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

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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_2
  - High combustion efficiency
  - Stable flame (no blowoff)
- Challenges with ammonia
  - Safety considerations with ammonia
  - Ammonia ignition and flameholding
  - NOx generation

	Methane	Hydrogen	Ammonia
Lower Heating Value (LHV)	Mass: 50 MJ/kg (21,500 BTU/lb) Volume: 915 BTU/scf	Mass: 120 MJ/kg (51,600 BTU/lb) Volume: 275 BTU/scf	Mass: 18.6MJ/kg (8,000 BTU/lb) Volume: 365 BTU/scf
Flame Speed (S_L)	37 cm/s (1.2 ft/s)	291 cm/s (9.5 ft/s)	7 cm/s (0.23 ft/s)
Flame Temperature (T_{ad})	1950°C (3542°F)	2110°C (3830°F)	1800°C (3272°F)

Comparison of fuel characteristics

IACT Plan & Key Roles

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

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Led Literature Review & Design Def.

UCF UNIVERSITY OF CENTRAL FLORIDA

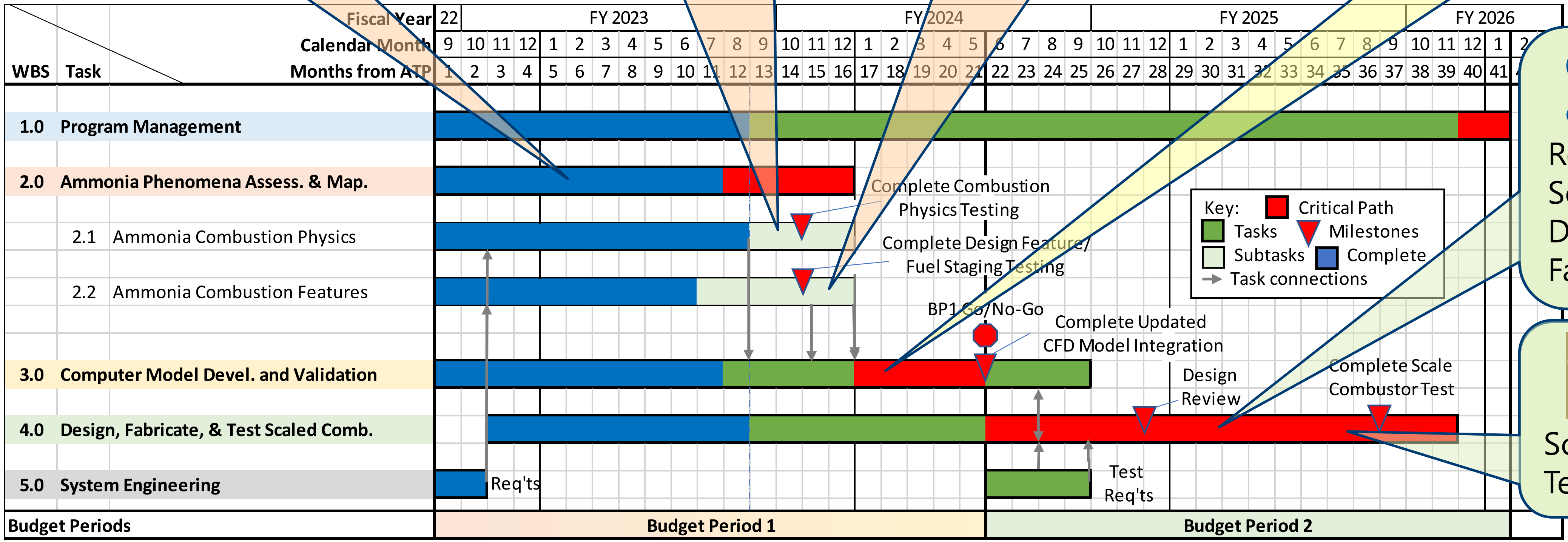
Shock Tube & Flame Speed Tests Kinetics mech.

Georgia Tech

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

CRAFT Tech

CFD Tool Devel.; Scaled Combustor Design



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Reqt's Def. & Scaled Comb. Design & Fabrication

Georgia Tech

Scaled Comb. Test

IACT Project Flow

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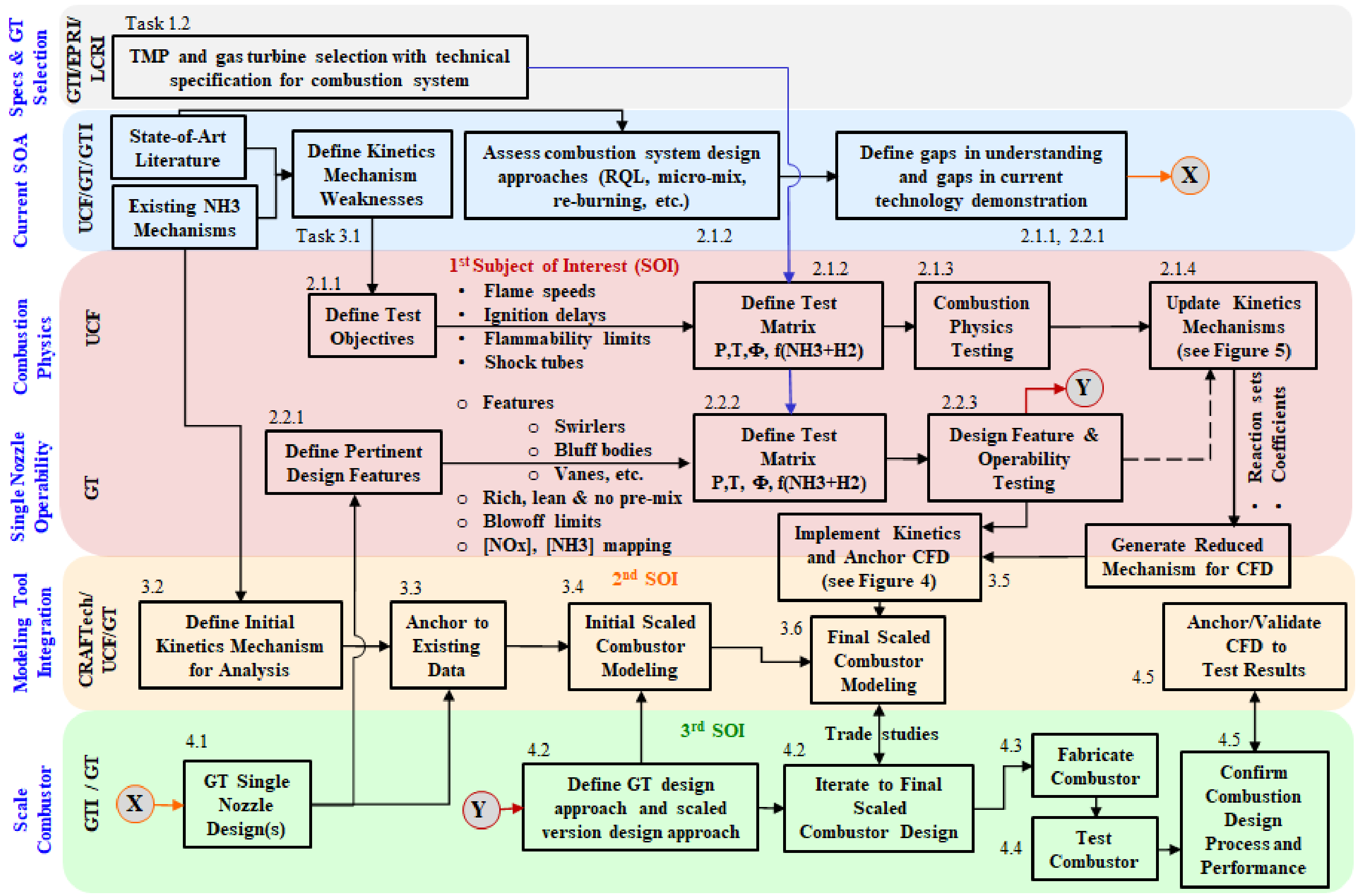


