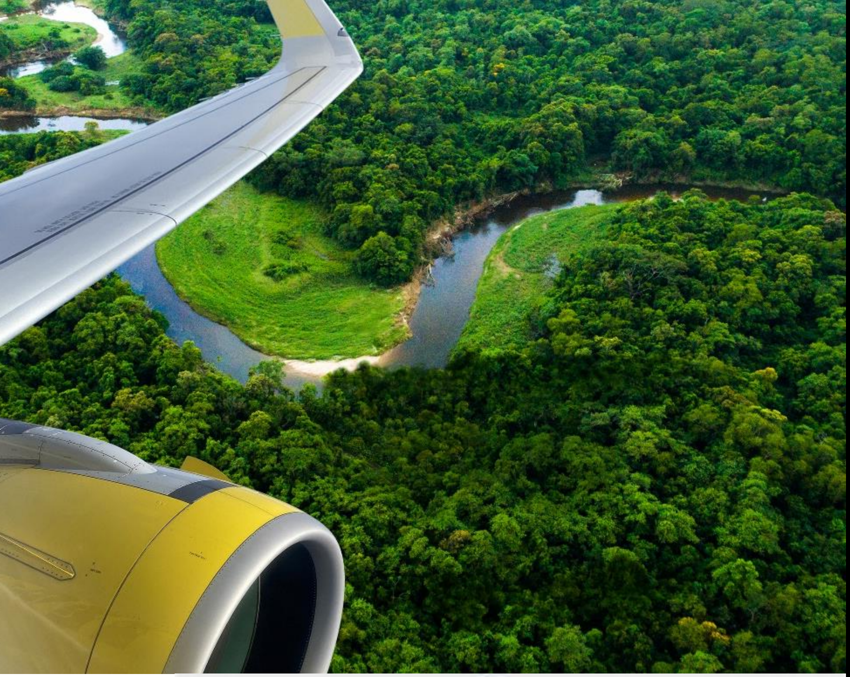

LOAD-Z

Low-NOx, **O**perable **A**mmonia Combustor **D**evelopment for **Z**ero-Carbon Power

FT4000® Aeroderivative Dual Fuel Gas Turbine Engine.

RTX

COLLINS AEROSPACE | PRATT & WHITNEY | RAYTHEON

RTX Technology Research Center

DOE/NETL University Turbine Systems Research (UTSR) Meeting
September 25, 2024

Prime Contractor: RTX Technology Research Center (RTRC)
Subcontractor: University of Connecticut (UConn)

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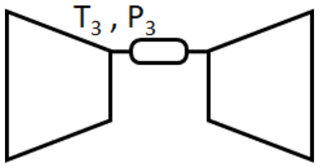
This material is based upon work supported by the Department of Energy under Award Number DE-FE0032169

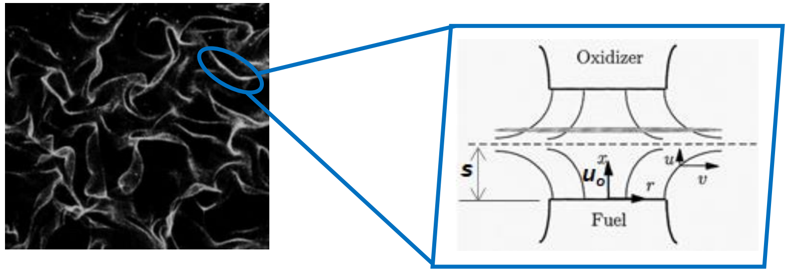
Key Project Goals …. WHAT / WHY

Low-NOx Operable Ammonia-Combustor Development (LOAD-Z)

(1) *EXPERIMENTS*
4 lab-scale facilities

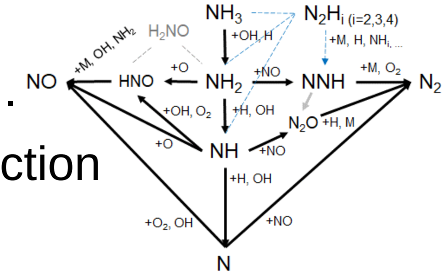
- Fundamental NH_3 flame data relevant to turbines:
  - P, T >> ambient → relevant to compressor exit conditions …..
  - strained & turbulent flames …. …. ….
    - *Targeted outcome*: expand published data w/ new, useful data (previously unreported)





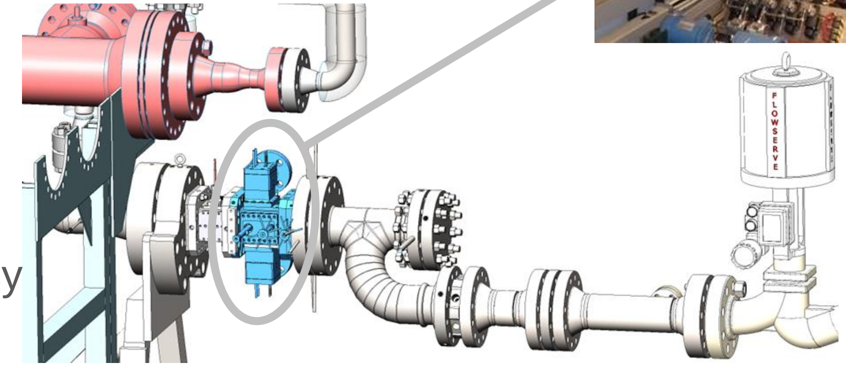
(2) *MODELING*

- Predictive capability for NH_3 combustion & emissions
  - NO_X formation kinetics integral w/ NH_3 comb. kinetics …..
  - CFD of turb. NH_3 flames w/ NO_x & NH_3 slip (η_{COMB}) prediction
    - *Targeted outcome*: capability for GT combustor design



(3) *DESIGN & DEMO.*

- Develop & test NH_3 gas-turbine combustor "@ scale"
  - Single-nozzle-rig (SNR) scale demo. @ high P, T ….
  - Pure NH_3 combustion @ 75% – 100% power
    - *Targeted outcome*: < 30ppm NOx** & >99.99% efficiency



**Note recent ETN recommendations for NOx reporting with hydrogen-containing fuels

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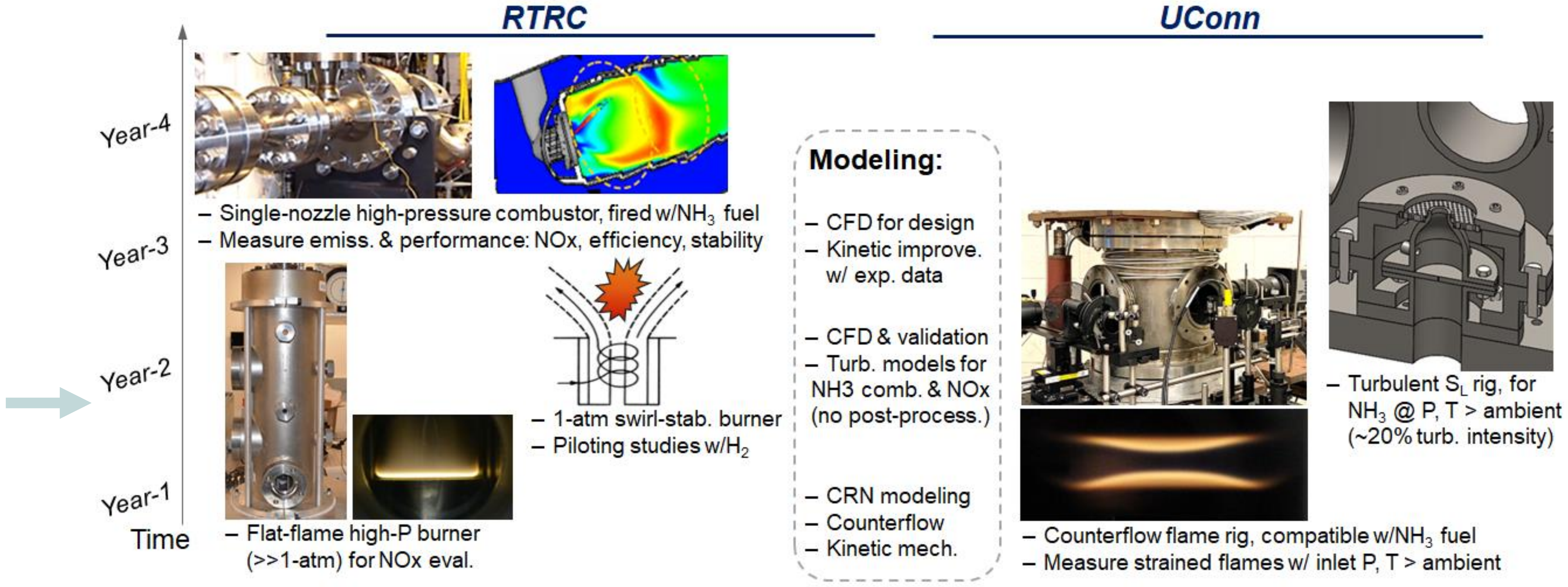
Approach & Work …. HOW



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Year-4

Year-3

Year-2

Year-1

Time

- Single-nozzle high-pressure combustor, fired w/NH_3 fuel
- Measure emiss. & performance: NOx, efficiency, stability

- 1-atm swirl-stab. burner
- Piloting studies w/H_2

- Flat-flame high-P burner (>>1-atm) for NOx eval.

Modeling:

- CFD for design
- Kinetic improve. w/ exp. data

- CFD & validation
- Turb. models for NH3 comb. & NOx (no post-process.)

- CRN modeling
- Counterflow
- Kinetic mech.

- Turbulent S_L rig, for NH_3 @ P, T > ambient (~20% turb. intensity)

- Counterflow flame rig, compatible w/NH_3 fuel
- Measure strained flames w/ inlet P, T > ambient

- **4 Lab Experiments -&- 1 Combustor Test:**
  - *Ongoing:* *2 laminar / fundamental rigs*
  - *Start Q4 & Q1:* *2 turbulent / applied rigs → complex fluid mechanics*
- **3 "Kinetics" Models -&- 1 CFD Model:**
  - *Kinetics validation:* *Counterflow-flame & Flat-flame*
  - *Combustor design:* *Chem. Reactor Network & CFD w/species transport*

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Fundamental Counterflow Data …. UCONN EXPERIMENTS

Low-NOx Operable Ammonia-Combustor Development (LOAD-Z)

(1)

UConn Experiments

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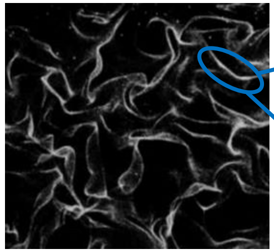

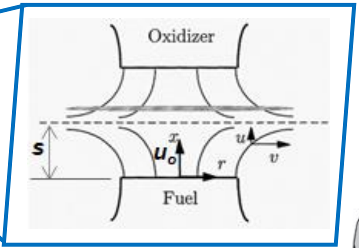

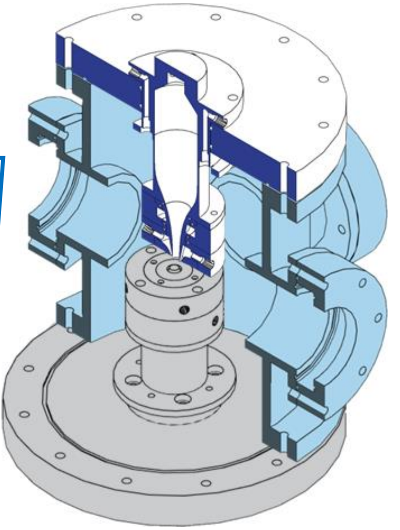

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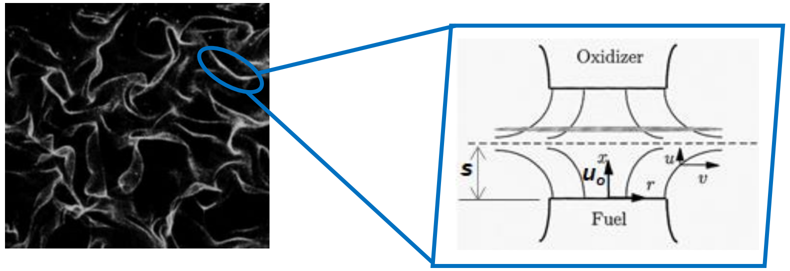
    - *Targeted outcome*: < 30ppm NOx** & >99.99% efficiency

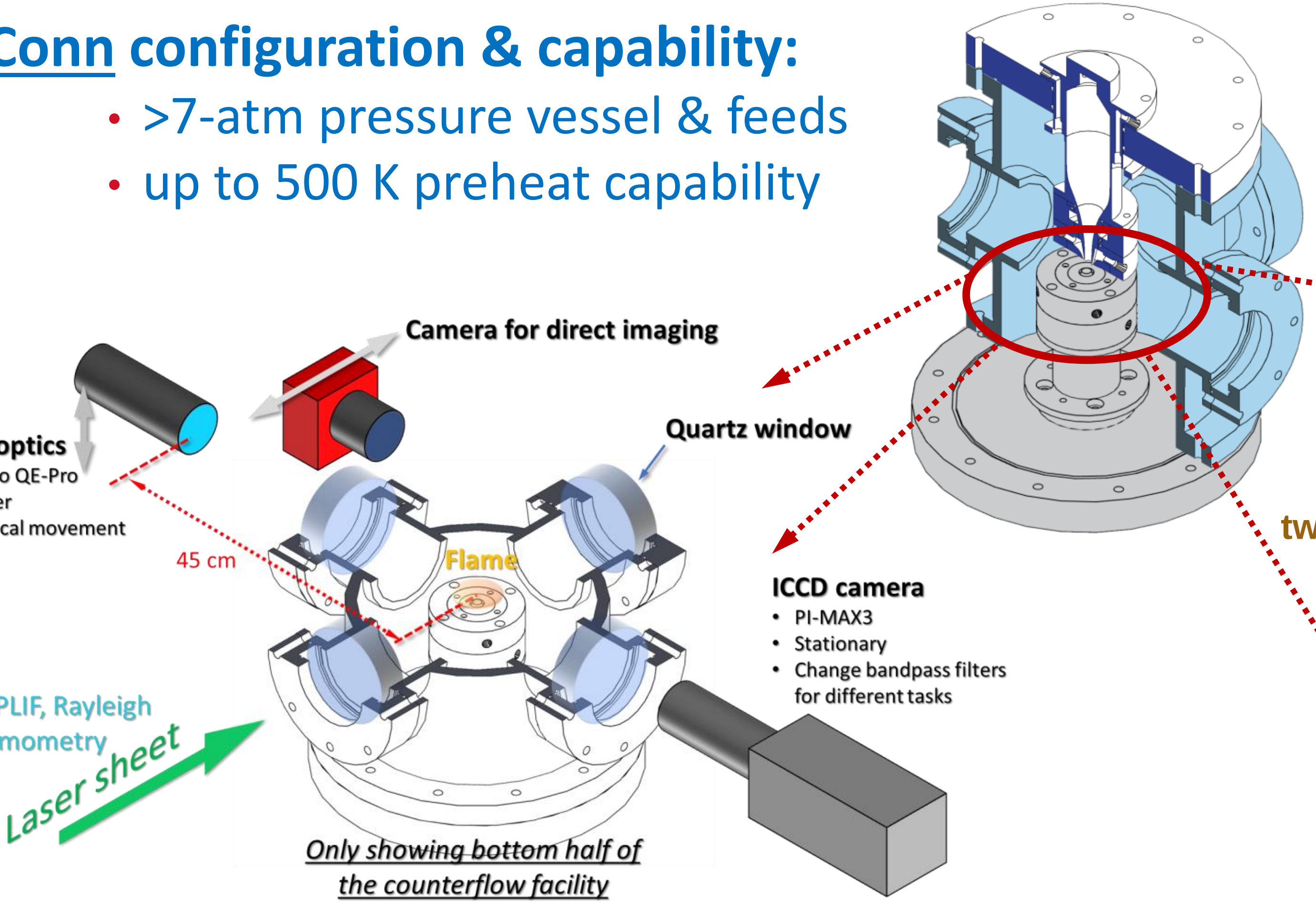
Lab-Scale Experiment: Counterflow Flame Rig | *Laminar (2D)*

Relevance:
- Scarce data on NH_3 flame extinction, esp. @ P, T > ambient.
- Stringent test of kinetic mechanisms, for comb. model development
- Canonical representation of turbulent "flamelet"

