



**GTI ENERGY**

*solutions that transform*

# Investigation of Ammonia for Combustion Turbines (IACT) - Summary DE-FE0032172

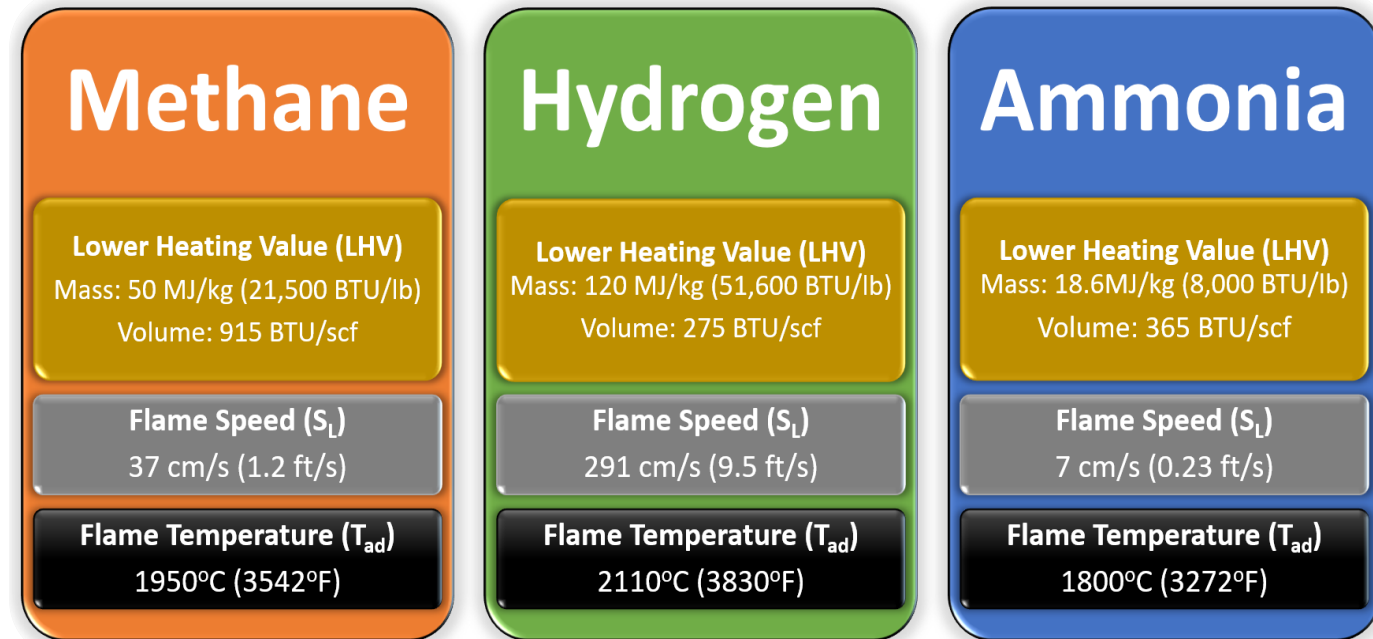
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Andrew O'Connell (DOE, NETL)

October 31<sup>st</sup>, 2023

# Investigation of Ammonia for Combustion Turbines (IACT)

- Goal - develop advanced combustor technology to utilize ammonia as a zero-carbon fuel for power generation applying an iterative physics, computational, and experimental approach resulting in a pilot combustor design validated through tests
- Testing Scaled Combustor
  - Design using updated mechanism/ validated model
  - NOX Target: 20 ppm at 15% O<sub>2</sub>
  - High combustion efficiency
  - Stable flame (no blowoff)
- Challenges with ammonia
  - Safety considerations with ammonia
  - Ammonia ignition and flameholding
  - NOx generation



Comparison of fuel characteristics



# IACT Plan & Key Roles

Schedule: 9/2022-1/2026; Funding: \$4.2M



**EPRI** | ELECTRIC POWER RESEARCH INSTITUTE

Led Literature Review & Design Def.

**UCF** | UNIVERSITY OF CENTRAL FLORIDA

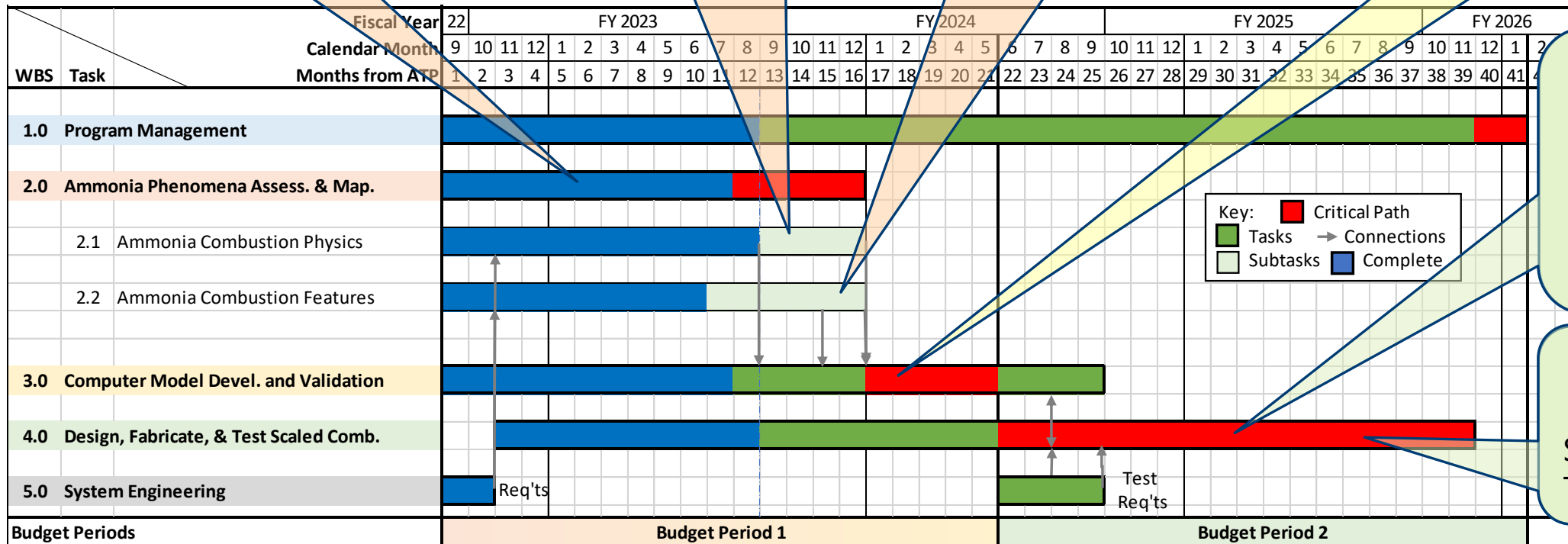
Shock Tube & Flame Speed Tests  
Kinetics mech.

