GTI ENERGY

solutions that transform

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

John Vega (GTI Energy)

Andrew O’Connell (DOE, NETL)

May 7th, 2024

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
- Challenges with ammonia
  - Safety considerations with ammonia
  - Ammonia ignition and flameholding
  - NOx generation
- Demonstration: Test Scaled Combustor
  - Design using updated mechanism/ validated model
  - NOX Target: 20 ppm at 15% O_2
  - High efficiency, Stable flame

	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

Project Objectives/Flow – Near End of BP1

GTI ENERGY

- Advance ammonia combustion technology from TRL 1-2 to TRL 3-4
- ✓ Assessment of ammonia and ammonia-hydrogen-nitrogen blend fuel combustion phenomena at relevant gas turbine conditions (BP-1)
- ✓ Development and validation of computational models (CFD) for ammonia combustion (BP-1 & 2)
  - Update and implement kinetics mechanisms
- Complete Design, Fabrication, and Testing of Scaled Combustor (BP2)
  - DOE NO_X Target: 20 ppm at 15% O2 – very challenging

- ✓ 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*
  - *Iterate with additional data*
- ✓ Develop computational CFD design tool implementing updated mechanisms
  - *Apply combustion physics knowledge and design tool*
- Design and test scaled combustor

IACT Plan & Key Roles
Schedule: 9/2022-1/2026; Funding: $4.2M

GTI ENERGY

EPRI ELECTRIC POWER RESEARCH INSTITUTE
Led Literature Review & Design Def.

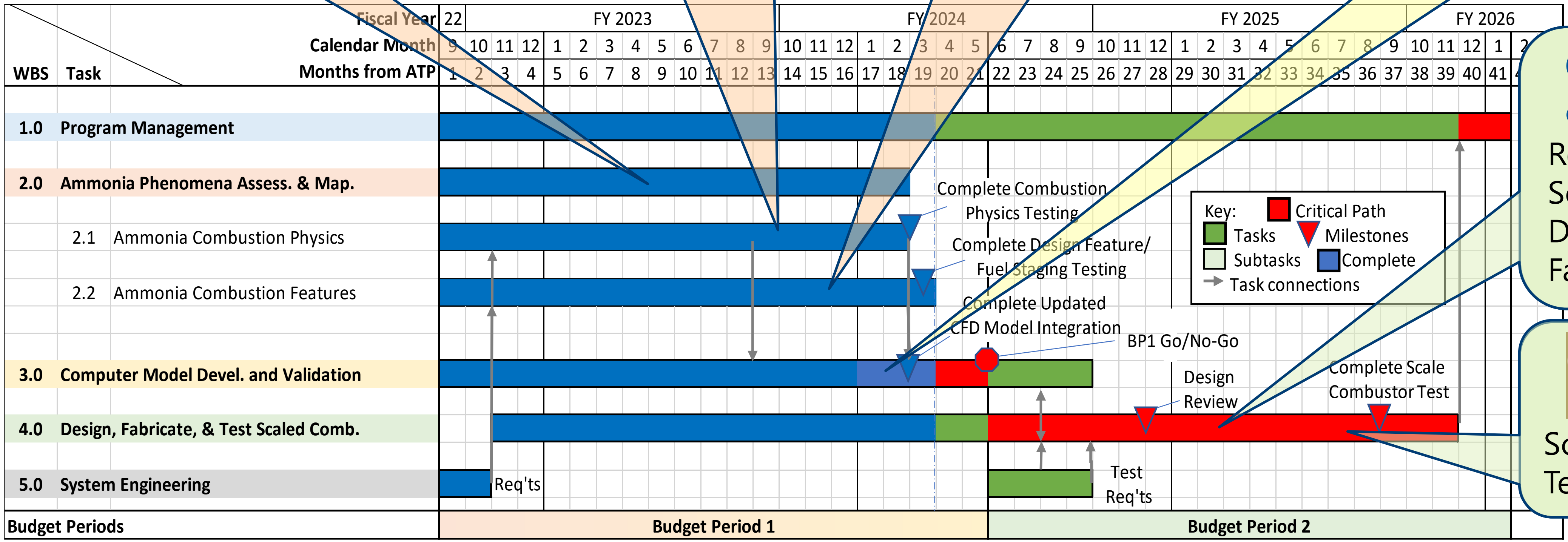
UCF UNIVERSITY OF CENTRAL FLORIDA
Shock Tube & Flame Speed Tests Kinetics mech.

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

CRAFT Tech
CFD Tool Devel.; Scaled Combustor Design

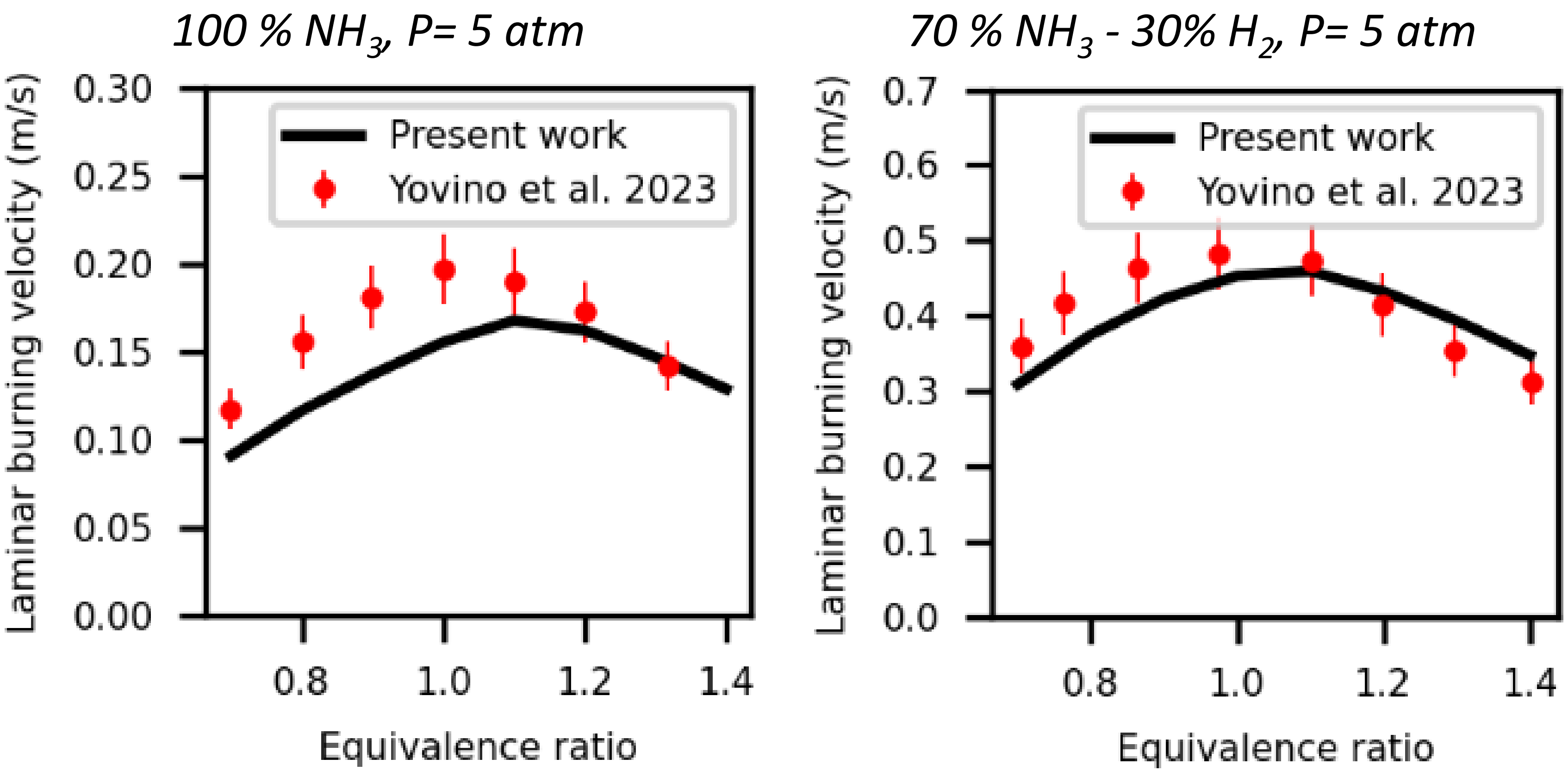
GTI ENERGY
Reqt's Def. & Scaled Comb. Design & Fabrication