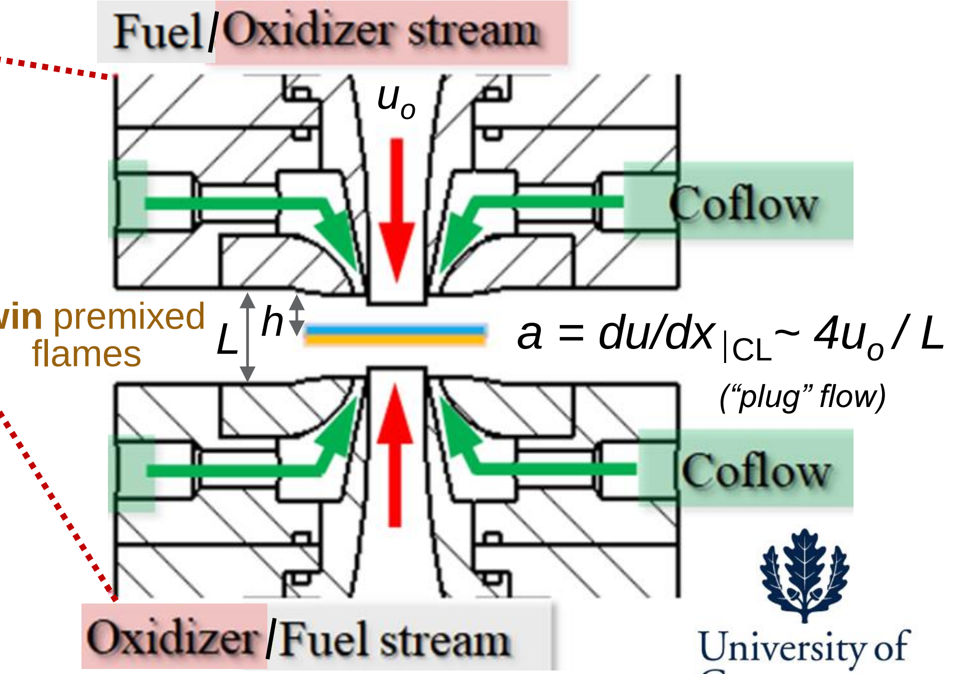


UConn configuration & capability:

- >7-atm pressure vessel & feeds
- up to 500 K preheat capability



Only showing bottom half of the counterflow facility



twin premixed flames

$a = du/dx_{|CL} \sim 4u_o / L$

("plug" flow)

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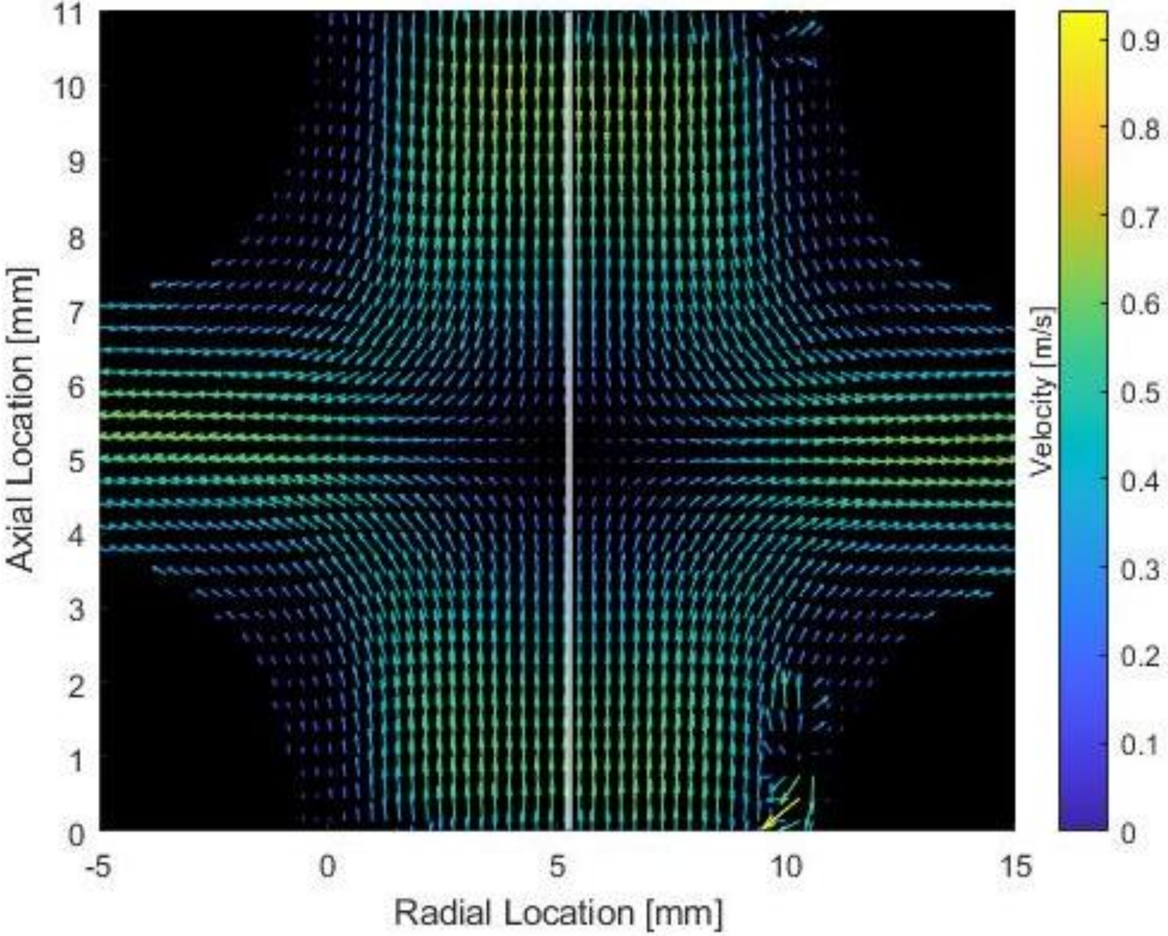
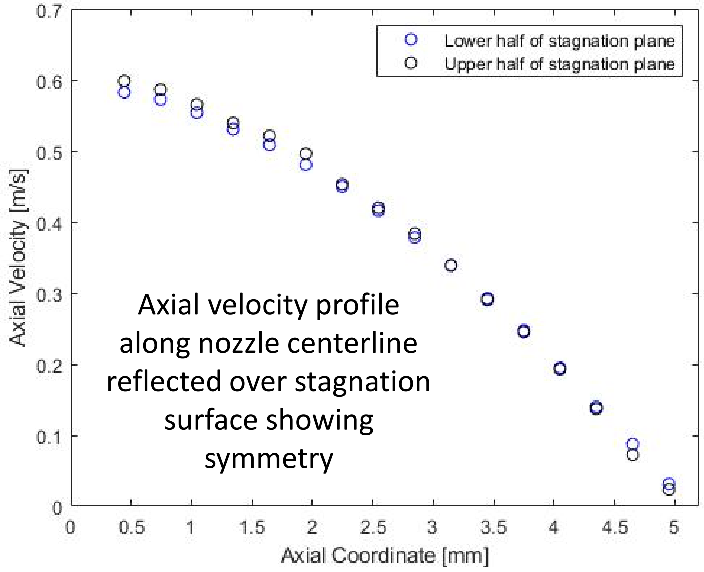
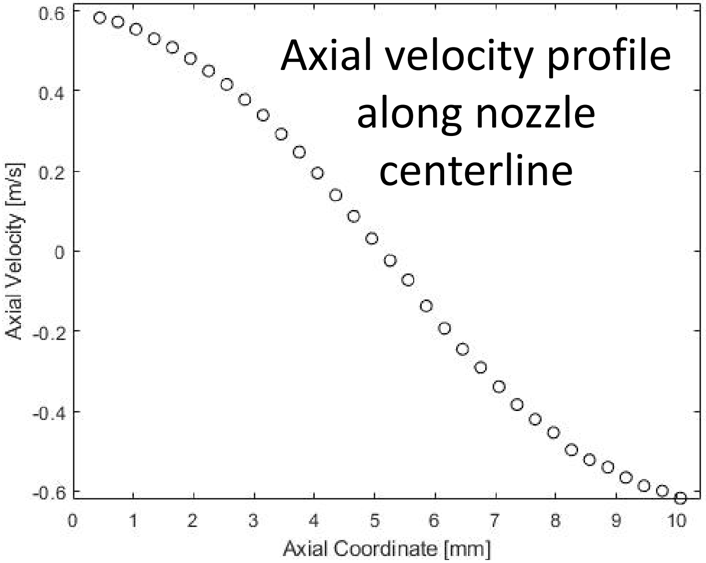
Counterflow Experiments – Measure Flow Uniformity & Strain

Velocity magnitude vector field

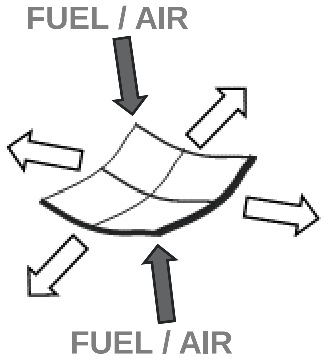




Axial velocity profile along nozzle centerline reflected over stagnation surface showing symmetry



Axial velocity profile along nozzle centerline



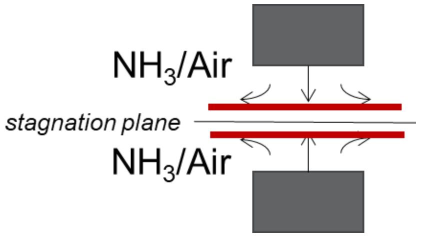
Flame stretch:

$$a_{STRETCH} = \frac{1}{A}\frac{dA}{dt}$$

Define:

Global / Centerline strain rate (for "plug" flow):

$$a_{GLOBAL} \sim \frac{4U_{JET}}{L}$$



Air at 5 SLPM flowrate + N_2 shroud (a ~ 200 s^{-1})
1 atm, 295 K
L = 10.4mm; D = 10mm

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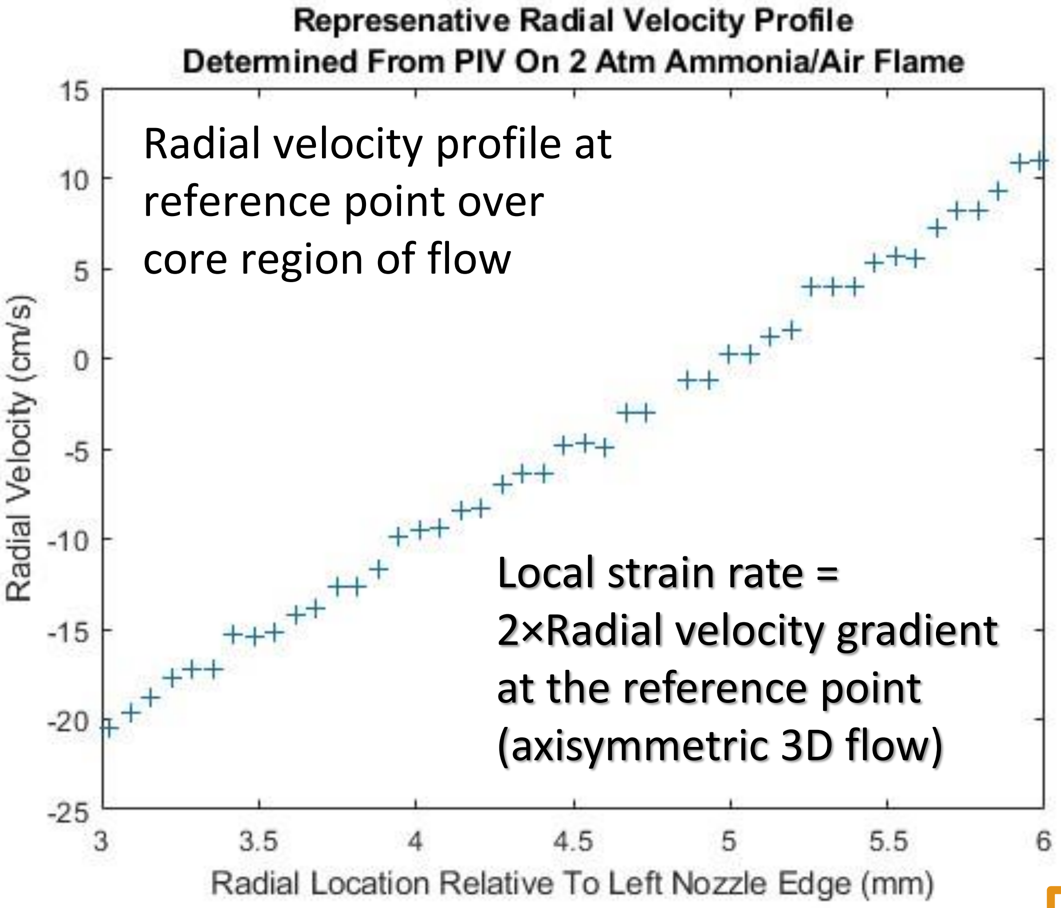
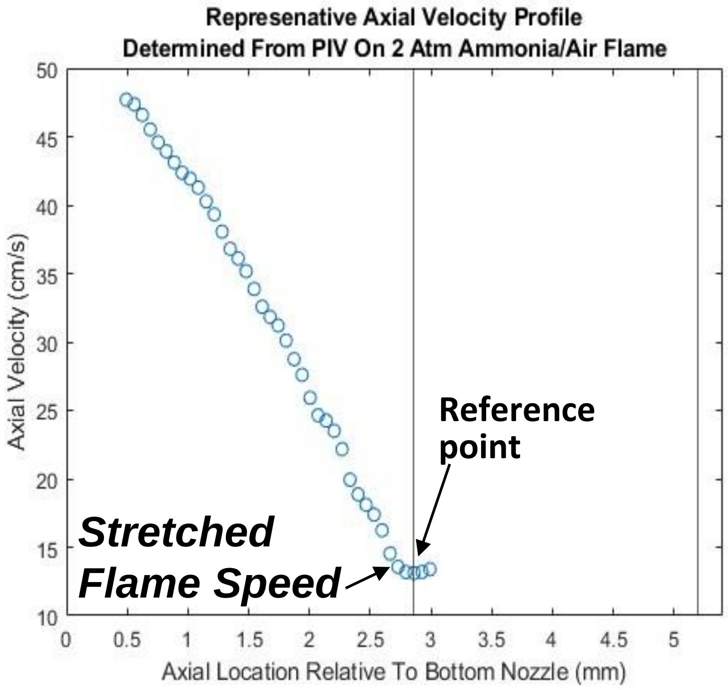
Counterflow Exp. – Global vs. Local Strain Rate in NH$_3$ flames



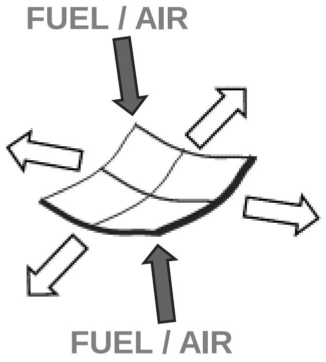
Radial velocity profile at reference point over core region of flow

Local strain rate = 2×Radial velocity gradient at the reference point (axisymmetric 3D flow)



Reference point

Stretched Flame Speed



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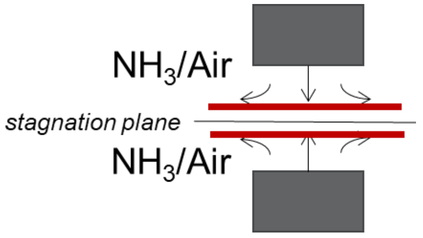