**Georgia Tech**

Hencken Burner & Fuel Staging Tests; Kinetics mech.; Analytical design

**CRAFT Tech**

CFD Tool Devel.; Scaled Combustor Design



**GTI ENERGY**

Req'ts Def. & Scaled Comb. Design & Fabrication

**Georgia Tech**

Scaled Comb. Test

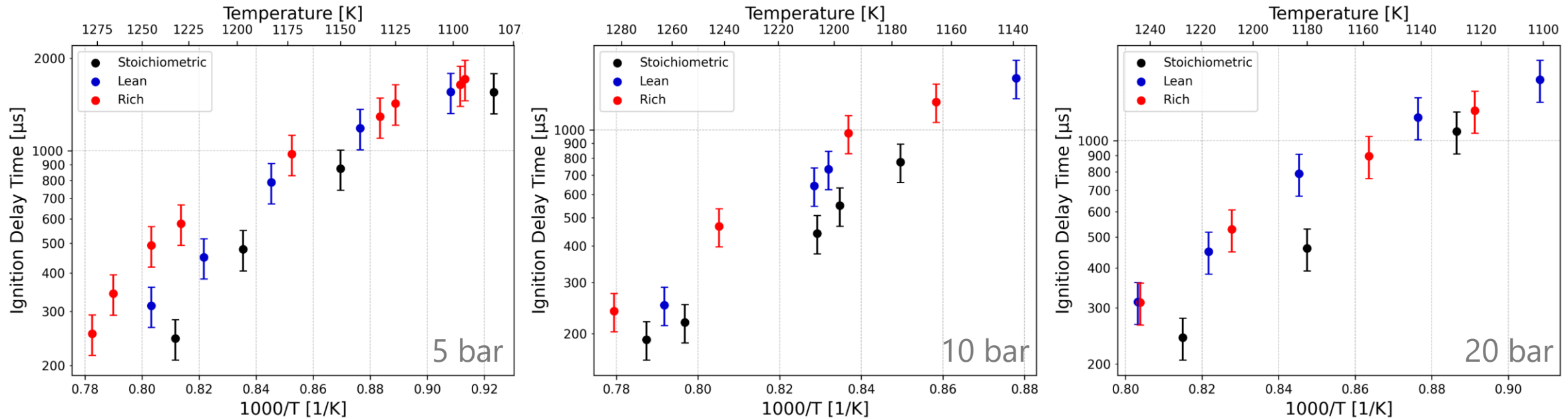
Key: ■ Critical Path  
■ Tasks → Connections  
■ Subtasks ■ Complete

# IACT Project Flow

- Literature search to understand SOA and identify knowledge gaps
  - ↓ – *Define test conditions to fill gaps*
- Fundamental  $\text{NH}_3$  &  $\text{NH}_3 + \text{H}_2$  combustion physics testing
  - ↓ – *Generate improved detailed and reduced kinetics*
- Develop computational CFD design tool implementing updated mechanisms
  - ↓ – *Apply combustion physics knowledge and design tool*
- Design and test scaled combustor

# 70/30 NH<sub>3</sub>/H<sub>2</sub> IDTs

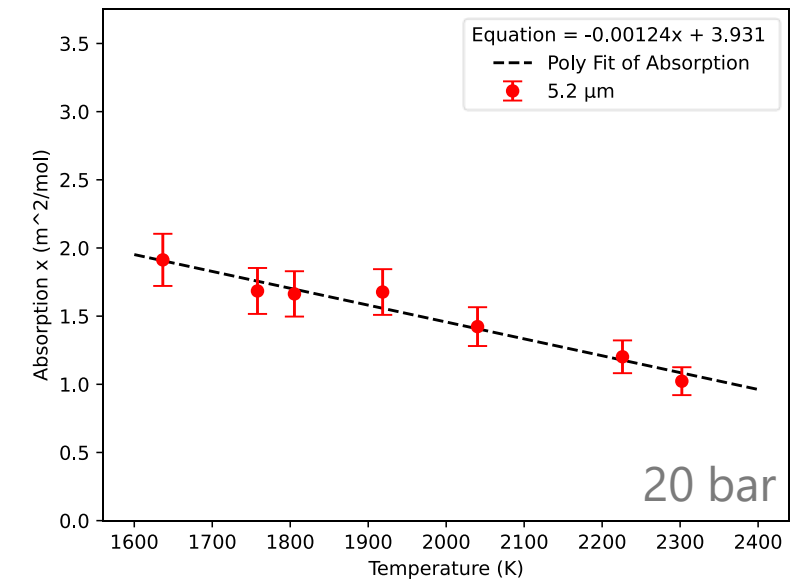
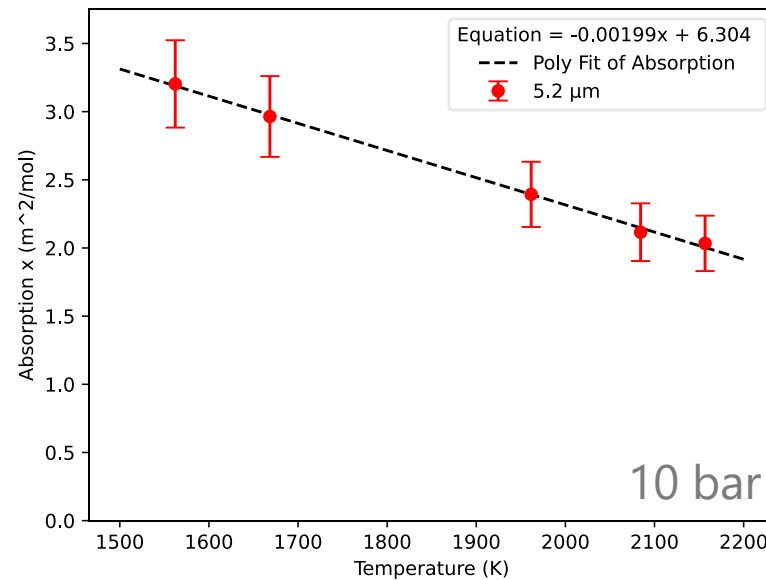
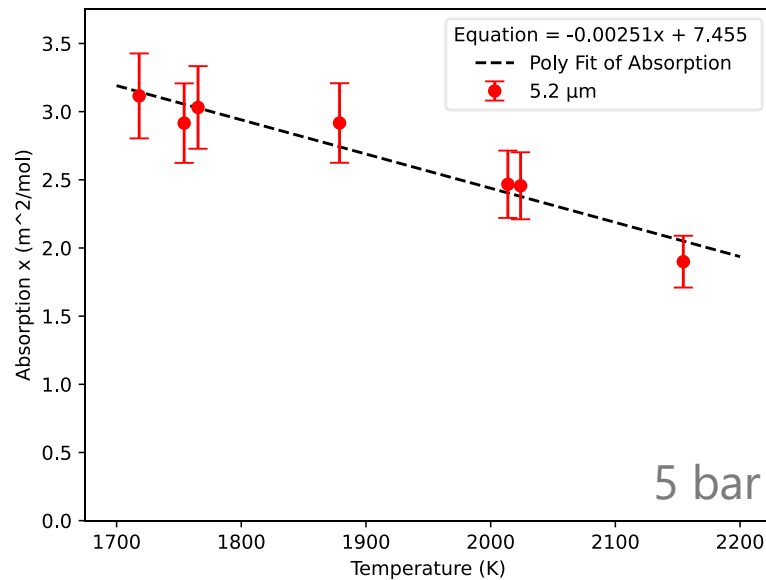
## Also Pure Ammonia and 50/50 Mix