Literature search to understand SOA and identify knowledge gaps

Define test conditions to fill gaps

Fundamental NH_3 & NH_3+H_2 combustion physics testing

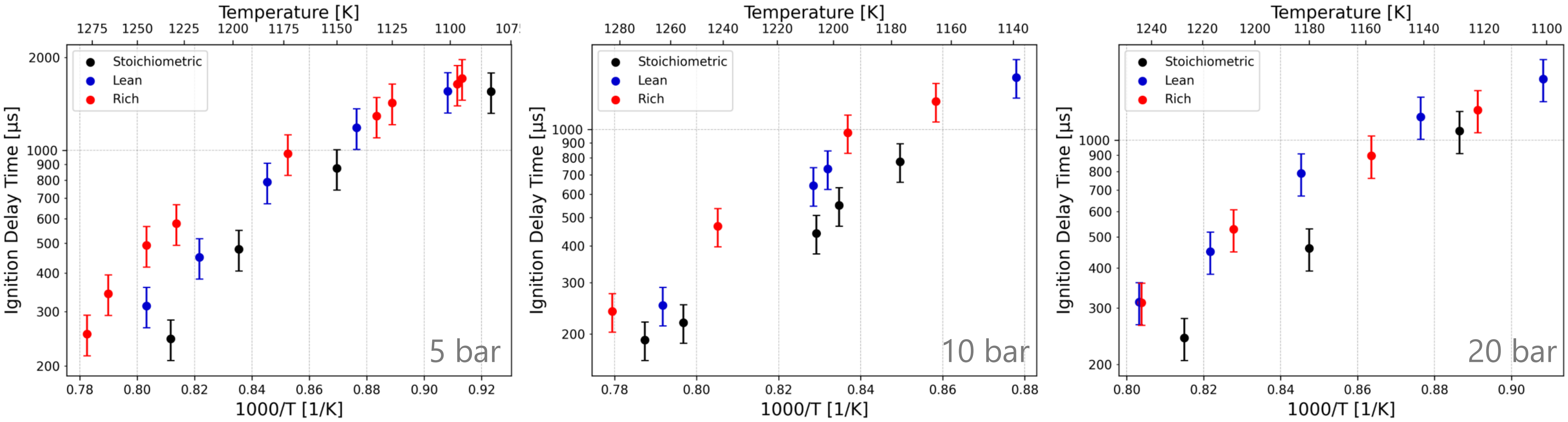
Generate improved detailed and reduced kinetics

Develop computational CFD design tool implementing updated mechanisms

Apply combustion physics knowledge and design tool

Design and test scaled combustor

70/30 NH_3/H_2 IDTs
Also Pure Ammonia and 50/50 Mix

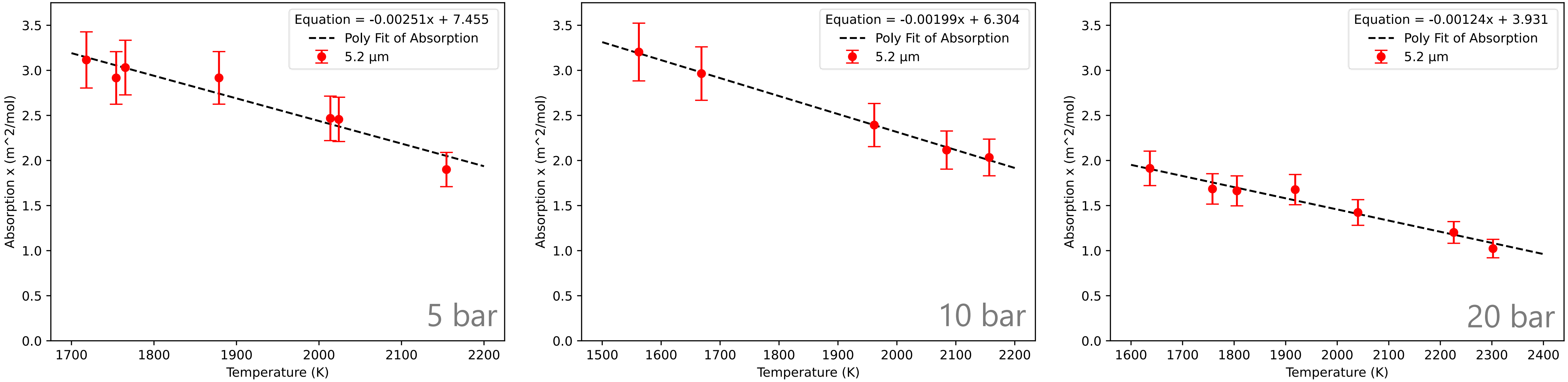


- At 5 bar and 10 bar, ignition order follows rich<lean<stoichiometric. However, at lower temperatures, all mixtures ignite nearly at same time.
- At 20 bar, lean and rich mixtures ignite slower than stoichiometric mixtures.

