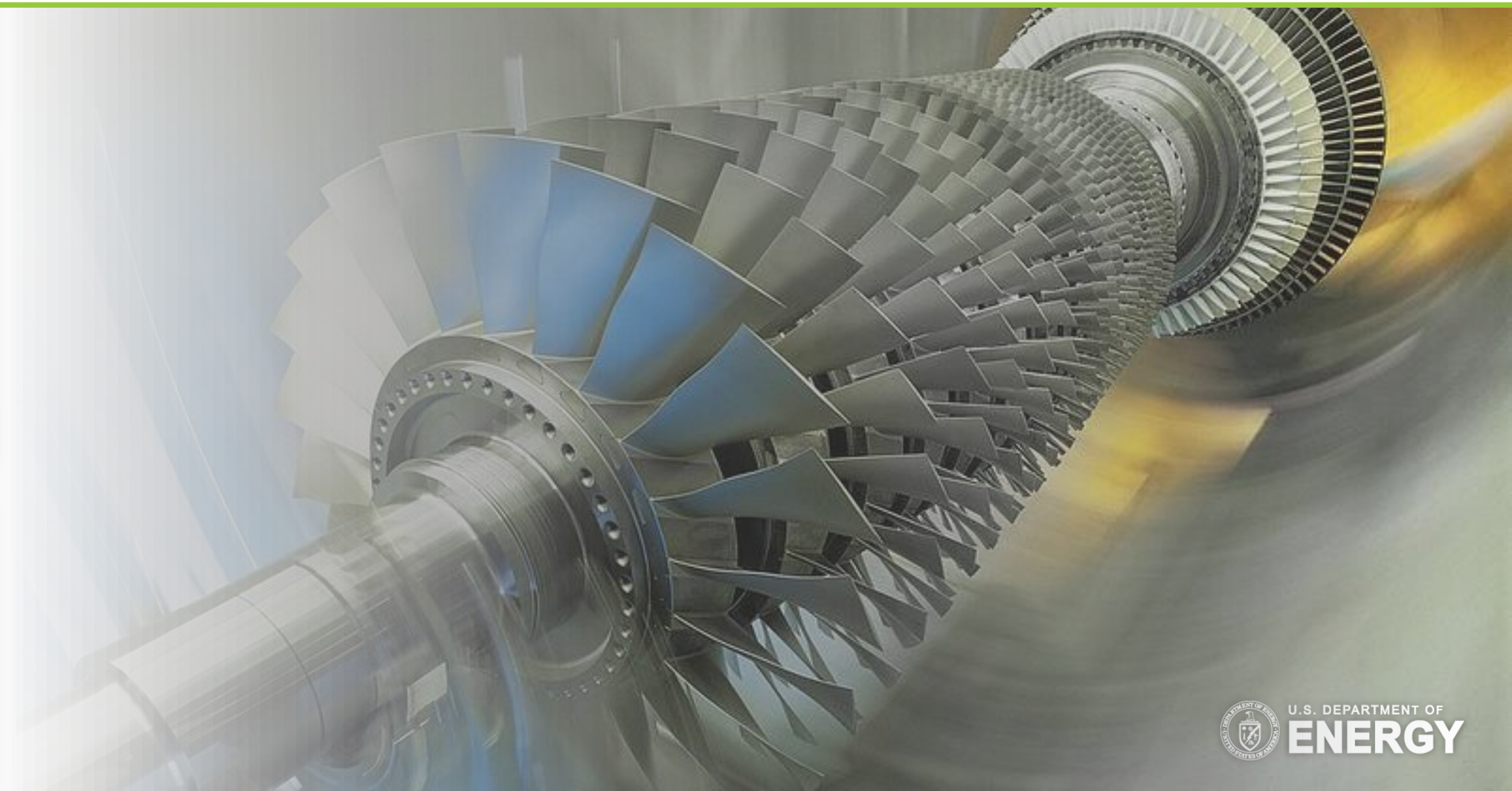
Ammonia Combustion for Gas Turbine Engines

Solutions for Today | Options for Tomorrow

Clinton Bedick

National Energy Technology Laboratory, Pittsburgh, PA, 15236



UTSR 2024
September 24-25, 2024
Tuscaloosa, AL

Outline

- Advanced Turbines Goal 2 Overview
- Motivation
- Fundamental Measurements
  - Laminar Flame Speed
  - Species Concentrations
- Modeling
- Applied Testing (atmospheric pressure)
- High Pressure Developments (2025)

Advanced Turbines MYRP – Goal 2

Data Dissemination	Atmospheric Experiments (PGH)	High Pressure Experiments (MGN)
Establish an ammonia combustion data repository on EDX (NETL data)	Conduct fundamental burner studies for model validation	Develop high-P NHG delivery system
Continue ammonia combustion working group	Develop engineering-level CFD models of candidate burner/combustor configurations	Modify the NETL PPC for NH3 (and H2) use up to 10 atm, 1MWth
Solicit external contributions to EDX repository	Perform atmospheric pressure testing in PGH FCL	Conduct high-P experiments – map combustor operability, global emissions
	Application of advanced diagnostics for comprehensive validation data sets	Application of advanced diagnostics for validation and combustor characterization
		Iterate burner/quick mix designs to achieve <25 ppm NOx, negligible NH3 slip

Motivation

- Hydrogen expected to play an important role in meeting U.S. net-zero 2050 goals
  - VRE
  - Reserve/peak power
  - Hard-to-electrify sectors (industrial decarbonization)
- Ammonia is an attractive hydrogen carrier due to favorable storage/ transport characteristics, existing industry, infrastructure
- H_2 to NH_3 must be worthwhile
  - Long distance transport
  - Long duration storage
- Direct utilization of NH_3 favorable vs. reconverting to H_2

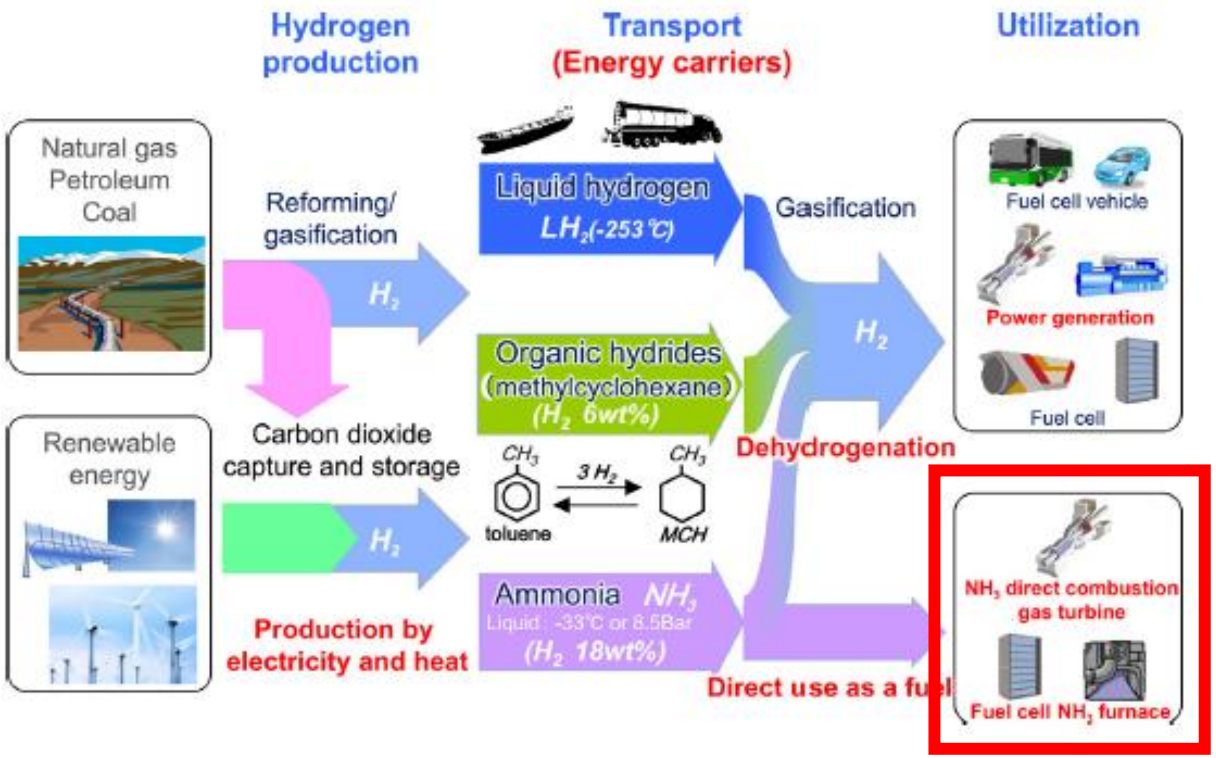
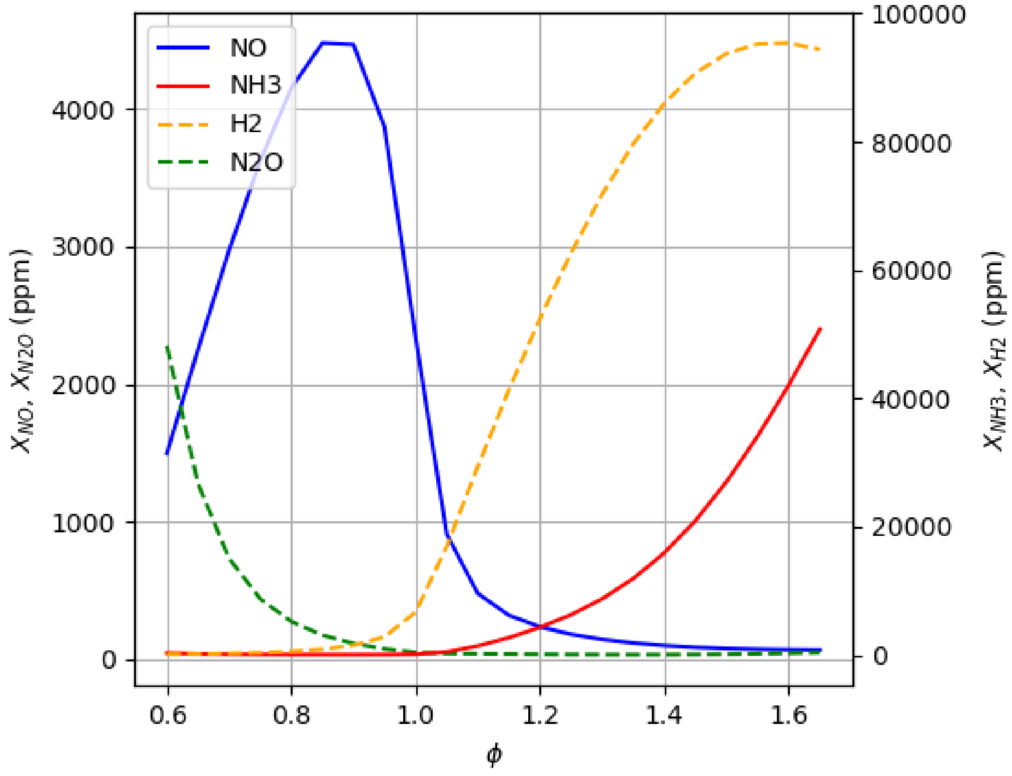


