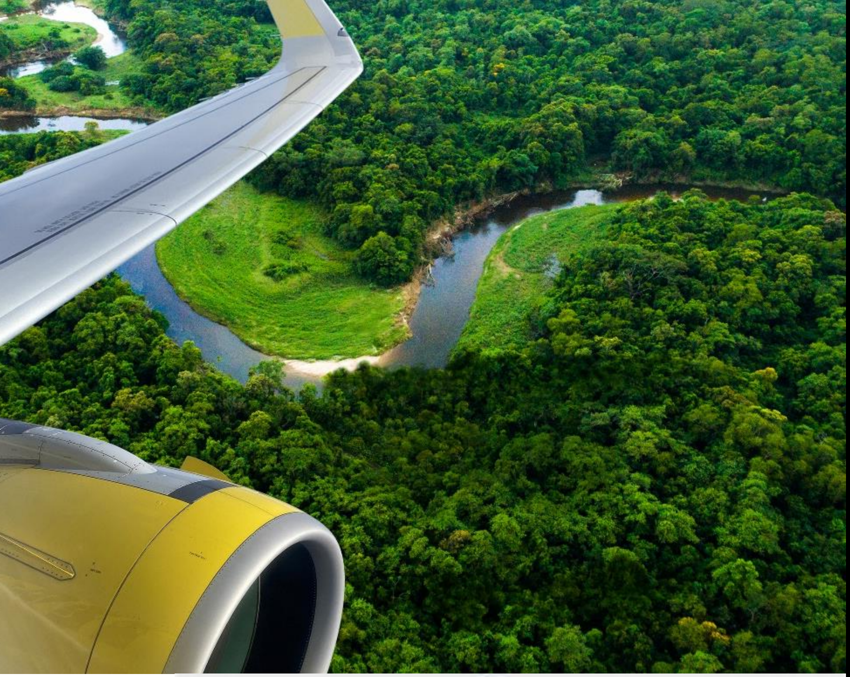

LOAD-Z

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

FT4000® Aeroderivative Dual Fuel Gas Turbine Engine.

RTX Technology Research Center

2024 FECM/NETL Spring R&D Project Review Meeting
April 24, 2024

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

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UNIVERSITY OF CONNECTICUT

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

RTX

COLLINS AEROSPACE | PRATT & WHITNEY | RAYTHEON

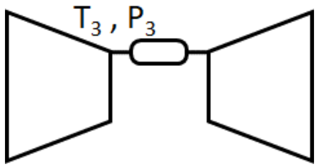
Key Project Goals …. WHAT / WHY

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

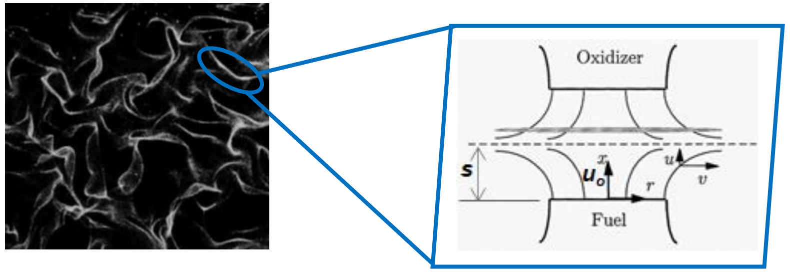
(1) *EXPERIMENTS* *4 lab-scale facilities*

– Fundamental NH_3 flame data relevant to turbines:

- P, T >> ambient → relevant to compressor exit conditions …..



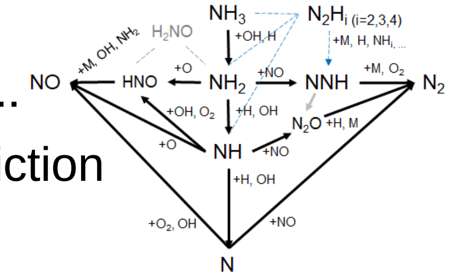
- strained & turbulent flames …. …. ….
  - *Targeted outcome*: expand published data w/ new, useful data (previously unreported)



(2) *MODELING*

– Predictive capability for NH_3 combustion & emissions

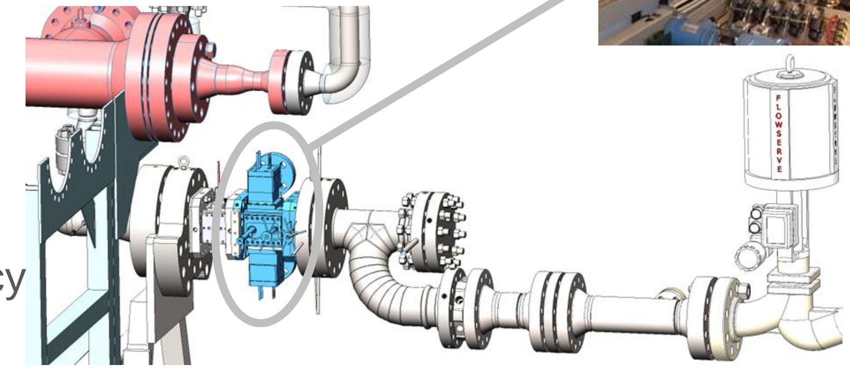
- NO_X formation kinetics integral w/ NH_3 comb. kinetics …..
- CFD of turb. NH_3 flames w/ NO_x & NH_3 slip (η_{COMB}) prediction
  - *Targeted outcome*: capability for GT combustor design



(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 & Progress …. HOW

- 4-year PoP: Oct. 2022 – Sept. 2026 (currently at year-1.5)
- \$3.3M Federal DOE funding
- \$0.9M Customer funding - RTRC & UConn (21.8% cost-share)

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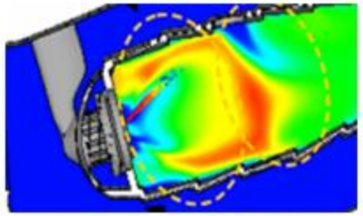
Year-4

Year-3

Year-2

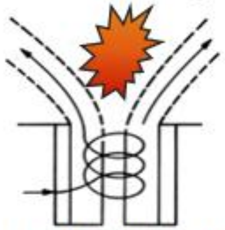
Year-1

Time

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


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



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

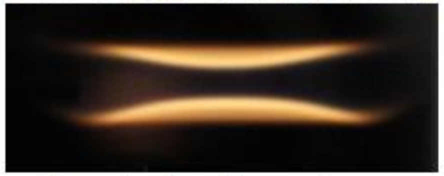
Modeling:

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

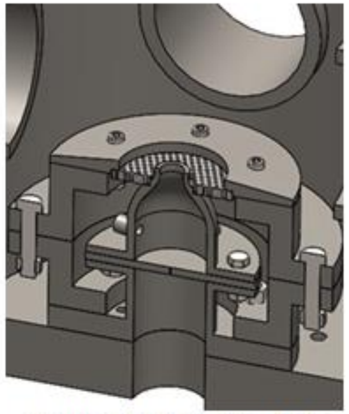
- CFD & validation
- Turb. models for NH3 comb. & NOx (no post-process.)

- CRN modeling
- Counterflow
- Kinetic mech.

UConn

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



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

- **Outcomes/Publications (to-date):**
  - *Proceedings of the Combustion Institute* – 40th CI Symposium paper in press for July 2024
  - *AIAA SciTech 2024* – paper # AIAA-2024-2019 (DOI:10.2514/6.2024-2019)
  - *Combustion Institute Meetings – 2023 US National & ESS Spring 2024* meeting papers

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1st Technical Task …. EXPERIMENTS ……………….

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

(1)
EXPERIMENTS
4 lab-scale facilities

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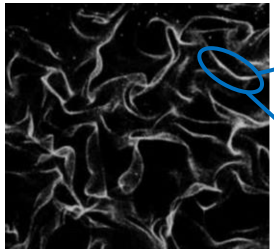

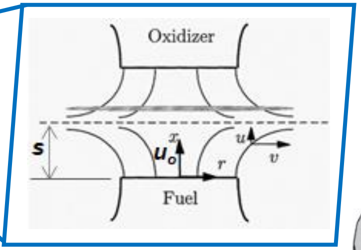

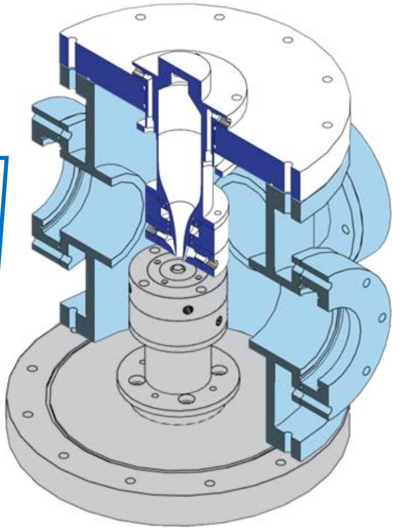

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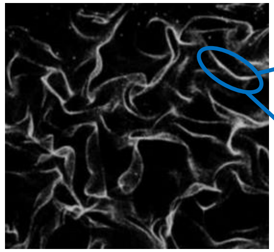
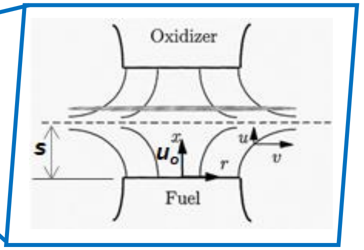
Lab-Scale Experiment #1: Counterflow Flame Rig | *Laminar (2D)*

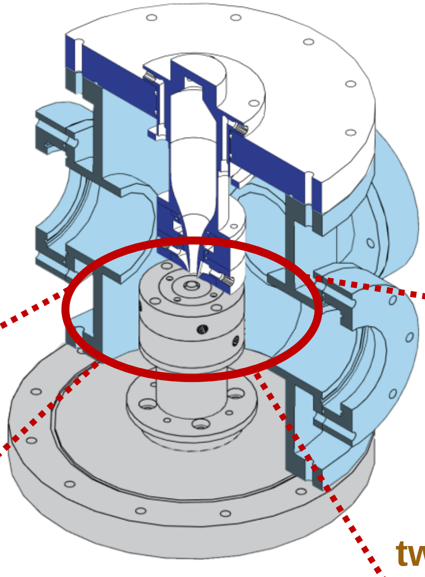
Relevance:
- Scarce data on NH_3 flame extinction, esp. @ P, T > ambient.
- Stringent test of kinetic mechanisms, for comb. model development
- Canonical representation of turbulent "flamelet"