Georgia Tech
Scaled Comb. Test



Completed Flame Speed Measurements

- Laminar flame speeds in spherical vessel
- 5, 10 and 20 bar
- Pure ammonia and ammonia/hydrogen blends
  - 100, 70, 50 % NH_3
- Range of E.R.
- Compared to IACT v1 mechanism (similar to Zhu et. al. 2024

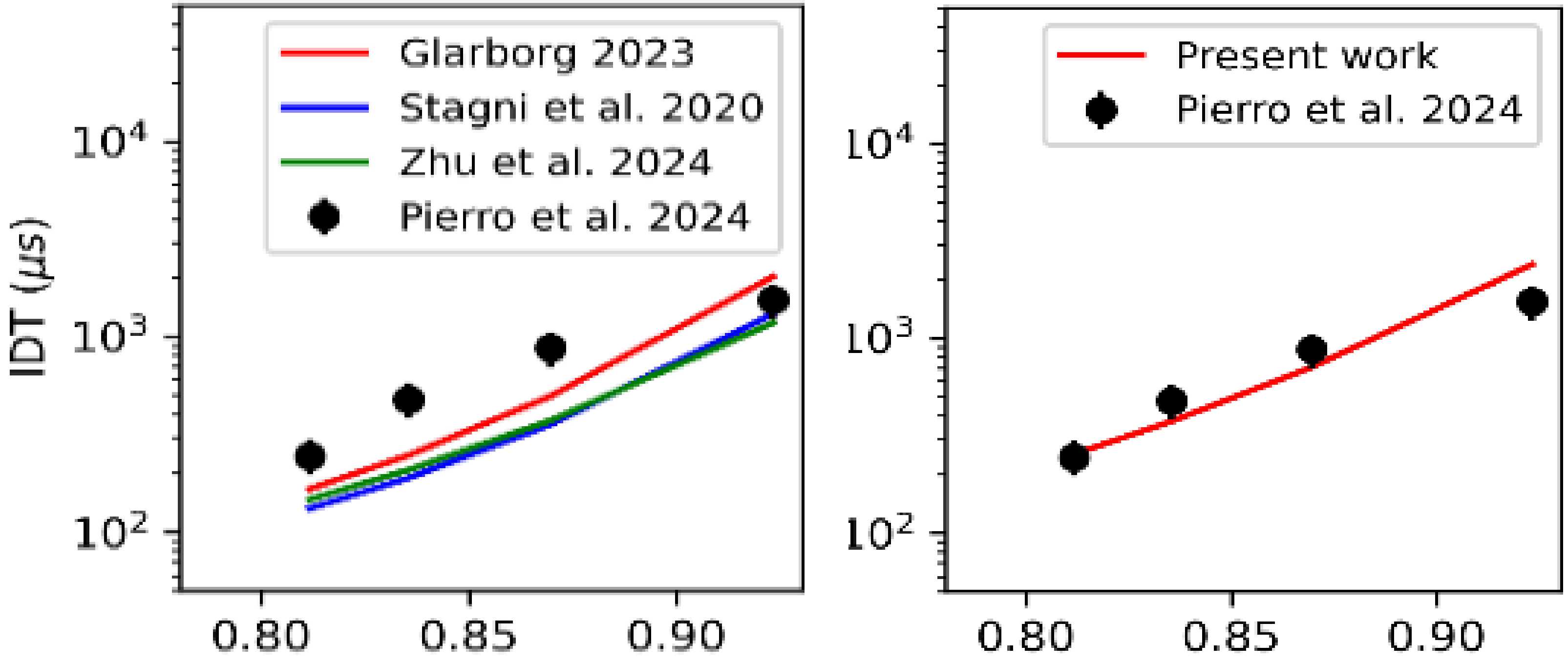


Data utilized to develop/improve chemical kinetic model for ammonia/hydrogen blends
Requires further improvement for lean 100% ammonia

Ignition Delay Time (IDT) Measurements

- Shock Tube
- 5, 10 and 20 bar
- Pure ammonia and ammonia/hydrogen blends
  - 100, 70, 50 % NH_3
- Range of Equivalence Ratios
- Multiple mechanisms shown