- 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, NO2, NH_3 and H_2O species time histories during NH_3/H_2 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.

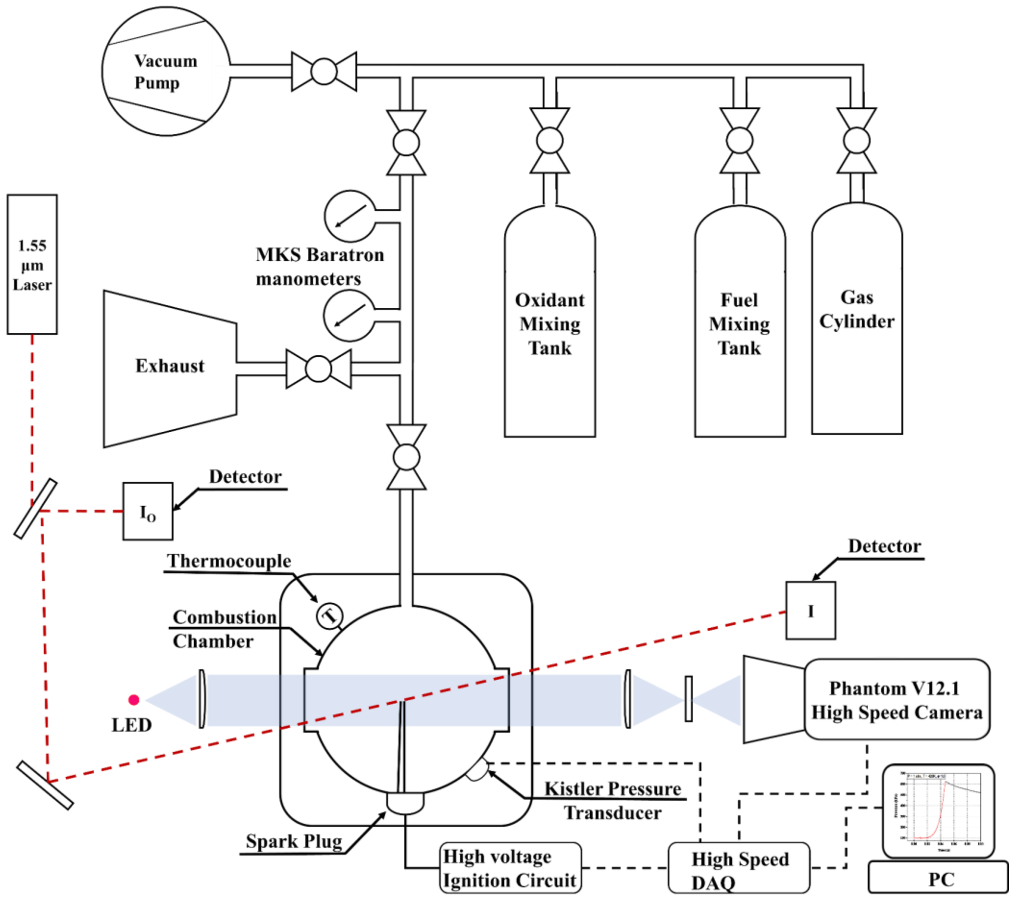
Flame speed measurements - Test matrix

- 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[1]				Phi	Temp. (K)	Pressures (atm)
		O_2	N_2	Ar	He			
H_2-NH_3	50	1	1	0	3	07 – 1.2	296	10
	70	1	1	0	3			
	100	1	2	0	1			
H_2-NH_3	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

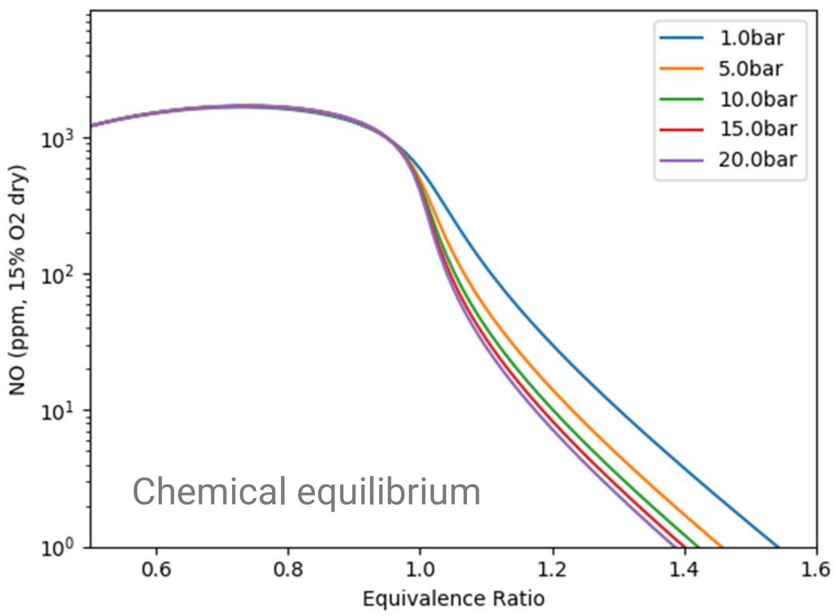


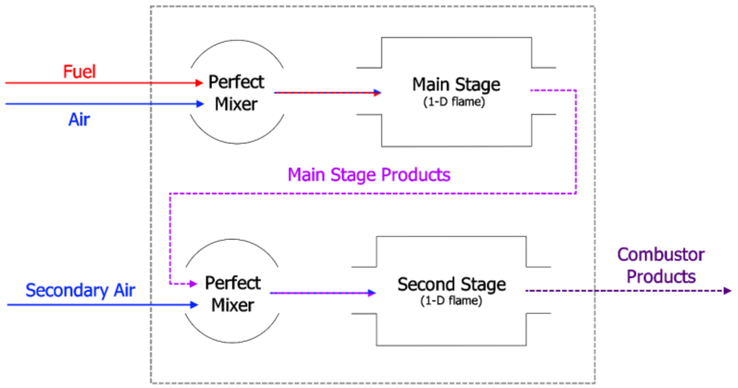
Theoretical Minimum NOx for Ammonia Combustion