Figure from Kobayashi et al. "Science and technology of ammonia combustion", Proceedings of the Combustion Institute 37 (2019) 109–133

Combustion Characteristics of Ammonia

- Two largest technical challenges
  - Low flammability
  - High NOx (+N_2O) or unburnt NH_3
- Chemistry differs considerably from HC fuels – requires new strategies
- Two-stage RQL proposed for low emissions
- Requires models which make accurate predictions over a wide range of equivalence ratios and compositions



PSR simulation, Otomo 2017 mech, 300K/1atm, tres=50ms

Chemical Kinetics

- Numerous kinetic mechanisms available for ammonia
  - Some specific to NH_3-CH_4 or NH_3-H_2 mixes
- Requires complex N-chemistry
- Validated reduced mechanisms needed for CFD
- Improved validation data needed
  - Laminar flame speeds
  - Ignition delay times
  - Species concentrations

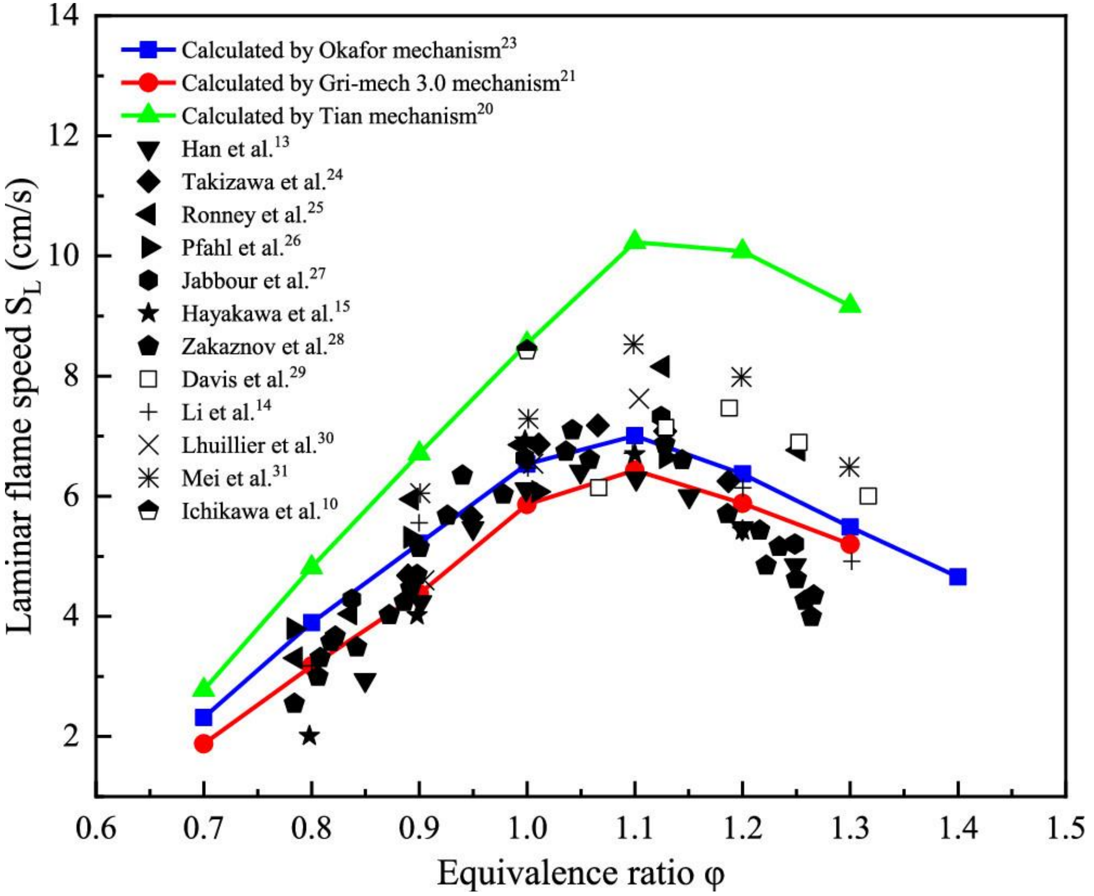
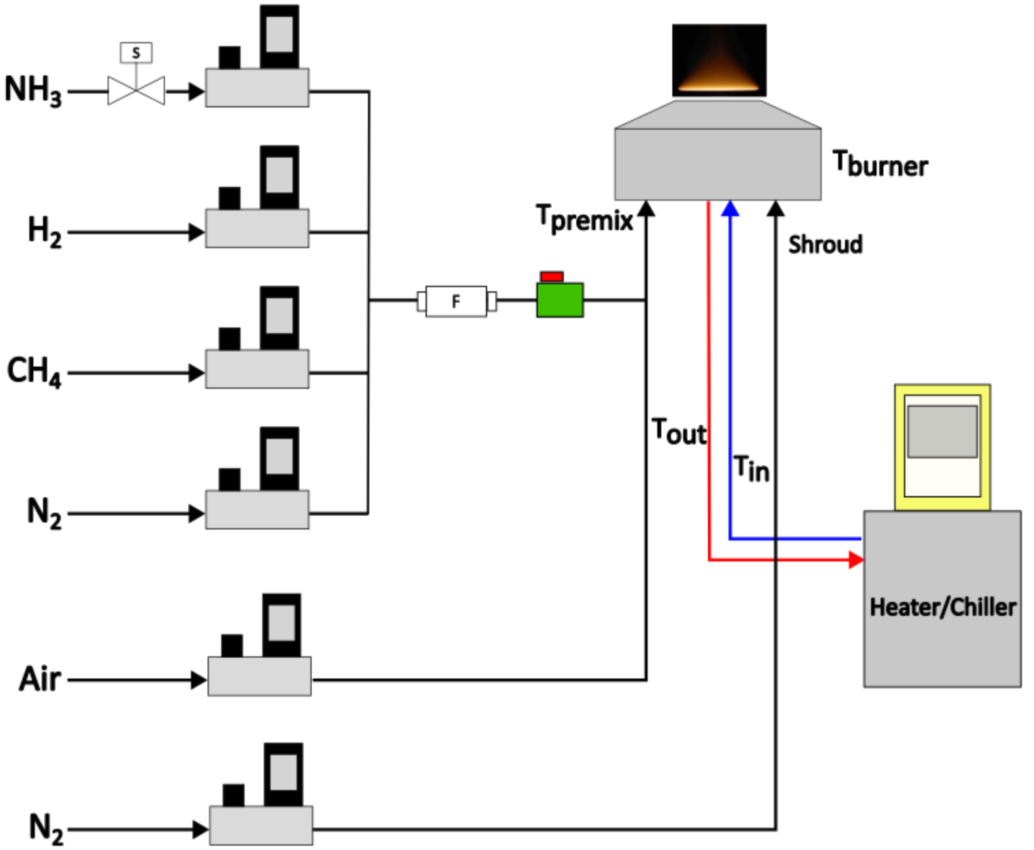


Figure: Zhang et al., “Effect of CH4, Pressure, and Initial Temperature on the Laminar Flame Speed of an NH3−Air Mixture”, ACS Omega 2021, 6, 18, 11857–11868

Experimental Setup

Laminar Flame Speed & Species

- Off-the-shelf stainless-steel McKenna burner
- UHP gases
  - Anhydrous NH3, vapor draw
- Alicat MFCs
  - Corrosive-compatible NH3
- Lauda circulating bath to regulate burner plug temp
- N_2 shroud



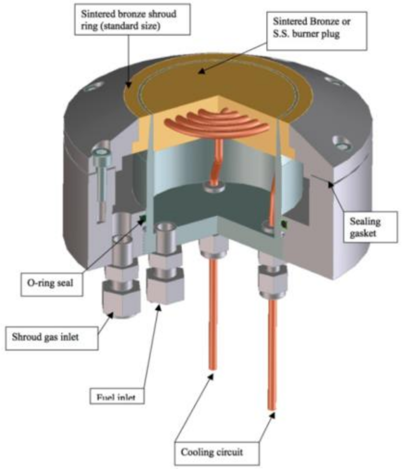
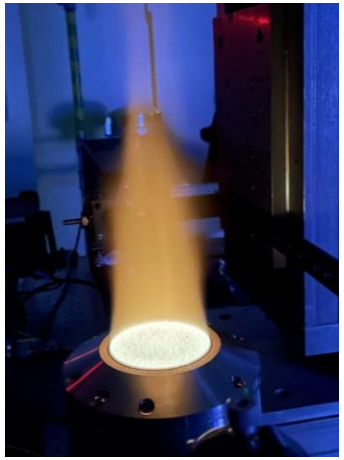


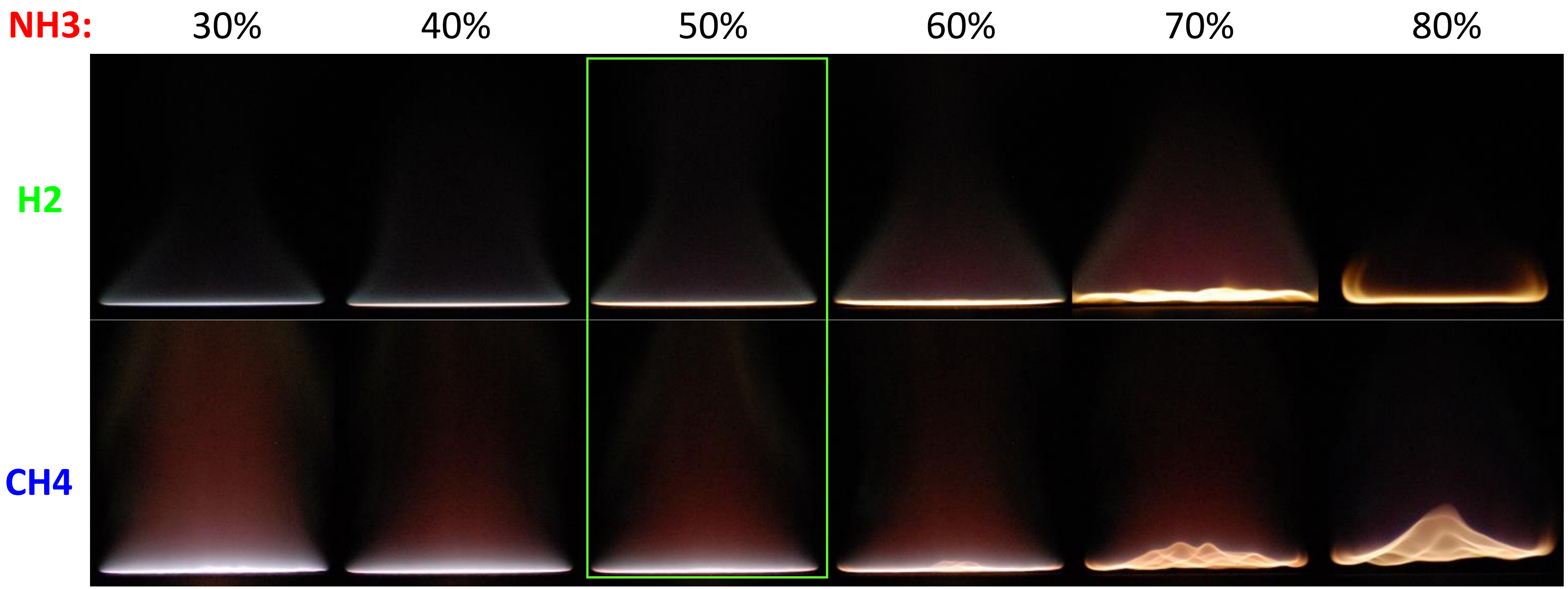
Image from Holthuis and Associates, flatflame.com