- At 5 bar and 10 bar, ignition order follows rich < lean < stoichiometric. However, at lower temperatures, all mixtures ignite nearly at same time.
- At 20 bar, lean and rich mixtures ignite slower than stoichiometric mixtures.
- IDT data new and will be utilized to develop a **validated ammonia/hydrogen chemical kinetic model for gas turbine operating conditions**

# NO Cross Sections

- For measuring species time histories, individual species absorption needs to be characterized.
- **Plan to measure NO, NO<sub>2</sub>, NH<sub>3</sub> and H<sub>2</sub>O species time histories during NH<sub>3</sub>/H<sub>2</sub> combustion at 5, 10 and 20 bar.**
- NO absorption characterization results are shown below:



- NO absorption cross-section is found to decrease with increase in temperature.
- NO absorption cross-section is found to decrease with pressure.
- A linear fit was developed at 5, 10 and 20 bar to fit experimental data.

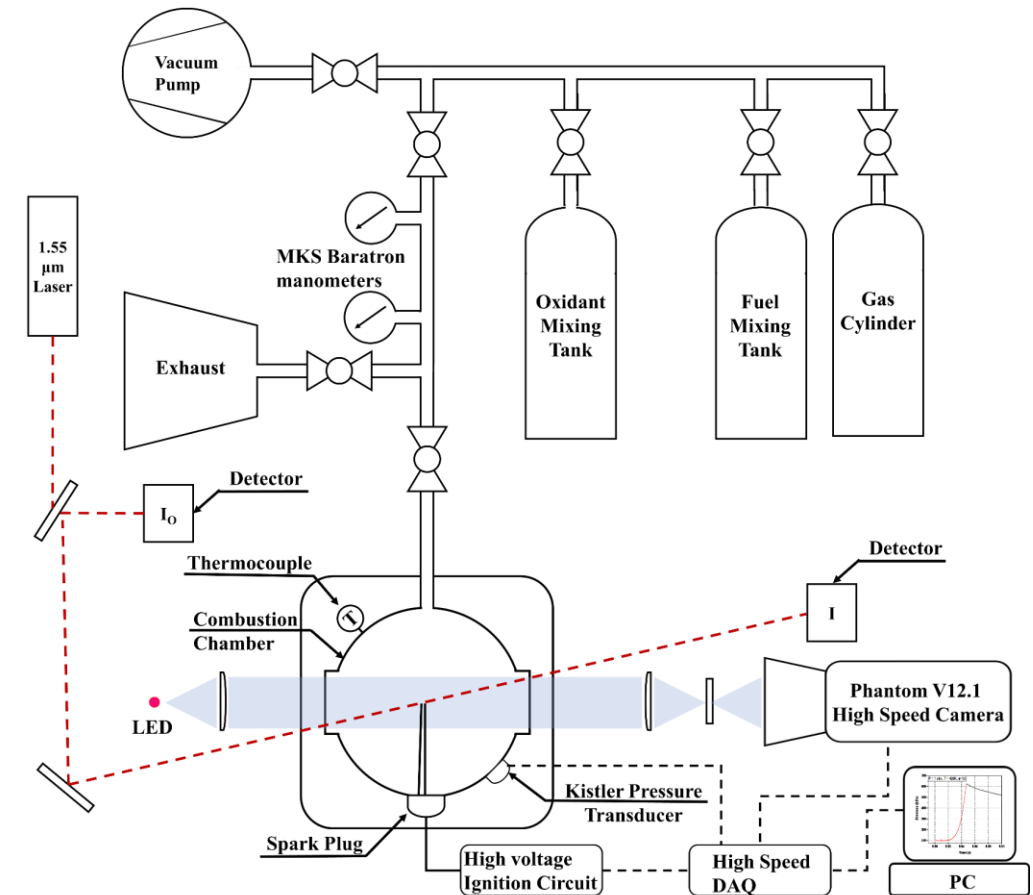
# Flame speed measurements - Test matrix

- Conduct flame speed measurements to acquire flame speed data at 10 and 20 bar for pure ammonia and ammonia/hydrogen blends