70 % NH_3 30% H_2, Φ – 1.0, 5 bar



Existing mechanisms

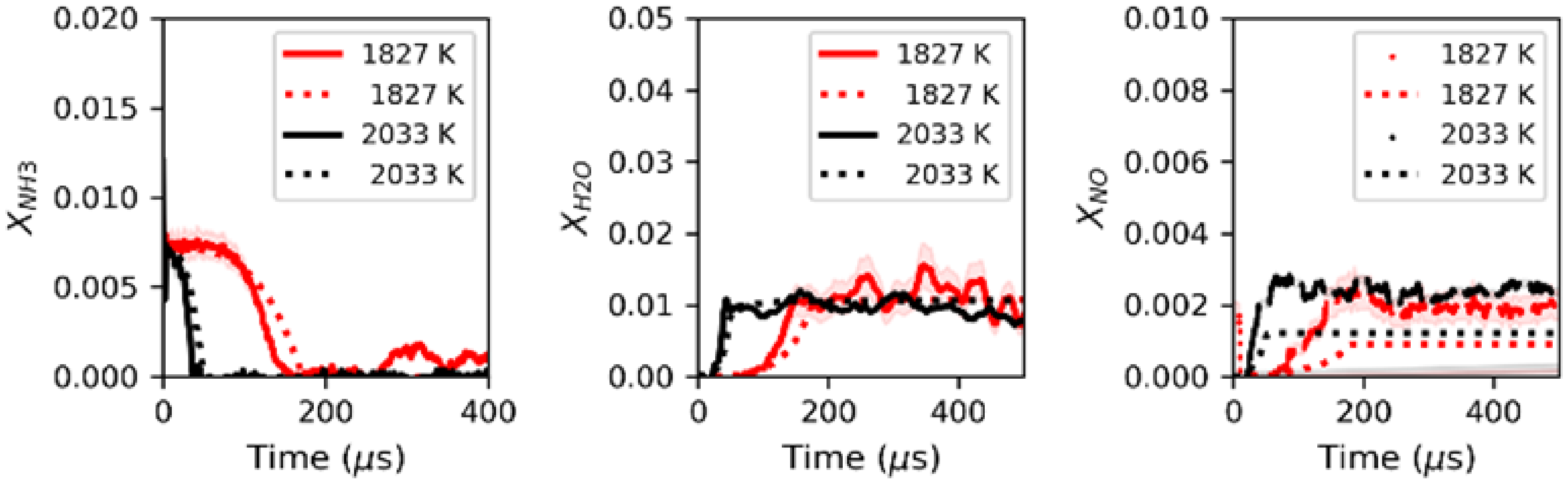
IACT v1 mechanism

Utilize data to develop/improve chemical kinetic model for ammonia/hydrogen blends
Improved, Requires further improvement in low pressure, fuel rich conditions

Develop Cross Sections and Measure Time Histories

- Characterize species absorption to determine species time histories
- Measured NO, NO_2, NH_3 and H_2O species time histories during NH_3/H_2 combustion at 5, 10 and 20 bar

20 bar NH_3 oxidation, Φ – 0.6, 95% Ar

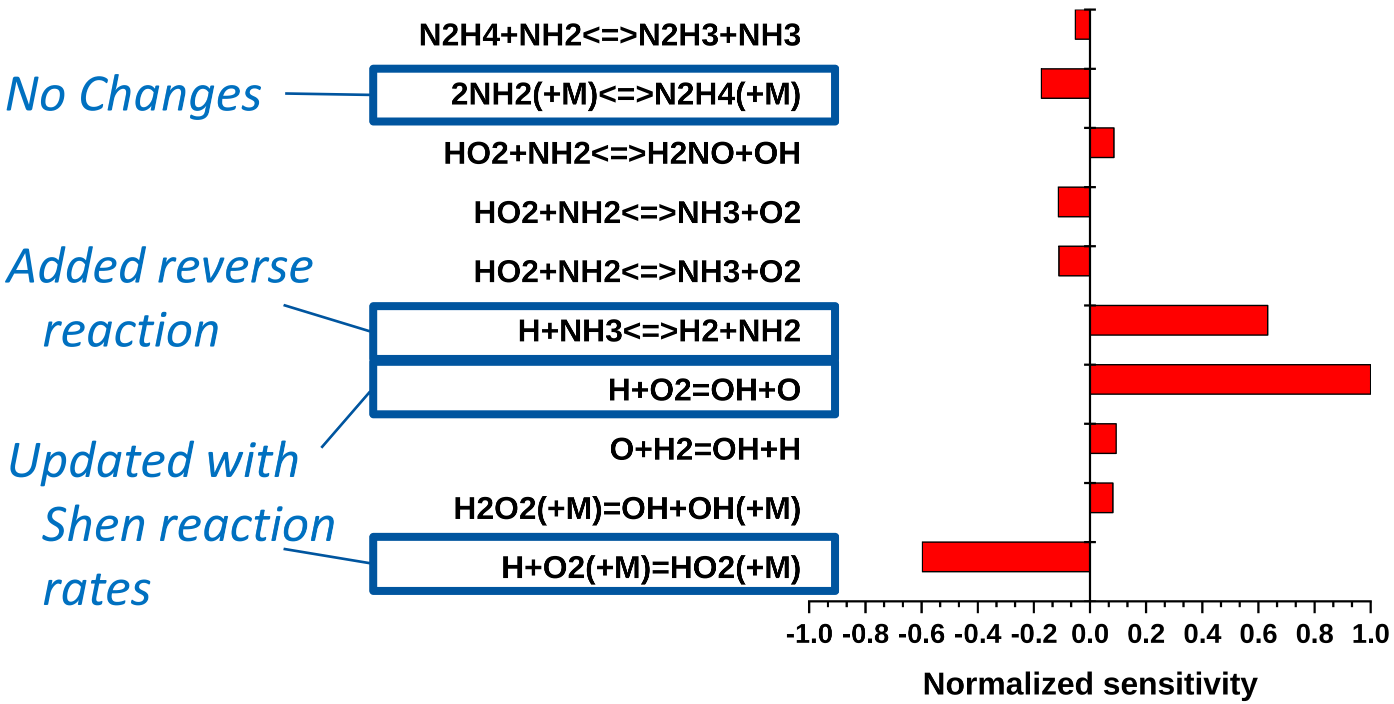


Dotted lines – simulation; Solid lines - experimental data

- New mechanism at 20 bar does not completely capture NO time histories

Accurate prediction of NO at gas turbine relevant conditions is key for optimizing the design to reduce emissions – NO requires further improvement