Flame Conditions

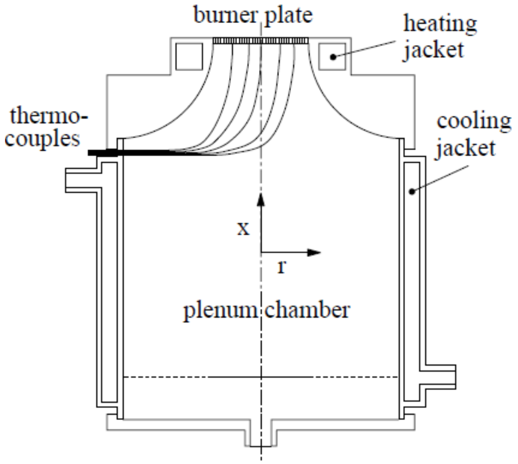
Laminar Flame Speed & Species

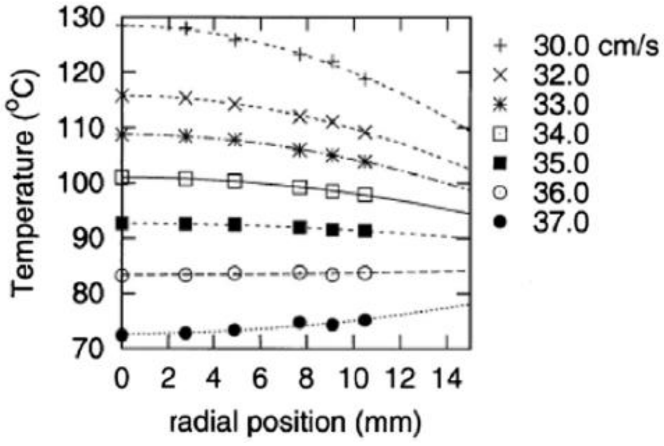
- Two flames selected for initial characterization



Diagnostic Approach for Laminar Flame Speed

- Burner heat flux method
  - Determine gas velocity which exactly opposes flame propagation speed
  - Heat added by burner plate equals flame heat loss
  - Adiabatic point = flat temperature profile
  - Requires measurement of burner face temperature profile
  - Interpolation vs. extrapolation
- Sources of uncertainty: flow controllers supplying gas, surface temperature measurement
- <u>Novel approach proposed to utilize IR imaging to derive complete 2D burner face temperature profile</u>





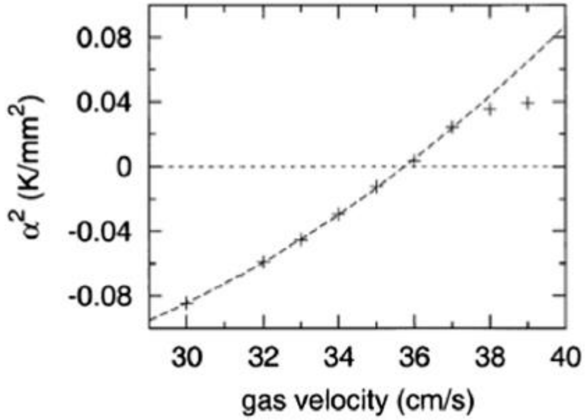


Figure from Bosschaart KJ, de Goey LPH. Detailed analysis of the heat flux method for measuring burning velocities. Combust Flame 2003;132:170e80.

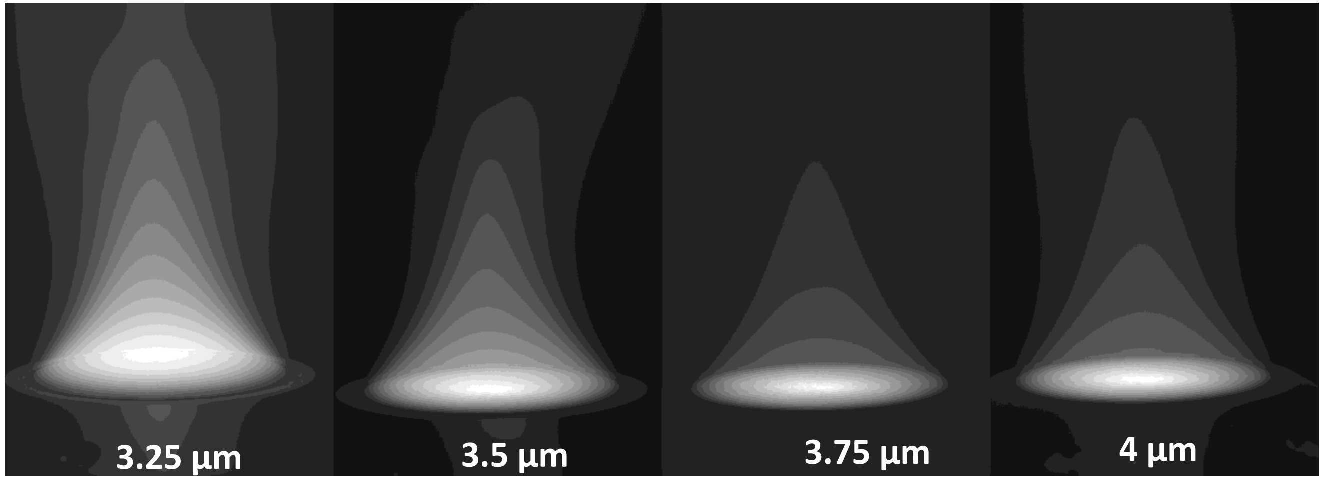
IR Imaging

- FLIR A8300SC IR camera
  - 3-5μm wavelength range
  - 50mm IR lens
- Can be calibrated via blackbody furnace for absolute measurements
- Nearly flat burner temperature profiles obtained without flame
- Minimal spatial emissivity effects
- Automated post-processing for perspective transform and corrections

Bedick, Clinton, Boyette, Wesley R., and Strakey, Peter, "Ammonia and Cracked Ammonia Laminar Flame Speed Measurements using the Burner Heat Flux Method and IR Thermometry", Presentation at the 2023 Clearwater Clean Energy Conference, Clearwater, FL, 2023.

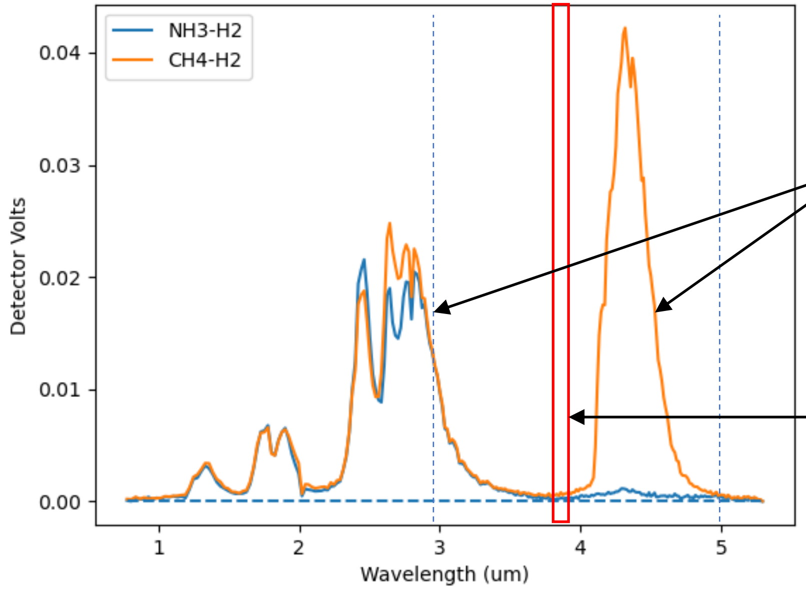
Flame Emission

- Flame emission is a major challenge
- Spectraline ES200 IR spectrometer used to determine optimal filtering strategies



Off-the-shelf 500nm FWHM filters

A8300sc range

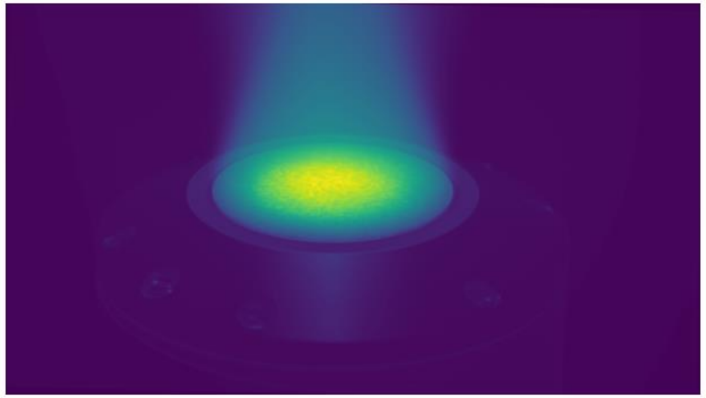


Must avoid wideband H2O and CO2 emission

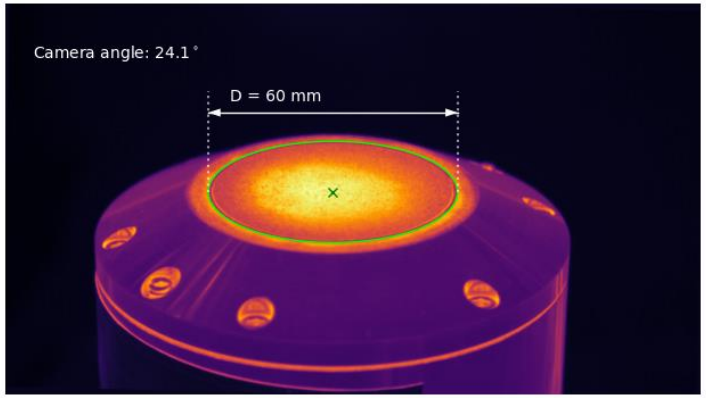
90nm FWHM filter selected at 3.9µm

Bedick, Clinton, Boyette, Wesley R., and Strakey, Peter, “Ammonia and Cracked Ammonia Laminar Flame Speed Measurements using the Burner Heat Flux Method and IR Thermometry”, Presentation at the 2023 Clearwater Clean Energy Conference, Clearwater, FL, 2023.

