Status of Ammonia Combustion Research at NETL

Ammonia Combustion Working Group
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Research and Innovation Center

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Ammonia Combustion

1. **Fundamental combustion lab capabilities**
2. **Initial flame characterization**
3. **Modeling**
   1. 1D flame models
   2. CRN models
4. **Diagnostics**
   1. Laminar flame speed via heat-flux method
   2. Species profiles, temperature via FTIR
   3. Hyperspectral imaging and UV/VIS spectrometer
5. **Future research activities and interests**

Approach: Generate novel data sets for model validation and combustion strategy development

Fundamental Combustion Lab Capabilities

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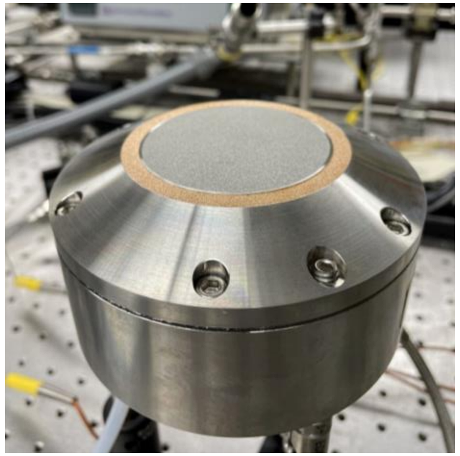
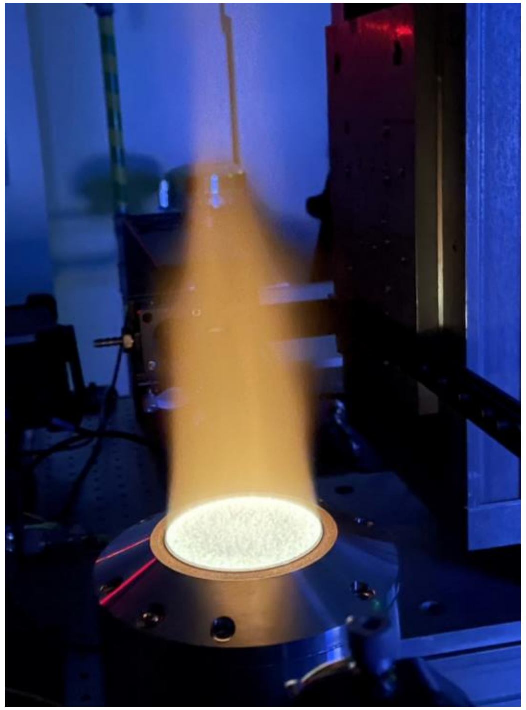
- **Operational since ~May 2022**
- **NH3 added to lab**
  - New NH_3 gas monitor
  - 100lb vapor draw anhydrous ammonia cylinder @ ~115 psig
  - Compatible Alicat flow controller
  - Premixed, flat-flame burner
- **Lab capabilities:**
  - NH_3, $NH_3/H_2(+N_2)$, NH_3/CH_4 mixes
  - Ability to heat air ahead of premixing (250C)
  - Ability to operate at elevated oxygen levels (21% to 100%)



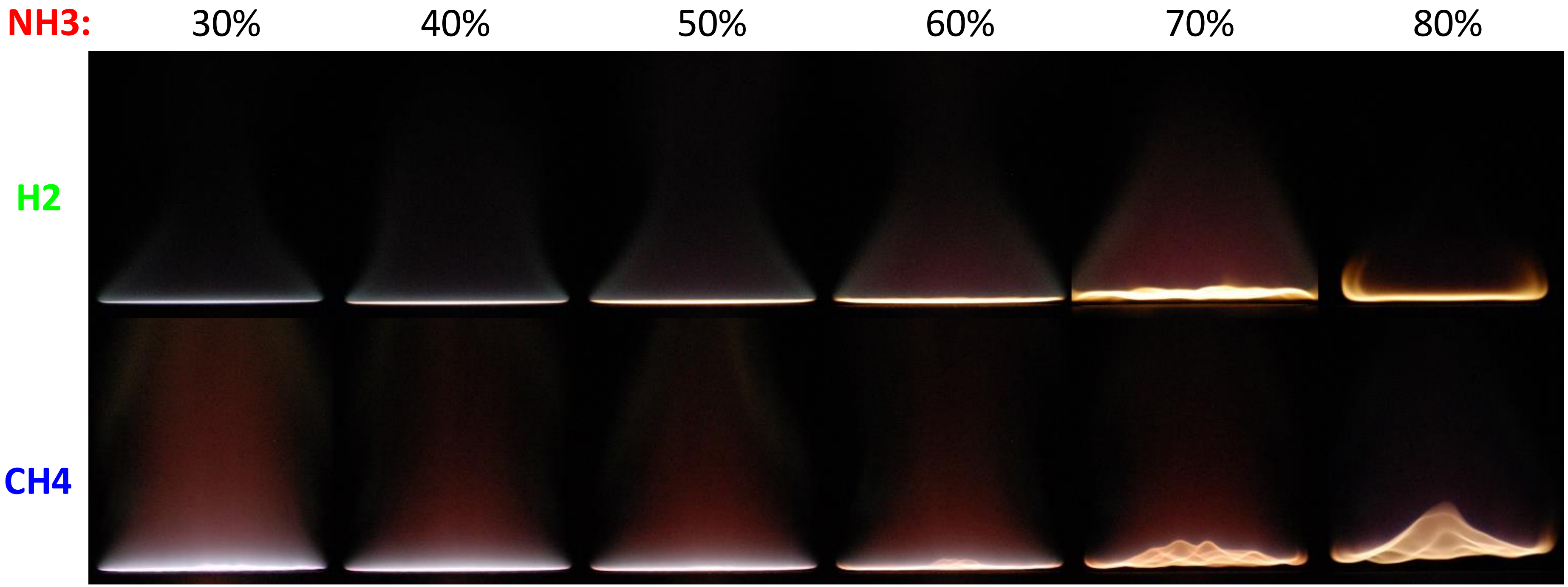
McKenna stainless steel flat flame burner (60mm)