Mixture	NH3 in fuel (%)	Oxidant <sup>1</sup>				Phi	Temp. (K)	Pressures (atm)
		O <sub>2</sub>	N <sub>2</sub>	Ar	He			
H <sub>2</sub> -NH <sub>3</sub>	50	1	1	0	3	0.7 – 1.2	296	10
	70	1	1	0	3			
	100	1	2	0	1			
H <sub>2</sub> -NH <sub>3</sub>	50	2	1	0	3			20
	70	2	1	0	3			
	100	2	1	0	3			

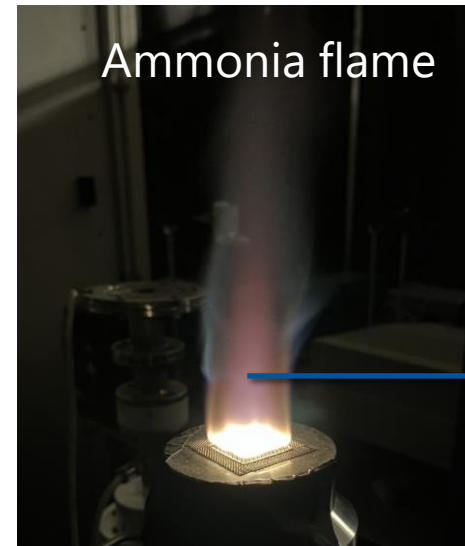
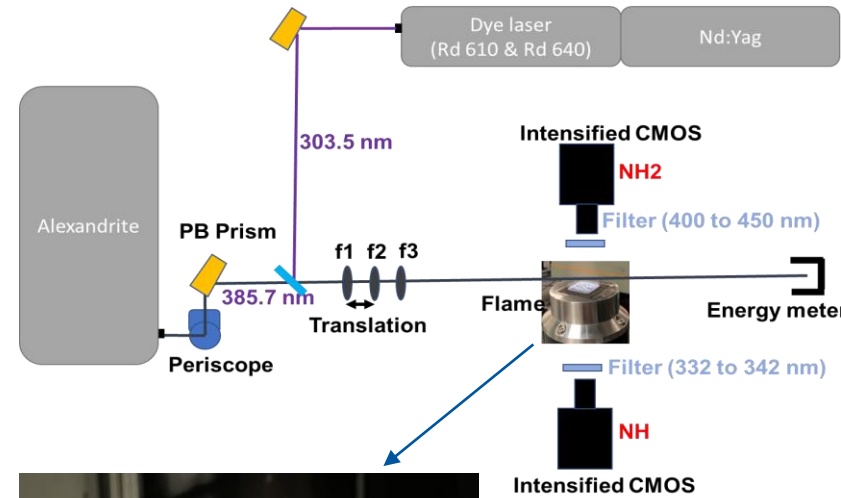
1. Oxidant ratio will be determined during experiments to get laminar flame speed.

- Utilize shock tube IDTs, speciation and flame speed experimental data to develop/improve chemical kinetic model for ammonia/hydrogen blends

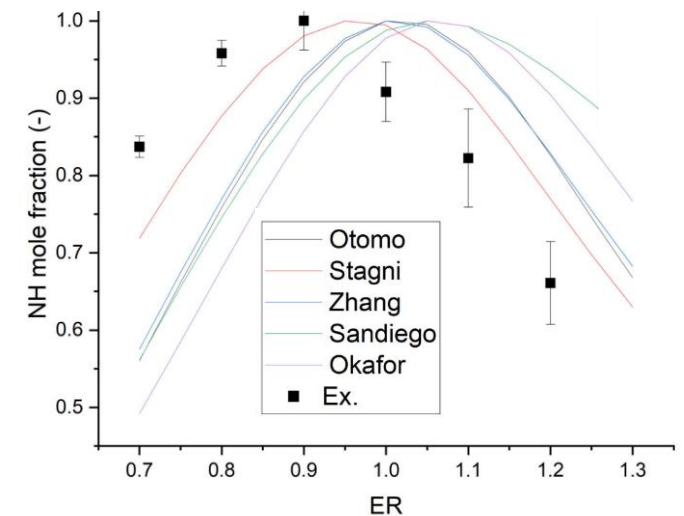
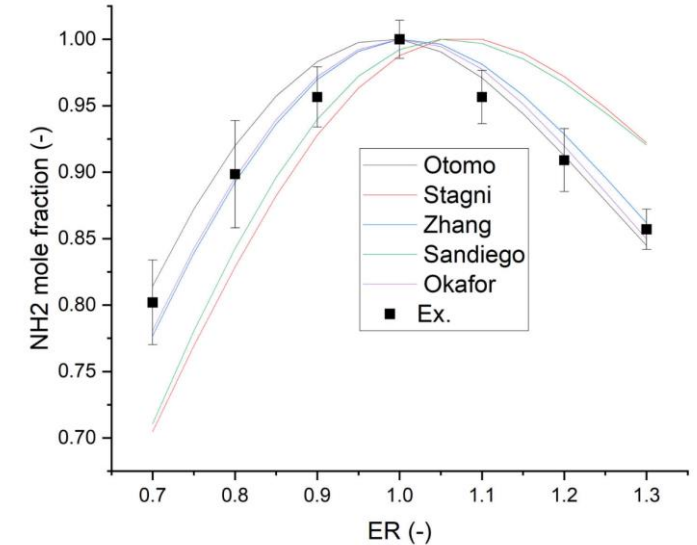


# Hencken Burner Test Setup

- Investigation of  $\text{NH}_2/\text{NH}$  laser-induced fluorescence (LIF)
  - Pure ammonia-air cases,  $\text{O}_2$  enriched air (50%  $\text{O}_2/50\%$   $\text{N}_2$ ) to help stabilize flame
  - Models seem to predict  $\text{NH}_2$  trend vs ER well
  - $\text{NH}$  trend vs ER is noticeably different
  - Work in progress
- New CAI Gas Analyzer commissioned and will measure  $\text{NO}$ ,  $\text{NO}_2$ ,  $\text{N}_2\text{O}$ , and  $\text{NH}_3$  at various equivalence ratios