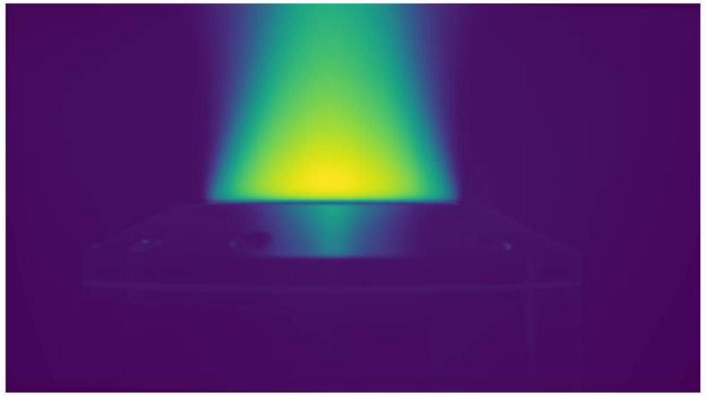
Image Post-Processing: Oblique and Side Views



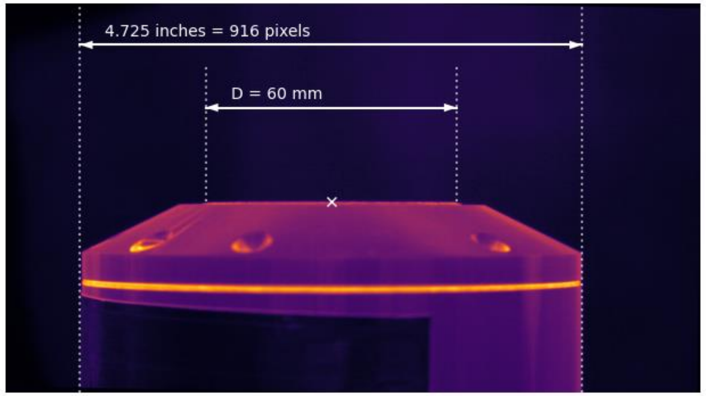
Oblique view: burner with emissions



Oblique view: burner only



Side view: emissions only

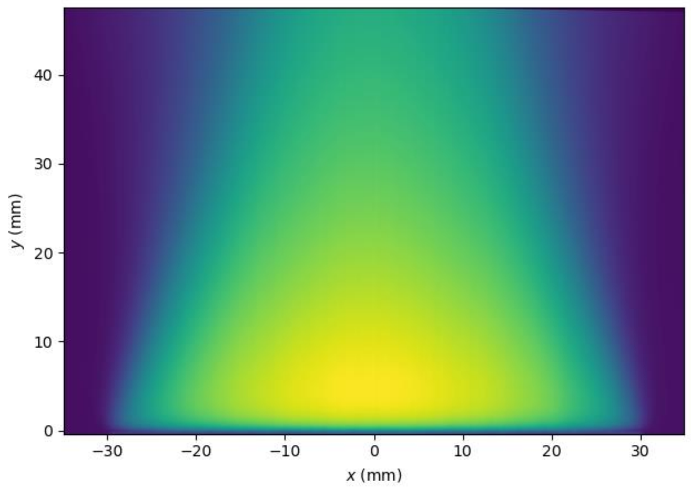


Side view: burner only

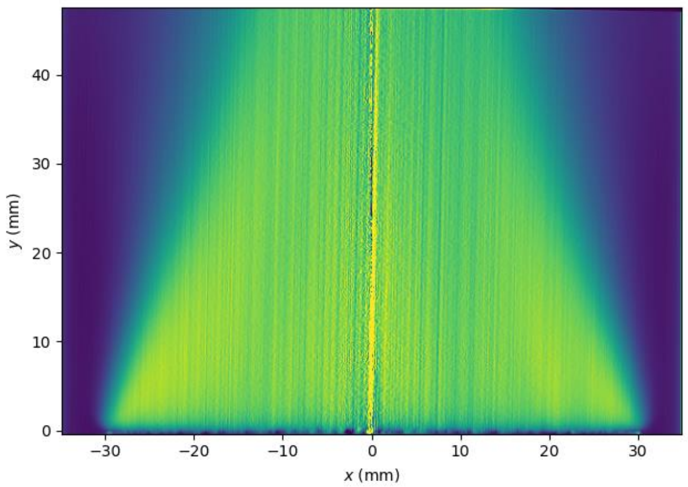
- Two orientations
  - Side view contains only emissions
  - Oblique view contains flame + burner emission
- Use side view to calculate line-of-sight emissions at any other camera angle
- Burner images for scaling, alignment, and calculation of camera angle

Bedick, Clinton, Boyette, Wesley R., and Strakey, Peter, "Ammonia and Cracked Ammonia Laminar Flame Speed Measurements using the Burner Heat Flux Method and IR Thermometry", Presentation at the 2023 Clearwater Clean Energy Conference, Clearwater, FL, 2023.

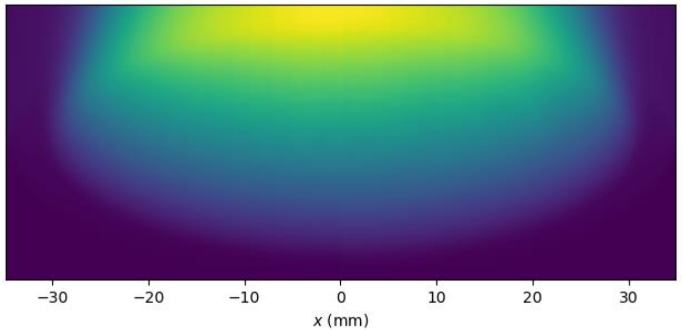
Image Post-Processing: Projected Flame Emissions



Mean side view emissions



Inverse abel transform



Projected emissions at required camera angle

- An inverse abel transform is applied to side-view emissions
- Abel transform used to create 3D flame emissions reconstruction
- Line-of-sight plane projection created from 3D emissions structure
- Verified at multiple angles
- Assumes negligible absorption effects

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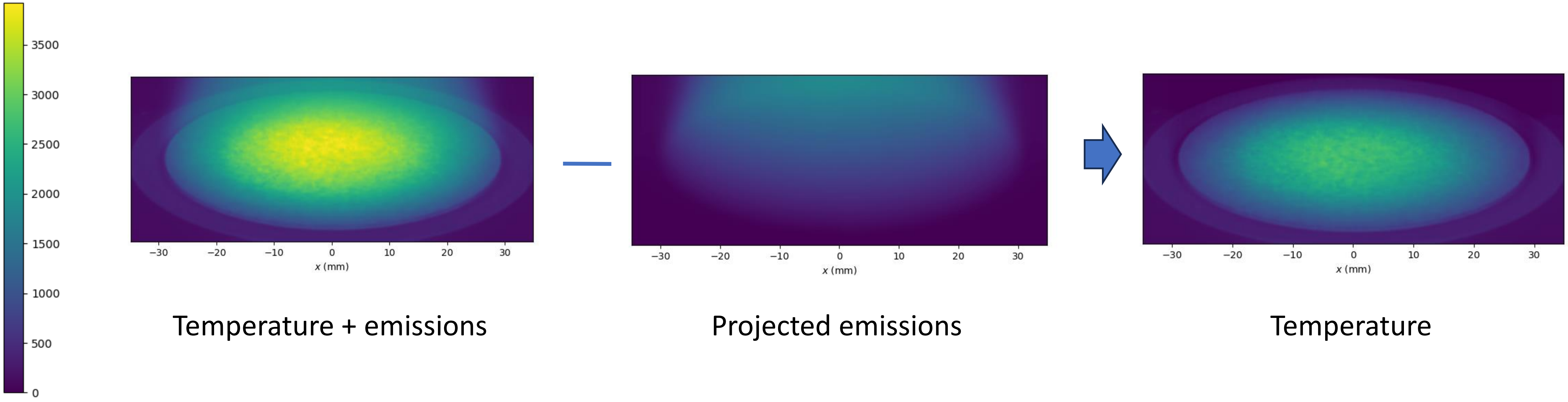
Image Post-Processing: Temperature Extraction

NATIONAL ENERGY TECHNOLOGY LABORATORY

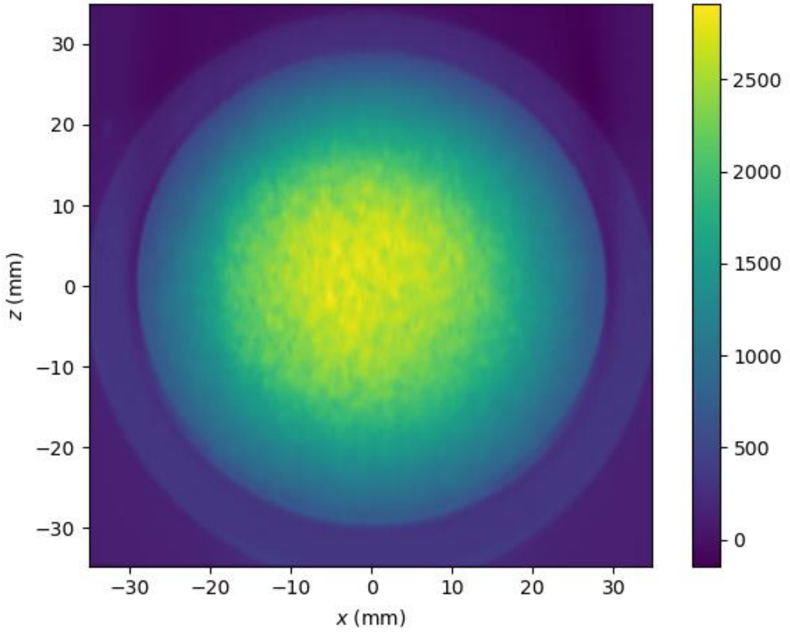


Temperature + emissions — Projected emissions → Temperature

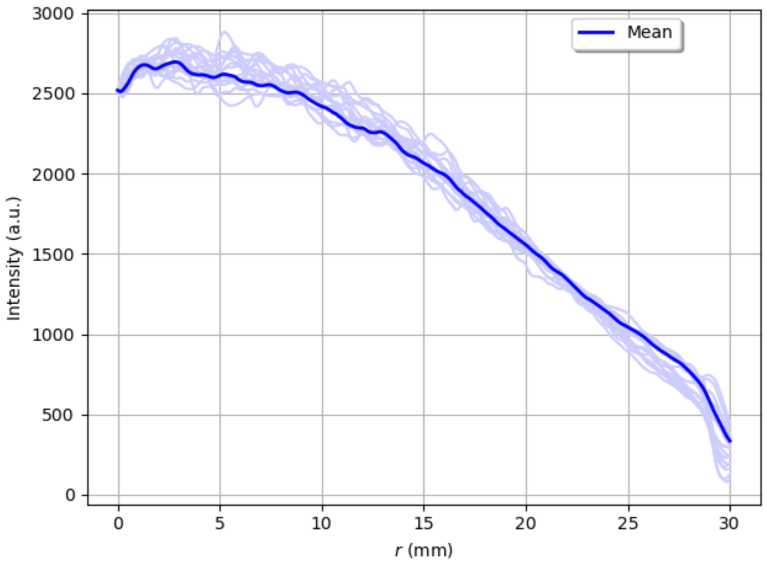
- Temperature + emissions from oblique view
- Projected emissions from side view
- Image subtraction results in temperature distribution (arbitrary units, future- absolute T calibration)