Local Extinction Strain Rate = 229 1/s

Global Extinction Strain Rate = 212 1/s

7% difference

Conditions

Pressure: 2 atm

Unburned Mixture Temperature: 25 ^{o}C

Equivalence Ratio: 1.0 (Ammonia/Air) → Quality PIV data in NH$_3$ flame

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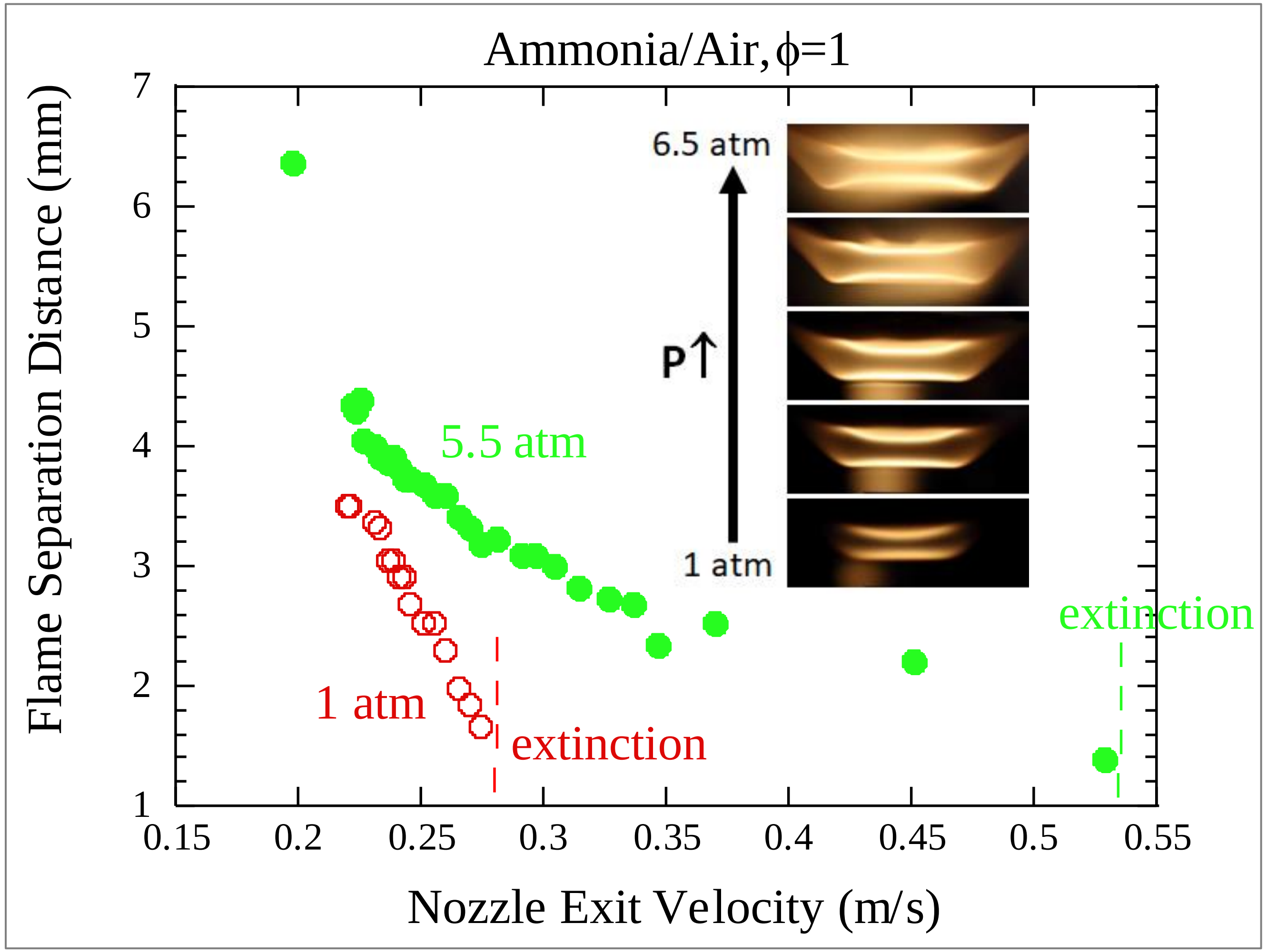
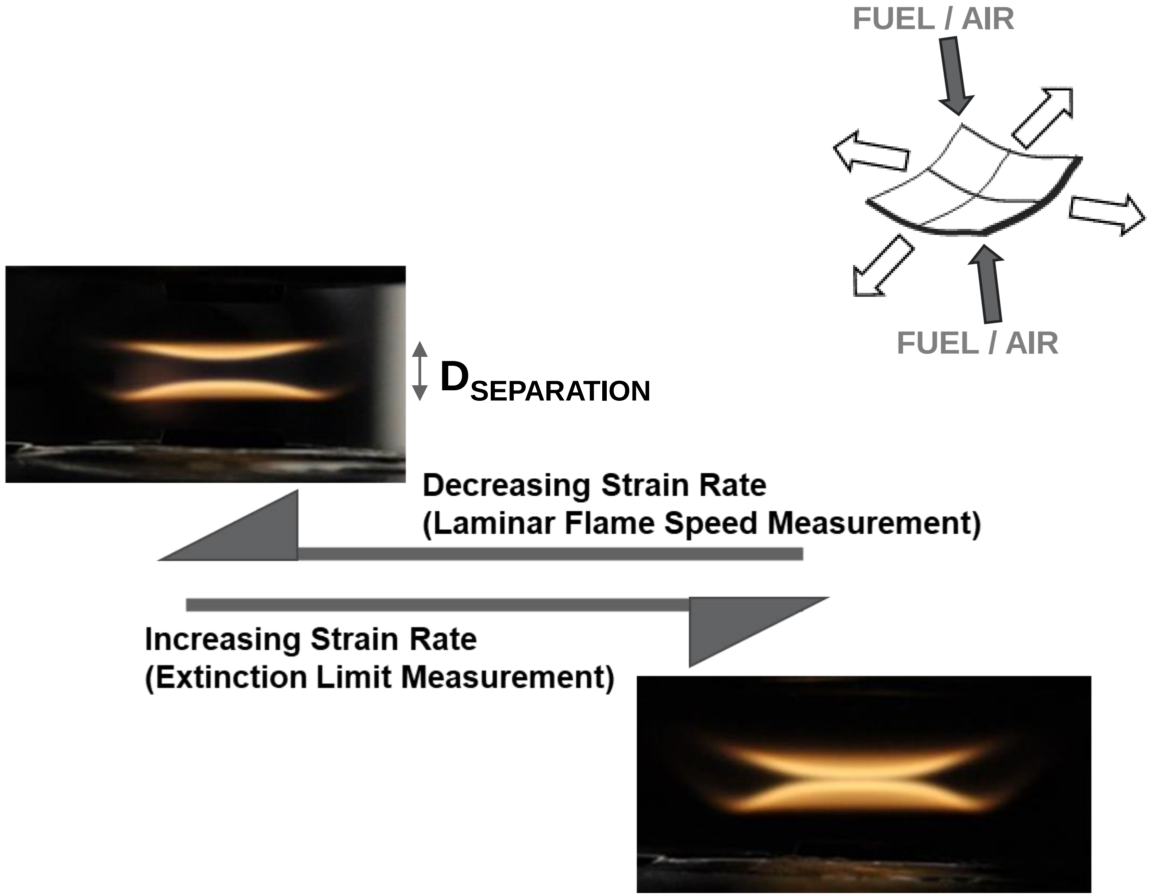
Counterflow Experiments – Procedure for Measuring Extinction





Decreasing Strain Rate (Laminar Flame Speed Measurement)

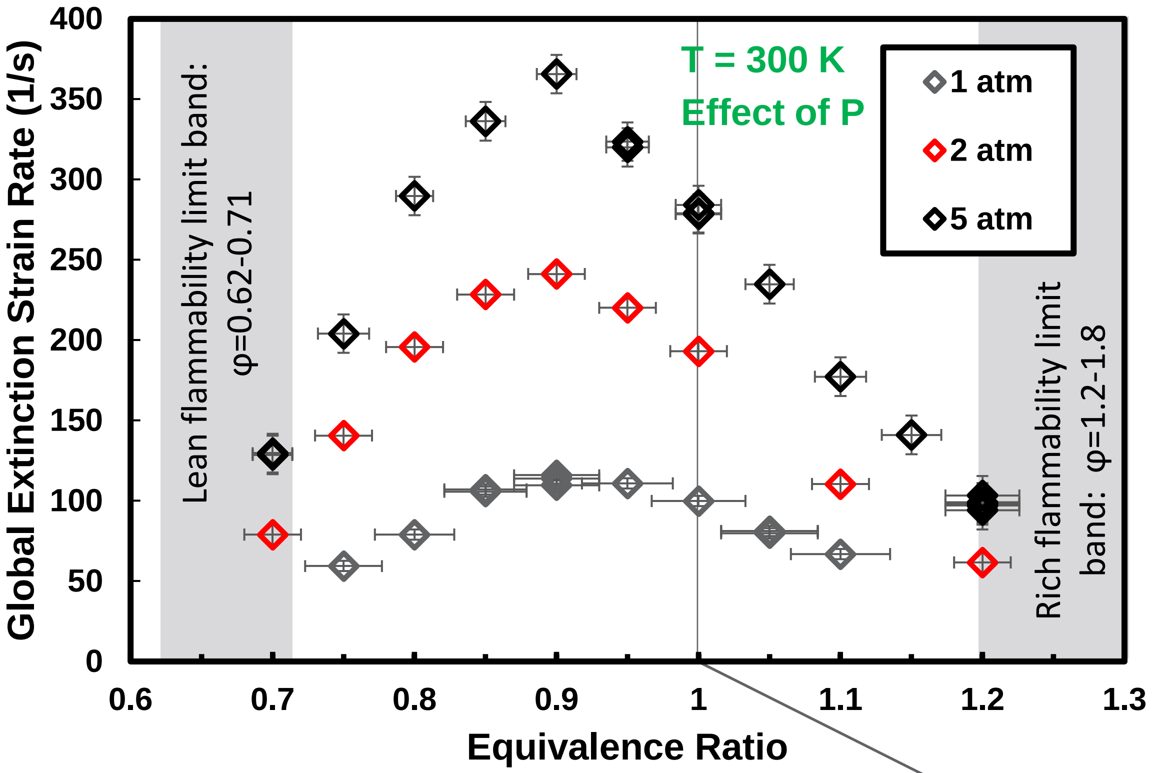
Increasing Strain Rate (Extinction Limit Measurement)

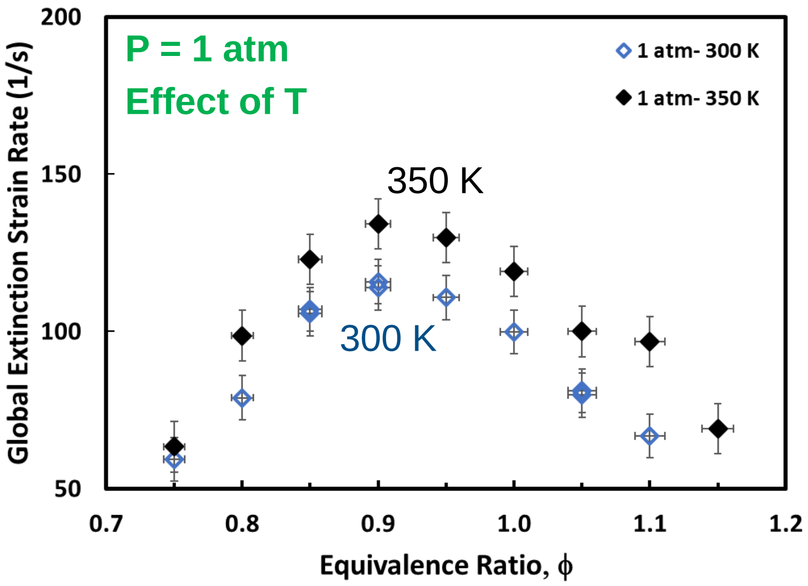
Sequence:

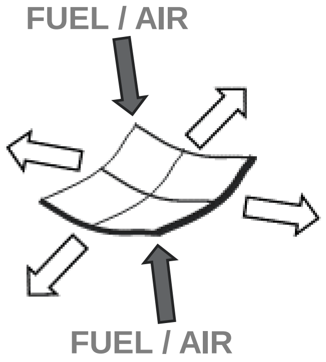
- Establish stable, premixed NH_3 / air flames @ initial $D_{SEPARATION}$ …… twin flames fixed in space
- At fixed P, ϕ: uniformly increase U_{JET} & observe $D_{SEPARATION}$ ↓
- Quasi-steady approach to U_{EXT} at extinction → $\frac{4U_{EXT}}{L} = a_{EXT\_GLOBAL}$

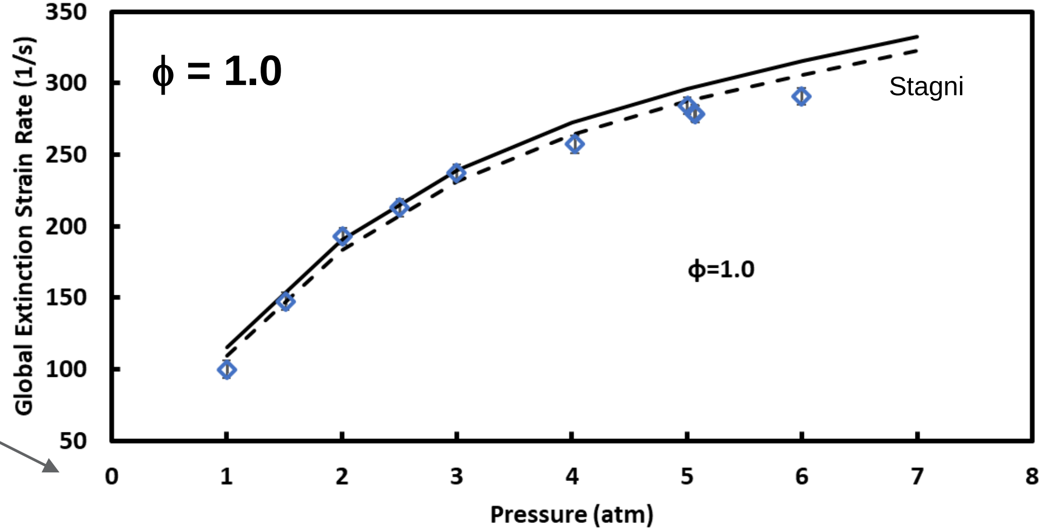
…for both experiments & modeling

Counterflow Experiments – Extinction Strain Rate vs. ϕ, p, T







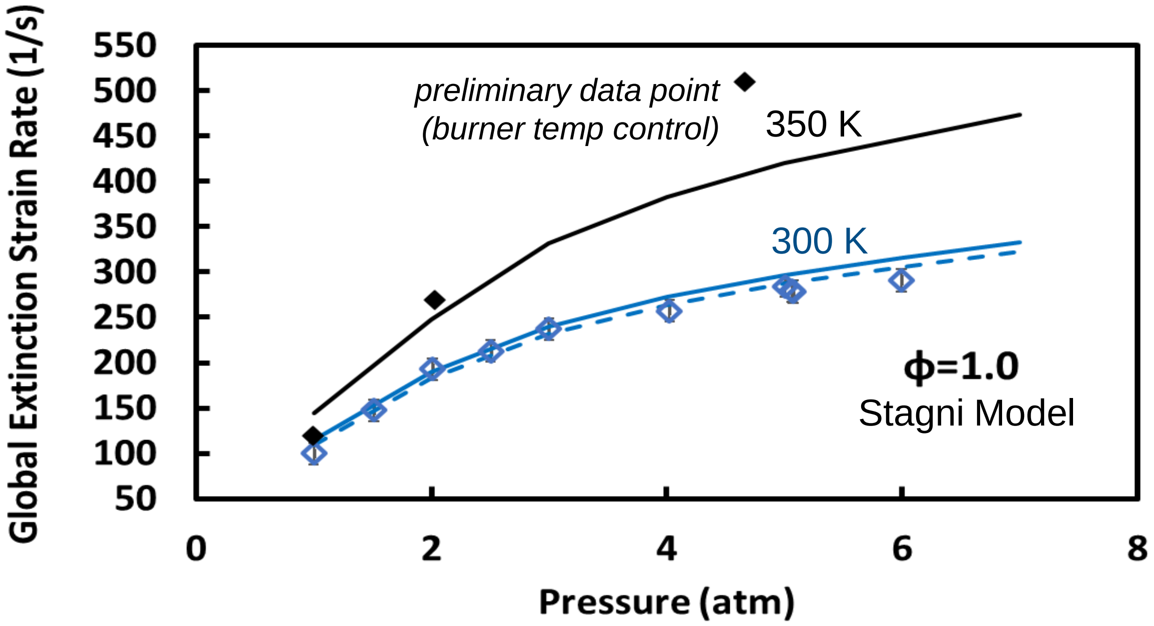


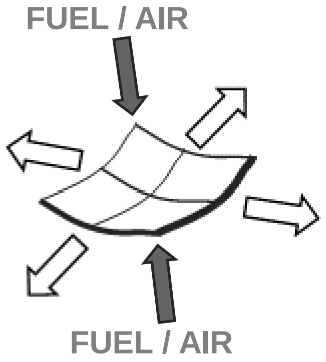
Accuracy / Error Assessment:

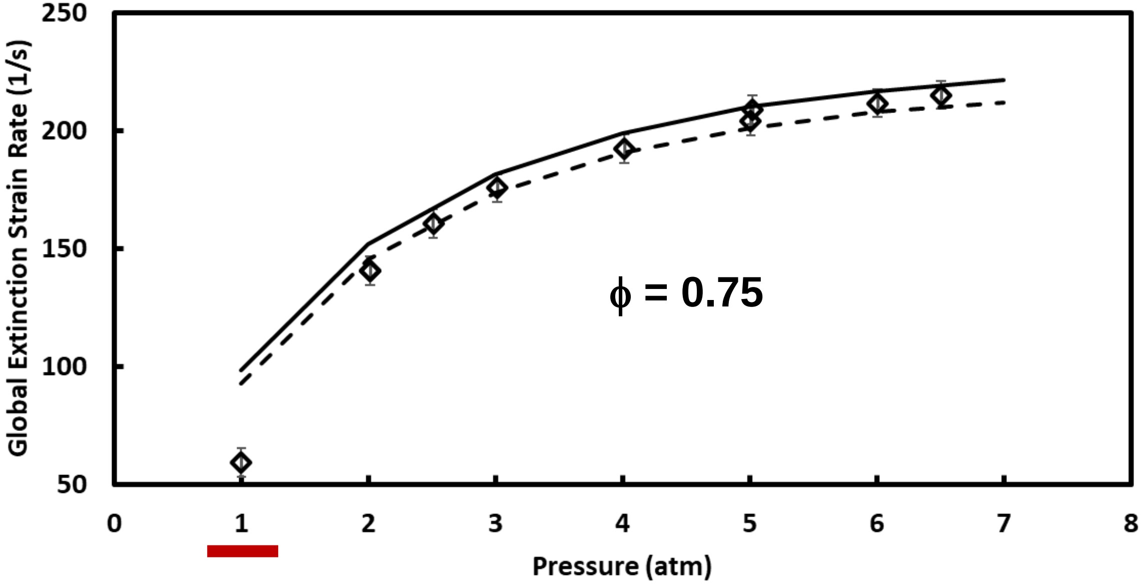
- Flowmeter precision incl. accuracy & calibration
- (Many) representative data points repeated to establish variability / repeatability

