# HIGH–TEMPERATURE LOW–$NO_X$ COMBUSTOR CONCEPT DEVELOPMENT

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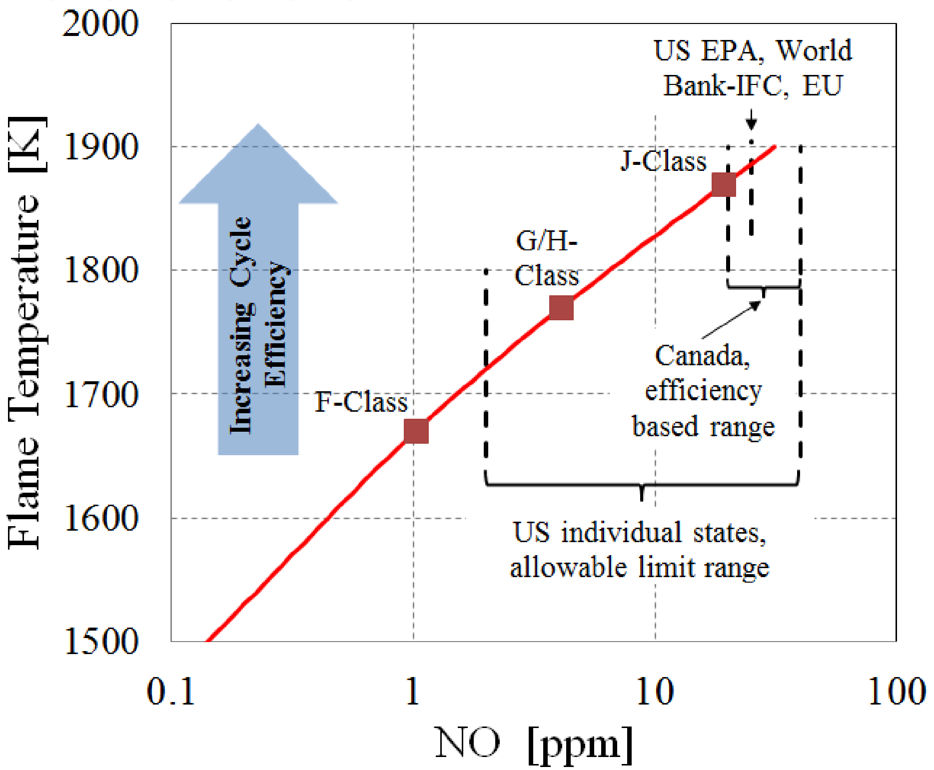
# MOTIVATION

- Gas turbine combined cycle efficiency has steadily increased from 47% to 62% over the past 3 decades
  - Driven by advances in materials and cooling methods
  - Simultaneous reduction in NOx emissions enabled by advanced combustion technologies
- Higher flame temperatures → higher efficiencies
- New combustor paradigm is needed
  - Current architectures (e.g. DLN) can't meet current emissions standards at elevated combustor temperatures




**New challenge: low NOx at high flame temperatures**

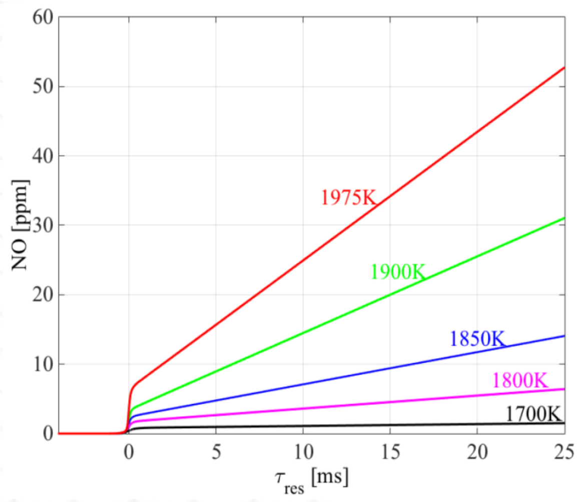
# PROPOSED APPROACH

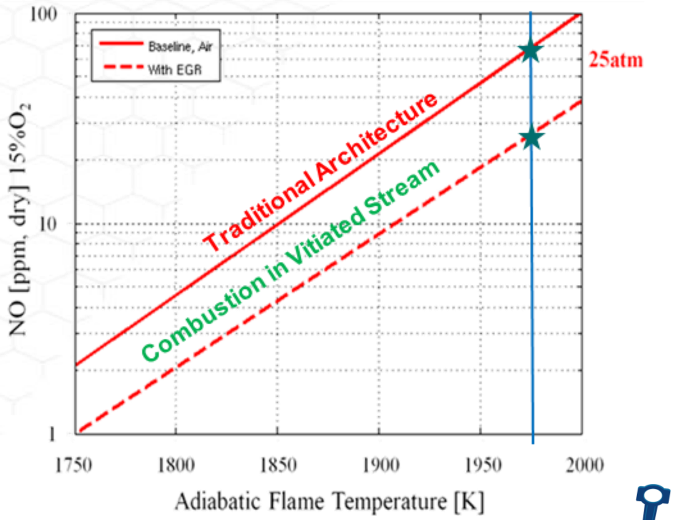
- Thermal NO formation dependent on temperature, residence time, and O radical concentration

$$O + N_2 \Leftrightarrow NO + N$$
$$[NO] \propto [O][N_2]e^{-38{,}379/T}\tau_{res}$$ (Bowman, 1992)

- Approach: Axial Staging
  - Reduce residence time @ high temperatures
  - Incorporate advantages of EGR (reduced [O])

- Reactor model studies have demonstrated advantages and potential pitfalls of axial staging (Ahrens et al., 2016 & Goh et al, 2017)
  - Highly sensitive to degree of mixing



# KEY RESEARCH QUESTIONS

(1) For a given firing temperature and residence time, what are the minimum theoretical NOx limits?

- How much lower is this fundamental limit than the limits achievable with current architectures?

(2) What do the actual fuel and air distribution patterns look like that attempt to achieve these theoretical values?

- Then, what are the operational behaviors of such a combustion system?

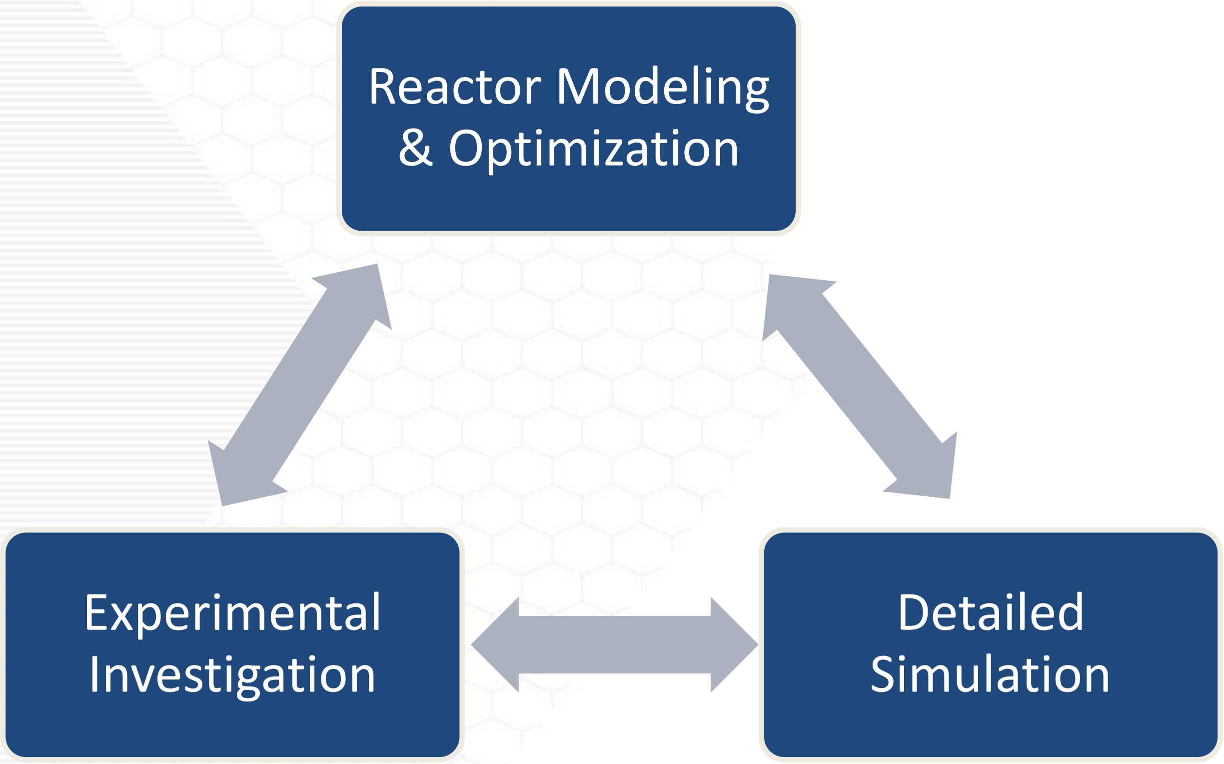
(3) What do local pre- & post-flame mixing patterns look like and how is the heat release distributed?

# EXECUTIVE SUMMARY

- Theoretical NOx floor enabled by axial staging is O(1 ppm)
- Measurements show NO production can vary significantly at a fixed rise in bulk average temperature ($\Delta T$) across the jet
- Crossflow entrainment with jet material/combustion products is critical to achieving low NOx emissions
  - NOx production primarily controlled by (1) stoichiometry of the jet and (2) lift-off of the flame from the jet exit
  - Vortical structures (shear layer, CVP) strongly influenced by flame lifting

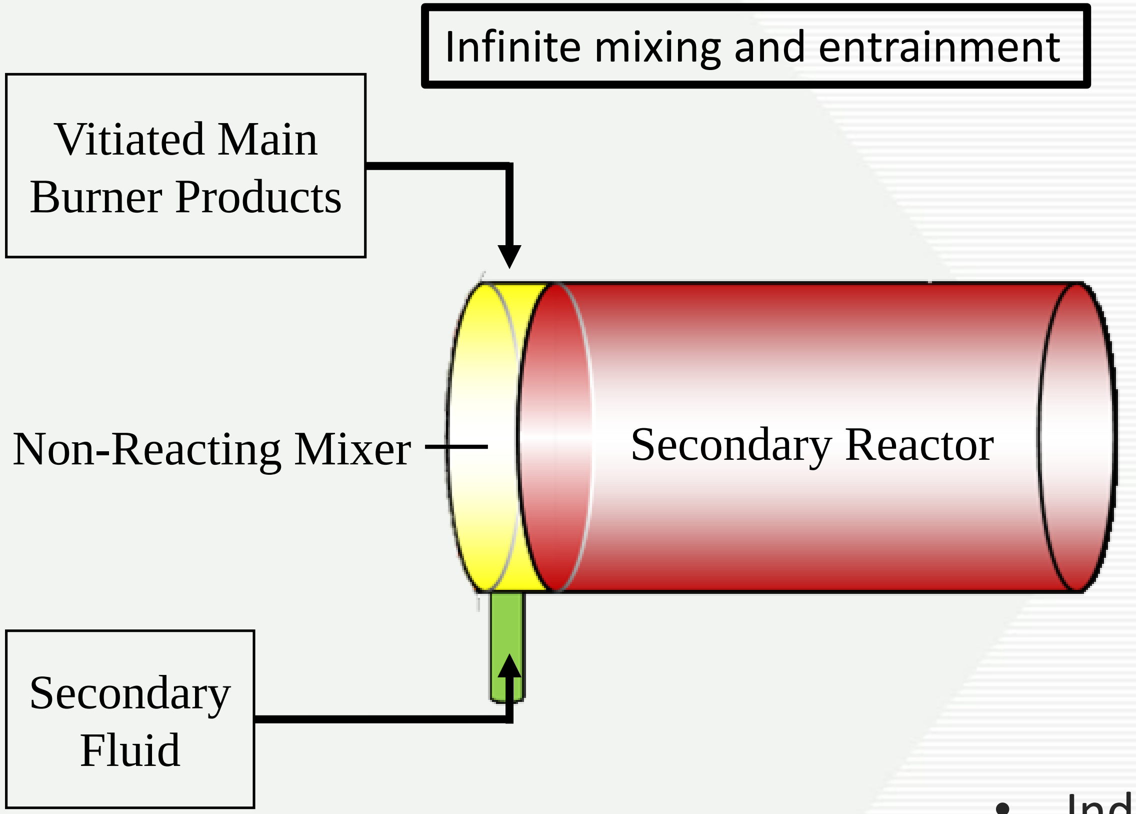
# TOP LEVEL METHODOLOGY

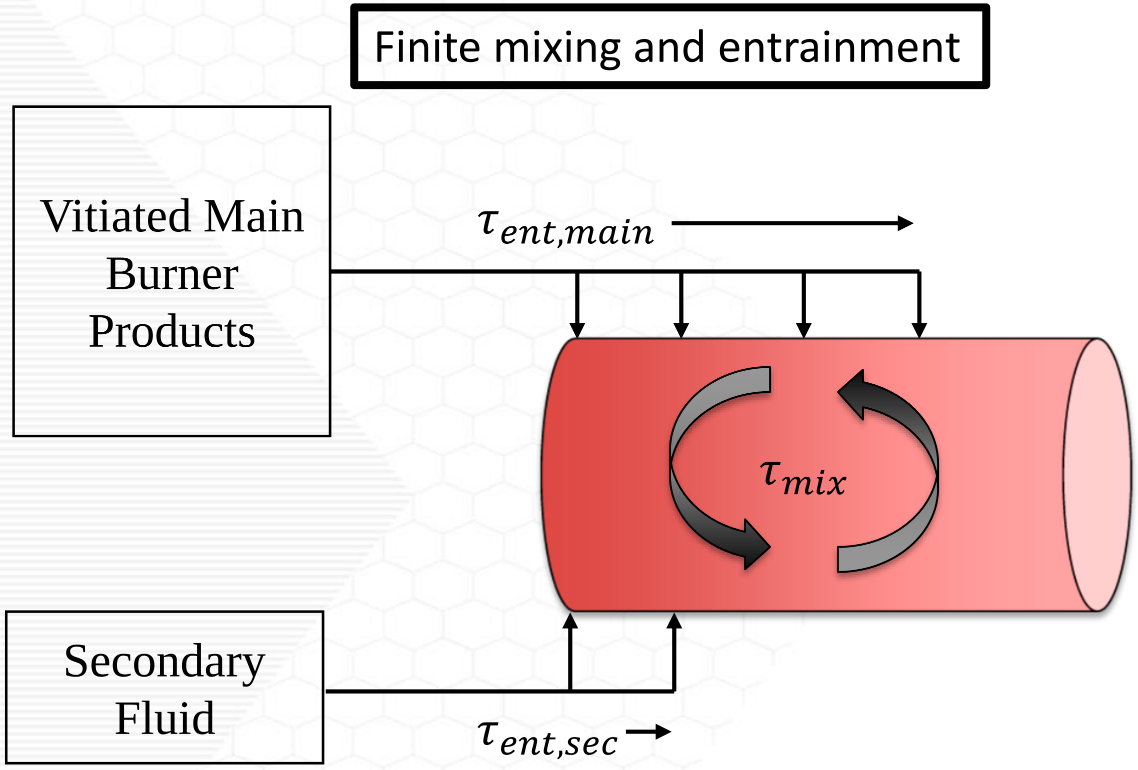
- Multi-pronged investigation with high degree of collaboration
  - Reactor modeling with theoretical and practical considerations as well as optimization
  - Experimental RJICF NOx emissions characterization with flame imaging
  - RJICF simulation using LES
- Results from each facet of investigation utilized to assist in interpreting results and informing next steps of the others



# DEVELOPED MODELING, EXPERIMENTAL, AND SIMULATION TOOLS

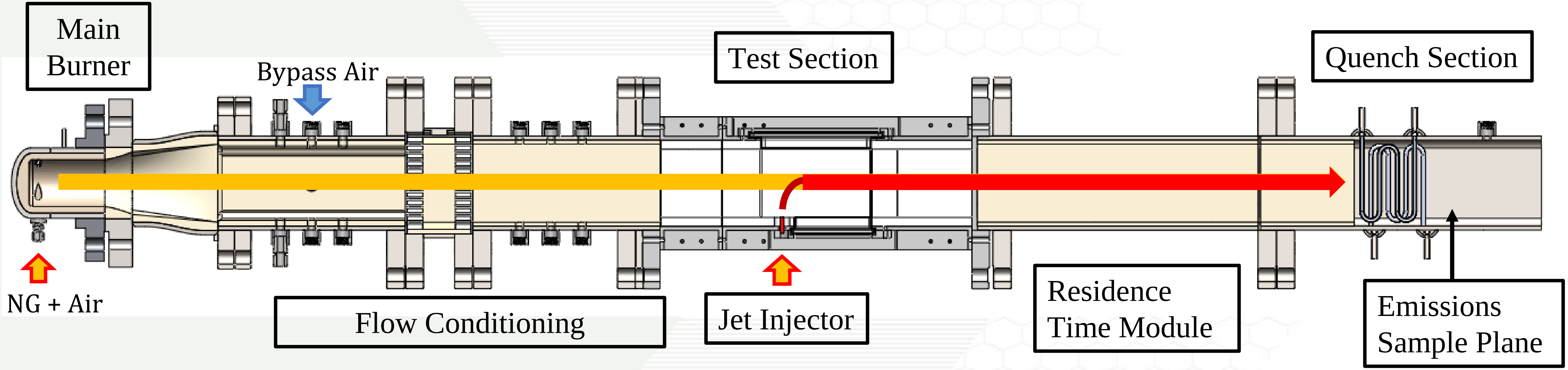
# REACTOR NETWORK MODELS



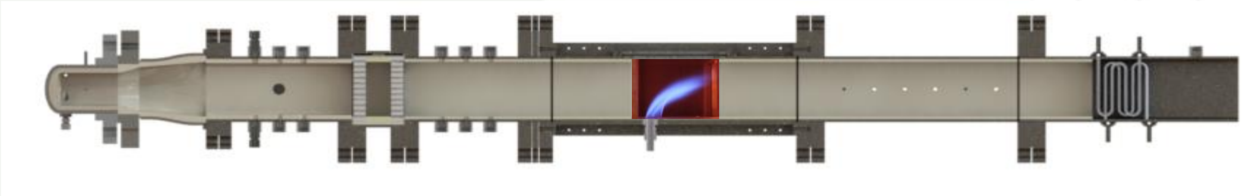

- Independent rates for mixing as well main burner product and secondary fluid entrainment: $1/\tau_{mixing}$ , $1/\tau_{ent,main}$ , $1/\tau_{ent,sec}$
- Finite mixing in reactor modeled using Interaction by Exchange with the Mean (IEM): $\psi(t+dt) = \psi(t) - \frac{C_\phi}{2\tau_{mix}}(\psi(t) - \langle\psi\rangle)$

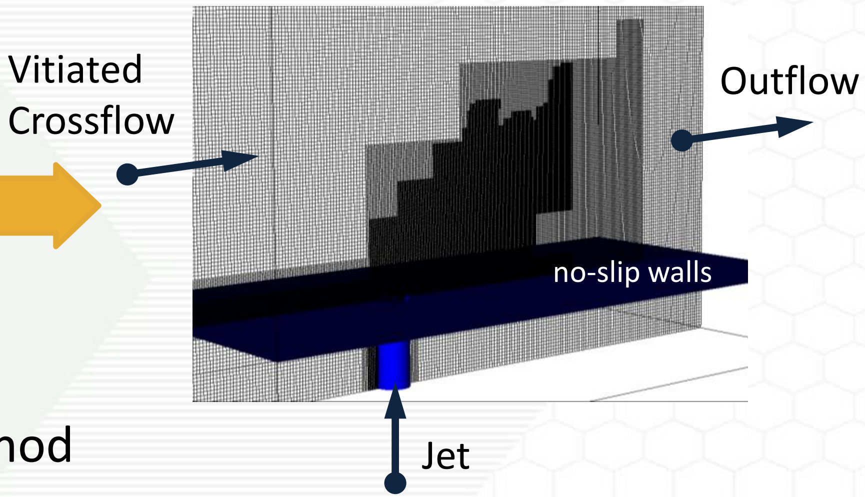
# CURRENT OPERATIONAL CAPABILITIES




- Main burner & bypass air provides crossflow of lean, combustion products at a wide range of equivalence ratios
- Multi-layer ceramic shielded flow conditioning section enable enthalpy retention yielding high cross flow temperatures
- Highly configurable jet injector allows choice of diameter, velocity profile, and 3 species selection
- Test section with 4 sided optical access
- Quench section rapidly cools exhaust to freeze NO chemistry prior to sampling
- Facility operated at P = 1atm

# LES DOMAIN AND SIMULATION PARAMETERS






- LESLIE simulation with AMR-CutCell[1] method employed to reduce cost
- Scaling factor of 3.0 applied to geometry and velocity
- Flame is resolved with 3 – 4 LES cells
- Physical flow-through time of $t_f \approx 1.54\ ms$ (mean)

- Simulation time:
  - ~24 hrs (512 cores) for 3-species cold flow
  - ~72 hrs (800 cores) for 19-species reacting flow
  - ~7 flow-through times (21 days) to complete one case

[1]Muralidharan, B. and Menon, S. JCP (321), 342-368, 2016

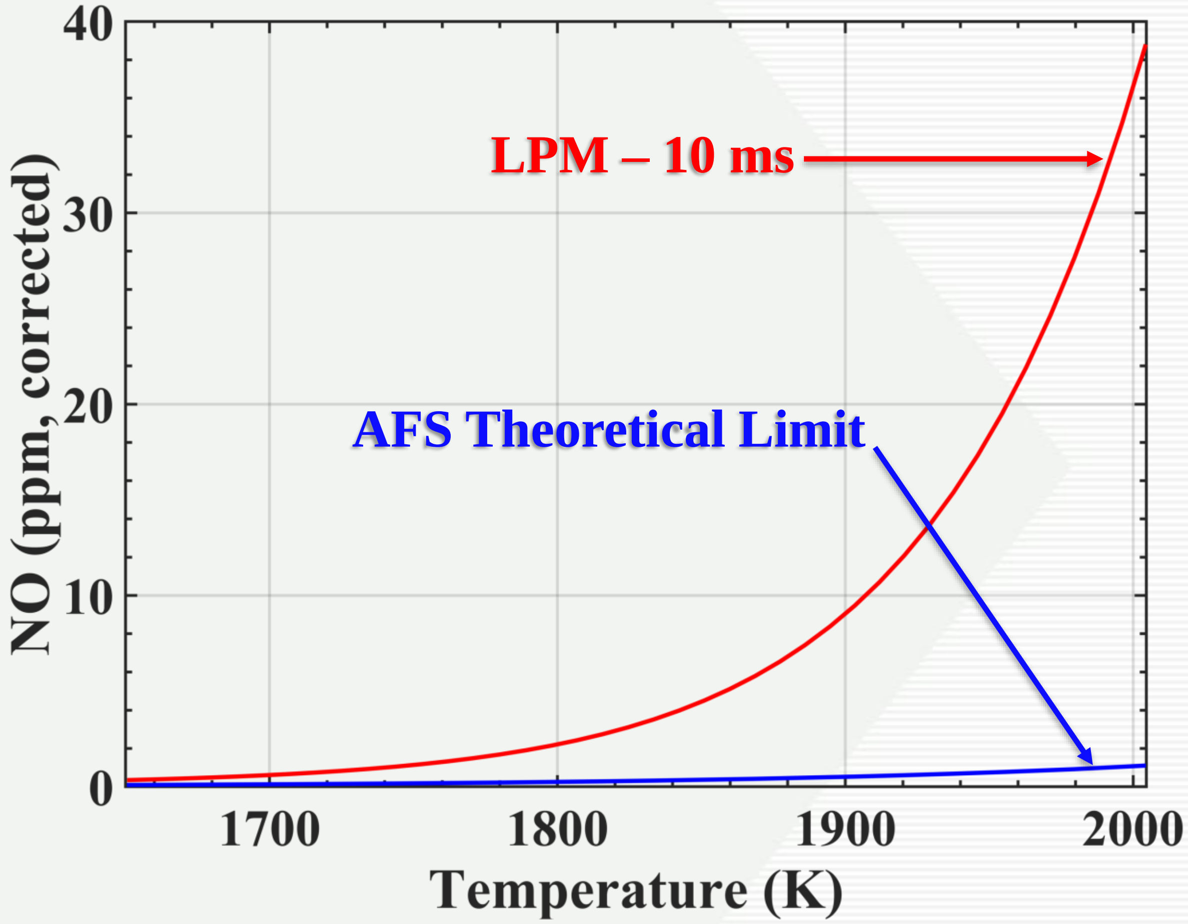
# THEORETICAL NOX FLOOR

# Key research questions

(1) For a given firing temperature and residence time, what are the minimum theoretical NOx limits?

- How much lower is this fundamental limit than the limits achievable with current architectures?