Image Post-Processing: Radial Temperature Profile

100% CH_4, Φ = 0.8, U = 22.1 cm/s



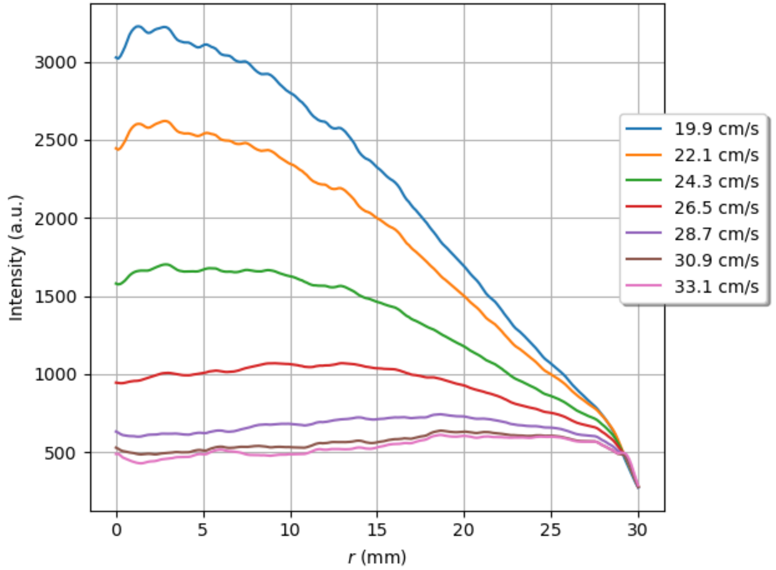
Transformed intensity (temperature)



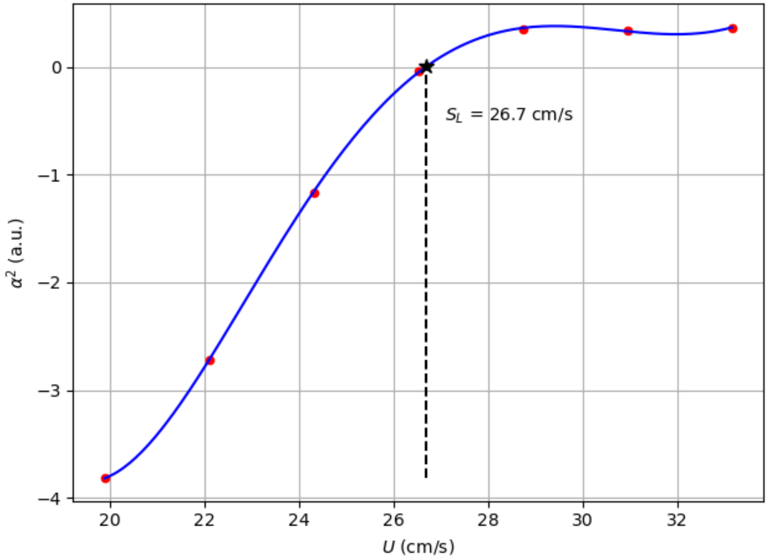
Radial intensity profiles

- Transformed intensity yields complete r-θ distribution
- Good top-bottom, left-right symmetry
- The mean of multiple profiles used for comparisons at different velocities

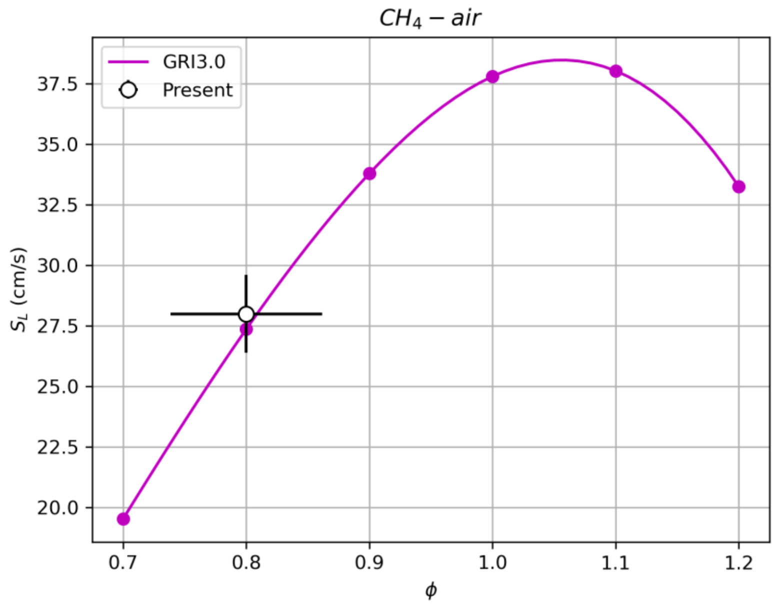
Image Post-Processing: 100% CH_4 Phi 0.8 Validation



Radial intensity profiles



Flame speed interpolation



Validation

- Mean radial profiles generated for multiple velocities
- Profiles fit to $\mathrm{I} = I_0 + \alpha^2 r^2$ for $r < 20$ mm
- $\alpha^2 = 0$, $U = S_L$
- Excellent agreement with prediction from GRI3.0 mechanism

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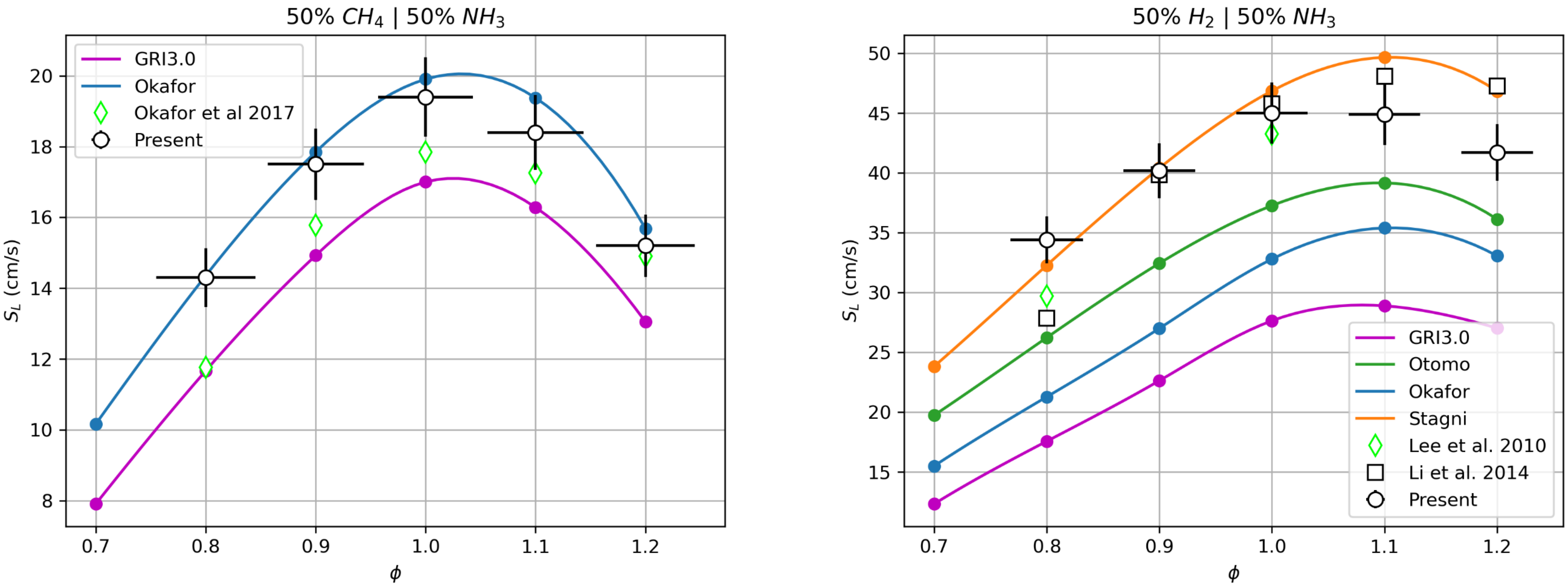
Results: NH_3-H_2 and NH_3-CH_4 mixes



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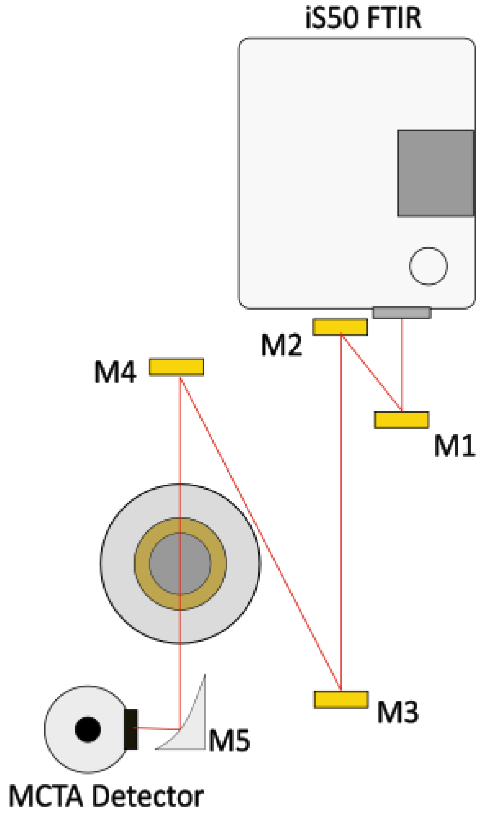
Diagnostic Approach for Species Concentrations

- Absorption spectroscopy used to measure post-flame species concentrations
  - Thermo-Fisher Nicolet iS50 FTIR spectrometer
  - External bean routing
  - LN2-cooled MCTA detector
- Enables wide spectral range, good SNR – at the expense of some resolution
  - 0.125 cm^{-1} resolution (0.015 cm^{-1} data spacing)
  - Happ-Genzel apodization function considered during lineshape fitting
- All measurements made 12 mm from burner surface
- Beam size ~2-5 mm through flame