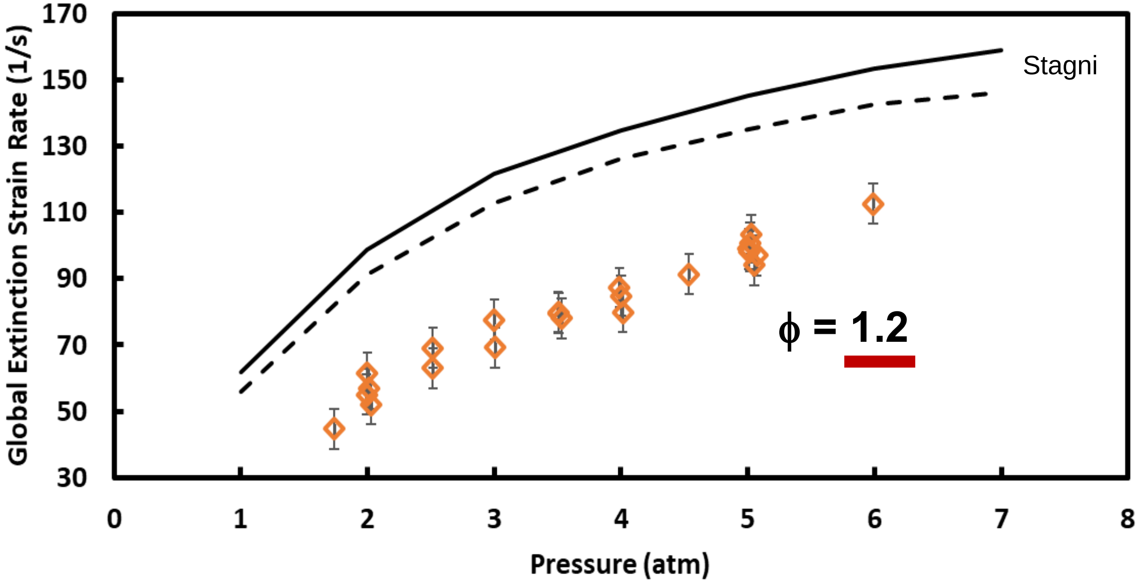
Roll–off in a_{EXT} with pressure (non–linear)

Counterflow Experiments – Press/Temp Effect on Extinction (3 ϕ's)









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UConn Next Steps – … Turbulent Flame Speed Rig for NH_3

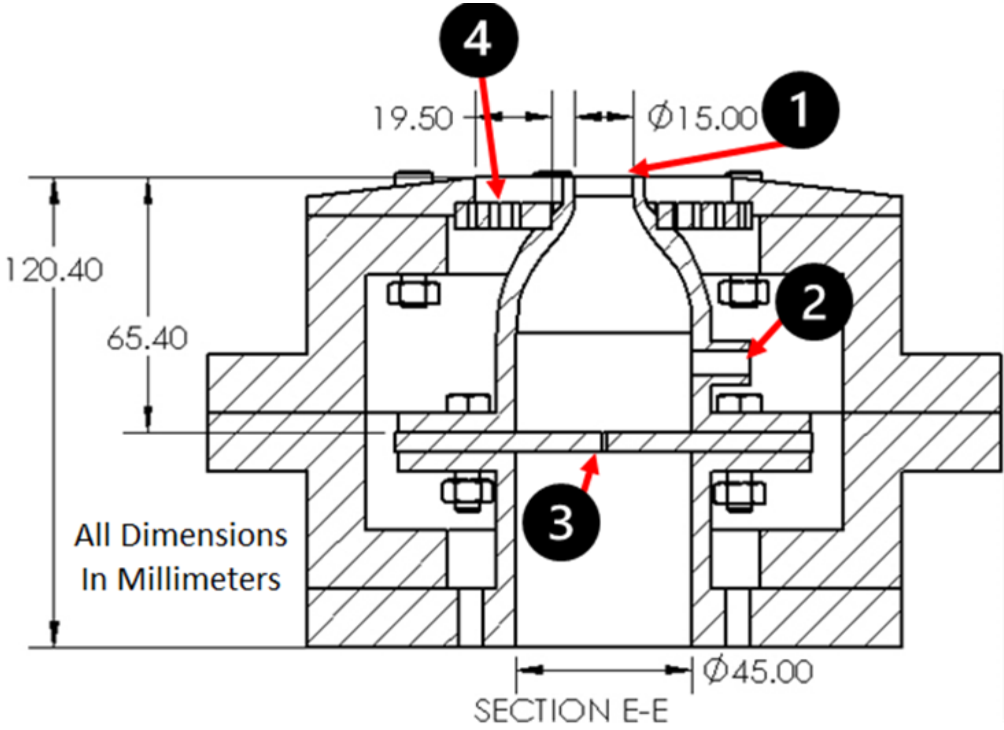
Q4- Fabricate **Turb. Flame Speed** Rig:

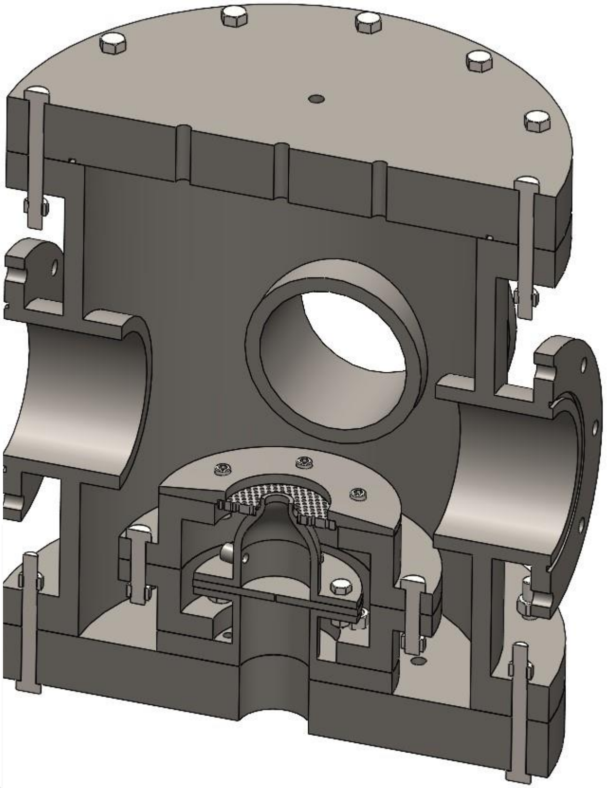
Turbulent intensity range: 15–25%

1. NH_3 Bunsen Burner Outlet
2. Jet In Crossflow Port
3. Sharp-Edged Orifice Plate
4. H_2 Pilot Burner Plate

- **NH PLIF for turbulent flame structure imaging**
- **High-speed PIV for turbulent flow-velocity characterization**
- **Turbulent intensity enhancement utilizing jet-in-crossflow & contraction section [e.g. Michigan*/Lund** Hi-Pilot/DRZ]**

*J.Driscoll, Univ. of Mich.; **M.Alden, Lund Univ.





Modeling NH3 Kinetics …. COUNTERFLOW & CHEM. REACTOR NETWORKS

Low-NOx Operable Ammonia-Combustor Development (LOAD-Z)

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  - strained & turbulent flames …. …. ….
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      w/ new, useful data
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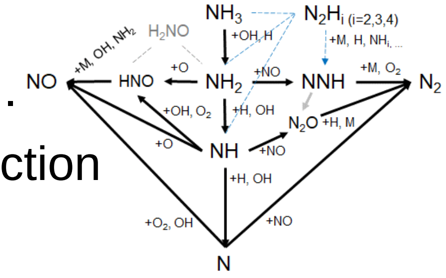

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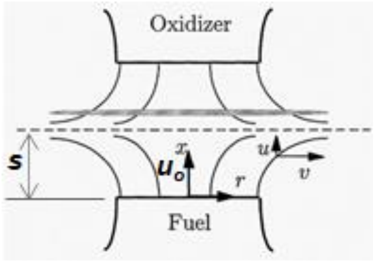

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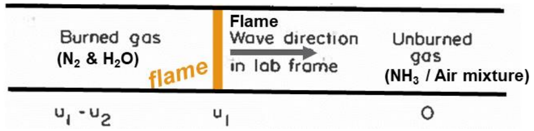
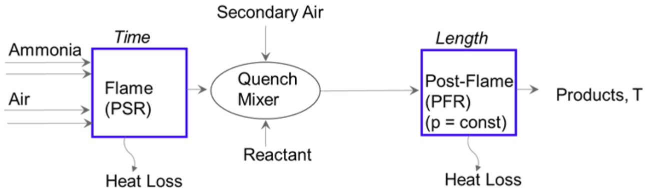
Computational Methods w/ Detailed Kinetics

- Cantera, open-source computational framework developed by Dave Goodwin at Caltech
- Models developed for flame speed, chemical reactor networks (CRN), and counterflow flames (premixed & non-premixed)
- Additional tools developed to perform sensitivity analysis, including feature sensitivity (e.g. extinction strain rate), reaction path, chemical mechanism reduction and other diagnostic tools

(i) **Freely Propagating Premixed** Flames (Flame Speed)



(ii) NH_3 Chemical Reactor Network (CRN) Models



(iii) NH_3 **Counterflow Flames**: Premixed and Non-Premixed

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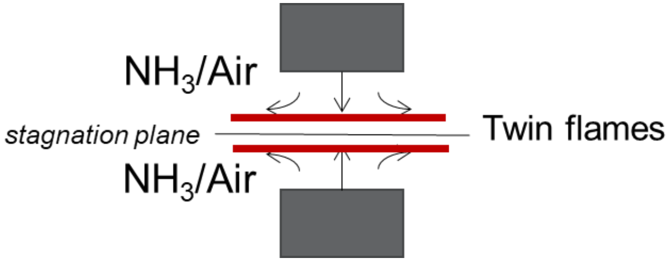
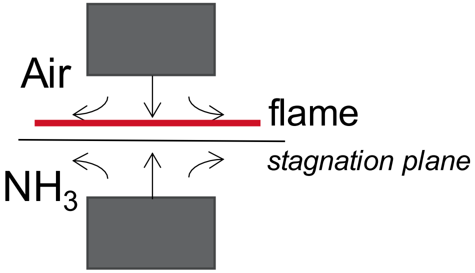
Premixed Counterflow Flames



Non-Premixed Counterflow Flames



Chemical Kinetic Mechanisms

Selected published, comprehensive N/H chemical mechanisms

- Open-source computational framework developed by Dave Goodwin at Caltech Cantera

- **Glarborg et al. Mechanism (2018 & 2022 versions)**

  [Glarborg, Miller, Ruscic, Klippenstein: Modeling nitrogen chemistry in combustion, Prog. Energy Combust. Sci. (2018) 31-68]
  [Glarborg: The $NH_3/NO_2/O_2$ system: Constraining key steps in ammonia ignition and N_2O formation, Combust. Flame, Vol. 257 (2023)]

- **Stagni et al. Mechanism (2020)**

  [Stagni, Cavallotti, Arunthanayothin, Song, Herbinet, Battin-Leclerc, Faravelli: React. Chem. Eng. 5 (2020) 696–711]

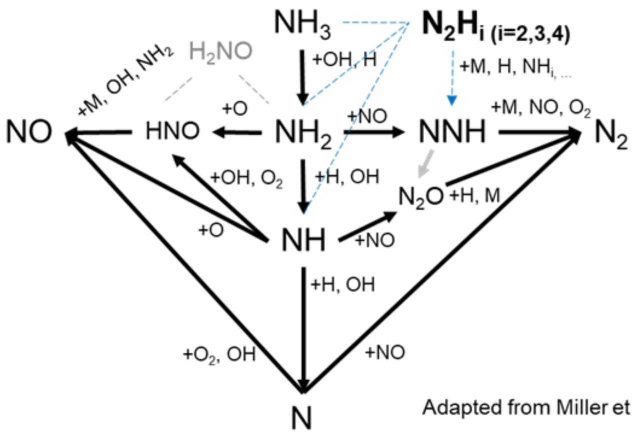
- **Powell & Papas et al. Mechanism- (2010 & 2011 versions) → RTRC**

  [Powell, Papas, Dreyer: Hydrogen- and C_1-C_3 Hydrocarbon-Nitrous Oxide Kinetics in Freely, Propagating and Burner Stabilized Flames, Shock Tubes, and Flow Reactors, Combust. Sci. Tech. 182 (2010) 252-283]
  [Powell, Papas, Dreyer: Flame Structure measurements of NO in Premixed Hydrogen-Nitrous Oxide Flames, Proc. Combust. Inst. 33 (2011) 1053-1062]

  - Two "Powell" mechanisms differ by only 3 different rate expressions for amine radical reactions:

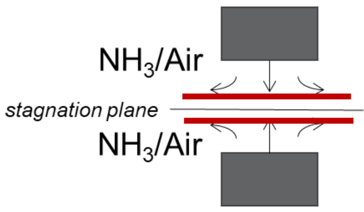
$$(1)\ NH_2 + NO \leftrightarrow N_2 + H_2O$$
$$(2)\ NH_2 + NO \leftrightarrow NNH + OH$$
$$(3)\ NH_3 + NH_2 \leftrightarrow N_2H_3 + H_2$$

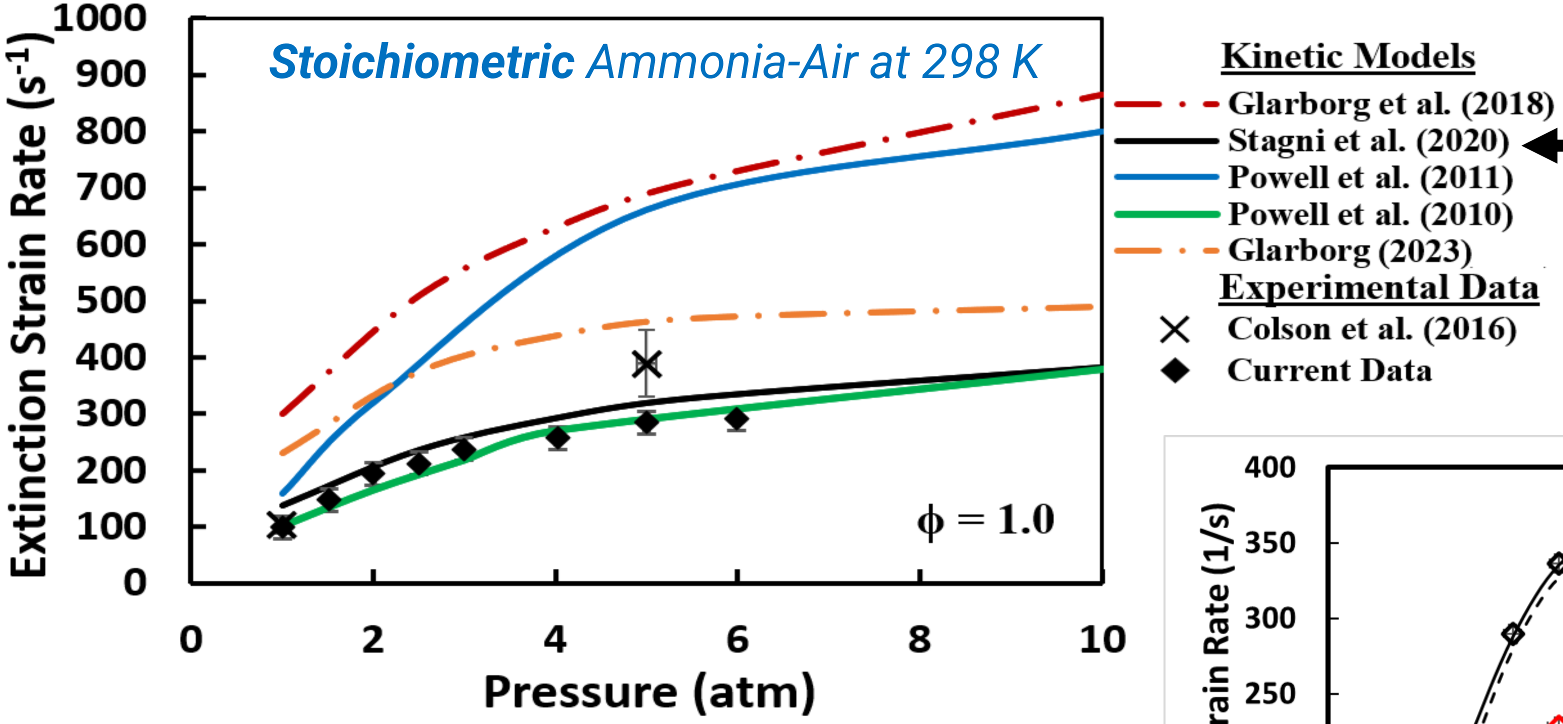
Ammonia Oxidation Pathway Schematic

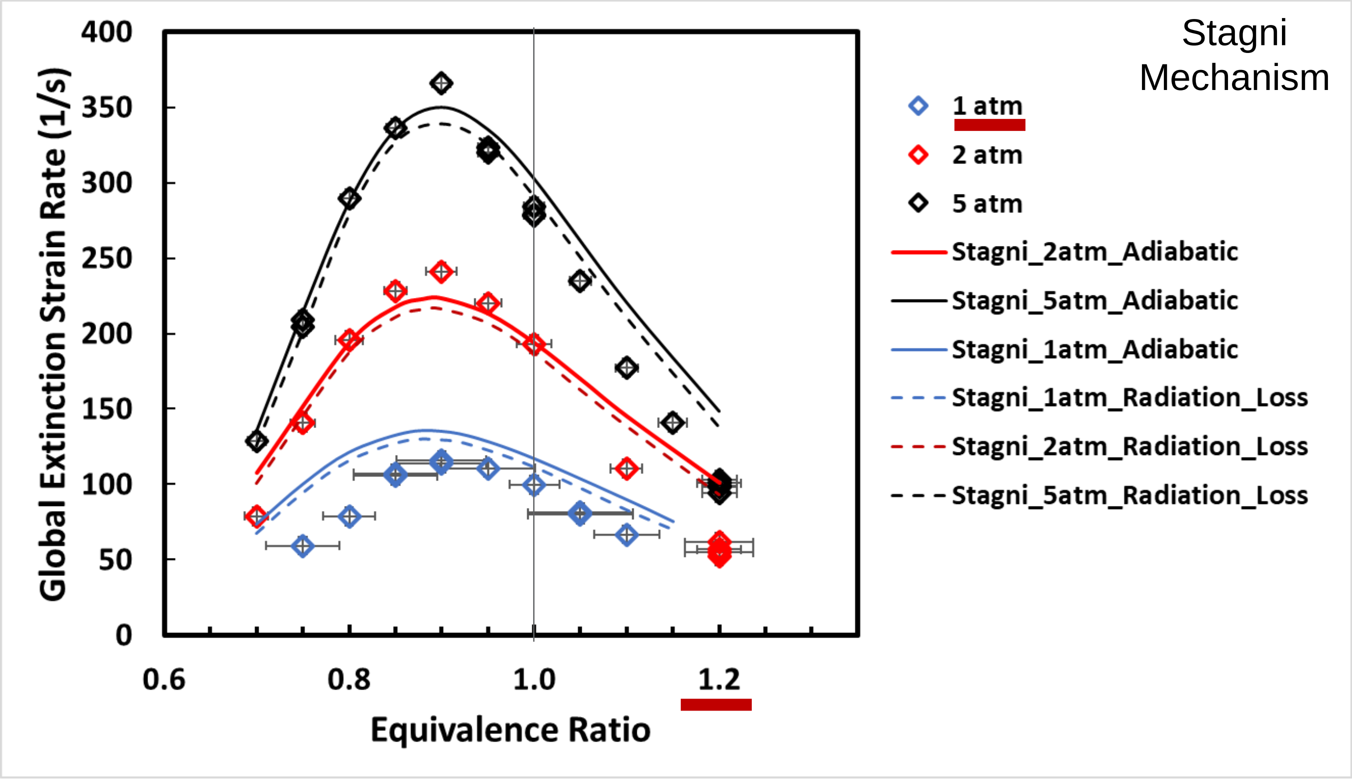


Adapted from Miller et al. (1983)