NH_3/H_2 flame in NETL PGH FCL

Initial Flame Characterization

- Flames generated for NH_3/H_2 and NH_3/CH_4 mixes
- Stability limits evaluated qualitatively (total flow, NH_3 fraction)



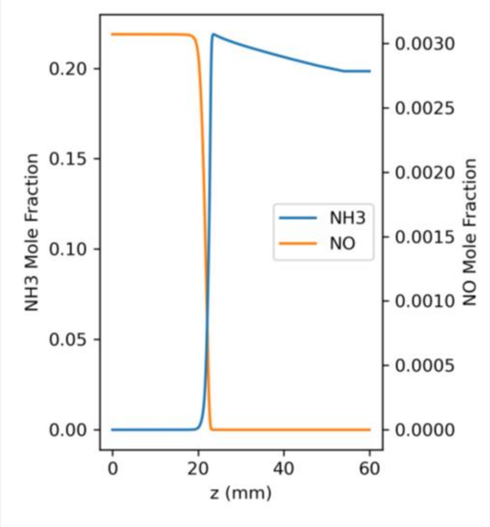
Ammonia Combustion Modeling

Accelerating development of viable ammonia combustion technologies

Model Validation

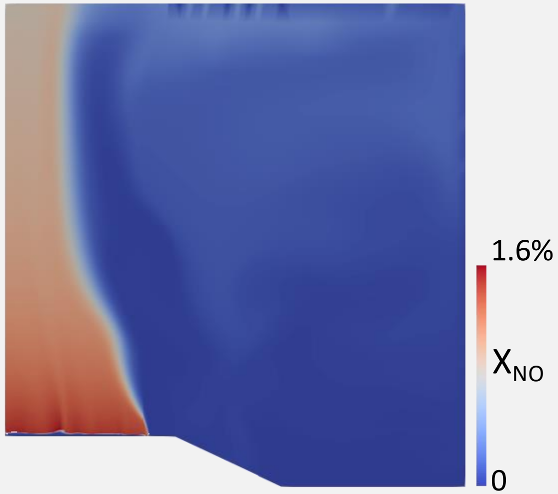
1D Flames

- Cantera flame models
- Flame speed, mechanism comparisons



2D CFD

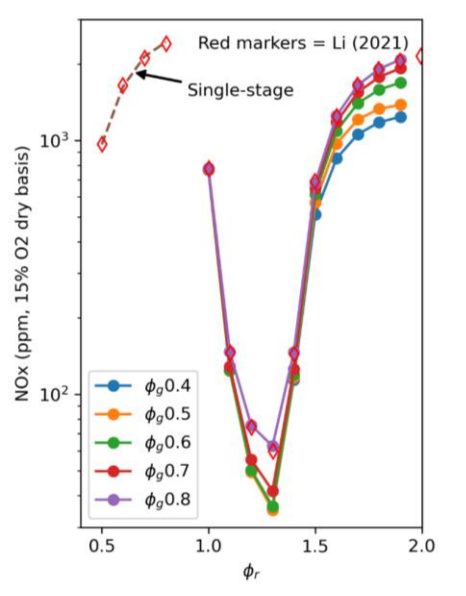
- OpenFOAM axis-symmetric
- Temperature/species profile comparisons



Combustion Strategy Development

CRN Models

- PSR-PFR, 2-stage rich-lean
- Identify candidate configurations



3D CFD

- Identify combustor configurations for experimental development/characterization