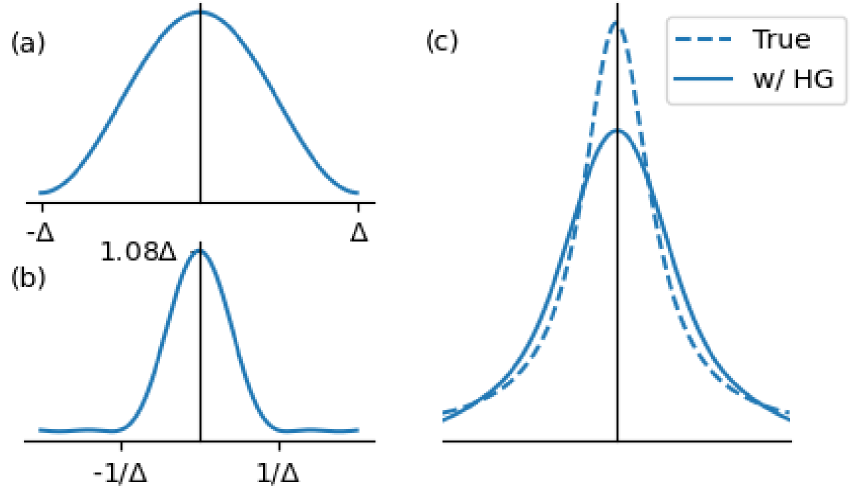


Lineshape Model

- Formulation follows past works in the literature
  - Beer-Lambert law
  - Voigt lineshape model w/ collisional/doppler broadening, pressure shift
  - HITEMP/HITRAN data
- Multi-spectral fitting routine via Python using Levenberg-Marquardt method
  - N-strongest lines considered
- Incorporates convolution of analytical Happ-Genzel apodization function, $a(v)$ (Δ=1/0.125cm^{-1})

$$\left(\frac{I_t}{I_0}\right)_v = exp\left[-S_j(T)\varphi_{v,j}(v,T,P)N_k l\right]$$

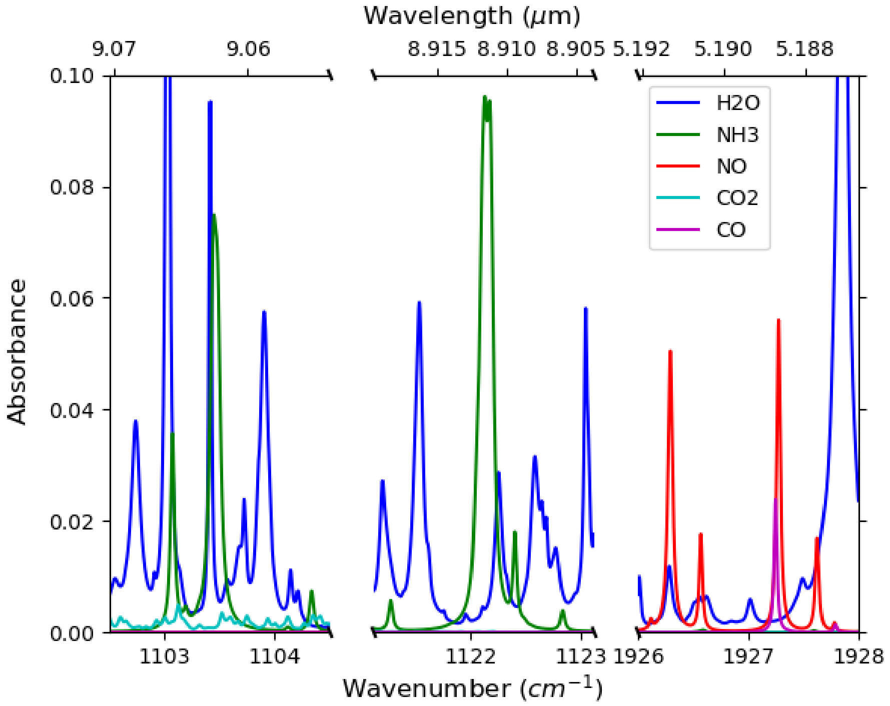
$$a(v) = \frac{0.54}{\pi v} + 0.46 \cdot \frac{4\pi v\Delta^2}{\pi^2 - (2\pi v\Delta)^2} \sin 2\pi v\Delta$$



Clinton Bedick, Andrew Tulgestke, Wesley Boyette, “In-situ species concentration measurements in ammonia-mix flames using FTIR spectroscopy”, ASME Turbo Expo, 2024.

Wavelength Selection

- <u>Primary species of interest: NO and NH_3</u>
- Overlapping H_2O a major challenge – but opportunity for H_2O thermometry
- Precedents in literature (most QCL/ICL laser-based):
  - NO – near 5.2 µm (v_1 fundamental band), exhaust/flue gas applications, lineshape measurements, Hanson/Goldenstein/others
  - NH_3 – near 1.6 µm OR ~9-10 µm (v_2 band), lineshape measurements, human breath, SCR applications, Farooq/Hanson/Peterson/others
  - H_2O – plenty of sources, ~2.5 µm from past thermometry experience



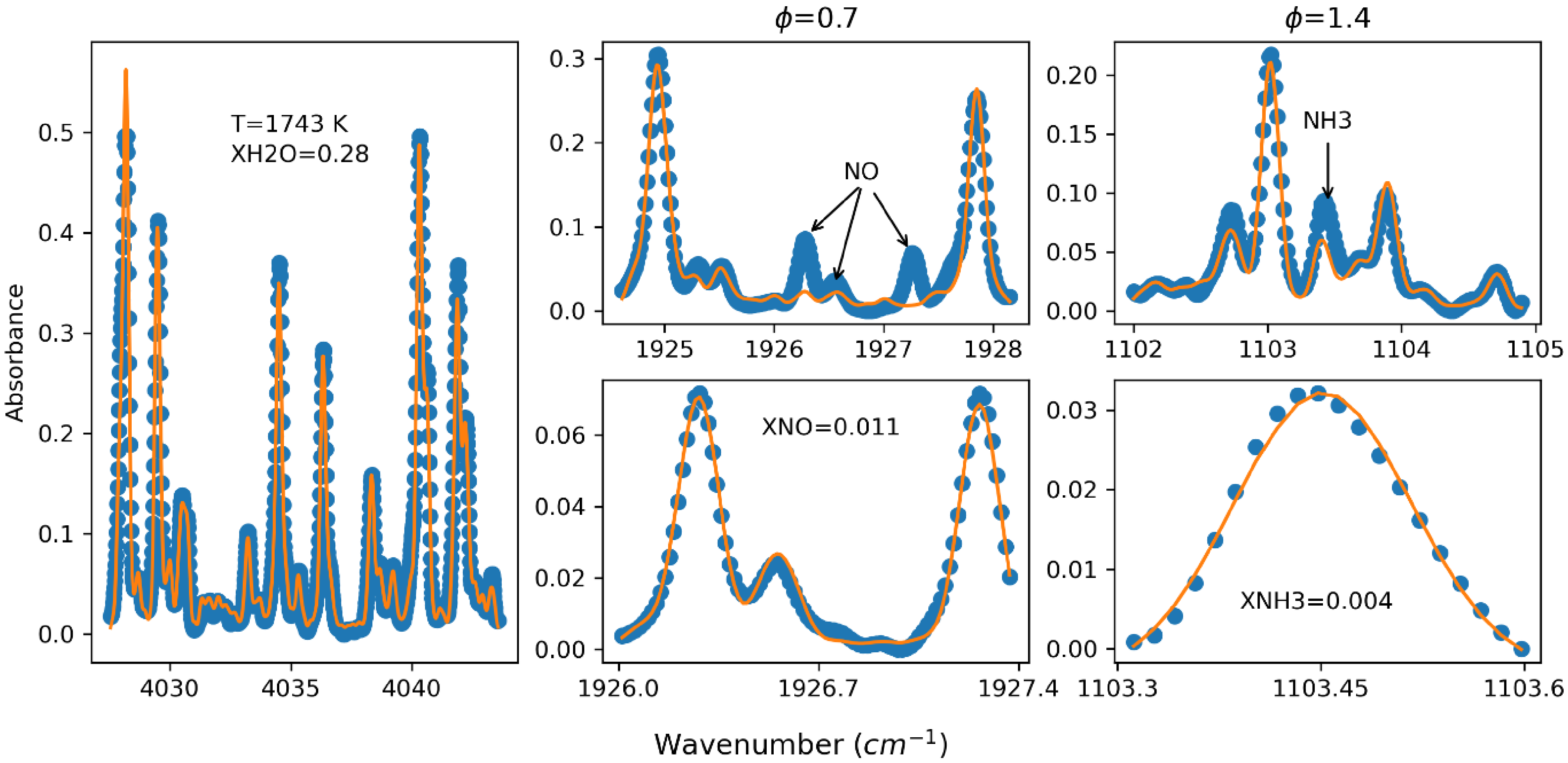
(2) Options for NH_3
- ~1103 cm^{-1}
- ~1122 cm^{-1}

~1926-1927.5 cm^{-1} for NO - (3) main features
- CO overlap near 1927.6 cm^{-1}

Clinton Bedick, Andrew Tulgestke, Wesley Boyette, “In-situ species concentration measurements in ammonia-mix flames using FTIR spectroscopy”, ASME Turbo Expo, 2024.

Example: Lineshape Fitting

50-50 NH_3-H_2



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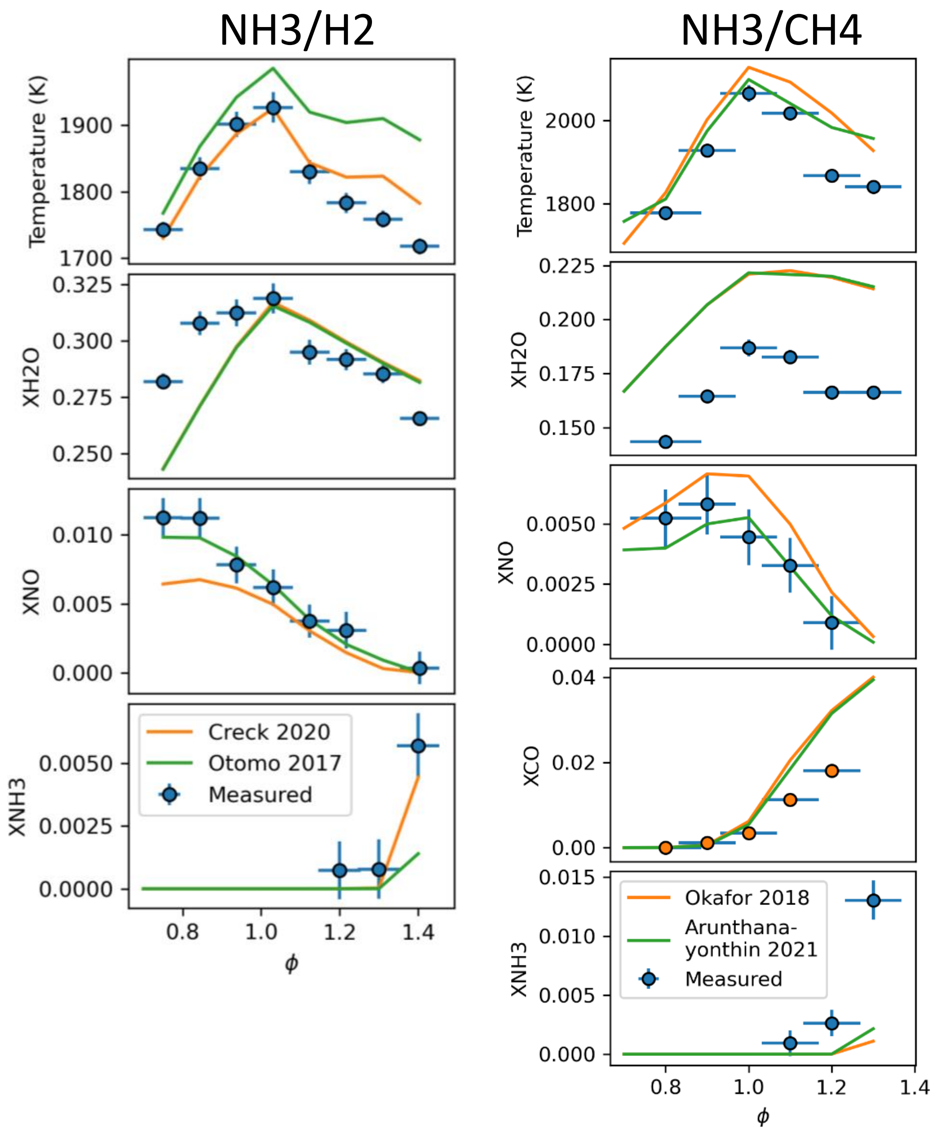
Results