Water cooled Sample Line

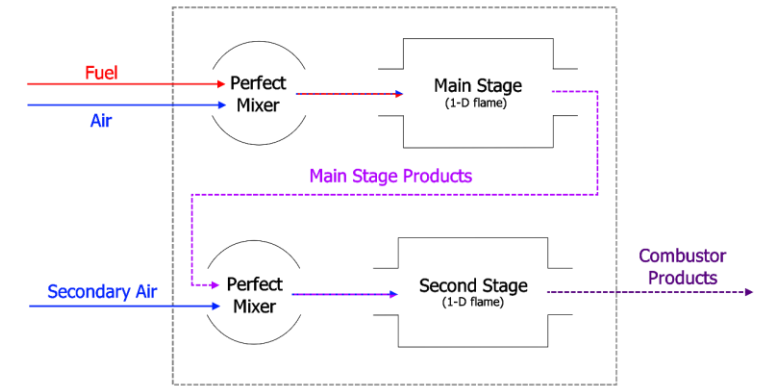
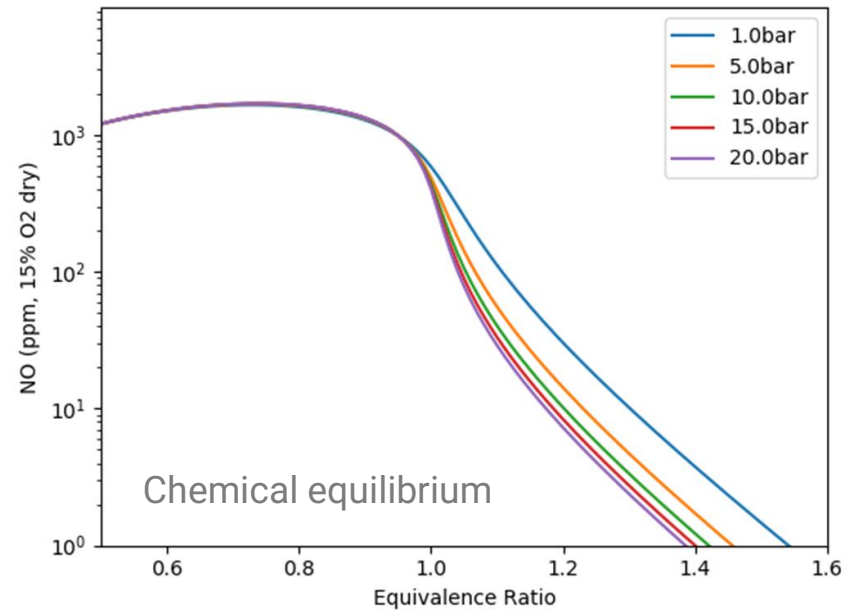




# Theoretical Minimum NO<sub>x</sub> for Ammonia Combustion

- A useful benchmark: what is the theoretical minimum possible NO<sub>x</sub> emission from ammonia combustion?
  - Not simulating a specific combustor, but rather what is possible with technology development

- Reactor network modeling (kinetic model from Mei et al. 2019)
- Acceptable NO<sub>x</sub> (O(10) ppm) possible
  - Rich front end, relaxation zone, lean zone
  - i.e., more than just RQL



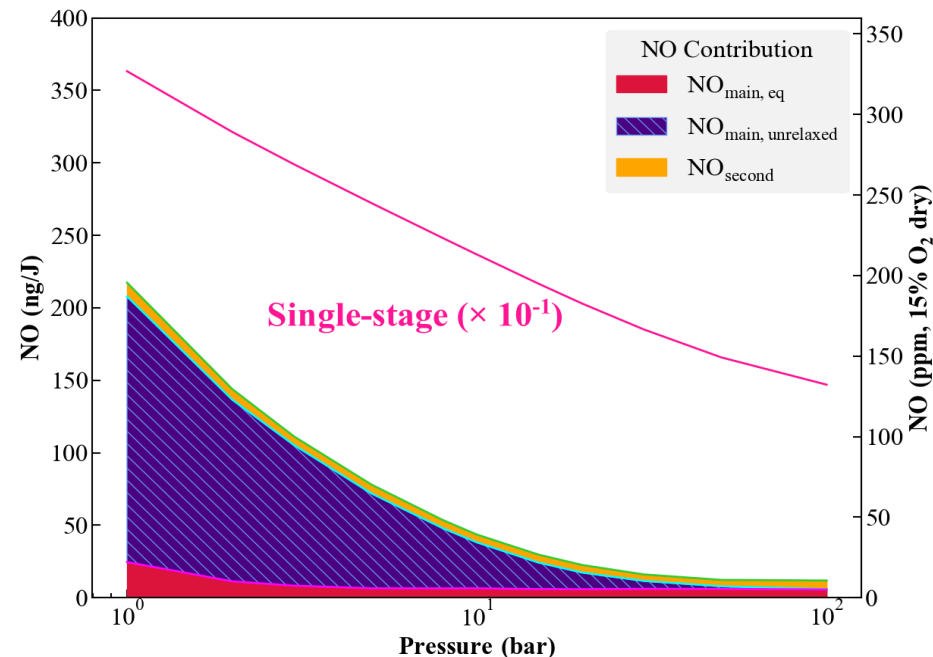
Schematic of staged combustor reactor network model

Gubbi, S., Cole, R., Emerson, B., Noble, D., Steele, R., Sun, W., & Lieuwen, T. (2023). Air Quality Implications of Using Ammonia as a Renewable Fuel: How Low Can NO<sub>x</sub> Emissions Go?. *ACS Energy Letters*, 8, 4421-4426.