- A useful benchmark: what is the theoretical minimum possible NOx 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_x (O(10) ppm) possible
  - Rich front end, relaxation zone, lean zone
  - i.e., more than just RQL





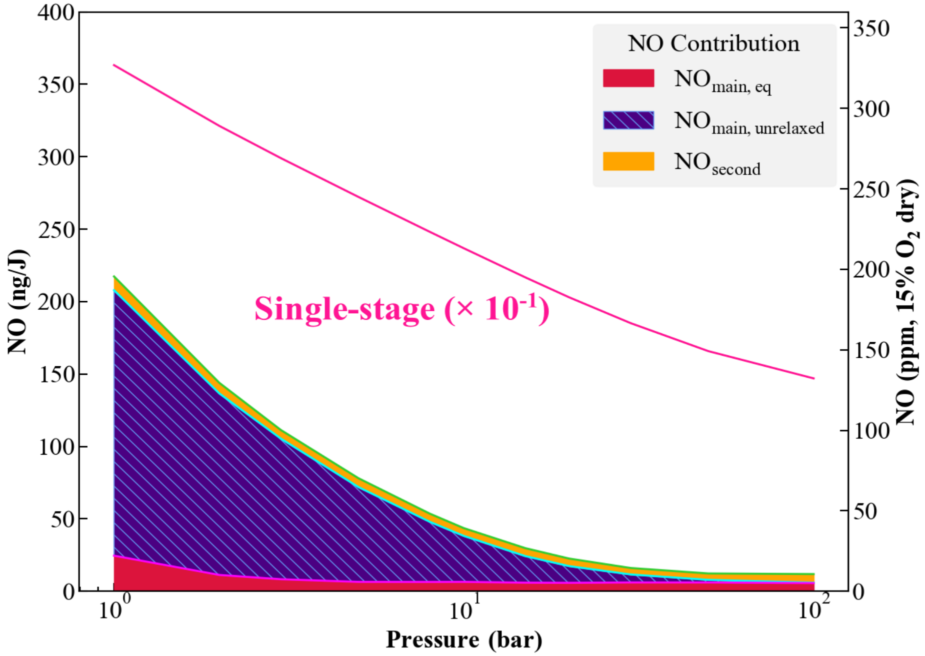
Schematic of staged combustor reactor network model

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 x Emissions Go?. *ACS Energy Letters*, *8*, 4421-4426.

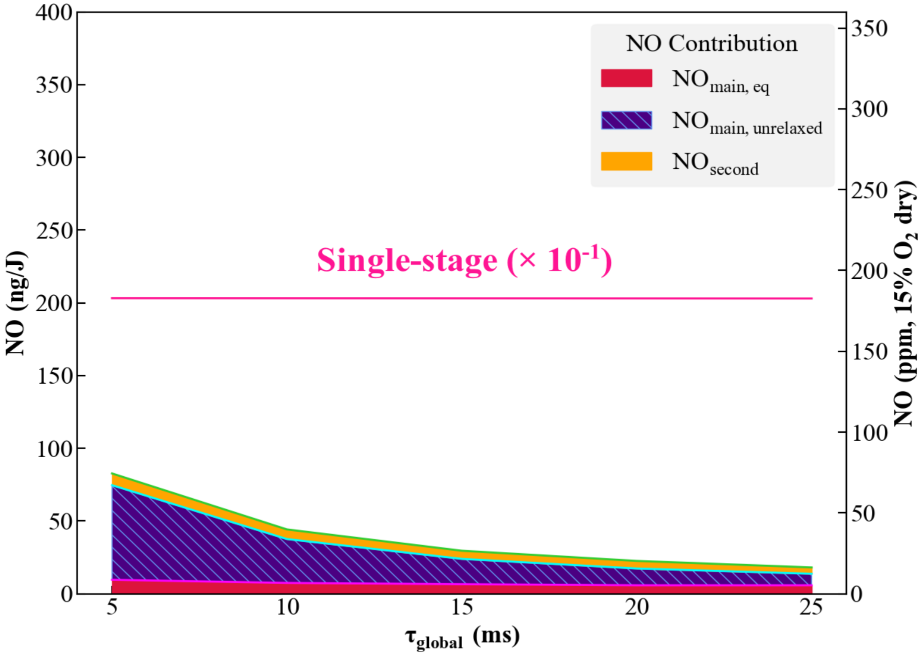
Optimized NO Emissions

- "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



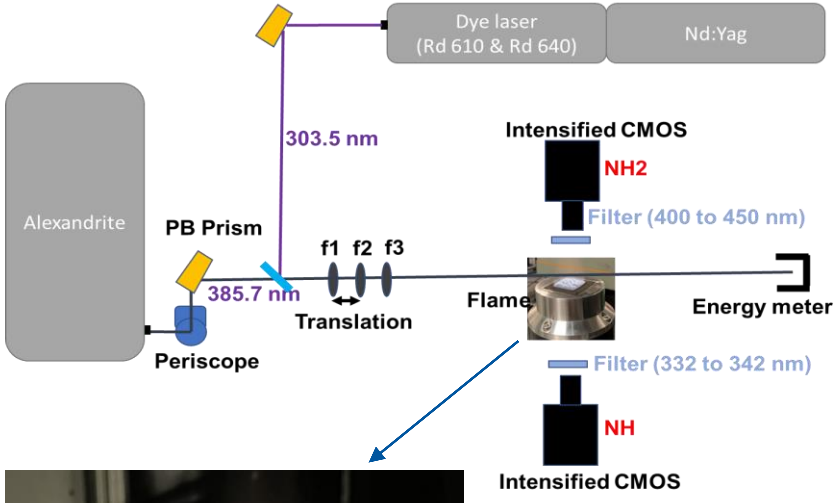
Minimum NO at various combustor pressures (T_{exit} = 1900 K, τ_{global} = 20 ms)

