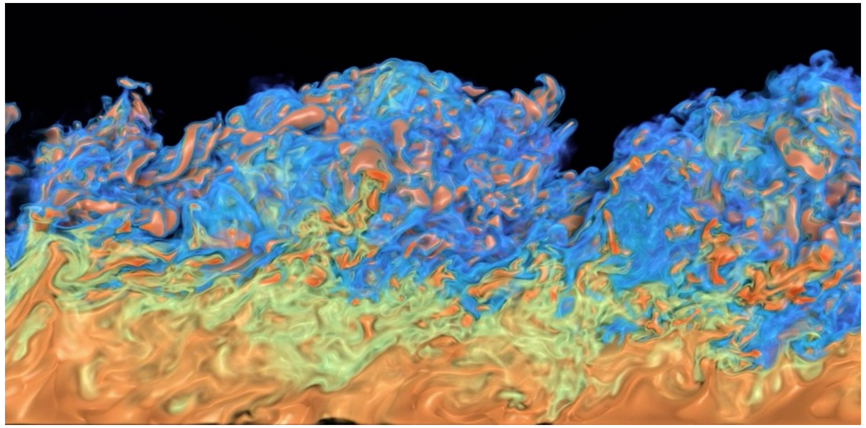
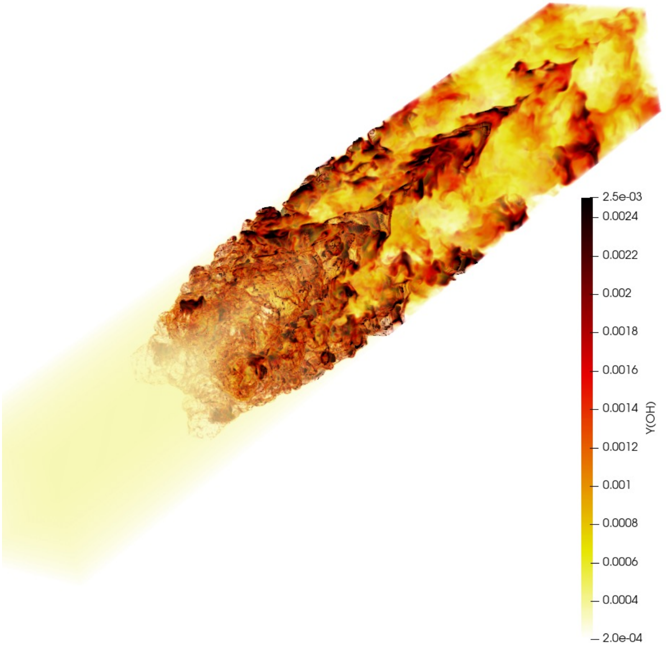
Turbulent Combustion: A Computational Perspective
Part 2. Ammonia/Hydrogen Flames



Temperature in a NH3/H2/N2-Air Premixed Flame in a Shear Layer at 10 atm



OH radical from second stage of a NH3-Air RQL jets-in-crossflow at 20 bar

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Ammonia/hydrogen has the potential to be an alternative **zero-carbon** fuel for hard-to-electrify sectors: long-haul shipping, power generation and agriculture

However, neat ammonia has a low reactivity compared to, e.g., natural gas (CH_4)


NH_3


CH_4

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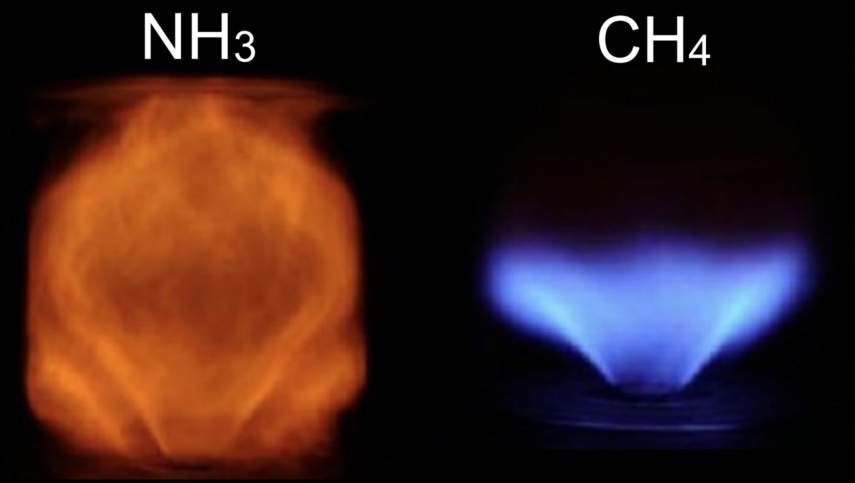
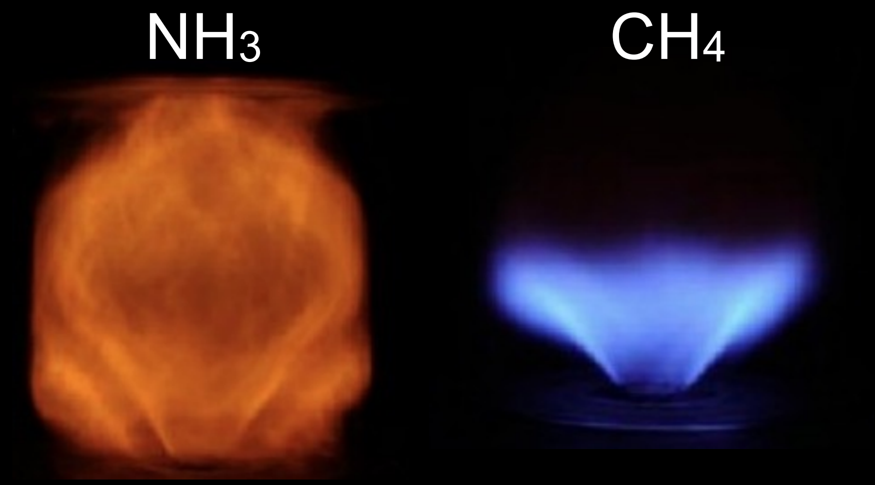


Valera-Medina et al., PECS, 2018.

The reactivity can be improved by adding hydrogen or partial cracking of ammonia to hydrogen and nitrogen

However, neat ammonia has a low reactivity compared to, e.g., natural gas (CH_4)



Valera-Medina et al., PECS, 2018.

The reactivity can be improved by adding hydrogen or partial cracking of ammonia to hydrogen and nitrogen

Combustion behavior of ammonia/hydrogen blends is poorly understood, especially behavior at high pressure

Outline of Part 2: Ammonia/hydrogen/nitrogen-air premixed turbulent flames relevant to gas turbines

- **Blow-out resilience**
- Pressure effects
- NO and N_2O emissions

A comparison of the blow-out behaviour of turbulent premixed ammonia/hydrogen/nitrogen-air and methane-air flames

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James Dawson[1], Jacqueline Chen[2]**

This work was supported by:

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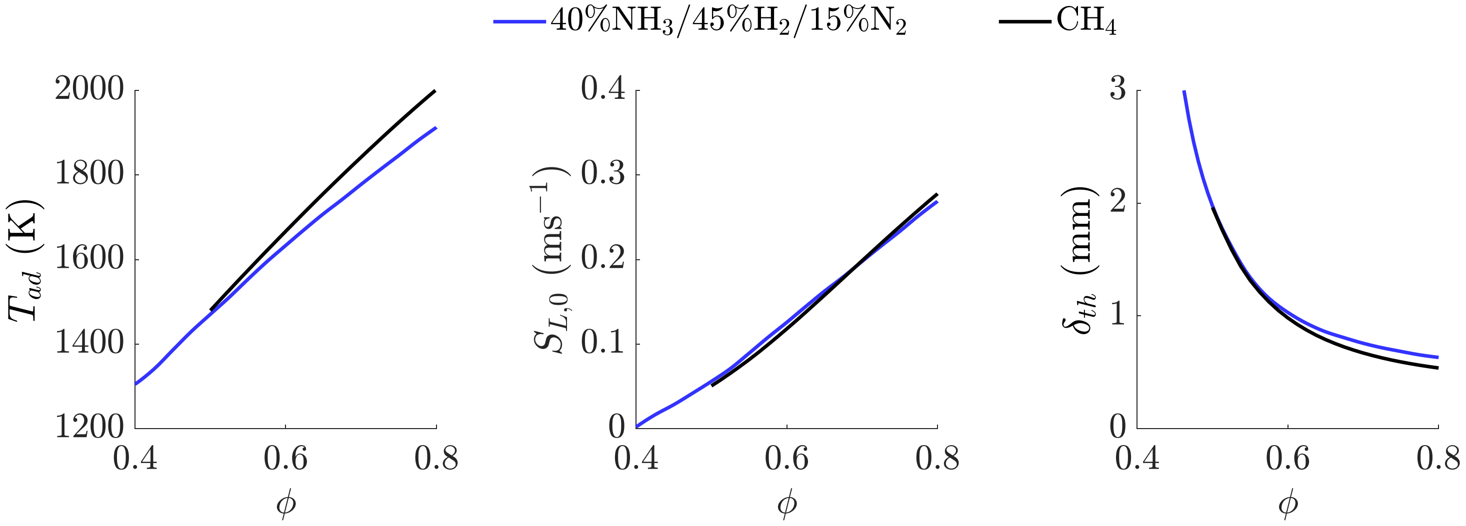
[2]*Combustion Research Facility, Sandia National Laboratories, Livermore, CA 94550, United States*
[3]*SINTEF Energy Research, 7465 Trondheim, Norway*

Wiseman et al. Proc. Comb. Inst. 2021

Why $NH_3/H_2/N_2$ blends?

- Ammonia Dissociation: $2NH_3 \longrightarrow 3H_2 + N_2$
- Extended flammability limits and higher flame speeds
- In this study, we use 40% NH_3 / 45% H_2 / 15% N_2 by volume
- The laminar flame properties of this blend is similar to methane over a wide range of lean equivalence ratios



Unstrained laminar premixed methane-air flame

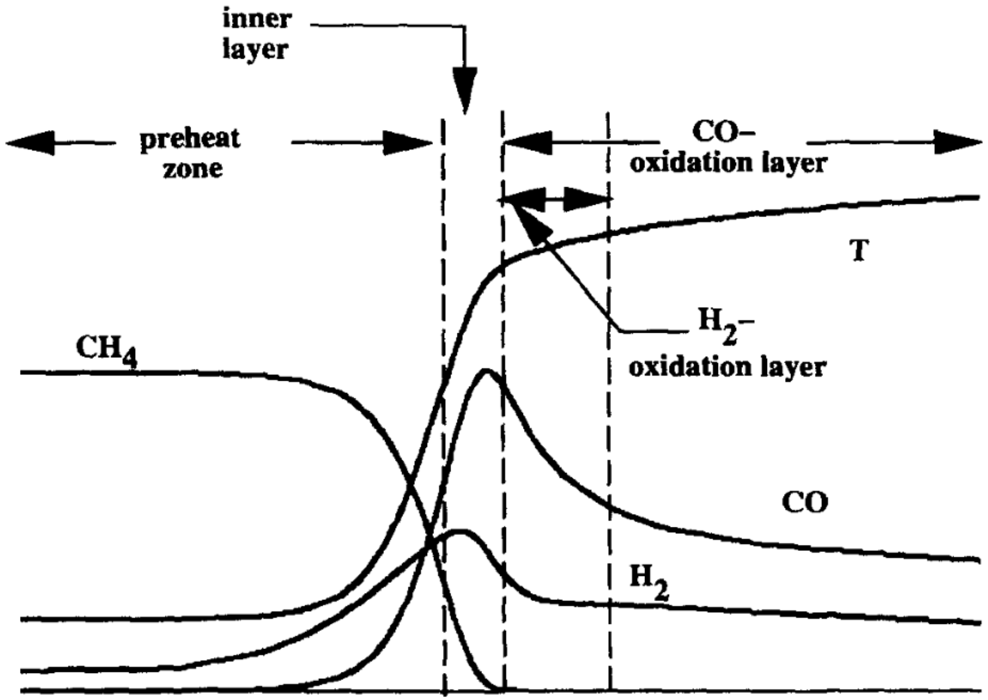
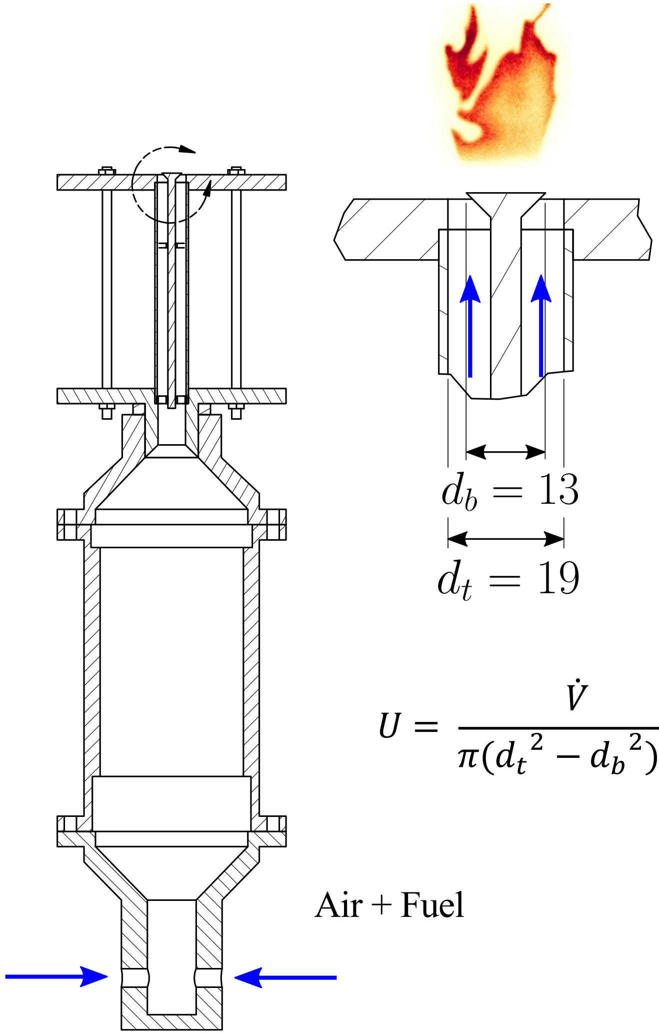


Fig. 1. Schematic of the overall structure of premixed methane–air flames.

Echekki and Chen, 1996

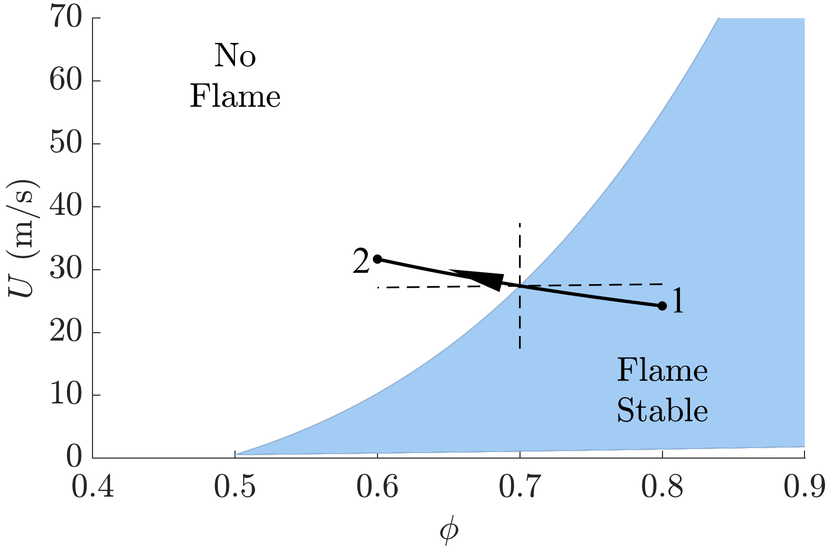
Blow-out Experiments



$$U = \frac{\dot{V}}{\pi({d_t}^2 - {d_b}^2)/4}$$

Blow-out Procedure:

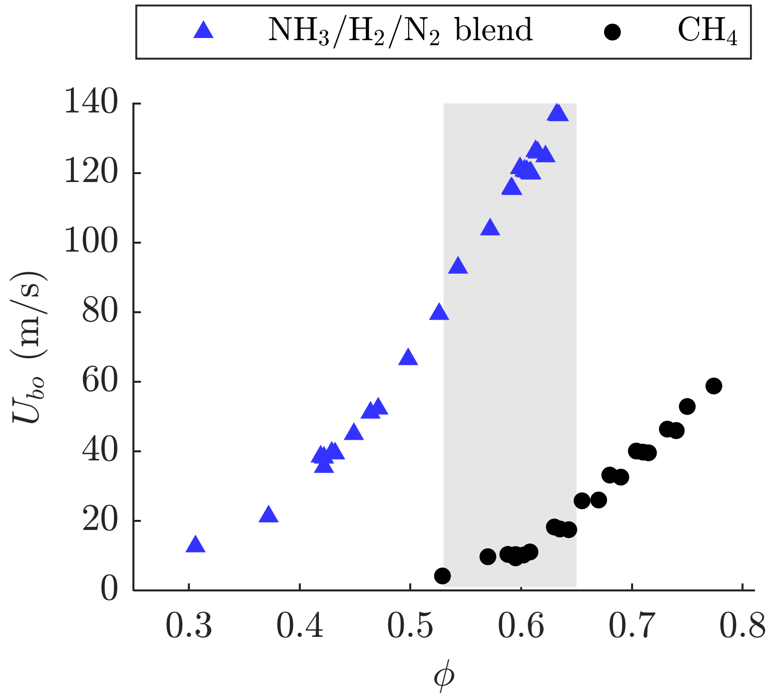
$\dot{m}_{fuel}$ fixed, $\dot{m}_{air}$ increasing **(chosen trajectory)**



Optical diagnostics:

- OH chemiluminiscence imaging at 10 kHz
- OH PLIF imaging at 10 kHz

Experiment Results and Blowout Criterion



Blow-out Criterion:

$$Da_{crit.} = \tau_{flow,bo}/\tau_{chem.}$$

$$\tau_{flow} \propto L/U$$

L – characteristic length scale
U – characteristic velocity

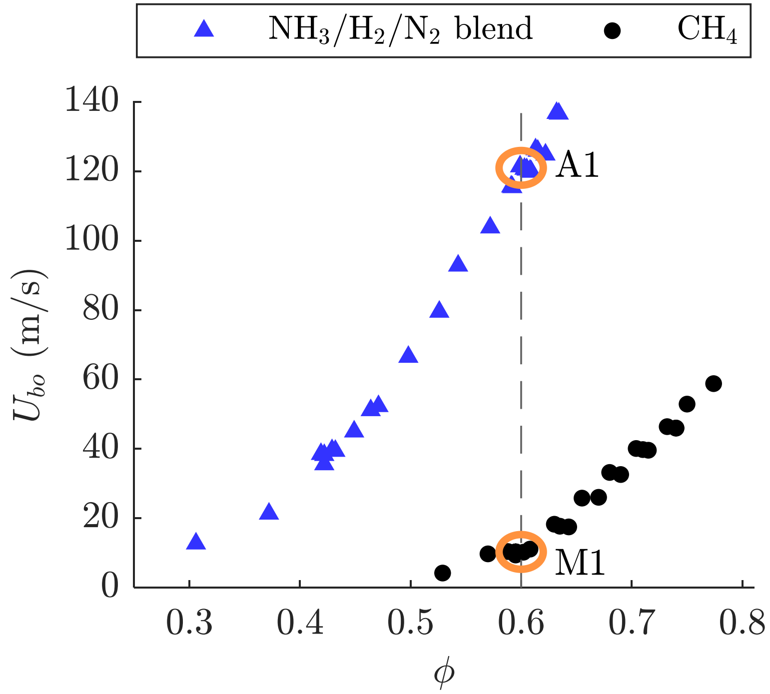
Assuming $\tau_{flow} \propto 1/U_{bo}$ and $Da_{crit.} =$ constant,

$$\boxed{\frac{U_{bo,1}}{U_{bo,2}} = \frac{\tau_{chem.,2}}{\tau_{chem.,1}}}$$

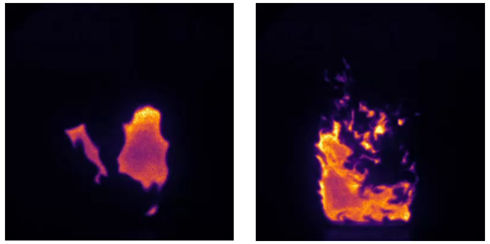
$\tau_{chem.}$?