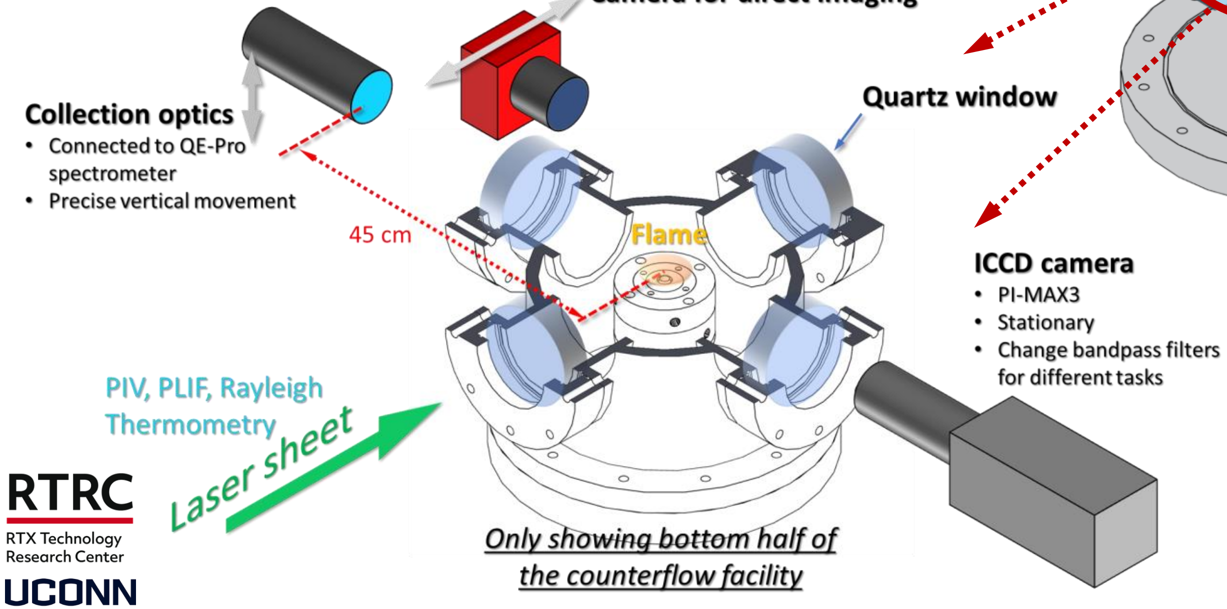


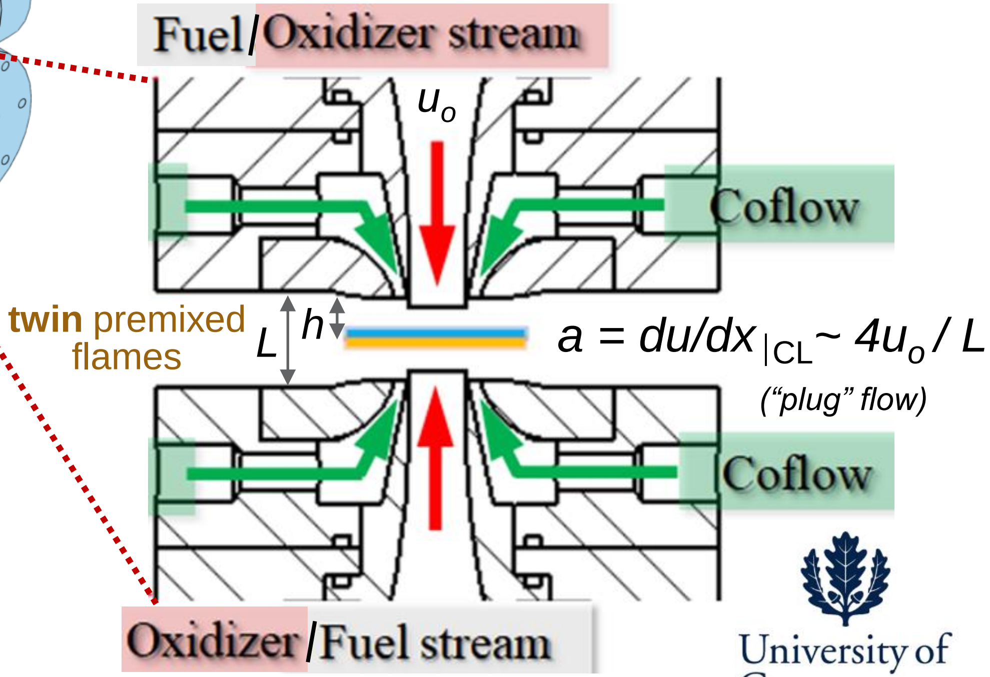


UConn configuration & capability:

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







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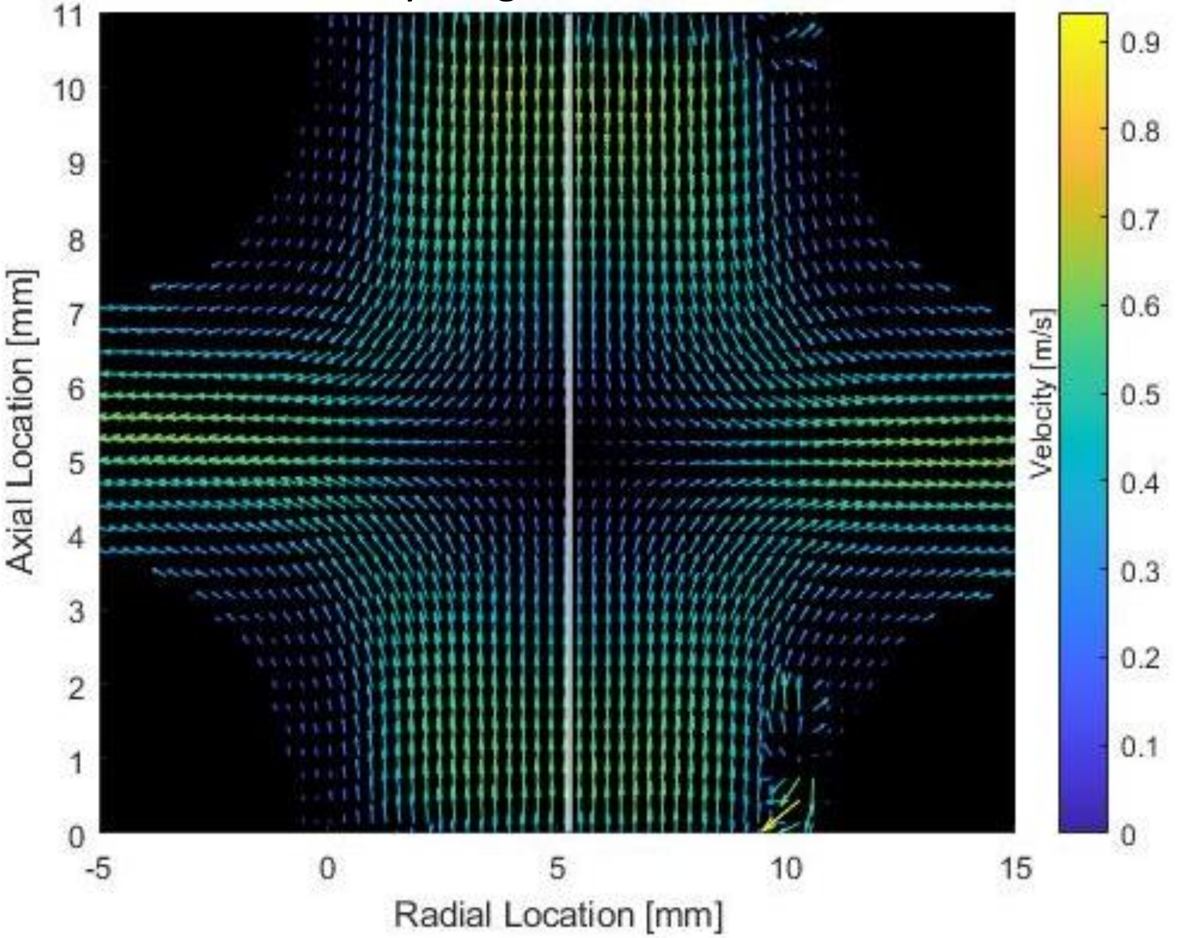
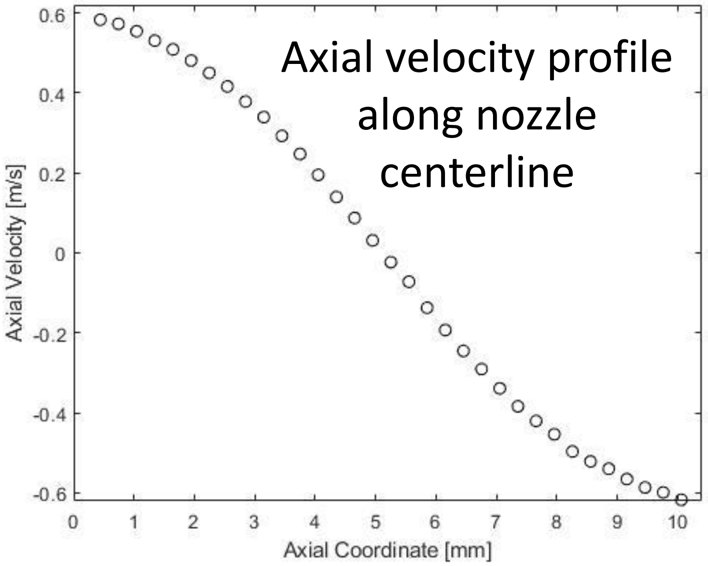
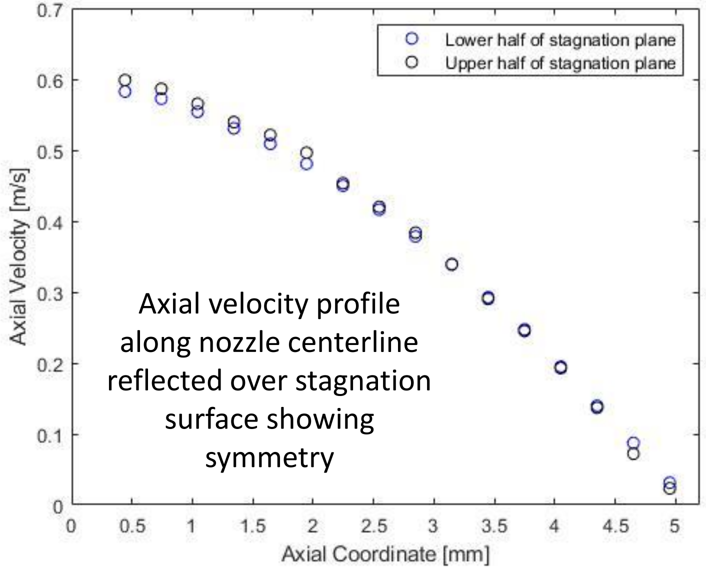
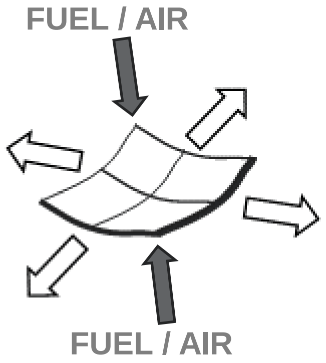
Counterflow Experiments – Measure Flow Uniformity & Strain

Velocity magnitude vector field









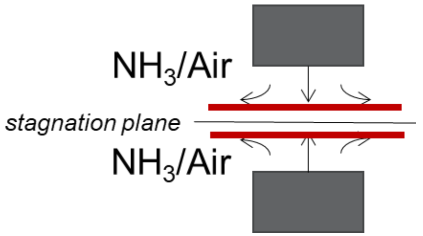
Flame stretch:

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

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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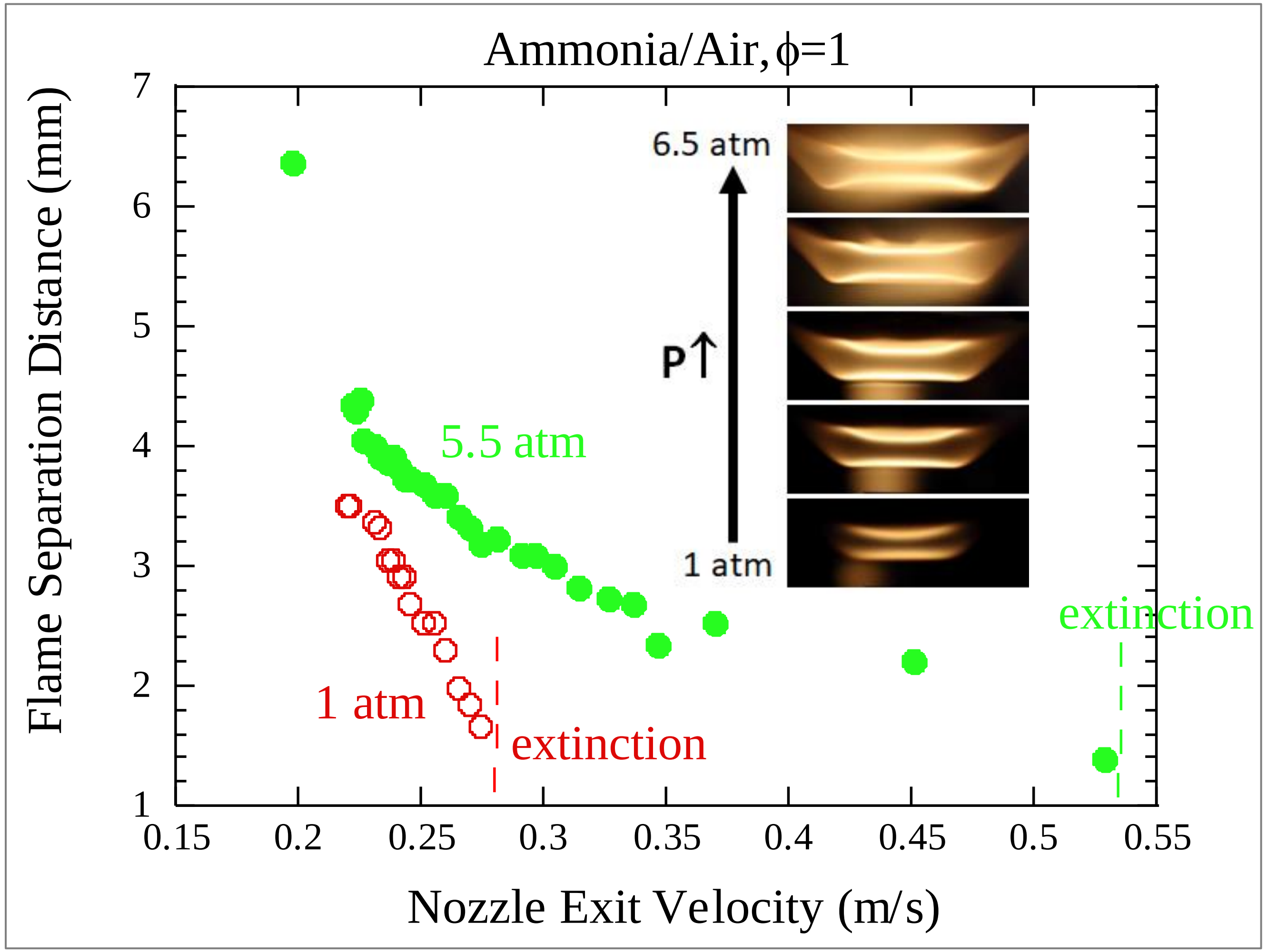
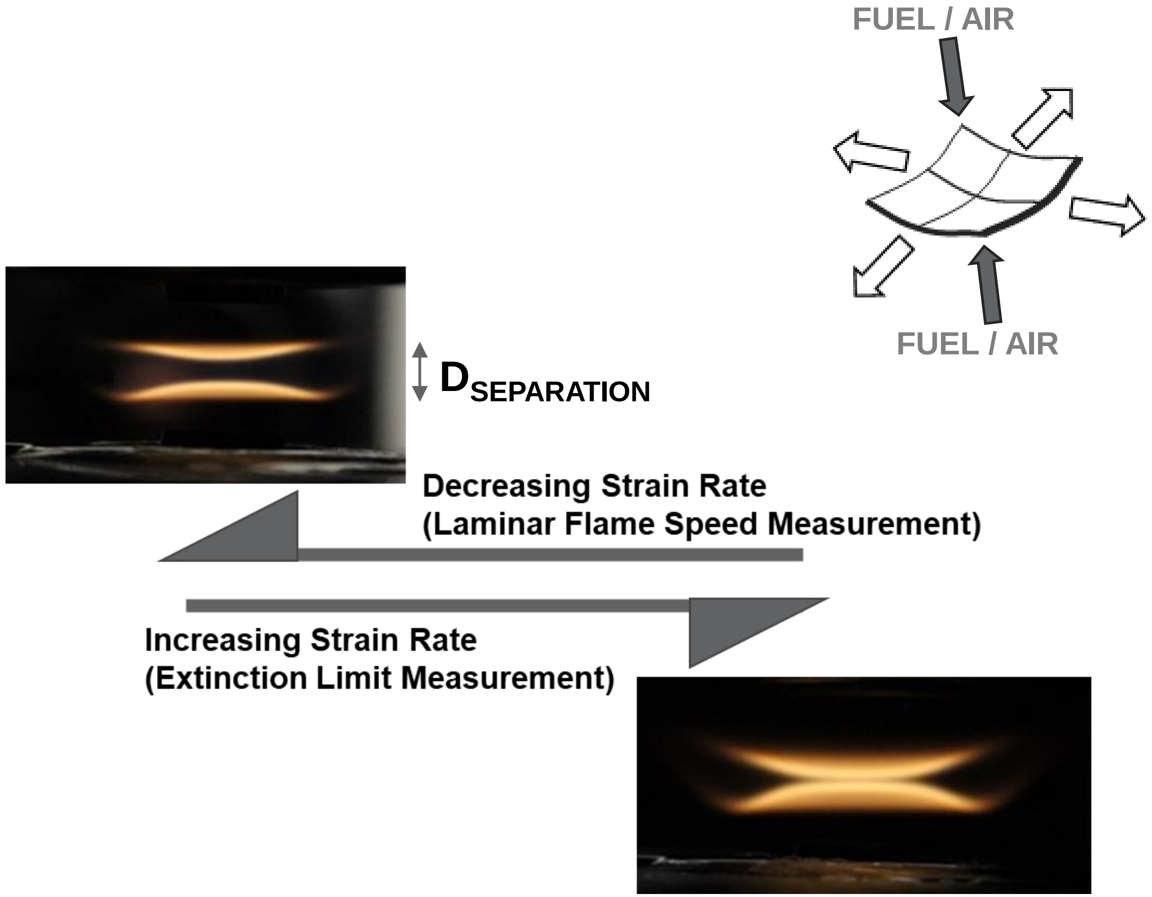
Counterflow Experiments – Procedure for Measuring Extinction





