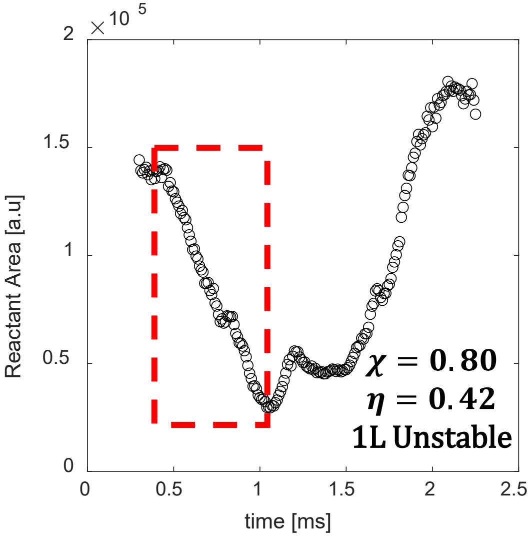
$$\chi\left[\eta\left(\frac{3}{2}H_2 + \frac{1}{2}N_2\right) + (1-\eta)NH_3\right] + (1-\chi)CH_4$$

χ = methane fuel fraction
η = hydrogen decomposition efficiency

$\chi = 0.90\ \eta = 1.00$ $\chi = 1.00\ \eta = 0.32$







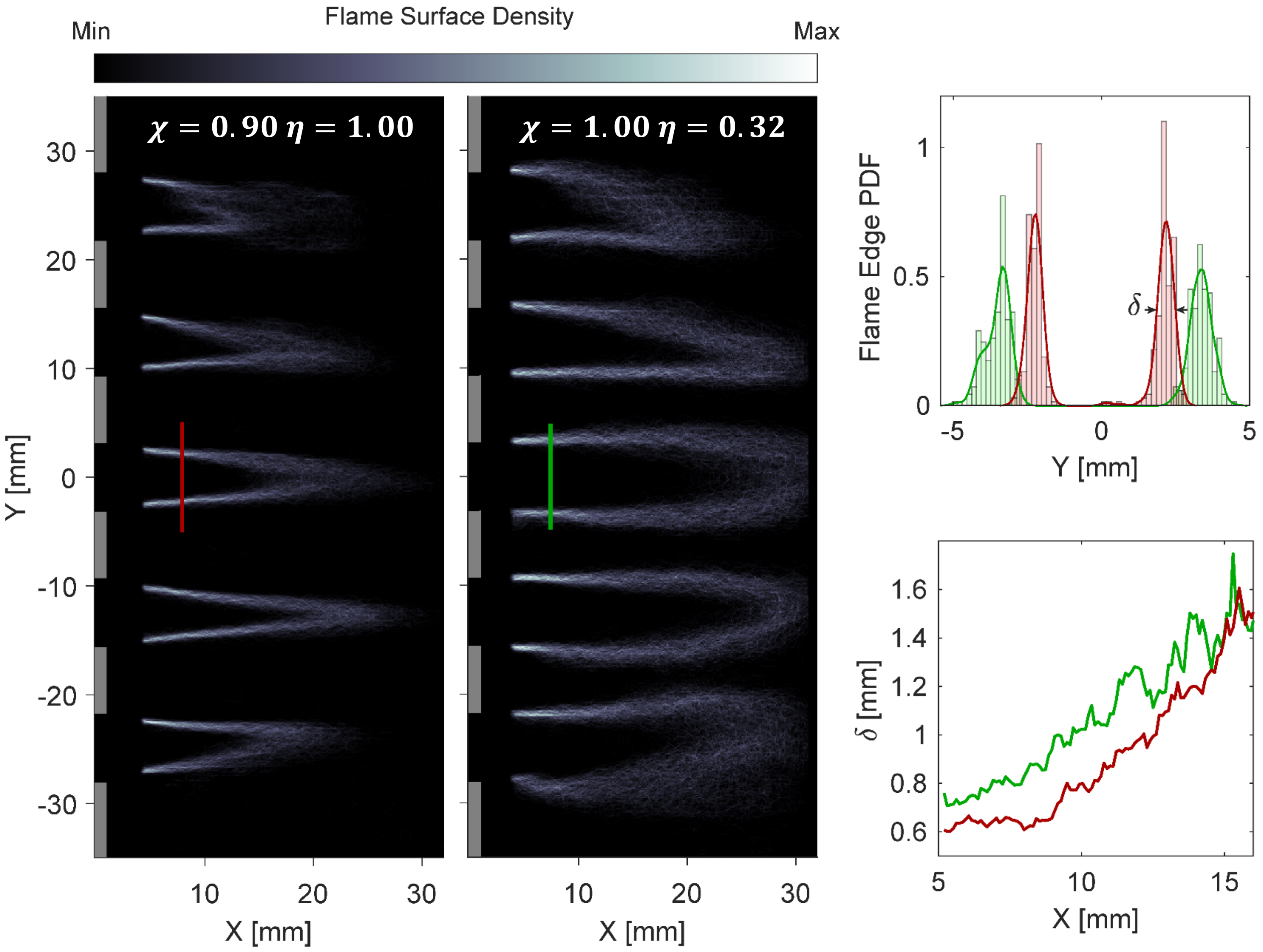
Effect of Ammonia Addition on Flame Structure