τ_{pf}	$= \delta_{th}/S_{L,0}$, i.e., the ratio of unstretched, laminar flame thickness to flame speed.
τ_{psr}	The blowout residence time of a perfectly stirred reactor.
τ_{ext}	$= 1/\kappa_{ext.}$, i.e., the inverse of the extinction strain rate.

Discrepancy Between Experiments and Blowout Criterion



$$\frac{U_{bo,A1}}{U_{bo,M1}} = 11.7$$

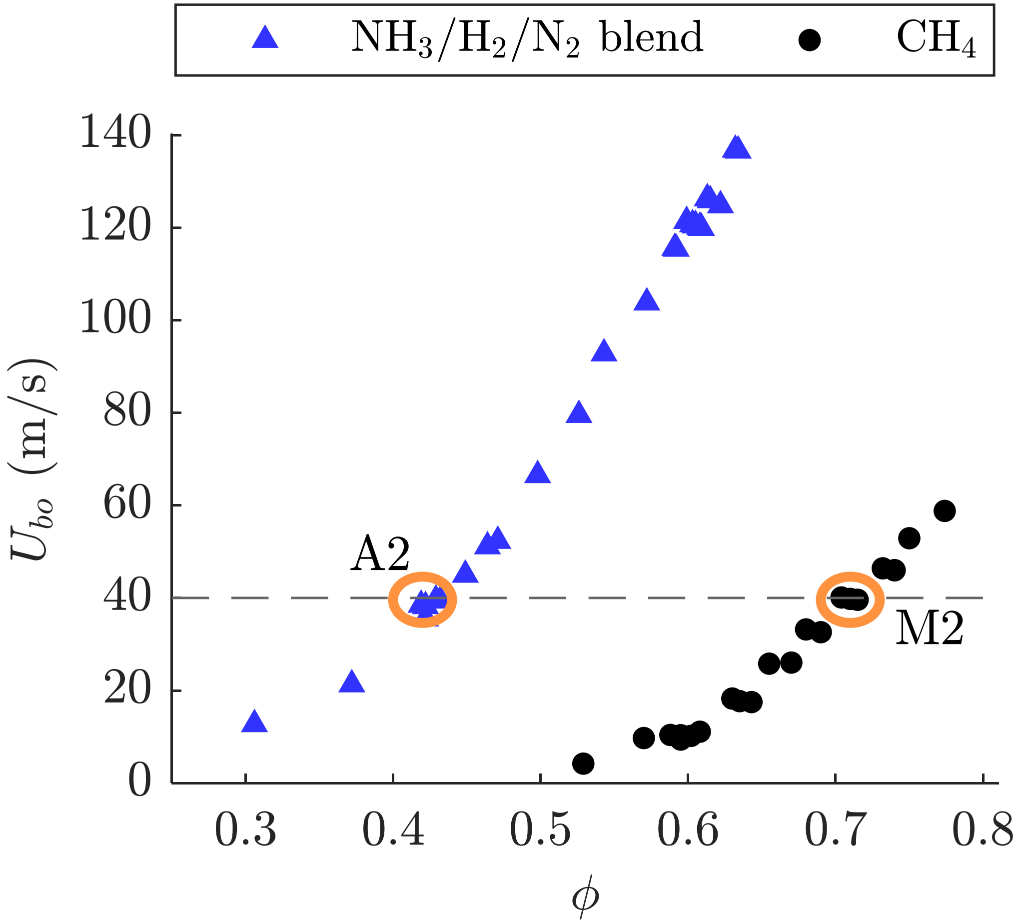


	Case M1	Case A1
T_{ad} (K)	1667	1633
$S_{L,0}$ (cm/s)	11.8	12.6
δ_{th} (mm)	0.98	1.02
Le_q (Le_D)	0.98	0.86 (0.53)

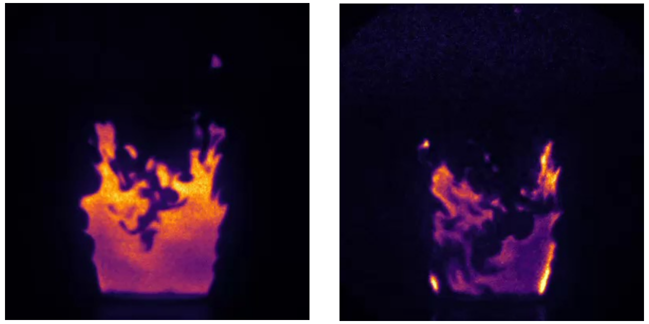
			$\tau_{chem.,M1}/\tau_{chem.,A1}$
τ_{pf}	8.32	8.19	1.0
τ_{psr}	0.34	0.13	2.6
τ_{ext}	1.75	0.46	3.8

$$\frac{U_{bo,A1}}{U_{bo,M1}} > \frac{\tau_{chem.,M1}}{\tau_{chem.,A1}}$$

Discrepancy Between Experiments and Blowout Criterion – Reynolds number Effect



$$\frac{U_{bo,A2}}{U_{bo,M2}} = 1.0$$



	Case M2	**Case A2**
T_{ad} (K)	1875	1350
$S_{L,0}$ (cm/s)	21.5	1.8
δ_{th} (mm)	0.67	3.6
Le_q (Le_D)	0.98	0.82 (0.50)

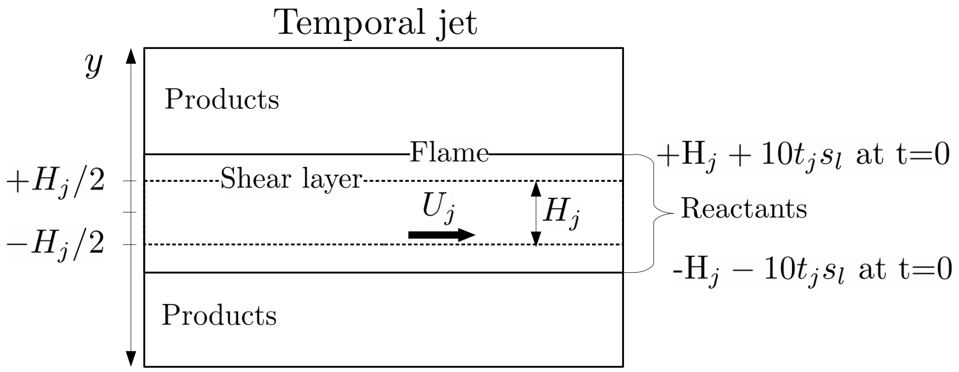
			$\tau_{chem.,M2}/\tau_{chem.,A2}$
τ_{pf}	2.87	370.8	0.077
τ_{psr}	0.13	1.48	0.088
τ_{ext}	0.75	4.46	0.17

$$\tau_{chem.,M2} \neq \tau_{chem.,A2}$$

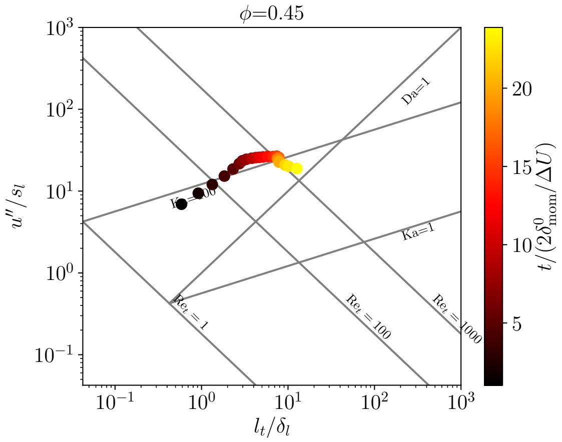
DNS Temporal Slot Jet Configuration

DNS of $NH_3/H_2/N_2$-air (40%/45%/15%) and CH_4-air:

- 750 K pre-heat temperature, 1 atm, $\phi=0.45$
- $Re_j=13,800$ ($NH_3/H_2/N_2$), 14,800 (CH_4), same domain size and velocity for both cases
- $Da_j=0.08$ for both cases
- Short chemical kinetics mechanism for H_2/NH_3 combustion in air, derived from San Diego mechanism
  (19 species, 63 elementary steps)[1]
- Short CH_4-air mechanism (16 species)[2]



Central jet within reactants, flame on both sides (in y direction)



DNS close to border of BRZ and TRZ regimes
(regime diagram computed at y location of maximum Re_t)

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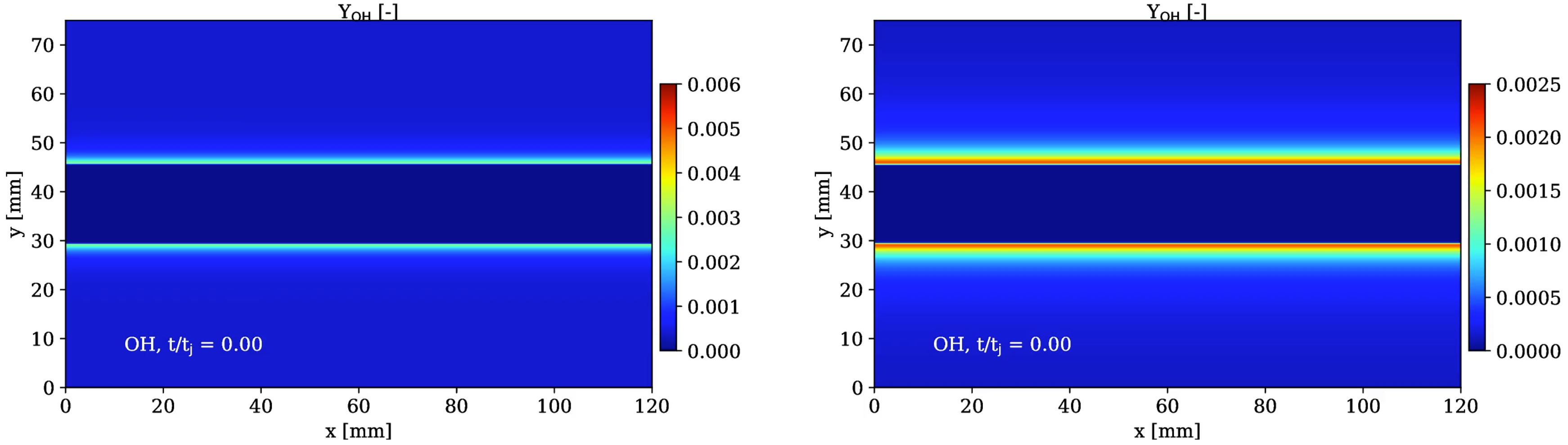
[1] Jiang et al, "An updated short chemical-kinetic nitrogen mechanism for carbon-free combustion applications", *Int J Energy Res*, vol. 44, pp.795-810 (2020).

[2] Smooke & Giovangigli, "Reduced Kinetic Mechanisms and Asymptotic Approximations for Methane-Air Flames", Springer, pp. 1–28 (1991).

Comparison of DNS of $NH_3/H_2/N_2$-air and CH_4-air flames

OH mass fraction in x-y-plane



$NH_3/H_2/N_2$-air

CH_4-air

- Faster flame surface generation and more wrinkling for $NH_3/H_2/N_2$-air flame
- Overall stronger burning for $NH_3/H_2/N_2$-air flame (also observed in heat release)

Turbulent burning velocity

Turbulent burning velocity, mass of fuel burned per unit time and per unit volume:

$$\langle \omega_R \rangle = (\rho_u Y_{Ru} \langle Sc \rangle_S) \langle \Sigma \rangle$$

Two contributions:

- Flame front surface area generation (wrinkling) through turbulent stretch results in *flame surface density*, $\langle \Sigma \rangle$:
- Modification of *flame structure* through stretch given by mean consumption rate per unit flame area, $\rho_u Y_{Ru} \langle Sc \rangle$ where *Sc* is the local integral of the reaction rate along the flame normal direction:

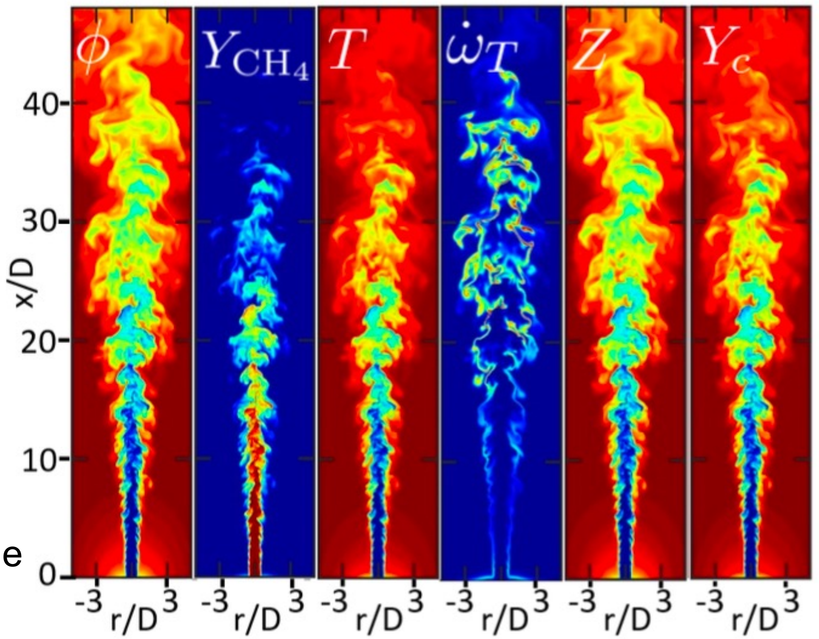
$$Sc = \int \omega_R \, dn \text{ (measure of the local burning rate)}$$

Stretch rate from flame theory measures the fractional rate of flame area growth

$$\frac{1}{\delta A} \frac{d(\delta A)}{dt} \equiv a_T + S_d \nabla \cdot \mathbf{n}$$

tangential strain rate

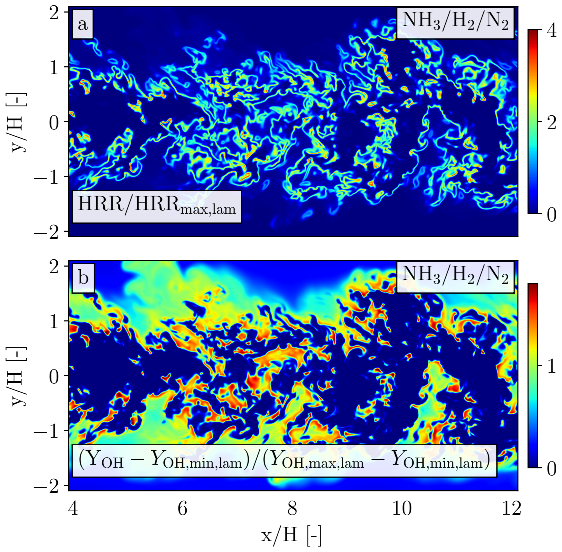
flame curvature x flame propagation



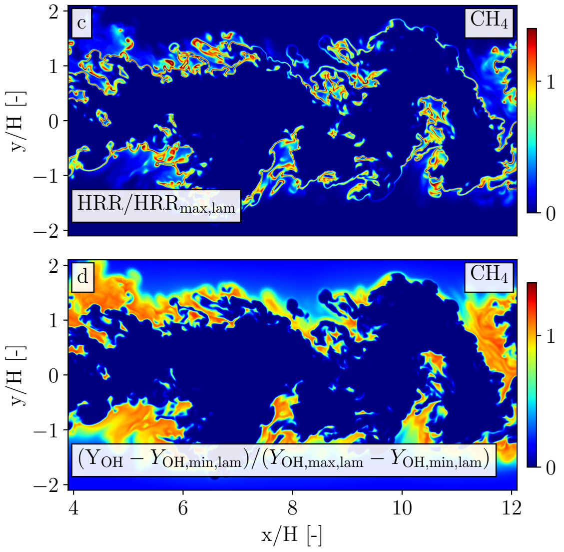
Turbulent premixed methane-air flame
Wang et al. 2019

DNS Results – Flame Surface Density and Consumption Speed

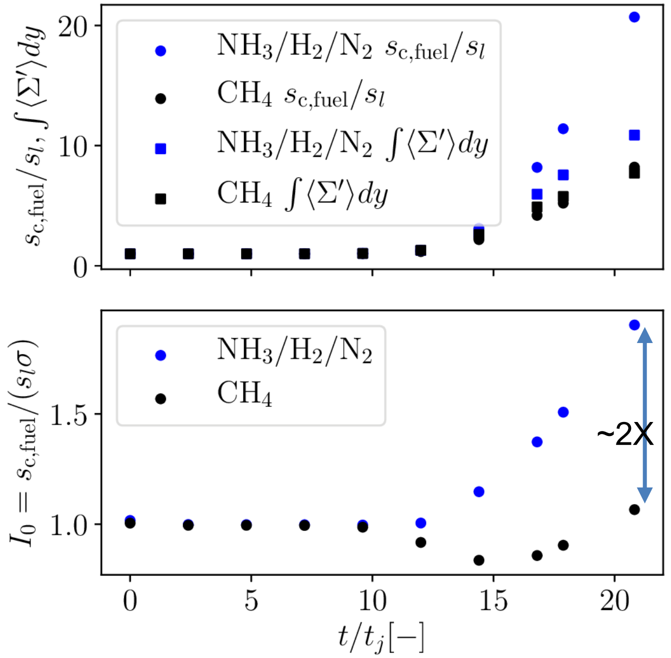
$NH_3/H_2/N_2$-air



CH_4-air



Fuel consumption, FSD & I_0

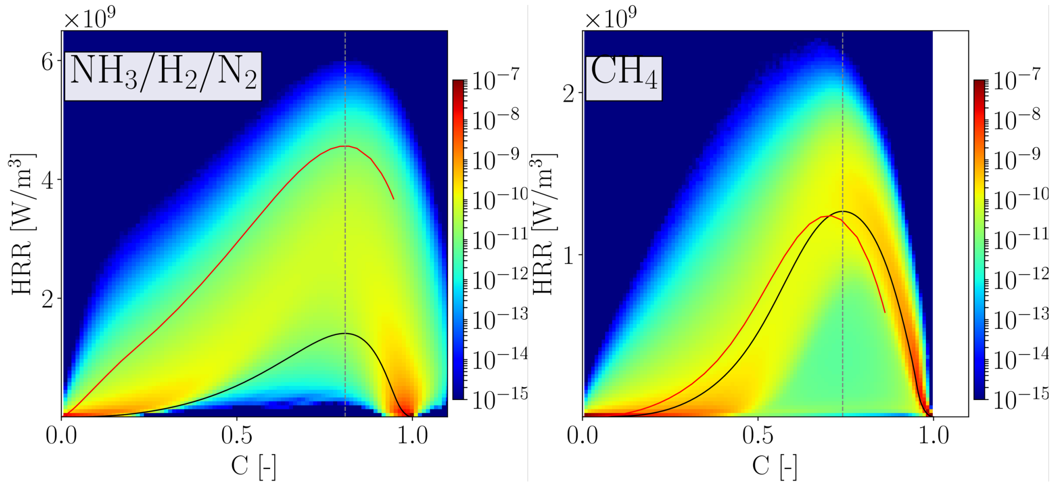


- Faster increase in flame surface density, consumption speed for $NH_3/H_2/N_2$-air flame compared to CH_4-air
- Ratio of turbulent to laminar burning rate per unit area (I_0) increases for $NH_3/H_2/N_2$-air flame, decreases first and slowly increases for CH_4-air flame