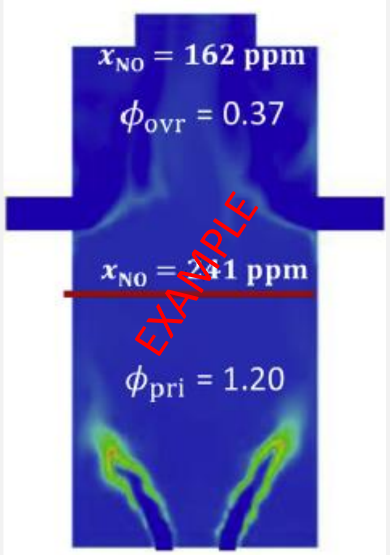


Image from https://doi.org/10.1016/j.ijhydene.2017.09.089

Evaluation of Chemical Kinetic Models

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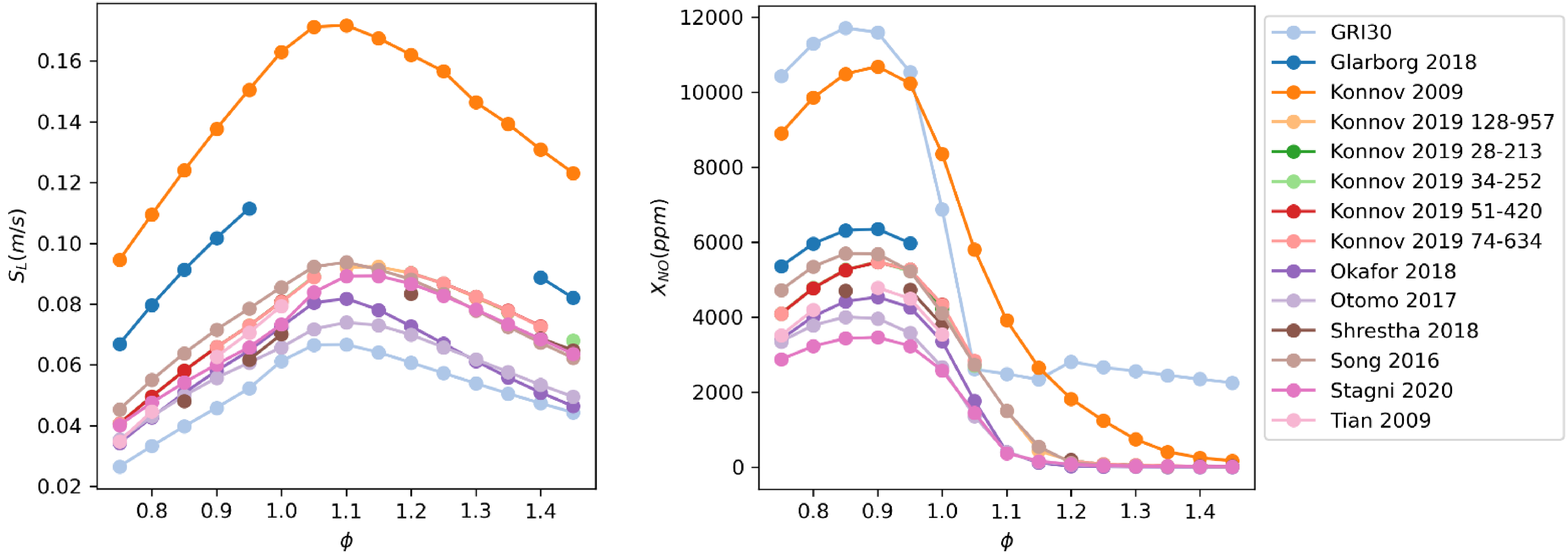
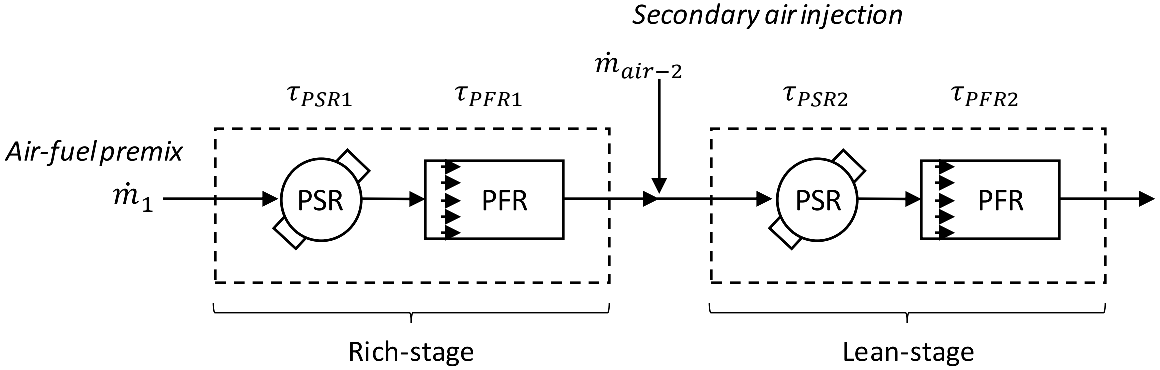
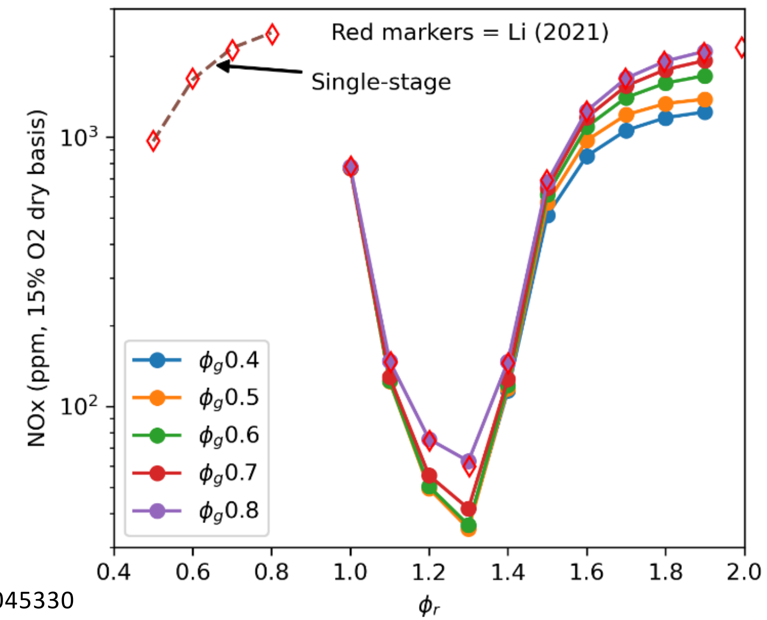