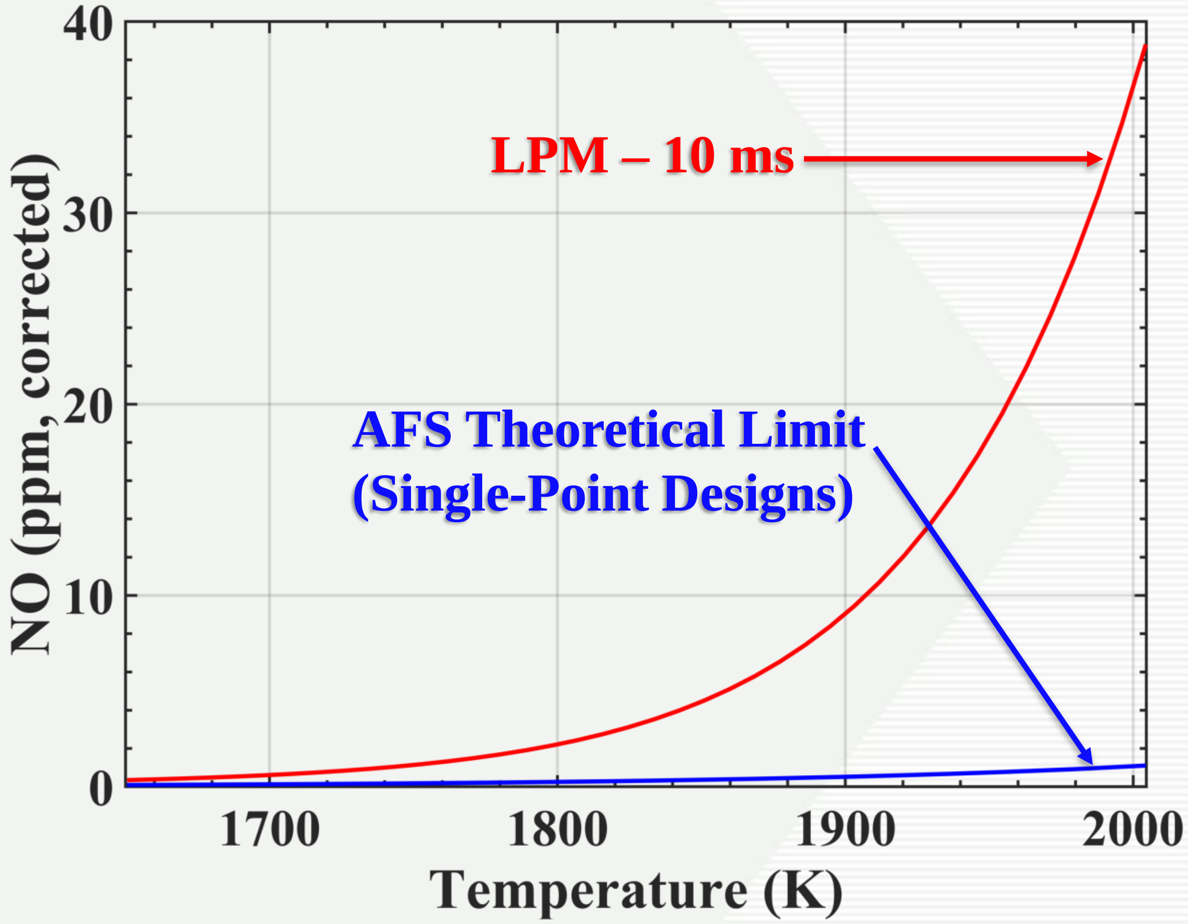
# MODELING: THEORETICAL NOX MINIMUM




- Infinite mixing for theoretical minimum limit
- CO constraint imposed:
  - 125% of Equilibrium level
- General rule for NO floor:
  - Main burner as lean as possible with remainder of fuel injected as late as possible
- Minimum NO levels insensitive to global $\tau_{res}$
- Konnov & UCSD mechanisms predict similar NO

**NOx floor at high flame temperatures ~O(1ppm) !!**

# MODELING: THEORETICAL NOX MINIMUM




- Theoretical limit a continuum of multiple designs
- Require a single geometric configuration for direct comparison of potential improvement over DLN architectures → Multi-point design
- Meeting CO constraint across entire turn down range → forces selection of design optimized for less that 1975K

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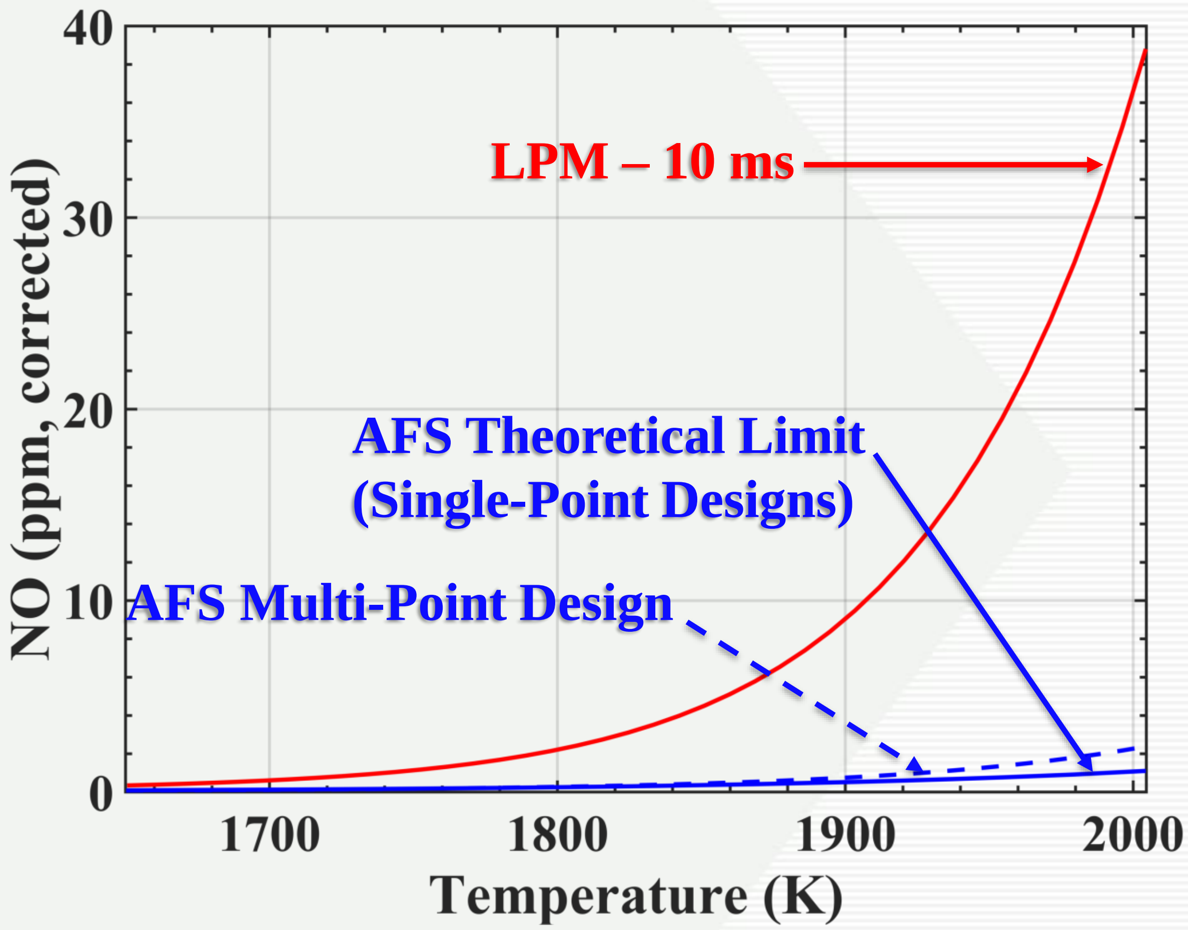


- Theoretical limit a continuum of multiple designs
- Require a single geometric configuration for direct comparison of potential improvement over DLN architectures → Multi-point design
- Meeting CO constraint across entire turn down range → forces selection of design optimized for less that 1975K

NOx floor still at ppm levels for multi-point optimum

# BEHAVIOR OF PRACTICAL AXIALLY STAGED COMBUSTION SYSTEMS

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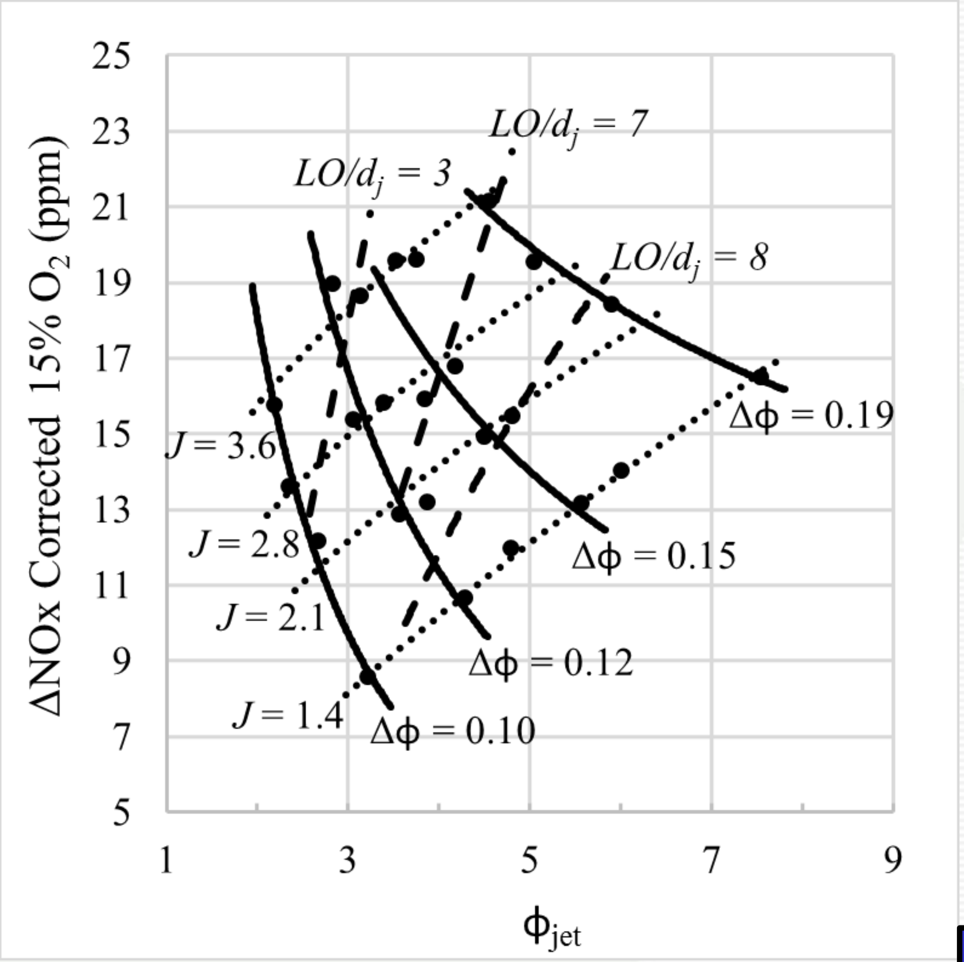
# Key research questions

(2) What do the actual fuel and air distribution patterns look like that attempt to achieve these theoretical values?

- Then, what are the operational behaviors of such a combustion system?

# EXPERIMENTAL: RICH PREMIXED JET EMISSIONS




ΔNOx as a function $\phi_{jet}$ for constant crossflow conditions at $\phi_{HE} = 0.525$

- Preliminary work experimentally demonstrated NOx benefit of axial staging with a RJICF at high combustor temperatures.

→ Most emissions efficient way to deliver ΔT with a RJICF?

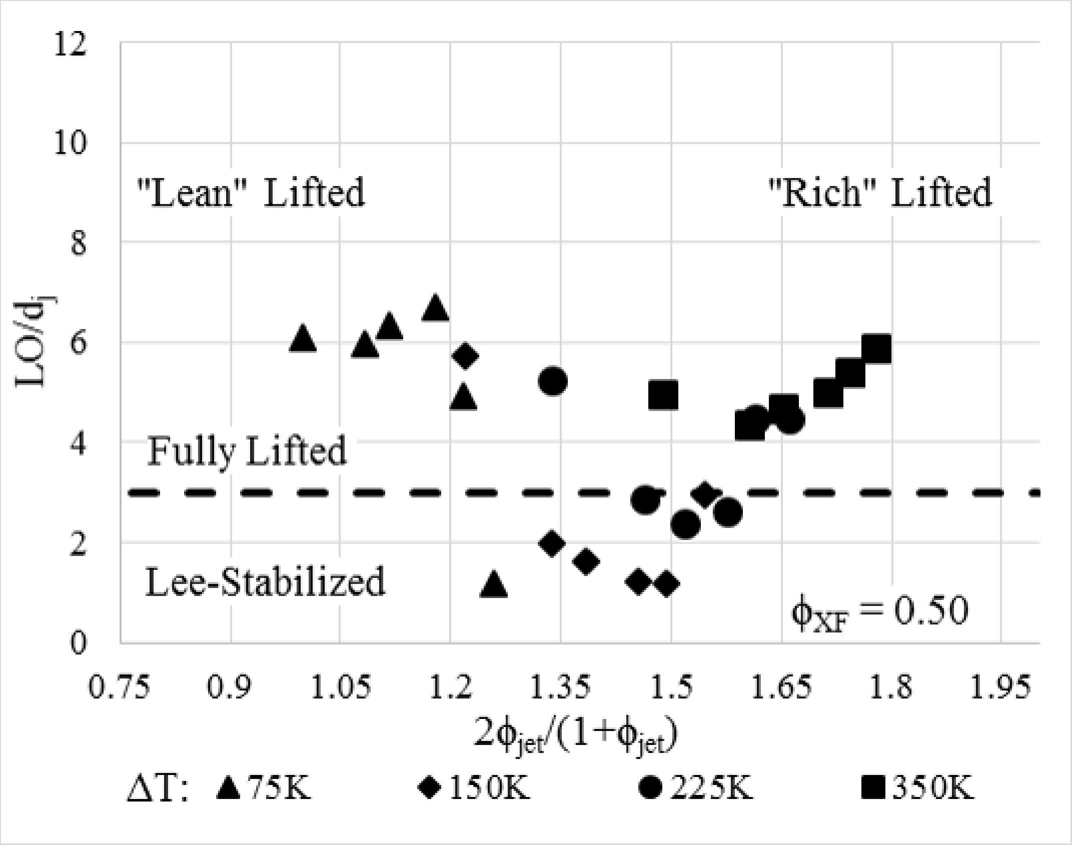
  - ΔNOx utilized to assess emissions efficiency of jets at similar ΔT

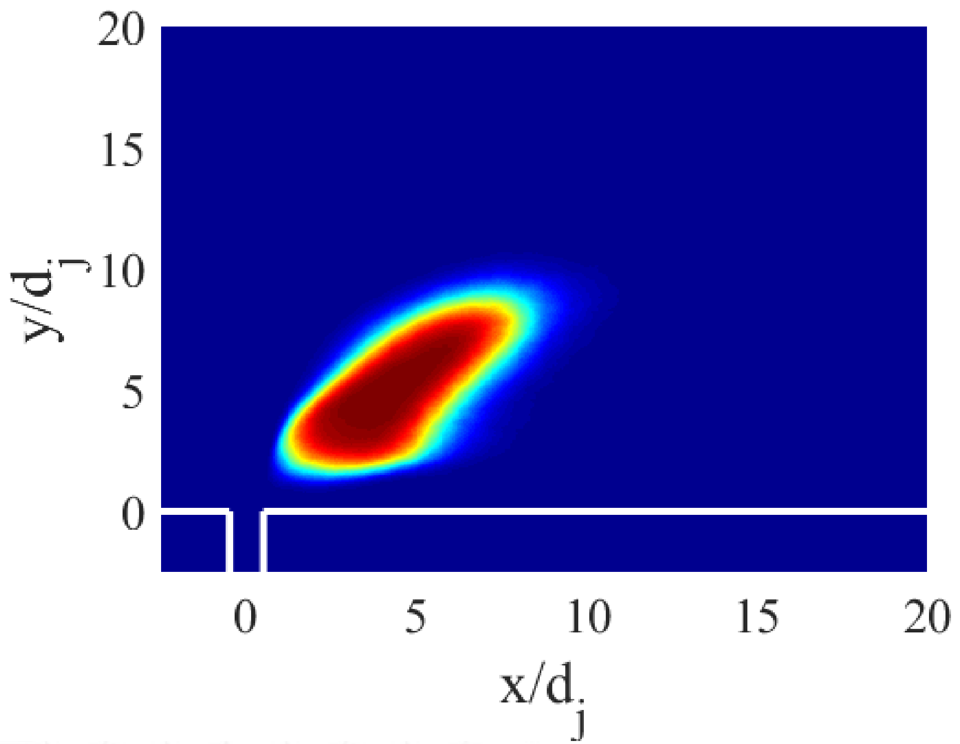
- Higher rise in system equivalence ratio (Δϕ) → higher ΔNOx
- For fixed Δϕ, higher jet equivalence ratio($\phi_{Jet}$) → lower ΔNOx
  - Higher $\phi_{Jet}$ is coupled with reduction in *J*
- For fixed Δϕ, higher lift-off height *($LO/d_j$)* → lower ΔNOx

**ΔNOx can vary up to 3x at constant Δϕ**

BEN T. ZINN COMBUSTION LAB

# EXPERIMENTAL: FLAME LIFTING



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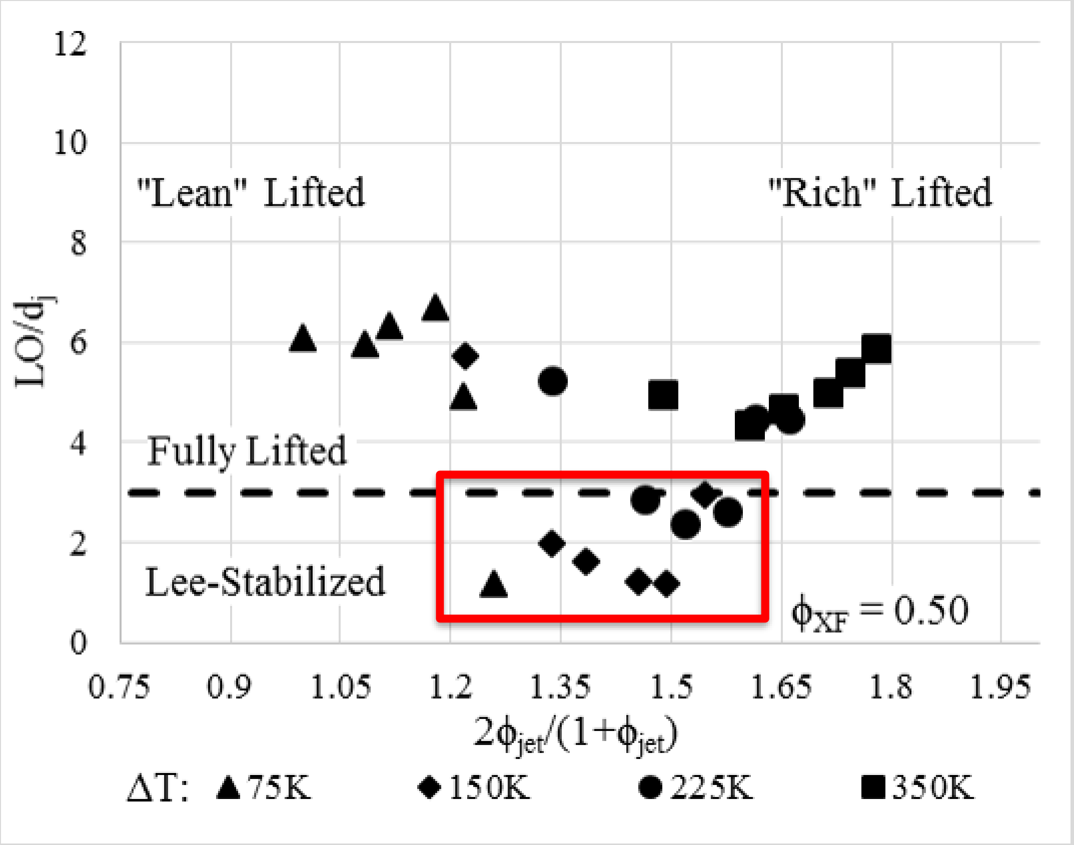


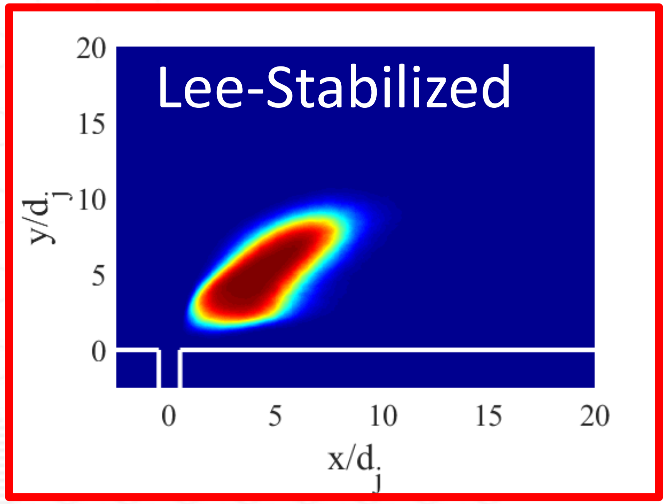

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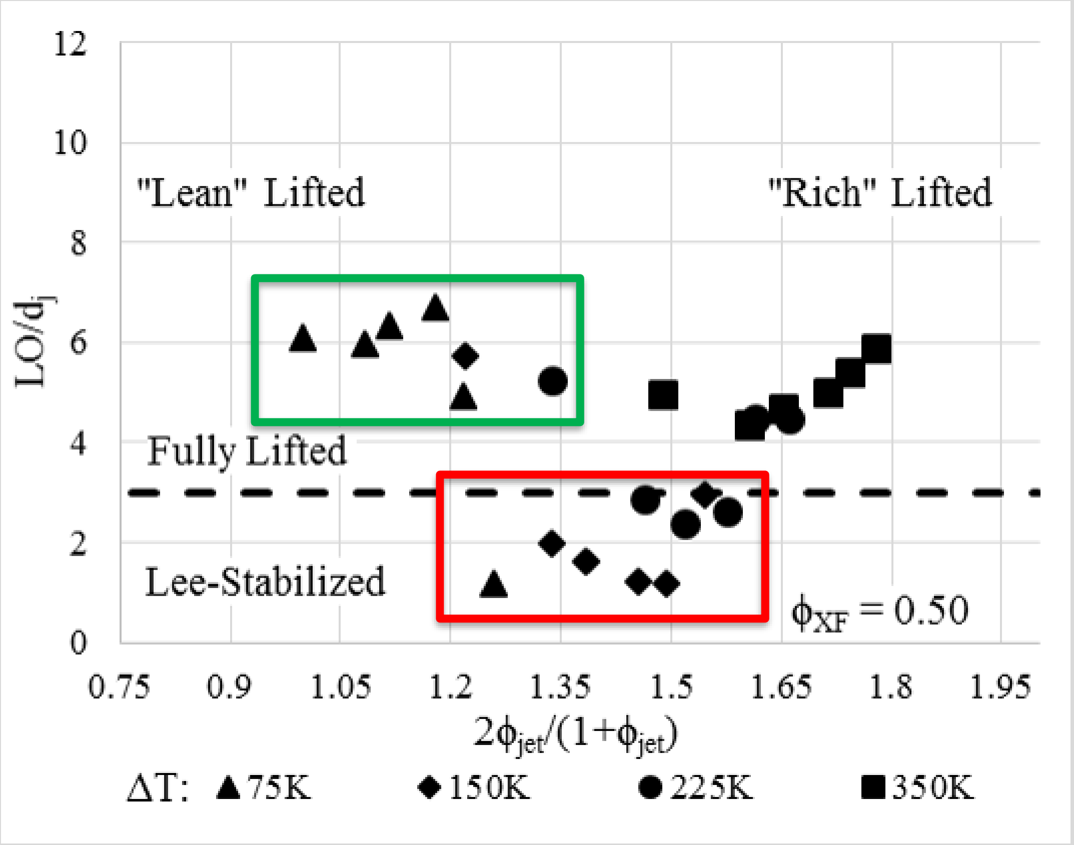