Developed Updated Kinetics Model



No Changes

Added reverse reaction

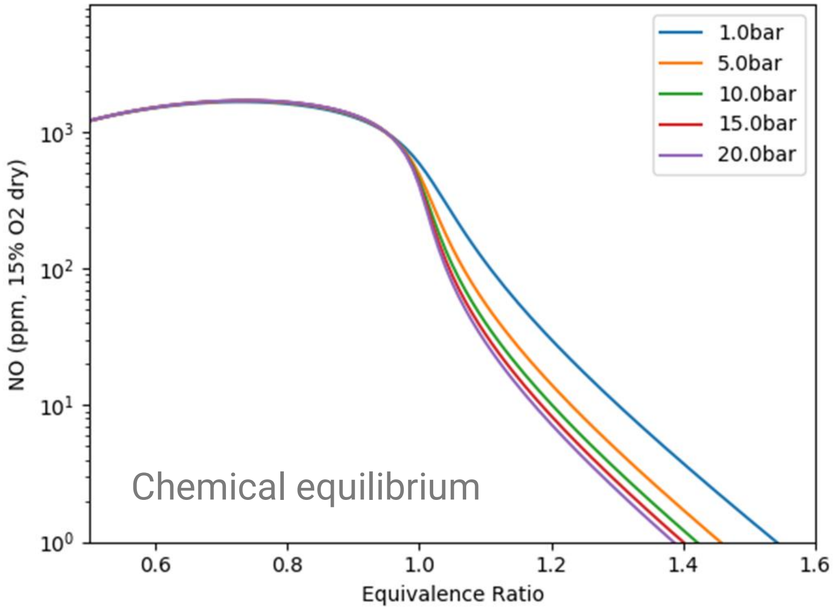
Updated with Shen reaction rates

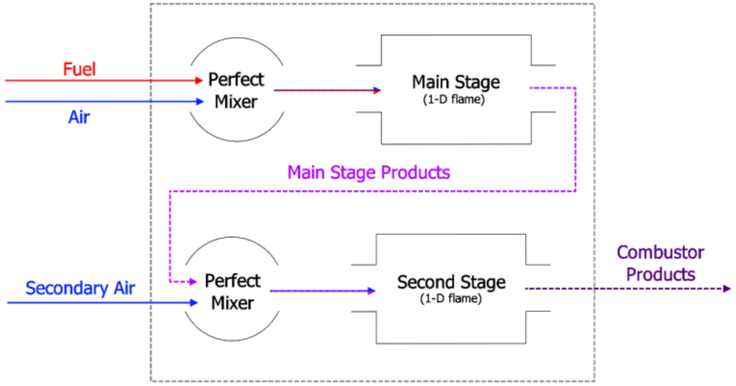
- Compared best mechanisms - Glarborg et al., Stagni et al. and Zhu et al
- Selected Zhu as base mechanism
  - Captures flame speed and pure hydrogen IDTs for ammonia/hydrogen blends better
  - Validated for shock tube species time histories for ammonia and N_2O
- Made modifications using recently gathered data

Data utilized to develop/improve chemical kinetic model for ammonia/hydrogen blends

Theoretical Minimum NOx for Ammonia Combustion - Focus

- Benchmark: what is the theoretical minimum NOx emission from ammonia combustion?
  - Not simulating a specific combustor, but rather what is possible
- Lower NOx
  - Higher E.R.
  - Higher pressure
  - Higher Temperature
  - Different than current DLN technology
- Acceptable NO_x (< 25 ppm) possible
  - Rich front end, relaxation zone, lean zone



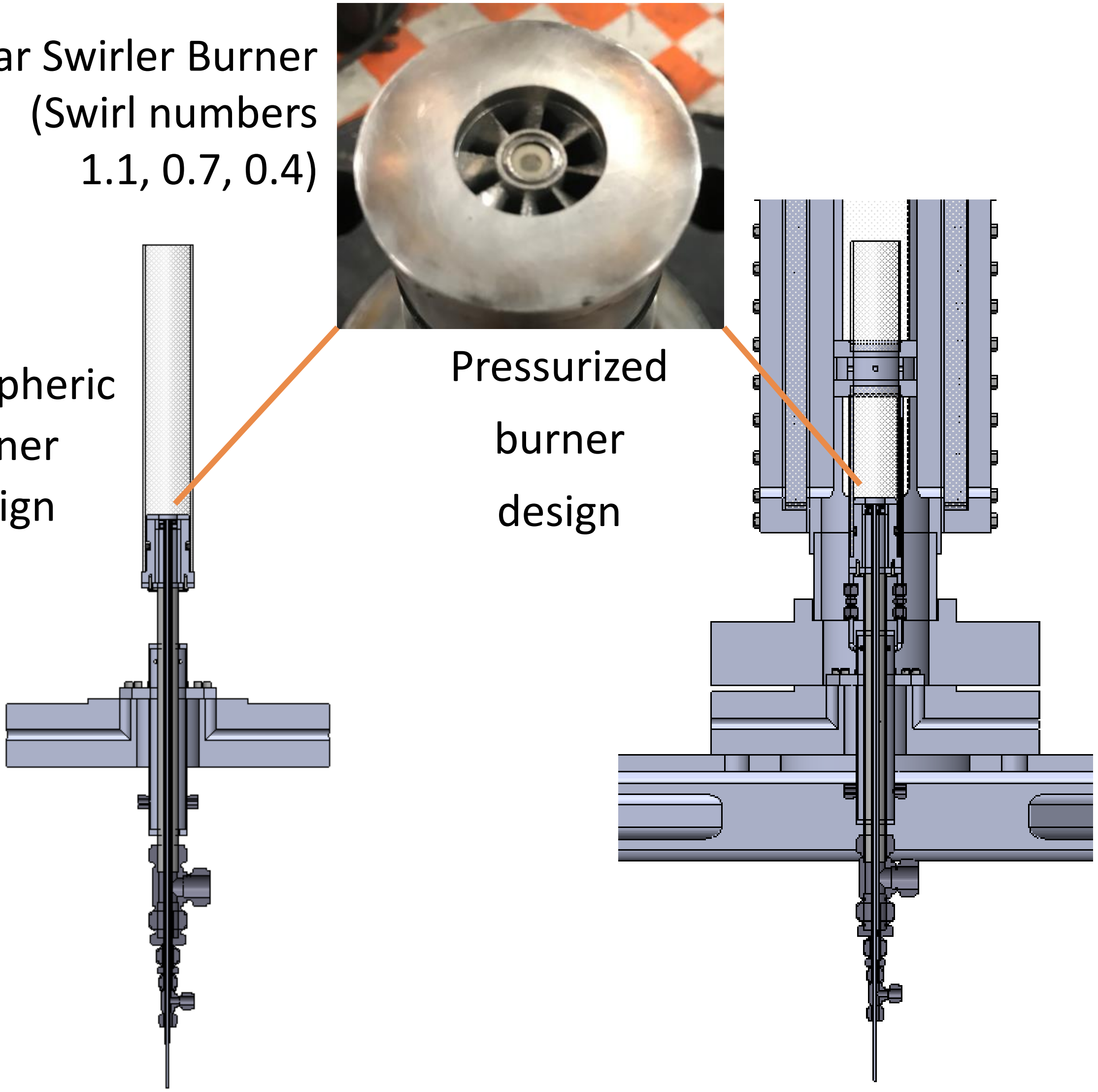


Schematic of staged combustor reactor network model

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.