Figure from: Bedick et al IJECE
10.1615/InterJEnerCleanEnv.2023045330

CRN Models

- **Useful to understand how to develop practical combustor configurations**
- **Developed in Cantera**
  - PSR-PFR to represent flame and post-flame zones
  - Two-stage approach w/ secondary air injection
    - Rich stage: low NOx, high NH_3-H_2 conversion
    - Lean stage: H_2, remaining NH_3 burnout, minimal fuel-N based NOx
  - Compared to Chemkin/literature results





Figures from: Bedick et al IJECE 10.1615/InterJEnerCleanEnv.2023045330

Diagnostics

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- **Laminar flame speed: fundamental parameter related to chemical kinetics**
- **Substantial variability among mechanisms, experimental data**
- **Methods include Bunsen, combustion bomb, <u>heat flux</u>, velocimetry**

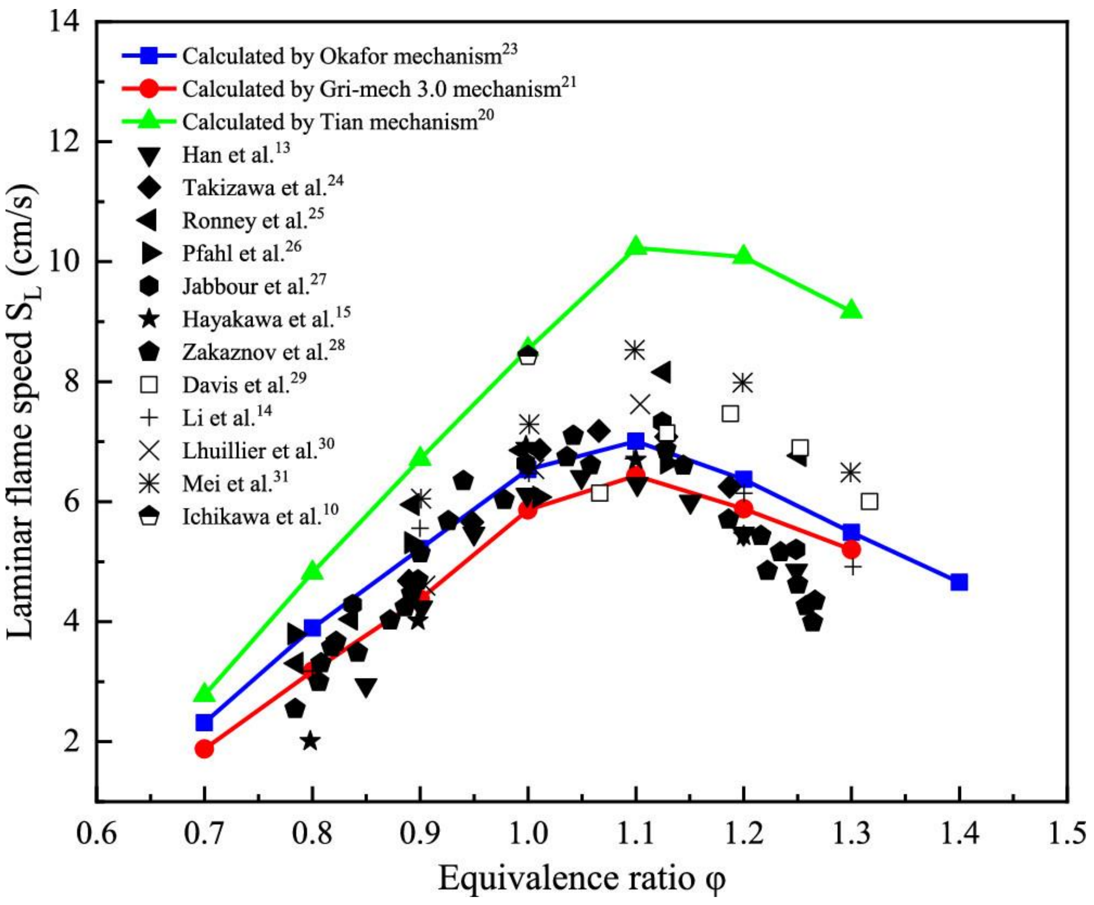

Figure from: Zhang et al ACS Omega 2021, 6, 18, 11857–11868

Diagnostics

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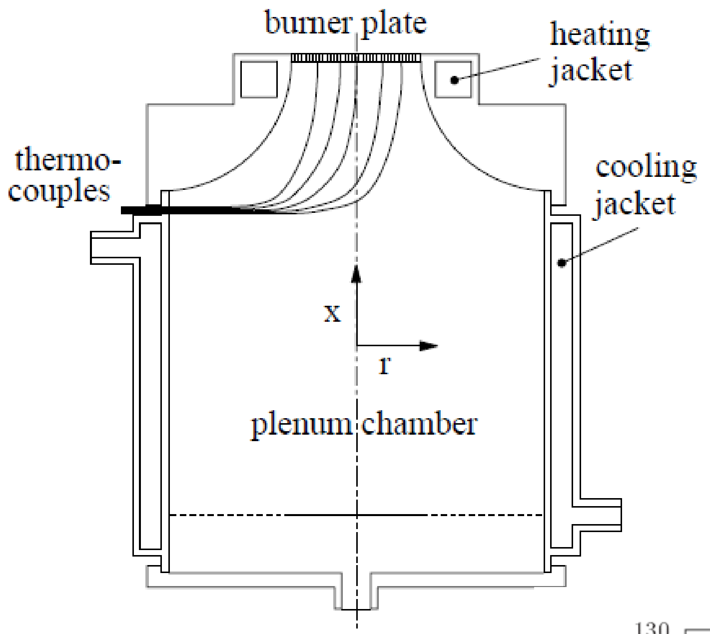
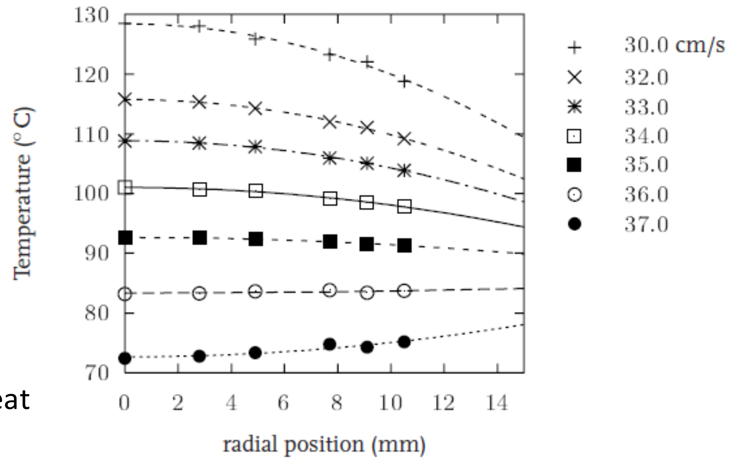
- **Burner heat flux method:**
  - Determine gas velocity where flame is not heating burner and burner is not heating gases (i.e. adiabatic point)
  - Requires measurement of burner face temperature profile
  - IR thermometry provides direct measurement of surface temp.