- Flame surface density (FSD) generated from flame fronts of all frames
- Upstream FSD width larger with more ammonia, indicating slower kinetics
- Downstream FSD width also larger with more ammonia, indicating larger amplitude flame front fluctuations

Fuel Composition

$$\chi\left[\eta\left(\frac{3}{2}H_2+\frac{1}{2}N_2\right)+(1-\eta)NH_3\right]+(1-\chi)CH_4$$

χ = methane fuel fraction
η = hydrogen decomposition efficiency



Effect of Ammonia Addition on Flame Structure

- Probability density functions (PDF) for radius of curvature (r) show the impact of NH_3 on flame structure
- Over entire FOV, slight bias towards negative curvature due geometry of the jet flames
- In upstream region, curvature more uniform with more H_2
  - H_2 induces thermo-diffusive instabilities that balance flame surface production from turbulent flow strain[1]
- In downstream region, this trend is reversed
  - Rapid surface annihilation near reactant core tip enhanced with more H_2, causing negative curvature bias

Fuel Composition

$$\chi\left[\eta\left(\frac{3}{2}\mathrm{H}_2+\frac{1}{2}\mathrm{N}_2\right)+(1-\eta)\mathrm{NH}_3\right]+(1-\chi)\mathrm{CH}_4$$

χ = methane fuel fraction
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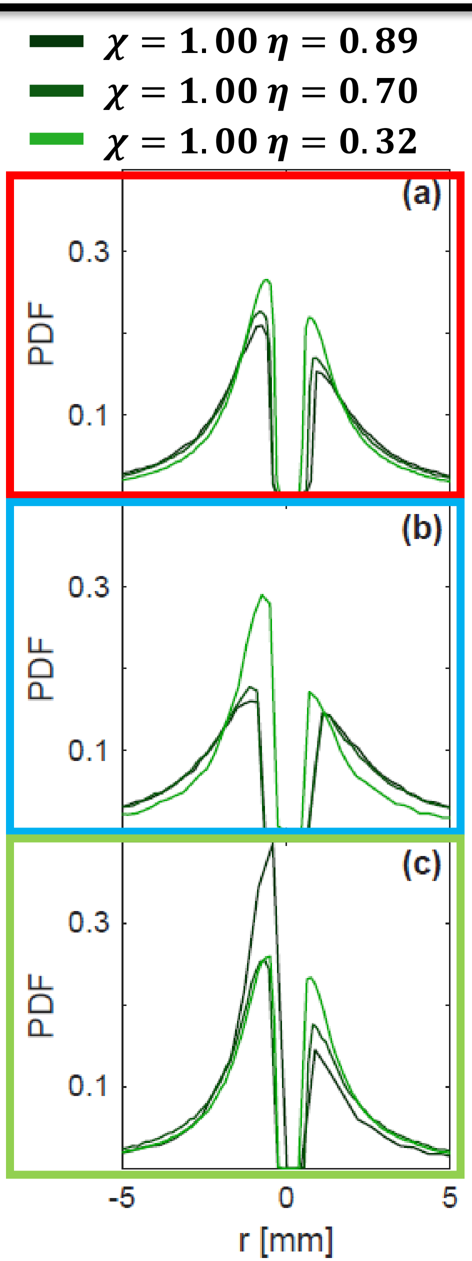
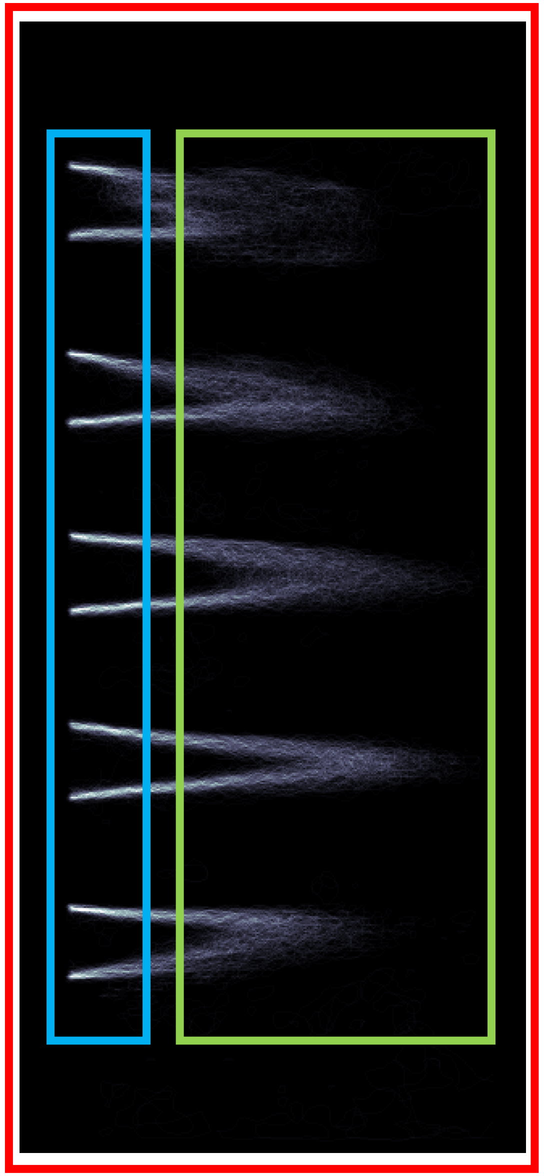
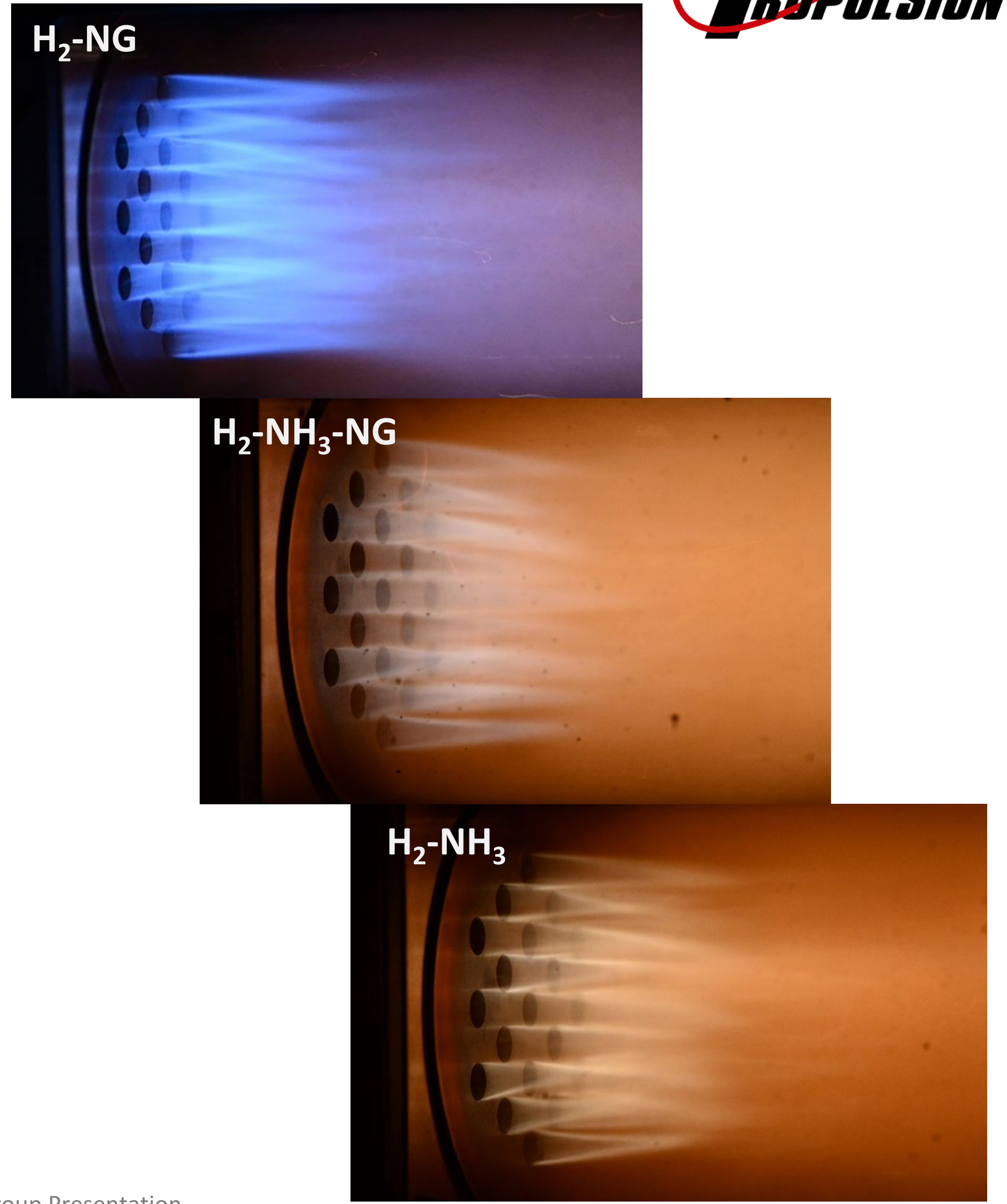




[1] *Coulon, V., Gaucherand, J., Xing, V., Laera, D., Lapeyre, C., and Poinsot, T., "Direct Numerical Simulations of Methane, Ammonia-Hydrogen and Hydrogen Turbulent Premixed Flames," Combustion and Flame, Vol. 256, 2023, p. 112933.* https://doi.org/10.1016/j.combustflame.2023.112933

Summary

- High pressure ammonia storage systems present novel challenges for safe and efficient use
- The addition of NH_3 and CH_4 alters the flame shape and distribution of reactions
- Combustion stability map shows sensitivity of thermoacoustics to NH_3 and CH_4 addition
- Time-resolved OH PLIF reveals how local flame behaviors affect the global dynamics
- Flame front tracking shows how fuel composition affects the turbulent flow-flame processes, leading to changes in combustion dynamics



This work was supported by the Department of Energy University Turbine Systems Research (UTSR) program grant DE-FE0032074 (Program Manager: Andrew O'Connell). The high-speed imaging equipment used in this work was purchased with Defense University Research Instrumentation Program grant FA9550-20-1-0226 (Program Manager: Chiping Li).