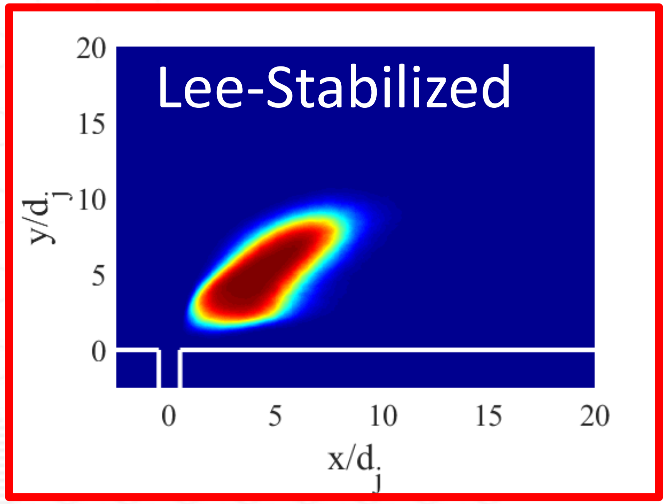


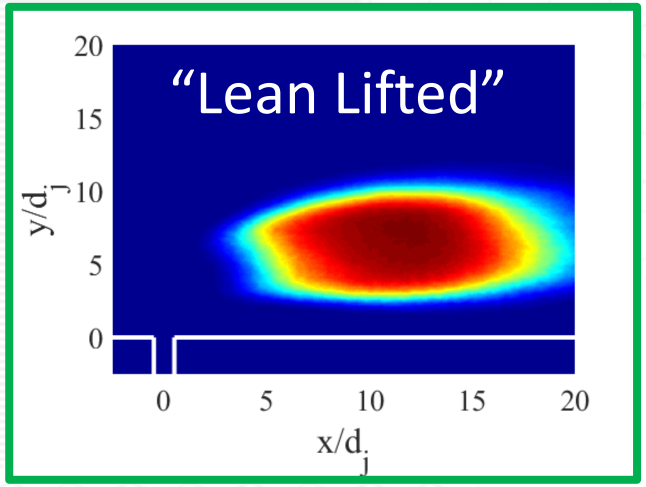

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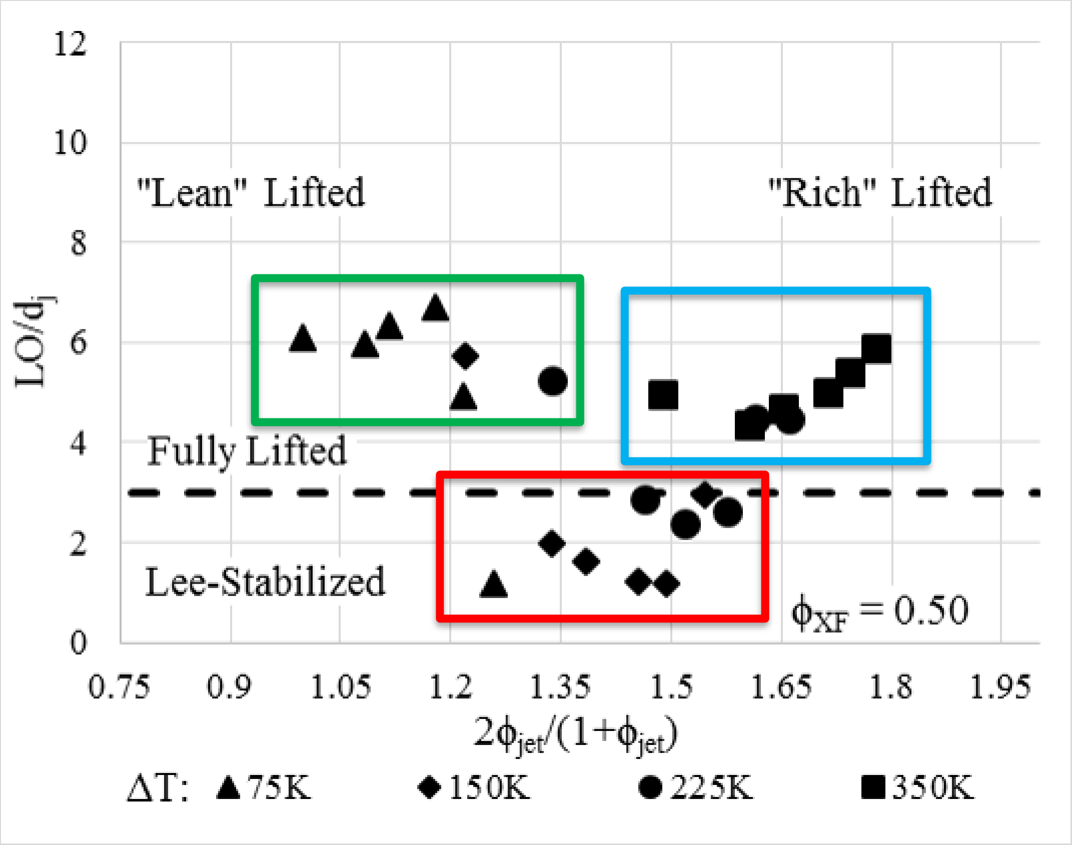
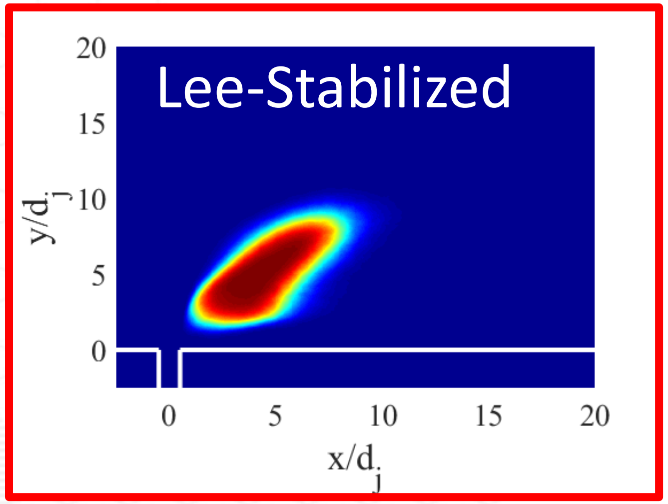
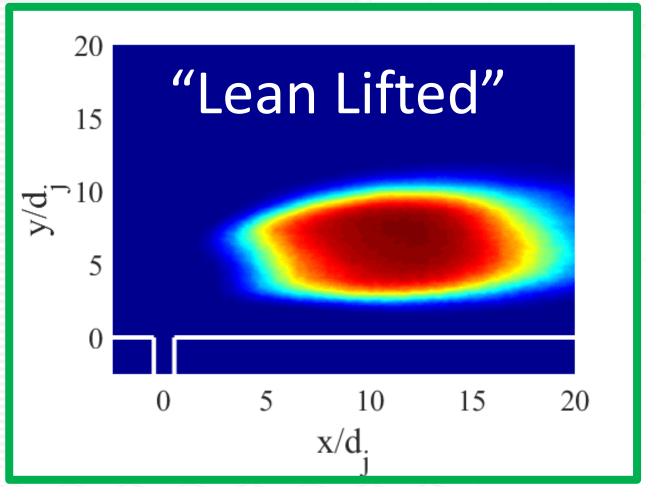
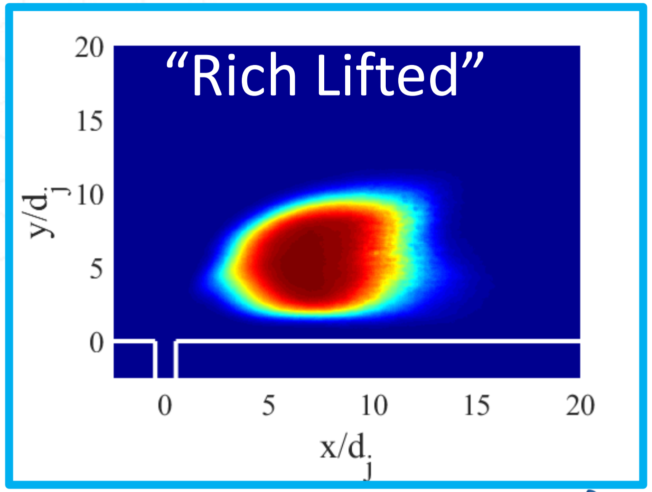
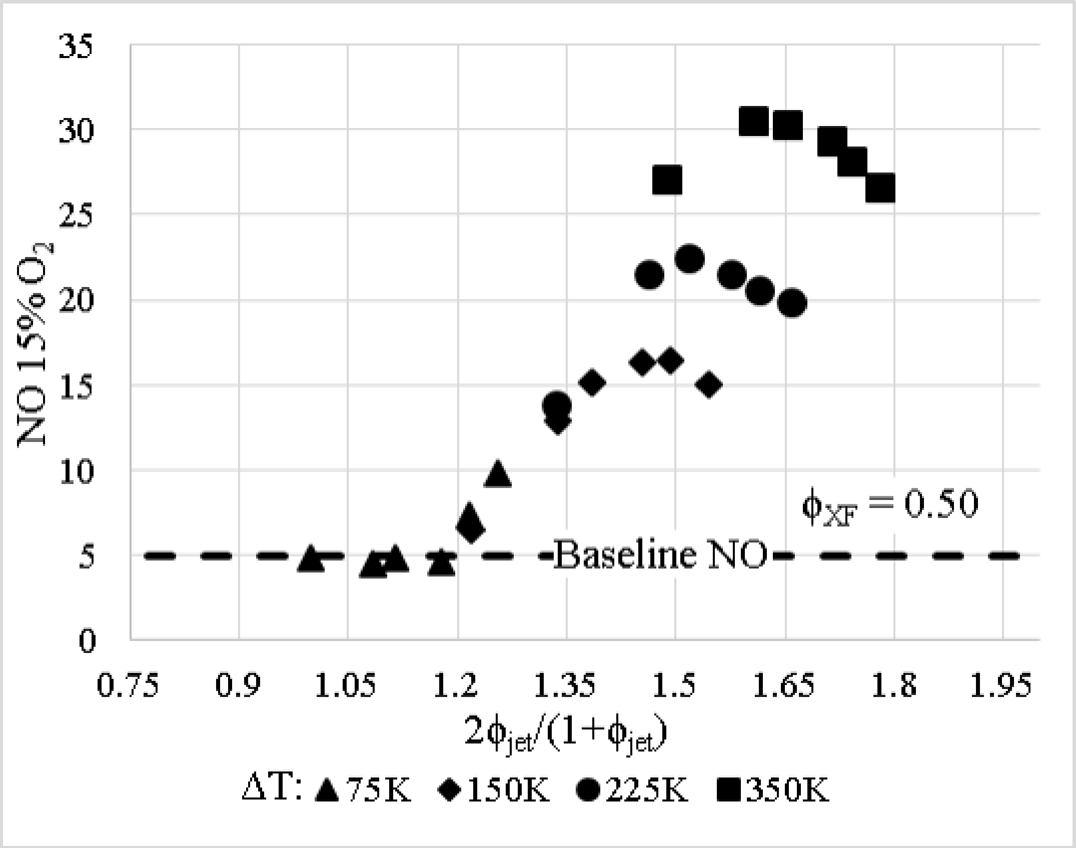


# EXPERIMENTAL: EMISSIONS




- Higher $\Delta$T → higher NO

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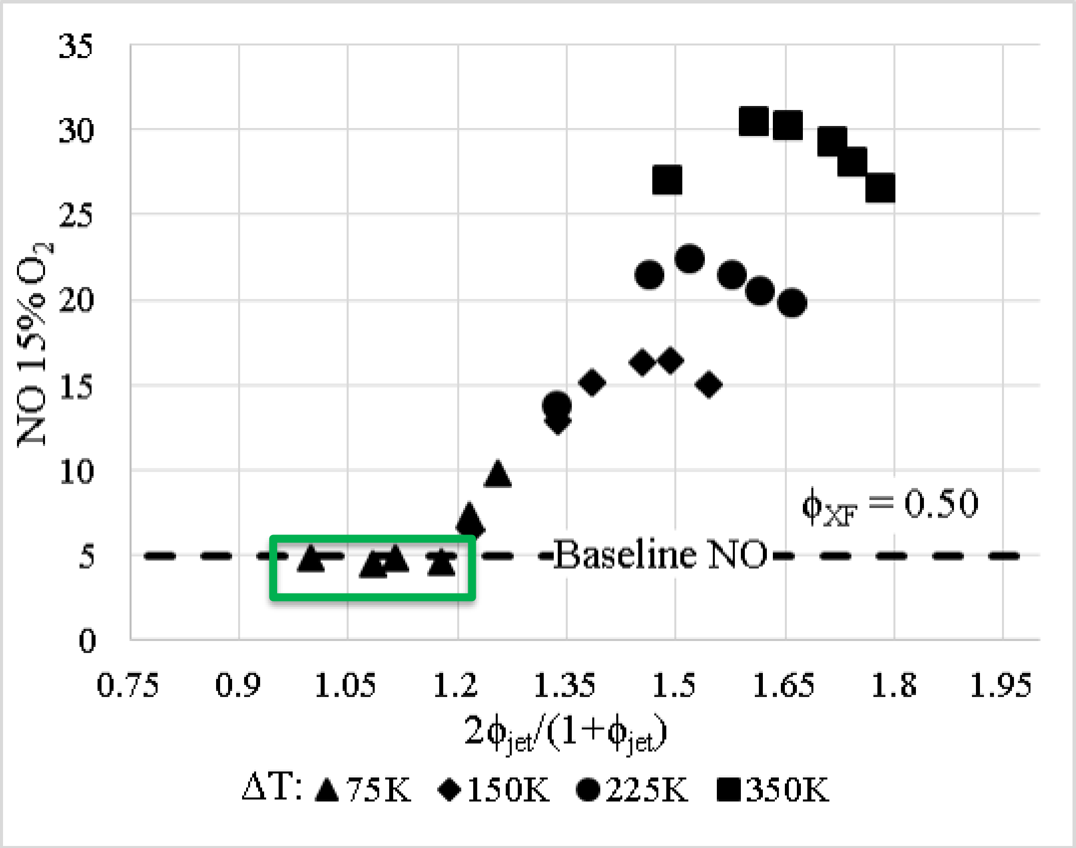


- Higher ΔT → higher NO
- Lean lifted flames:
  - Very little NOx production compared to baseline
  - NOx production insensitive to $\phi_{jet}$

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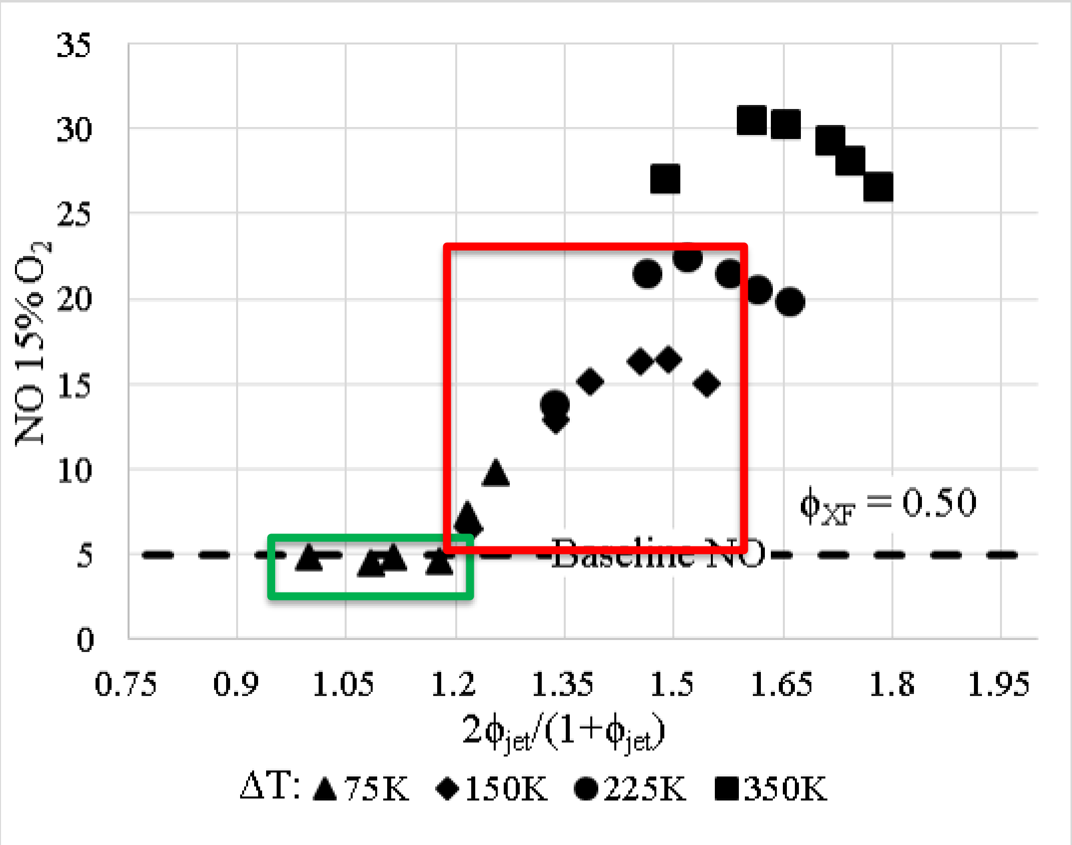


- Higher ΔT → higher NO
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- Attached flames:
  - Significant increase in NOx production is observed compared to lean lifted cases
  - NOx production increases with $\phi_{jet}$ for attached flames until $\phi_{jet}$~2.5 then plateaus

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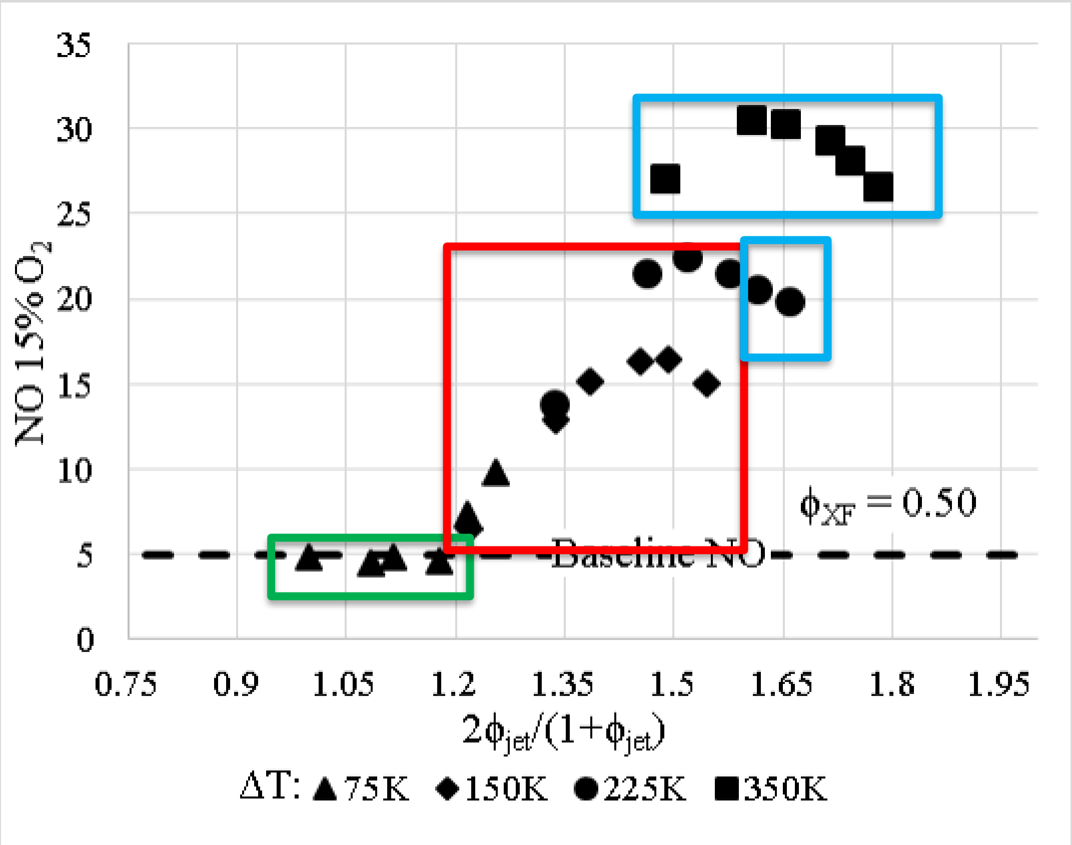


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- Lean lifted flames:
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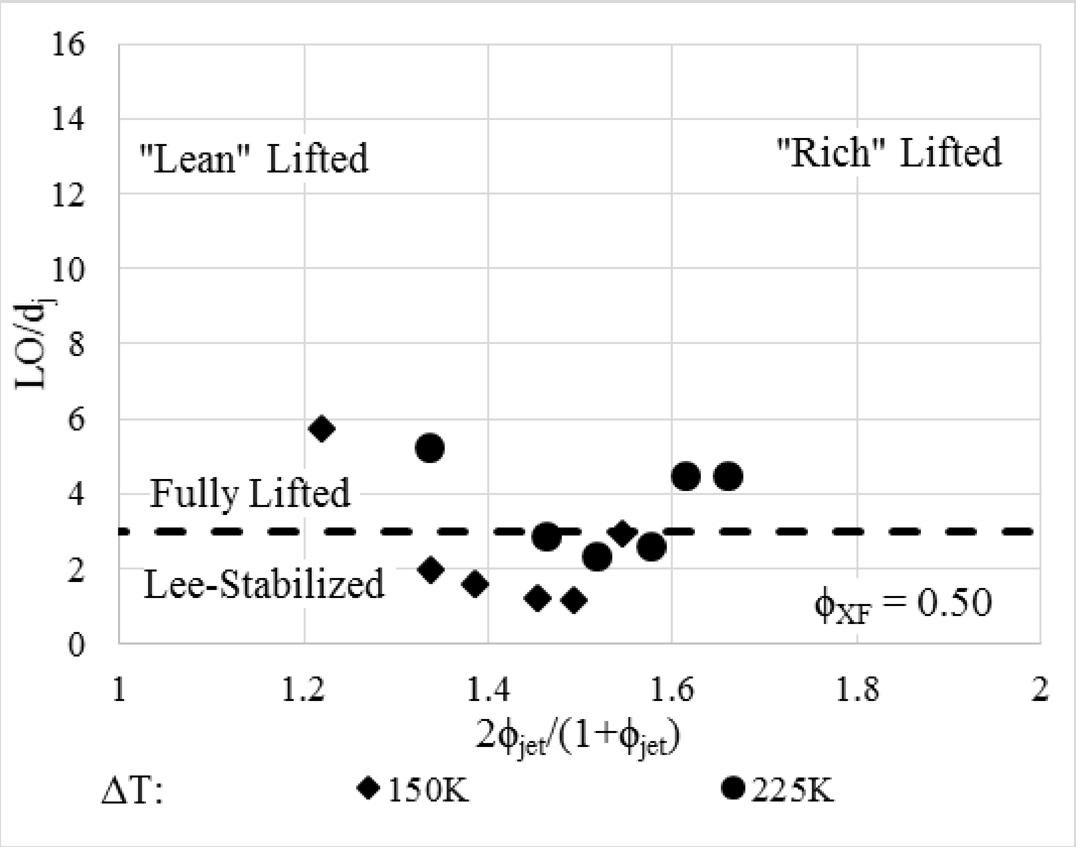
  - NOx production insensitive to $\phi_{jet}$
- Attached flames:
  - Significant increase in NOx production is observed compared to lean lifted cases
  - NOx production increases with $\phi_{jet}$ for attached flames until $\phi_{jet}$~2.5 then plateaus
- Rich lifted flames:
  - Reduction in NOx production compared to attached cases

# EXPERIMENTAL: DOPING IMPACT ON LIFTING




- 150K and 225K series doped with methane until fully lifted behavior was observed for each data point

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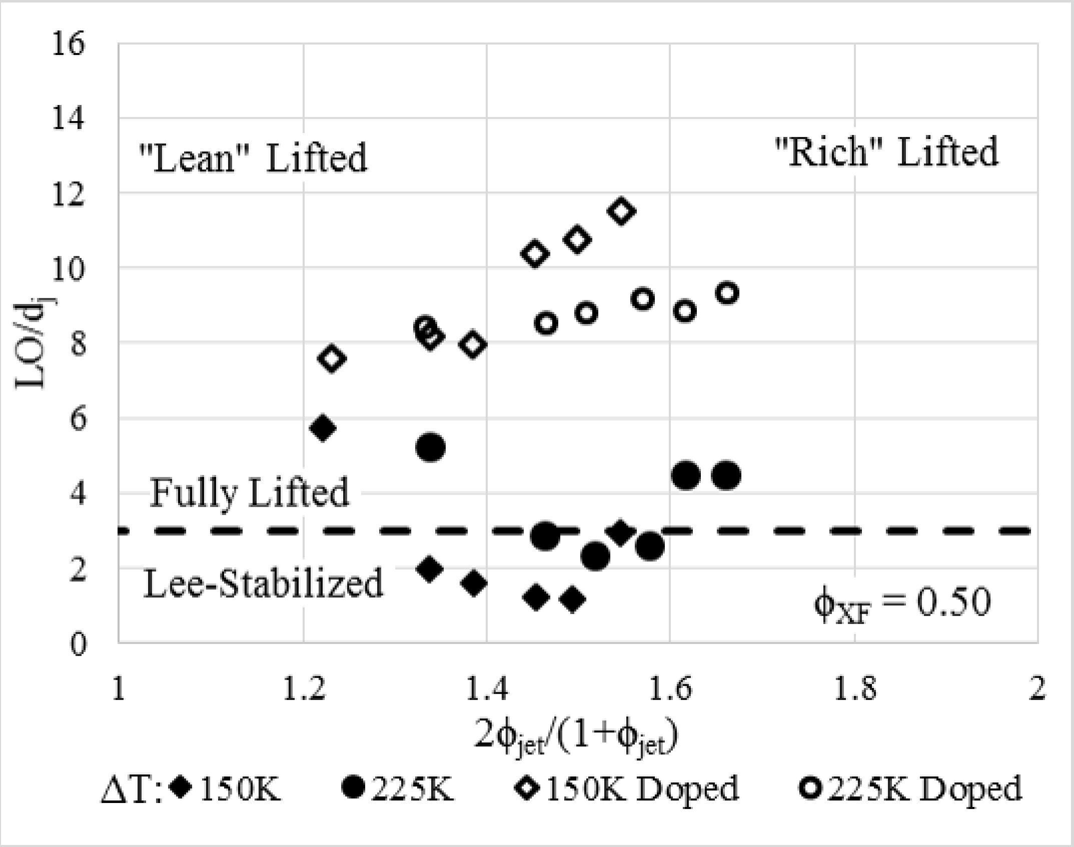


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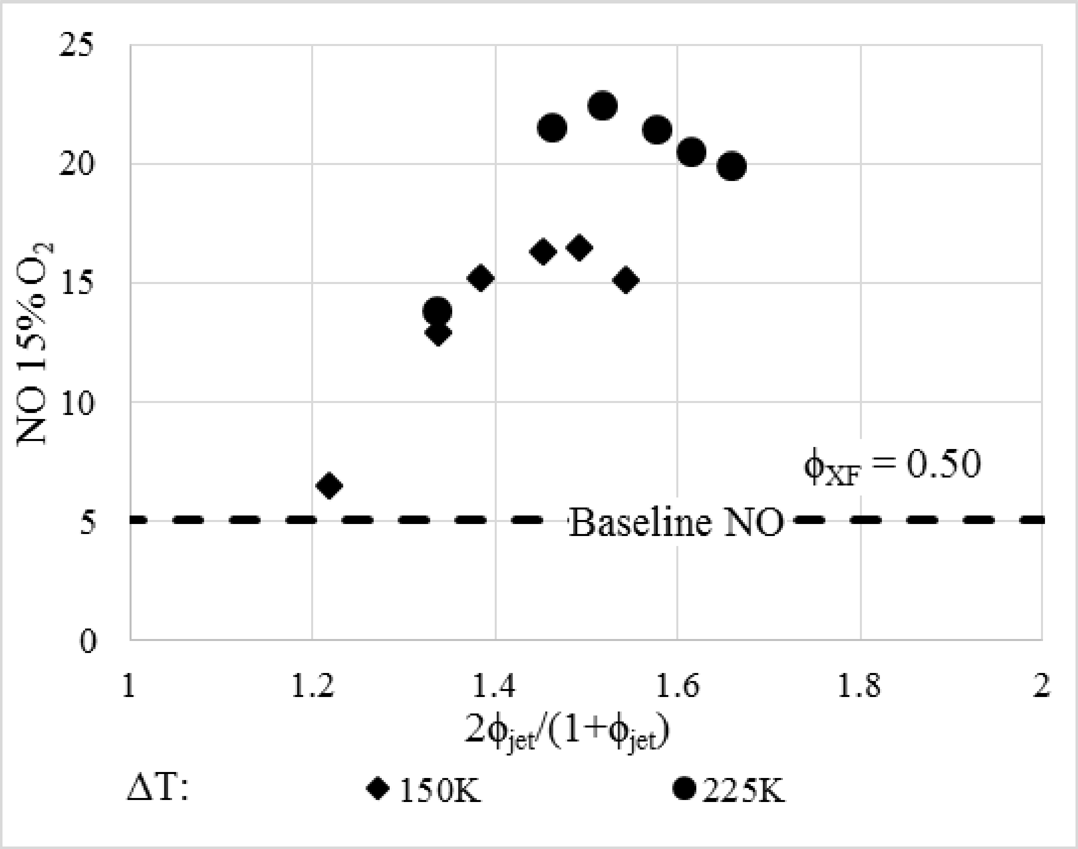