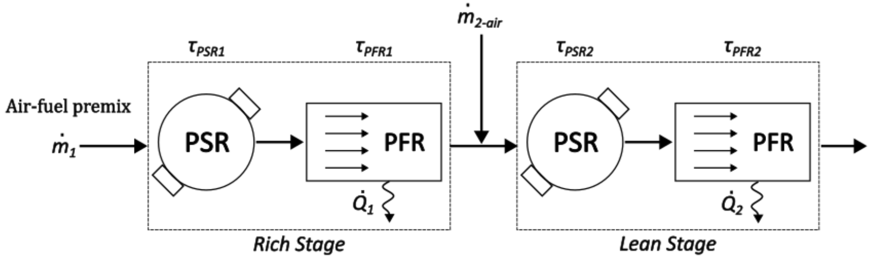
- Equivalence ratios swept from 0.7-1.4
- 25 C burner temperature
- Results compared to Cantera burner-stabilized flame simulations
  - Required due to heat-loss stabilized flames generated by McKenna burner
- Data only reported for SNR>5

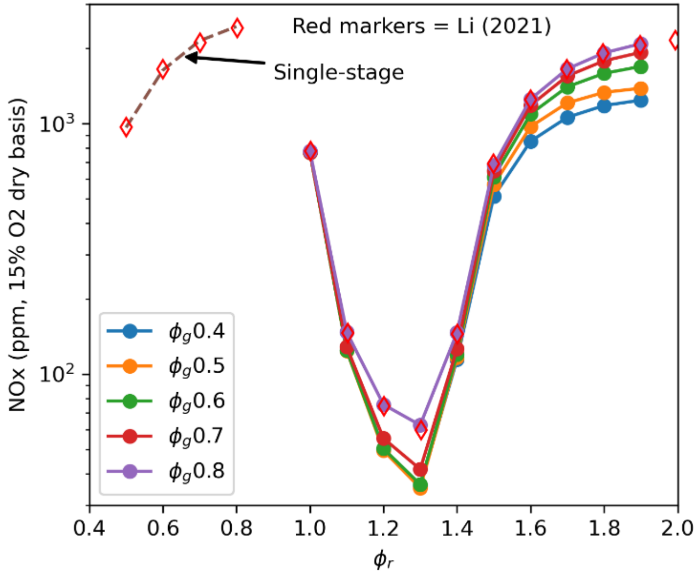


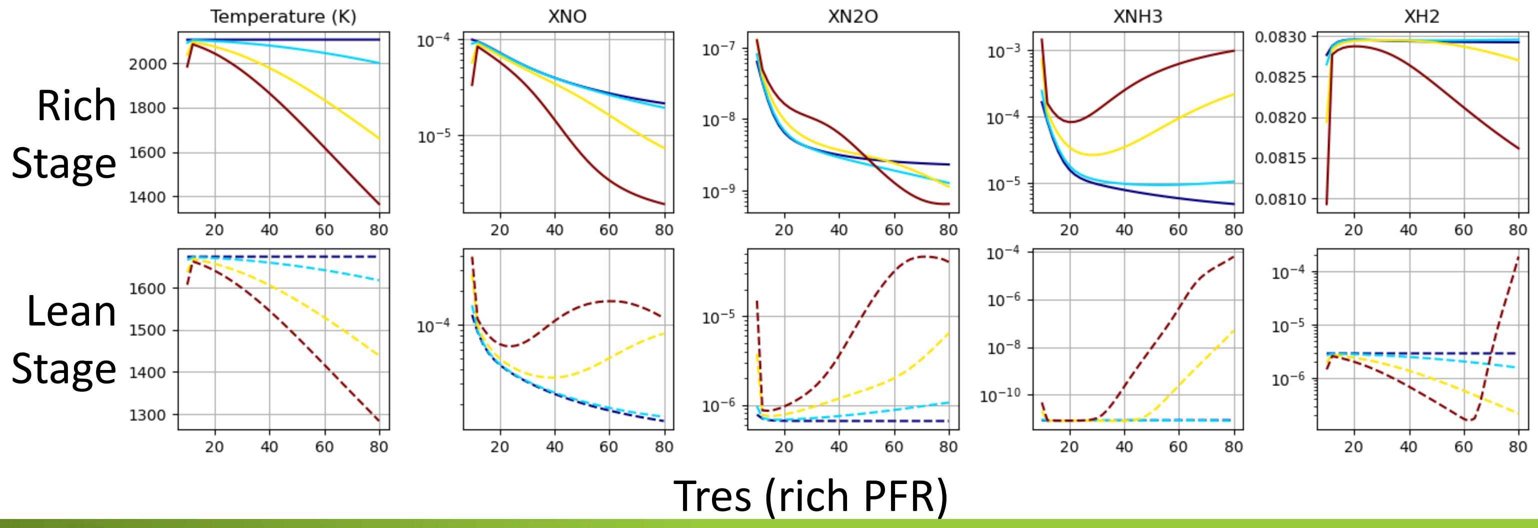
Y-error bars consider shot noise, fitting uncertainties, x-error bars consider MFC uncertainties (~10-20% total)

Chemical Reactor Network Modeling

- Custom CRN models developed in Python/Cantera
- Used to understand practical Rich-Quench-Lean (RQL) approaches
- Impacts of heat loss considered – important during rich relaxation phase

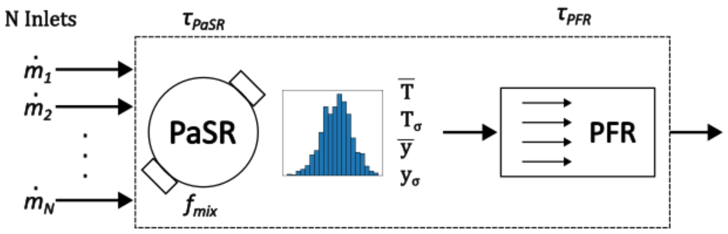






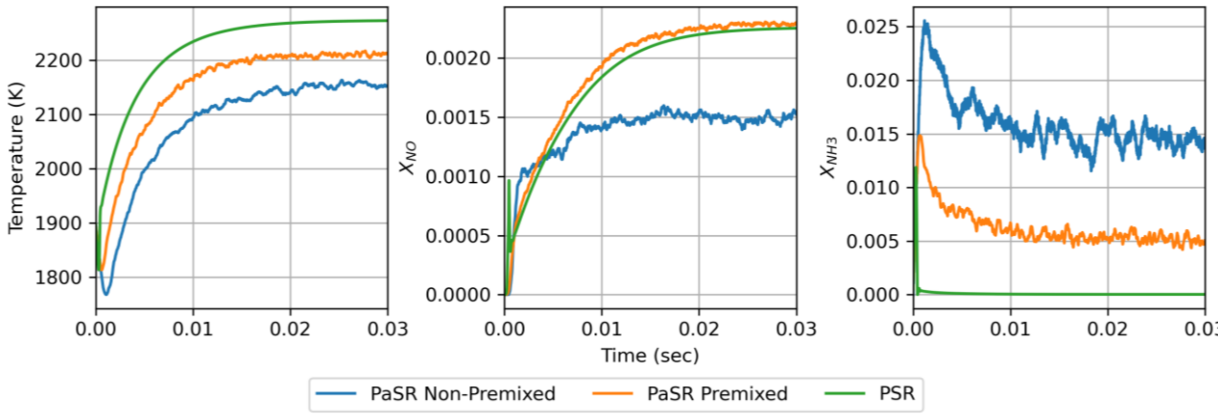
Chemical Reactor Network Modeling

- Models extended to consider impacts of mixing via Partially-Stirred-Reactor (PaSR) model
  - Reduce computational expense vs. Chemkin via use of pyjac and parallelization
- Allows consideration of non-premixed operation
- Primary interest – understanding impacts of mixing in lean burn phase



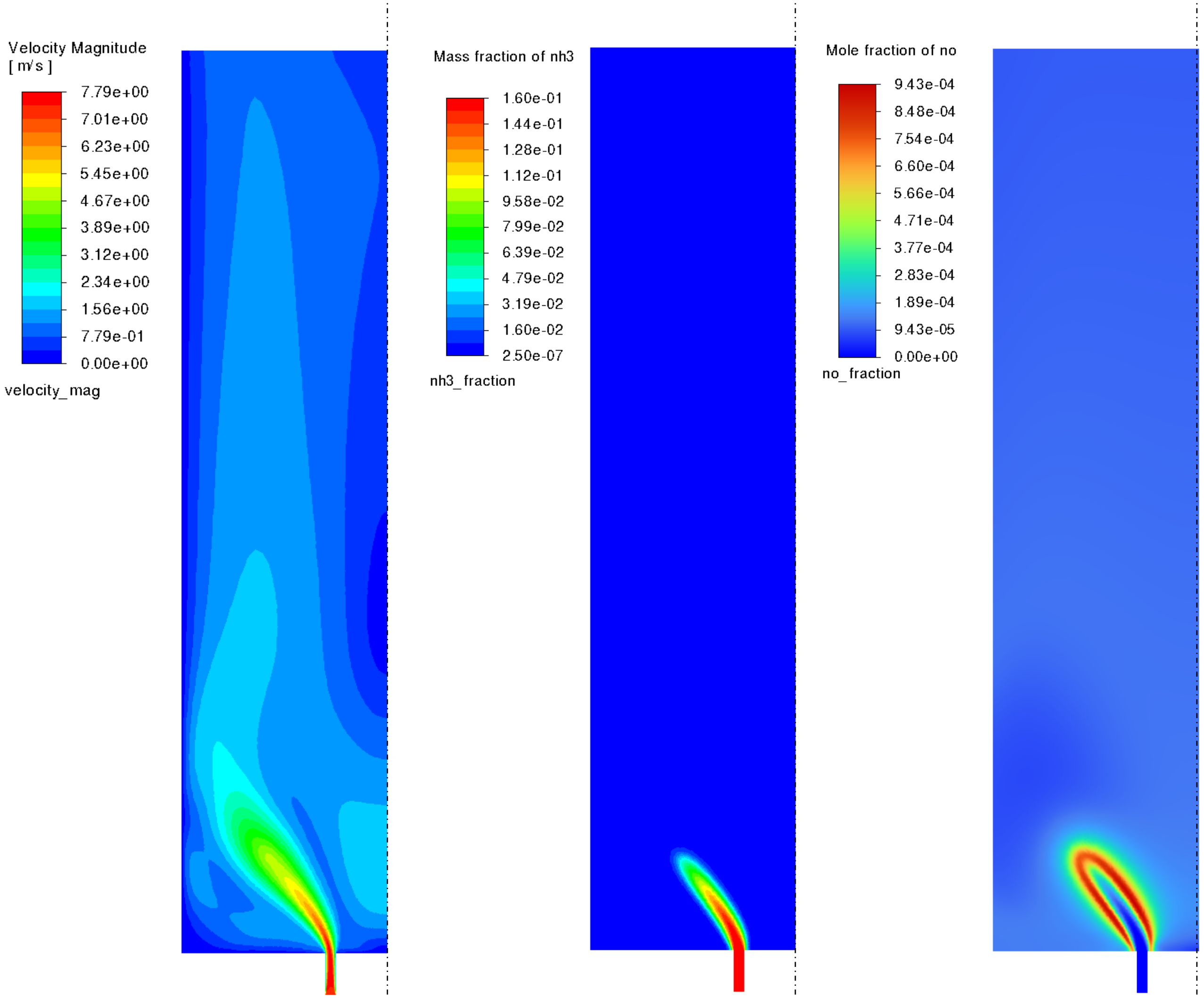
(top) Generic gas turbine combustor configuration with PaSR