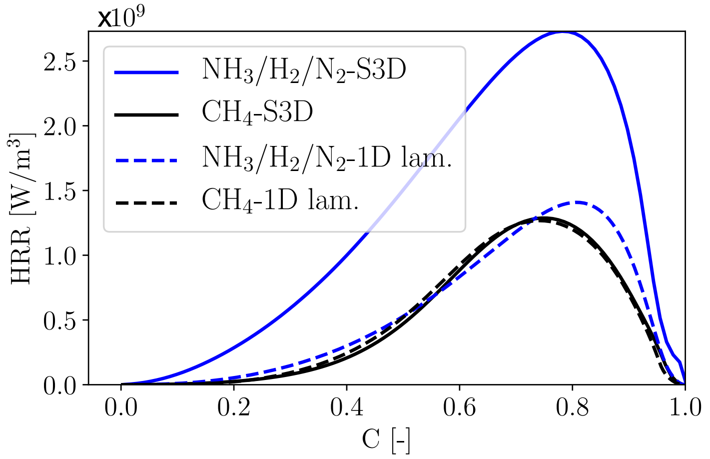
DNS Conditional Heat Release Statistics

JPDF of Heat Release Rate and Progress variable

Black line laminar flame
Red line strained flame near extinction



Heat Release Rate Conditional Mean

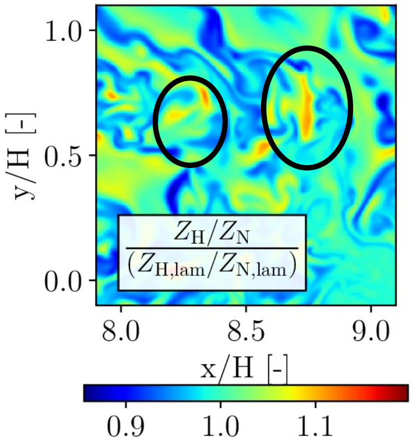


- Heat release increase across all progress variables for $NH_3/H_2/N_2$-air flame, considerable amount of heat release for low progress variable values
- Heat release conditioned on progress variable shows large departure from laminar flame solution for $NH_3/H_2/N_2$-air flame

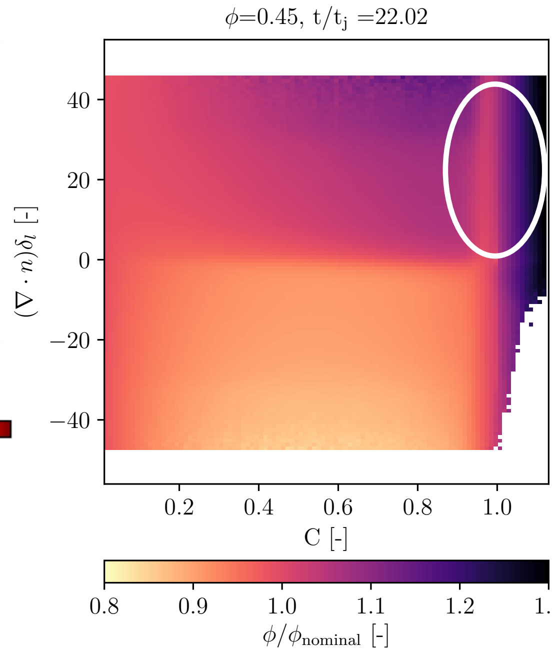
*C is based on H_2O mass fraction

DNS Reveals Preferential Diffusion

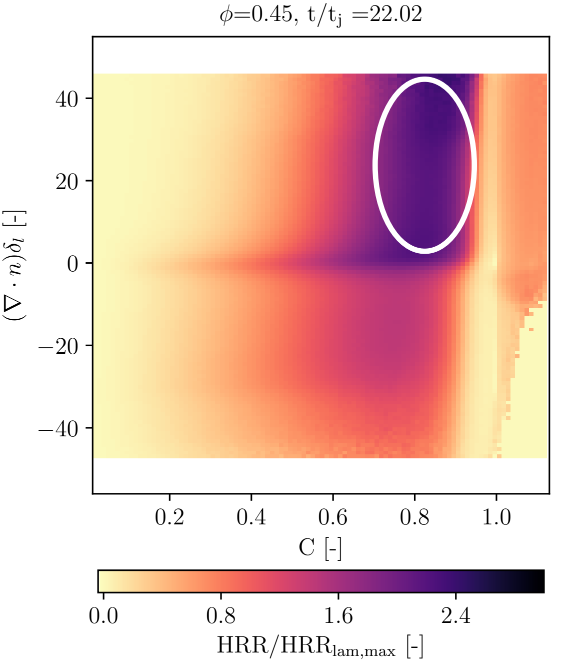
Local atomic H to N ratio for $NH_3/H_2/N_2$-air flame



Local equivalence ratio vs curvature and C



Local heat release rate vs curvature and C



- Strong preferential diffusion observed for $NH_3/H_2/N_2$-air flame
- Local enriched regions coincide with higher OH and heat release
- Richer regions with high heat release found mostly in positively curved flame regions (center of curvature in products)
  → Thermodiffusive instability, enhanced burning rates & higher strain resilience

Conclusions

- A joint experimental and numerical study was conducted of the blow-out behaviour of $NH_3/H_2/N_2$-air flames, blended such that the flame exhibits similar premixed, unstretched laminar flame properties as lean methane-air flames
- In the experiment, blow-out curves for the ammonia blend and methane-air flames were measured in an axisymmetric, unconfined, bluff-body stabilized burner, showing an order of magnitude difference in blowout velocity
- DNS of a slot jet configuration revealed that the $NH_3/H_2/N_2$-air flame exhibits strongly enhanced heat release rates compared to a methane-air flame and points towards preferential diffusion of hydrogen as the main reason for increased burning rates and resistance to strain

Pressure Effects on Turbulent Premixed Lean Ammonia/Hydrogen Flames

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Visualization: Tyson Neuroth[1], Qi Wu[1], Kwan-Liu Ma[1]

[1] University of California, Davis, [2]Sandia National Laboratories, [3]SINTEF Energy Research, [4]Univerisity of California at San Diego

Rieth et al. Comb Flame 2022

Motivation

High Pressure Premixed Combustion

- Gas turbine combustors operate at ~20-30 atm
- Premixed combustion at pressurized conditions is not fully understood and studied to a limited extent due to cost
- Previous studies: larger normalized turbulent burning velocity (e.g., Kobayashi et al., 2000; Venkateswaran et al., 2014)

Ammonia/hydrogen/nitrogen combustion

- Ammonia (NH3) is a promising energy carrier for zero-carbon combustion
- Blends of NH3/H2/N2 can be optimized to have unstrained laminar flame behavior close to that of natural gas
- However, lean turbulent combustion behavior of NH3/H2/N2 differs to that of natural gas (Wiseman et al., 2021) due to the thermo-diffusive nature → not fully understood yet, especially at elevated pressure

Outline of Part 2: Ammonia/hydrogen/nitrogen-air premixed turbulent flames relevant to gas turbines

- Blow-out resilience
- **Pressure effects**
- NO and N_2O emissions

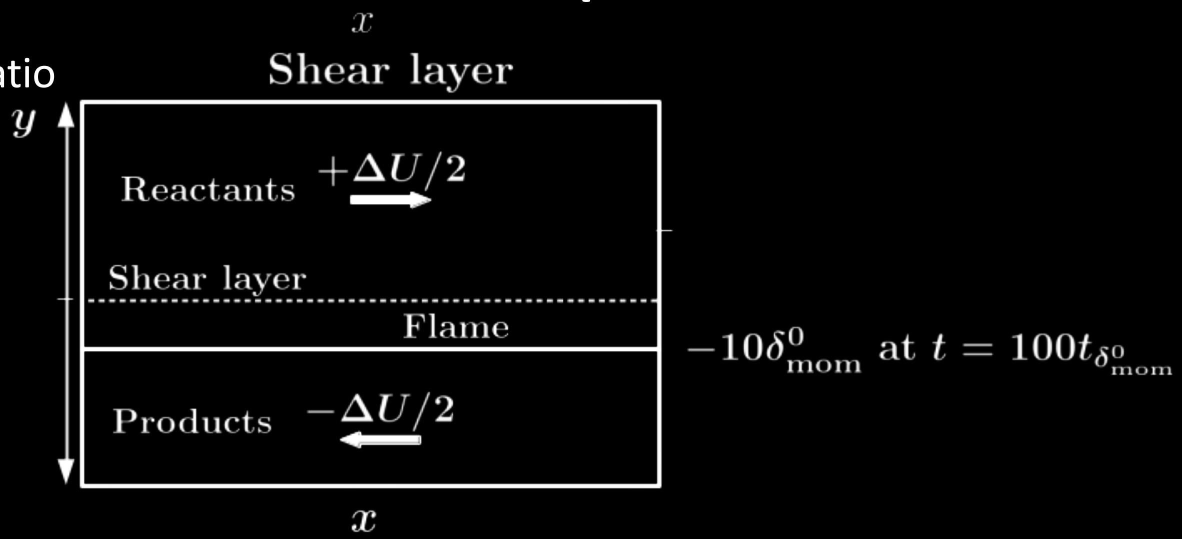
Pressure effects on ammonia/hydrogen premixed flames: direct numerical simulations in a temporal planar shear layer configu[illegible]n

Simulation Parameters

- Lean premixed $NH_3/H_2/N_2$-air (40%/45%/15% vol) with equivalence ratio of 0.45 at **1 and 10 atm**
- Reactants are preheated to 750 K
- Flames are nominally in the broken reaction zone regime (Karlovitz # (Ka)>600, turbulent Re # (Re_t)>1000)
- Simulations are designed such that normalized parameters (Re_t, Ka, Damköhler #) are consistent between 1 and 10 atm
- Growing grid size with 11 B grid points on the final grid
- 19 species chemical mechanism (Jiang et al., 2020)
- DNS using S3D-Legion run on OLCF's 200 Pflop Summit supercomputer on ~1000 nodes using a DOE INCITE allocation

More information: Rieth et al., *Comb. Flame*, 2022

Simulation setup



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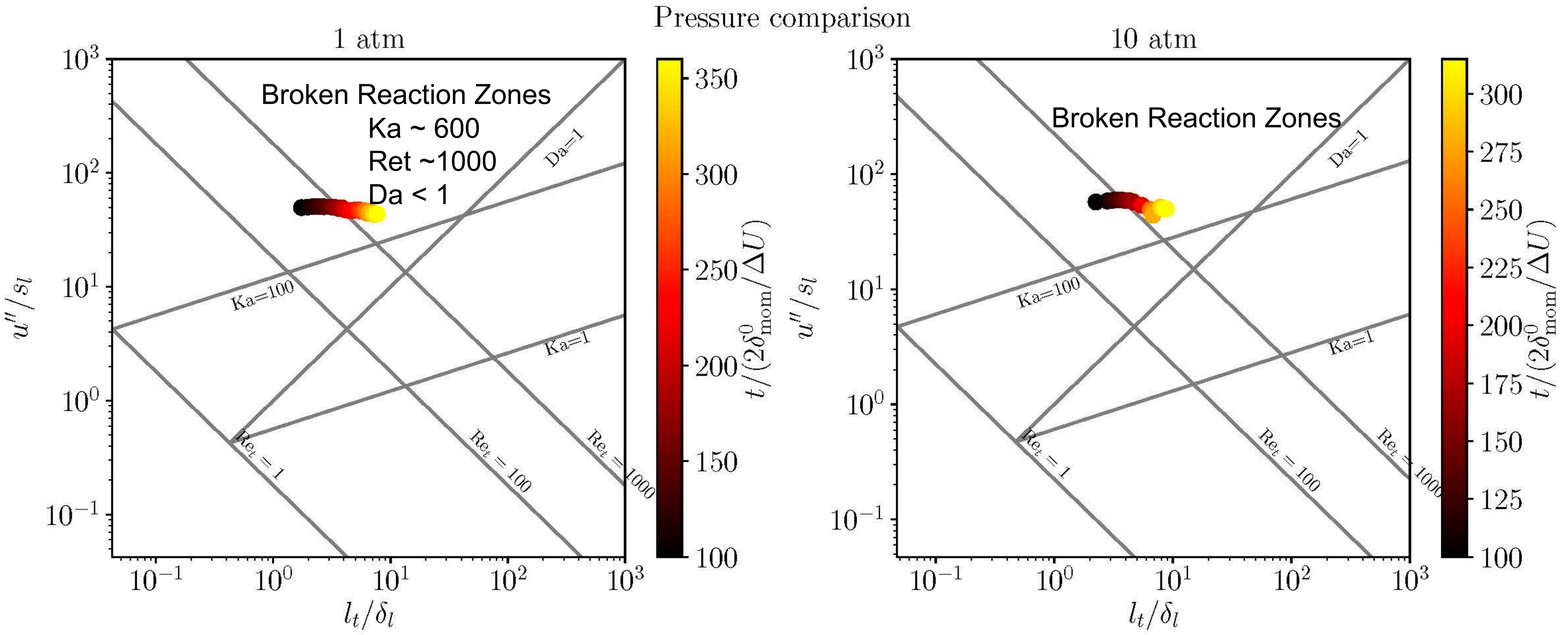
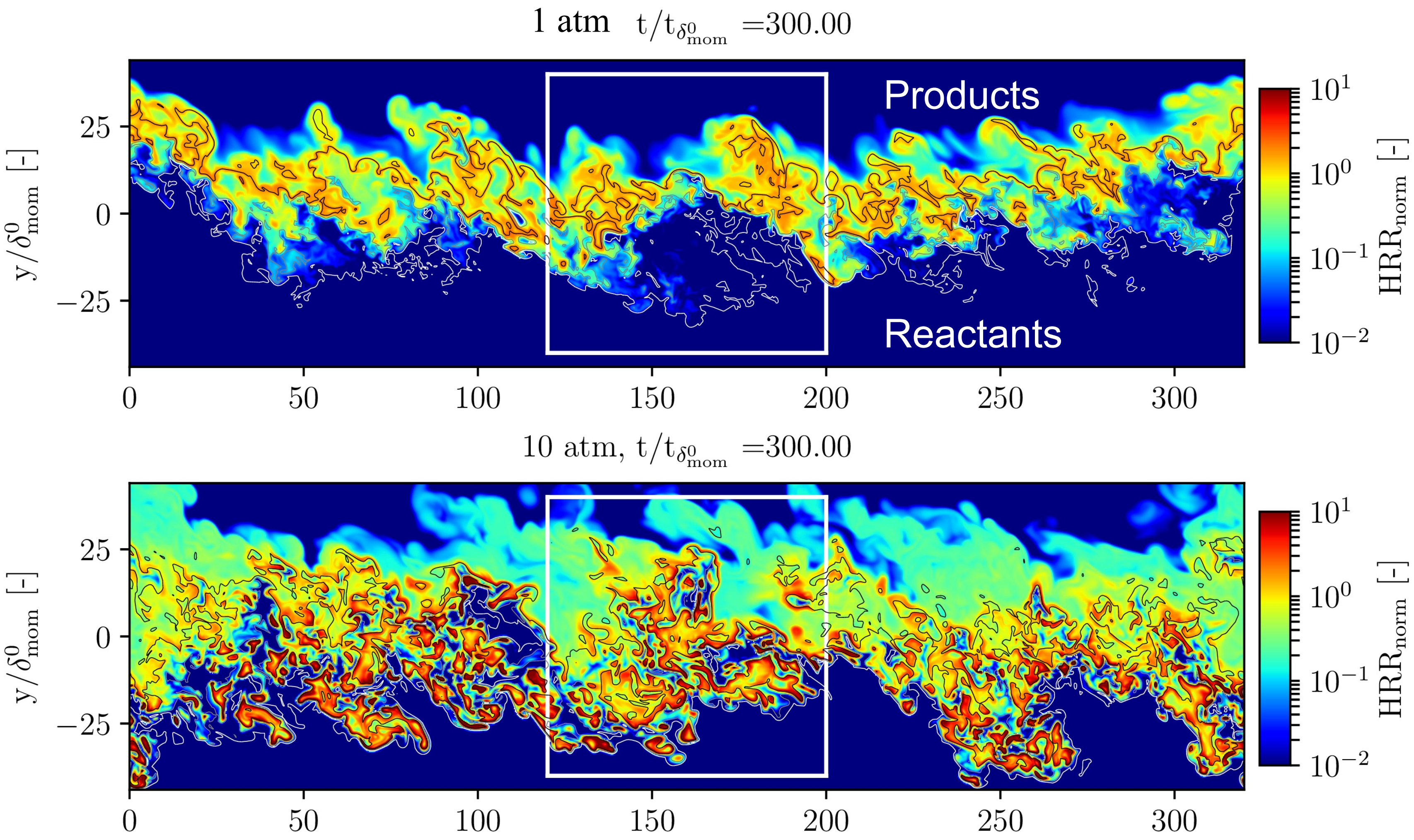
Premixed Flame Regime Diagram



Broken Reaction Zones
Ka ~ 600
Ret ~1000
Da < 1

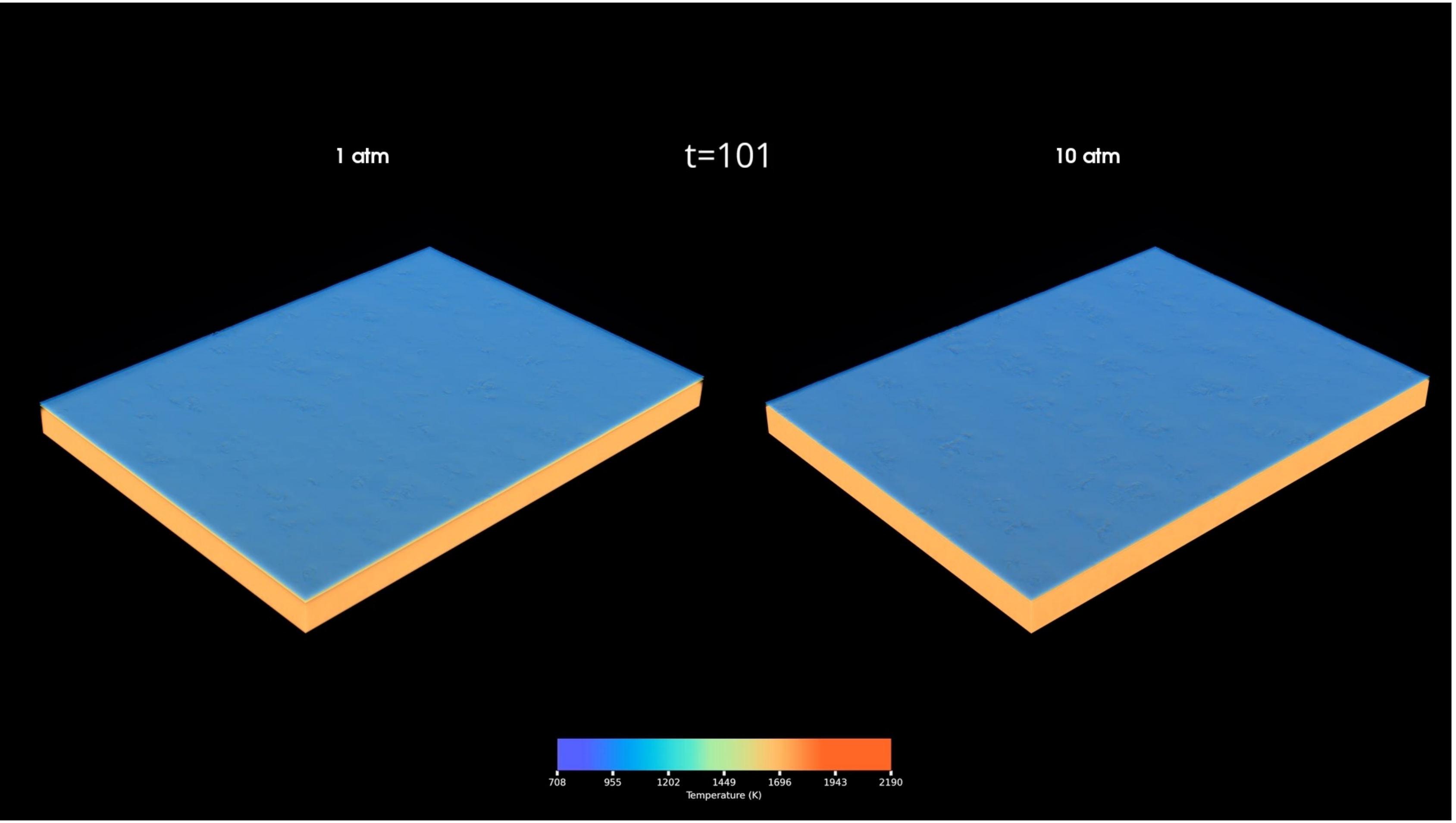
Broken Reaction Zones

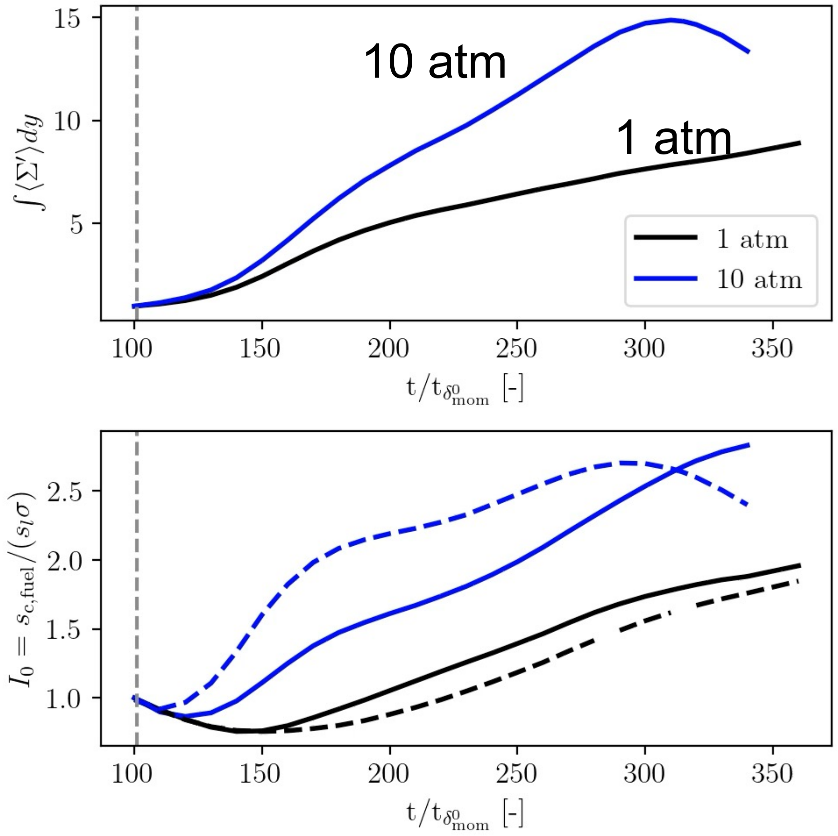
Heat release rate from $NH_3/H_2/N_2$/air premixed flame in turbulent mixing layer at 1 and 10 atm