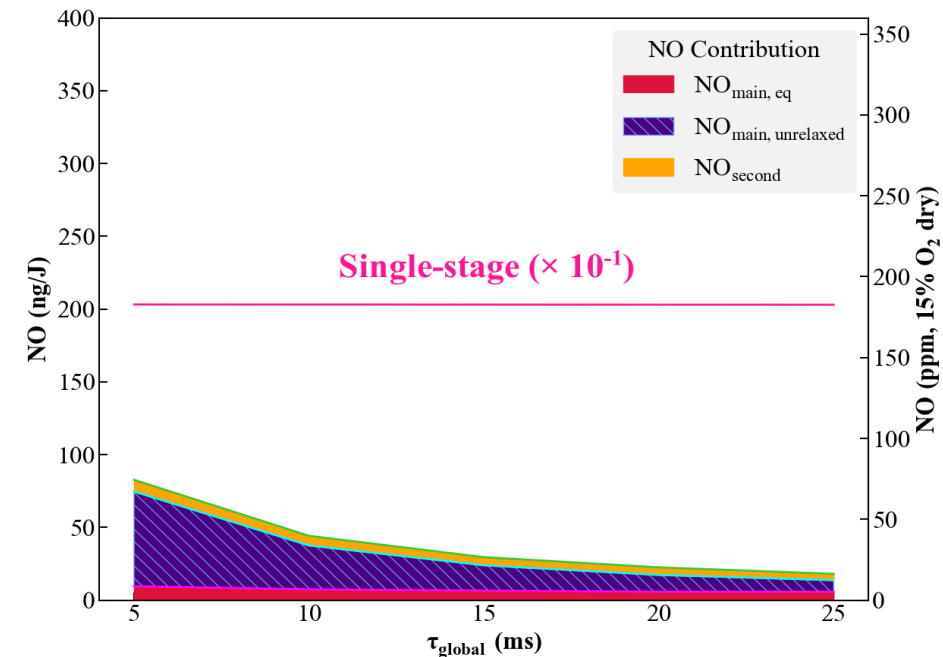
# Optimized NO Emissions

- “Unrelaxed” NO dominates, manage by:
  - Increasing pressure (reduces equilibrium NO, increases relaxation rates)
  - Increasing temperature (increasing relaxation rates)
  - Increasing residence time
- Sensitivities are flipped for current DLN technologies!
- Theoretically, it is possible to be EPA compliant without SCR for ammonia combustion

Pressure and residence time dependence of NOx emission breakdown

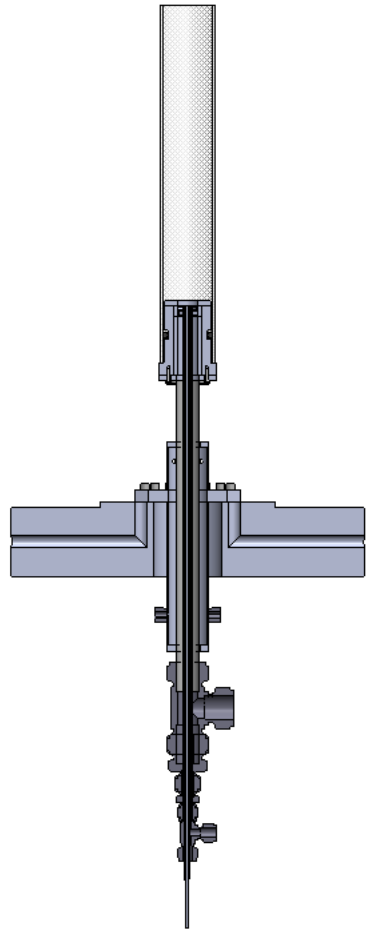


Minimum NO at various combustor pressures ( $T_{\text{exit}} = 1900 \text{ K}$ ,  $\tau_{\text{global}} = 20 \text{ ms}$ )

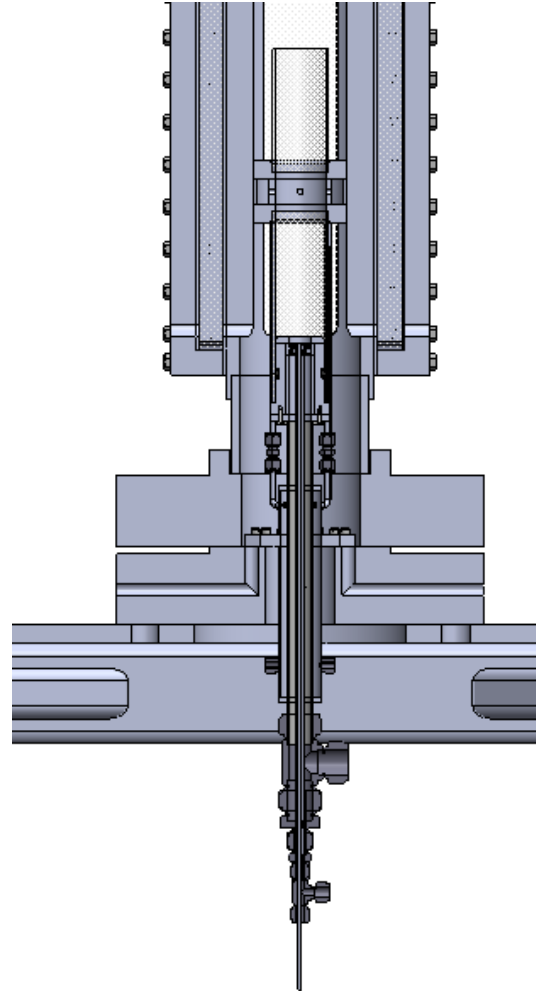


Minimum NO at various global residence times ( $T_{\text{exit}} = 1900 \text{ K}$ ,  $P = 20 \text{ bar}$ )

# Atmospheric/Pressurized Tests Staging Tests



Atmospheric burner  
design



Pressurized burner design

- Design for atmospheric and pressurized ammonia testing is complete
  - Tests will share the burner
- Experiments will investigate flame stability, blow-off, and emissions
  - Various swirl configurations
- Atmospheric tests will characterize the emissions profiles in the primary zone at various residence times
  - Investigate the NO relaxation vs. theoretical minimum NO<sub>x</sub> calculations