(bottom) Example temperature, NO, and NH3 results for NH3/air combustion using the PaSR model w/ intermediate mixing (fmix=1E4 1/s), for premixed and non-premixed operation, compared to perfectly-mixed (PSR) case; results illustrate higher unburnt NH3 for finite mixing cases



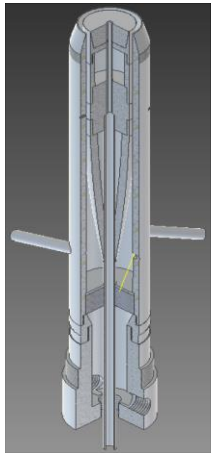
CFD Modeling

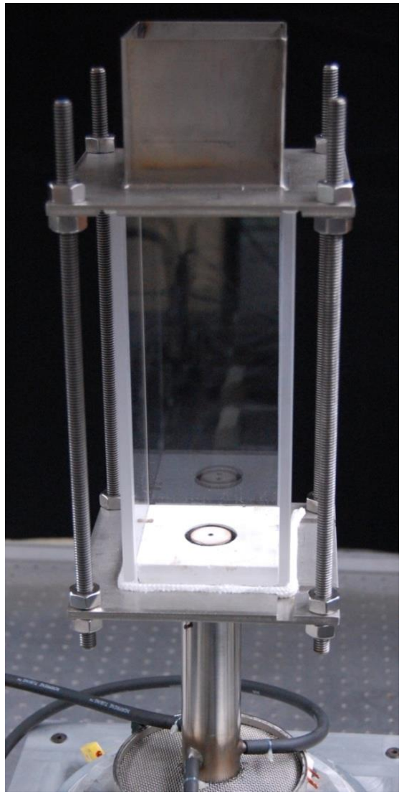
- Engineering-level modeling of various burner configurations
  - Inform burner and RQL designs for upcoming applied studies
- OpenFOAM and Fluent
- Collaboration with Argonne National Lab for additional modeling support

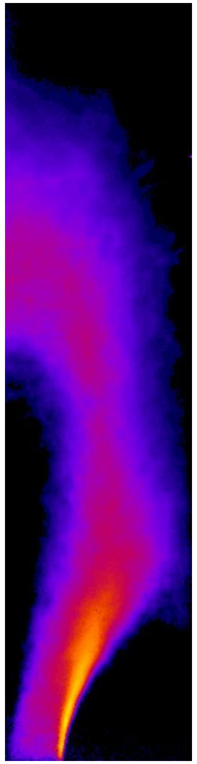


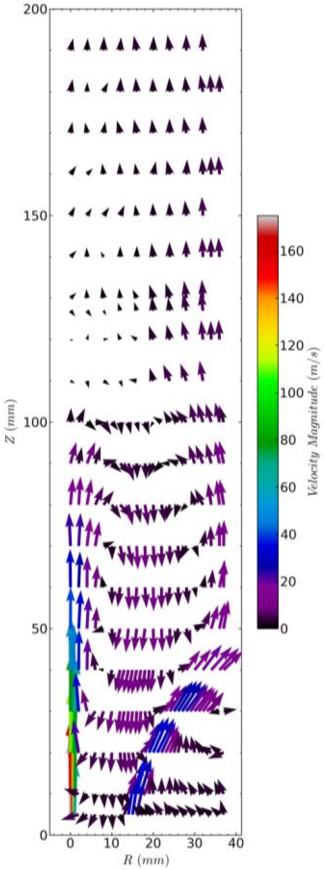
Applied Testing

- Leverage existing burner platform to study swirl-stabilized NH3 flames
  - Premixed operation
- Repeat prior measurements done for CH4 and H2
  - Stability mapping
  - Global emissions(FTIR) - NO/NO2/N2O/NH3/H2O
  - PLIF/PIV/LDV
  - Thermal BCs
- Modify burner for RQL operation (in progress)
  - Baseline secondary air ring



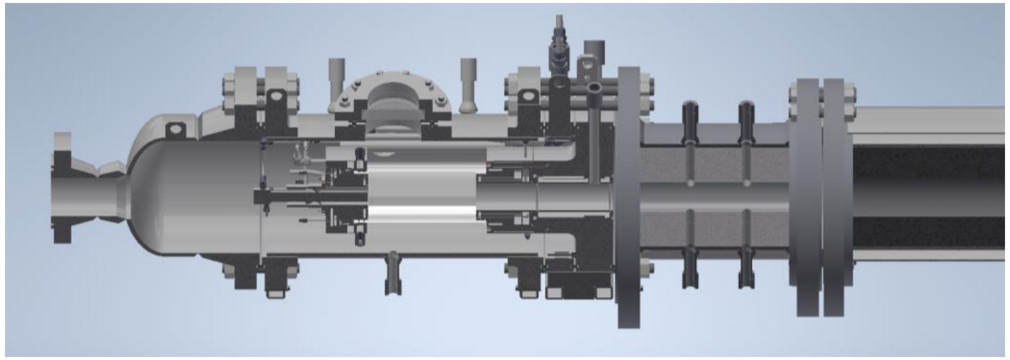






High Pressure Developments

- Adding H_2 & NH_3 capabilities to existing NETL PPC rig (1MWth, 10 atm)
- Development of high T&P storage/delivery system underway
  - 150 lb liquid-draw anhydrous cylinder
  - Piston-pump accumulators
  - Off-the-shelf electric vaporizer (~80kW)
- Will provide ~30 min run time at full power
- Combustor mods for RQL
  - NG (current) and NH_3 (when available)



NETL RESOURCES

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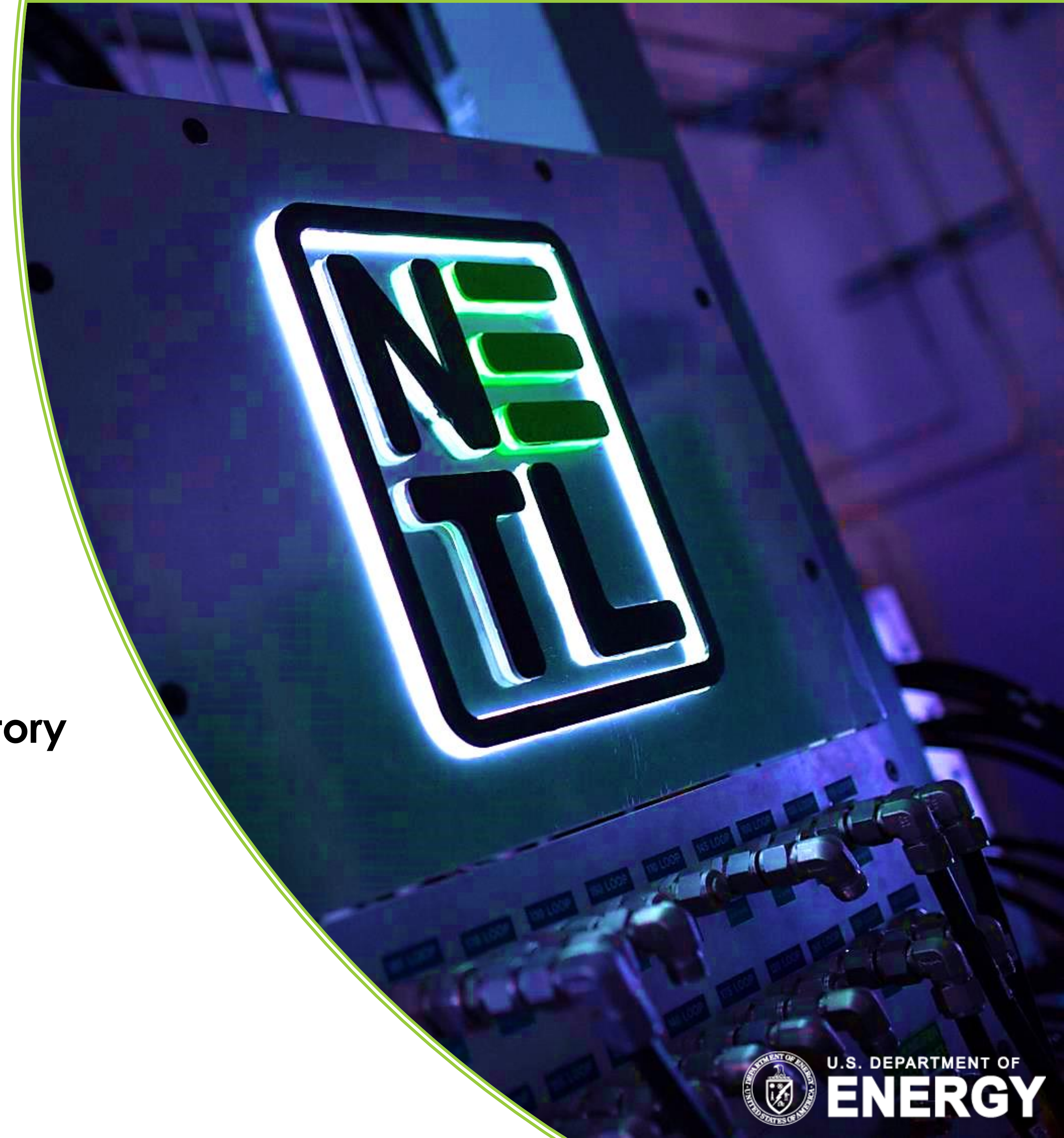
Dr. Clinton Bedick
Clinton.Bedick@netl.doe.gov



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