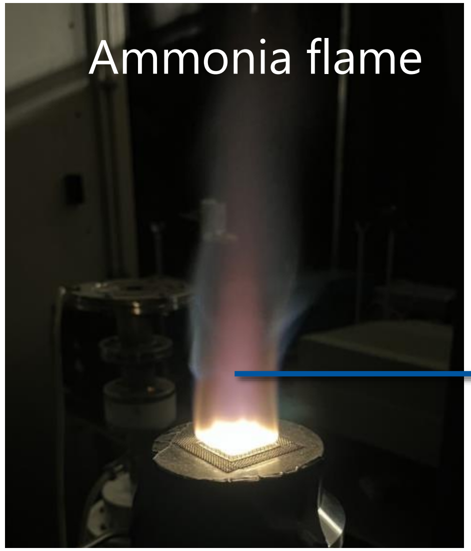


Minimum NO at various global residence times (T_{exit} = 1900 K, P = 20 bar)

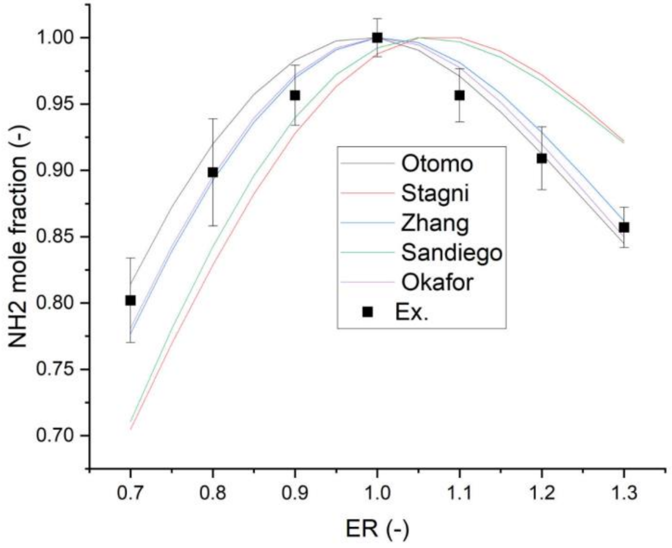
Hencken Burner Test Setup

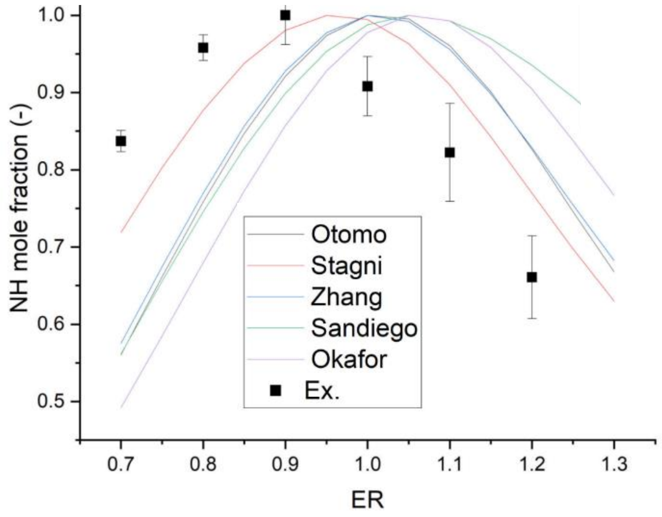
- Investigation of NH_2/NH laser-induced fluorescence (LIF)
  - Pure ammonia-air cases, O_2 enriched air (50% O_2/50% N_2) to help stabilize flame
  - Models seem to predict NH_2 trend vs ER well
  - NH trend vs ER is noticeably different
  - Work in progress
- New CAI Gas Analyzer commissioned and will measure NO, NO_2 N_2O, and NH_3 at various equivalence ratios