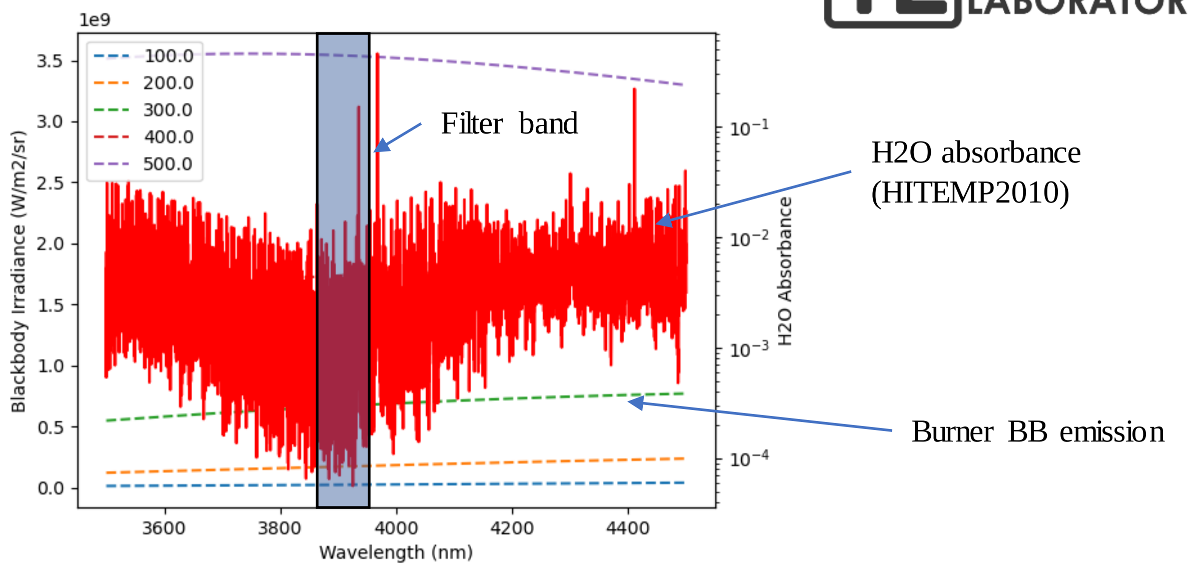


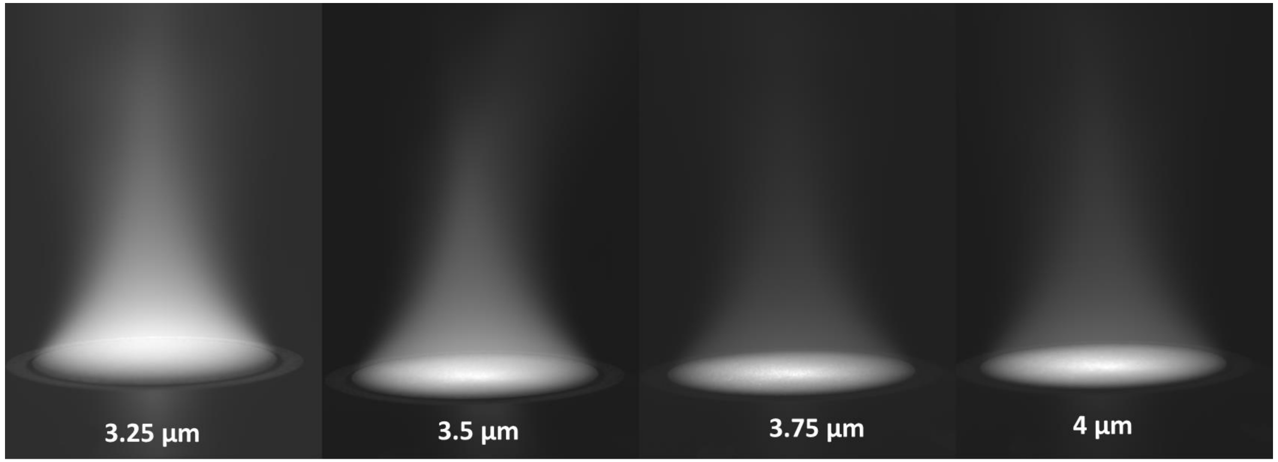


Images from: Bosschaart, Karel J., “Analysis of the heat flux method for measuring burning velocities”, Eindhoven : Technische Universiteit Eindhoven, .

Diagnostics

- **Burner face temperature thermometry:**
  - FLIR A8303sc camera (3-5µm)
- **Flame emission impacts ability to image burner emission**
  - Eliminated/reduced via filtering and post-processing corrections
  - Off-the-shelf 500nm FWHM filters provided some improvement
  - Custom 3900 nm narrow-band filter recently acquired for further reductions
- **Relative difference between burner and flame emission helps – heated via silicone oil**





Diagnostics

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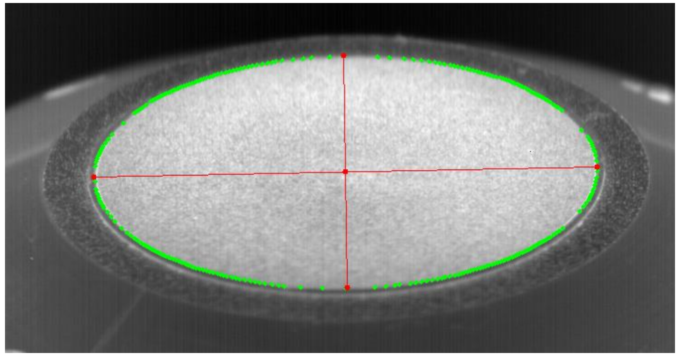
- **Image processing via Python**
  - Perspective correction
  - Nonlinear correction for I to T and surface emissivity
  - T-profile fitting:

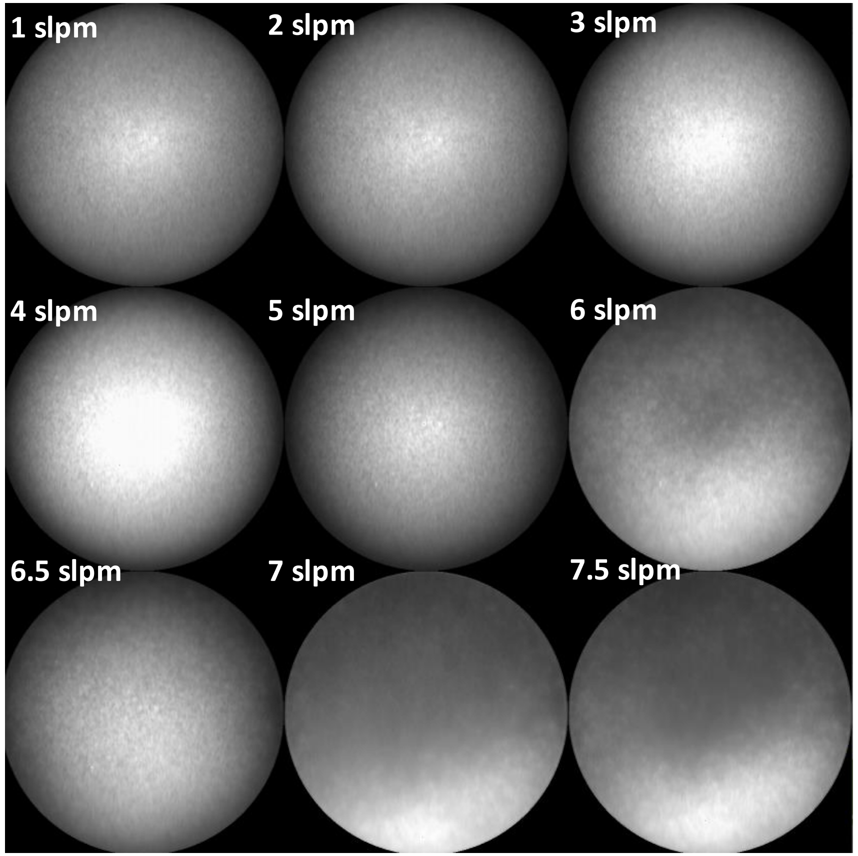
$$T(r) = T_{center}(1 - ar^2)$$

- **Interpolation of parabolic coefficient (a) vs. flow rate determines laminar flame speed**

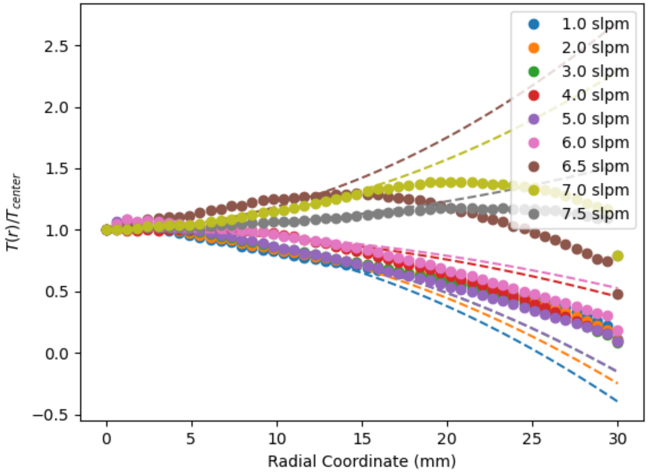
Automated burner detection and transform calculation



Corrected top-down images vs. flow rate



T-profile fitting example



Diagnostics

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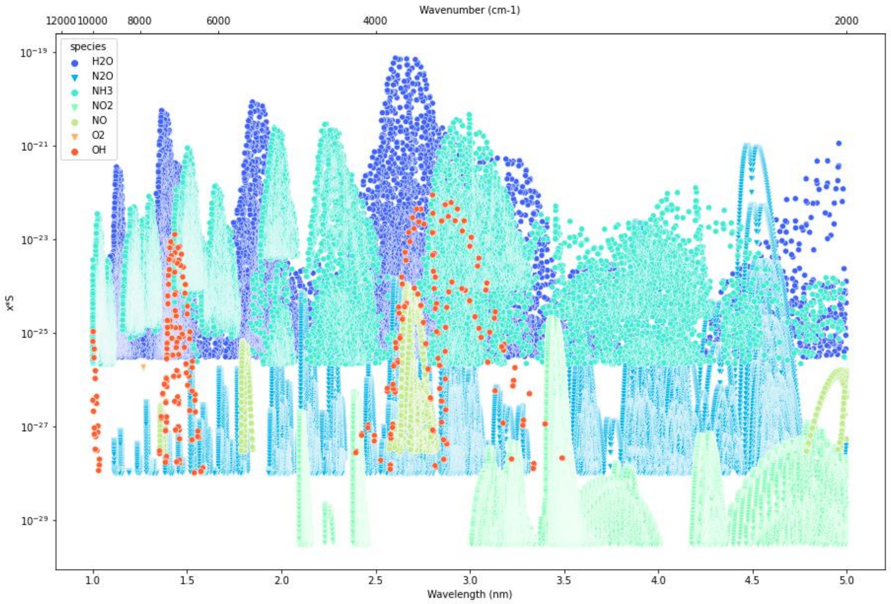
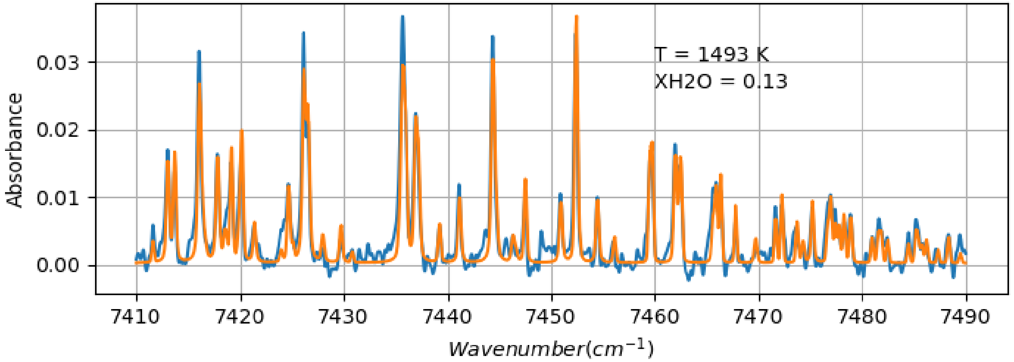
- **Detailed species data very limited in literature**
- **Of interest: NH_3, $NO/NO_2/N_2O$, H_2O, (CO/CO_2 if CH4 mix), NH, NH_2, OH (and T)**
- **FTIR spectrometer for quantitative NH3, NOx species, H2O, and T**
  - External beam passed through flame
  - Burner translated to vary measurement location
  - Abel inversion to extract centerline values
  - Lineshape fitting to determine absolute concentrations
- **Leverage new HTP gas cell for lineshape data generation as needed**
  - TDLs for future applications