Sequence:

...for both experiments & modeling

- 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 → $\frac{4U_{EXT}}{L} = a_{EXT\_GLOBAL}$

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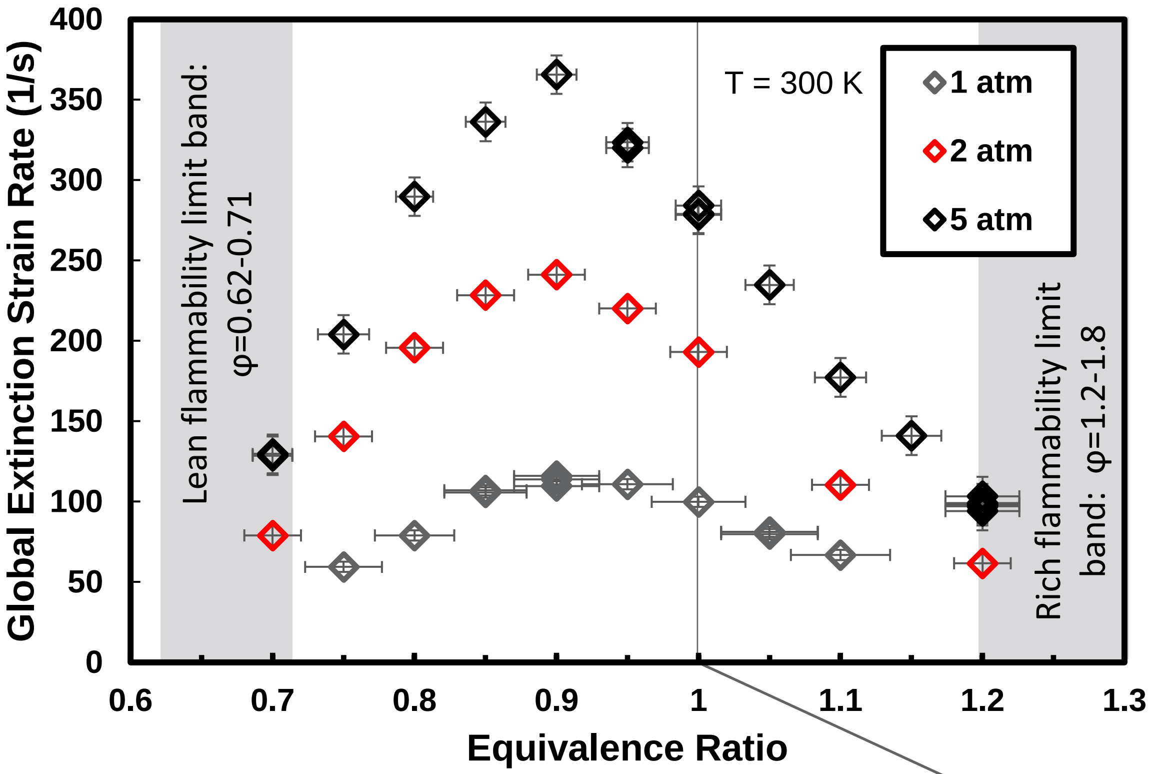
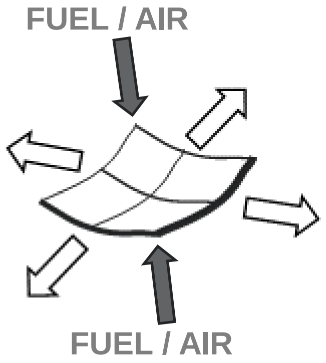
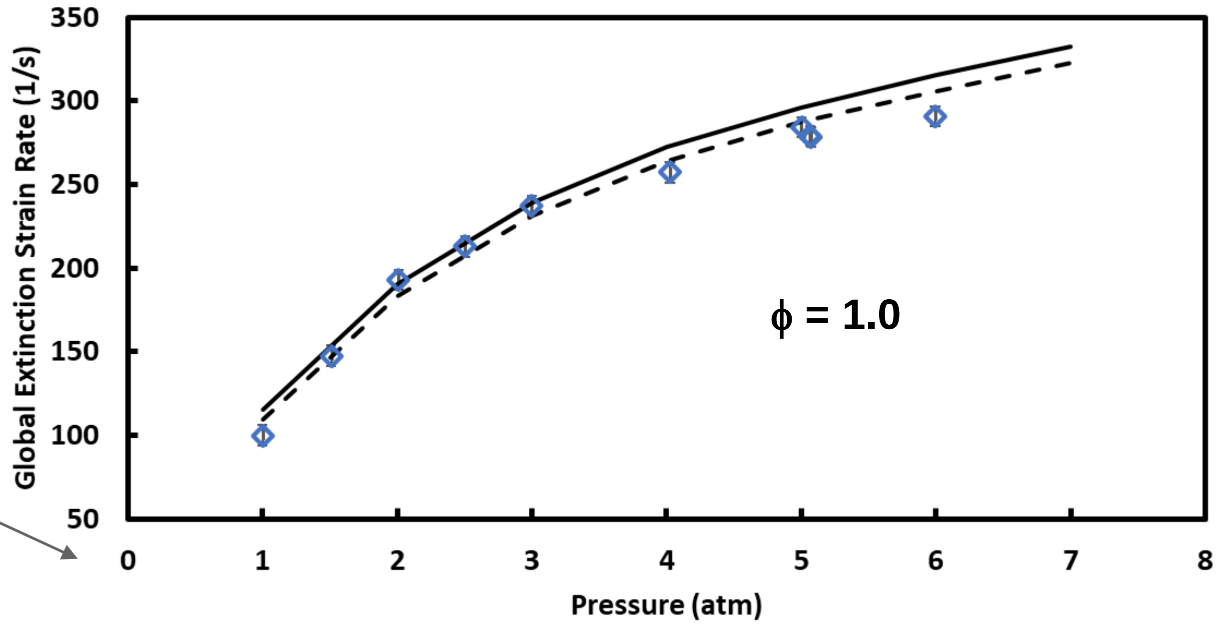
Counterflow Experiments – Extinction Strain Rate vs. ϕ, p







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

Accuracy / Error Assessment:

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

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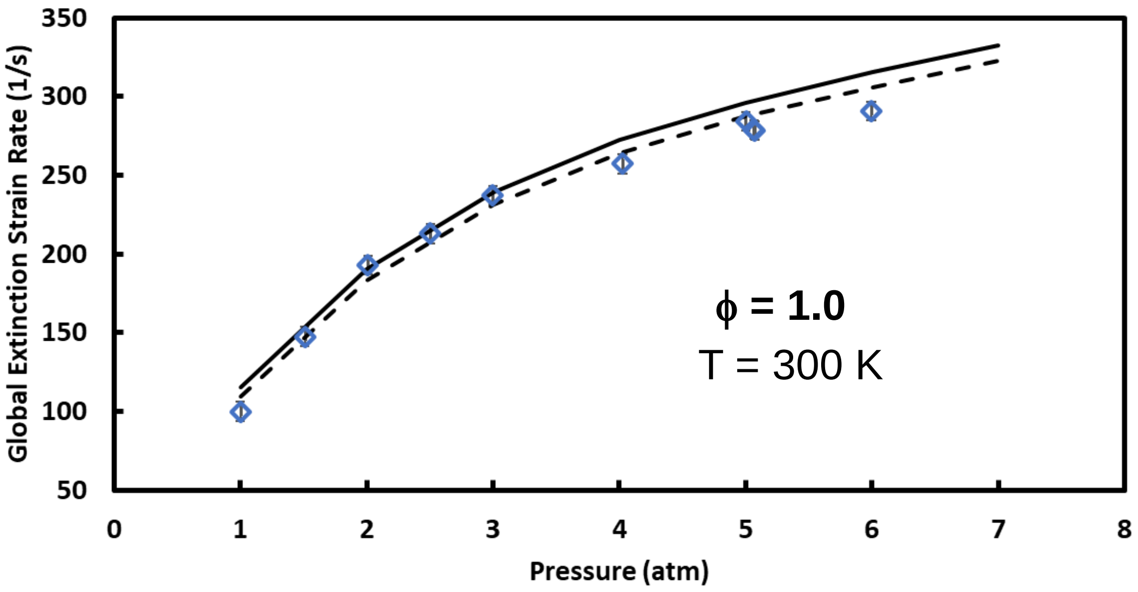
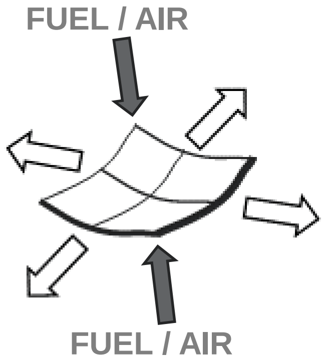
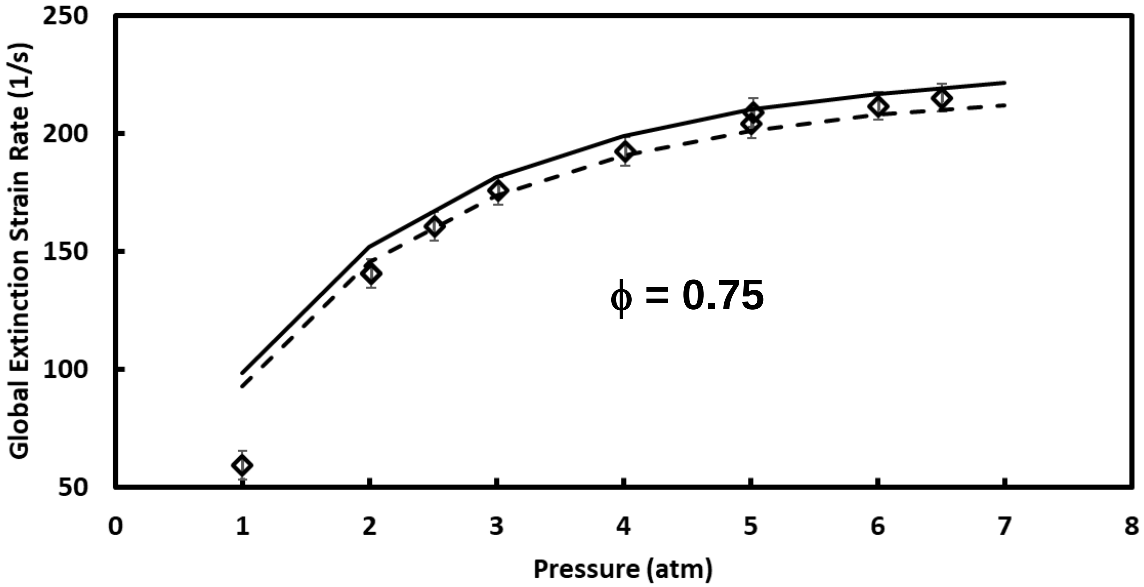
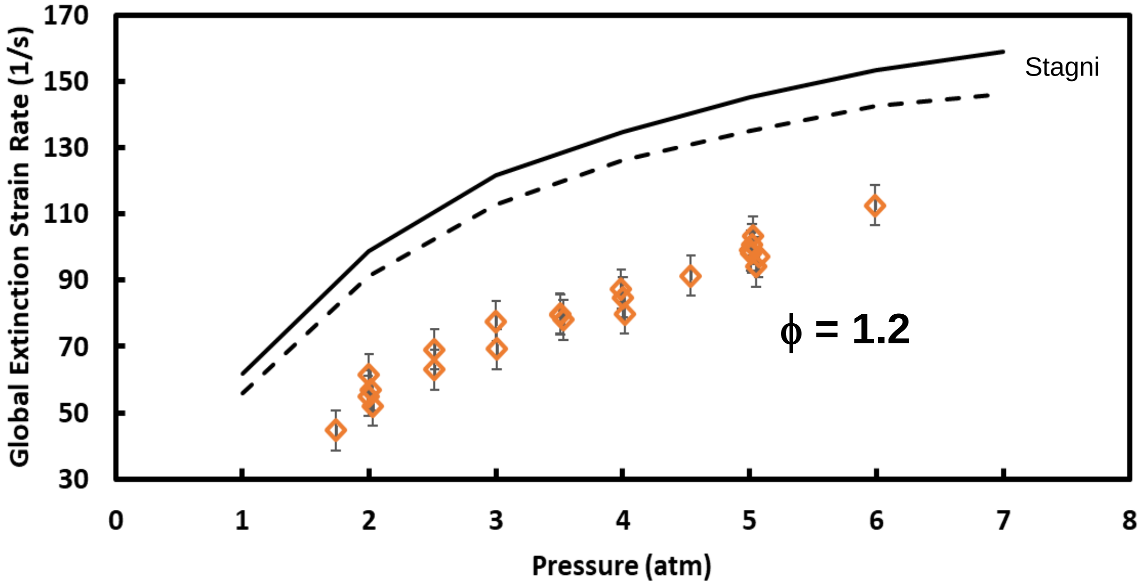
Counterflow Experiments – Pressure Effect on Extinction (3 ϕ's)









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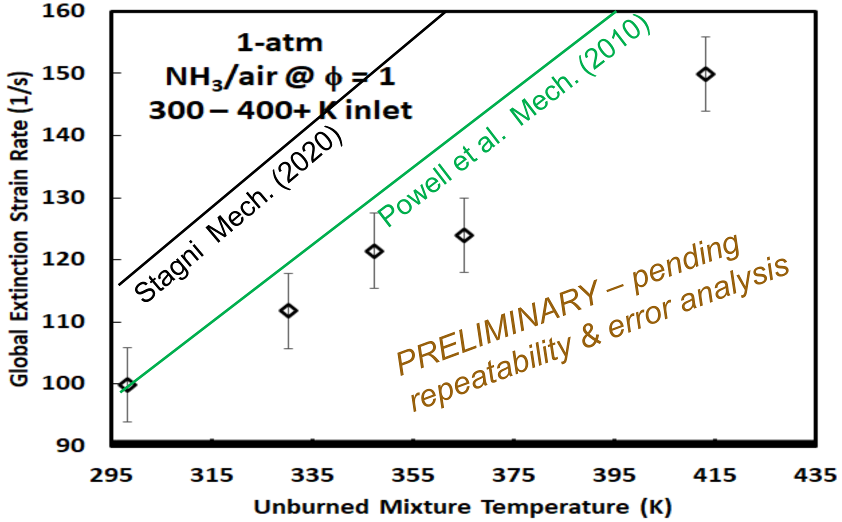
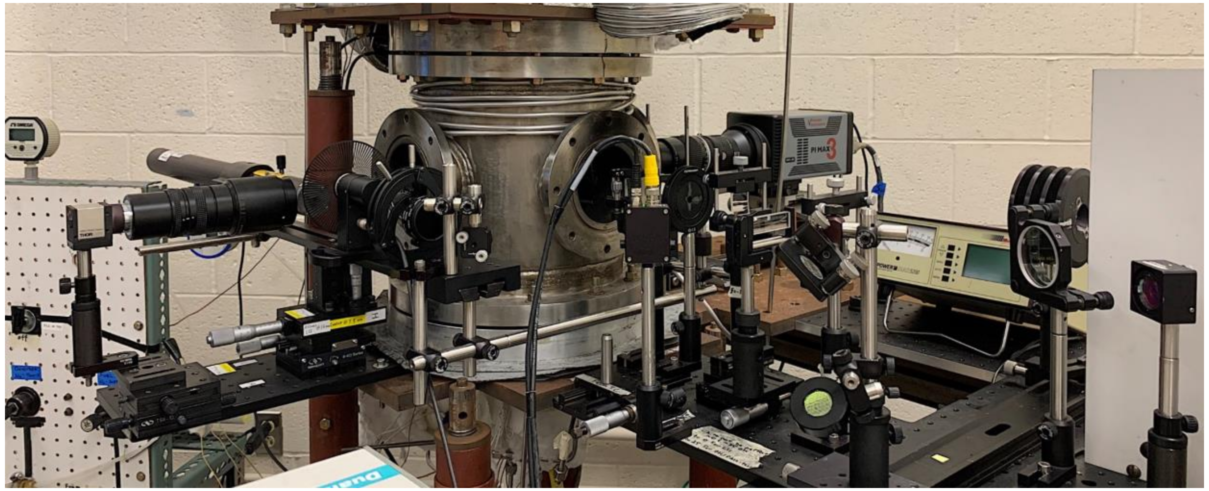
UConn Next Steps – T_{INLET}↑, PIV … Turb. Flame Speed Rig

Ongoing Counterflow Flame Rig Work:

- PIV measurements for local velocities → S_L & a_{EXT}
- 300K to 500K T_{INLET} experiments → a_{EXT} vs. T, P, ϕ





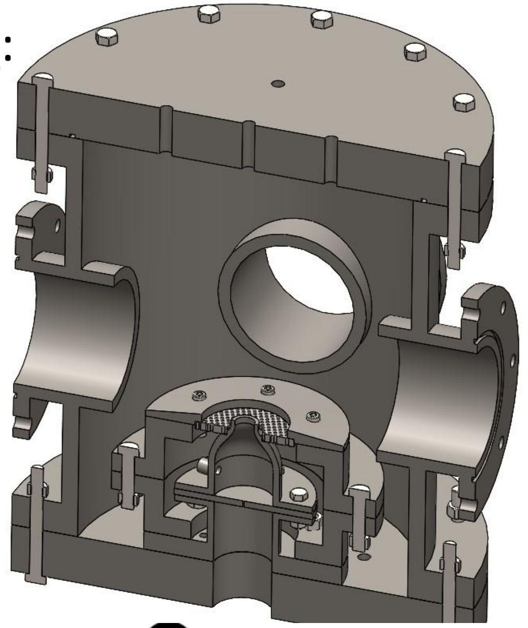
Q3- Fabricate **Turb. Flame Speed** Rig:

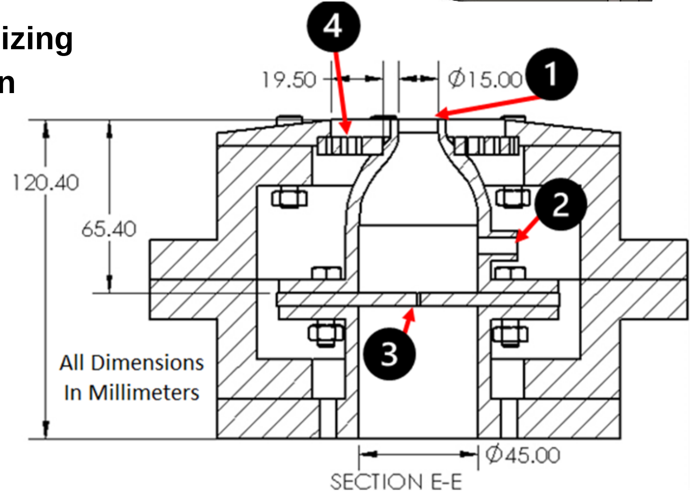
Turbulent intensity range: 15–25%

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.



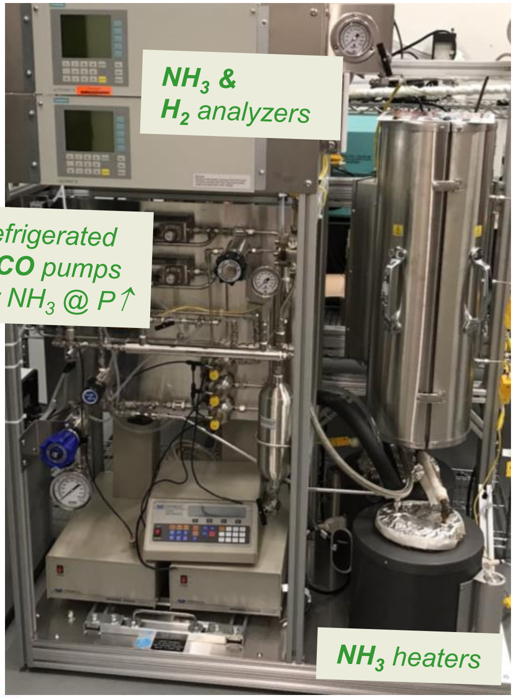


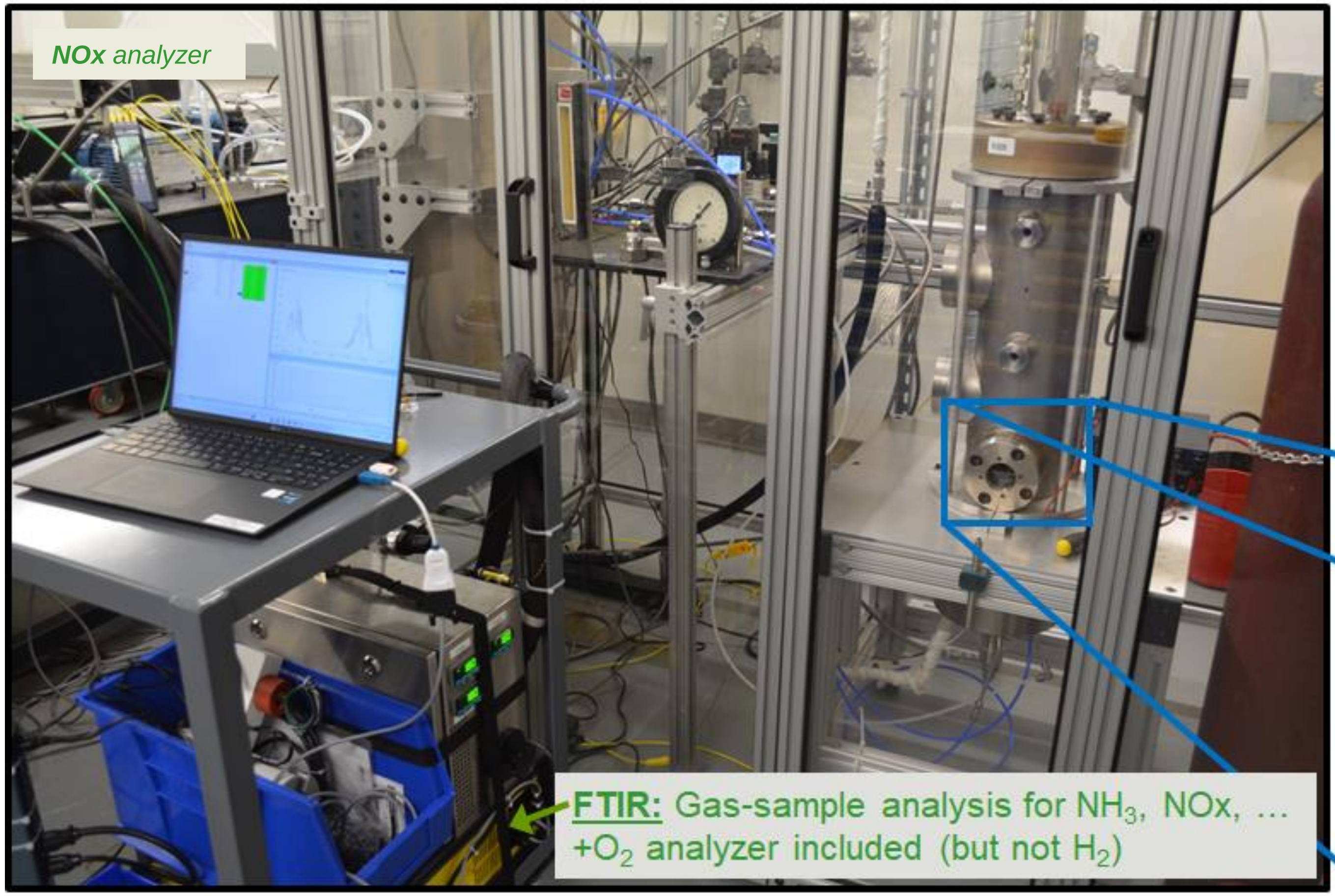
Lab-Scale Experiment #2: High-P Flat-Flame Rig | *Laminar (1D)*