RTRC Predictions vs. UConn Measurements







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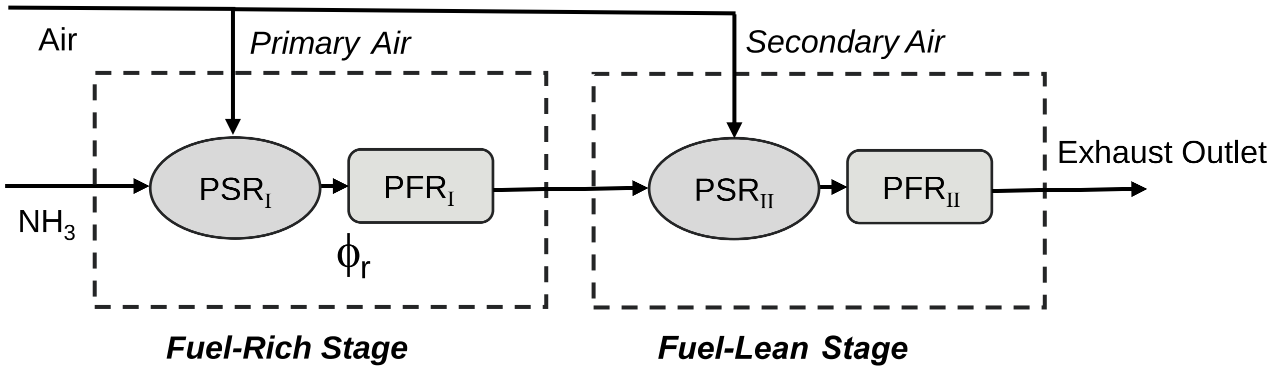
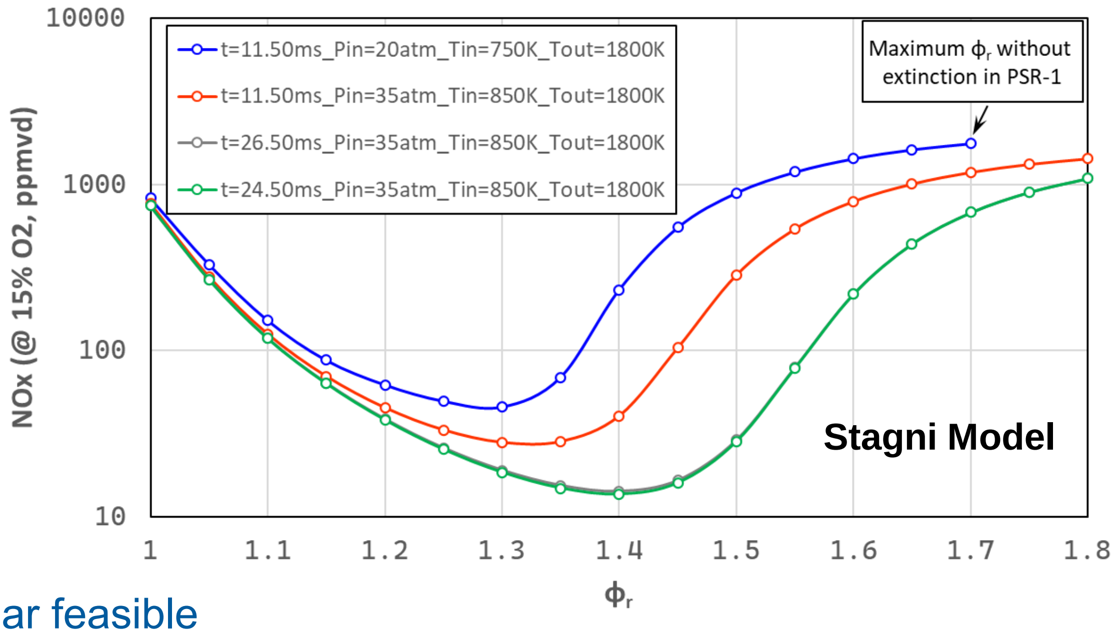
Chemical Reactor Network (CRN) Model → ROM Design Tool

CRN Model Schematic for RQL Combustor





- Outlet temperature fixed at 1800 K.
- Overall "theoretical" NOx levels <30 ppm for a RQL architecture appear feasible

Total Residence time τ (ms)	τPSR_I (ms)	τPFR_I (ms)	τPSR_II (ms)	τPFR_II (ms)	Pressure (atm)	Inlet Temp. (K)	Rich Stage		Lean Stage**		
							NH_3 (ϕ_r = 1.25) (ppm_wet)	NO (ϕ_r = 1.25) (ppm_wet)	NO (ϕ_r = 1.25) (ppm_wet)	NO_x* (ϕ_r = 1.25) (ppm)	$NO_{x,min}$* (ppm)
11.50	0.50	5.0	1.0	5.0	20	750	9.5	**121.6**	68.0	49.8	**46.0**
11.50	0.50	5.0	1.0	5.0	**35**	850	8.1	**75.7**	40.6	33.3	**28.0**
26.50	0.50	**20.0**	1.0	5.0	35	850	6.5	**57.3**	31.5	26.0	**14.2**
24.50	0.50	20.0	1.0	**3.0**	35	850	6.5	57.3	30.9	25.5	**13.7**

** NH_3 slip <1E-5 ppm at exhaust

* 15% O_2 dry

RTX

Modeling NH3 Combustor …. CFD for NH3 NOx Estimates & Combustor Design

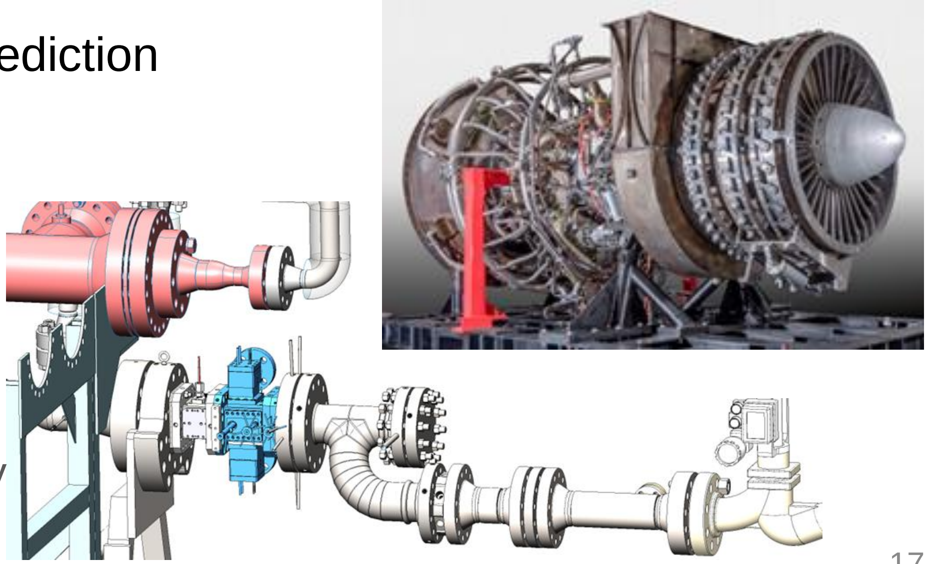
Low-NOx **O**perable **A**mmonia-Combustor **D**evelopment (LOAD-Z)

- Fundamental NH_3 flame data relevant to turbines:
  - P, T >> ambient → relevant to compressor exit conditions …..
  - strained & turbulent flames …. …. ….
    - *Targeted outcome*: expand published data
      w/ new, useful data
      (previously unreported)

- Predictive capability for NH_3 combustion & emissions
  - NO_X formation kinetics integral w/ NH_3 comb. kinetics …..
  - CFD of turb. NH_3 flames w/ NO_x & NH_3 slip (η_{COMB}) prediction
    - *Targeted outcome*: capability for GT combustor design

(3)
DESIGN & DEMO.

- Develop & test NH_3 gas-turbine combustor "@ scale"
  - Single-nozzle-rig (SNR) scale demo. @ high P, T ….
  - Pure NH_3 combustion @ 75% – 100% power
    - *Targeted outcome*: < 30ppm NOx** & >99.99% efficiency



**Note recent ETN recommendations for NOx reporting with hydrogen-containing fuels

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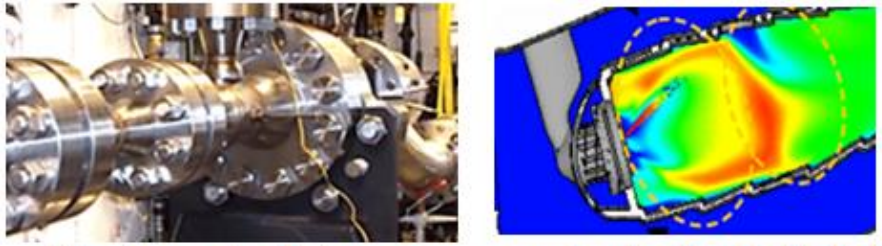
Modeling Activities & Next Steps …… Toward GT Design



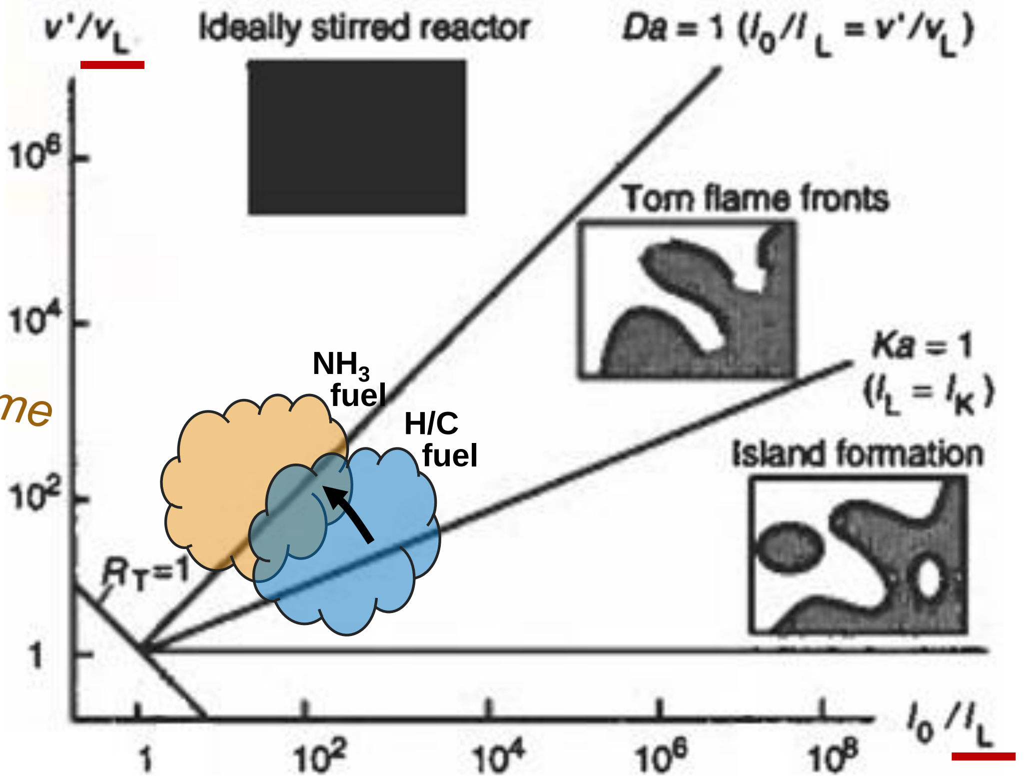
– Single-nozzle high-pressure combustor, fired w/NH_3 fuel

Turbulent combustion regime for NH_3-fueled gas turbines:

- v’ & ℓ_o ~independent of fuel type (only aero dependent)
- $v_L \downarrow$ w/ NH_3 fuel
- $\ell_L \uparrow$ w/ NH_3 fuel
- shift by ~5 – 10x

CFD modeling of NH_3-fueled gas turbine combustor:

- Challenges:
  - Efficient flamelet models uncertain (regime => stirred)
  - NOx cannot be post-processed (integral to comb. rxns)
- For efficient GT design calculations, *possible approach*:
  - Reduced NH_3/NOx kinetics w/transport, e.g. EDC**
  - Steady RANS turbulence model saves computational power for chemistry/transport



validate w/ turb. flame rig measurements

**Eddy Dissipation Concept, Magnussen et al., Norwegian Inst. of Technol.*

Developing CFD Approach for NH_3 Combustor Aero Design

Begin CFD methodology evaluation w/H_2 combustion case from existing RTRC exp. rig:

- Change ***from*** LES turbulence model ***to*** steady-RANS (realizable k-eps.)
- Change ***from*** 2-mixture-fraction/Zimont combustion model ***to*** EDC w/species transport
- Start w/complete H_2 combustion chemical mechanism (10-species)
- Then add NOx mechanism (coupled w/H_2 mechanism) & evaluate emiss. predict. (12-species)
- Then add NH_3 combustion mechanism (31-species)

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Proceedings of ASME Turbo Expo 2024
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GT2024
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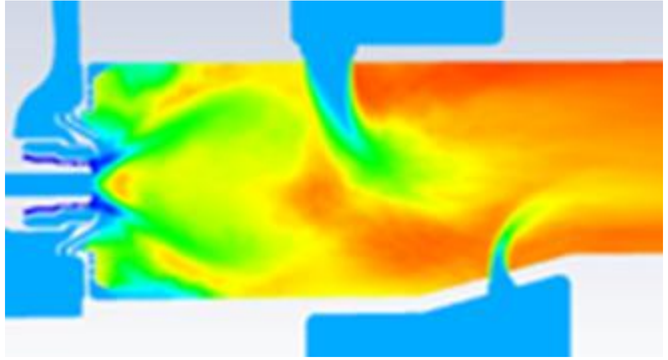
LES/2mf/Zimont (partially premixed St)



LES w/out NOx prediction capability (no species transport)

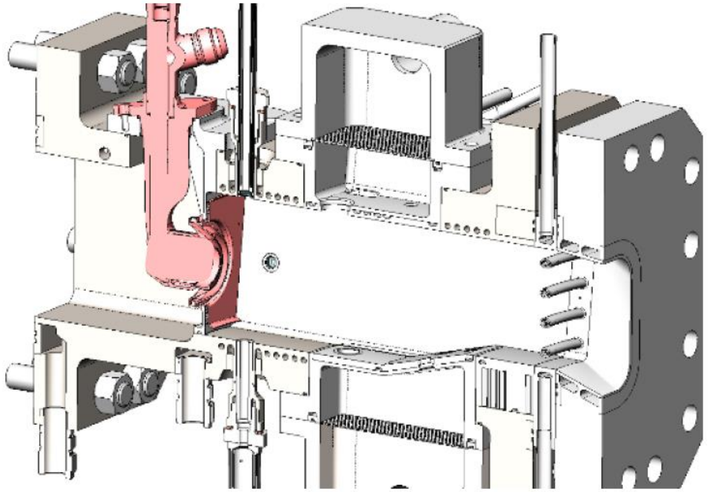
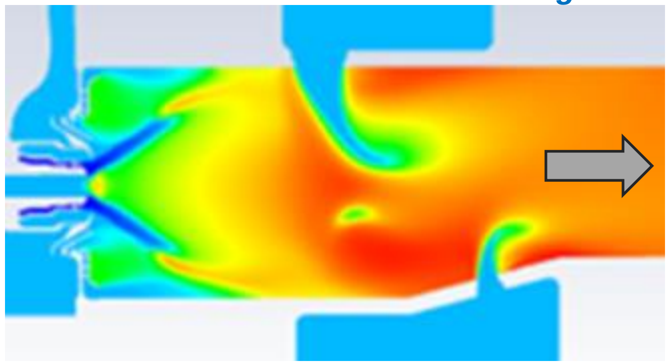


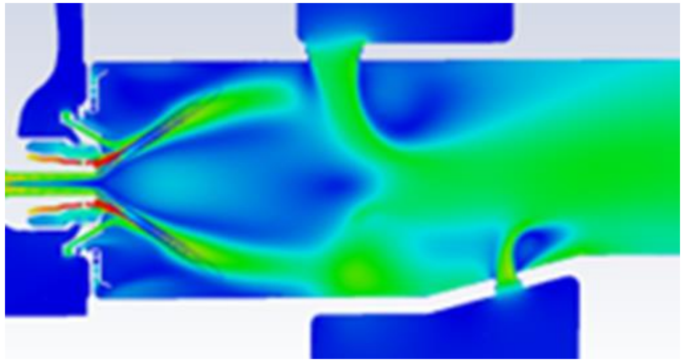
FIGURE 5. FT4000 Single Nozzle Combustor Rig (SNR).