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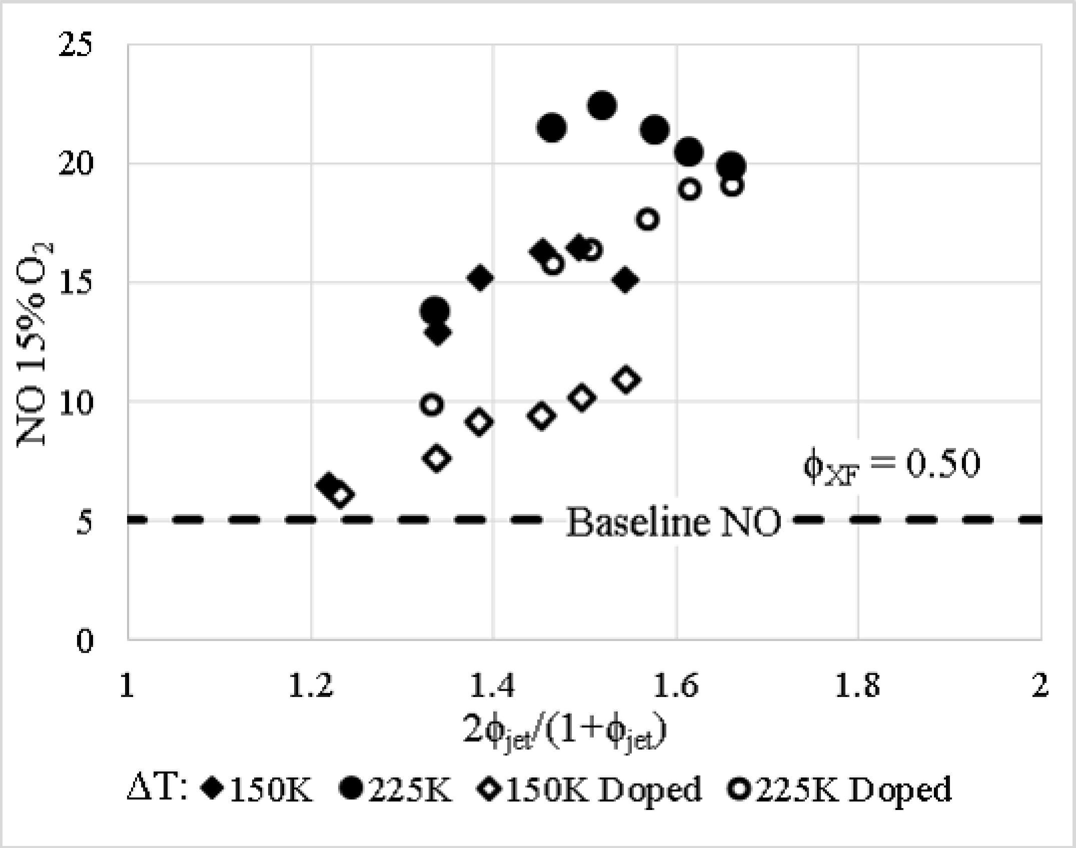


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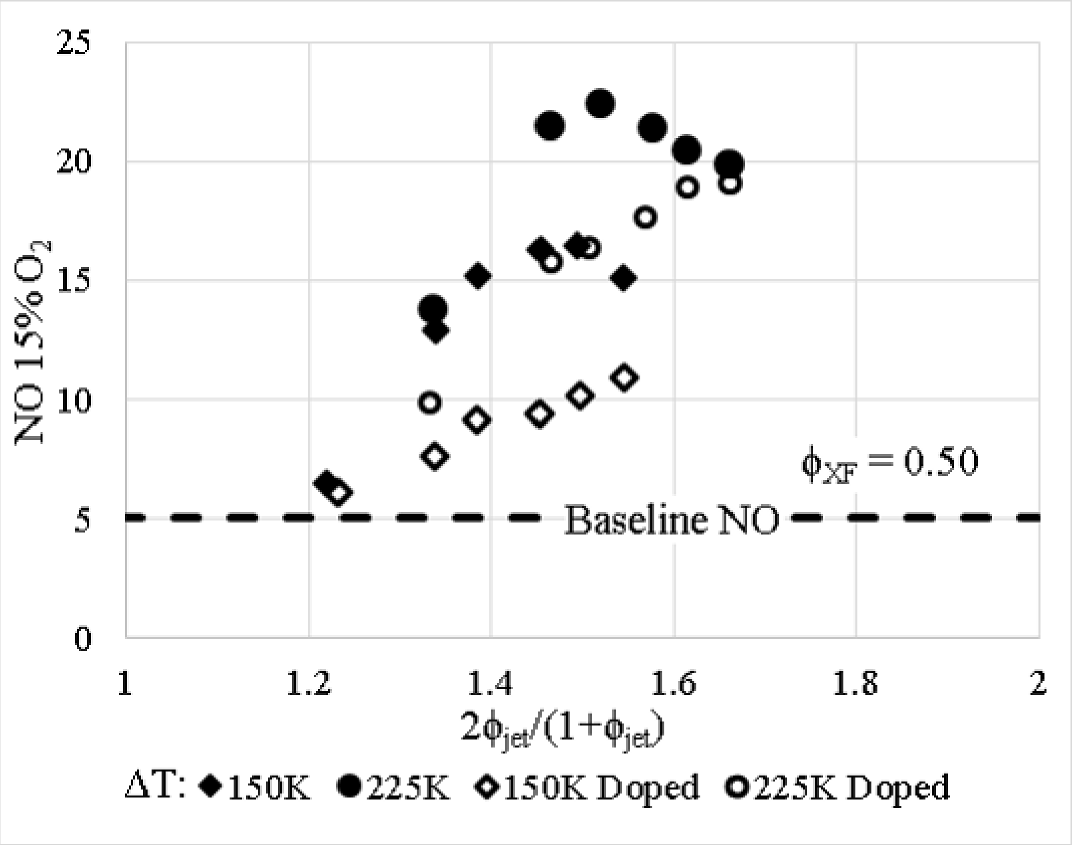


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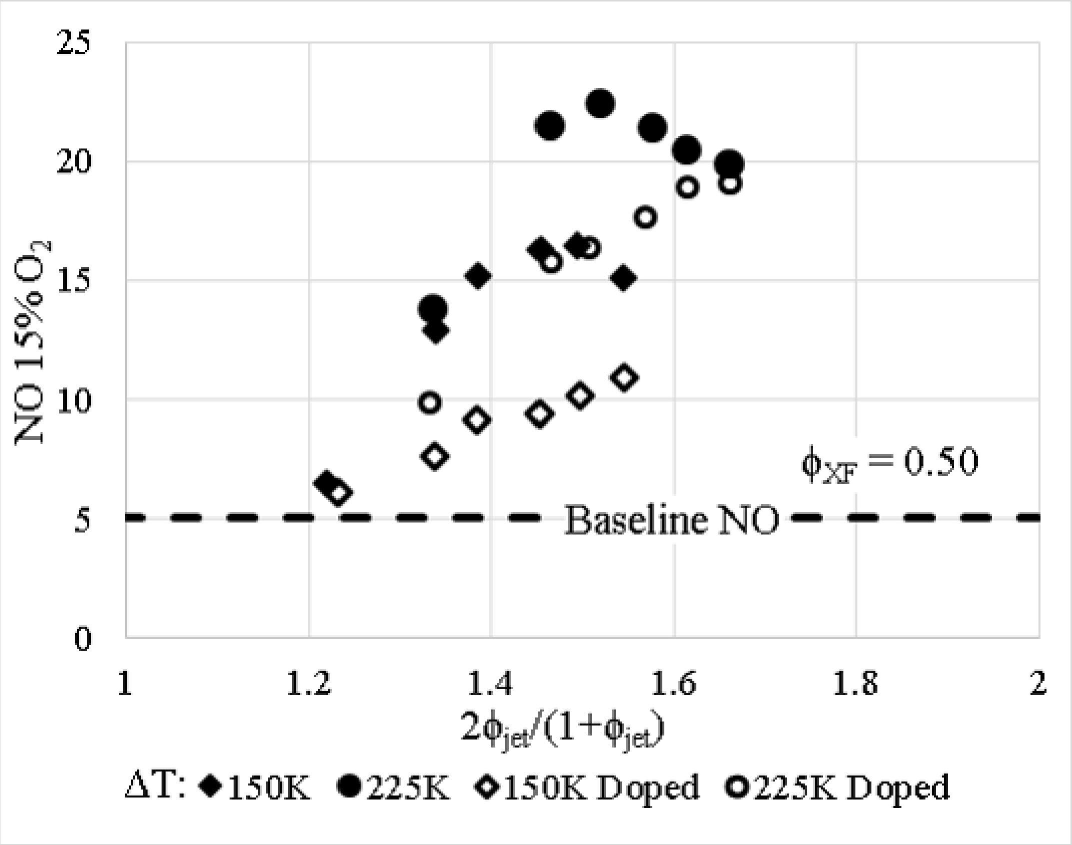
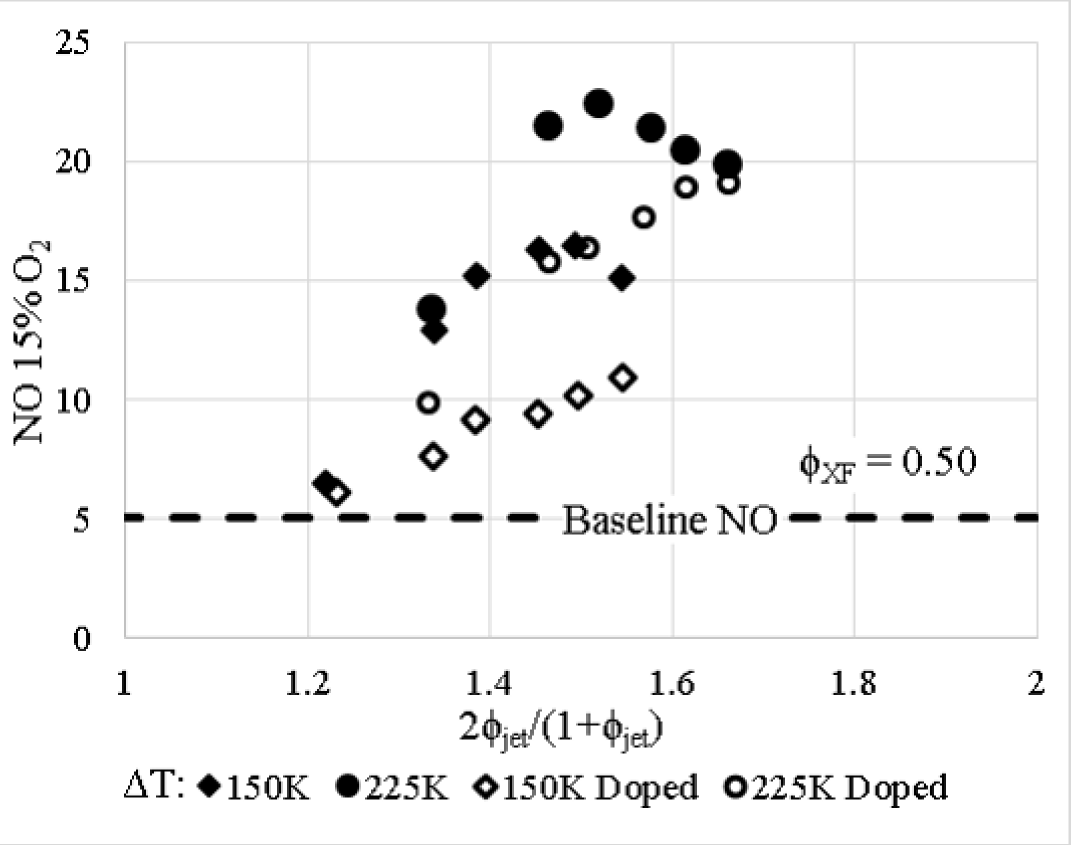
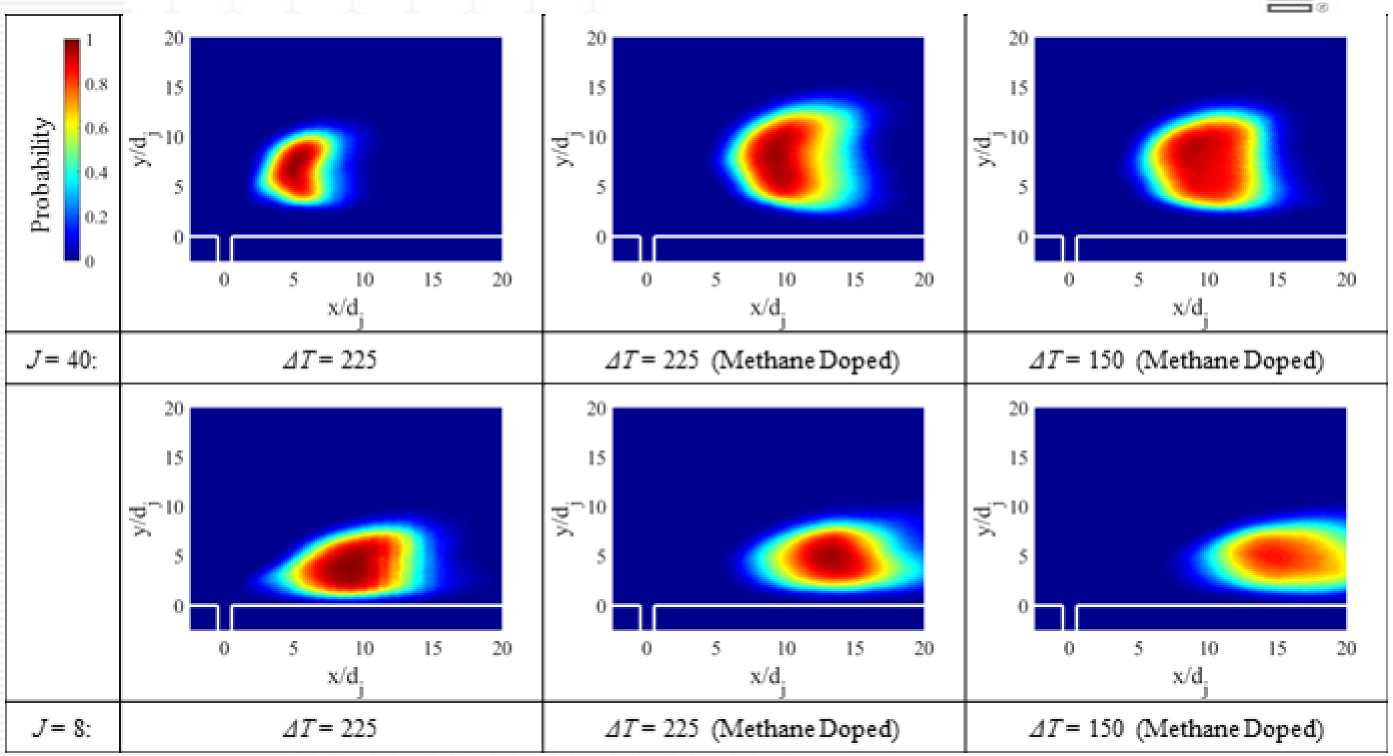



- 150K and 225K series doped with methane until fully lifted behavior was observed for each data point
- 150K series shows significant reduction in NO
- 225K had significant reduction for low $\phi_{jet}$ but not for high $\phi_{jet}$
  - Highest $\phi_{jet}$ cases already fully lifted for 225K series

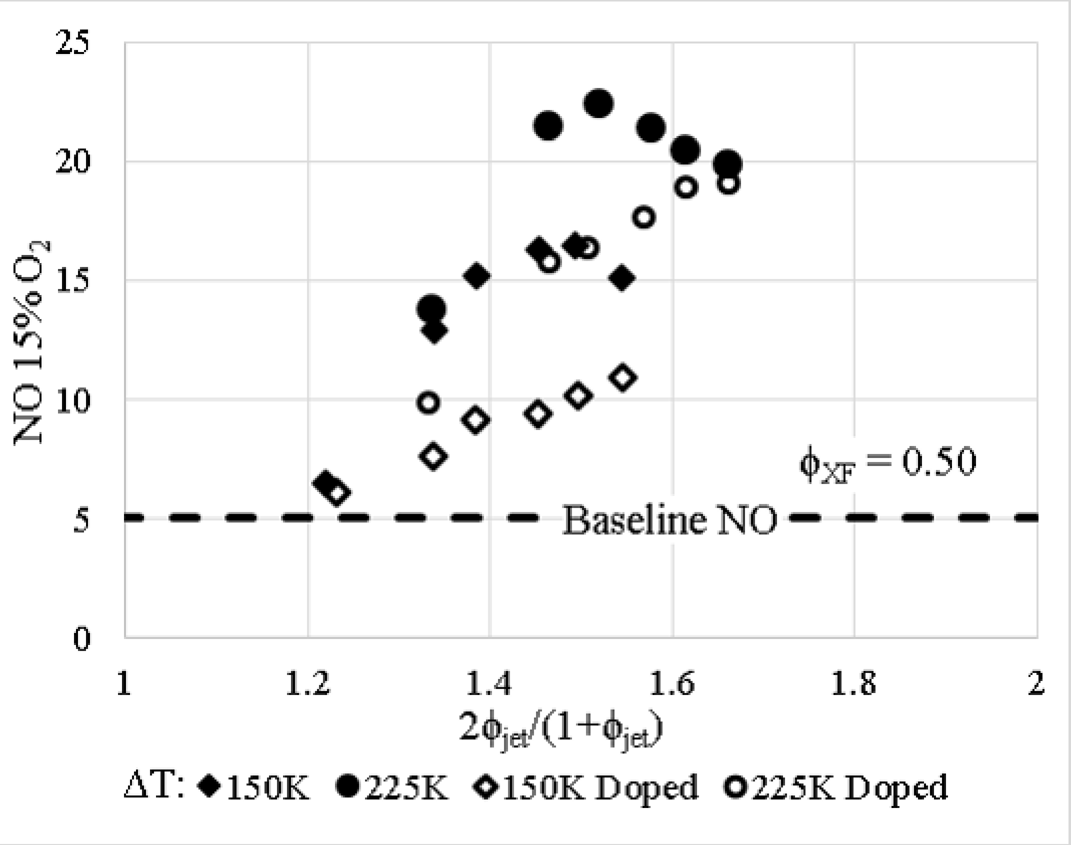
# EXPERIMENTAL: LIFTING IMPACT ON EMISSIONS

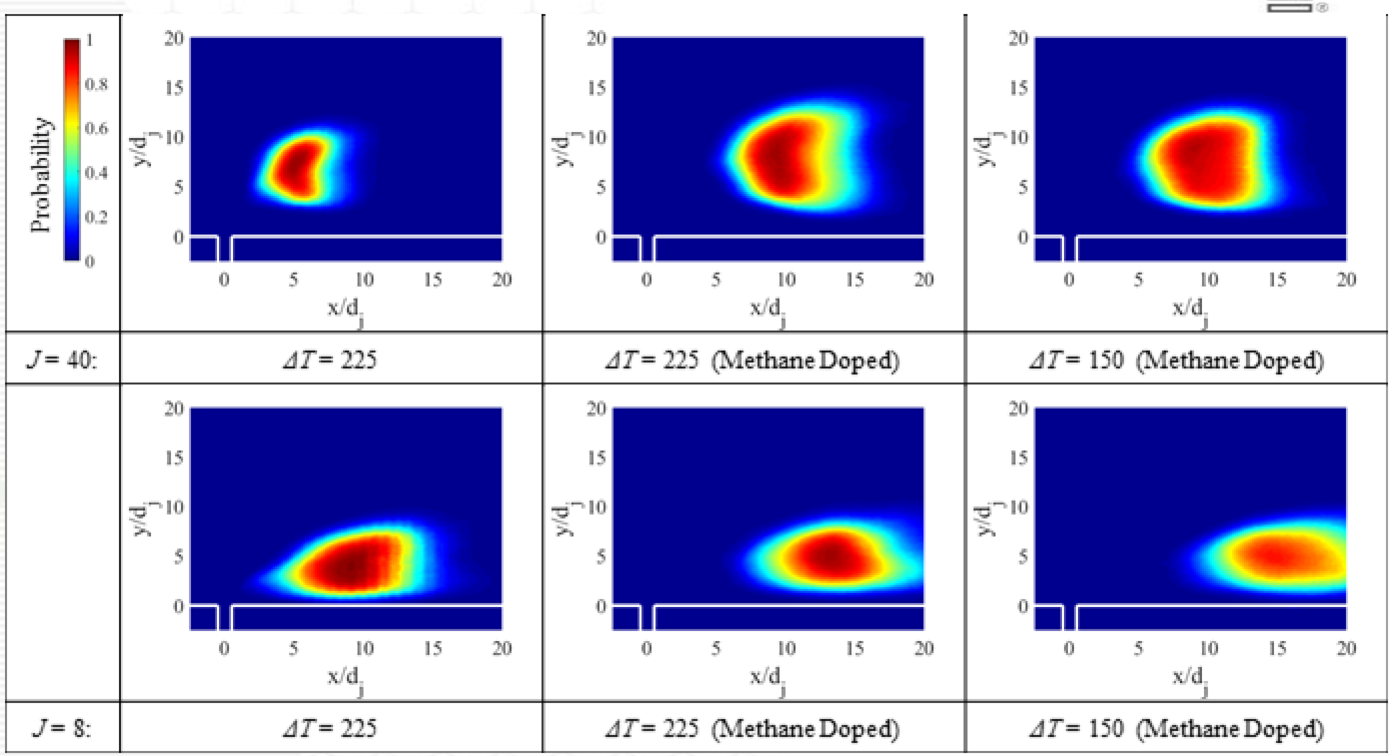



- Methane doping is forcing towards lean lifted behavior, but transition not always complete

# EXPERIMENTAL: LIFTING IMPACT ON EMISSIONS

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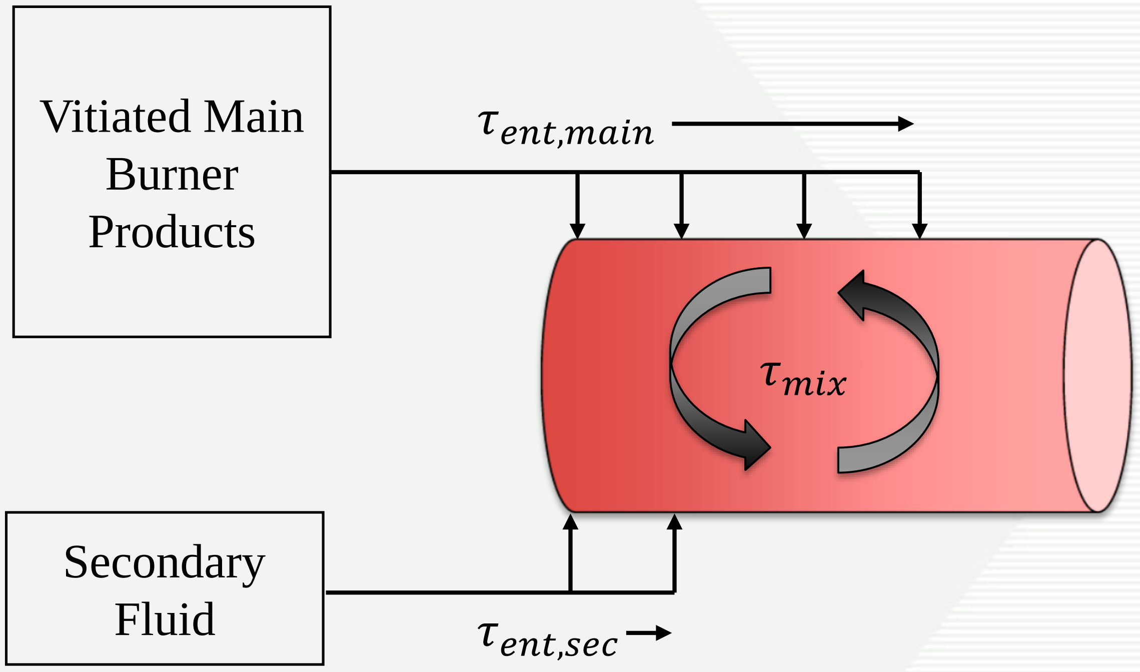
**Different lifting regimes impact NO in different ways → connection to entrainment sensitivity shown by reactor modeling**

# MODELING: PRACTICAL CONSIDERATIONS




- Finite mixing and entrainment model used to isolate and analyze the impact of entrainment and mixing on theoretical NOx minimums
- Can also help de-convolute experimental results by isolating sensitivities

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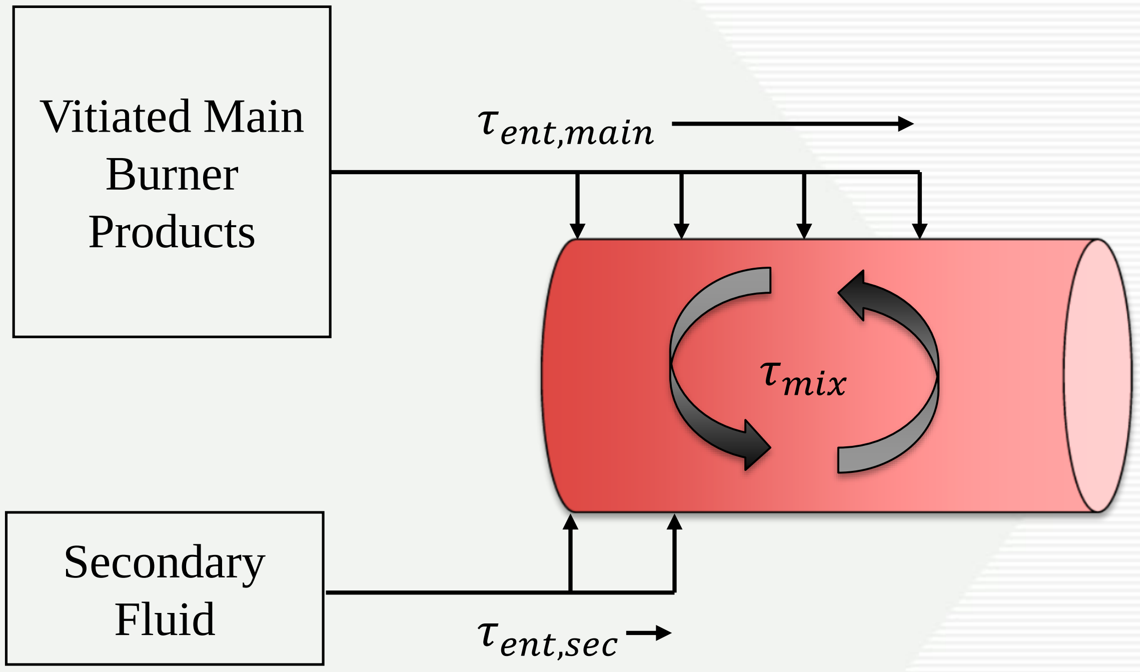