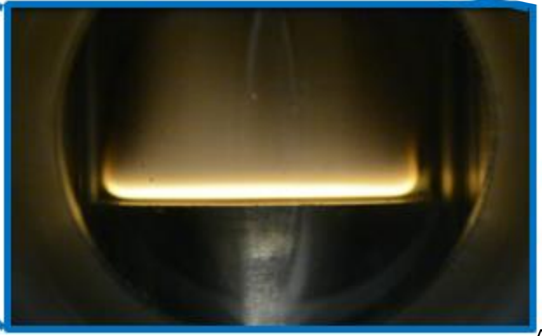
Relevance:
- Scarce data on NH_3 flames & NOx formation at >>10-atm.
- Capability to evaluate staged (RQL or "RRQL") combustion of NH_3

RTRC configuration & capability:

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

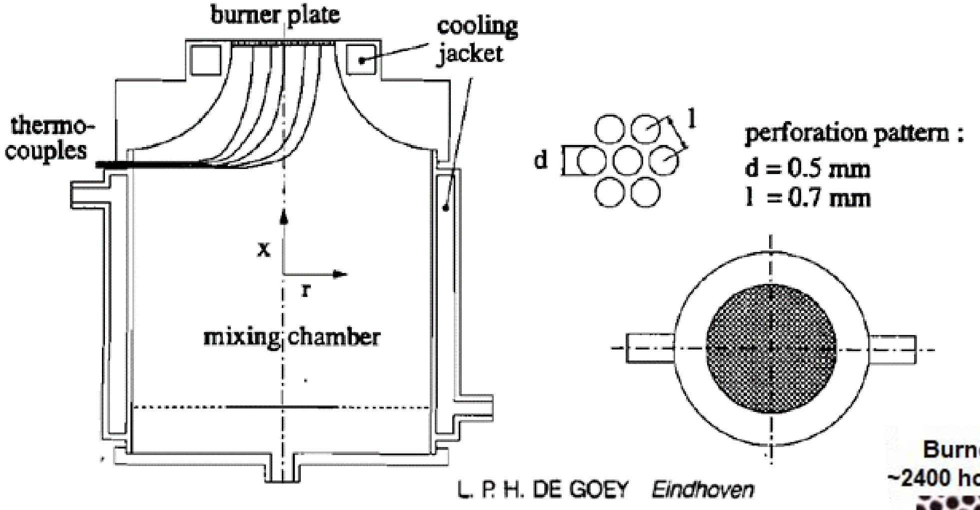




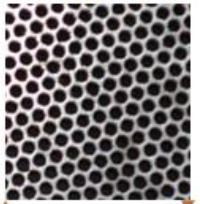


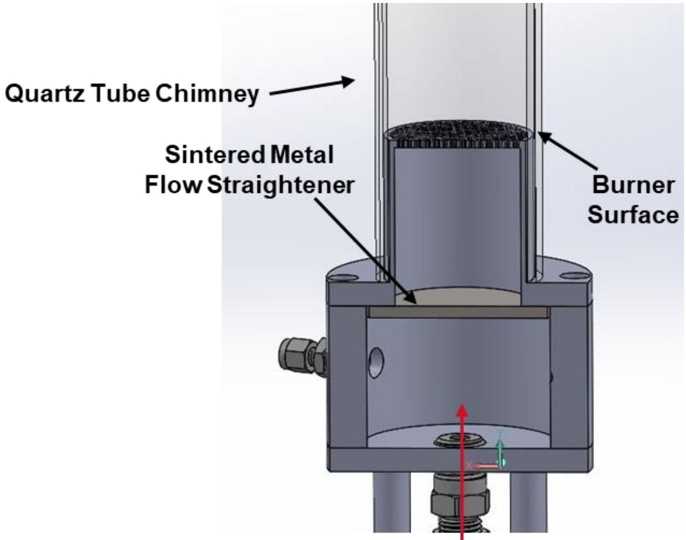
Viewport
NH_3 flame (ϕ = 1.0) at 3-atm pressure

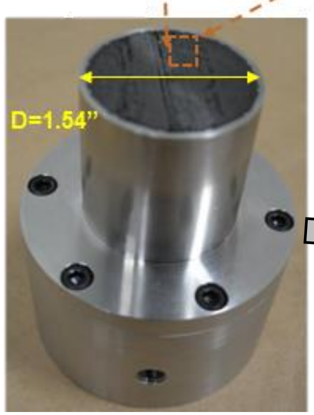
Flat-Flame Exper. – Premixed “Adiabatic” Burner & Emissions



Burner Surface
~2400 holes, d=0.020”

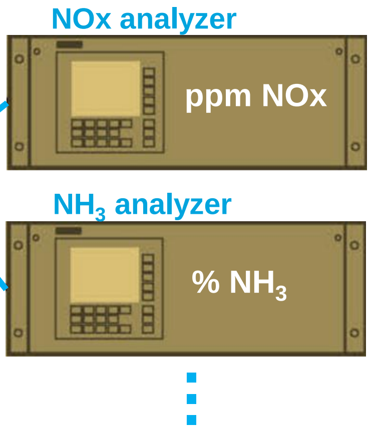






Traversable Emissions Probe (Air-Cooled)

FUEL / AIR



CH_4-Air	100% NH_3-Air
	
Ambient Inlet Temp. (<100F)	Heated Inlet Temp. (~200F)

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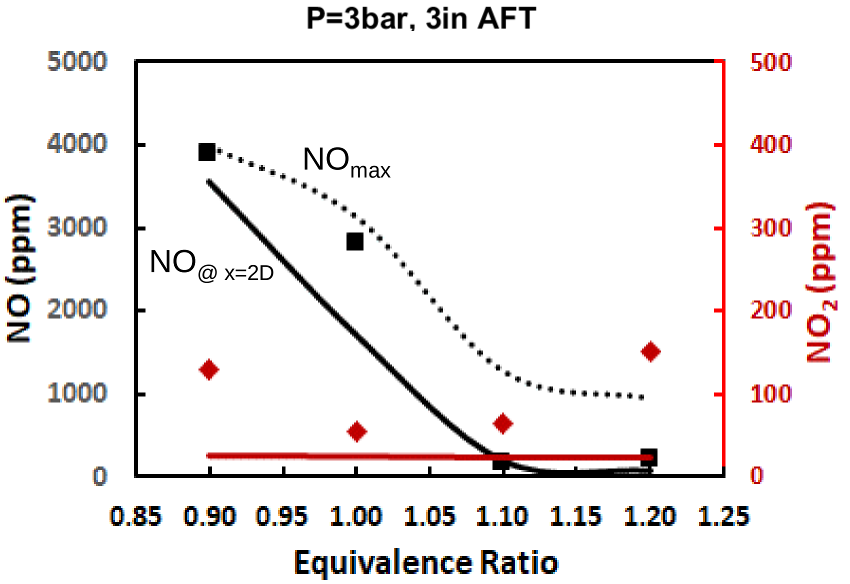
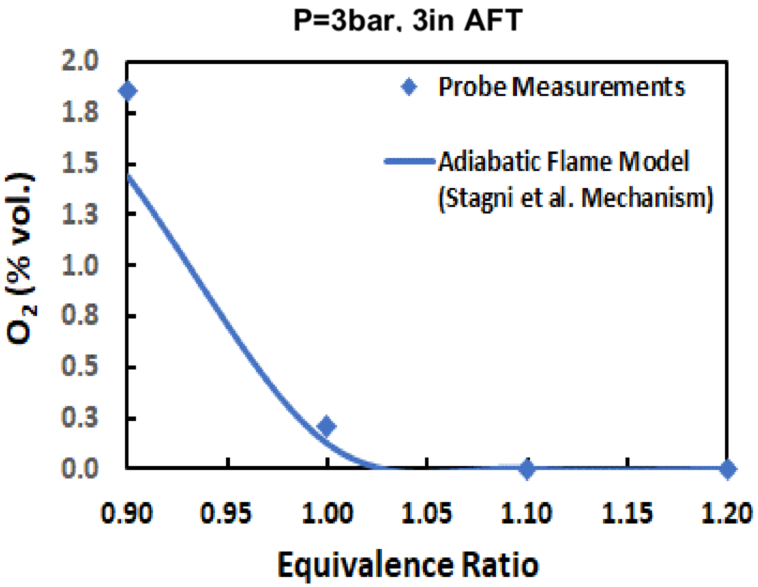
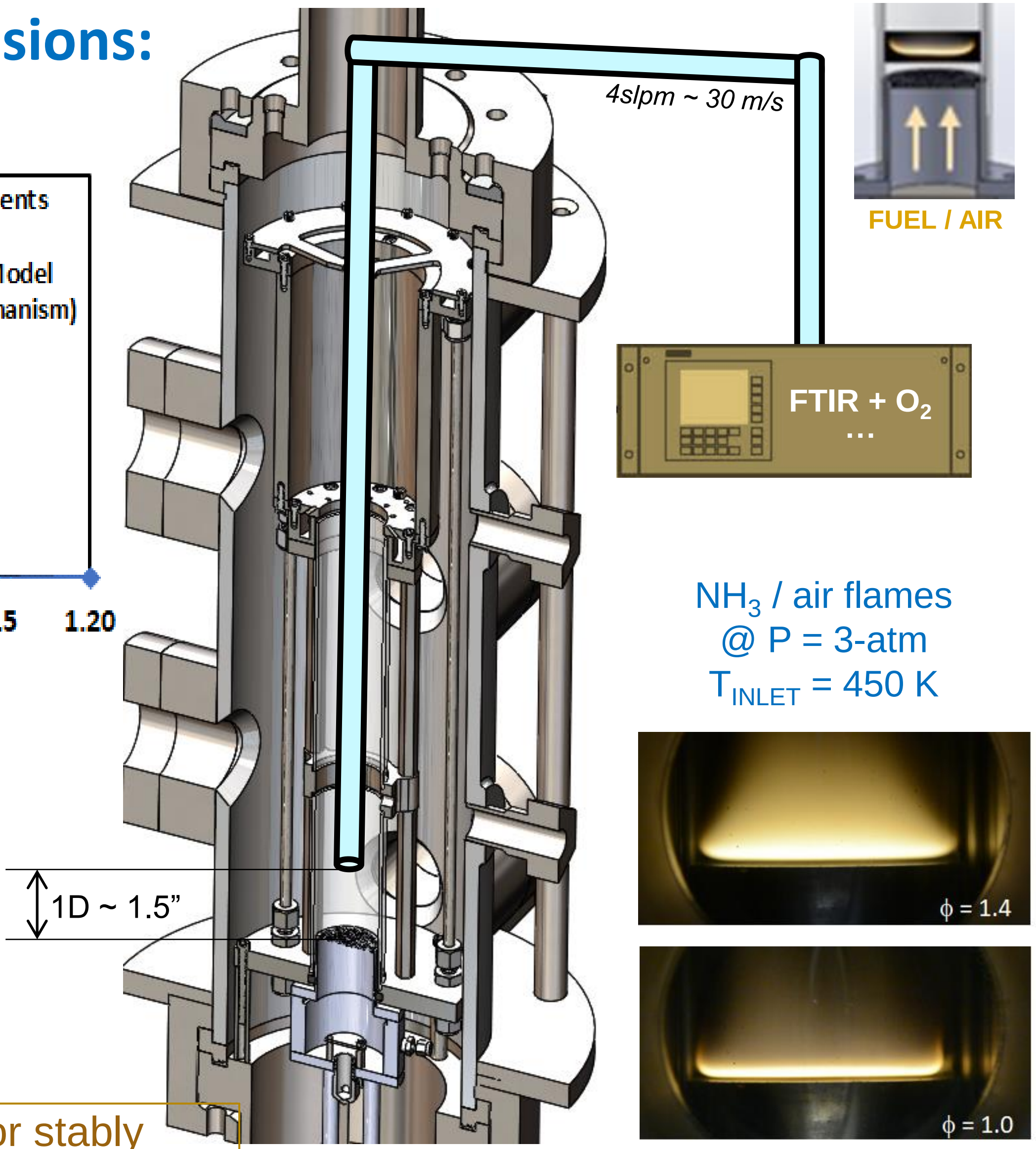
Flat-Flame Experiments – FTIR Measurements of NOx & NH_3