Iso-lines correspond to temperatures of 800 (white), 1000(grey) and 1500 K (black)

Pressure Effect on $NH_3/H_2/N_2$-air Premixed Flame Turbulent Burning Velocity



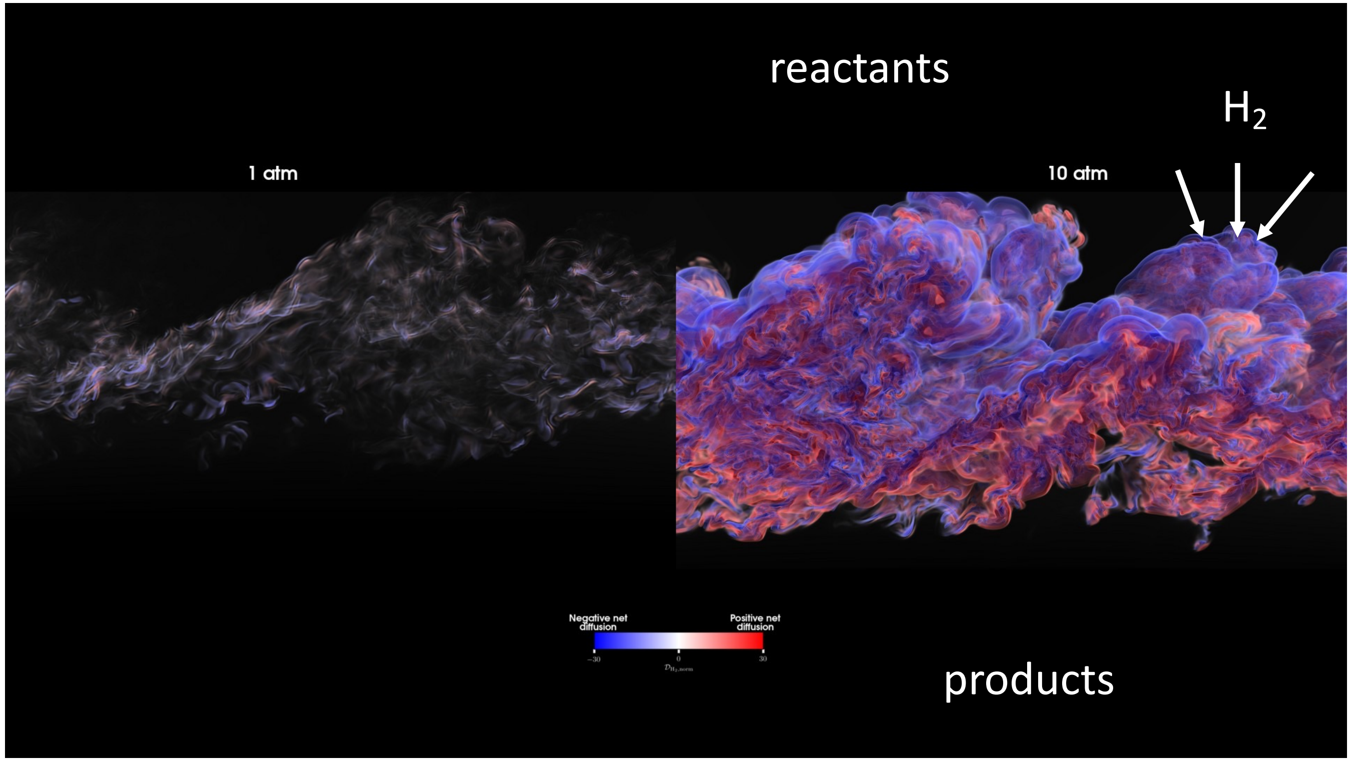


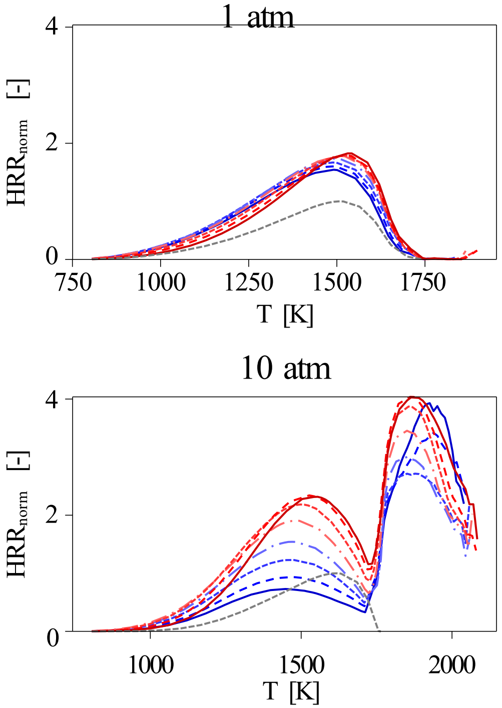
- Faster increase in flame surface density, fuel consumption rate, burning intensity (I_o)
- Weaker thinner flames at high pressure, greater preferential diffusion and thermodiffusive effect

Thermo-diffusive instabilities and preferential diffusion

Preferential/Differential Diffusion Effects at 1 & 10 atm ($t/t_{\delta_0} = 300$)

Diffusion rates of H_2





convex concave towards reactants

- Preferential diffusion rates are amplified at elevated pressure
- Flame at 10 atm responds more strongly to preferential diffusion, i.e., is more equivalence ratio sensitive (corroborated by simplified 2D studies)

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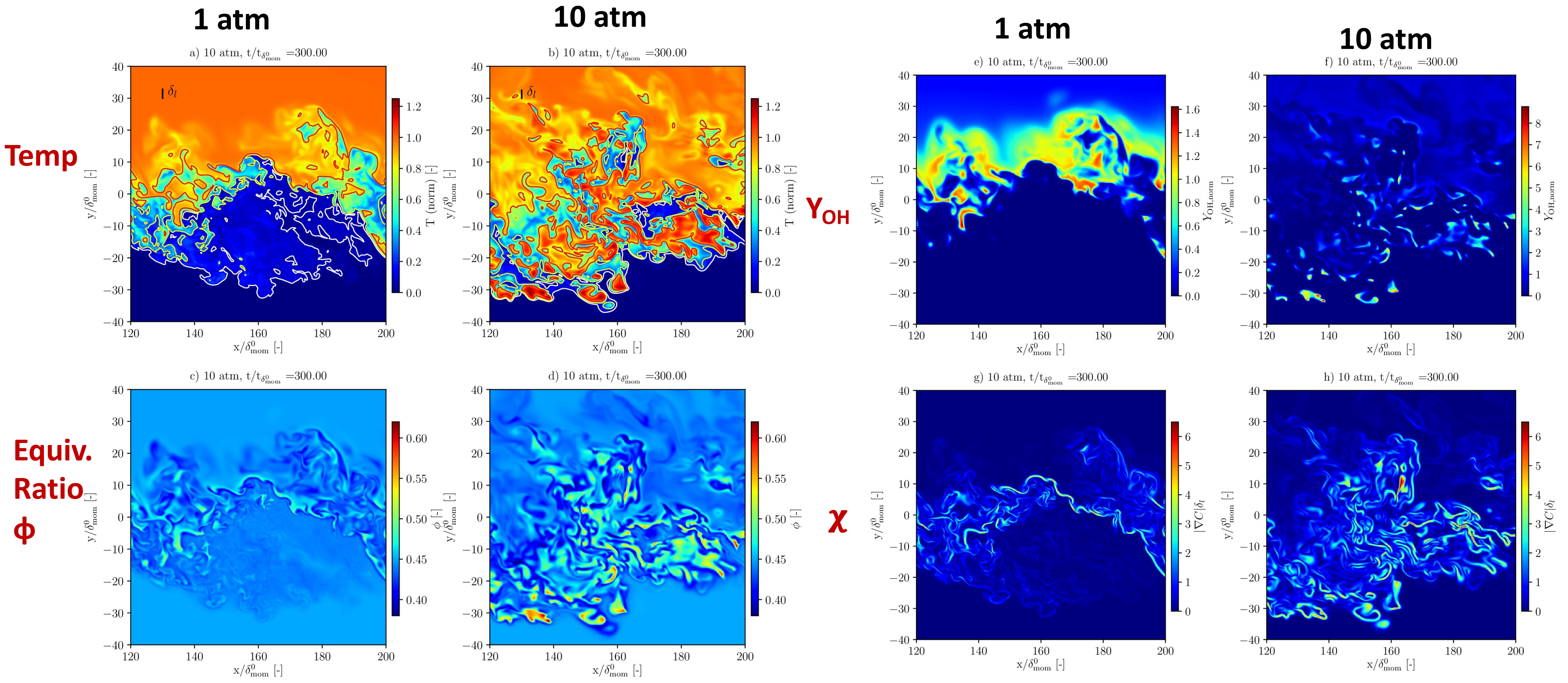
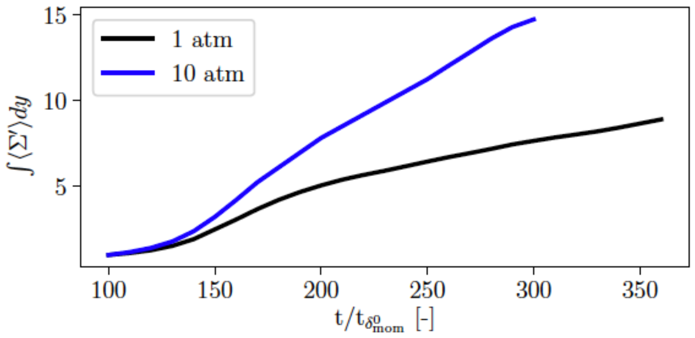
Comparison of flame structure and mixing rates



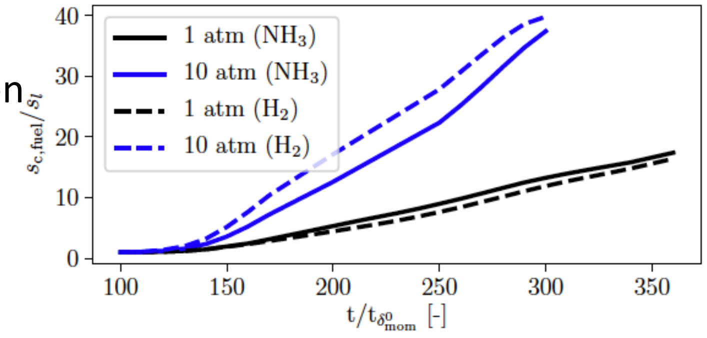
Temperature (top)and equivalence ratio (bottom) (left panel) OH mass fraction(top) and scalar dissipation rate (bottom)(right panel) Iso-lines correspond to temperatures of 800 (white), 1000(grey) and 1500 K (black)

Flame Surface Area and Burning Rate

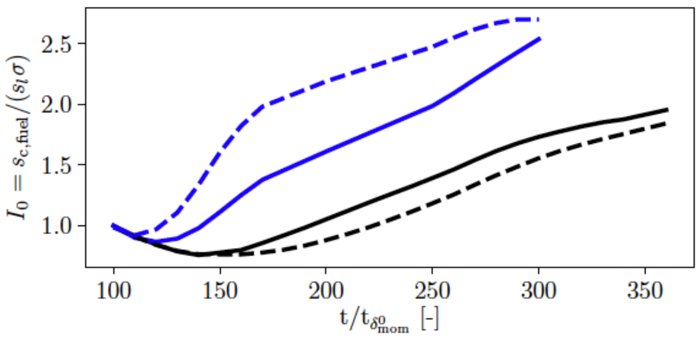
Flame surface density



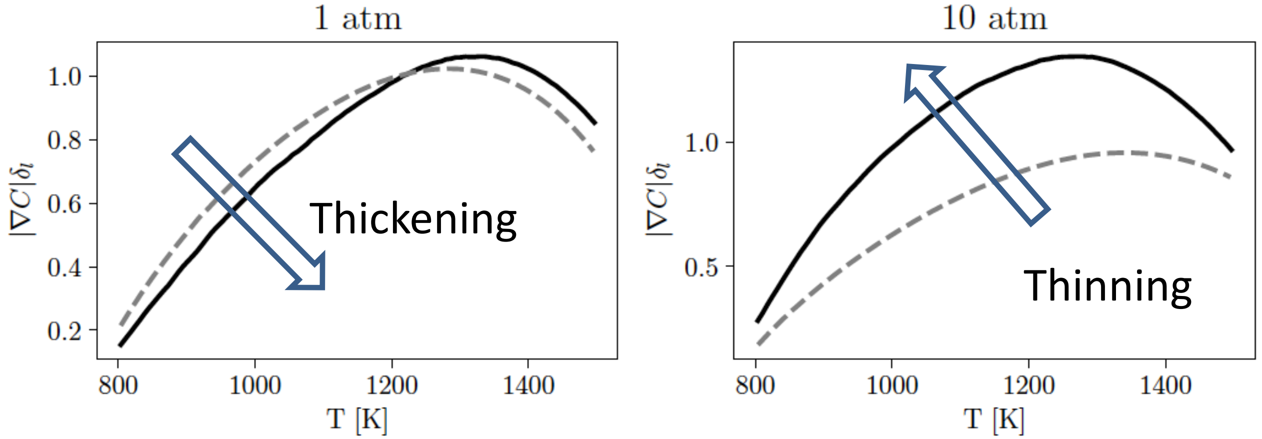
Fuel consumption speed



Burning Intensity



Flame thickness

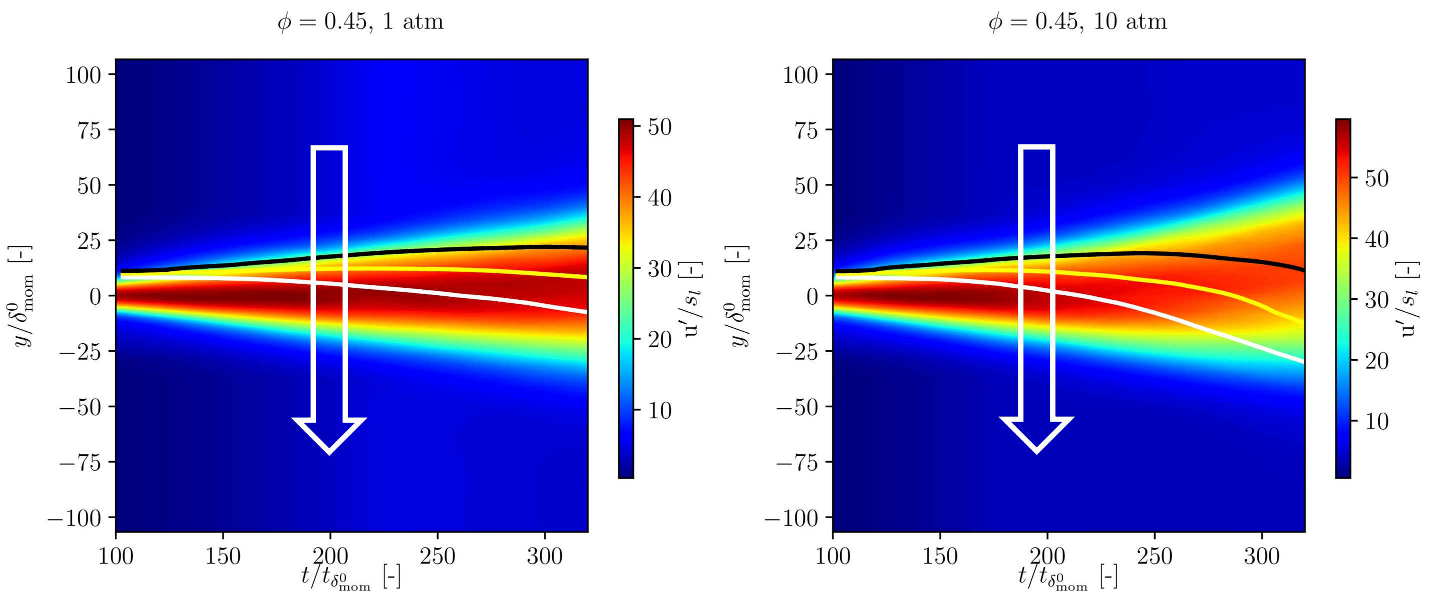


Black lines represent DNS solution at $t/t_{\delta^0_{mom}} = 300$. Grey dashed lines represent laminar flame solution.

- Faster increase of flame surface density ($\int\langle\Sigma'\rangle dy$), overall fuel consumption speed ($s_{c,fuel}/s_l$) and burning intensity (I_0)
- Thinner flames at 10 atm (larger $|\nabla C|\delta_l$)

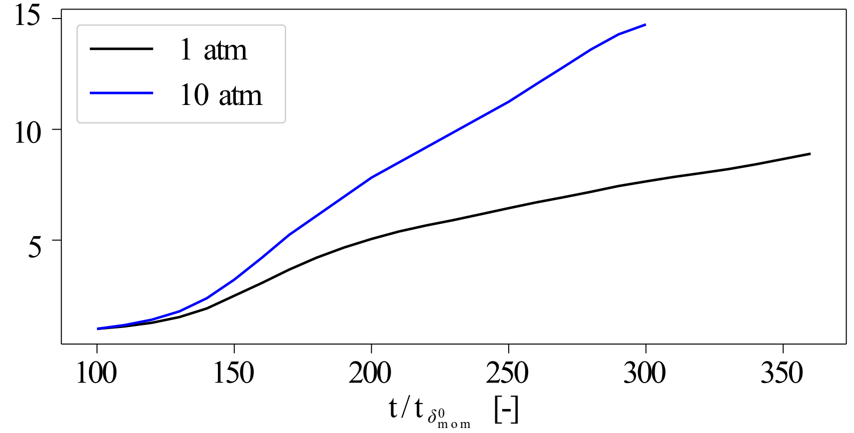
General Flame Behavior at 1 and 10 atm

U_{rms} vs. normalized y and t



Flame Surface Density

$(\int \langle \Sigma' \rangle dy)$ vs. time



C=0.2 (white), C=0.5 (yellow), C=0.8 (black)

- Turbulent flame brush propagates through shear layer faster at 10 atm, flame surface generation is faster.