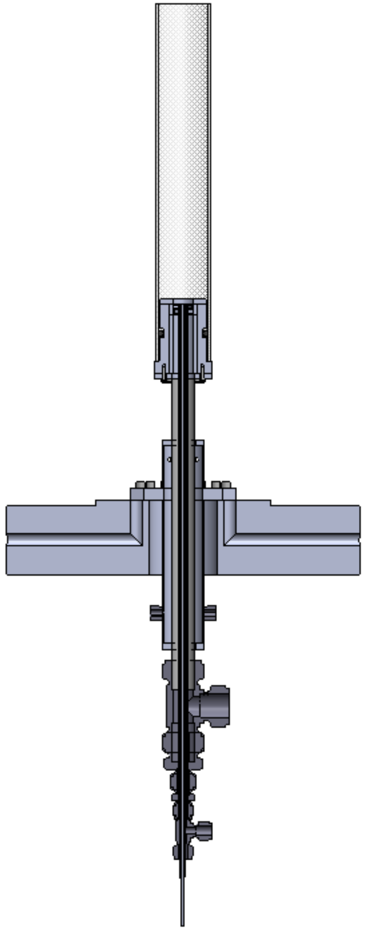


Water cooled Sample Line

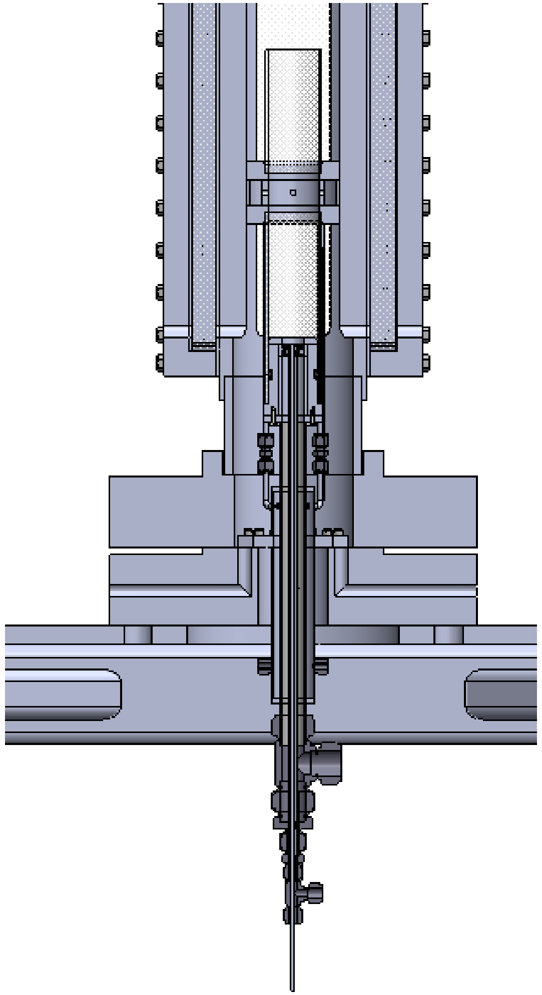




Atmospheric/Pressurized Tests
Staging Tests



Atmospheric burner design



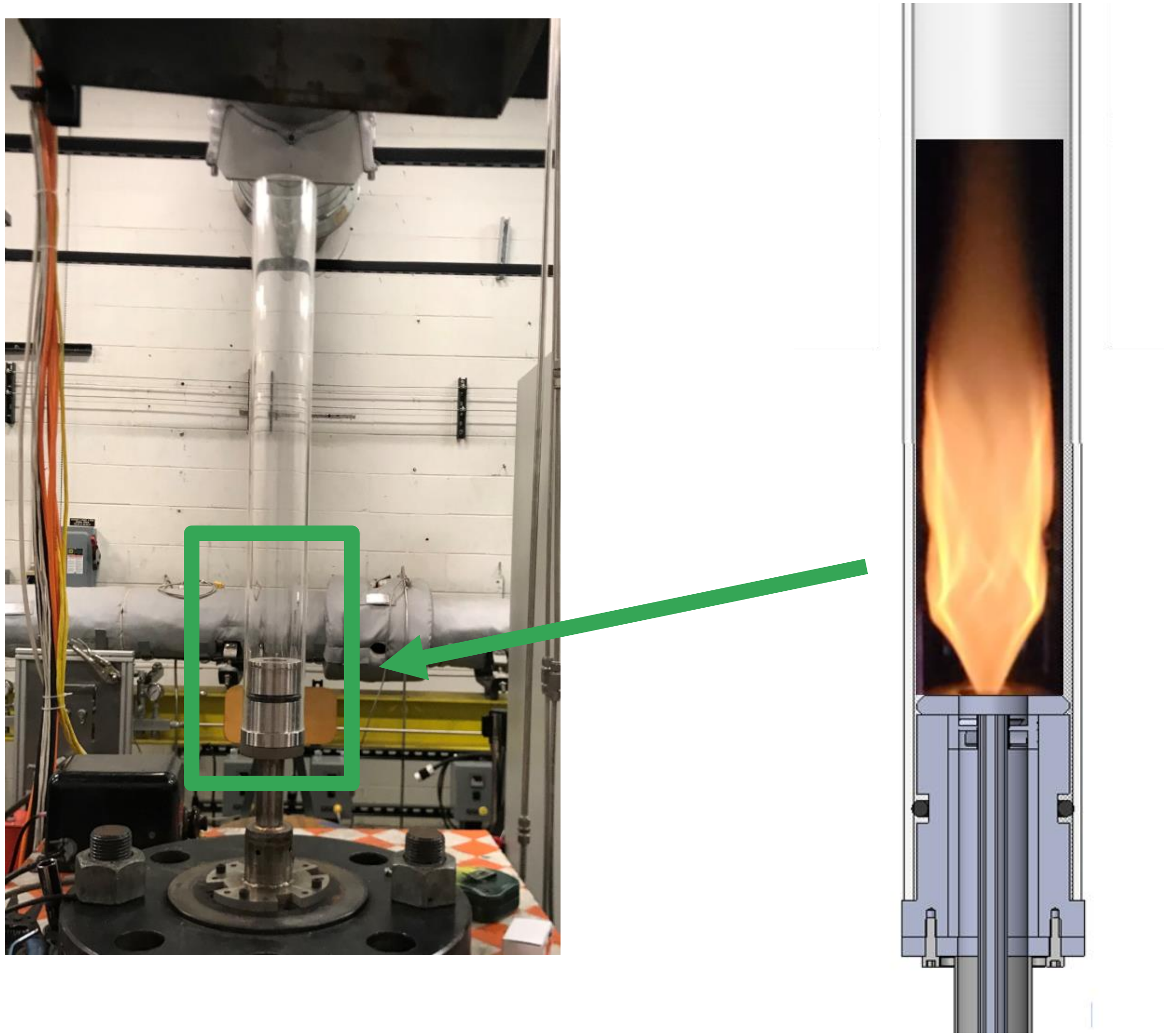
Pressurized burner design

- 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 NOx calculations