RANS/EDC/LLNL H2/Air Mech. & Stagni NOx



EDC-predicted NOx qualitatively matches rig meas. …within factor of 1 to 1.5 for three different FARs…

RANS/EDC/LLNL H2/Air Mechanism



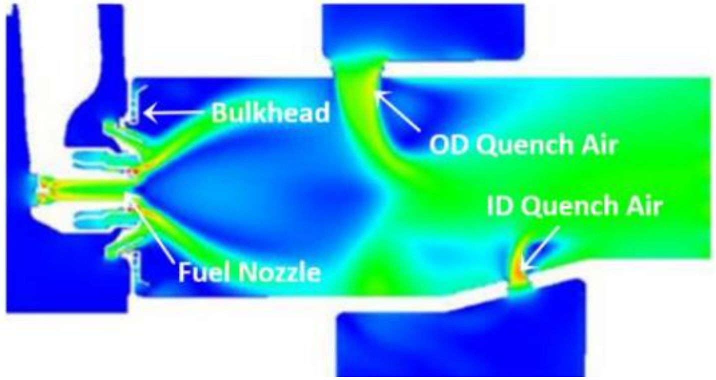
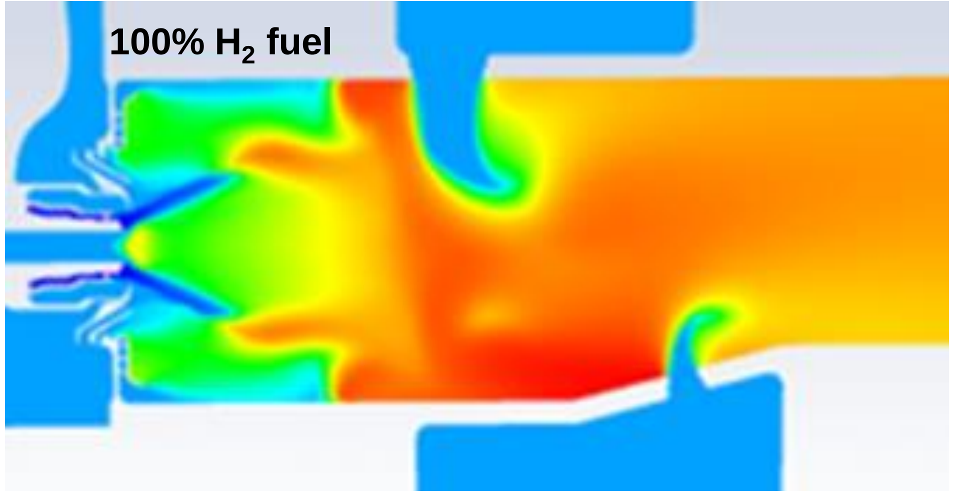


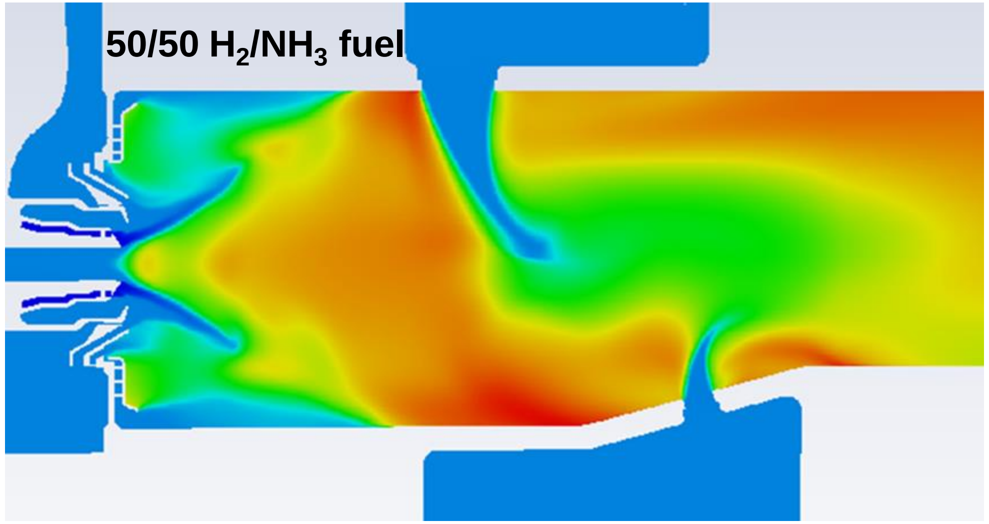
FIGURE 7. CFD analysis of engine (a) and rig (b) combustor velocity flowfields.

Initial CFD Simulation of NH_3 Combustion in Existing Geom.

RANS/EDC/LLNL H2/Air Mech. & Stagni NOx



RANS/EDC/Stagni Mech. for Combustion & NOx



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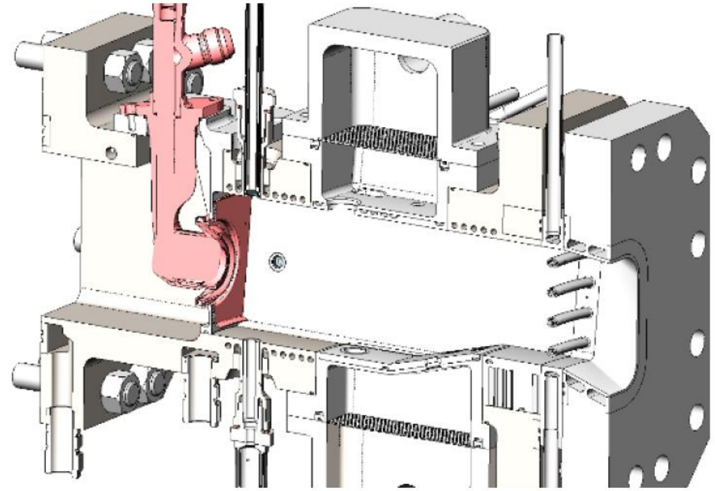

FIGURE 5. FT4000 Single Nozzle Combustor Rig (SNR).

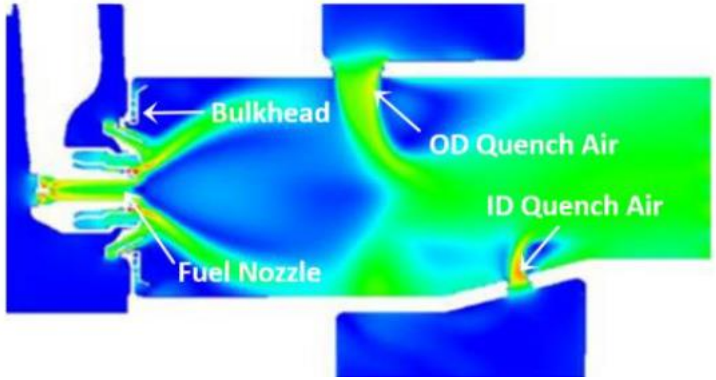

FIGURE 7. CFD analysis of engine (a) and rig (b) combustor velocity flowfields.

Fundamental Flat-Flame Data …. RTRC EXPERIMENTS

Low-NOx Operable Ammonia-Combustor Development (LOAD-Z)

(1)

RTRC Experiments

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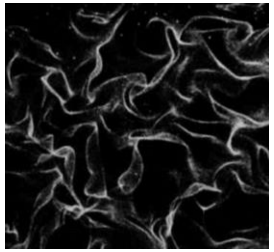
- Fundamental NH_3 flame data relevant to turbines:
  - P, T >> ambient → relevant to compressor exit conditions …..
  - strained & turbulent flames …. …. ….
    - *Targeted outcome*: expand published data w/ new, useful data (previously unreported)



- Predictive capability for NH_3 combustion & emissions
  - NO_X formation kinetics integral w/ NH_3 comb. kinetics …..
  - CFD of turb. NH_3 flames w/ NO_x & NH_3 slip (η_{COMB}) prediction
    - *Targeted outcome*: capability for GT combustor design
- Develop & test NH_3 gas-turbine combustor "@ scale"
  - Single-nozzle-rig (SNR) scale demo. @ high P, T ….
  - Pure NH_3 combustion @ 75% – 100% power
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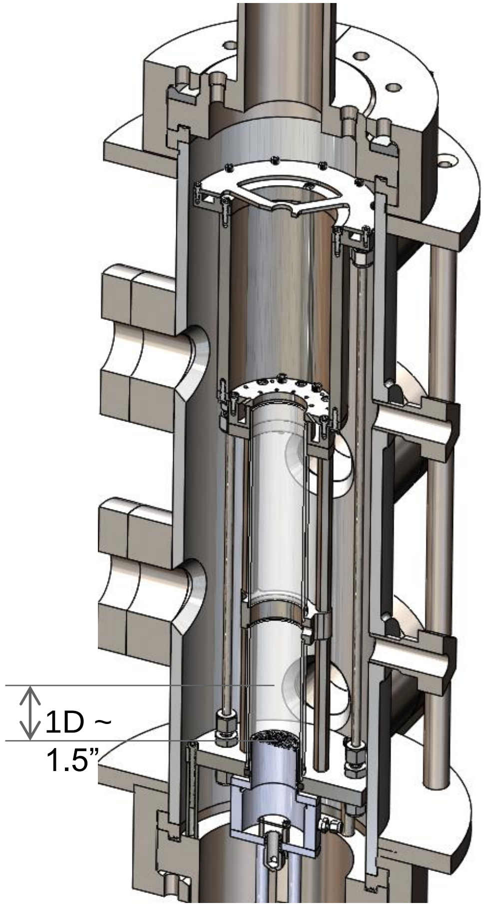

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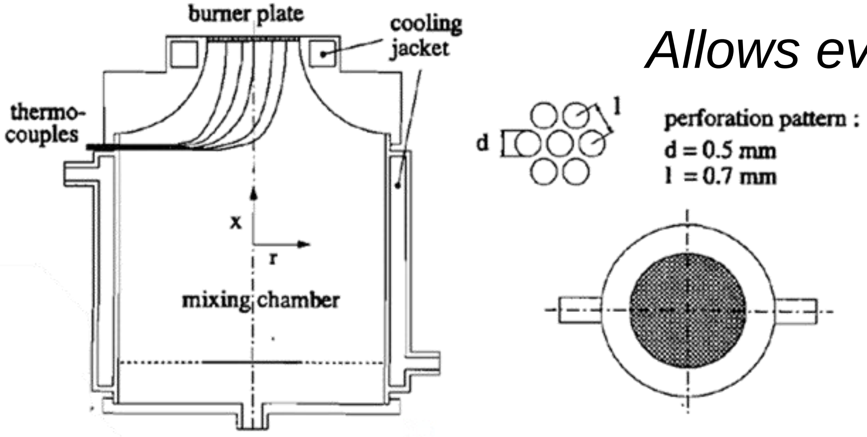
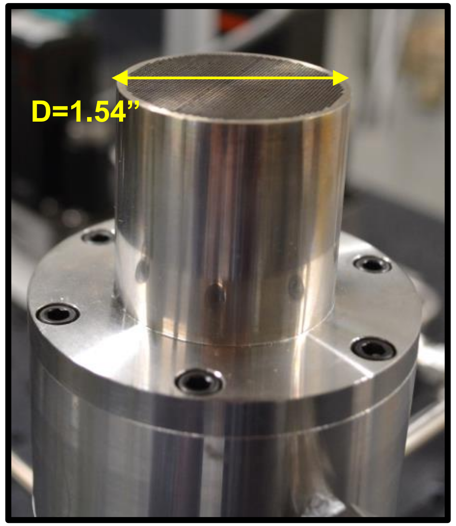
High-Pressure Flat-Flame Burner Rig

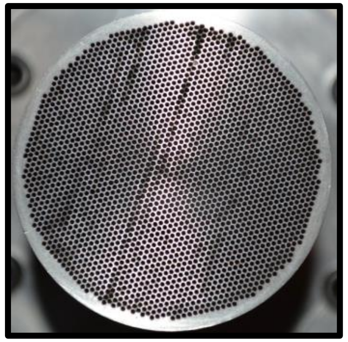
Goal: Characterize NO_X emissions from laminar flame at high pressure for model validation

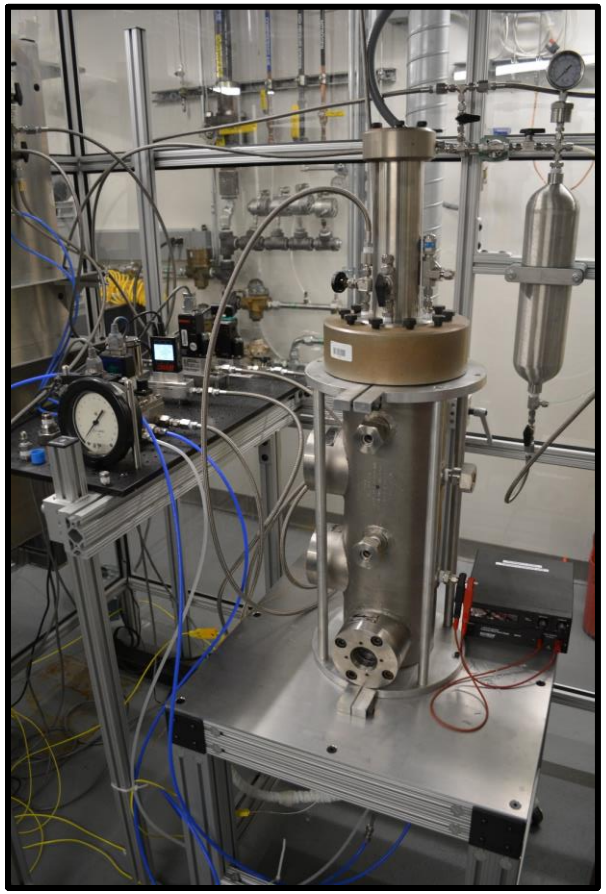
Scarce data available on NO_X formation in NH_3 flames at >>10 atm
Target system operation >20 atm
Allows evaluation of staged (RQL) NH_3 combustion



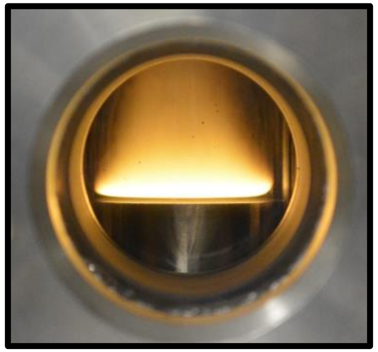


Burner Surface
~2400 holes, D=0.020”





Methane Combustion



Ammonia Combustion

Facility Preparations for High-Pressure Operation

RTRC configuration & capability:

- **425** to >500+ K preheat capability (>25-atm w/new heater install.)
- **10** to >20-atm pressure vessel & feeds … fuel, air, & N_2 chamber flow