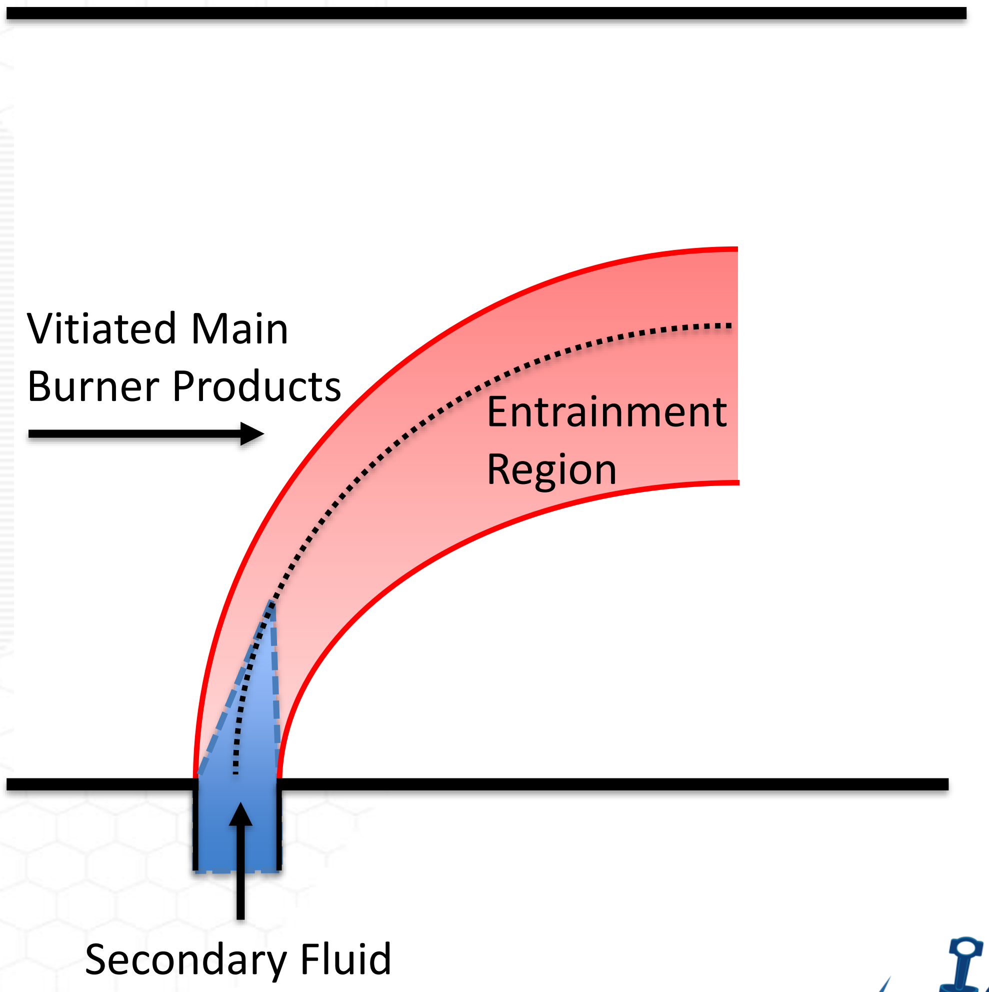


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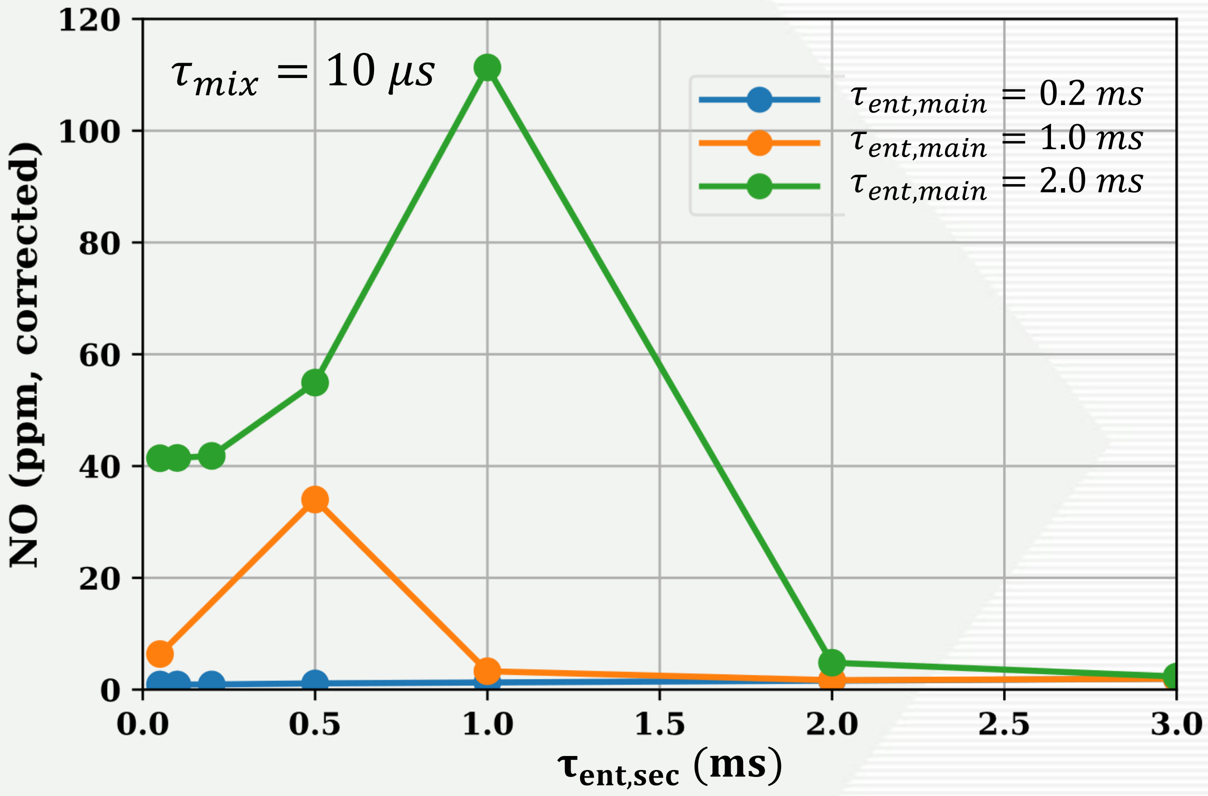
# MODELING: FINITE ENTRAINMENT RATE EFFECTS



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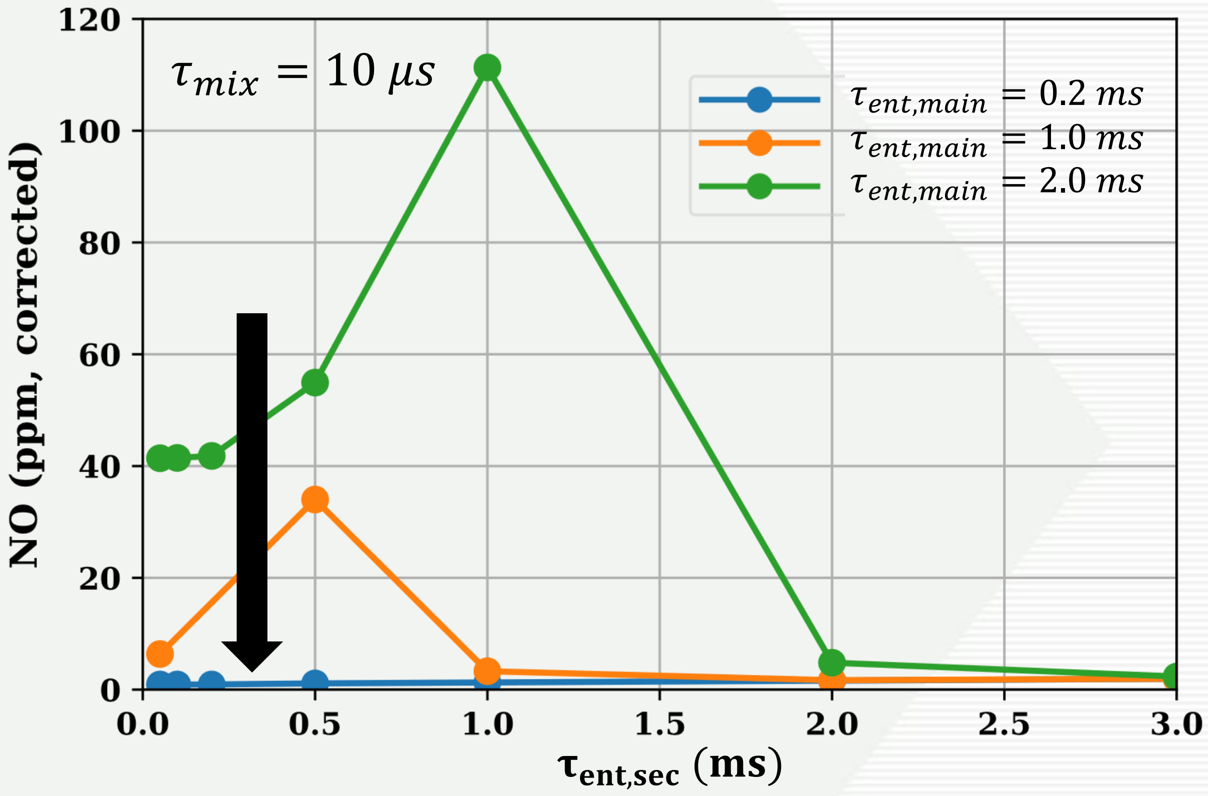
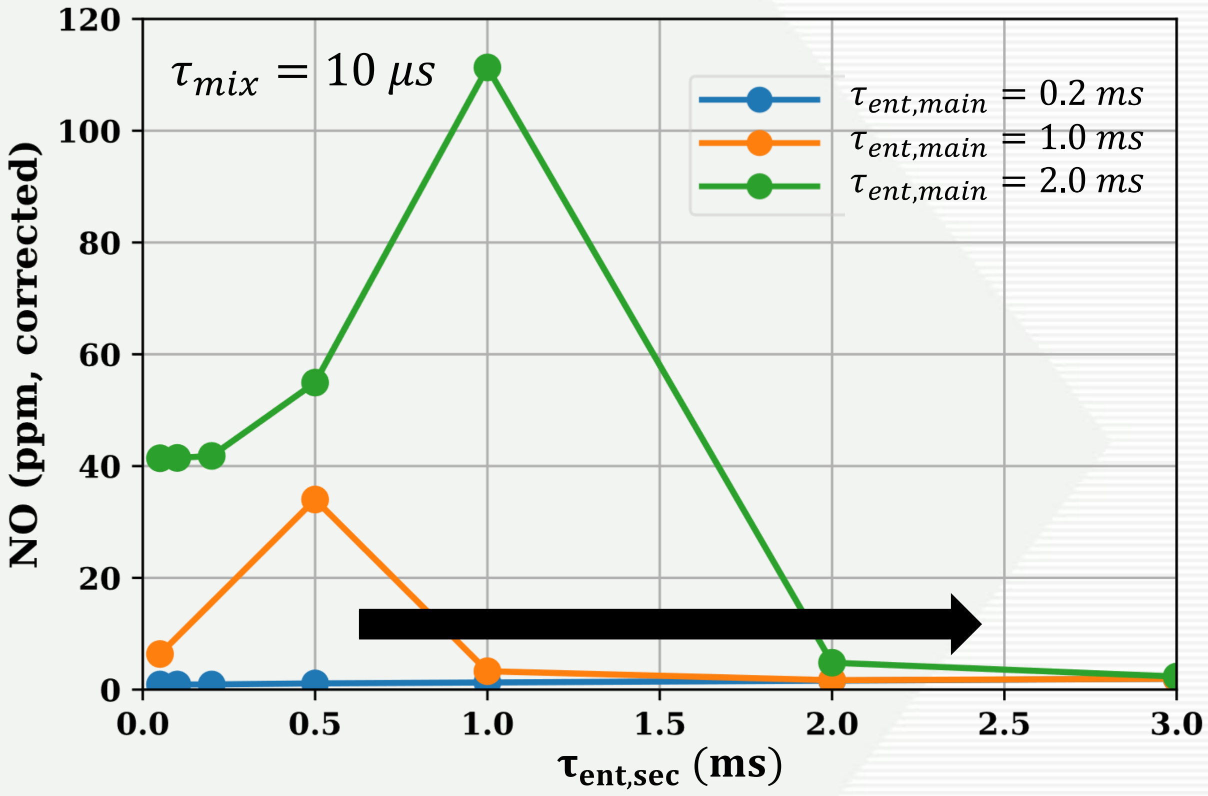



- With fast mixing, reduce $NO_x$ by:
  - Increasing main product entrainment rate ($^1/_{\tau_{ent,main}}$)

# MODELING: FINITE ENTRAINMENT RATE EFFECTS




- With fast mixing, reduce $NO_x$ by:
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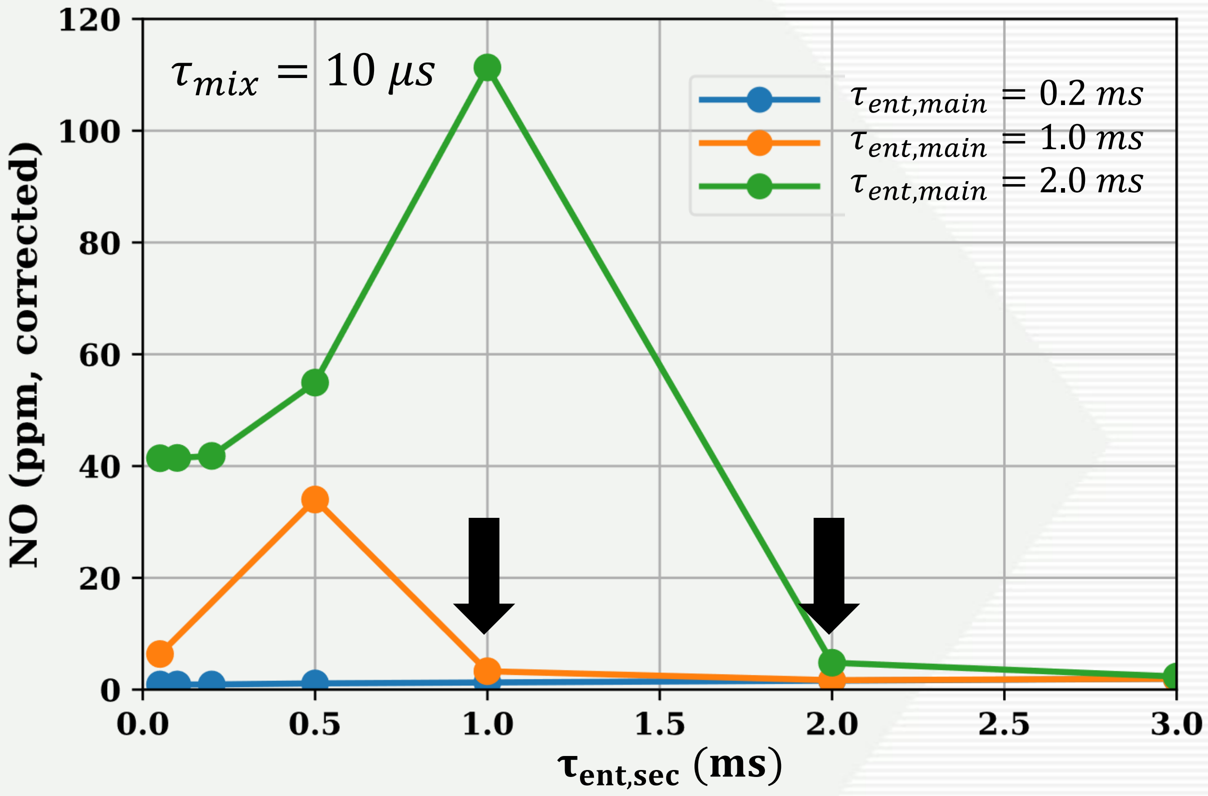
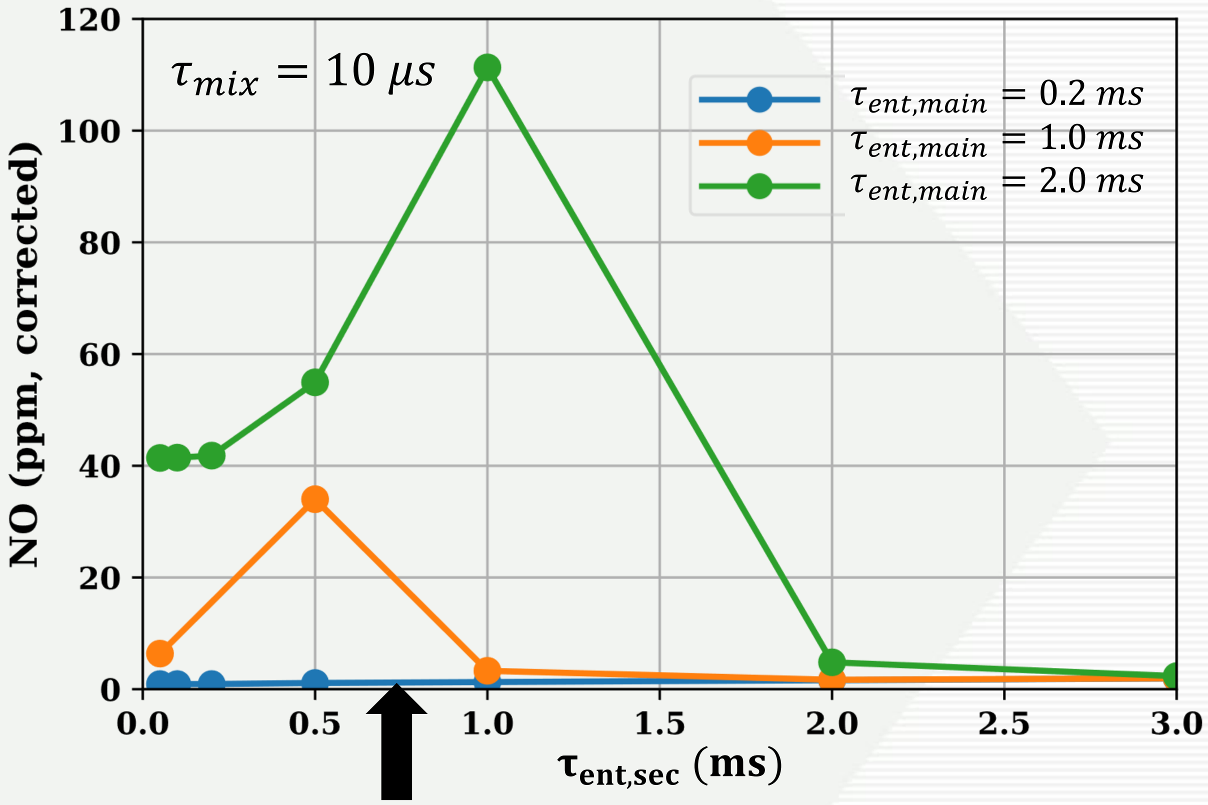



- With fast mixing, reduce $NO_x$ by:
  - Increasing main product entrainment rate ($^1/\tau_{ent,main}$)
  - Reducing secondary fluid entrainment rate ($^1/\tau_{ent,sec}$)
  - Threshold for NOx performance when entrainment rates are matched ($^1/\tau_{ent,main}$ = $^1/\tau_{ent,sec}$)

# MODELING: FINITE ENTRAINMENT RATE EFFECTS

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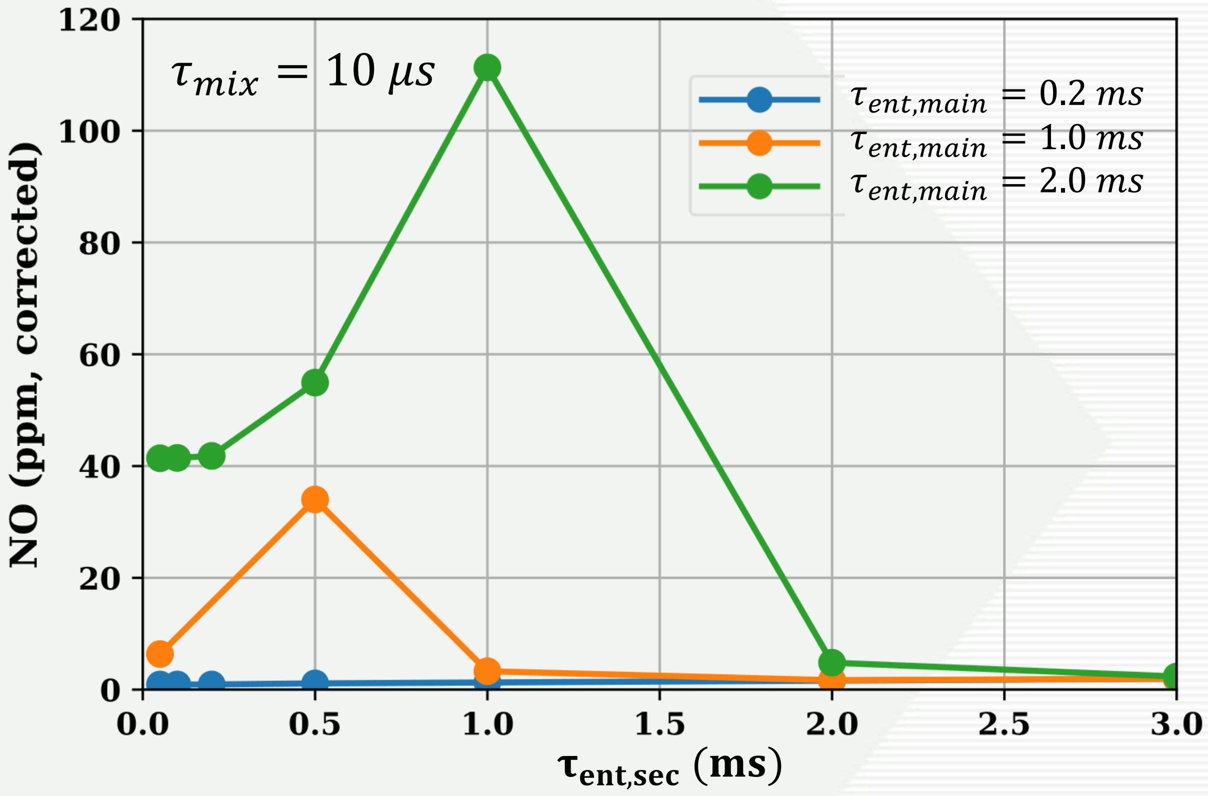
  - Threshold for NOx performance when entrainment rates are matched ($^1/\tau_{ent,main}$ = $^1/\tau_{ent,sec}$)
  - Very rapid main entrainment rate ($^1/\tau_{ent,main}$) → low NOx regardless of secondary entrainment rate ($^1/\tau_{ent,sec}$)

## MODELING: FINITE ENTRAINMENT RATE EFFECTS

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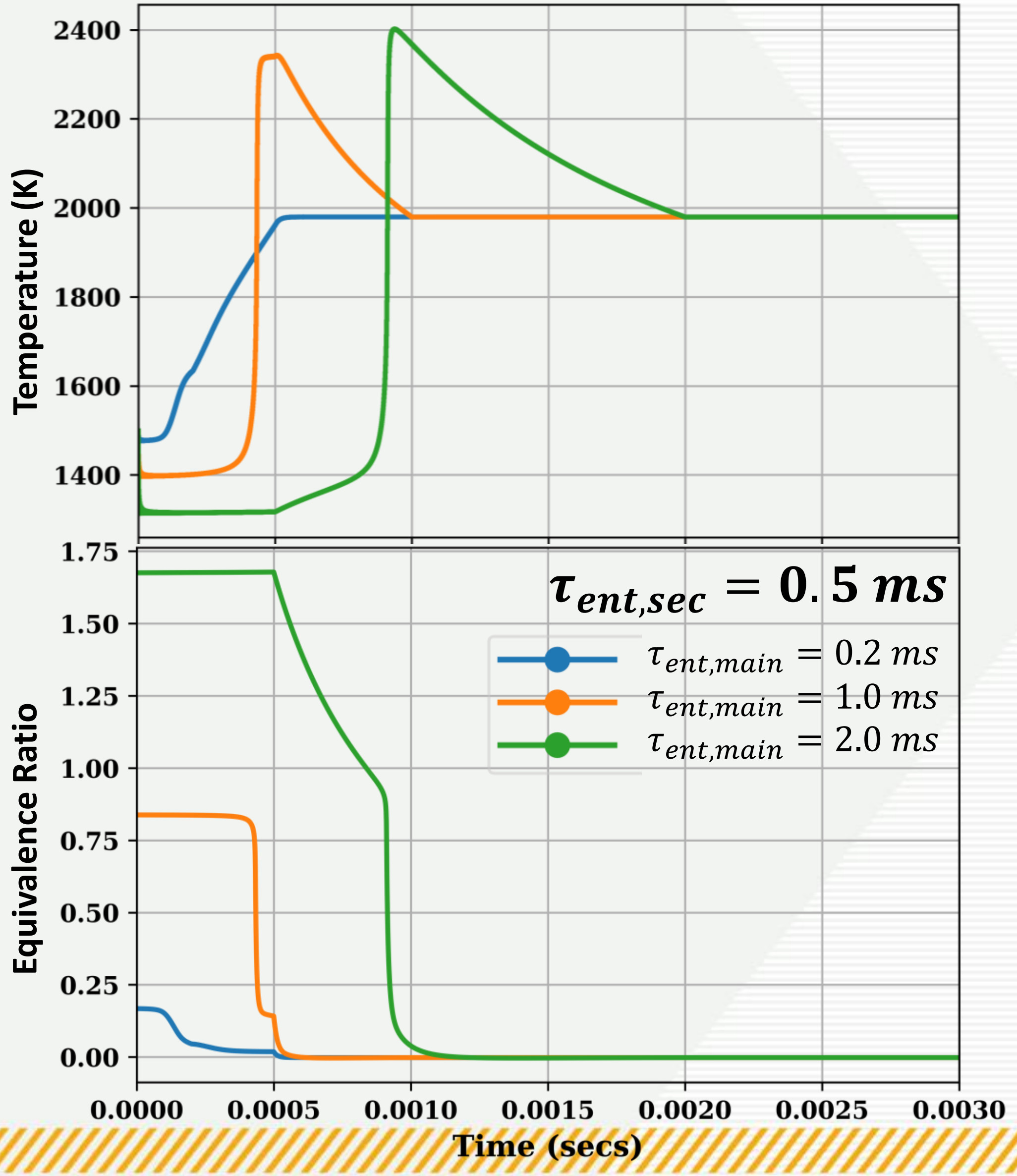
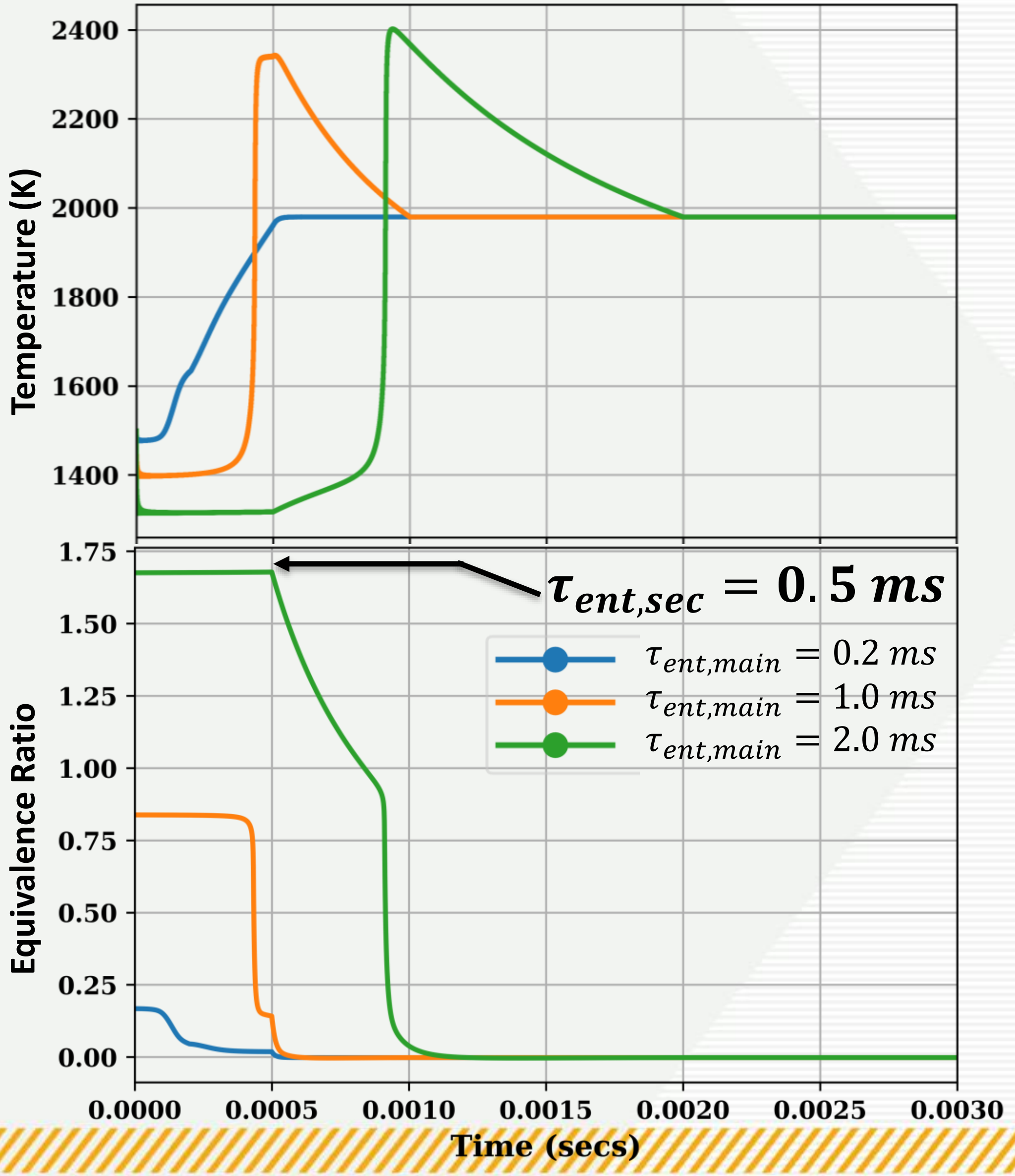
  - Reducing secondary fluid entrainment rate ($^1/\tau_{ent,sec}$)
  - Threshold for NOx performance when entrainment rates are matched ($^1/\tau_{ent,main}$ = $^1/\tau_{ent,sec}$)
  - Very rapid main entrainment rate ($^1/\tau_{ent,main}$) → low NOx regardless of secondary entrainment rate ($^1/\tau_{ent,sec}$)