Measured NOx Values – Rich vs. Lean NH_3 Flame Emissions:







- 450 K preheat
- 12 cm/s burner face velocity
- τ ~ 60 ms to 1D sample-probe location

- NEXT STEPS: - NH_3 & air preheat ↑ as P ↑ for stable flat flames
  - Rich, lean, & staged NOx / NH_3 studies vs. P, T
  - Burner instrumentation & Q_{LOSS} characterization / control

Note NH_3 flames do not anchor stably w/out preheat, especially @ P > $P_{AMBIENT}$

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2^{nd} Technical Task …. MODELING ………………

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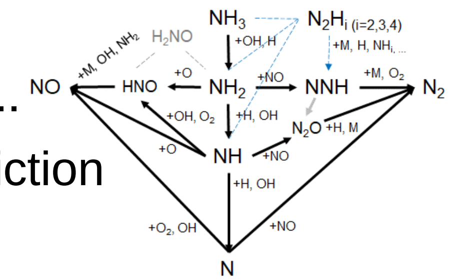

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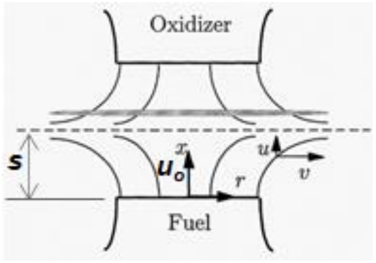

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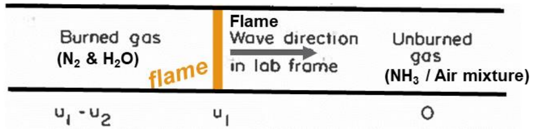
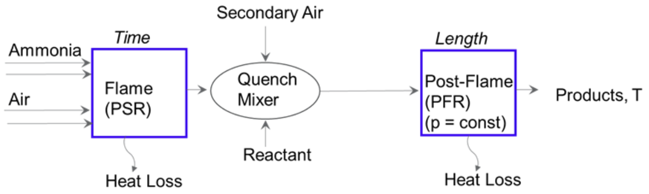
Computational Methods

- 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)



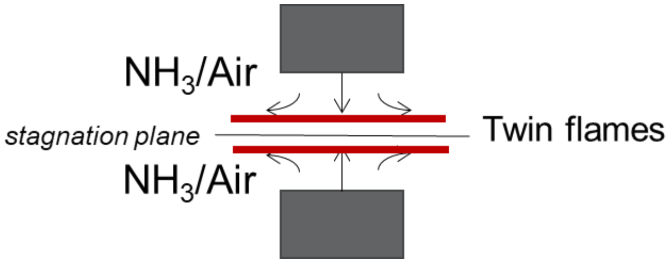
(ii) NH_3 Chemical Reactor Network (CRN) Models



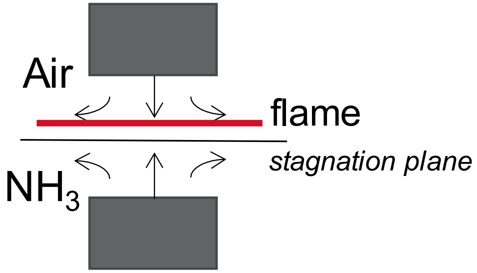
(iii) **NH_3 Counterflow Flames**: Premixed and Non-Premixed

FOCUS HERE

Premixed Counterflow Flames



Non-Premixed Counterflow Flames



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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)**

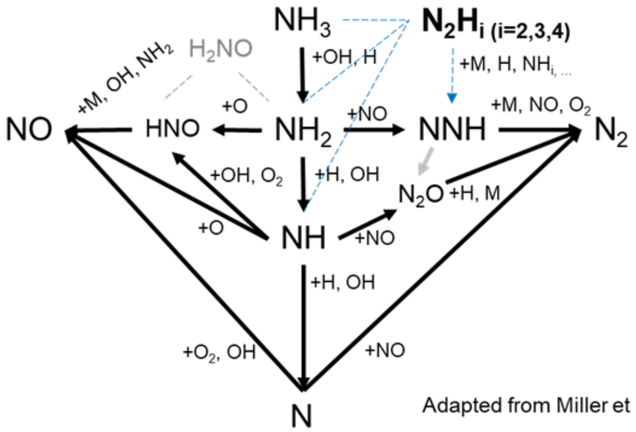
  [Stagni, Cavallotti, Arunthanayothin, Song, Herbinet, Battin-Leclerc, Faravelli: React. Chem. Eng. 5 (2020) 696–711]

- **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)

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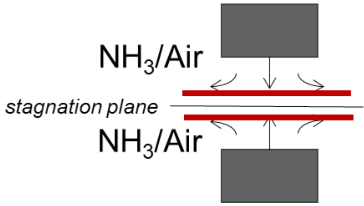
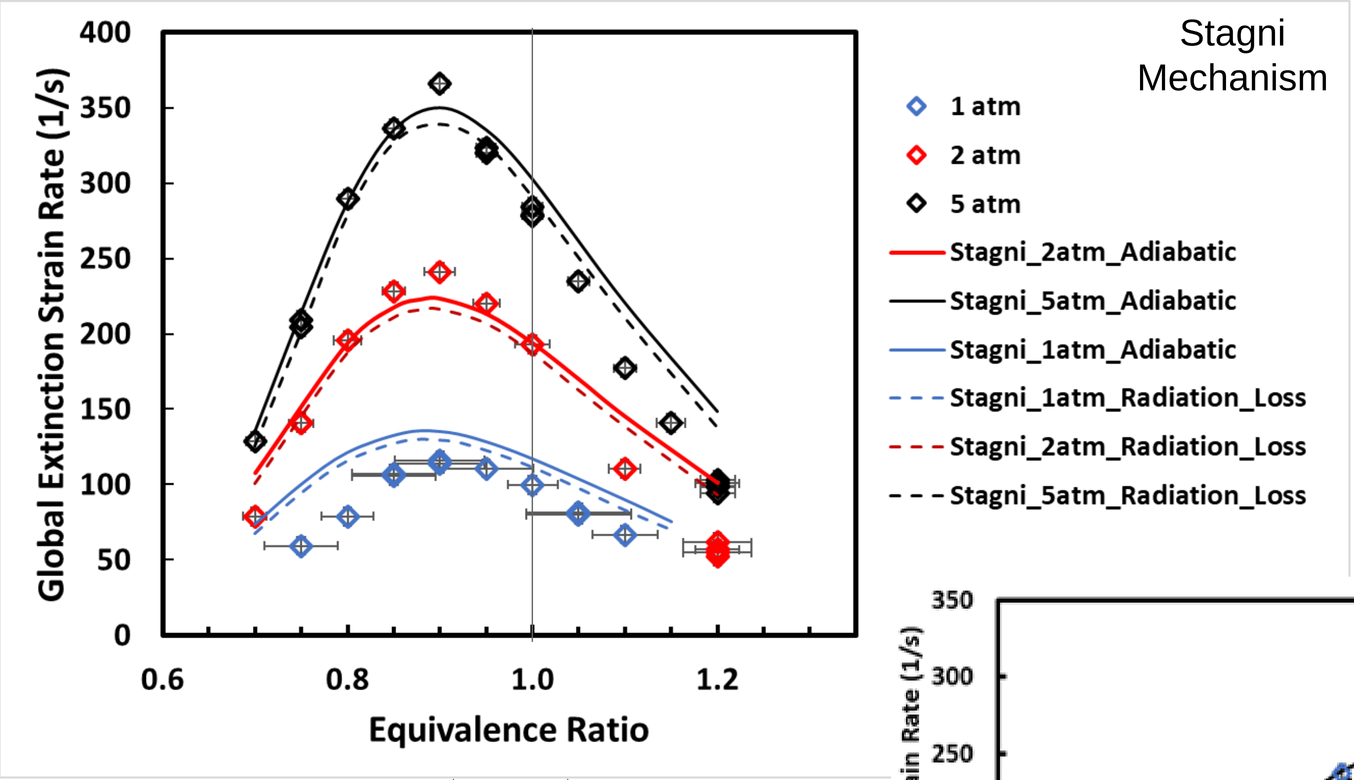
RTRC Predictions vs. UConn Measurements (1/2)



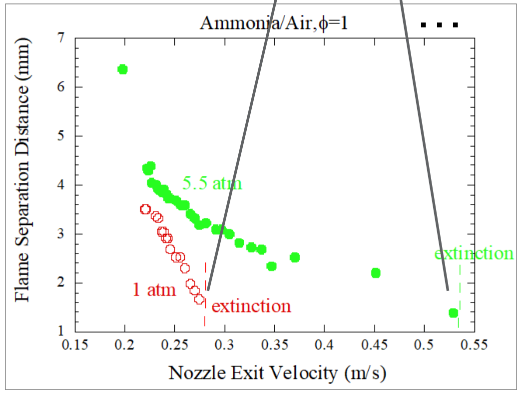


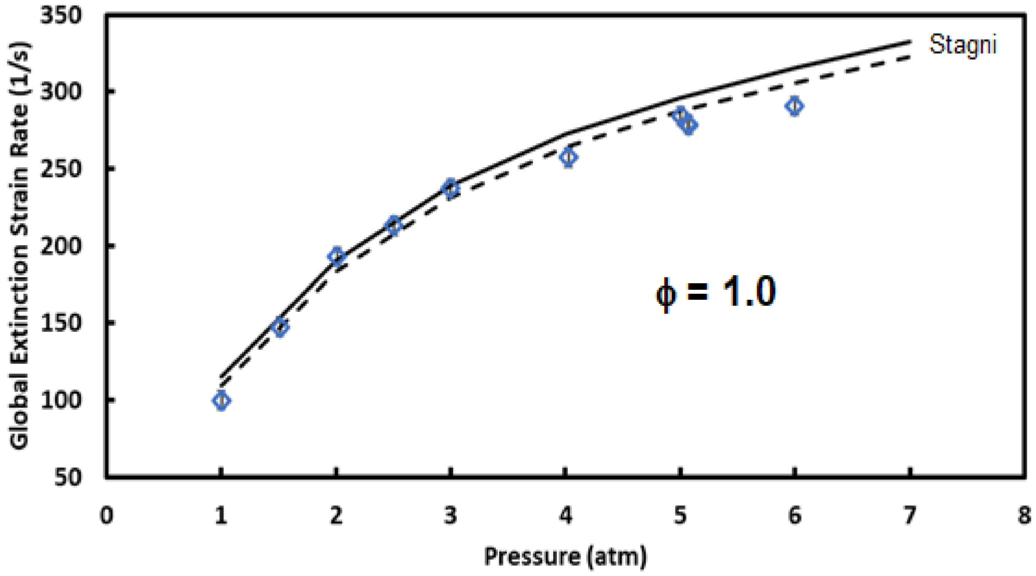
$$q_r = -4\sigma\kappa_p(T^4 - T_o^4)$$

Modified Counterflow Model scripts to account for radiative heat loss

Radiative heat loss per unit volume

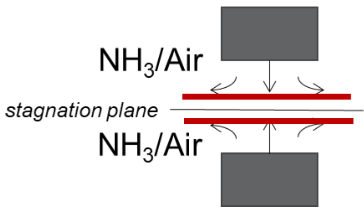
(σ = Stefan-Boltzmann constant, T_o = ambient unburnt reactant temp., κ_p = total Planck's mean absorption coefficient)