Rieth *et al., Comb. Flame* 2022

Summary

- Performed DNS of lean (ϕ=0.45) $NH_3/H_2/N_2$-air flames at 1 and 10 atm in intense sheared turbulence

- Despite nominally similar 'turbulence-flame' interaction parameters, both flames behave very differently:
  - 1 atm flame exhibits significant preheat zone broadening and strongly disrupted flame surface
  - 10 atm flame features cellular structure, strong super-adiabaticity, faster flame surface area growth, faster fuel consumption and thinner flames despite the high Karlovitz number

Outline of Part 2: Ammonia/hydrogen/nitrogen-air premixed turbulent flames relevant to gas turbines

- Blow-out resilience
- Pressure effects
- **NO and N_2O emissions**

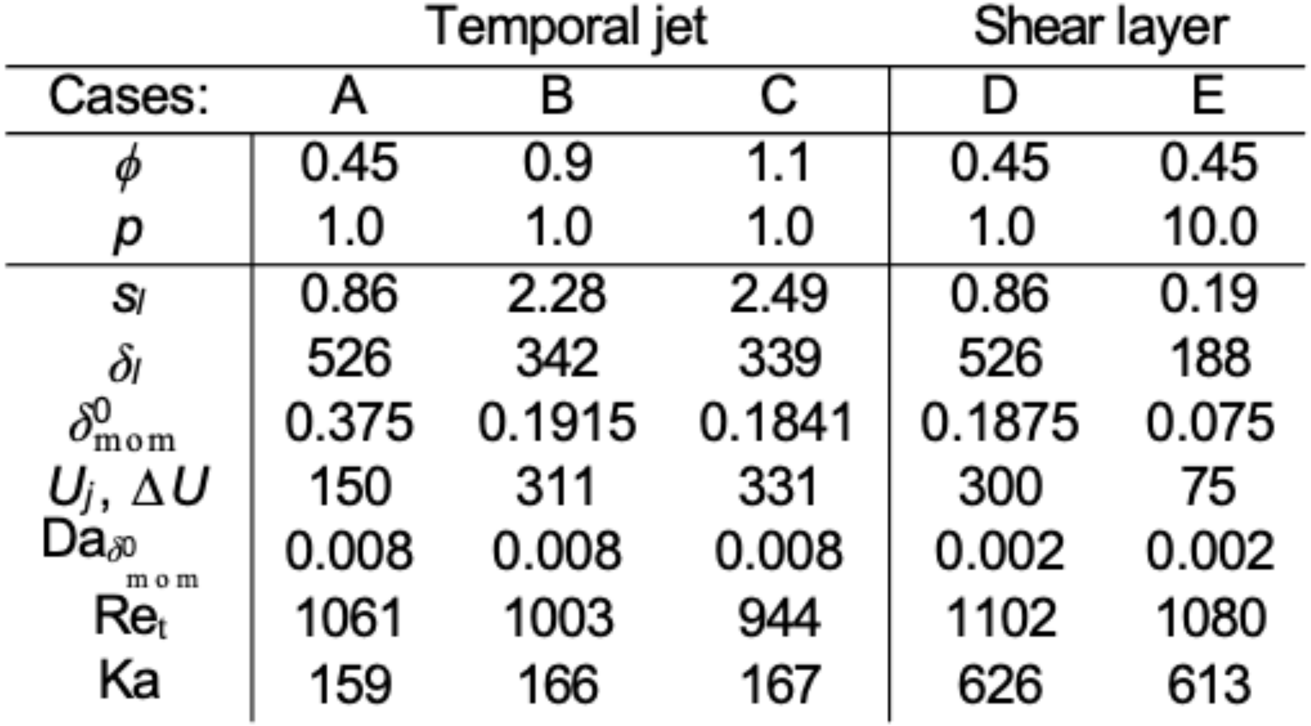
A direct numerical simulation study on NO and N_2O formation in turbulent premixed ammonia/hydrogen/nitrogen-air flames

M. Rieth[1], A. Gruber[2], J.H. Chen[1]

[1]Sandia National Laboratories, [2]SINTEF Energy Research

Rieth et al. (2022) Proc. Comb. Inst.

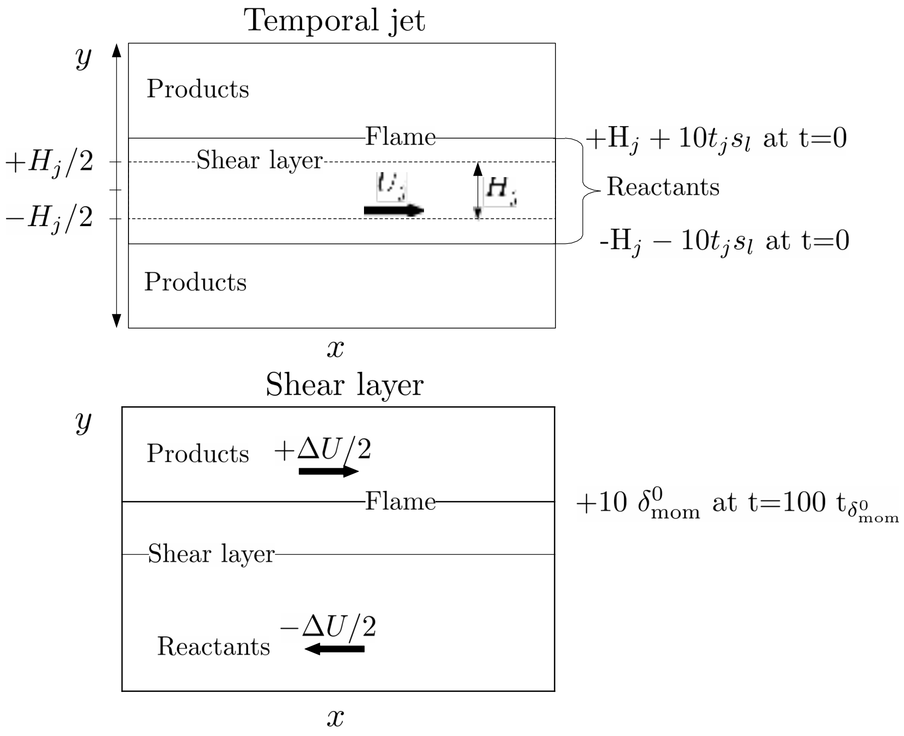
Problem Configuration and Parameters



	Temporal jet			Shear layer	
Cases:	A	B	C	D	E
ϕ	0.45	0.9	1.1	0.45	0.45
p	1.0	1.0	1.0	1.0	10.0
s_l	0.86	2.28	2.49	0.86	0.19
δ_l	526	342	339	526	188
δ^0_{mom}	0.375	0.1915	0.1841	0.1875	0.075
U_j, ΔU	150	311	331	300	75
$Da_{\delta^0_{mom}}$	0.008	0.008	0.008	0.002	0.002
Re_t	1061	1003	944	1102	1080
Ka	159	166	167	626	613

- Fuel: $NH_3/H_2/N_2$-air (40/45/15% vol)
- Reactants are preheated to 750 K
- DNS using S3D-Legion on up to ~ 1000 nodes on OLCF's Summit
- DNS feature up to 11 B grid points
- DNS use UCSD reduced chemical mechanism by Jiang et al. (IJER, 2020)

Temporally-evolving shear layer and temporal jet configurations



Flame is placed close to shear layer in all cases.

Pressure Effects on NO and N_2O production for lean $NH_3/H_2/N_2$-air premixed turbulent flames

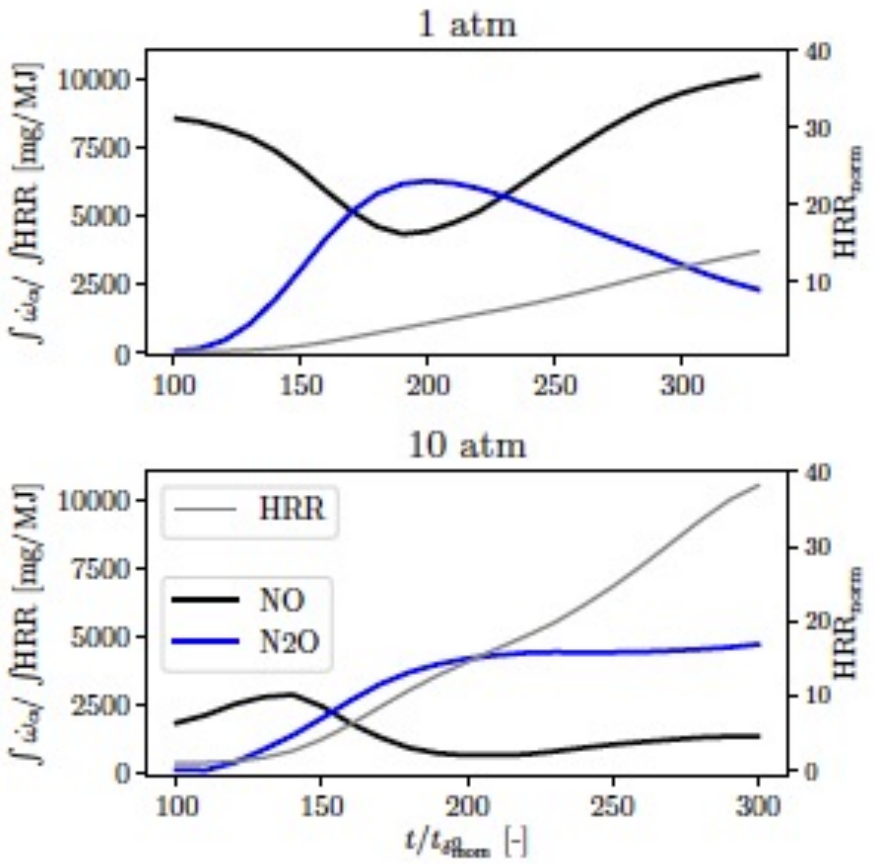
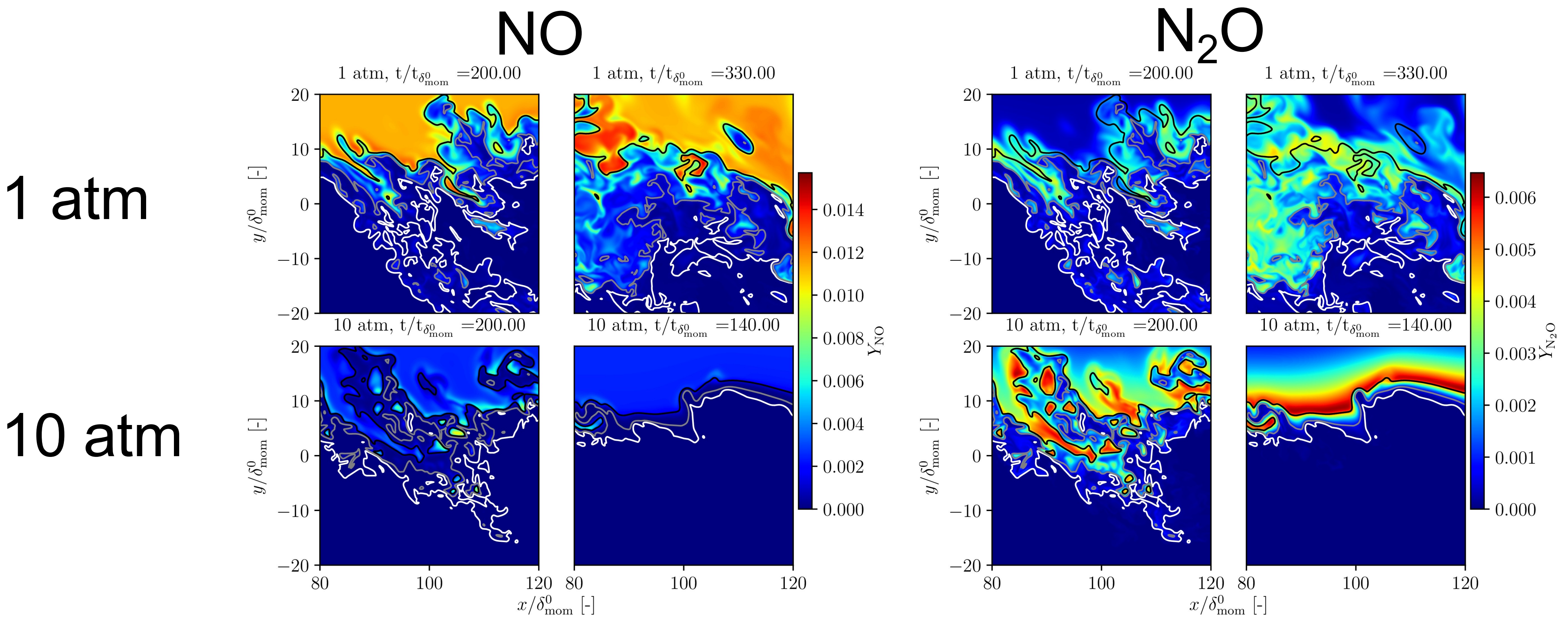


Fig. 2: Volume-integrated NO and N_2O net production rates per unit of heat released and normalized volume-integrated heat release rate for cases D and E versus time.

Rieth et al. (2022) Proc. Comb. Inst.

- The turbulent flame for $\phi = 0.45$, 10 atm is significantly more unstable and accelerates faster compared to the $\phi = 0.45$, 1 atm flame
- At 10 atm, the net NO production is reduced compared to 1 atm and approaches a steady-state value that is well below the values observed at 1 atm (8 fold reduction) and laminar 10 atm conditions; however, N_2O production is elevated

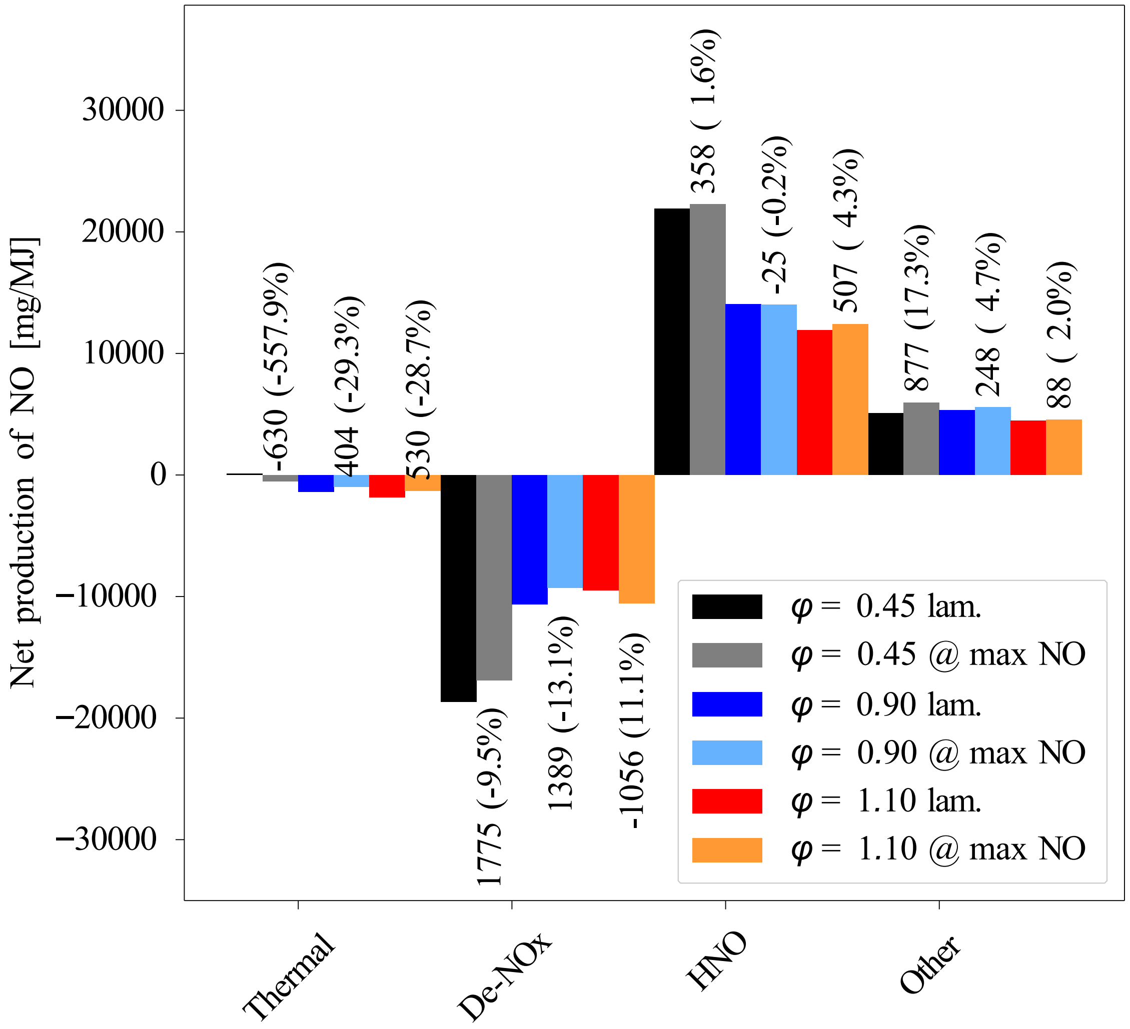
Topological dependence of instantaneous NO and N_2O



- The $\phi =$ 0.45, 10 atm case features overall lower NO mass fractions (through a decrease in the radical pool by chain-terminating three-body reactions)
- However, local NO mass fractions can significantly exceed laminar peak values at turbulent conditions
- NO and N2O mass fraction peaks in positively curved flame elements (convex towards the unburnt side) which is pronounced at 10 atm
- Strong role of thermo-diffusive effects driving increase in availability of H atom in the consumption N_2O

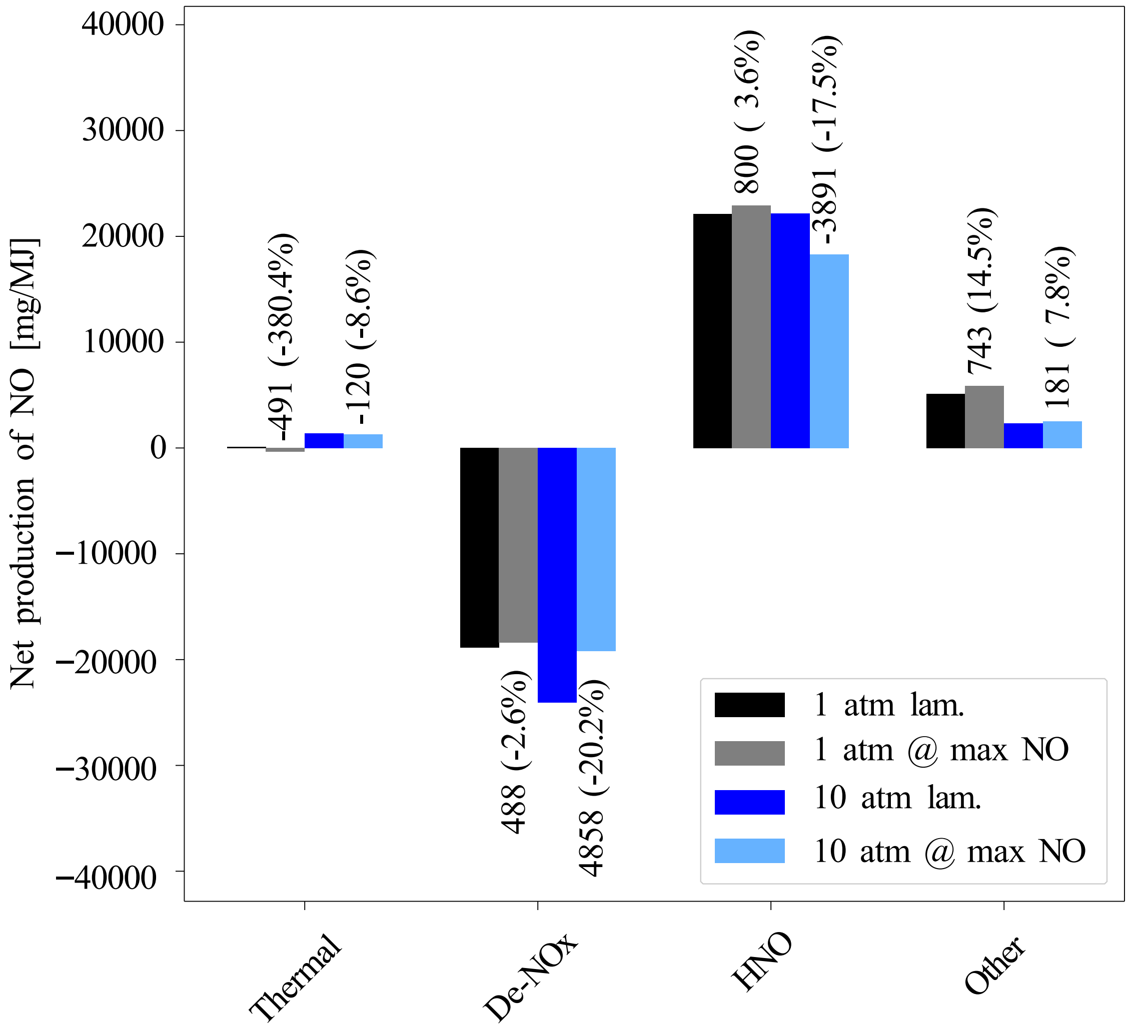
R42: $NH+NO \rightleftharpoons H+N_2O$; R61: $H + N_2O \rightleftharpoons OH + N_2$