# Atmospheric/Pressurized Tests Staging Tests

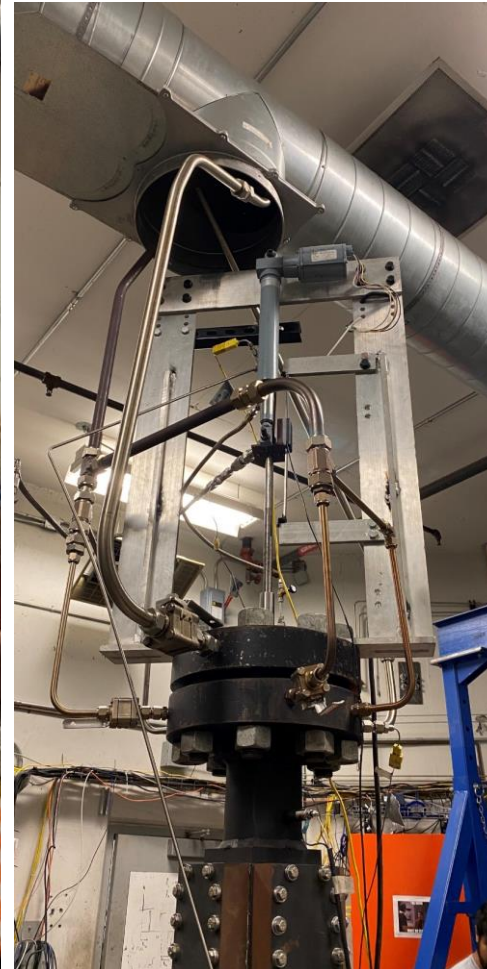
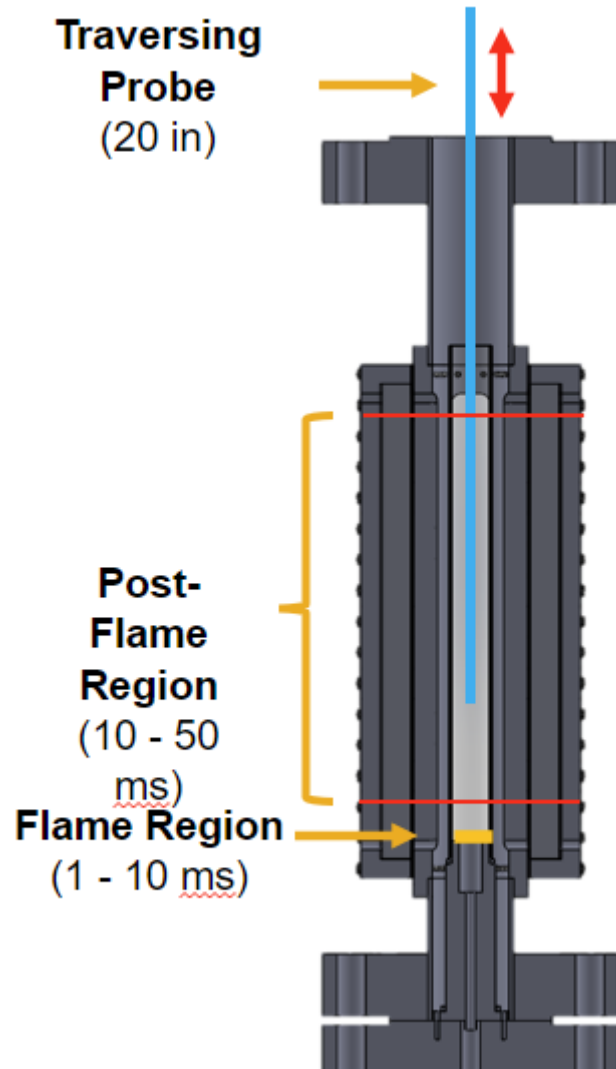
- Burner manufactured, passed safety review, shakedown, and first fire
- Planning atmospheric and 6 bar tests



Modular Swirler Burner (Swirl numbers 1.1, 0.7, 0.4)



# Scaled Combustor Test Planning



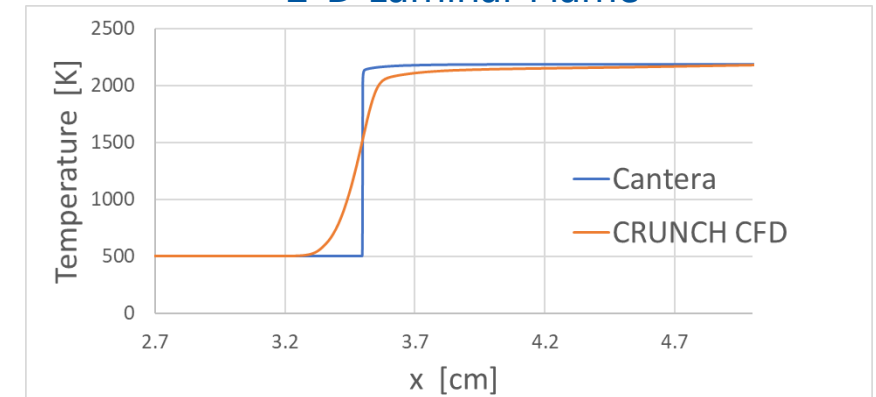
- 20 bar experiments planned for 2024

# Modeling Upgrades for Turbulent Premixed Flames

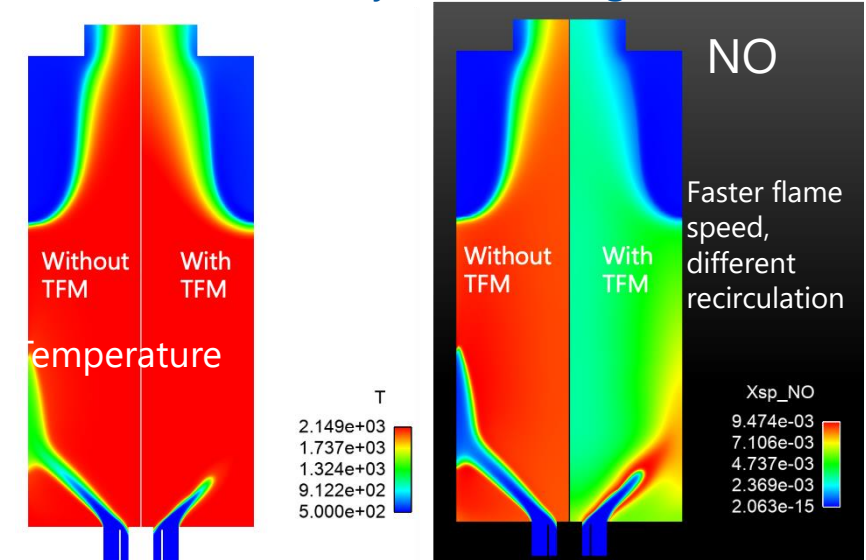


- CRAFT Tech completed code development related to Thickened Flame Model (TFM) implementation in CRUNCH CFD
- TFM: Well-established turbulent combustion model for application to premixed flows using finite-rate chemistry
  - “Flame front” artificially thickened to be properly resolved locally on computational grid
  - Effects of turbulent flame interactions and flame stretch included by modifying flame speed of thickened flame front
- Initial TFM evaluation complete (operation/robustness):
  - 2-D Laminar freely-propagating flame
  - 2-D Tohoku University/AIST configuration
- Application to GA Tech test configuration in progress
- Leveraging on MTS-FPV tabulated chemistry capabilities to reduce computation cost and turn-around time of simulations