Possible to be EPA compliant without SCR for ammonia combustion

Prototypic Swirl Burner Tests



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

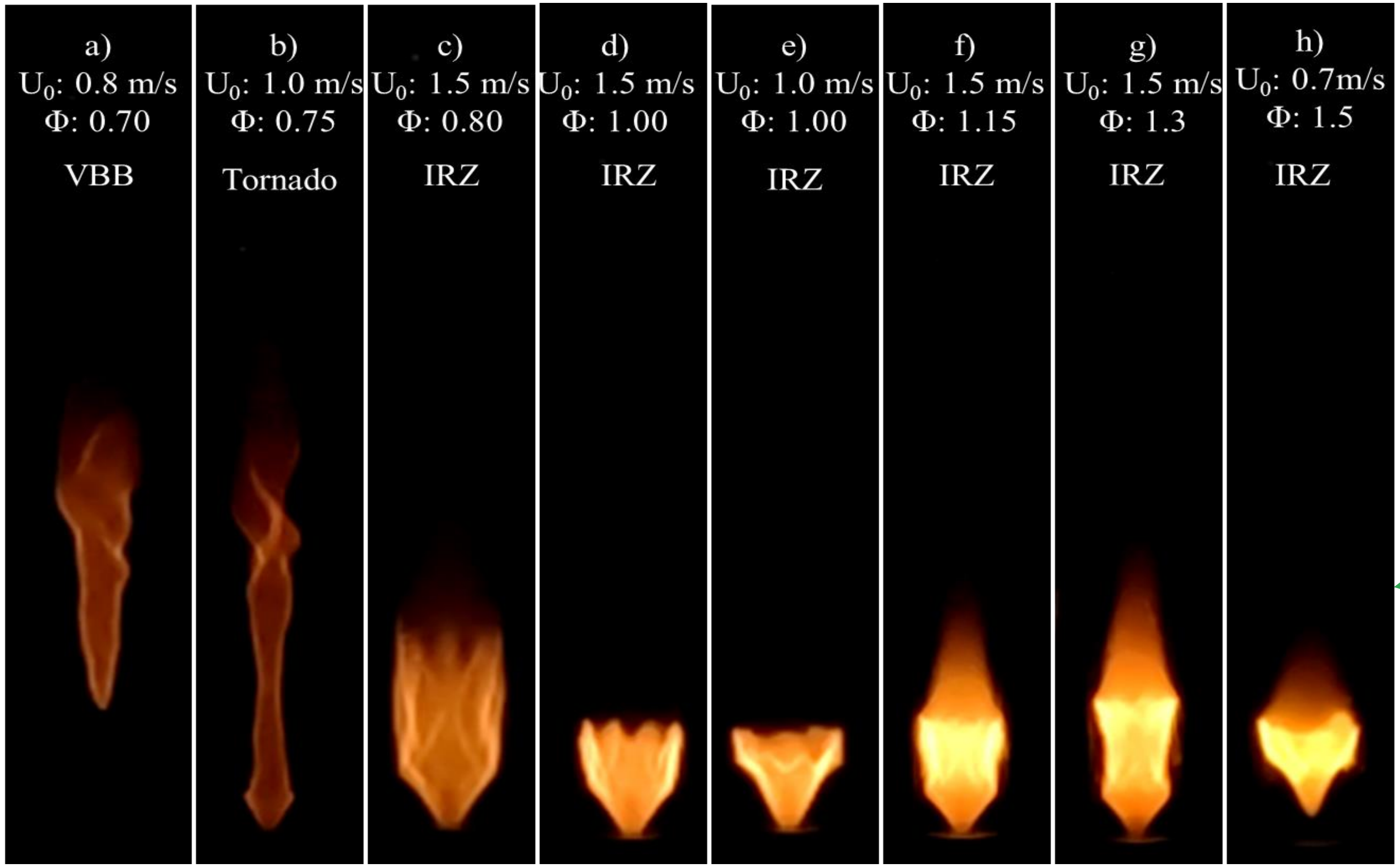
Atmospheric burner design

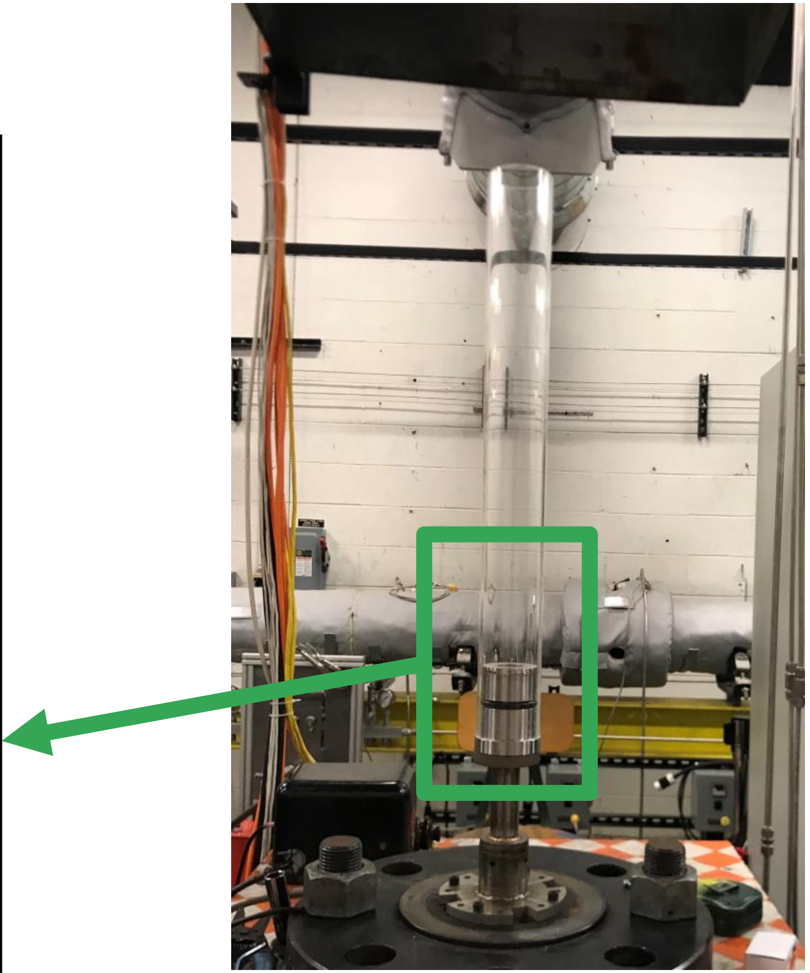
Pressurized burner design

- Atmospheric and pressurized (to be completed) ammonia testing
  - Tests will share the burner
- Investigated 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