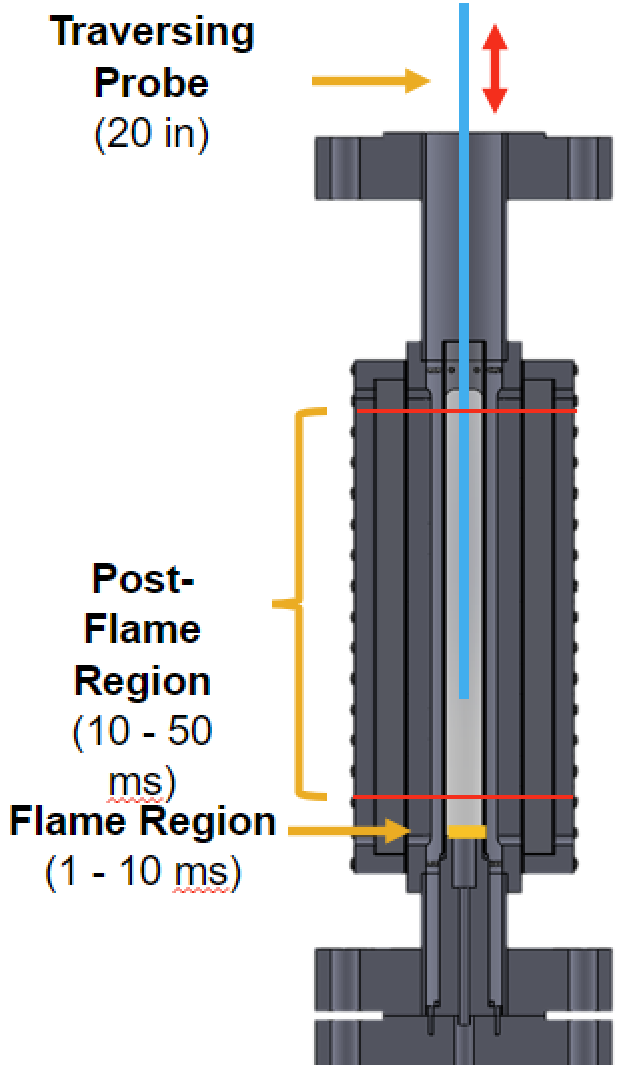
Atmospheric/Pressurized Tests
Staging Tests

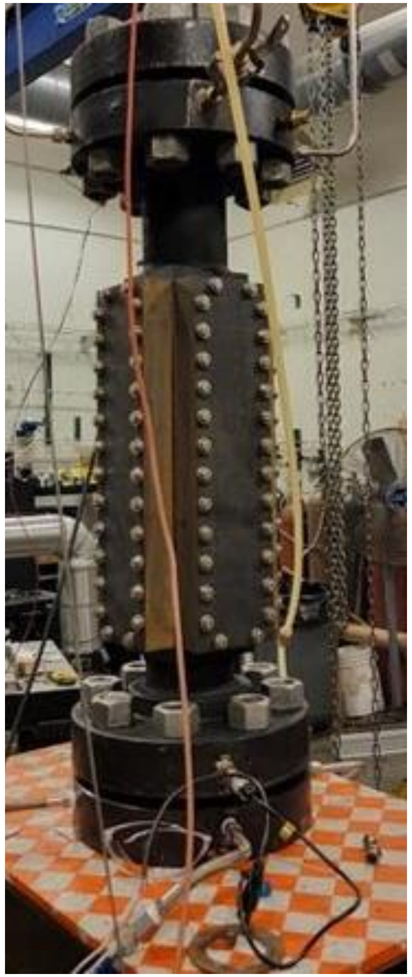
- Burner manufactured, passed safety review, shakedown, and first fire
- Planning atmospheric and 6 bar tests

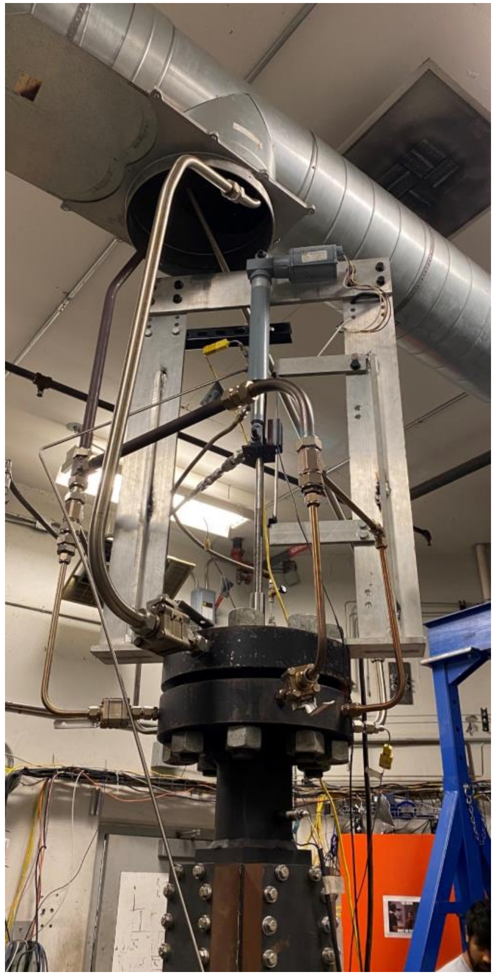

Modular Swirler Burner (Swirl numbers 1.1, 0.7, 0.4)