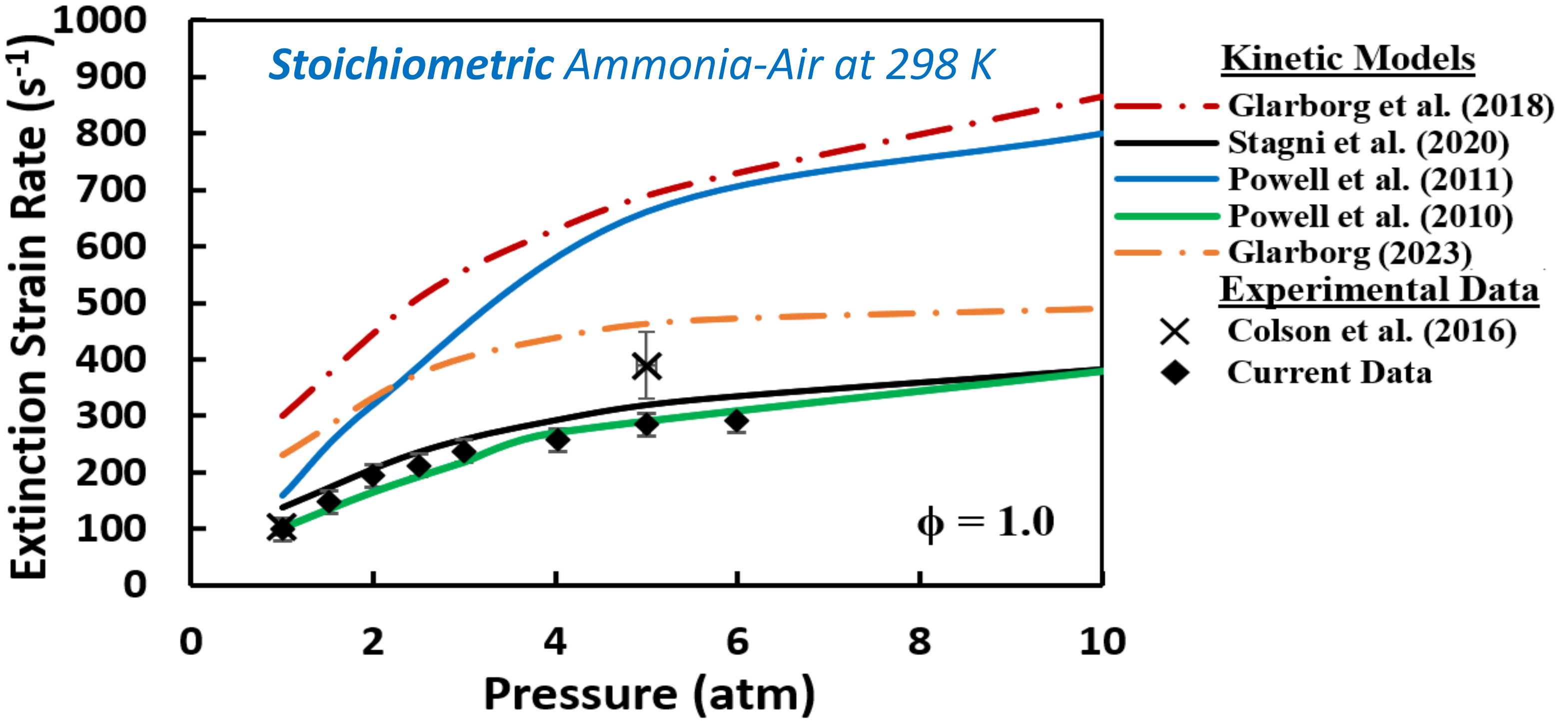


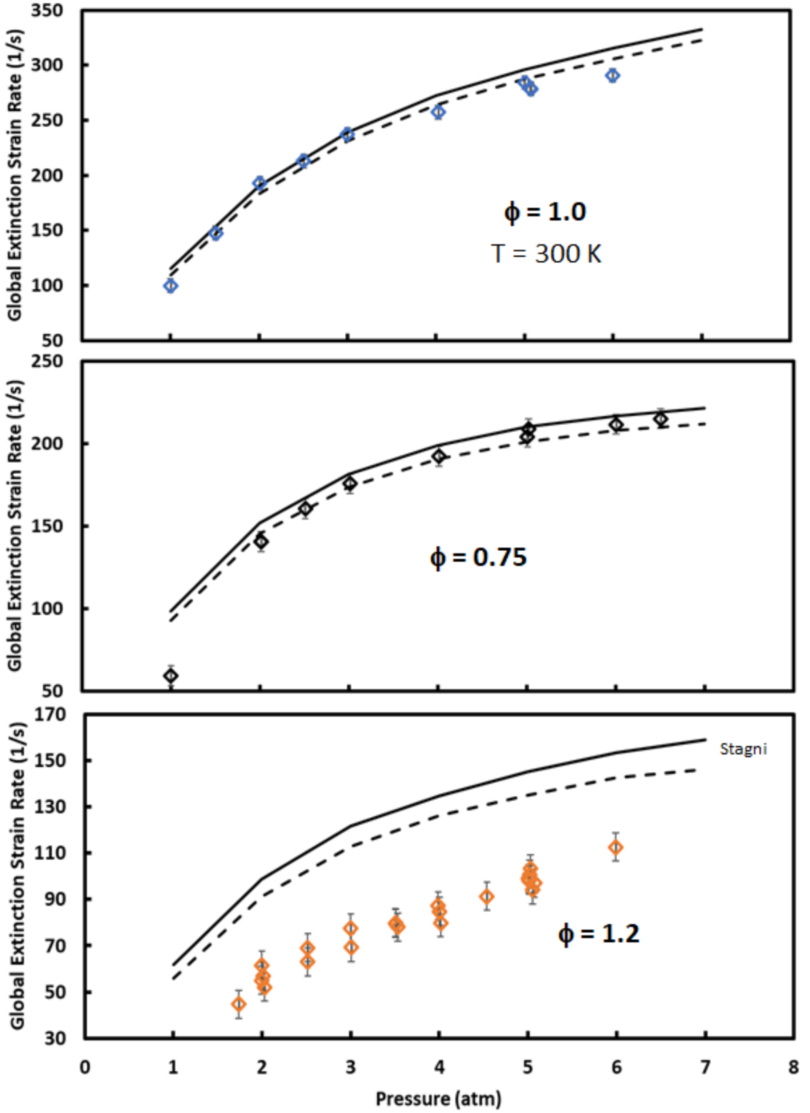


Roll−off in a_{EXT} with pressure (non−linear)

RTRC Predictions vs. UConn Measurements (2/2)







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

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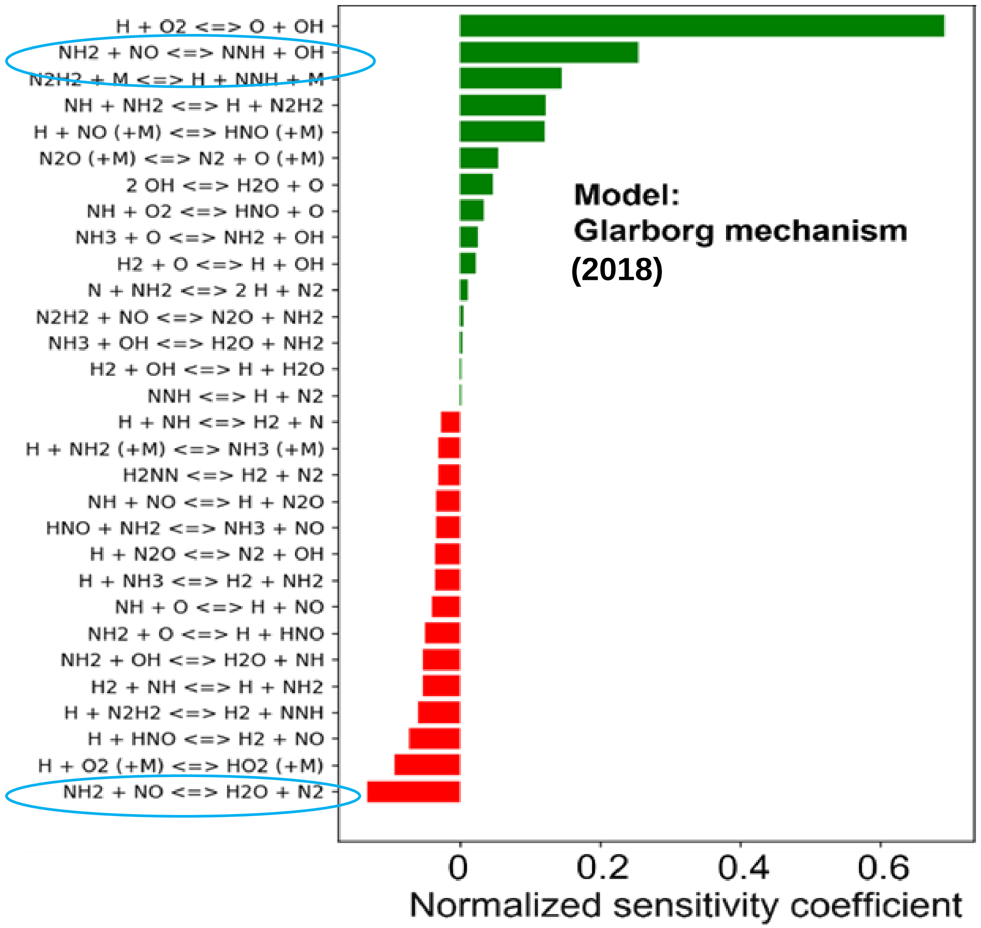
Feature Sensitivity to Extinction Strain Rate

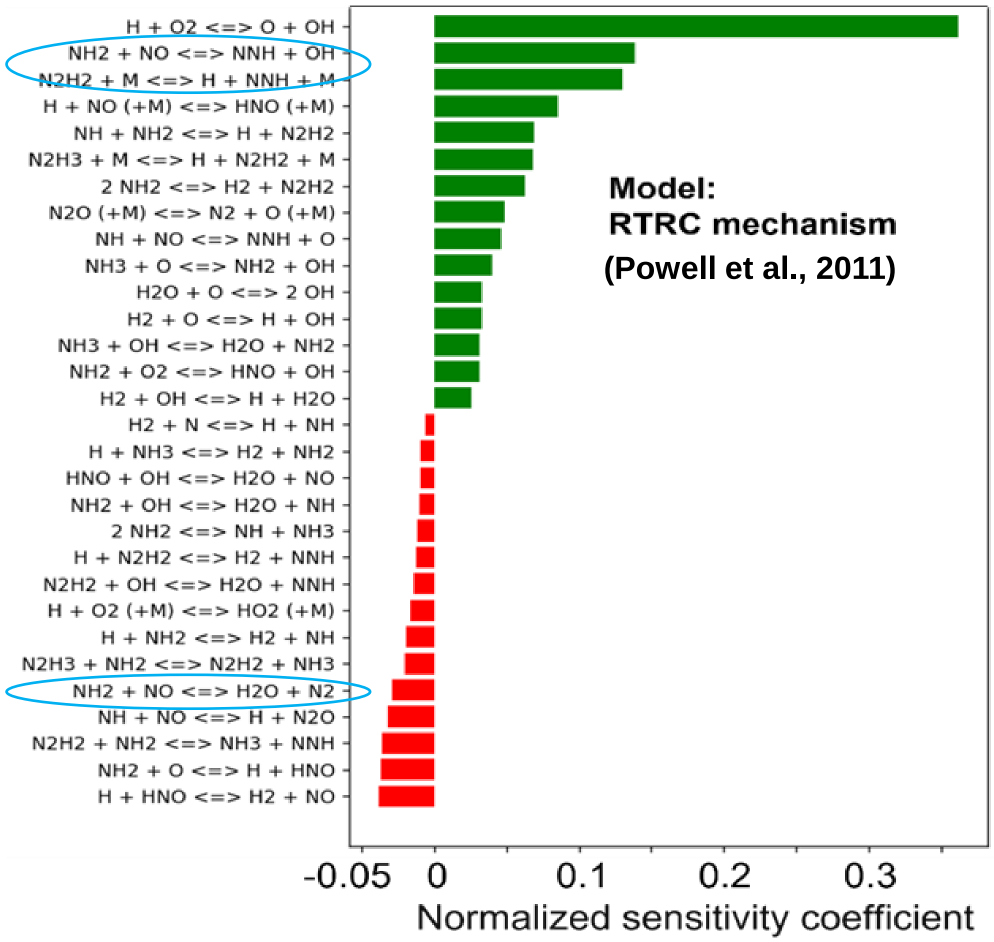
$(1)\ NH_2 + NO \leftrightarrow N_2 + H_2O$
$(2)\ NH_2 + NO \leftrightarrow NNH + OH$
$(3)\ NH_3 + NH_2 \leftrightarrow N_2H_3 + H_2$

NH_3/Air Counterflow Flame

T_i = 301/333 K; P = 0.1 MPa



T_i = 301/333 K; P = 0.1 MPa



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 <u>and</u> Uncertain rate constants