Facility Preparations – Completed

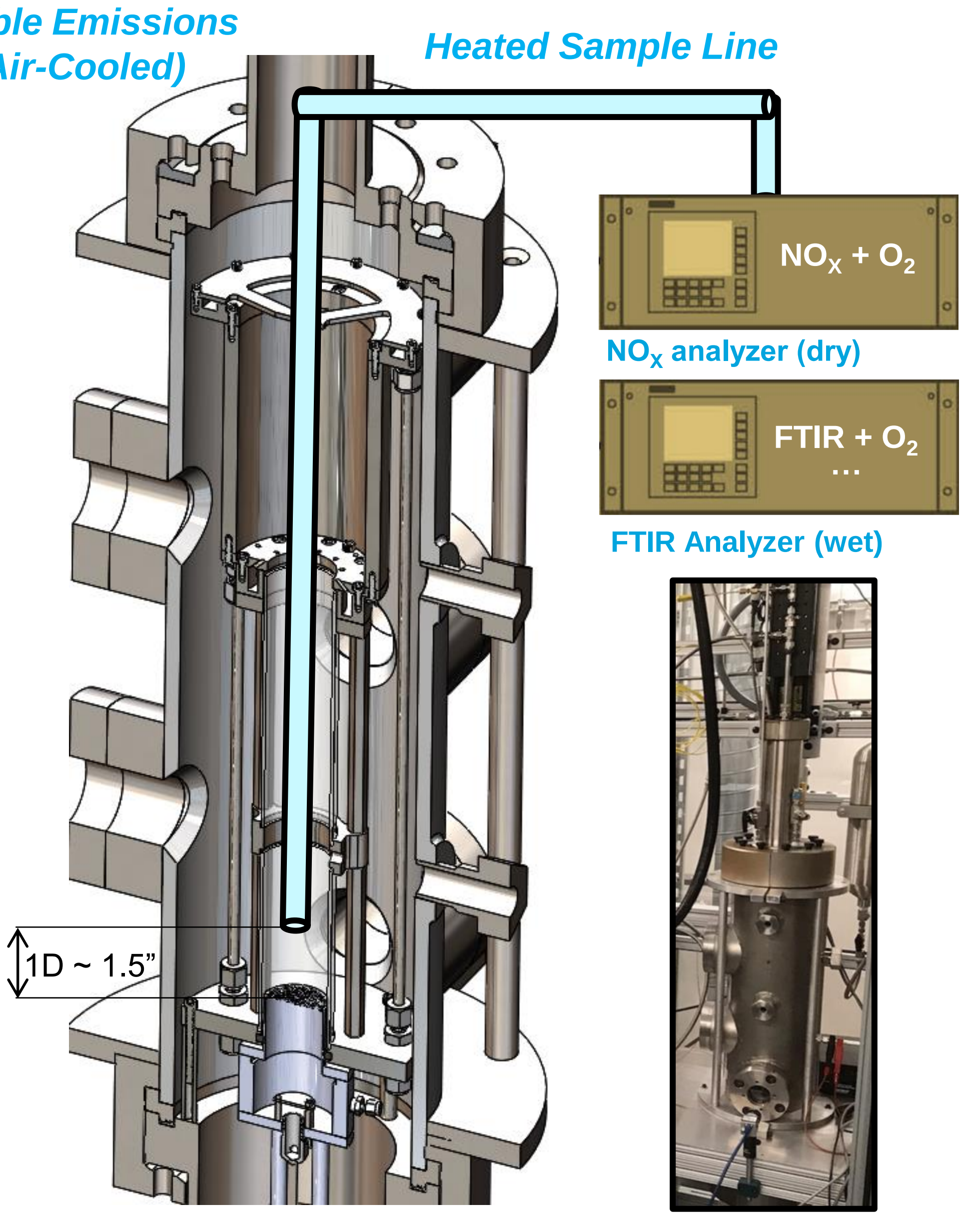
- High-pressure vessel w/ pass-throughs
- Ventilated experiment enclosure
- Interlocked PLC control system
- High-pressure air & N_2 supply
- Inlet air heater (low pressure)
- Remote flow control system for air, CH_4, NH_3, and N_2
- Backpressure valve for chamber pressure control

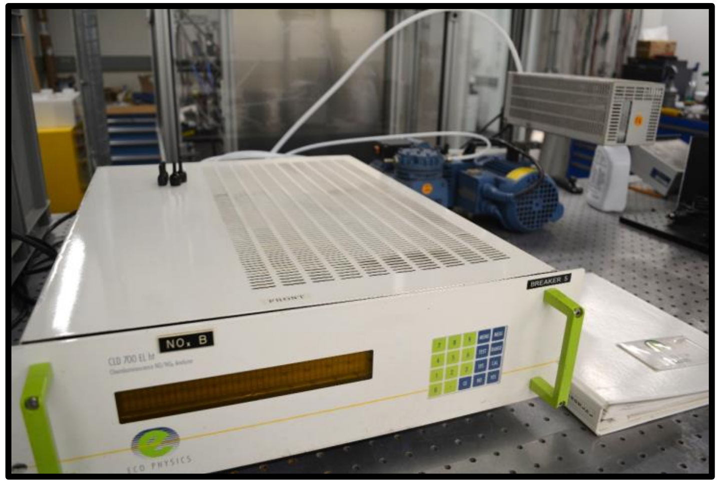
Facility Preparations – In Progress

- *Inlet air heater (high-pressure)*
- *High-pressure liquid ammonia pumping cart w/ refrigerated pumps*
- Heater controllers for air and NH_3 heaters

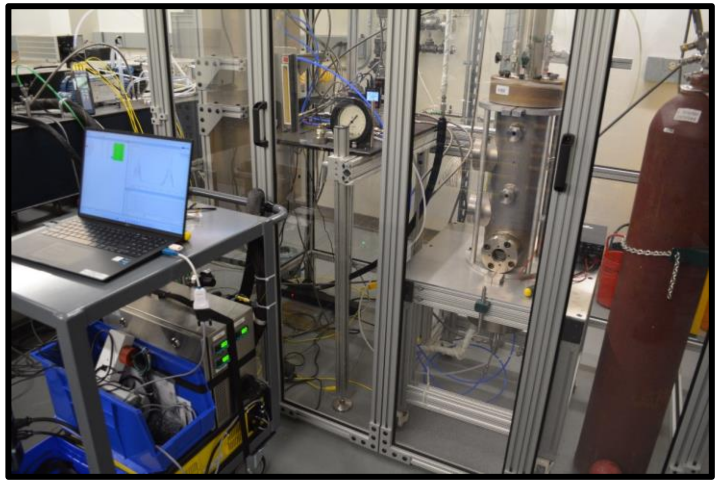
Emissions Sampling System

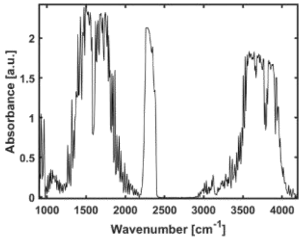
Emissions Sampling
- Air-cooled sample probe
- Probe traversable using translation stage system
- Heated sample line to prevent condensation
- NO_X analyzer system with ammonia scrubber & dryer
- Heated, NH_3 compatible FTIR system accepts wet sample
  - FTIR species: H_2O, NH_3, NO, NO_2, N_2O
- Sample chain can be easily swapped from conventional analyzer to FTIR system
- Sample probe can be swapped with B-type TC-probe for heat loss characterization





Conventional NO_X Analyzer

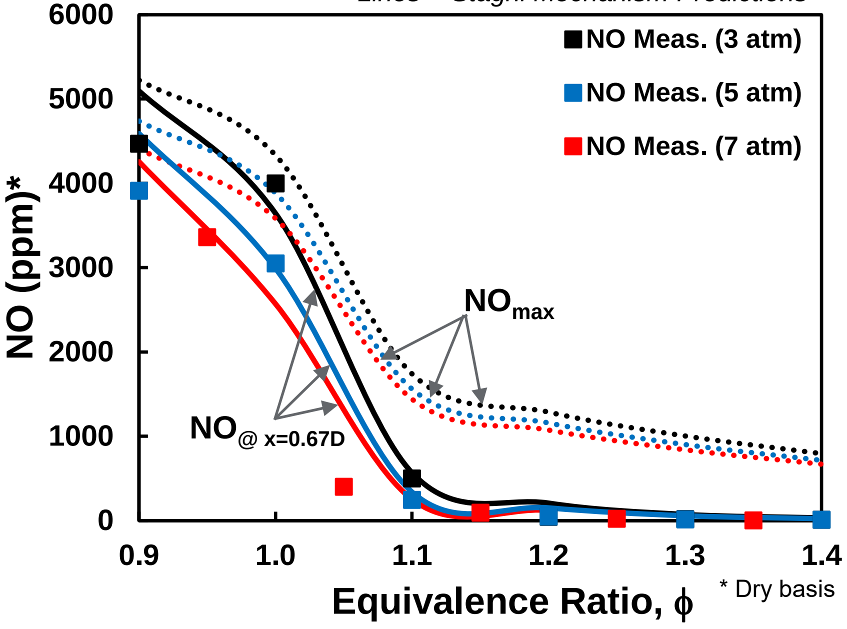




FTIR Analyzer & Sample FTIR Spectrum

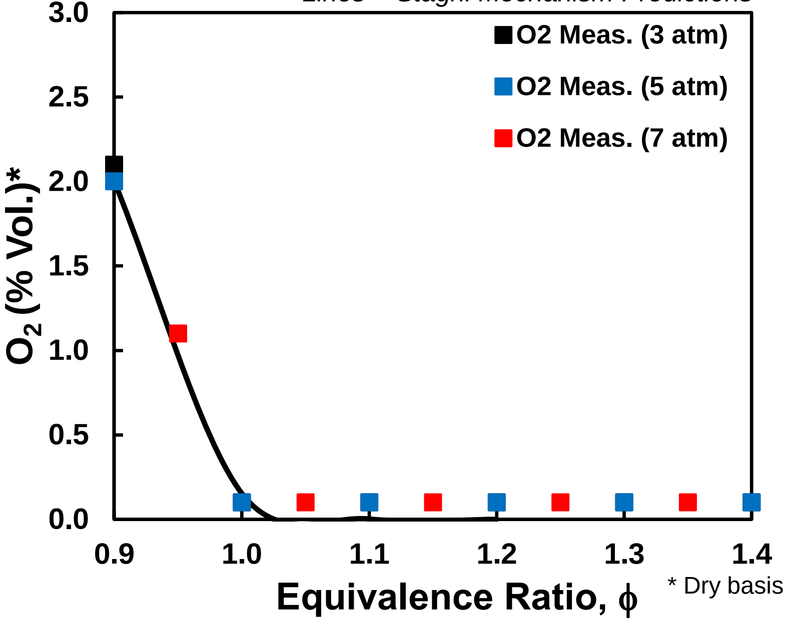
Flat-Flame NO_X Emissions Results – Moderate Pressure

Lines = Stagni Mechanism Predictions



* Dry basis

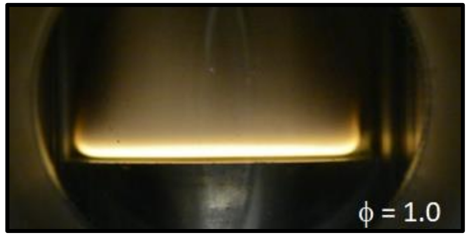
Lines = Stagni Mechanism Predictions

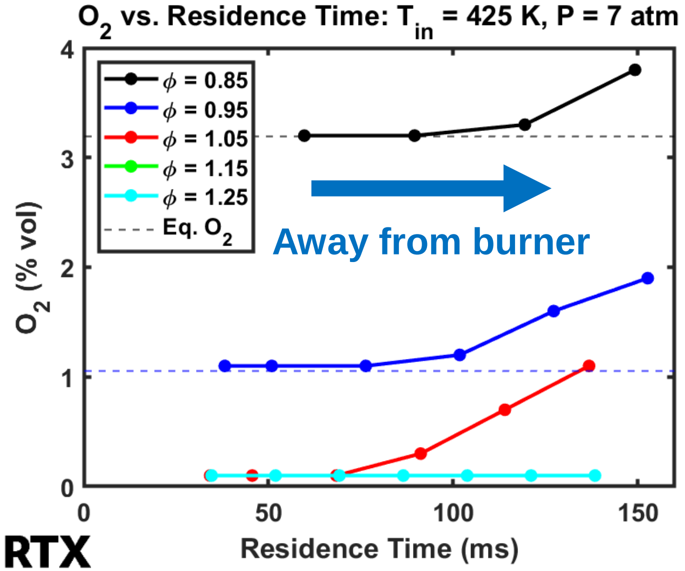


* Dry basis

- **NO_X analyzer used to collect emissions data across multiple pressure conditions**
- 425 K preheat, 9-15 cm/s burner velocity
- *x=0.67D* - 1D sample-probe location
- Stable burner operation achieved across pressures and equivalence ratios at 425 K
- Adiabatic flame model used w/ Stagni mech.
- FTIR data at select 7-atm conditions shows high NH_3 comb. efficiency (<75 ppm NH_3)

NH_3 / air flames
@ P = 3-atm





- Experimental challenges observed when translating probe to locations further from burner surface
- Measured oxygen concentration increases at locations further from surface
- Downstream cooling air entrainment is likely occurring
- **Further system optimization needed to reduce pathways for entrainment before additional measurements**

Next Steps for High-Pressure NO_X Measurements

Next Steps for Improved Emissions Data

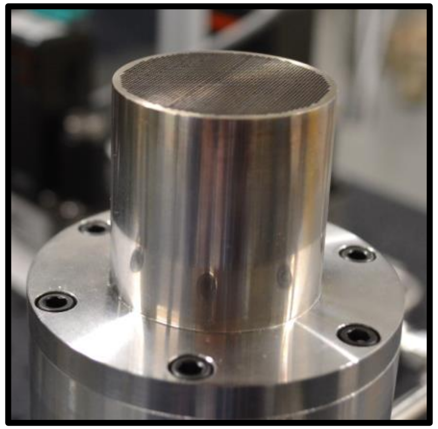
- Improve sampling/burner system for reduced air entrainment
- Collect additional data using NO_X/O_2 analyzer system to confirm reduced entrainment
- Collect temperature profile along centerline to characterize burner heat loss
- Collect additional emissions data using FTIR to measure other species

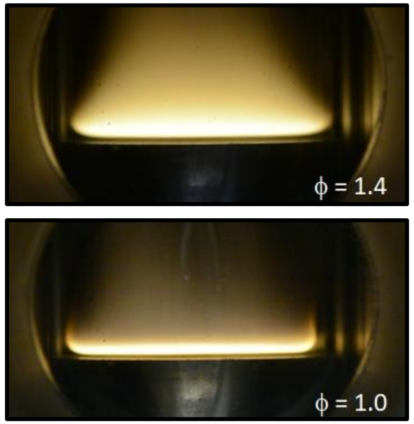
Improvements for Higher Pressure Operation

- Integrate high-pressure liquid pumping cart to allow higher-pressure gaseous NH_3 input
- Integrate liquid-pumping cart with existing PLC infrastructure
- Finish installing high-pressure-rated heater & controllers

Laminar burner operating well up to 7 atm

Further improvements underway to improve & validate data quality and achieve higher pressure operation >20 atm





BACKUP

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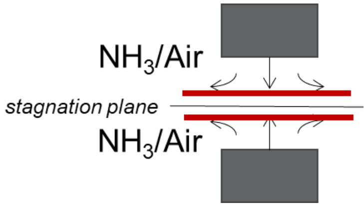
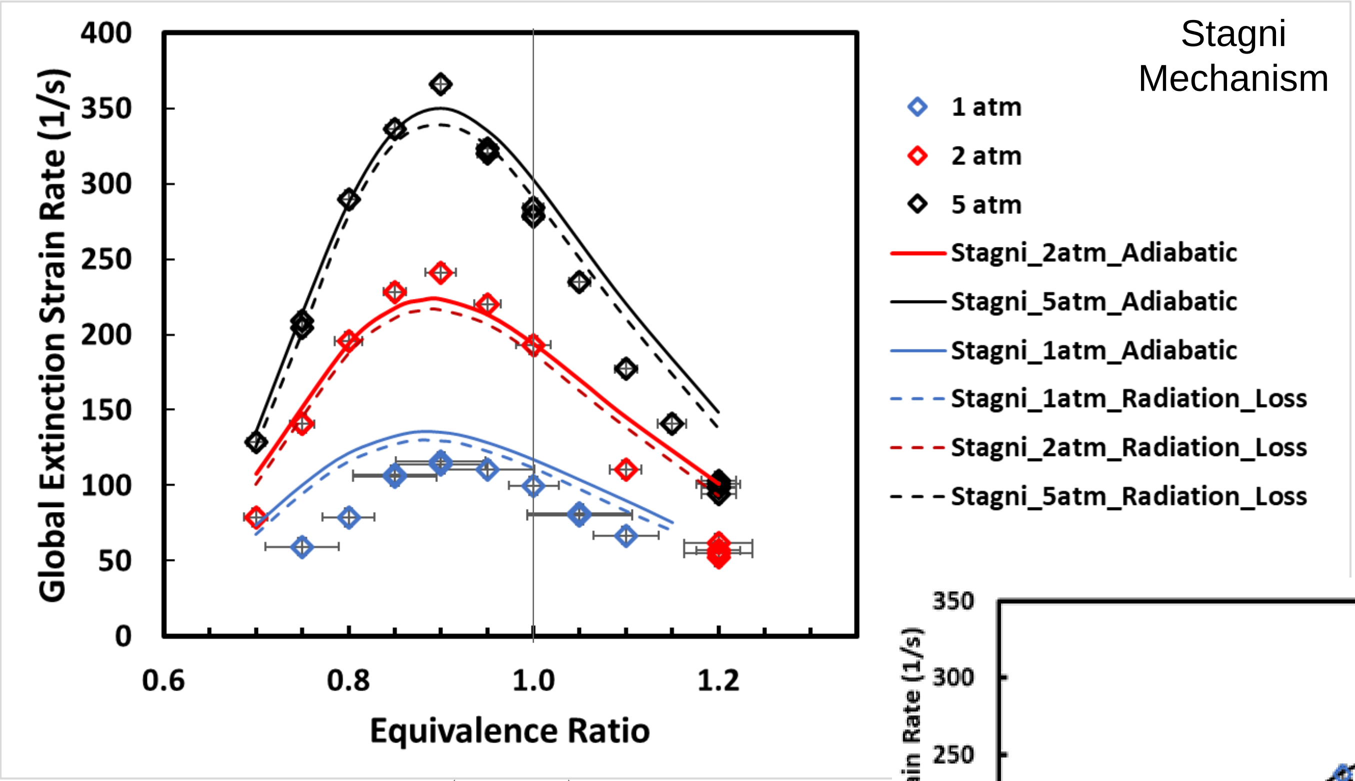
RTRC Predictions vs. UConn Measurements (1/2)