Prototypic Swirl Burner Tests

- Atmospheric testing complete
- 6 bar tests next – facility preparation ongoing

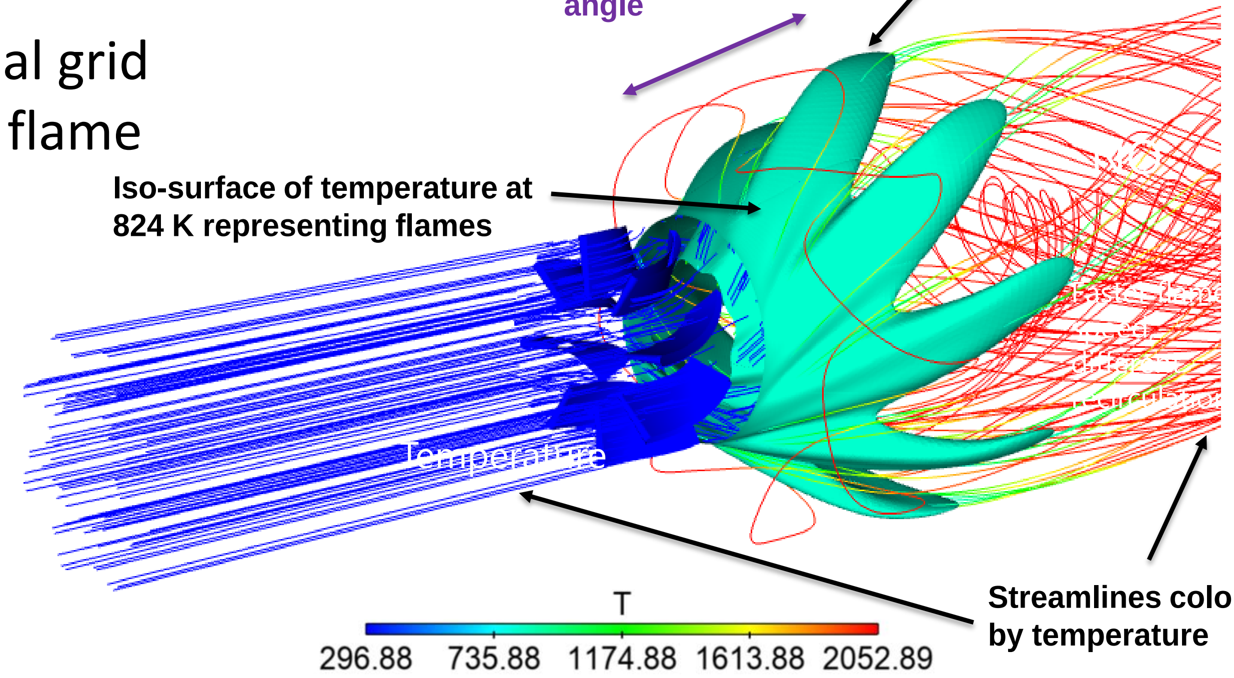




Modeling Upgrades for Turbulent Premixed Flames

- Completed code development implementing Thickened Flame Model (TFM) 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
  - Leveraging on MTS-FPV tabulated chemistry capabilities to reduce computation cost and turn-around time
- Modeling GA Tech burner configuration complete and compared to test data

CFD Model: Leveraged on periodicity: 45 degree wedge (one vane)



Flames rotate with swirling flow and impinge against side walls

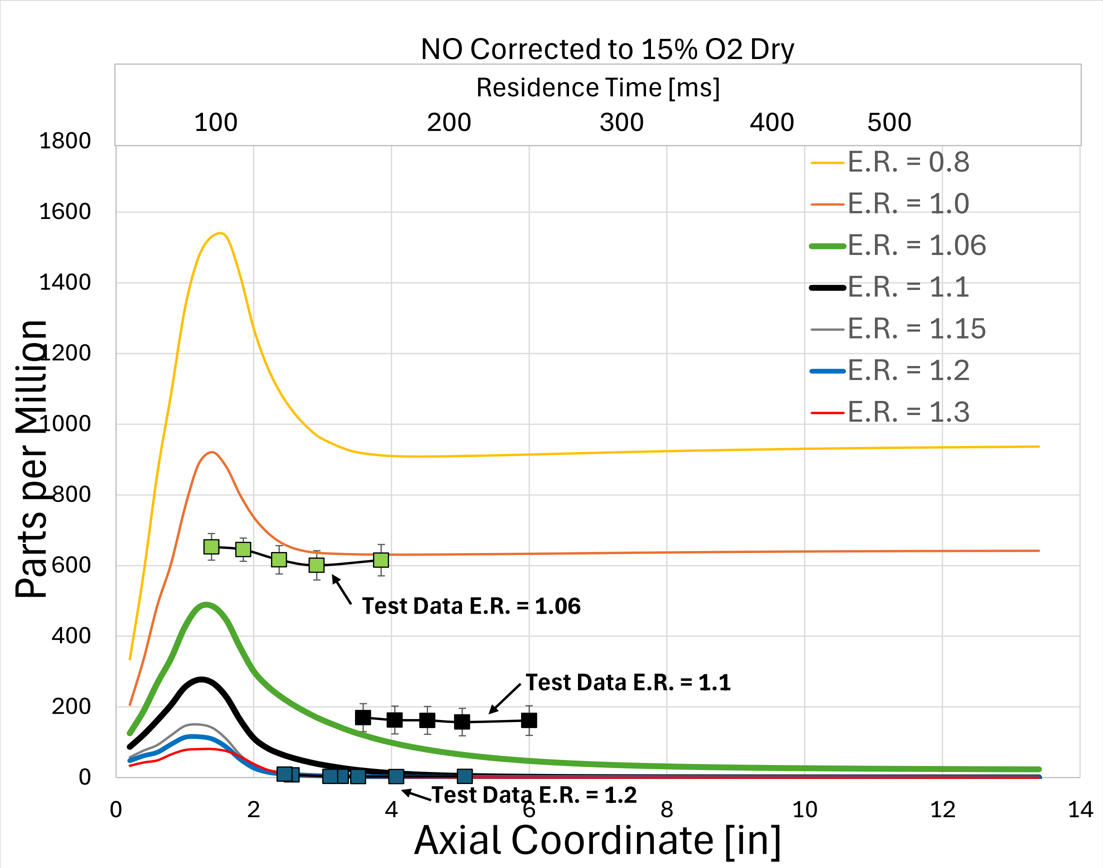
Attached flames extend ~2 in downstream at an angle