NO pathways - equivalence ratio comparison



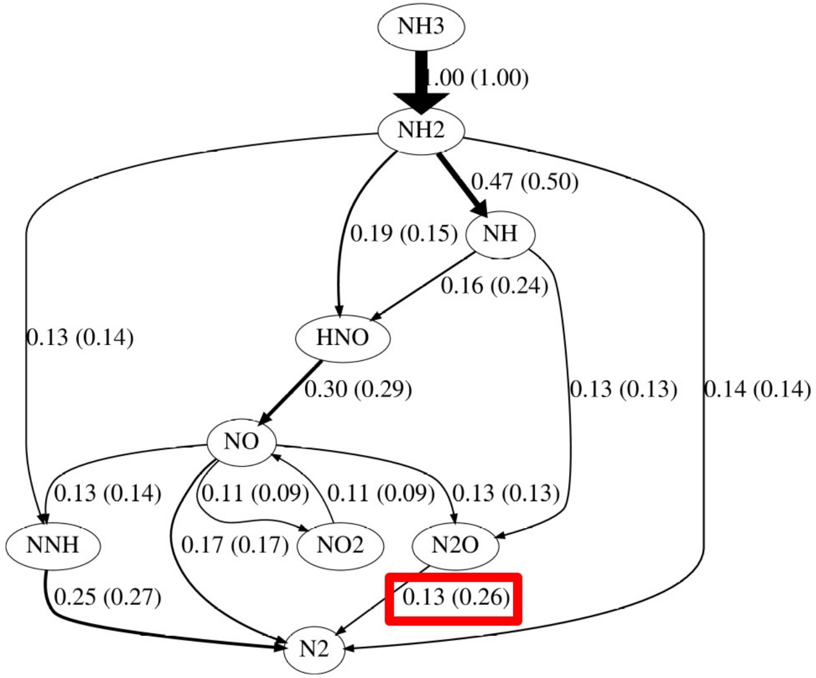
- Thermal pathway is relatively insignificant at $\phi = 0.45$ (case A), becomes more important at $\phi = 0.9$ (B) and $\phi = 1.1$ (C)
- The De-NOx pathway is responsible for the majority of the consumption of NO; for $\phi = 0.45$ and $\phi = 0.9$ NO consumption decreases, while it increases during the turbulence-chemistry interaction at $\phi = 1.1$
- The HNO pathway to NO production is large at $\phi = 0.45$ compared to $\phi = 0.9$ and $\phi = 1.1$, and it is only marginally affected by the turbulence-chemistry interaction

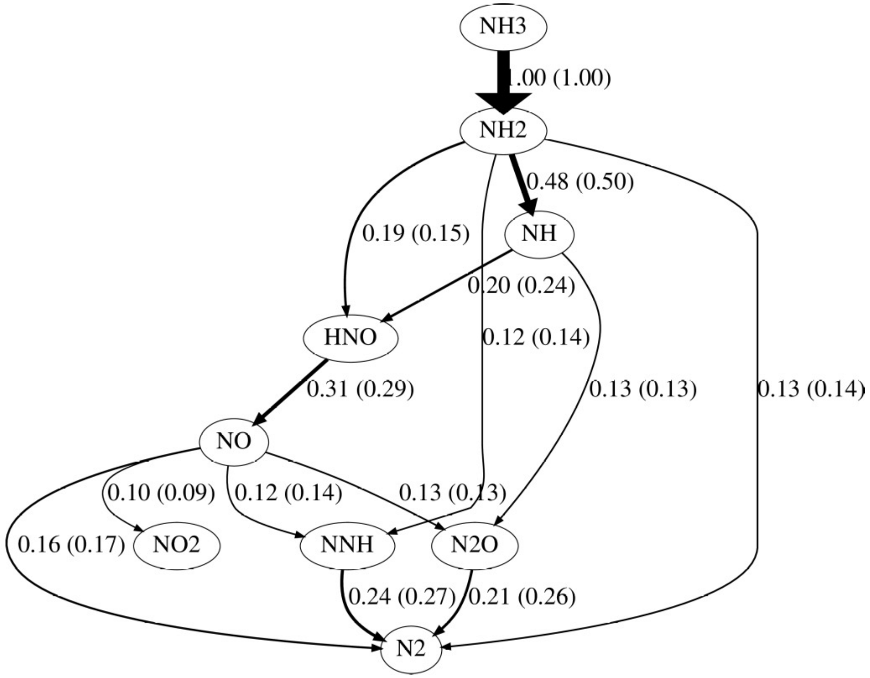
NO pathways - pressure comparison



- Comparison of cases D (1 bar, $\varphi = 0.45$) and E (10 bar, $\varphi = 0.45$) suggests that the relative importance of the thermal pathway increases at elevated pressure, but is weakened under turbulent conditions
- A decrease in NO consumption by De-NOx, a decrease in NO production through the HNO pathway and a slight increase in NO production through the “other” pathways result in overall lower NO emissions at 10 bar compared to atmospheric pressure conditions

Nitrogen flux for case E (10 atm)


Max N2O prod, t/t_j=200.0

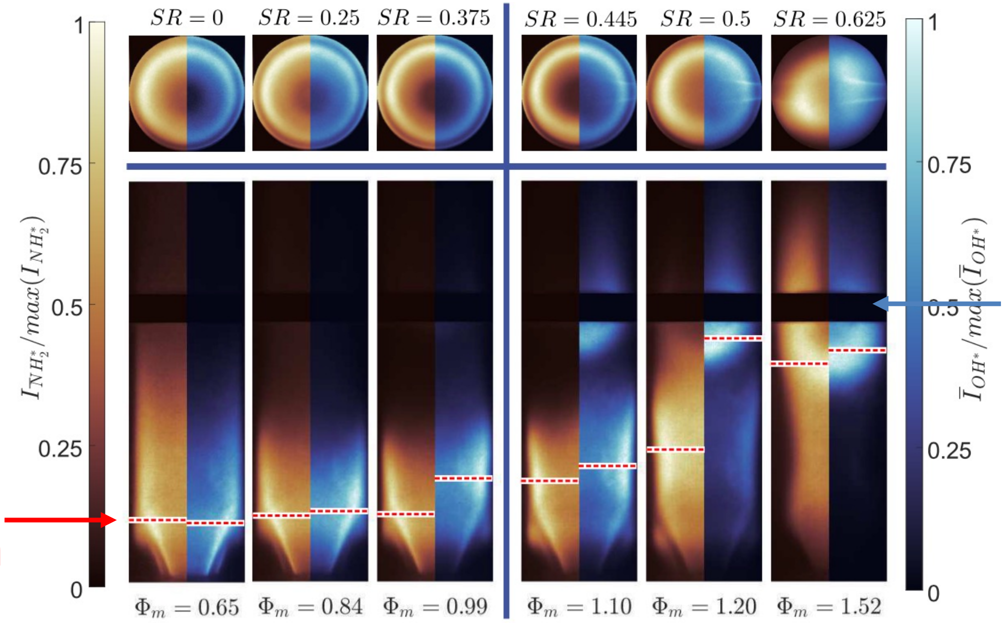

Max NO prod, t/t_j=140.0

- Clear difference is observed in the nitrogen flux at time $t^{\max}_{N_2O}$; while the formation of N_2O from NO and NH is only slightly amplified at 10 bar, the formation of N_2 via N_2O is significantly lower
- Largest contributing reaction is $H + N_2O \rightleftharpoons OH + N_2$, while $NH+NO \rightleftharpoons H+N_2O$ is the leading reaction producing N_2O

NTNU NH_3/H_2 Axially Staged Lab-Scale Burner

- NTNU (Norway) RQL 2-stage burner configuration: NH_3/H_2 + air [1]
- 1bar, 298 K at inlet
- Experimental data available: OH* and NH_2*
- Detailed study of NO and N_2O formation in realistic configuration

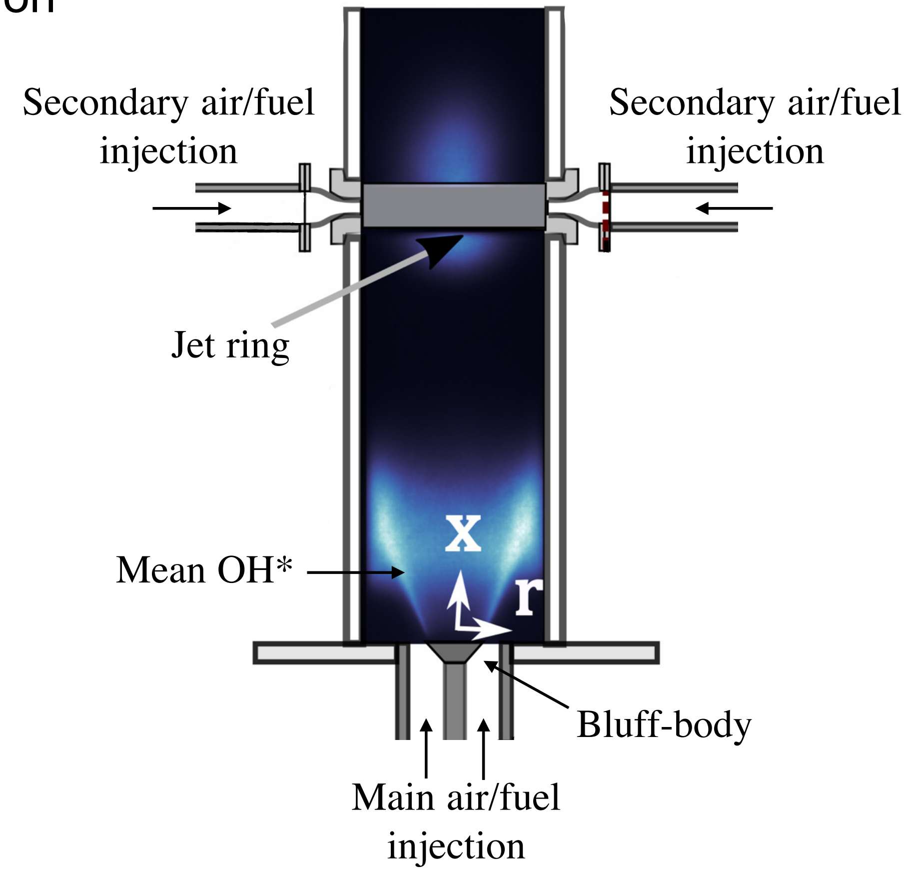
NH_2* (left) and OH* (right)
chemiluminescence for 6 different split ratios



Max location

Secondary air injection

NTNU experimental set up



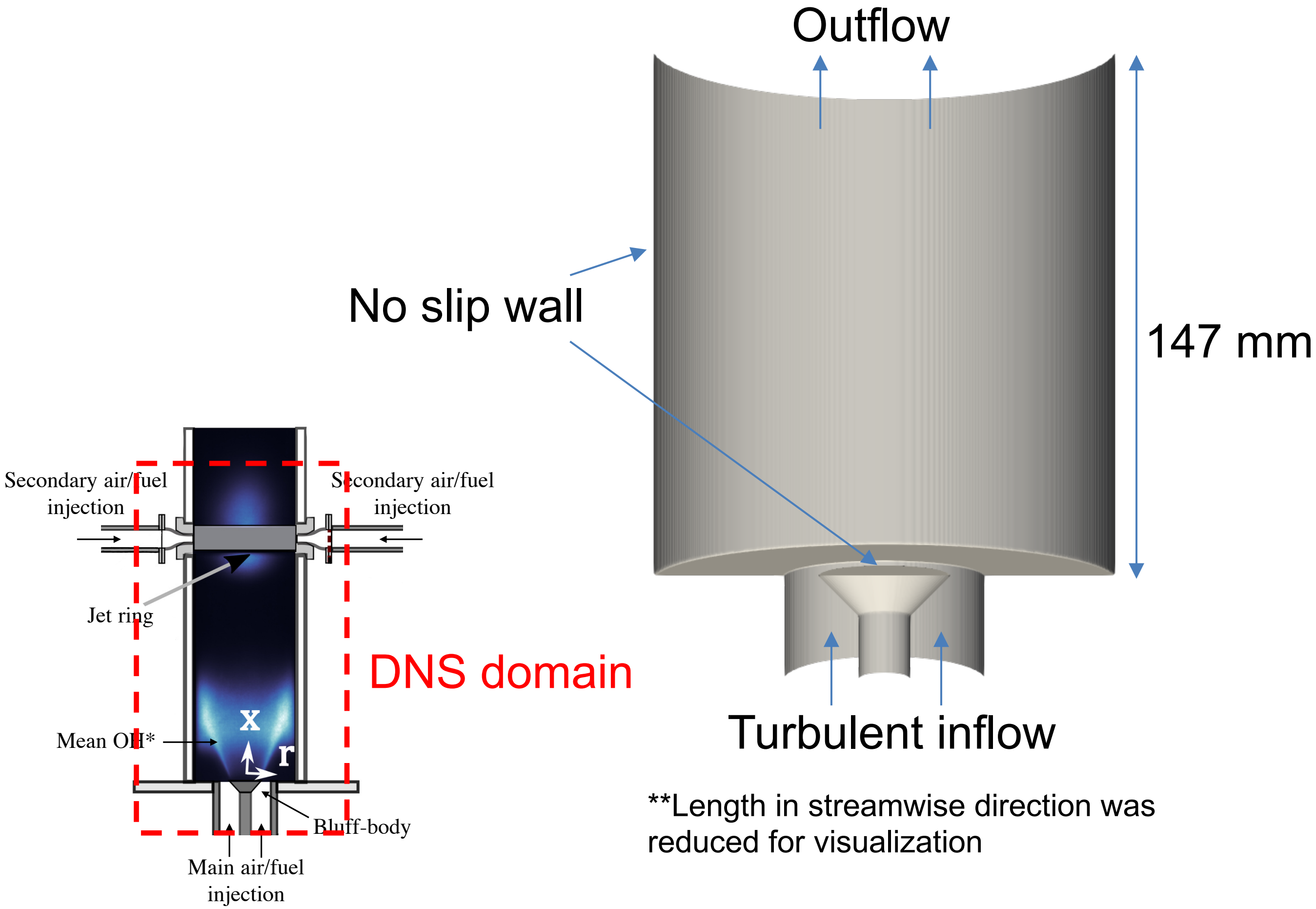
[1] Ånestad, Aksel, et al. "The Structure and Stability of Premixed CH4, H2, and NH3/H2 Flames in an Axially Staged Can Combustor." *Turbo Expo: Power for Land, Sea, and Air*. Vol. 86960. ASME, 2023

DNS of the Rich-Quench-Lean (RQL) Burner

- DNS simulation of a real combustor using PeleLMeX
- Combustor geometry captured with Embedded Boundary (EB) treatment

Conditions	
Pressure	1 bar
Inlet temperature	298 K
Inlet bulk velocity	15 m/s
Re number	10,540
Kolmogorov length	45 µm
Split ratio	0.0
Equiv. ratio	1.15
Fuel composition	$X_{NH3} = 0.75; X_{H2} = 0.25$
Chem. mechanism	Jiang et al

PeleLMeX domain with boundary conditions



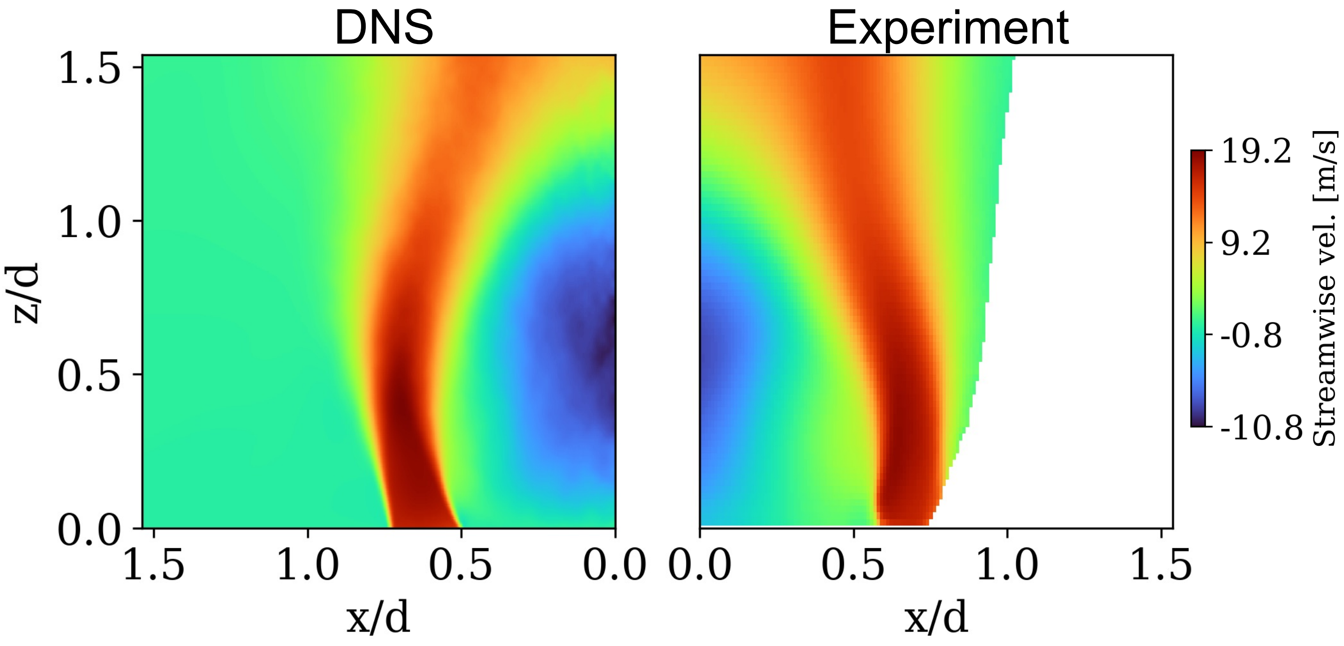
**Length in streamwise direction was reduced for visualization

B. Soriano, in prep. 2024

DNS of the RQL Burner: validation

- Non-reacting and reacting flow field validation using a hydrogen-air configuration with the same bluff-body geometry