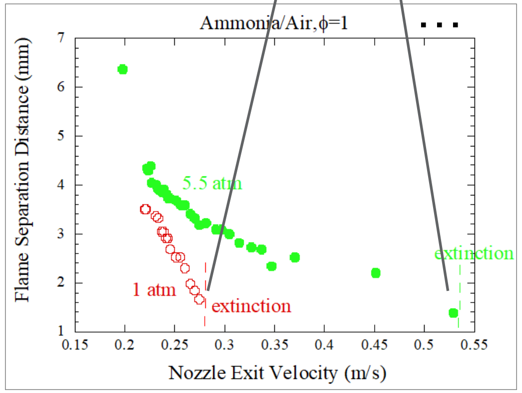


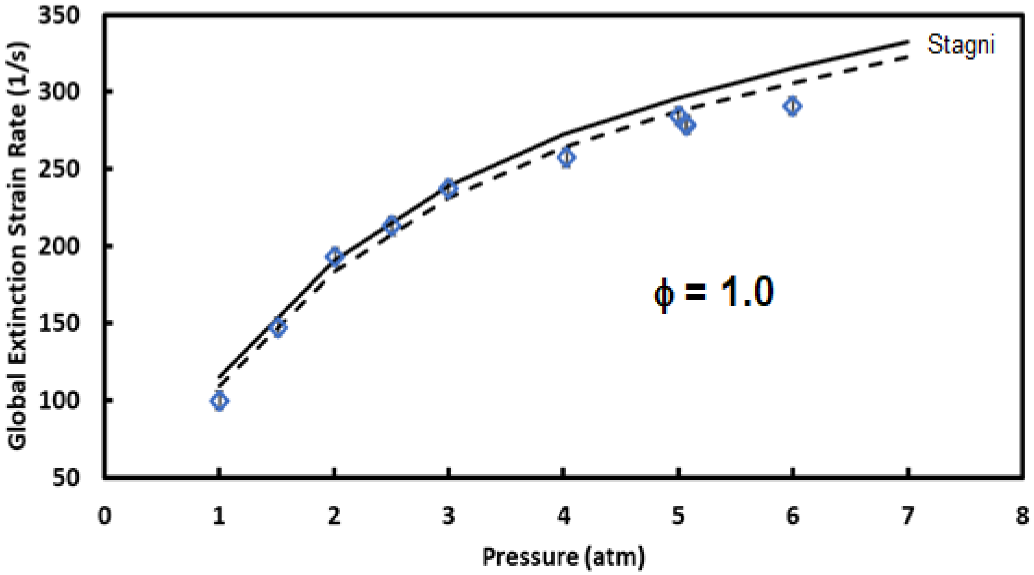
$$q_r = -4\sigma\kappa_p(T^4 - T_o^4)$$

Modified Counterflow Model scripts to account for radiative heat loss

Radiative heat loss per unit volume

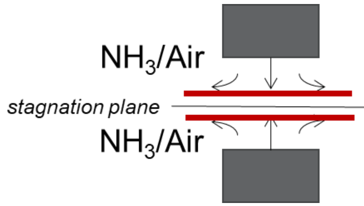
(σ = Stefan-Boltzmann constant, T_o = ambient unburnt reactant temp., κ_p = total Planck's mean absorption coefficient)

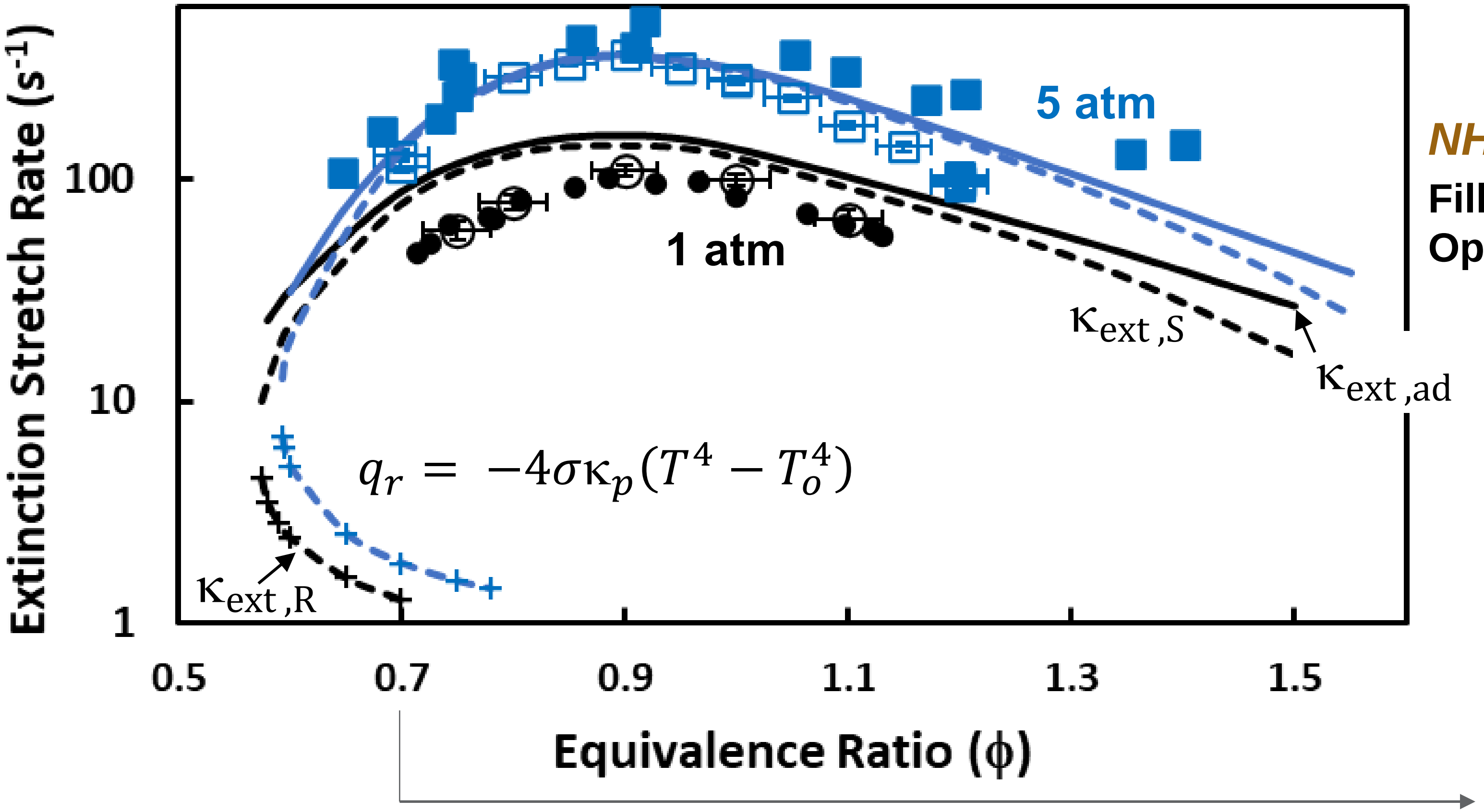




Roll–off in a_{EXT} with pressure (non–linear)

Counterflow NH_3 Flames w/Heat Loss → Impact & Lean Limit

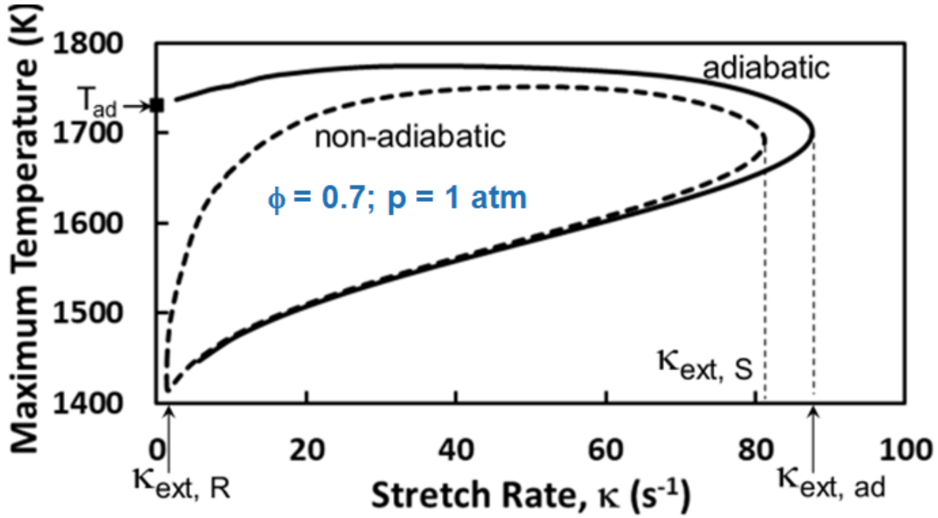




NH_3/Air Counterflow Flames

Filled Symbols: Colson et al. (2016)

Open Symbols: UConn Data (2023-4)



C-shaped curve for counterflow premixed fuel-lean, ammonia-air flames showing:

- **i.** adiabatic stretch-induced stretch rate $\kappa_{ext,ad}$ (solid line),
- **ii.** non-adiabatic stretch-induced stretch rates $\kappa_{ext,S}$ (dashed line), and
- **iii.** radiative-induced stretch rates $\kappa_{ext,R}$ (+ symbols).

Take-Away:

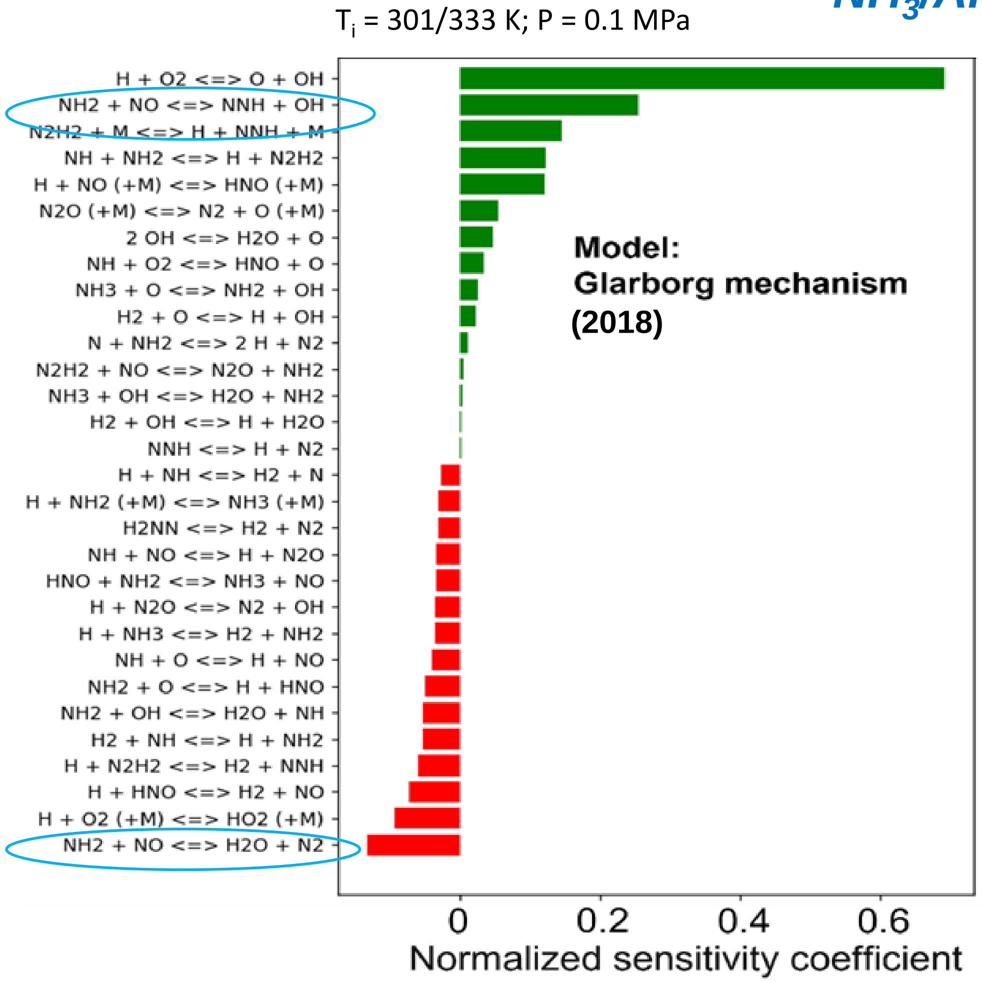
- **Heat-loss weakens low-burning-rate NH_3 flames**
- **Stretched high-burning-rate flames more robust**

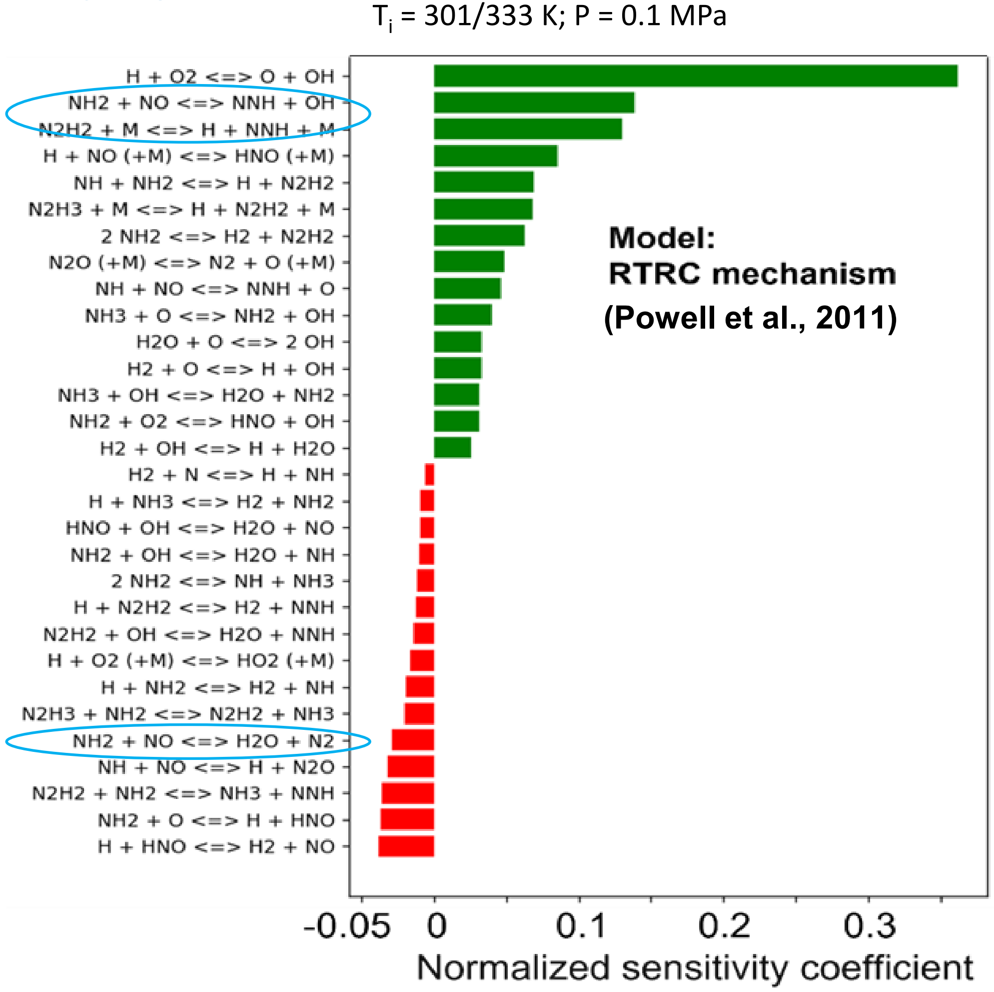
Fang, Papas, Sung, Stevens, & Smith, "Effects of radiative heat loss on extinction limits of counterflow premixed ammonia-air flames," Proceedings of the Combustion Institute, Vol. 40, doi: 10.1016/j.proci.2024.105569 (2024).

Feature Sensitivity to Extinction Strain Rate

$(1)\ NH_2 + NO \leftrightarrow N_2 + H_2O$
$(2)\ NH_2 + NO \leftrightarrow NNH + OH$
$(3)\ NH_3 + NH_2 \leftrightarrow N_2H_3 + H_2$

NH_3/Air Counterflow Flame





Sensitive rate constants:

NH_2/NO Interactions

$(1a)\ NH_2 + NO \leftrightarrow N_2 + H_2O$
$(1b)\ NH_2 + NO \leftrightarrow NNH + OH$

NH_i/N_2H_i Reactions

$(2a)\ N_2H_2 + M \leftrightarrow NNH + H + M$
$(2b)\ N_2H_3 + M \leftrightarrow N_2H_2 + H + M$

Sensitive and Uncertain rate constants

END