2-D Laminar Flame



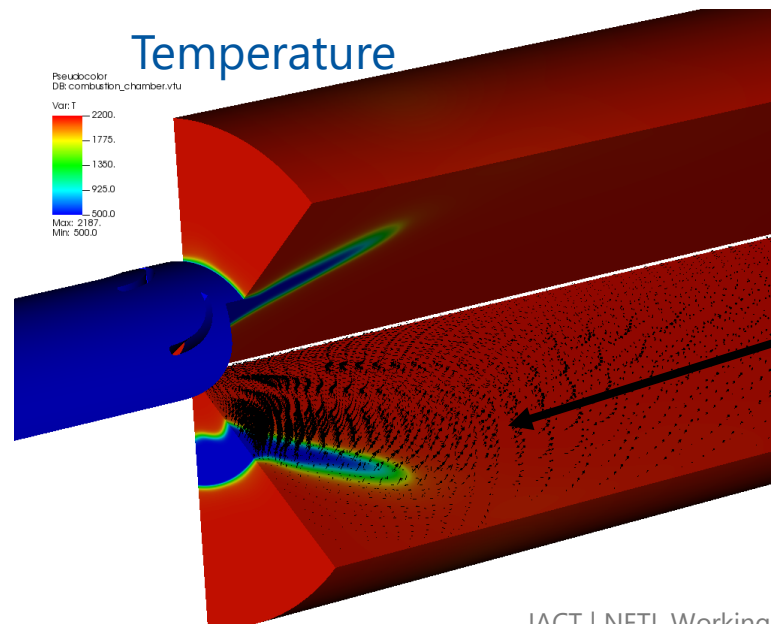
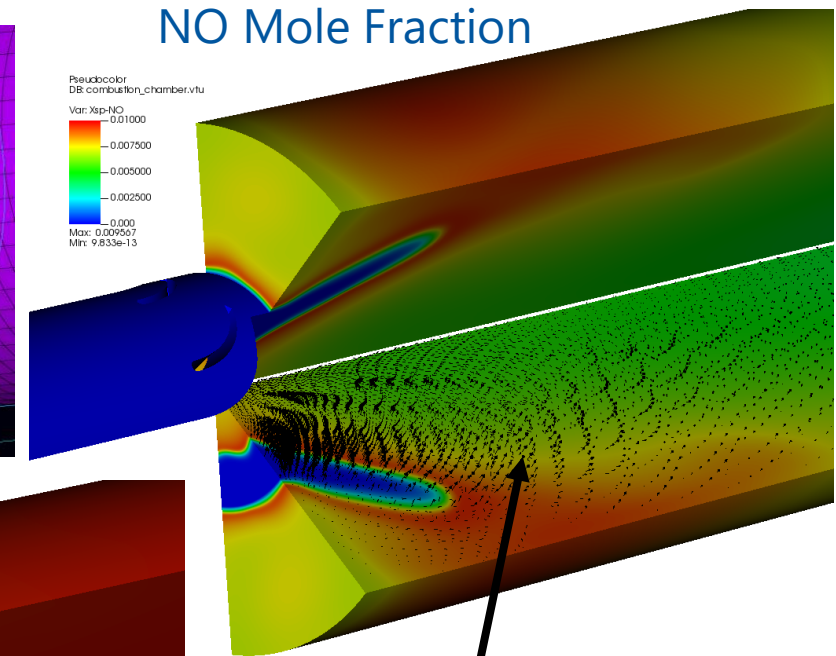
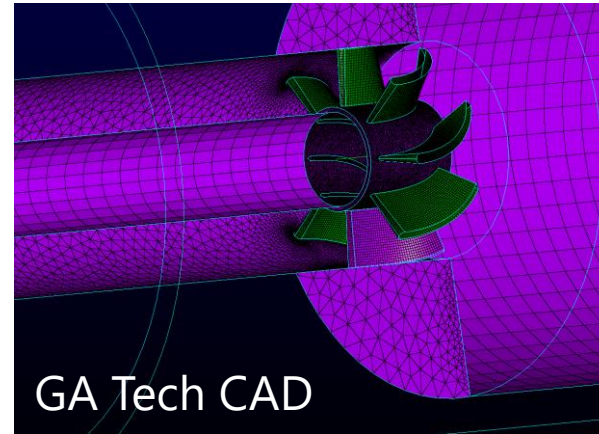
Tohoku University/AIST Configuration



Strong effects of kinetics and turbulence

# Modeling of GA Tech Test Configuration

- Completed calculation setup on HPC systems:
  - Leveraged on periodicity: 45 degree wedge (one vane)
  - Used placeholder chemistry model
- Established **computationally efficient** procedure for steady-state solution:
  - Non-reacting swirl flowfield with FPV approach
  - Ignition in combustor via FPV table lookup (detailed species mapping and temperature field initialization)
  - Reacting flowfield with TFM approach
- Next: Test planning calculations



Velocity vectors

- Swirl number of 1.1
- Stoichiometric  $\text{NH}_3$ -air mixture (premixed) at 1 atm pressure

# Summary/Next Steps

- Selected for 41 month, \$4.2M project to advance NH<sub>3</sub> combustion technology
  - Ammonia is an alternative low-carbon energy carrier
- Completed detailed Literature Review and analyses indicating a preferred path forward
- Ammonia combustion physics testing is ongoing (UCF) over a range of relevant gas turbine conditions to fill in high pressure data
- Hencken Burner and staged fuel tests ongoing (GTRC)
- Initial CFD model updates ongoing and analysis of configurations ongoing
- Ongoing preparations for higher pressure Scaled Combustor tests at GTRC
- Thanks to DOE NETL for supporting this work