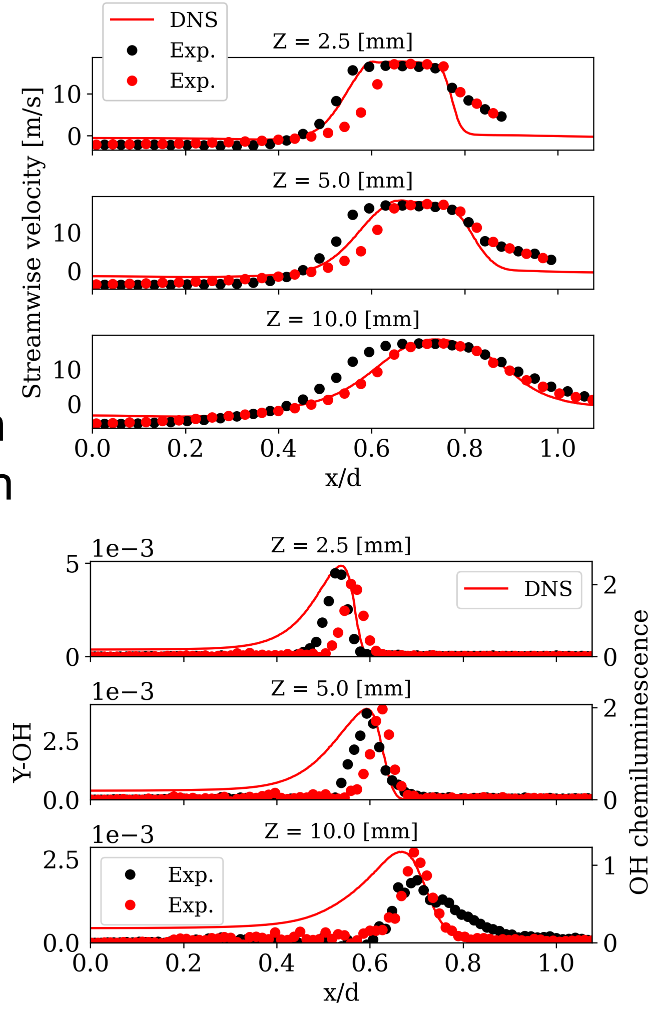
Non-reacting



Comparison ensemble average streamwise velocity

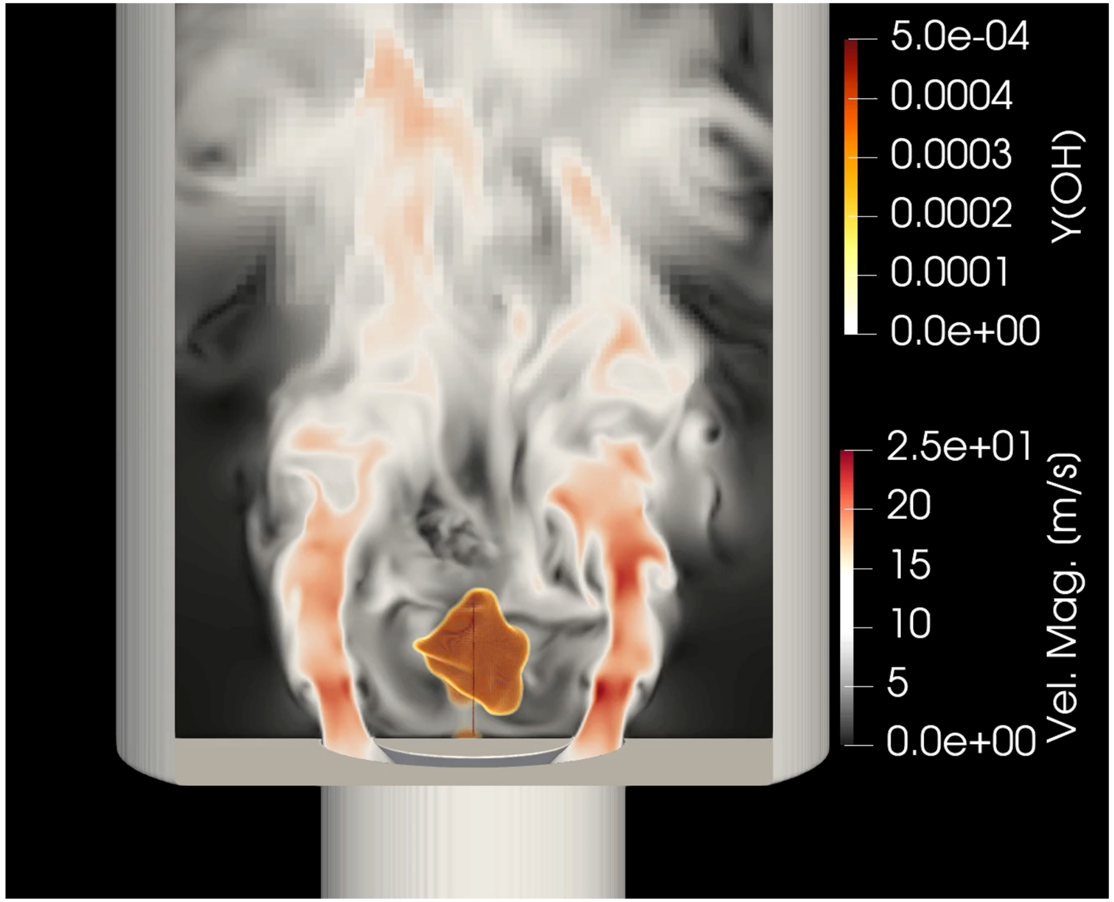
- Two experimental means correspond to each side of the combustor along vertical symmetry plane
- Good agreement with streamwise velocity in the reacting flow field
- OH peak correctly captured in the shear layer

Reacting



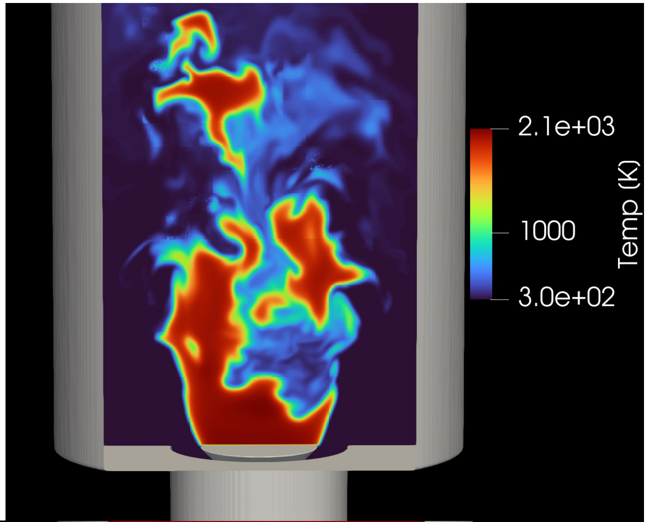
DNS of the RQL Burner: preliminary results

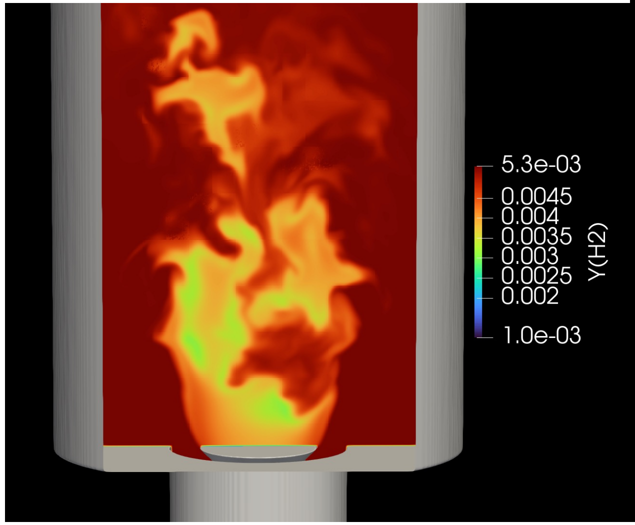
Ignition and early stages of combustion

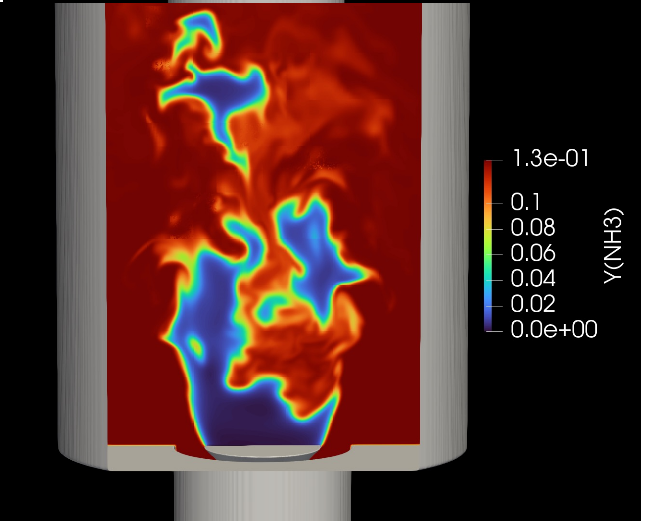


Preliminary instantaneous analysis:

- Ammonia is mostly consumed in the recirculation zone
- H_2 persists in the flame products side
- Potential increase in H_2 contribution to flame stabilization

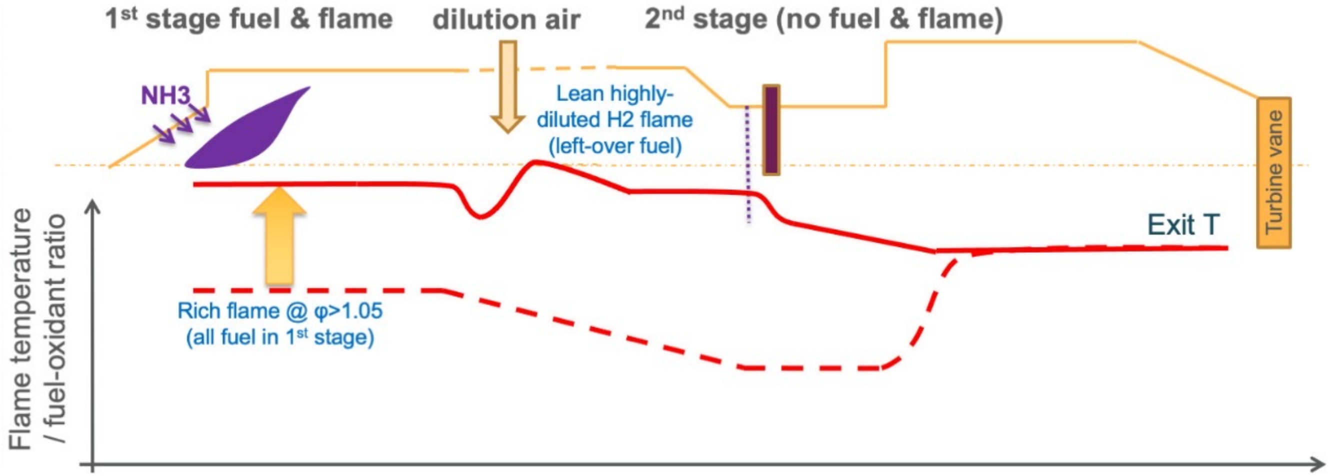






Ammonia Rich-Quench-Lean (RQL) Operation

- Reactivity and NO_x emissions are a challenge for ammonia combustion
- Promising strategy: 2-stage rich-quench-lean (RQL)
  - 1st stage fuel-rich NH_3-air flame (good for NO_x[1])
  - 2nd stage air injection to burn off remaining hydrogen



Heggset et al., Proc. of ASME Turbo Expo 2023.

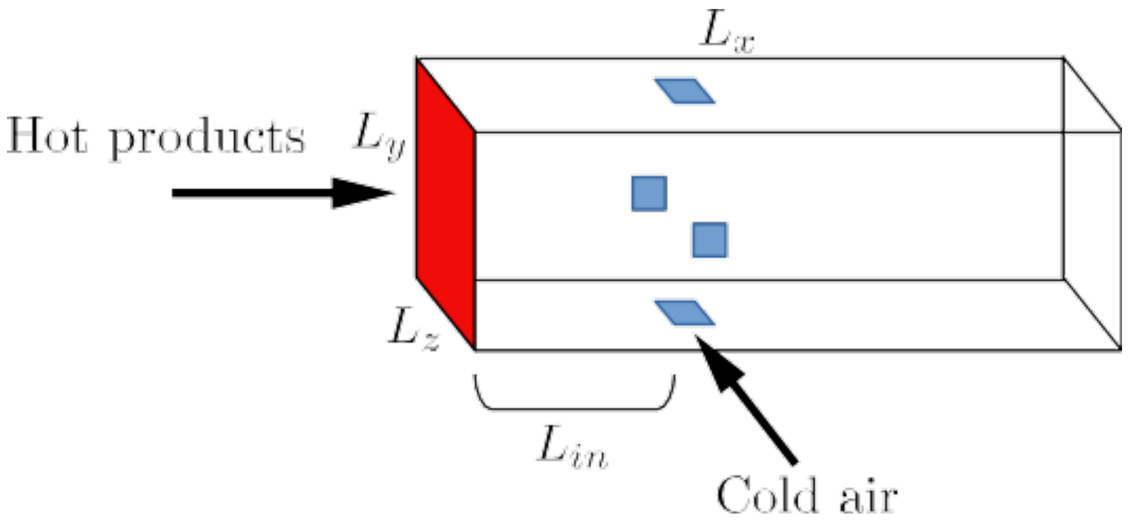
NO_x depends on 2nd stage combustion, mixing & residence times

→ unravel details with DNS

[1] Kobayashi et al, PROCI, 2019.

Numerical Setup: Dilution air jet into cross-flow of equilibrium products

- Cross-flow: hot equilibrium products of rich ammonia-air flame
- 3 cases for ϕ=1.1, 1.2 and 1.3 plus case with ammonia slip at ϕ=1.3
- 4 air jets in cross-flow
- Air/unburned temperature is 780 K
- 25 atm pressure, 1900 K outlet target
- Timescales based on Heggset et al. LES[1], Re scaled down to 20,000
- 19 species NH_3/H_2 mechanism by Jiang et al.[2]



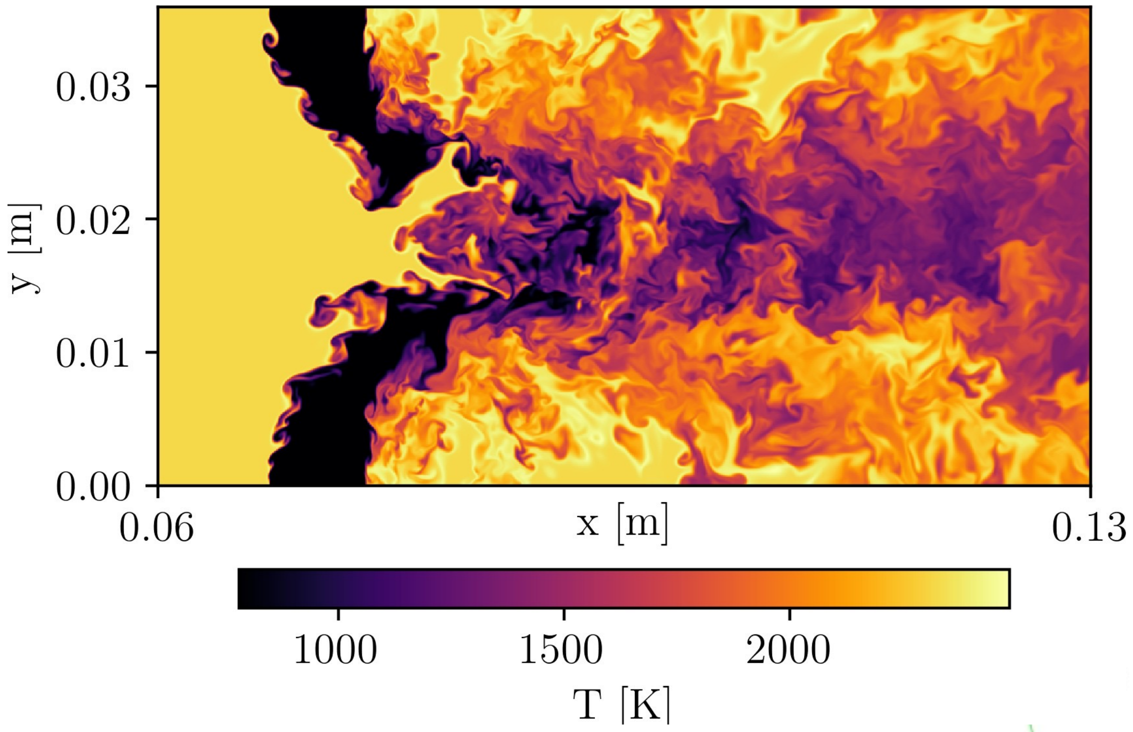
Code:

- PeleLMeX[2] - low-Mach AMR
- > 30B grid cells
- Frontier up to 768 nodes

[1] Heggset et al., Proc. of ASME Turbo Expo 2023. [2] Jiang et al., Int. J. Energy Res., 2020.

[2] https://github.com/AMReX-Combustion/PeleLMeX

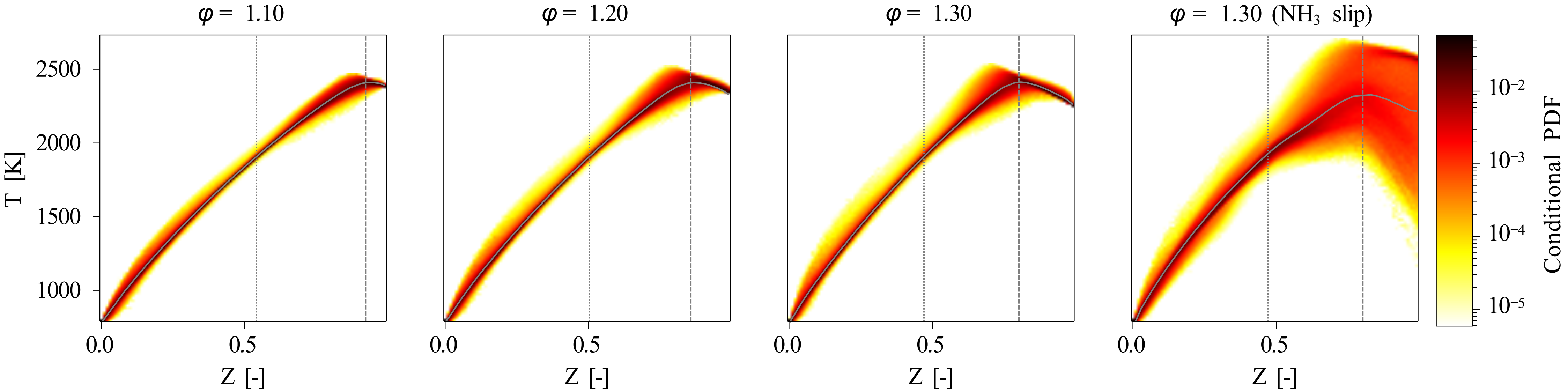
General Observations



- Rapid combustion as rich H_2-containing products come into contact with air jets
- Richer 1st stage ⟶ higher amount of H_2 ⟶ higher HRR
- Interesting 'inverted' diffusion flame (fuel on hot side)