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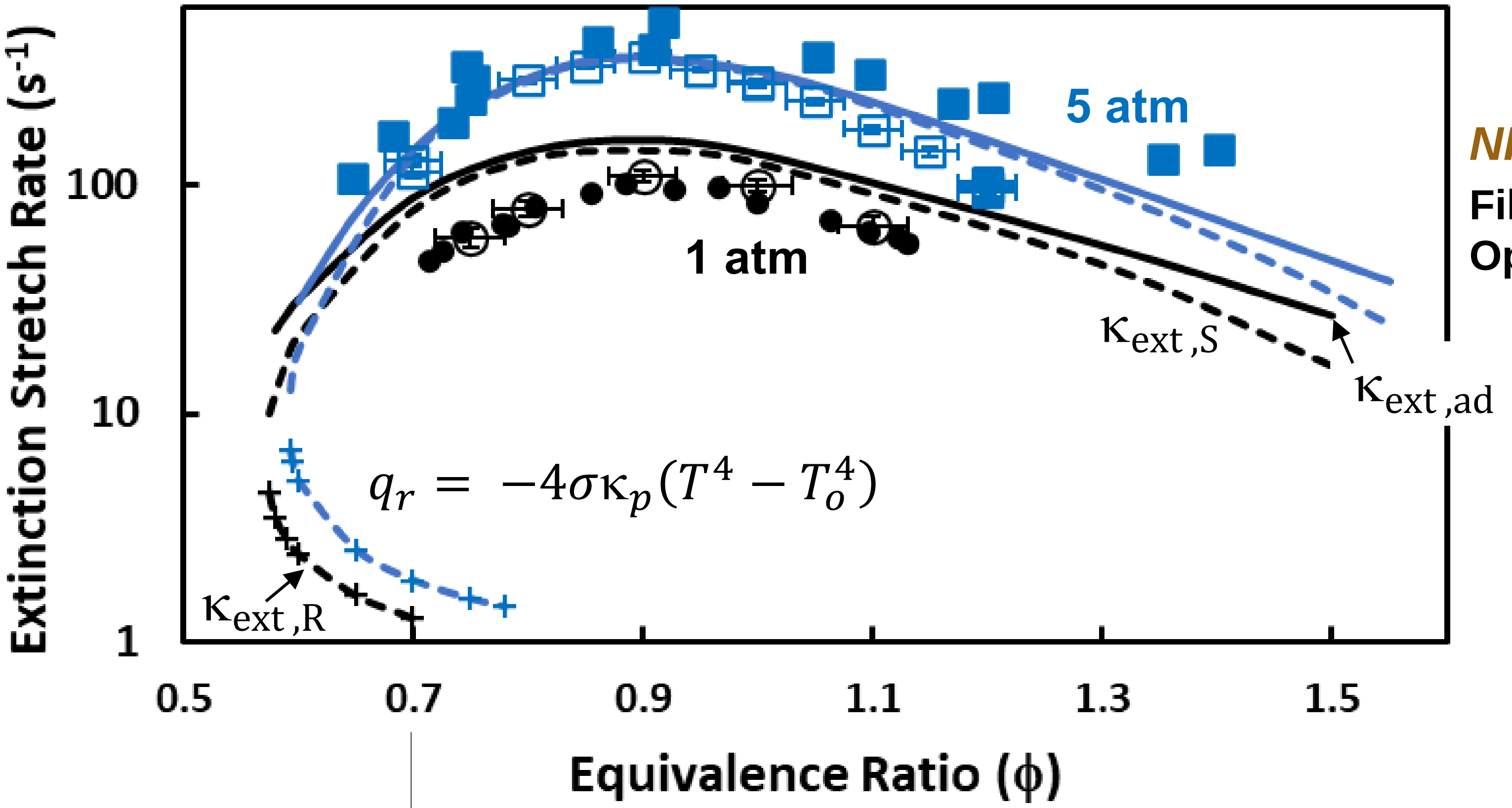
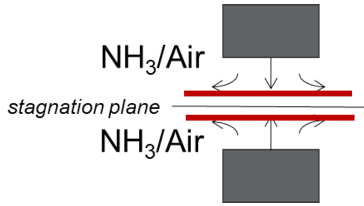
Counterflow NH_3 Flames w/Heat Loss → Impact & Lean Limit

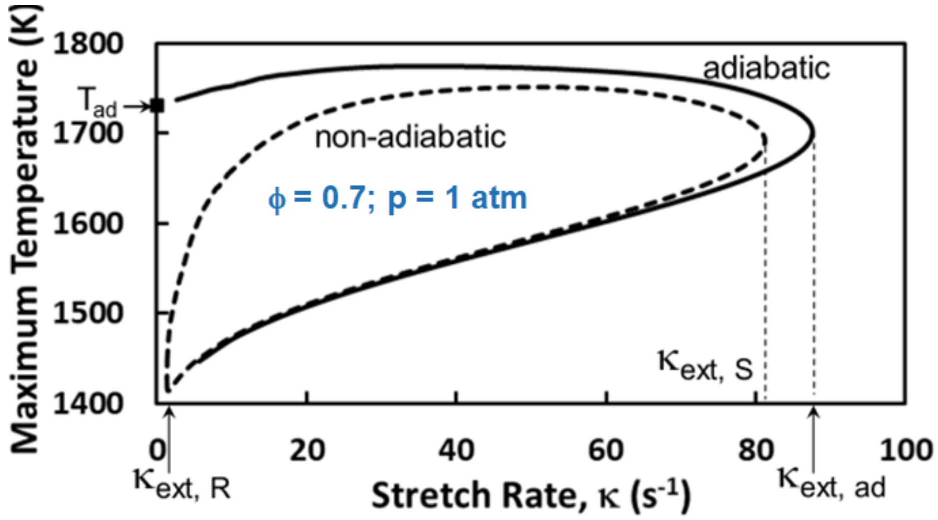




NH_3/Air Counterflow Flames

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).

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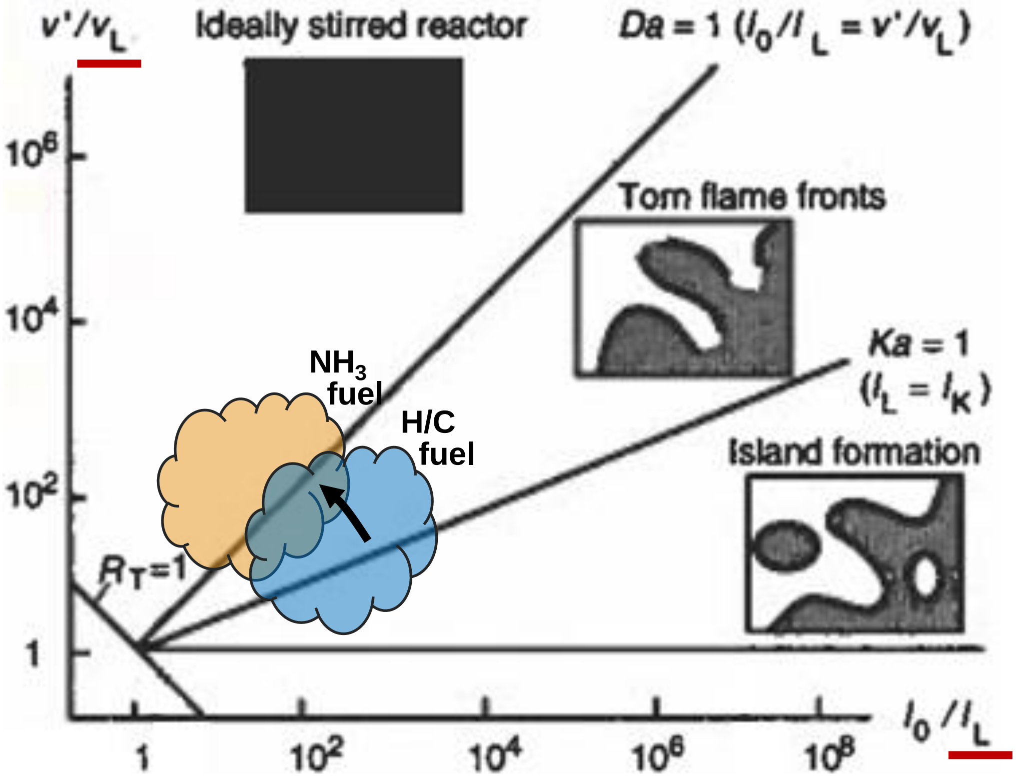
Modeling Activities & Next Steps ...... Toward GT Design

- **Outcomes/Publications (to-date):**
  - *Proceedings of the Combustion Institute* – 40th CI Symposium paper in press for July 2024
  - *AIAA SciTech 2024* – paper # AIAA-2024-2019 (DOI:10.2514/6.2024-2019)
  - *Combustion Institute Meetings – 2023 US National & ESS Spring 2024* meeting papers

Turbulent combustion regime for NH_3-fueled gas turbines:

- v' & ℓ_o ~independent of fuel type (only aero dependent)
- v_L ↓ w/ NH_3 fuel
- ℓ_L ↑ w/ NH_3 fuel
- shift by ~5 – 10x

validate w/ turb. flame rig measurements



CFD modeling of NH_3-fueled gas turbine combustor:

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

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

3rd Technical Task …. GAS TURBINE COMBUSTOR DESIGN (PREP) …………

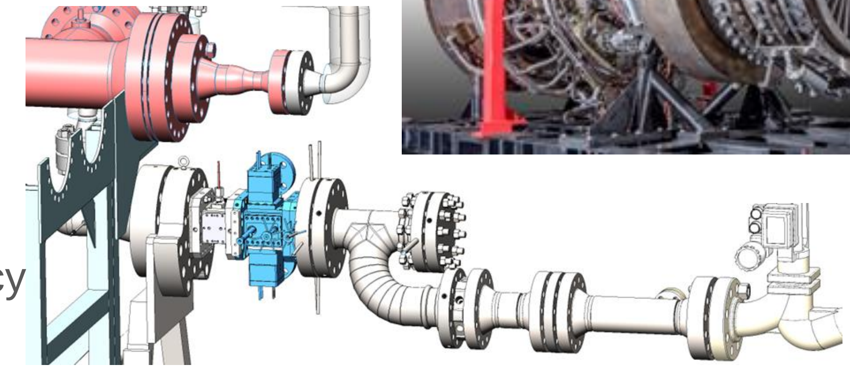
Low-NOx **O**perable **A**mmonia-Combustor **D**evelopment (LOAD-Z)

- 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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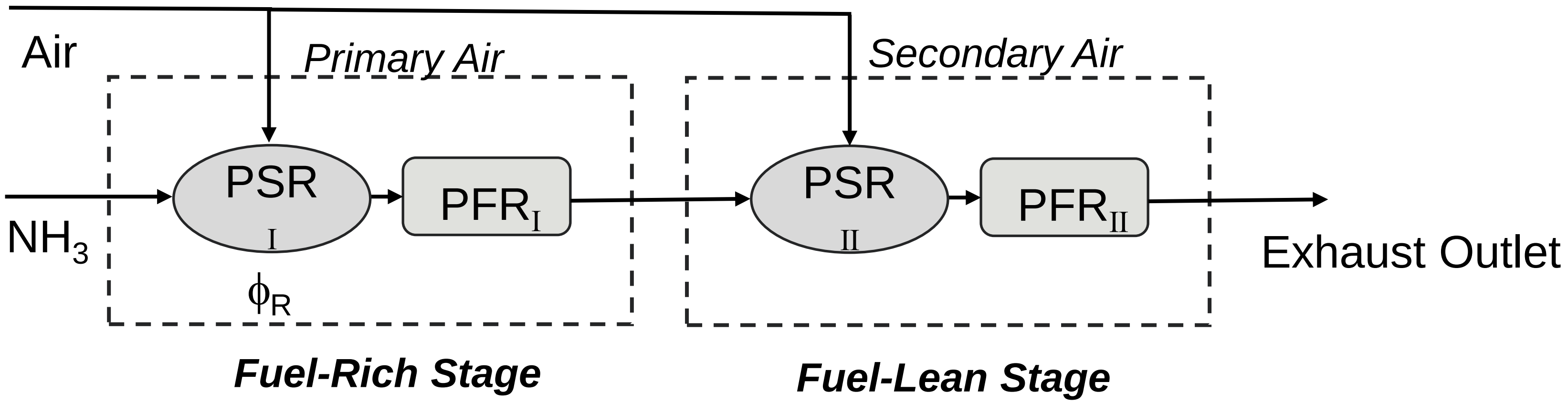
Chemical Reactor Network (CRN) Modeling

CRN Model Schematic for RQL Combustor



- Validation against available simulation data from Li et al., Fuel 355 (2024) 129509.
- **Overall "theoretical" NOx levels <30 ppm for a RQL architecture appear feasible**
- Established N/H mechanisms show wide variability for NOx

$\phi_R = 1.25$

Total Residence time τ (ms)	τ_{PSR_I} (ms)	τ_{PFR_I} (ms)	τ_{PSR_II} (ms)	τ_{PFR_II} (ms)	Pressure (atm)	Inlet Temp. (K)	Outlet Temp. (K)	NOx* (ppm)
20	3	14	2	1	12	600	1850	38.5
20	3	14	2	1	30	700	1850	30.1
30	3	24	2	1	30	700	1850	22.9

* 15% O_2 dry

RTX

END