**Rapid entrainment of crossflow → lean stoichiometry of burning**

# MODELING: FINITE ENTRAINMENT RATE EFFECTS



# MODELING: FINITE ENTRAINMENT RATE EFFECTS



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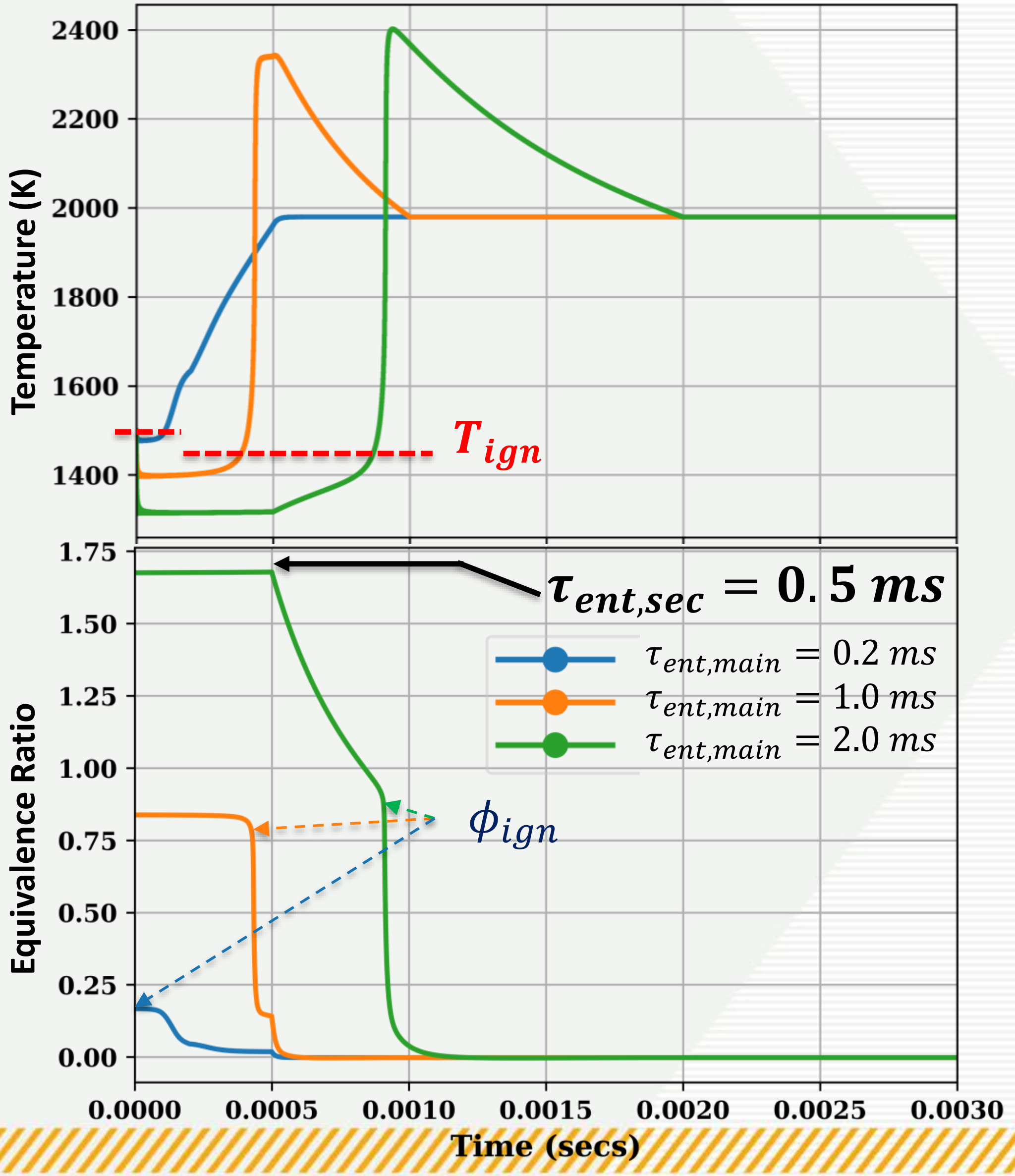


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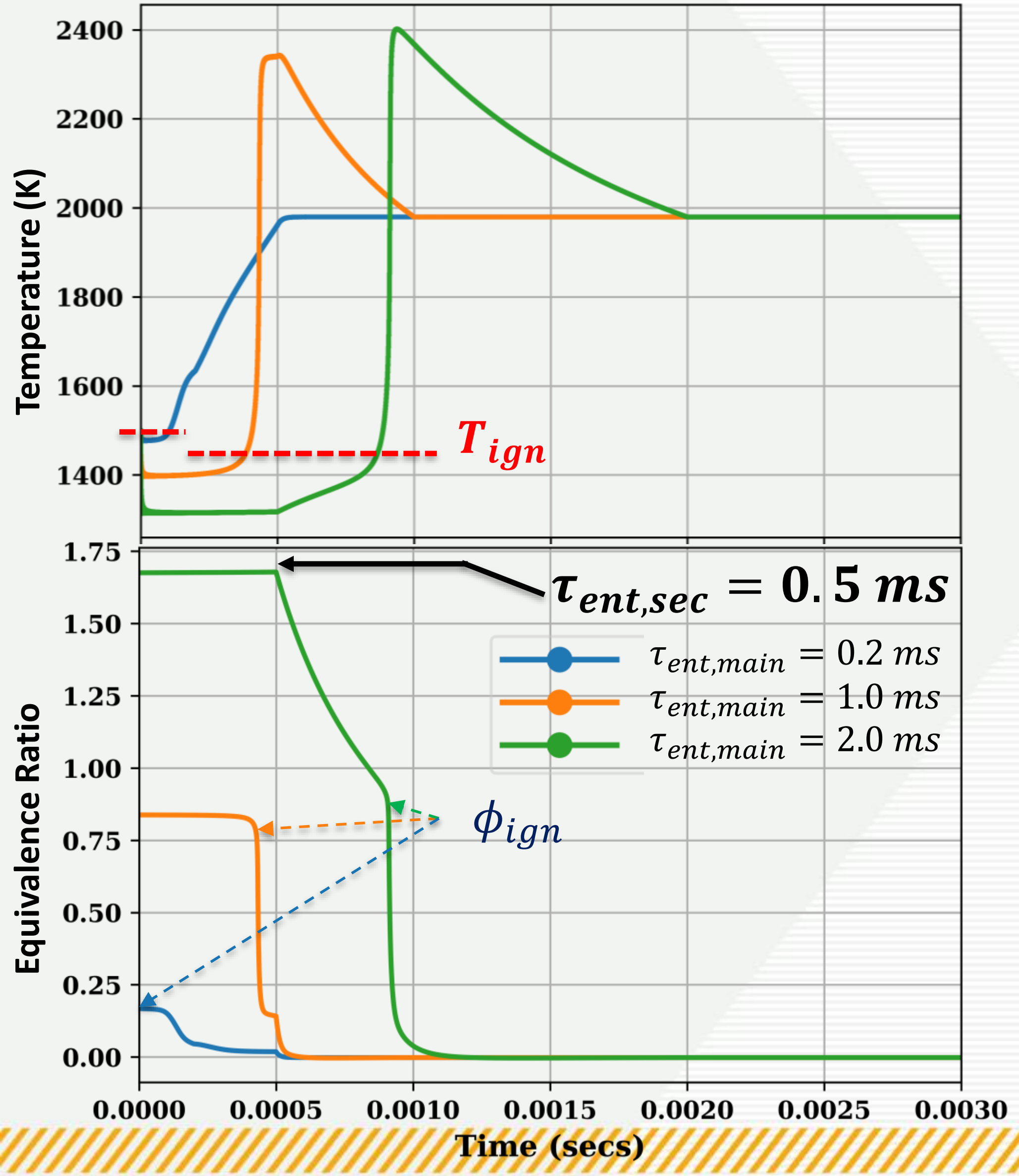
# MODELING: FINITE ENTRAINMENT RATE EFFECTS




- High main entrainment rate ($^1/_{\tau_{ent,main}}$) relative to secondary entrainment rate ($^1/_{\tau_{ent,sec}}$)
  - Start lean and hot → rapid autoignition
  - System ramps up to $\phi_{global}$ as fuel is entrained
    - ***Always lean!***
- No temperature overshoot = **Low NOx**

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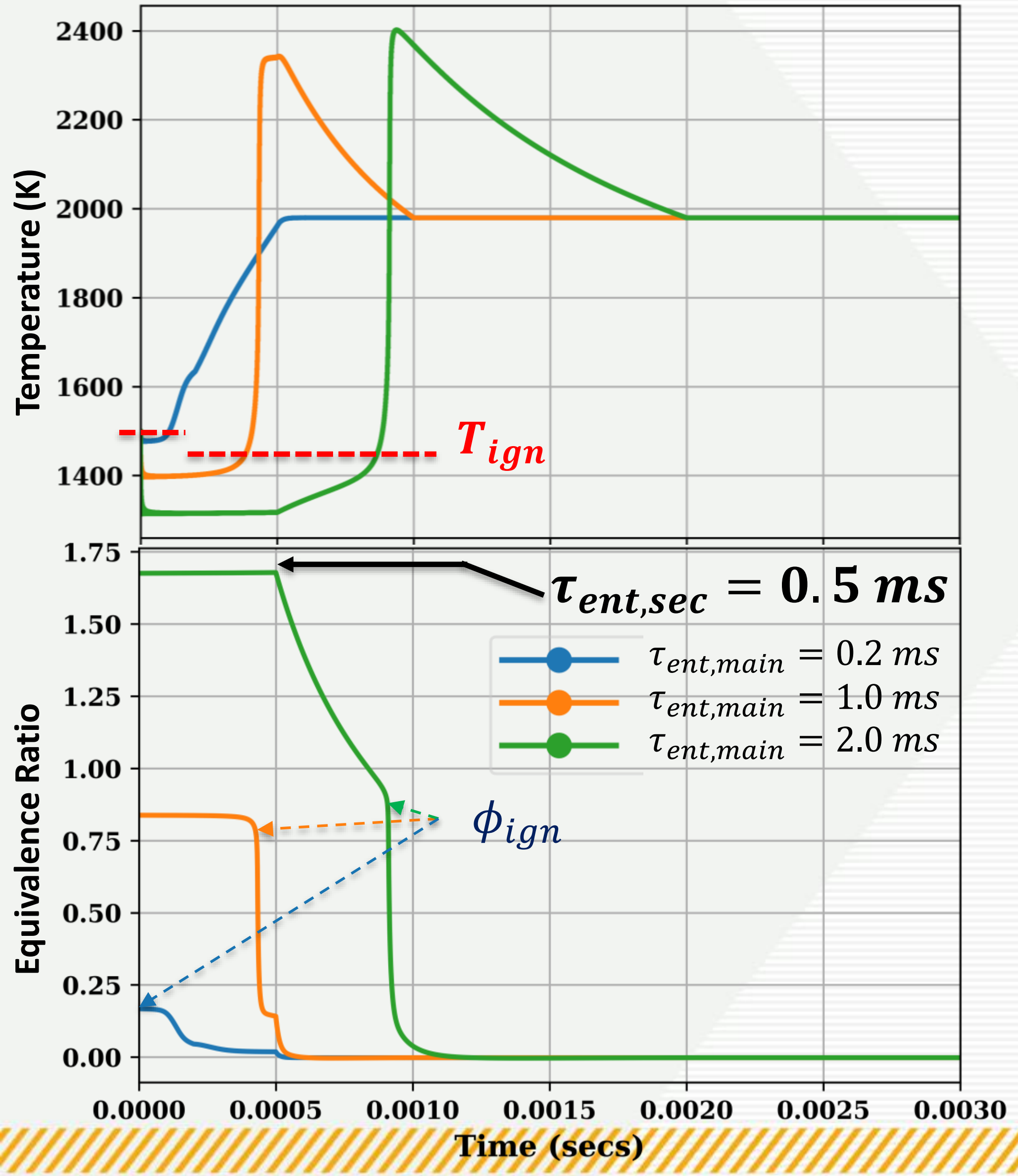
# MODELING: FINITE ENTRAINMENT RATE EFFECTS

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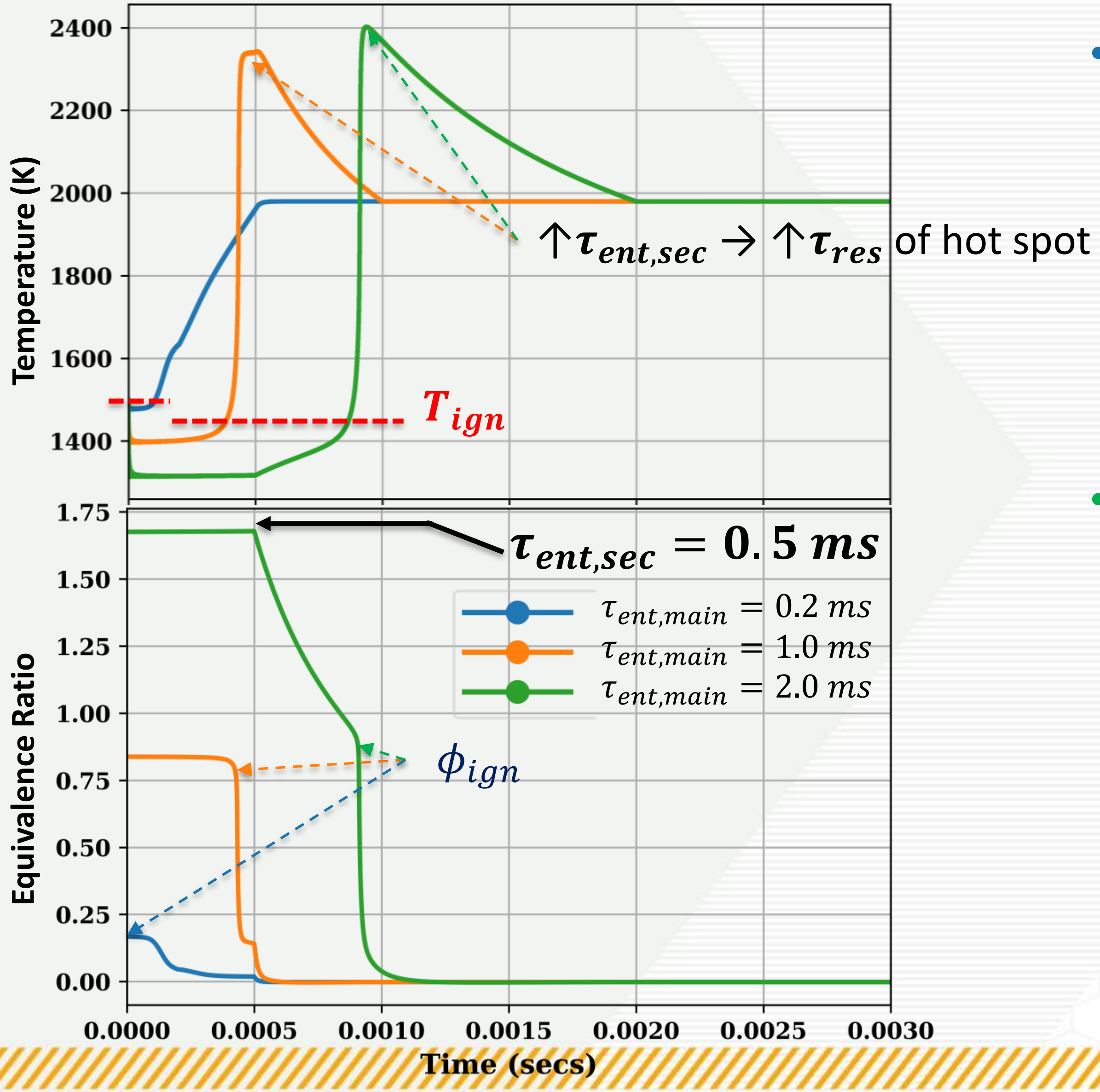
  - System ramps up to $\phi_{global}$ as fuel is entrained
    - ***Always lean!***
  - No temperature overshoot = **Low NOx**
- Low main entrainment rate ($^1/\tau_{ent,main}$) relative to secondary entrainment rate ($^1/\tau_{ent,sec}$)
  - Start rich (or near stoich) and cooler → delayed autoignition
  - $\boldsymbol{\phi} \approx 1$ for reaction time
    - High flame temp and prompt contributions
  - Temperature overshoot & time to dilute = **High NO**

# MODELING: FINITE ENTRAINMENT RATE EFFECTS

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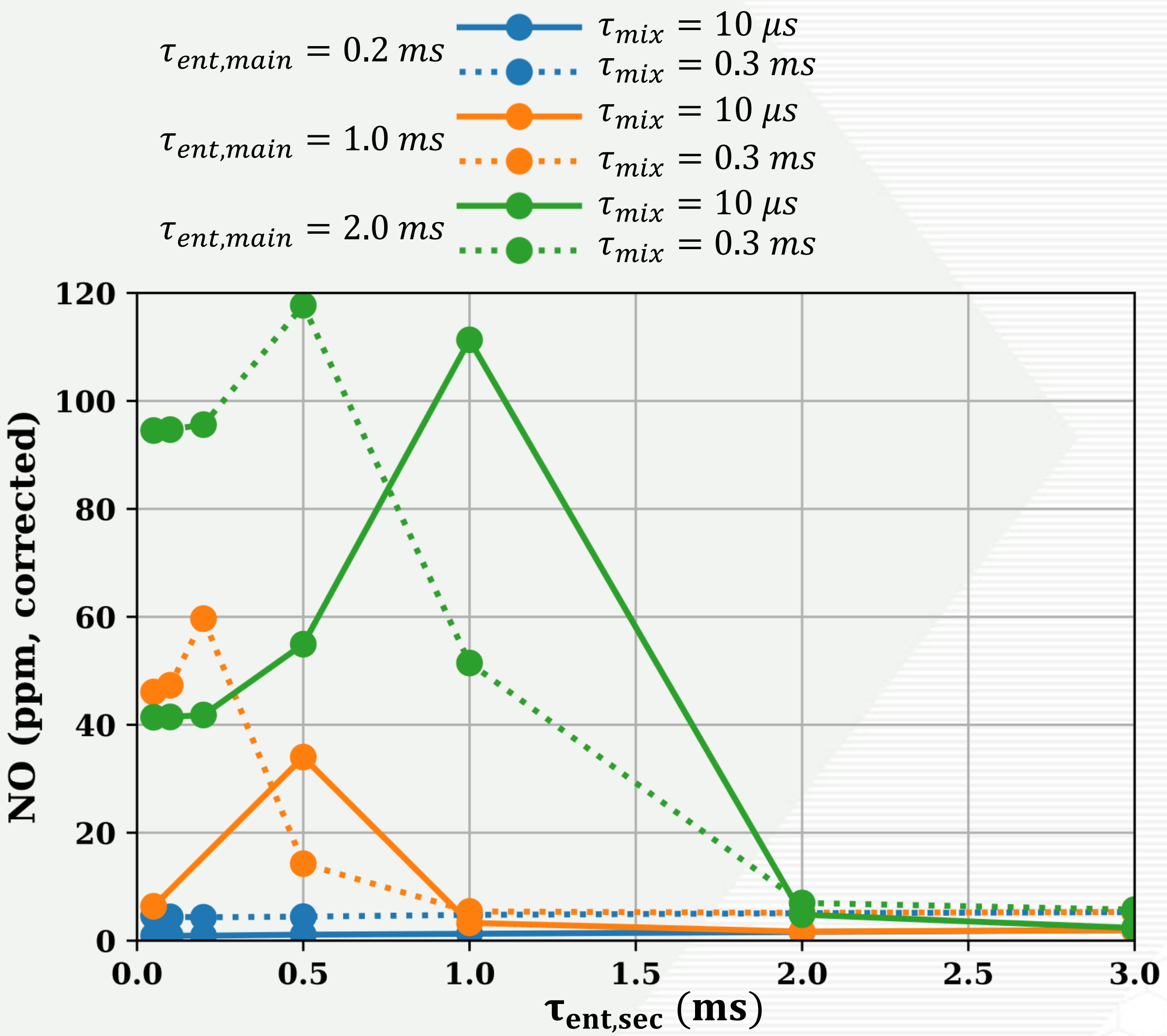
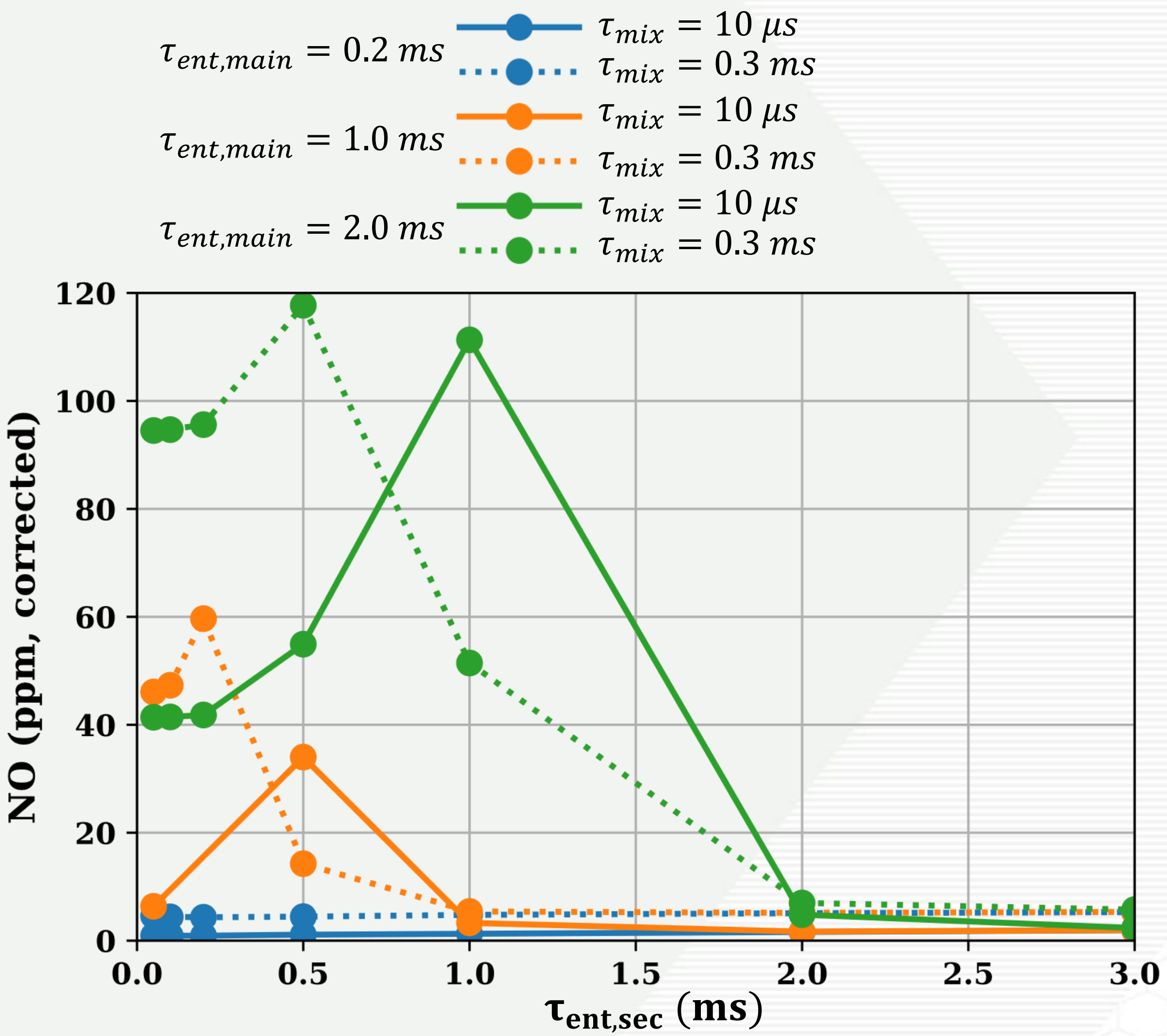
# MODELING: FINITE MIXING RATE EFFECTS