Rieth et al., PROCI, 2024, in press

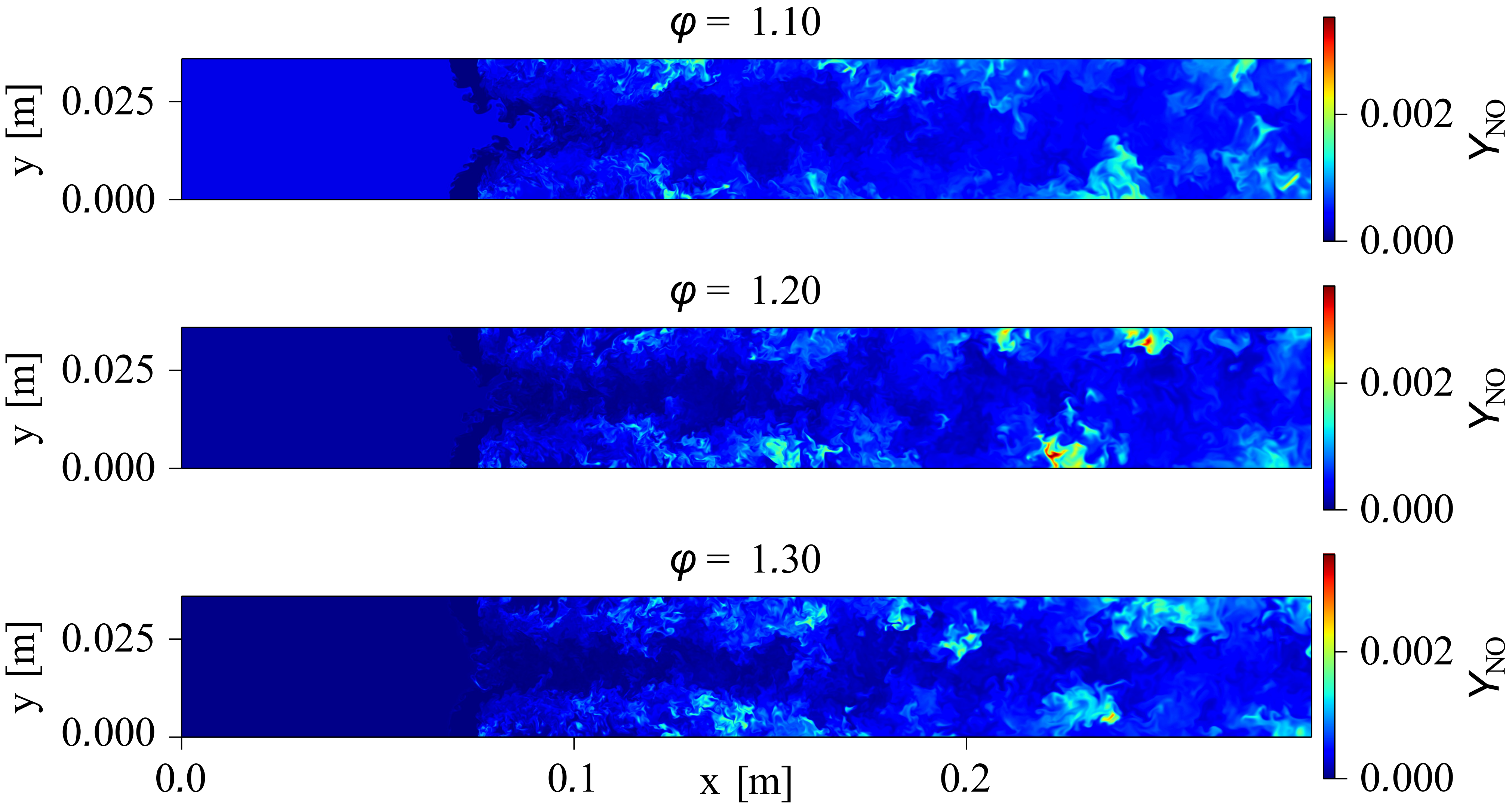
Temperature statistics



- Z=0: cold air, Z=1: cross-stream
- Richer 1st stage: larger temperature variation, especially close to stoichiometric mixture fraction
- Large temperature variation for NH_3 slip case

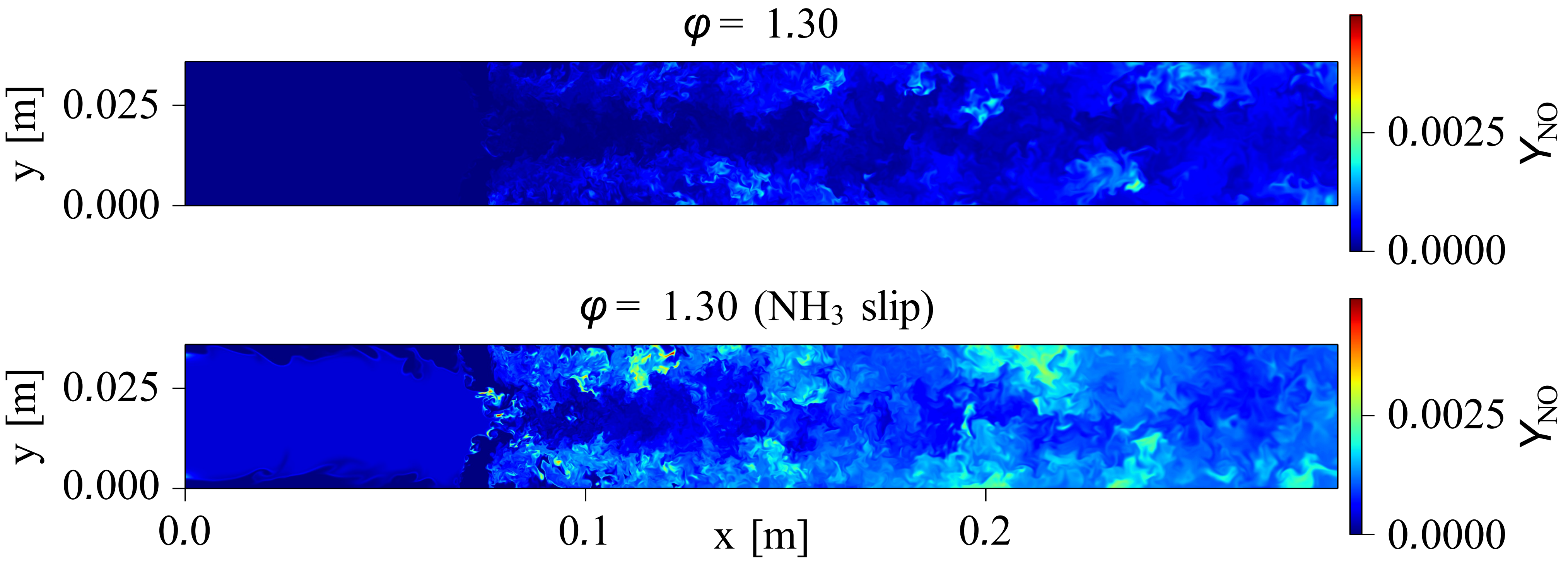
Rieth et al., PROCI, 2024, in press

NO formation



- Leaner 1st stage ⟶ higher NO at inlet
- NO appears in pockets downstream of air injection

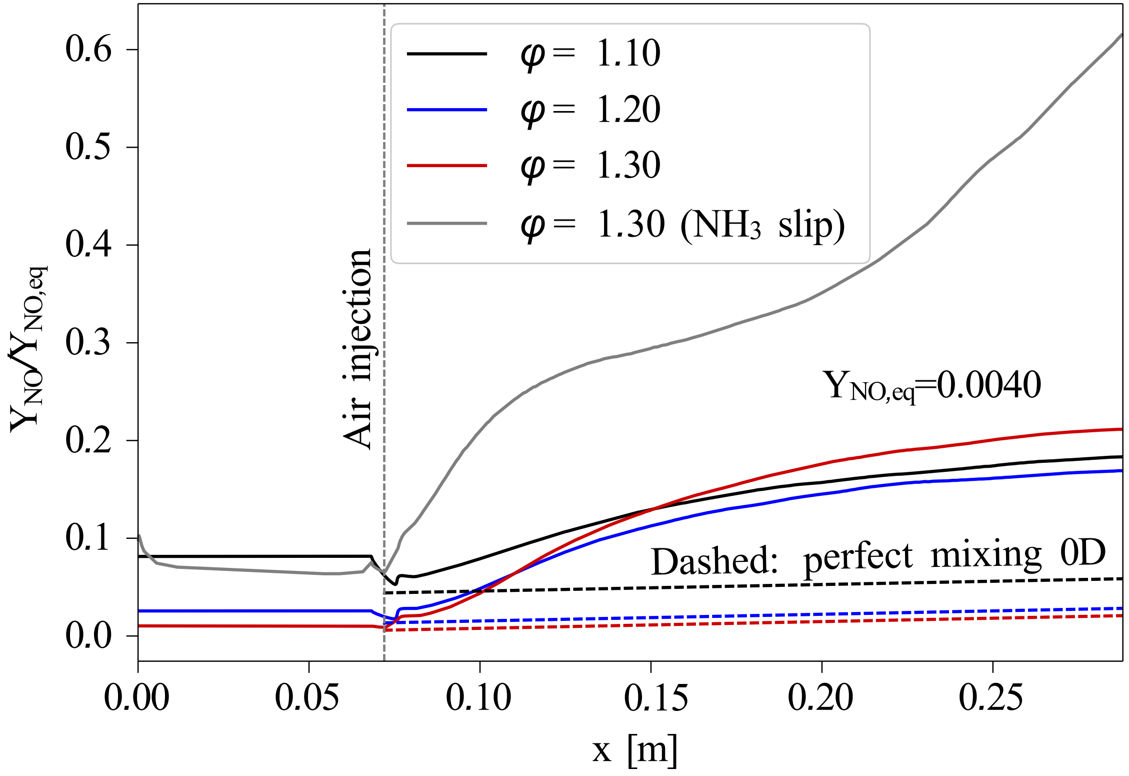
NO formation (with NH_3 slip)



- Additional DNS with ammonia slip in boundary regions of the cross-flow (4% of ammonia at air injection location)
- Significant increase of NO formation, NO produced in flame & downstream of air injection in regions of fast mixing

Rieth et al., PROCI, 2024, in press

Global NO emissions: averaged NO mass fraction profiles

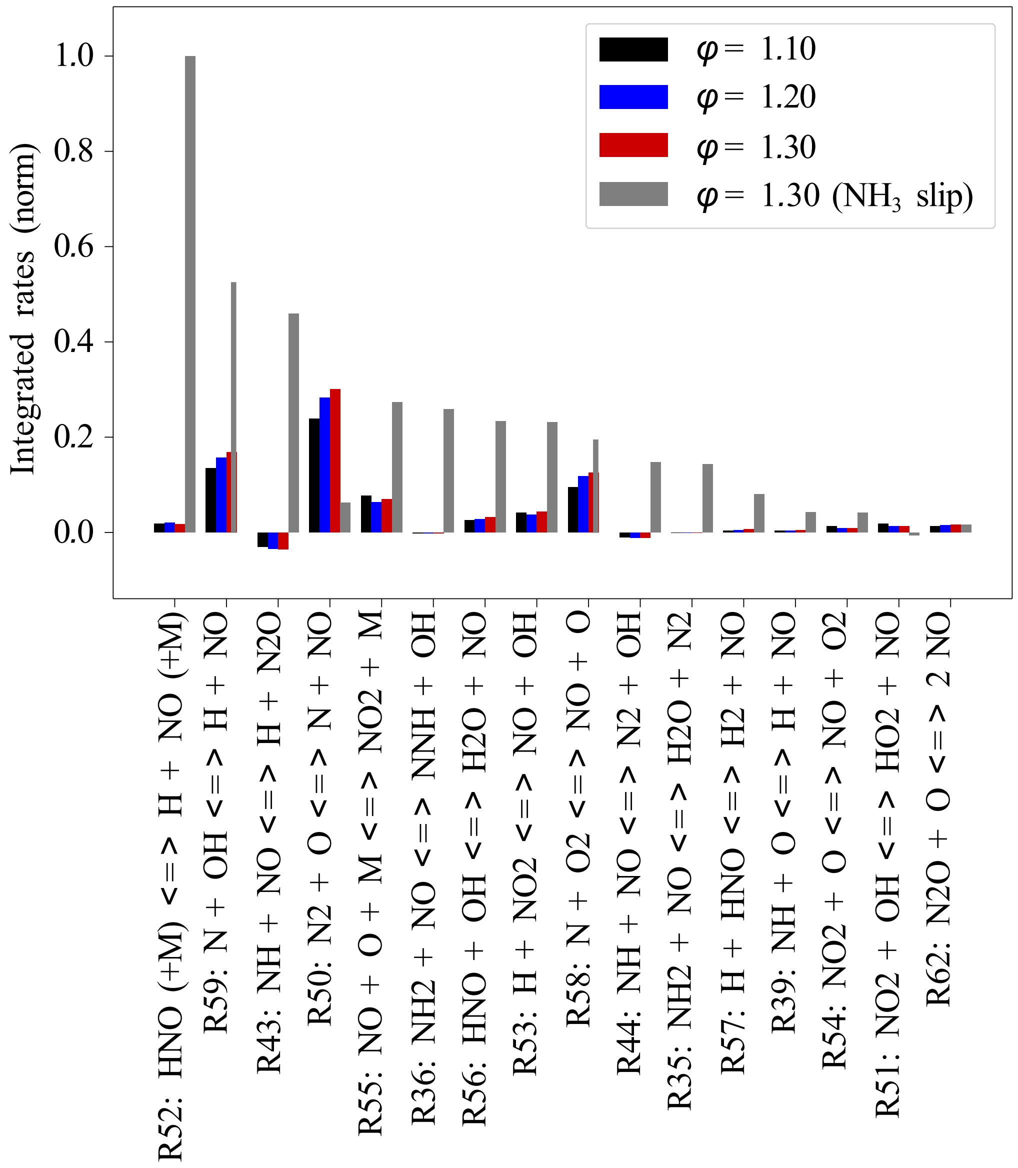


- Outlet NO depends on (1) inlet NO, (2) NO produced post air injection
- Richer 1st stage ⟶ lower inlet NO, faster NO production
- Ammonia slip leads to significantly faster NO production
- All cases show NO lower than equilibrium

- Through which pathways is NO produced?

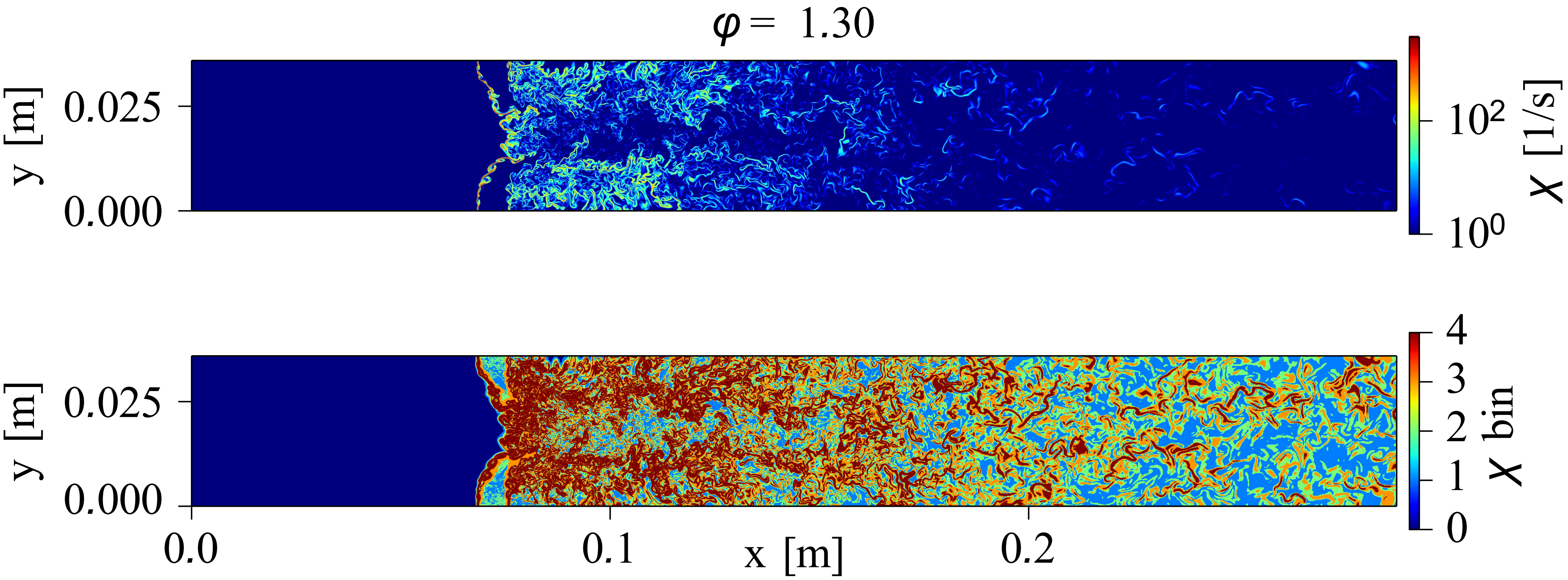
Rieth et al., PROCI, 2024, in press

NO formation pathways



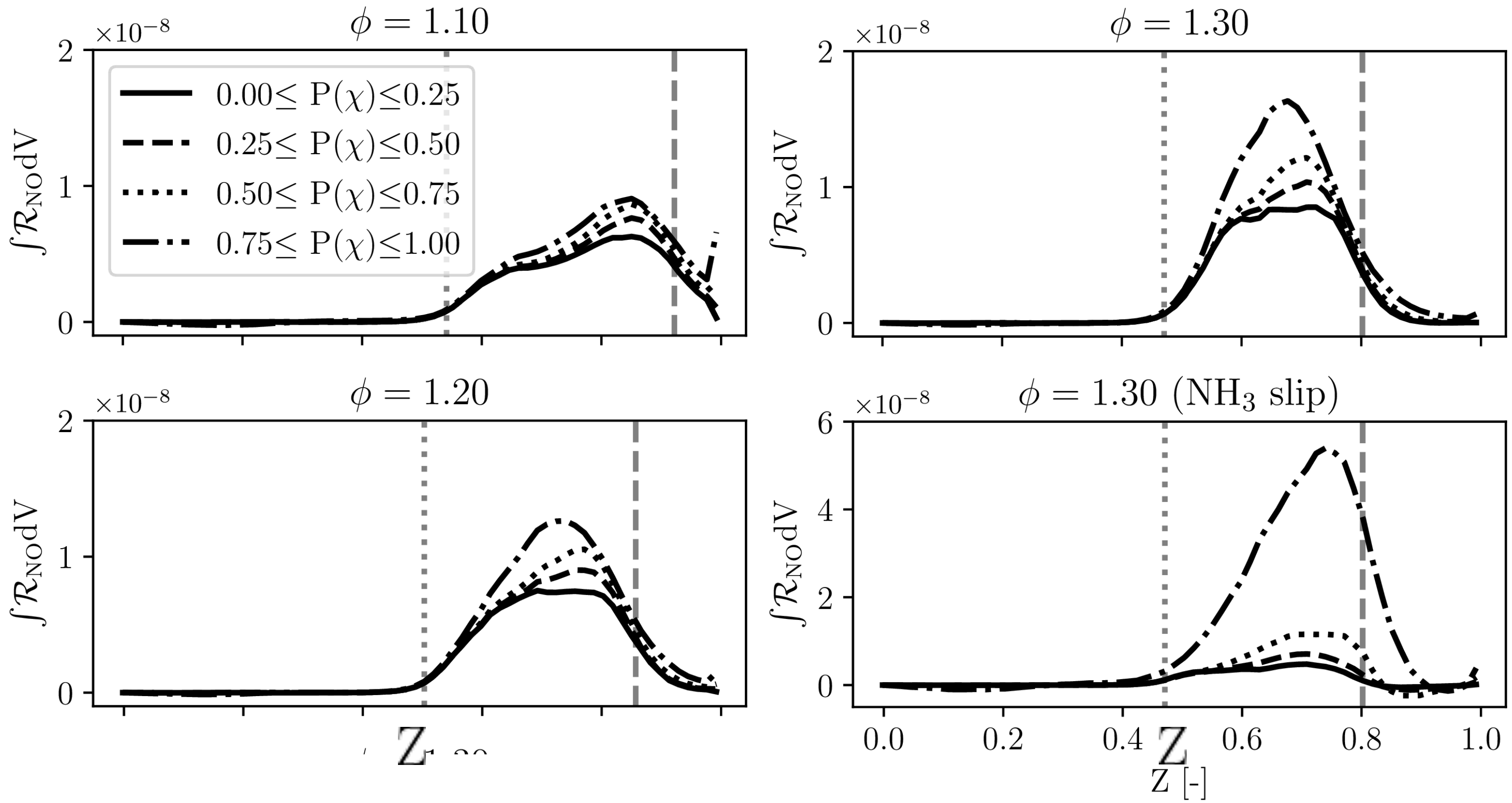
- NO formation for cases without ammonia slip is dominated by thermal pathway
- Higher H_2 content coming from 1st stage leads to larger temperature variation due to heat release and higher probability for hot regions
- Significant NO production through HNO pathway with ammonia slip (mainly: HNO(+M) = H + NO(+M)) from fuel-bound nitrogen, shifts in thermal production rates

NO formation dependence on mixing rates



- High scalar dissipation rate → high mixing rates
- Bins based on quartiles of the conditional scalar dissipation rate PDF (conditioned on the mixture fraction) to examine different regions of mixing in the jet

NO formation dependence on mixing rates



- Z=0: cold air, Z=1: cross-stream
- Higher first stage equivalence ratio: more NO production in strong mixing regions (due to higher T variation through heat release)
- Significantly higher NO production in ammonia slip case

Conclusions

- Increase in pressure amplifies thermo-diffusive instabilities in lean premixed flames when hydrogen is present
- Latest bluff-body flame simulations show promising results in simulating flames in more complex geometries
- RQL simulations at high pressure demonstrate NO emission reduction, but also show detrimental impact of ammonia slip