Future Work – bench scale

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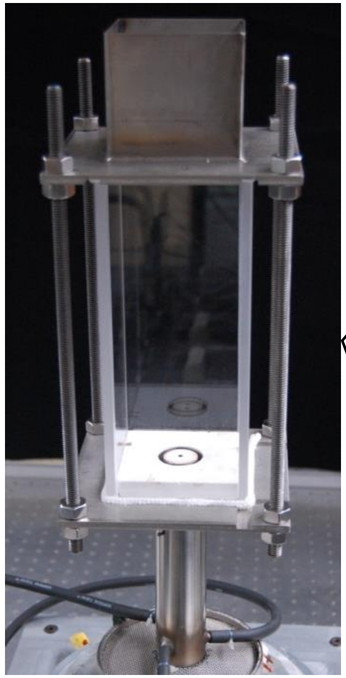
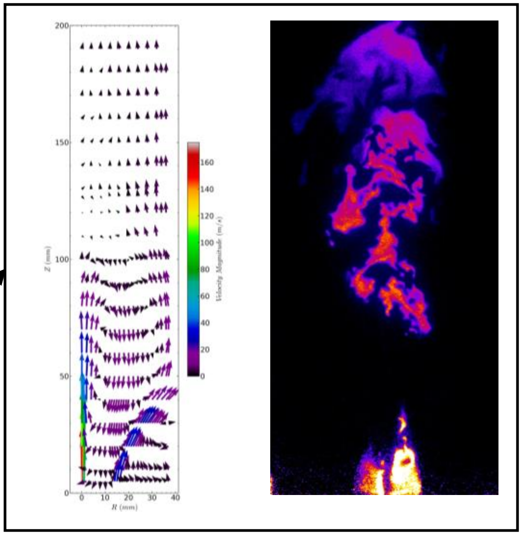
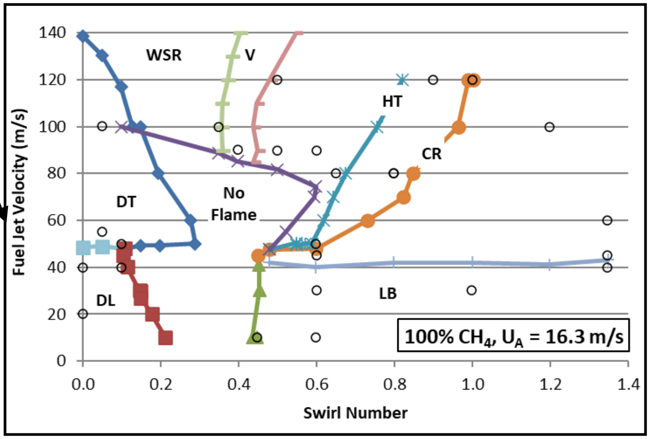
- **Reformer considerations (2023)**
  - Characterize flame speeds, emissions characteristics for reformer exit comps.
- **Model combustor development and characterization (2024)**
  - Leverage existing optically accessible burner platforms, modified for ammonia
  - RQL approaches
  - Informed by 3D CFD
  - Global emissions sampling
  - Additional diagnostics (existing: OH-PLIF, PIV/LDV, new: NO-PLIF)
- **Additional interests- Non-thermal plasma for stability enhancement, NOx control**



Example model gas turbine combustor from past CH_4/H_2 work at NETL (a)



Advanced LDV/OH-PLIF diagnostics (left-b, right-a)



Global emissions/stability (c)

Future Work – increased scale

- **Interests include atmospheric pressure industrial furnaces and high pressure gas turbine combustion**
- **New furnace test facility being considered at NETL MGN for ~2024+**
- **Leverage existing ~MW high pressure (10-30 atm) combustion facilities at NETL MGN, adapted for NH_3**
  - Requires liquid NH_3 storage, vaporization, delivery

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Questions?