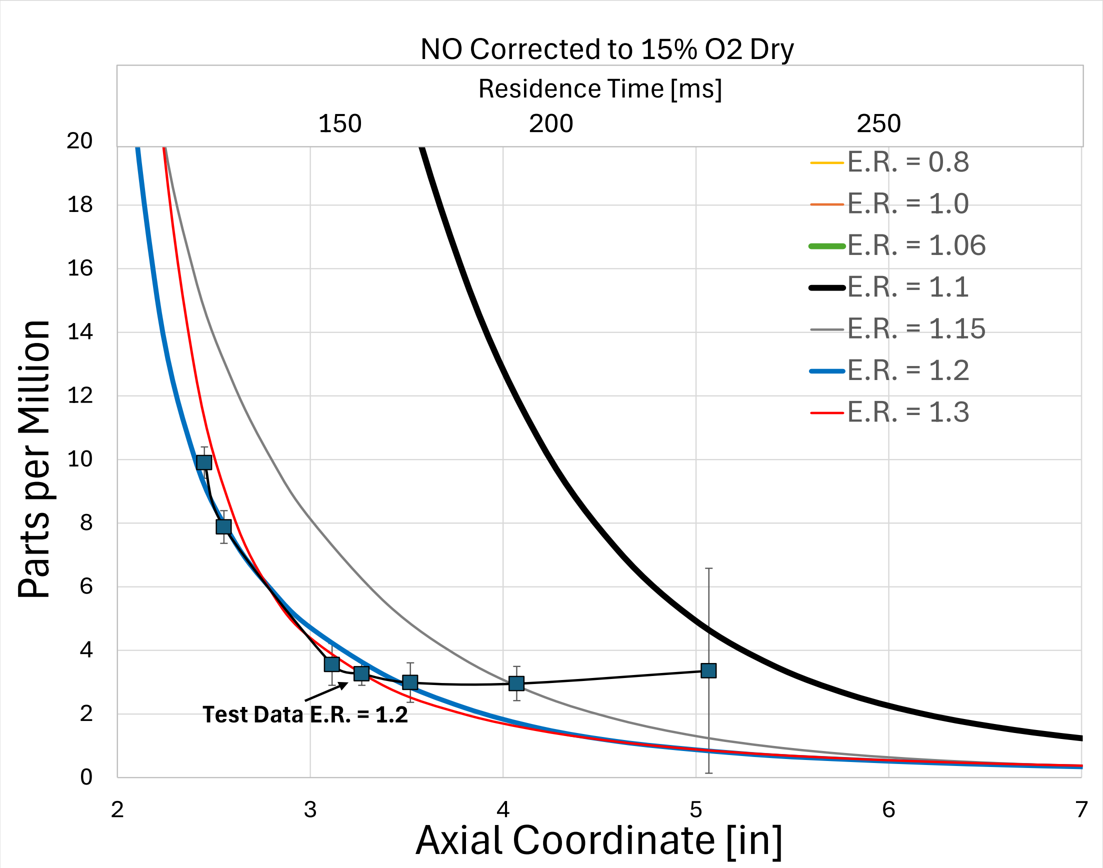
Iso-surface of temperature at 824 K representing flames

Streamlines colored by temperature

NO Model Predictions Compared to Test Results

NO Emission Profiles Corrected to 15% O_2 Dry for P = 1 bar, U_{bulk} = 1 m/s – IACT v1 mechanism