Scaled Combustor Test Planning





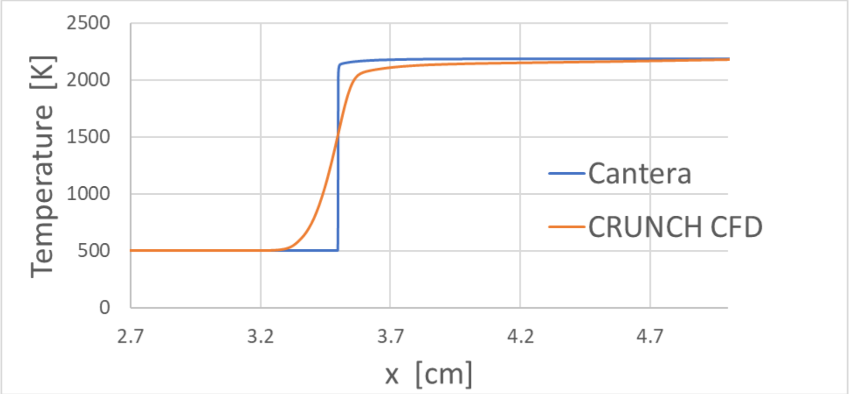


- 20 bar experiments planned for 2024

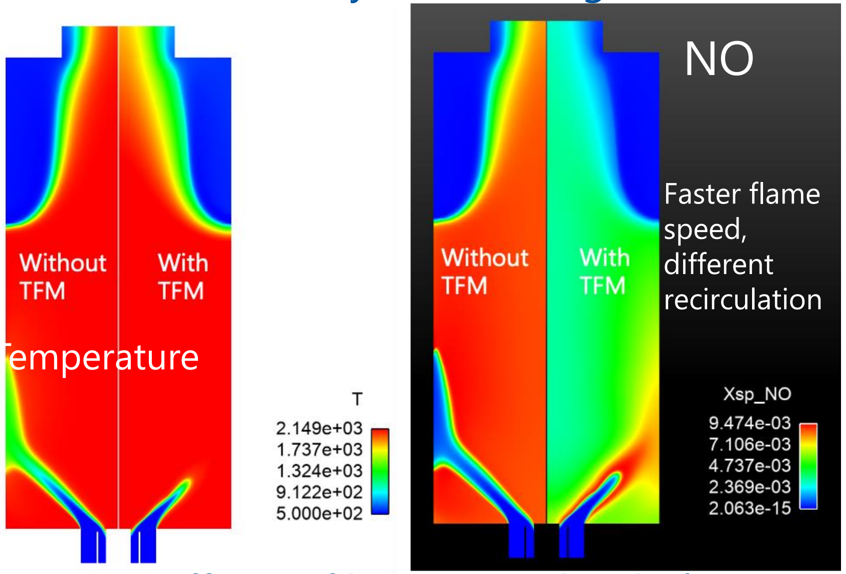
Modeling Upgrades for Turbulent Premixed Flames

- 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



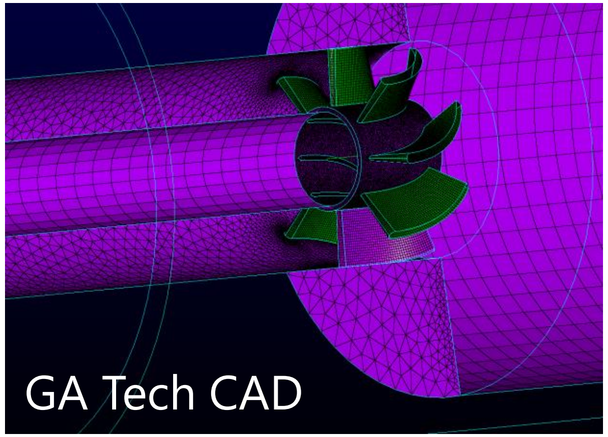
Tohoku University/AIST Configuration



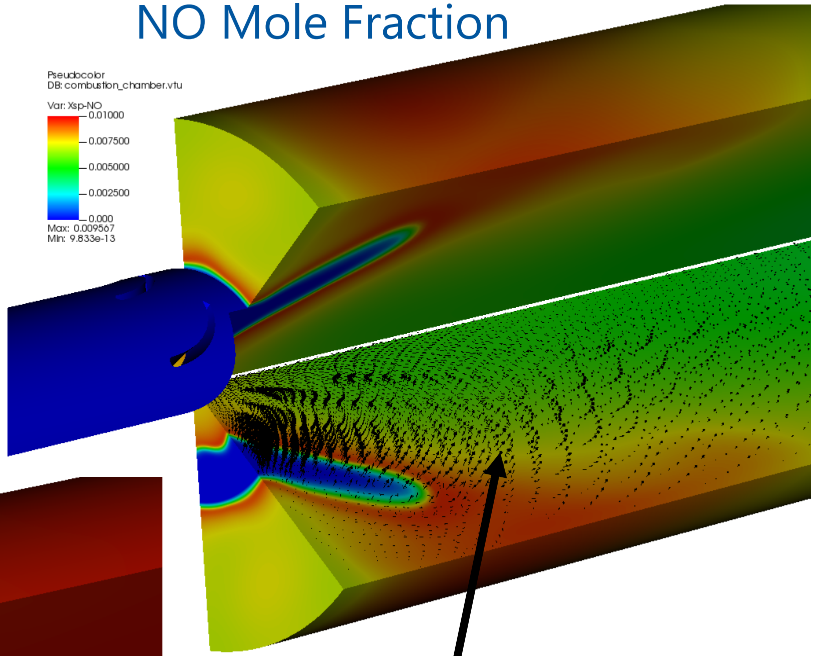
Strong effects of kinetics and turbulence

Modeling of GA Tech Test Configuration

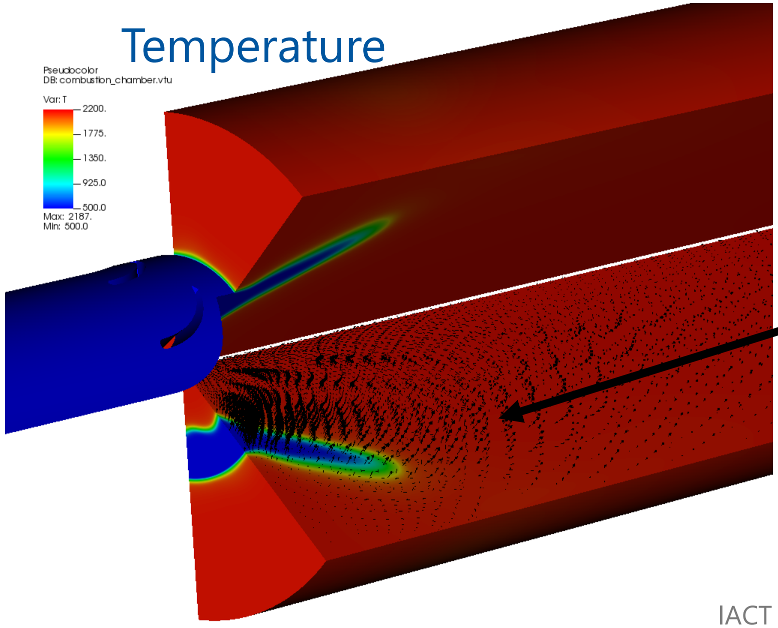
- Completed calculation setup on HPC systems:
  - Leveraged on periodicity: 45 degree wedge (one vane)
  - Used placeholder chemistry model
- Established **computationally efficient** procedure for steady-state solution:
  - Non-reacting swirl flowfield with FPV approach
  - Ignition in combustor via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



NO Mole Fraction



Temperature



Velocity vectors

- Swirl number of 1.1
- Stoichiometric NH_3-air mixture (premixed) at 1 atm pressure

Summary/Next Steps

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- Selected for 41 month, \$4.2M project to advance NH3 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

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