- Entrainment constant, reduce $^1/_{\tau_{mix}}$ by 30x

# MODELING: FINITE MIXING RATE EFFECTS




- Entrainment constant, reduce $^1/_{\tau_{mix}}$ by 30x
- NOx reduction still present if main entrainment rate is greater than secondary ($^1/_{\tau_{ent,main}} > {}^1/_{\tau_{ent,sec}}$)

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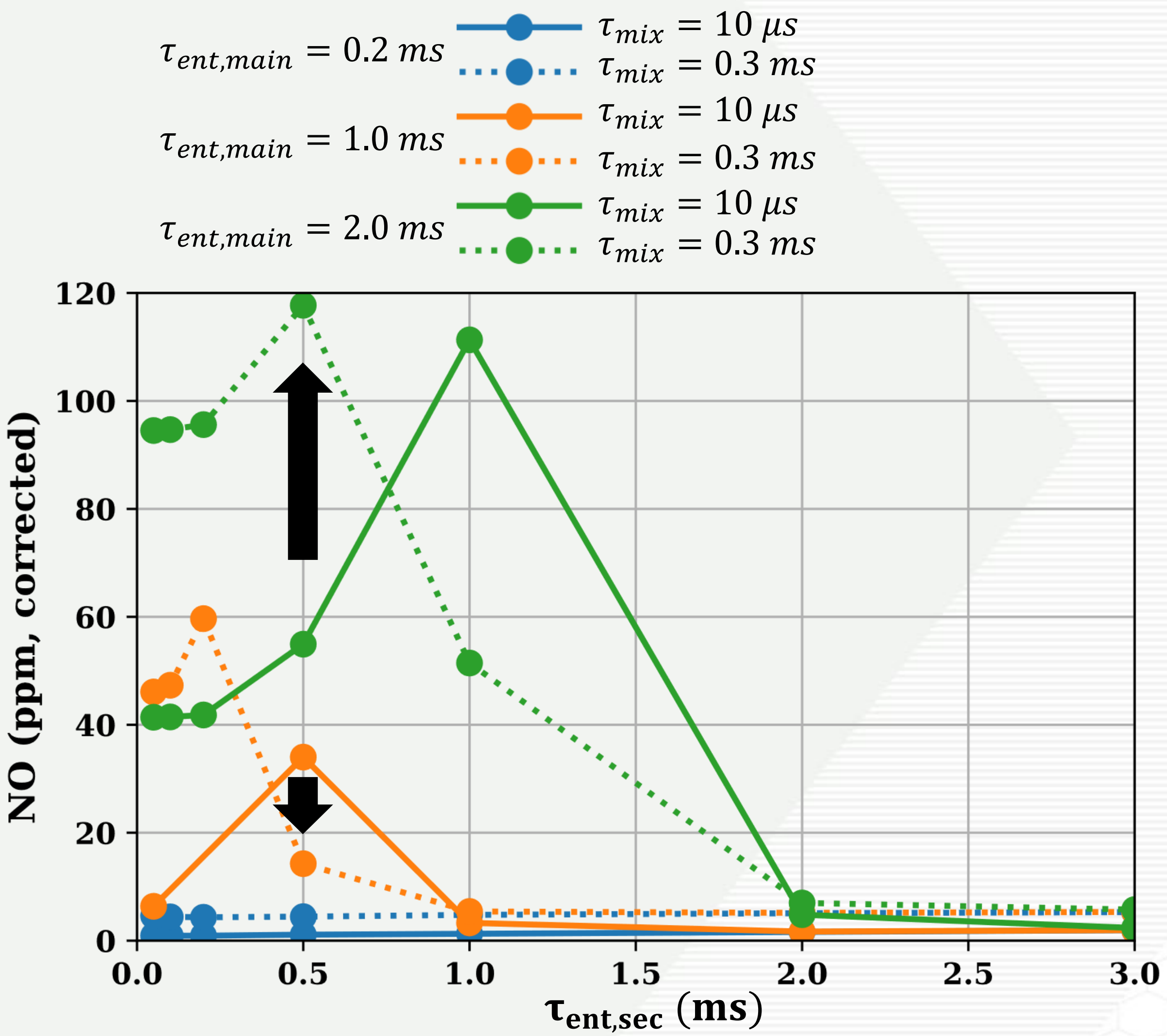
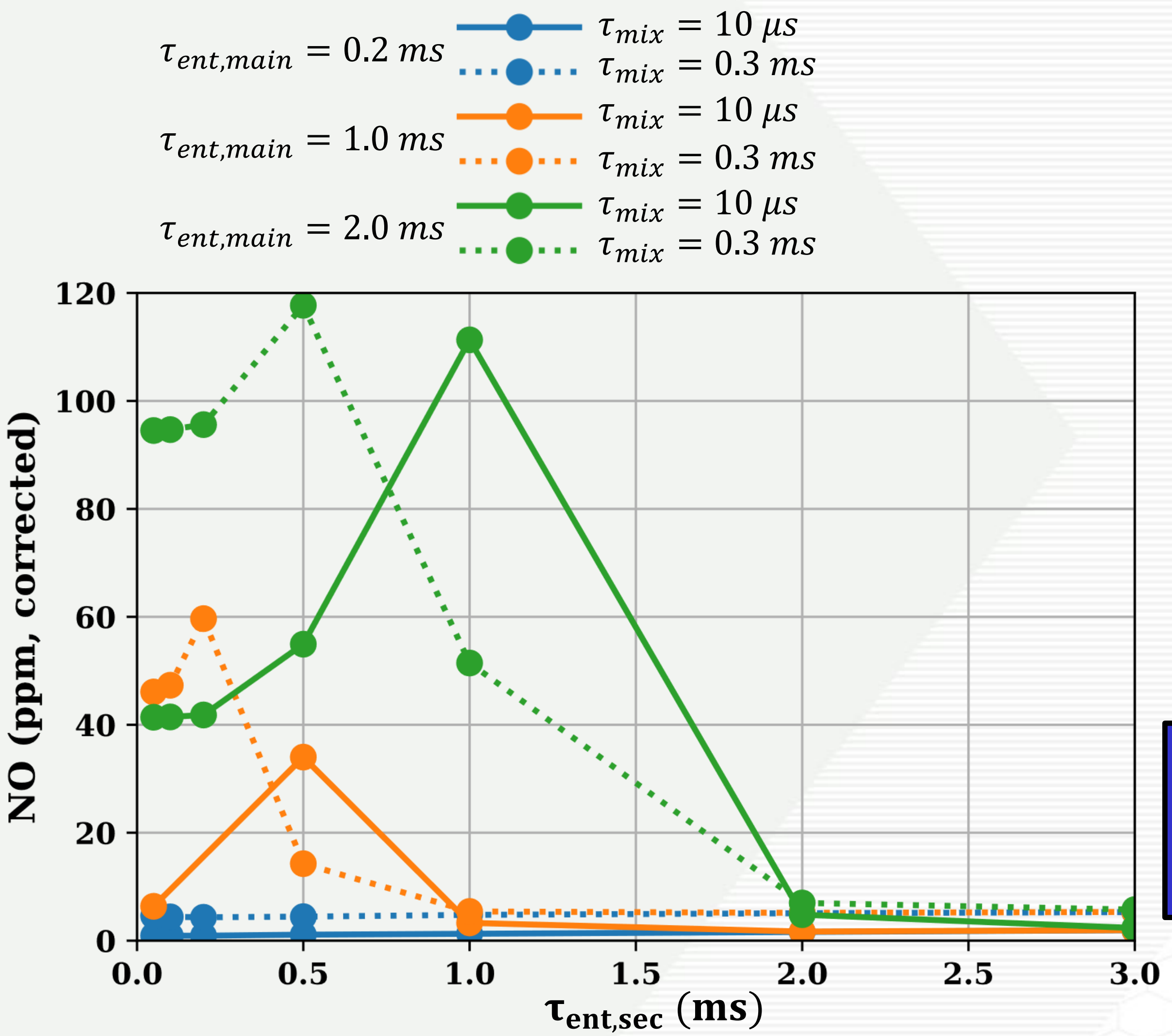



- Entrainment constant, reduce $^1/_{\tau_{mix}}$ by 30x
- NOx reduction still present if main entrainment rate is greater than secondary ($^1/_{\tau_{ent,main}} > {}^1/_{\tau_{ent,sec}}$)
- Finite mixing becomes significant when secondary entrainment rate becomes greater than main

  ($^1/_{\tau_{ent,main}} < {}^1/_{\tau_{ent,sec}}$)
- Mixing impact can be either beneficial or detrimental

# MODELING: FINITE MIXING RATE EFFECTS

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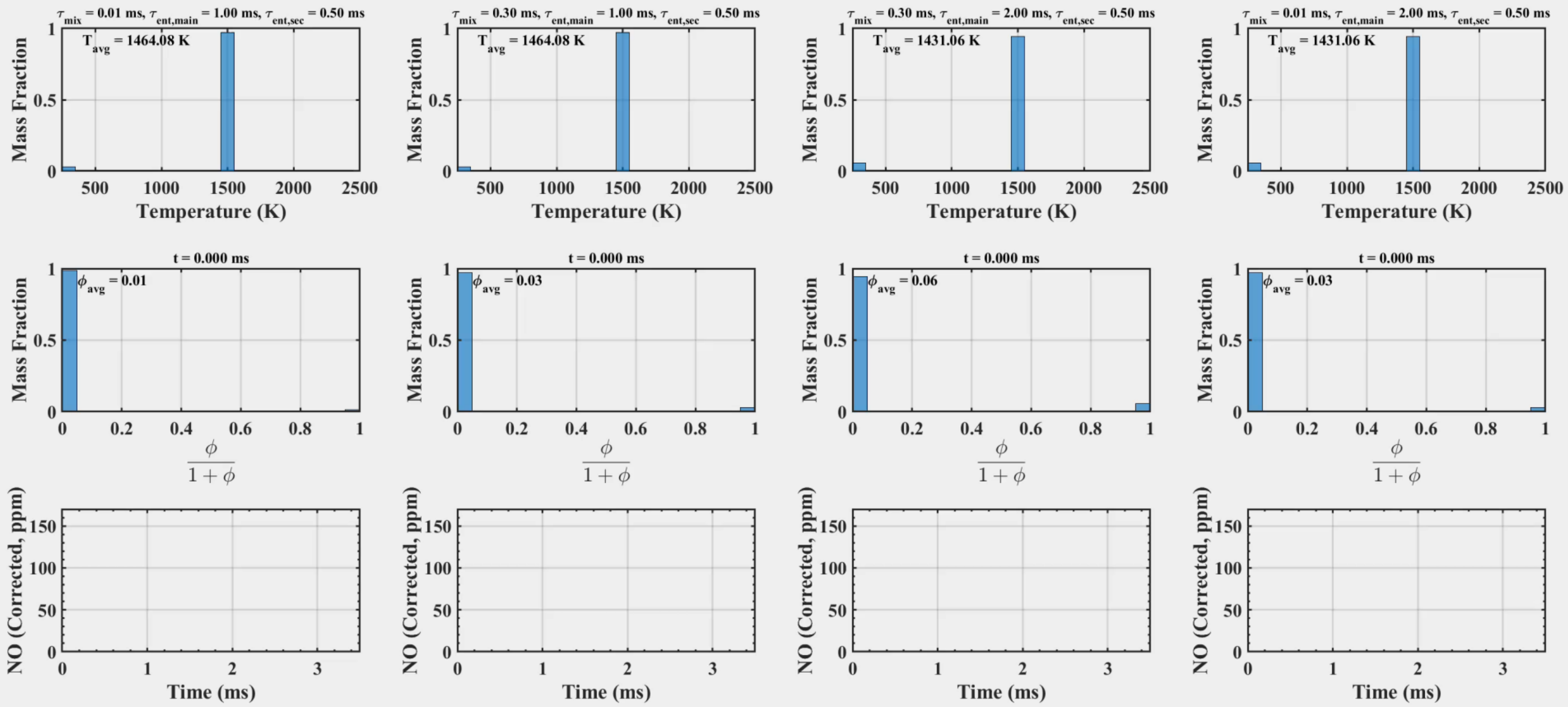
**Rapid entrainment of crossflow critical for NOx reduction**

# MODELING: FINITE MIXING RATE EFFECTS




Rapid entrainment of crossflow is dominant compared to mixing

# MODELING & EXPERIMENT TIE INS

- Modeling of finite rate axial staging behaviors can inform experimental results
- Low NOx levels found in “lean lifted” case suggest similarities to high crossflow entrainment results
  - Sufficient mixing occurs prior to combustion to drastically reduce or eliminate temperature overshoot
- For “rich lifted”
  - Flame most likely occurs near stoichiometric equivalence ratio creating temperature overshoot that must be then diluted
- For lee-stabilized increase in NOx vs “rich lifted” cases potentially due to
  - Impact on dilution rate of temperature overshoot from proximity of flame to jet exit
  - Impact on modality of combustion of rich products (synthesis gas):diffusion vs partially premixed

# DETAILED INVESTIGATION OF LOCAL MIXING AND HEAT RELEASE

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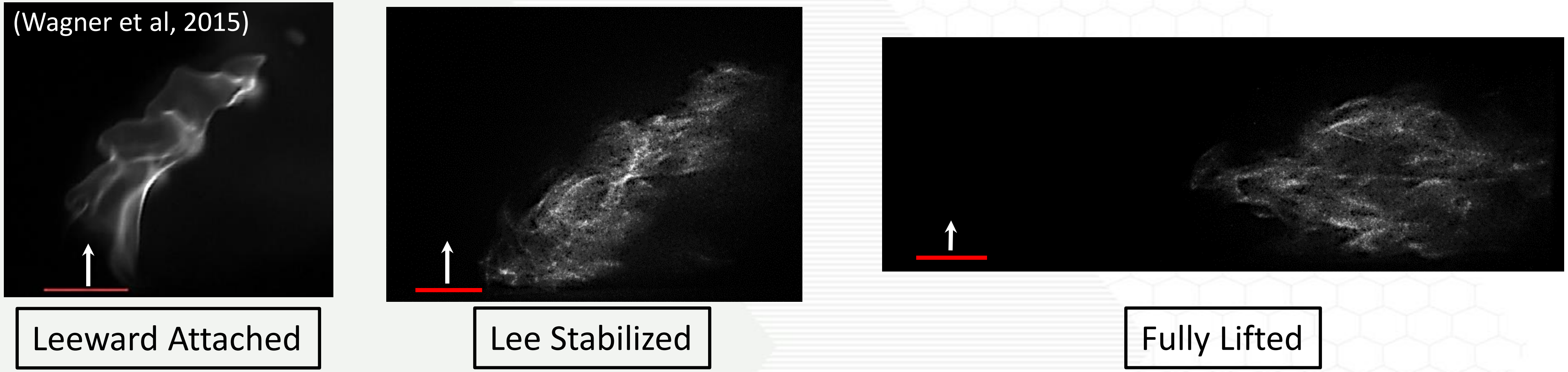
# Key research questions

(3) What do local pre- & post-flame mixing patterns look like and how is the heat release distributed?

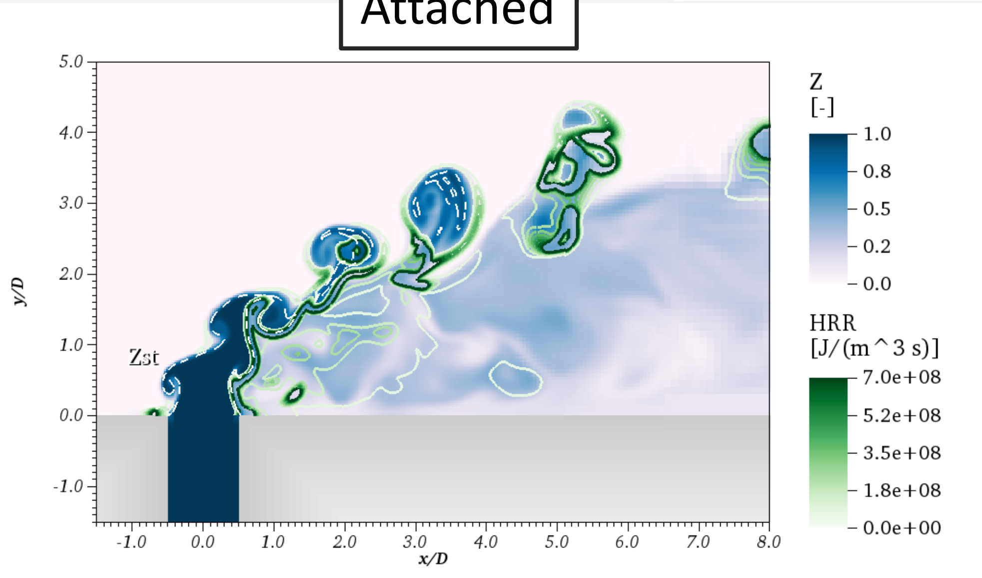
# RJICF: FLAME ATTACHMENT




- Simulations conducted to investigate local structure of RJICF under a variety of attachment conditions
- $\phi_{jet}$ = 1.1
- Leeward attached achieved with adiabatic wall boundary condition
- Lee stabilized achieved with isothermal boundary condition
- Fully lifted achieved by additionally doubling $\phi_{jet}$

# SIMULATION: ATTACHED VS LEE-STABILIZED

Attached



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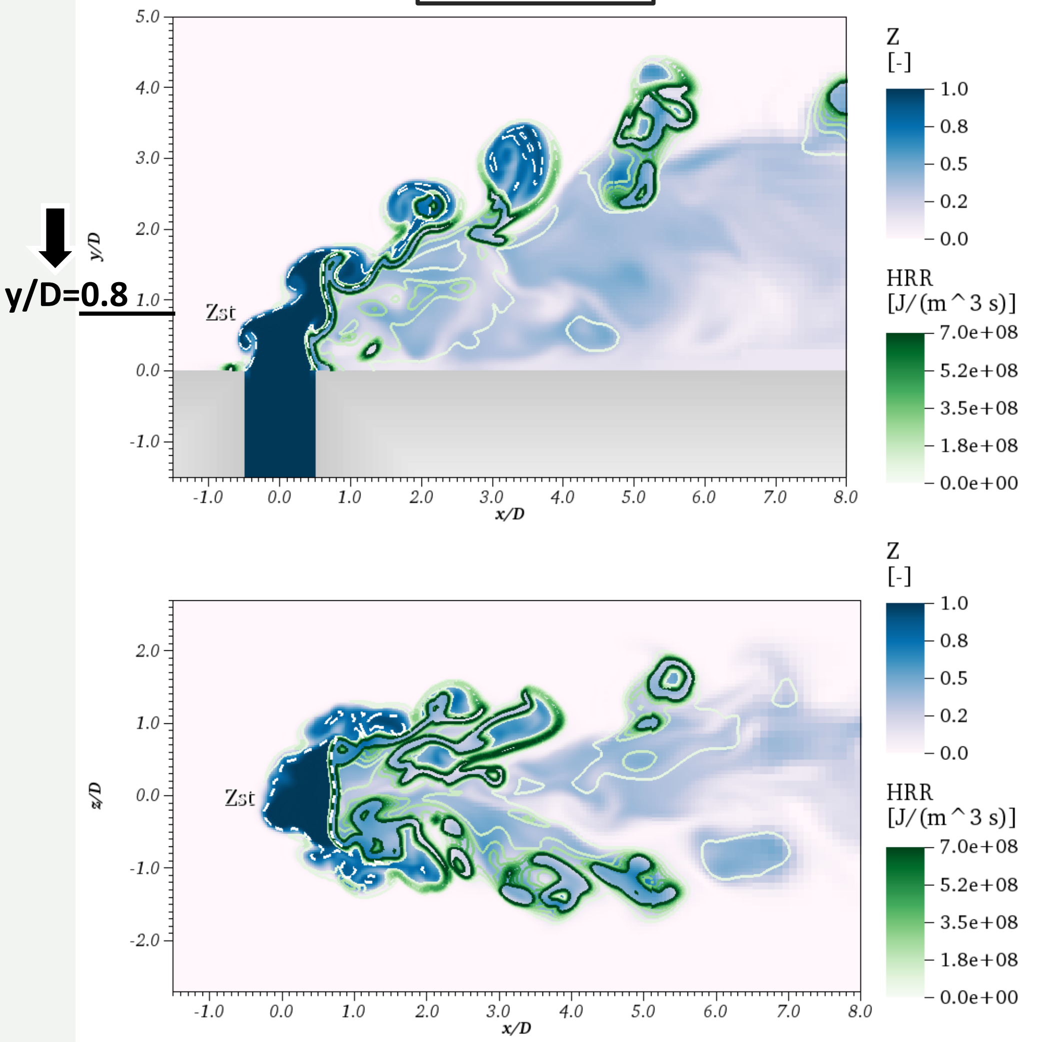

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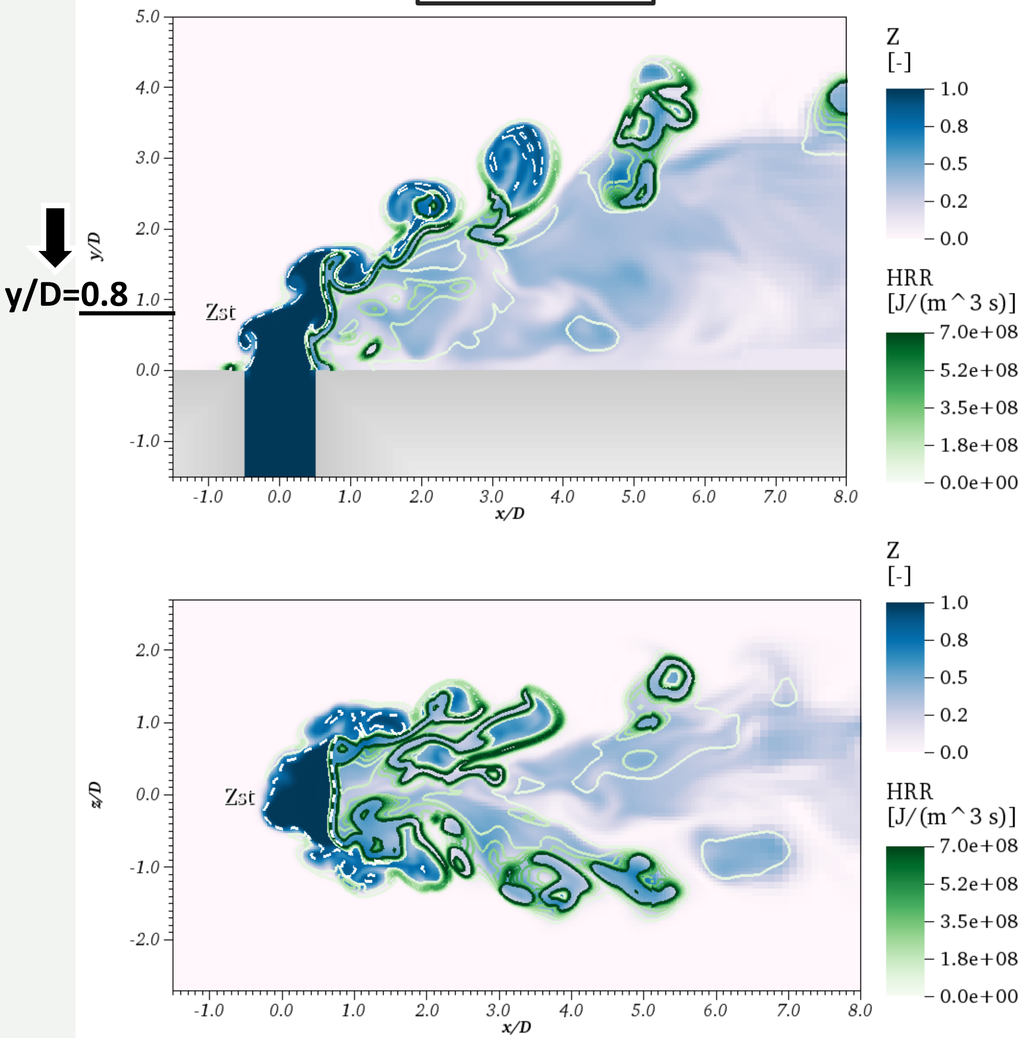
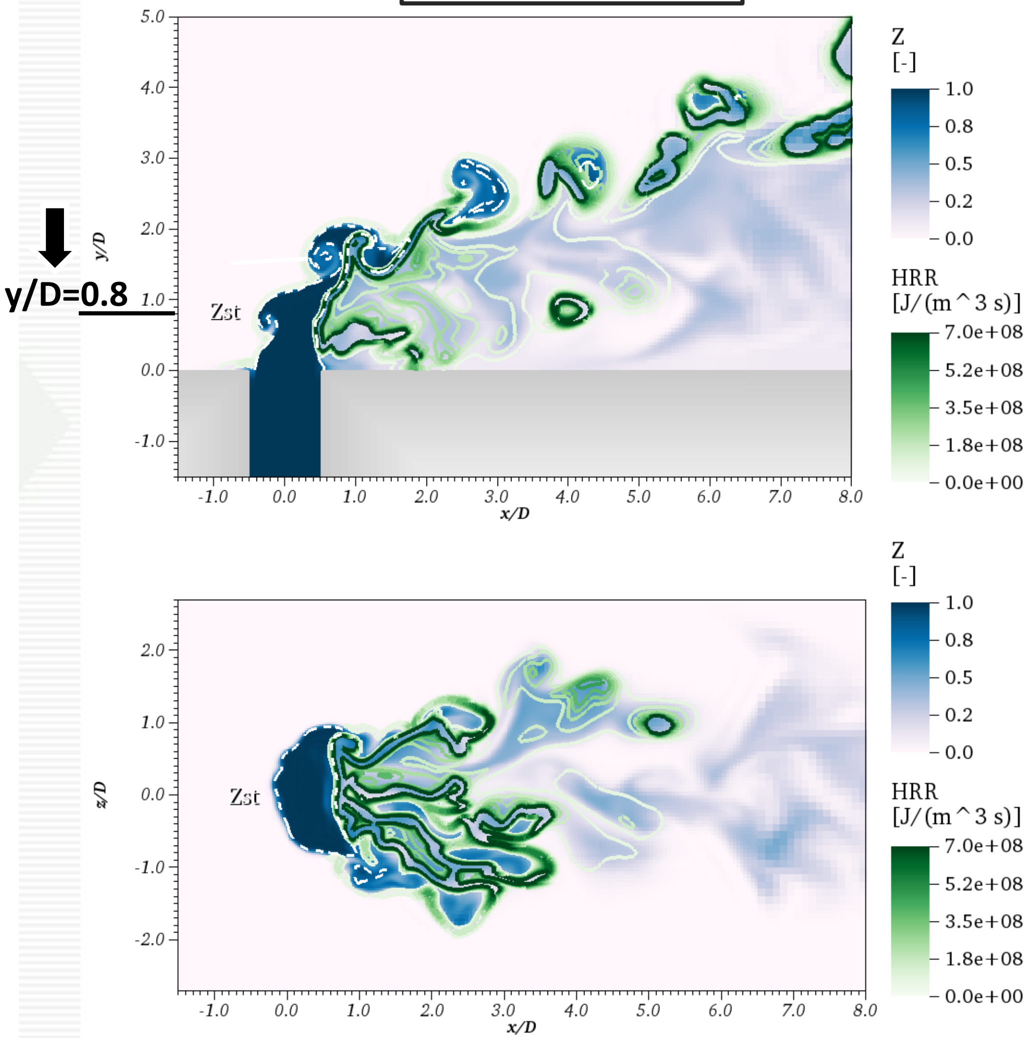