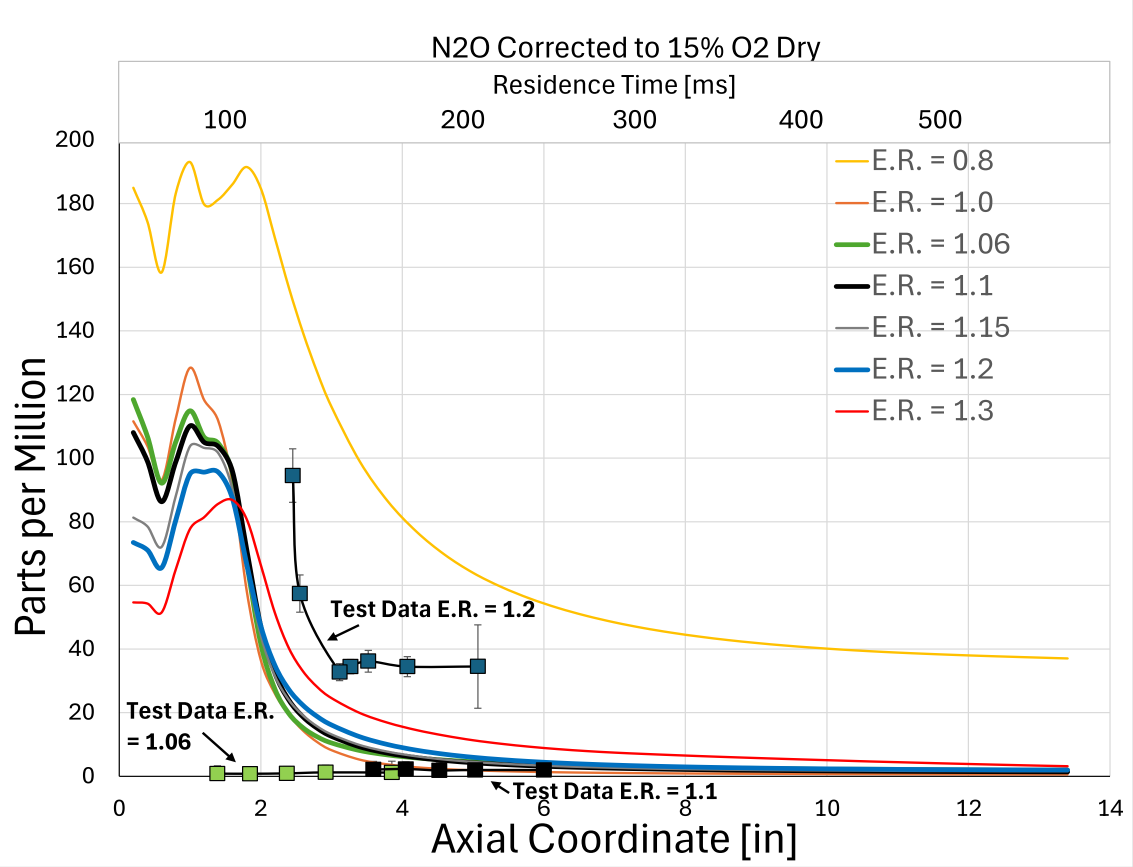


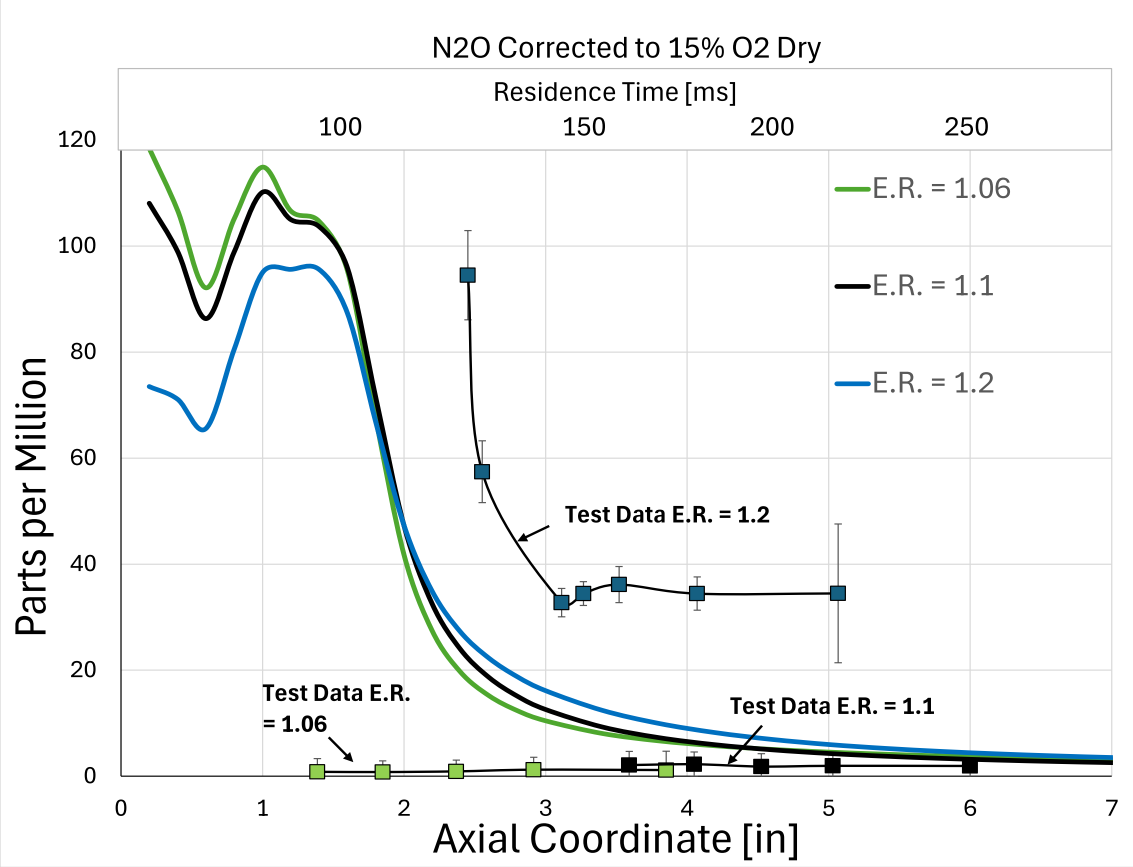


Model/Data trends match – Absolute values also agree remarkably well

N_2O Model Predictions Compared to Test Results

N_2O Emission Profiles Corrected to 15% O_2 Dry for P = 1 bar, U_{bulk} = 1 m/s – IACT v1 mechanism

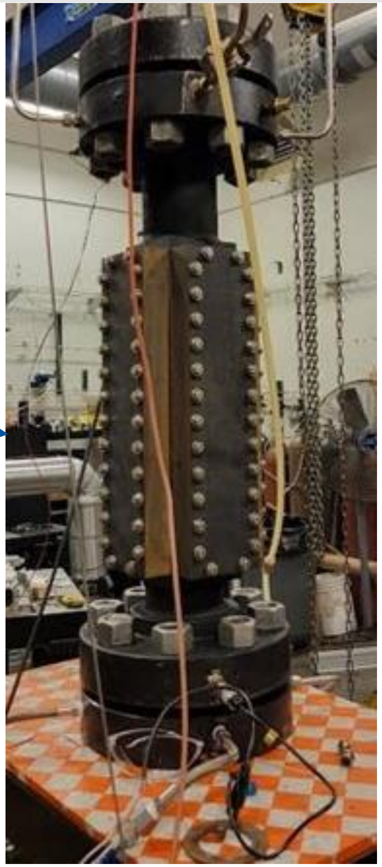




Model/Data trends match – Absolute values need improvement

Summary/Next Steps

GTI ENERGY



- Selected for 41 month, \$4.2M project to advance NH_3 combustion technology
  - Ammonia is an alternative low-carbon energy carrier/gas turbine fuel
- Completed Literature Review with analyses indicating a preferred path forward
- Ammonia combustion physics testing complete over a range of relevant gas turbine conditions to fill in high pressure data and update kinetics mechanism
- Prototypic burner tests complete at atmospheric conditions – 6 bar next
- CFD model updates incorporating new mechanism complete
- Prototypic swirl burner modeling is complete and matches data well
- Go/No-Go Report/Continuation Application just delivered
  - Next: BP2 effort - apply model/data to design/build/test Scaled Combustor
- Thanks to DOE NETL for supporting this work
- This research used resources of the National Energy Research Scientific Computing Center (NERSC), a Department of Energy Office of Science User Facility

GTI ENERGY

EPRI ELECTRIC POWER RESEARCH INSTITUTE

UCF UNIVERSITY OF CENTRAL FLORIDA

Georgia Tech

CRAFT Tech

LCRI LOW-CARBON RESOURCES INITIATIVE