Lee-Stabilized



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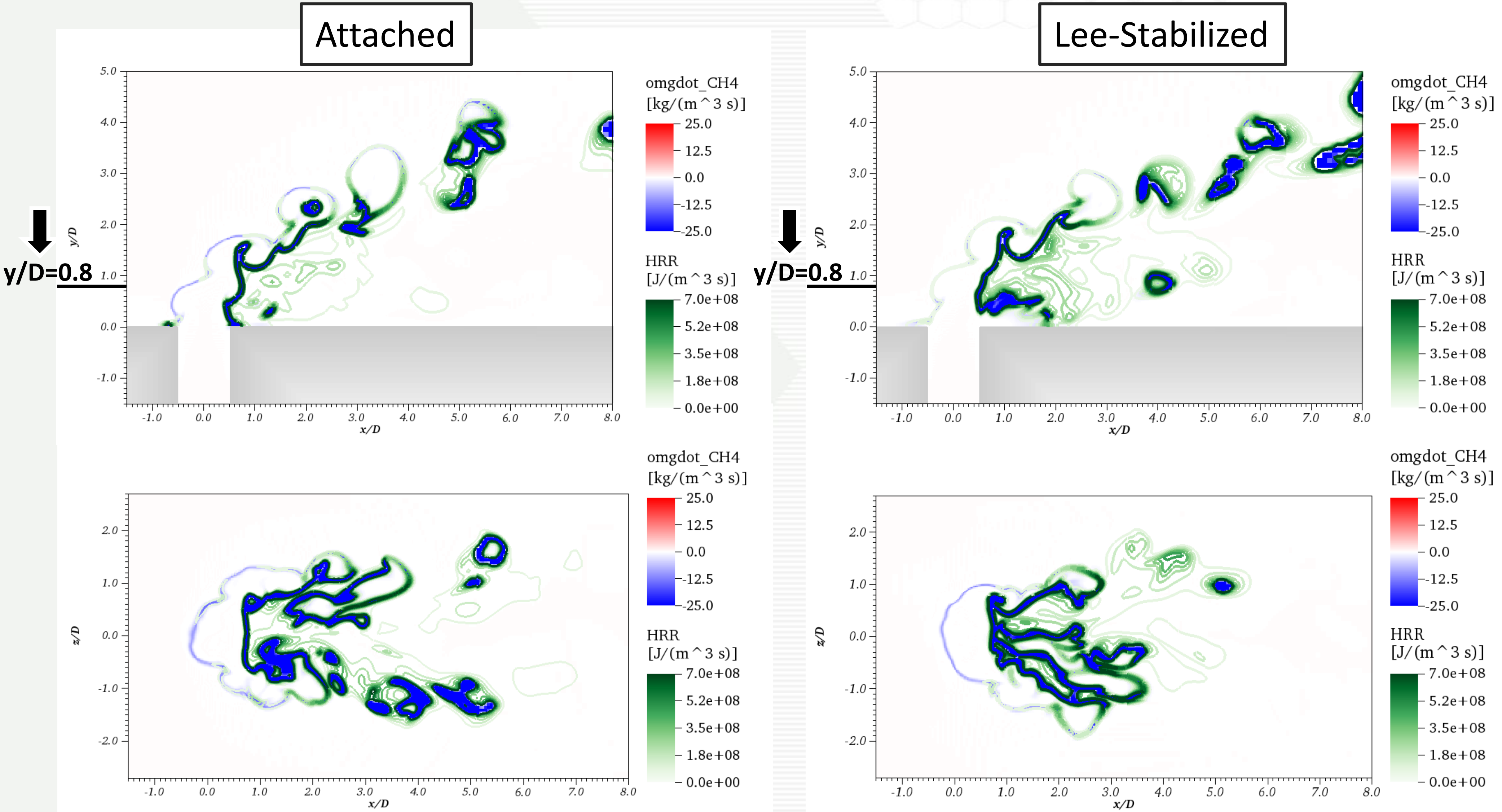
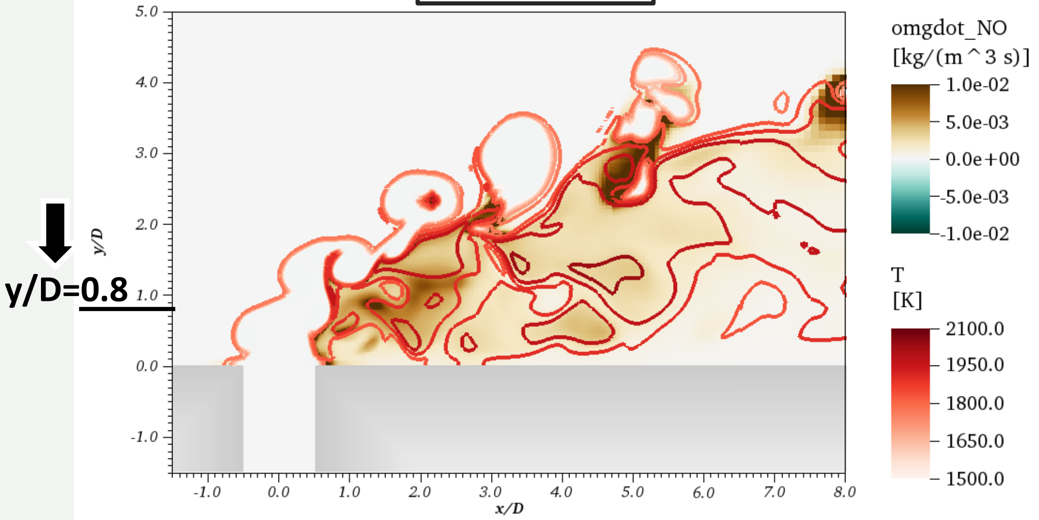
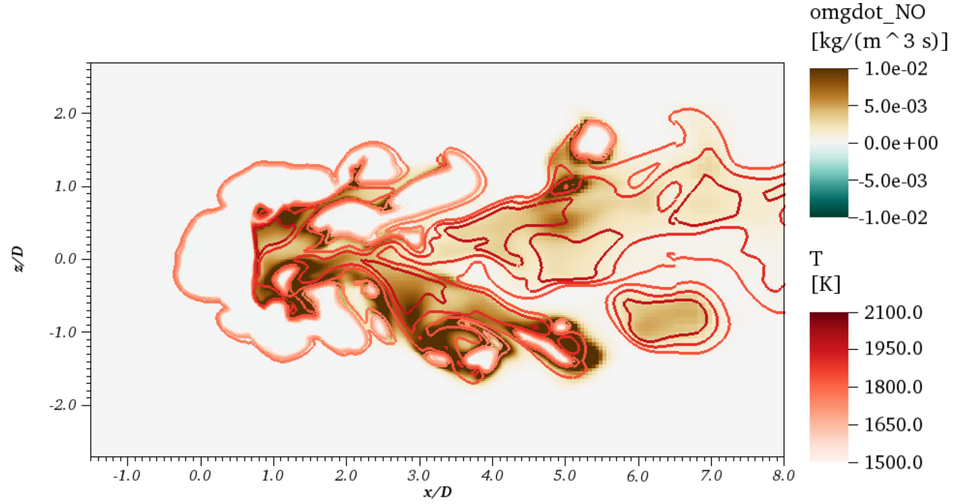


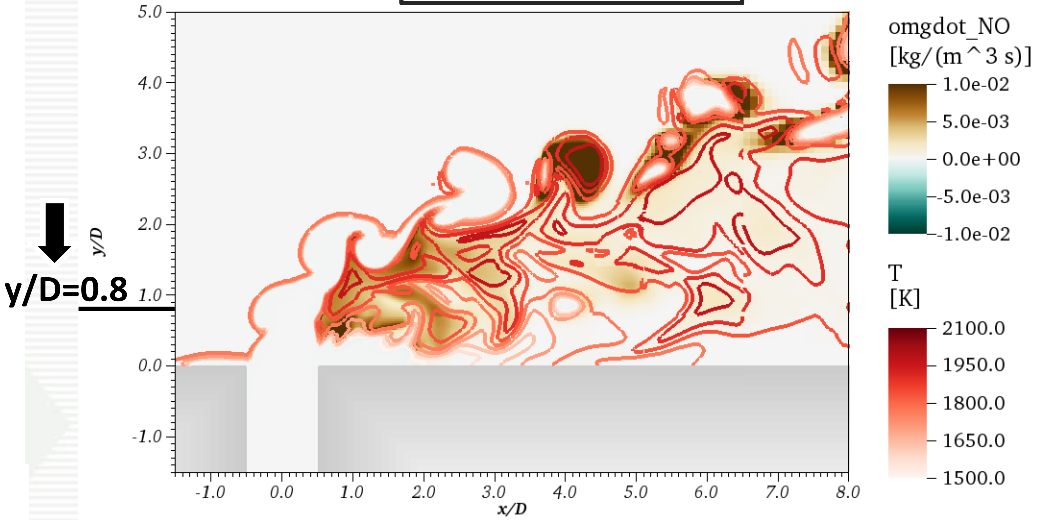
# SIMULATION: ATTACHED VS LEE-STABILIZED

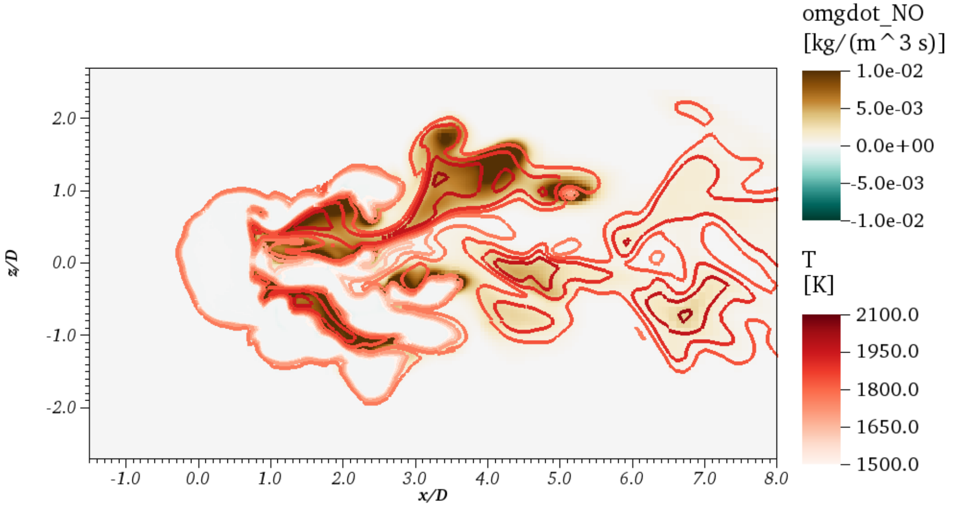
**Attached**




**Lee-Stabilized**



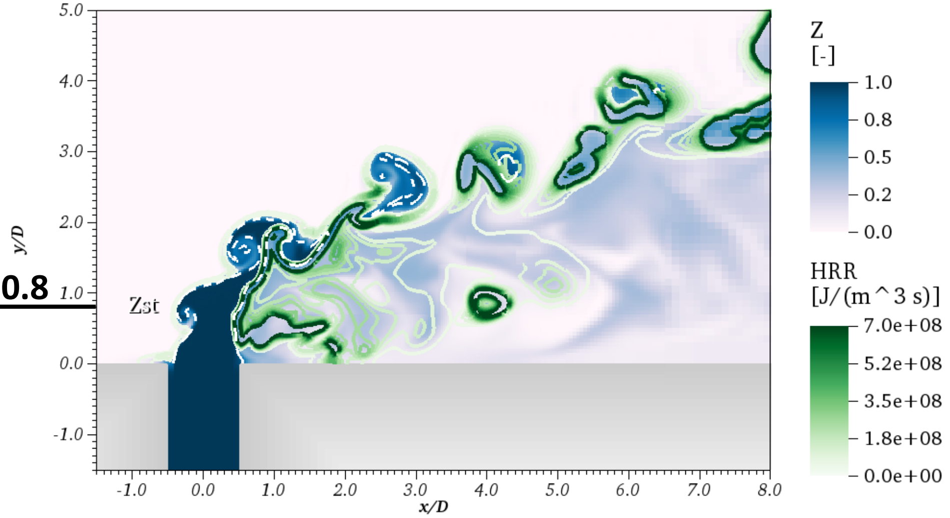
# SIMULATION: LEE-STABILIZED VS LIFTED

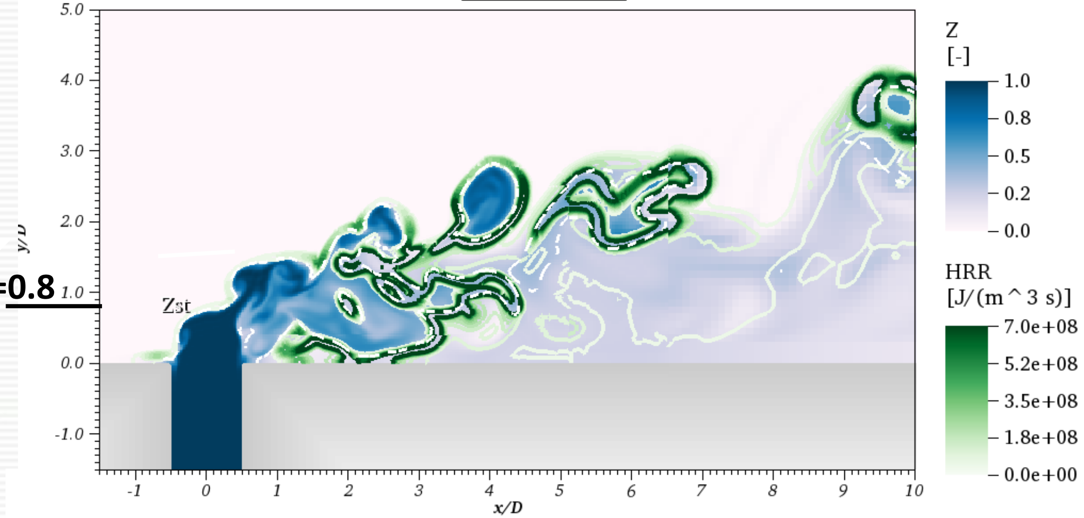
Lee-Stabilized

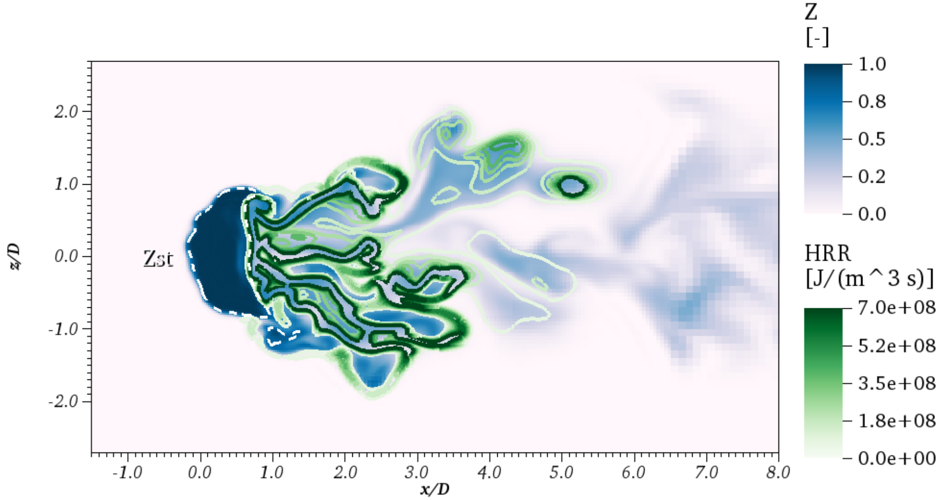
Lifted

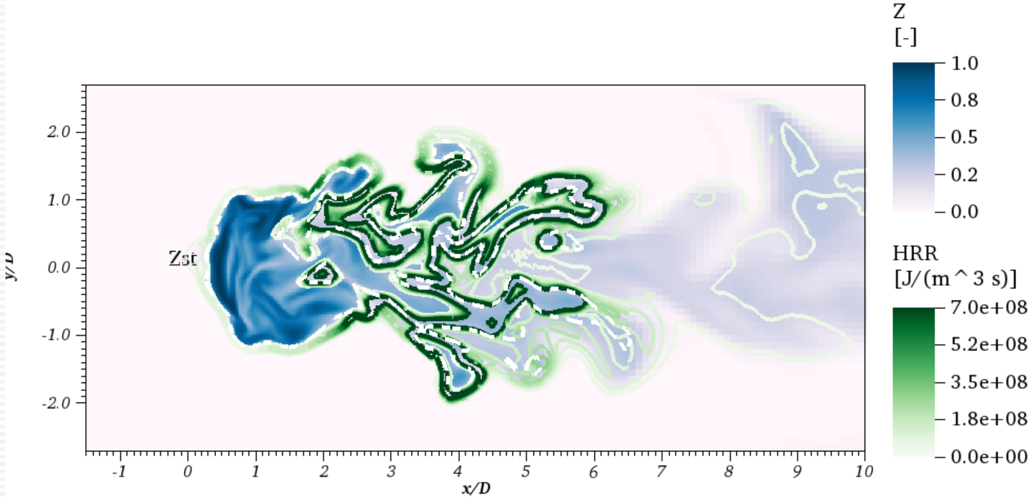
y/D=0.8

y/D=0.8



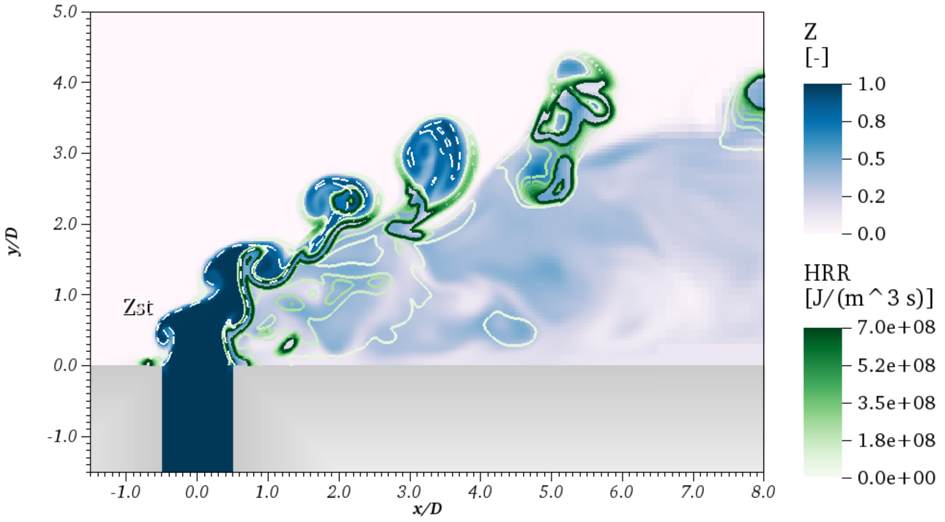



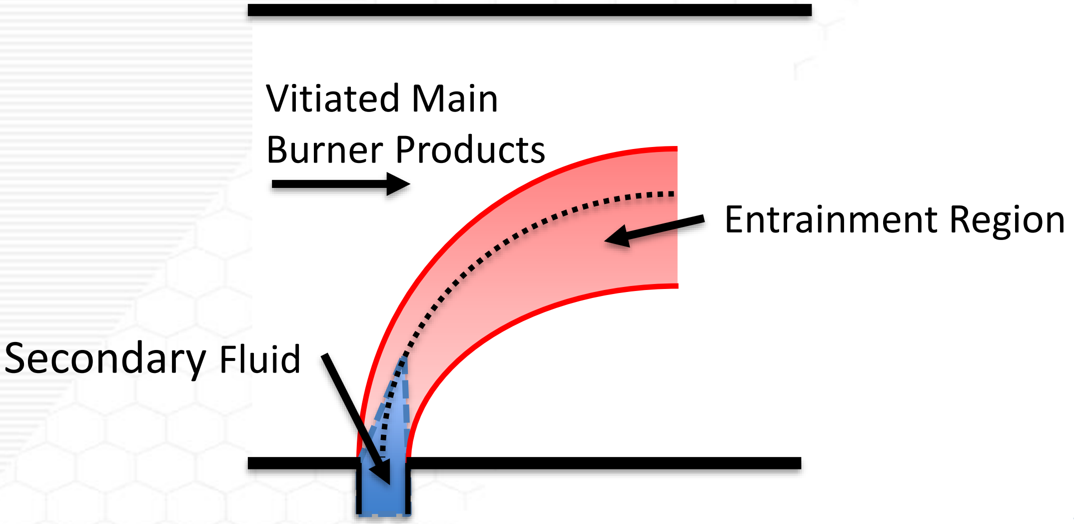



# SIMULATION TIE INS TO MODELING & EXPERIMENT

- Single RJICF:
  - Main entrainment rate less than secondary ($^1/\tau_{ent,main} < {}^1/\tau_{ent,sec}$) → Not ideal for low NOx
- Lifted rich flames still initiate at near-stoichiometric equivalence ratios
  - Supports hypothesis regarding rich lifted flames
- Detachment is critical for crossflow access to products of RJICF flame
  - Impact on dilution of hot spots and burning of produced syngas from rich RJICF



# SUMMARY

- Axial staging has great potential due to a theoretical NOx floor of O(1 ppm) at high flame temperatures (>1975K)
- Entrainment rate, specifically of main burner products, is critical parameter for successful axial staging implementation
  - Single RJICF does not rate well against this criteria → other configurations necessary
- Practical NO levels are highly sensitive to controlling parameters
- Regardless of specific configuration, lifting of RJICF flames from jet exit is critical in enabling the necessary entrainment and mixing to reduce NOx
- RJICF flames tend to establish themselves near stoichiometric equivalence ratios, creating hot spots

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# QUESTIONS?

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# BACKUP

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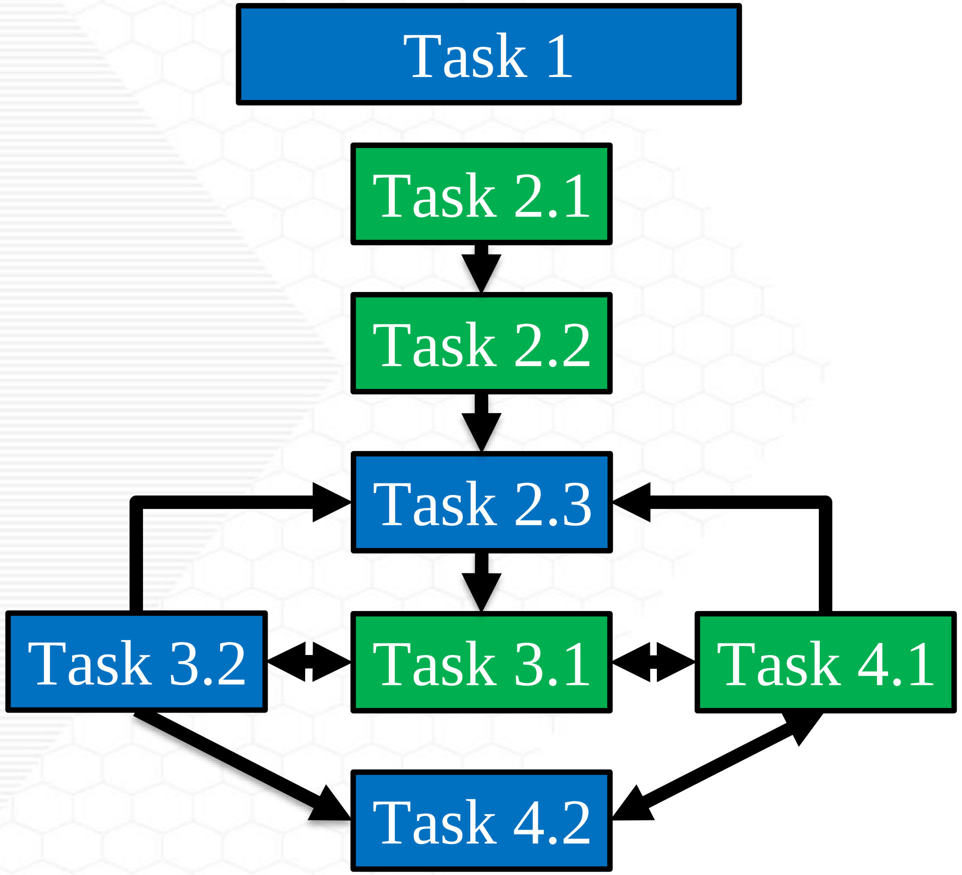
# WORK FLOW

- Task 1: PMP
- Task 2: Kinetic modeling & optimization
  - 2.1 Fundamental Kinetic Studies
  - 2.2 NOx Optimization Studies
  - 2.3 Constrained NOx Optimization Studies
- Task 3: Experimental characterization of distributed combustion concept
  - 3.1 Facility Development
  - 3.2 Experimental Characterization
- Task 4: Detailed experimental & computational investigation of mixing & heat release distributions
  - 4.1 Large Eddy Simulations (LES)
  - 4.2 Experimental Characterization using High-Speed Laser Diagnostics

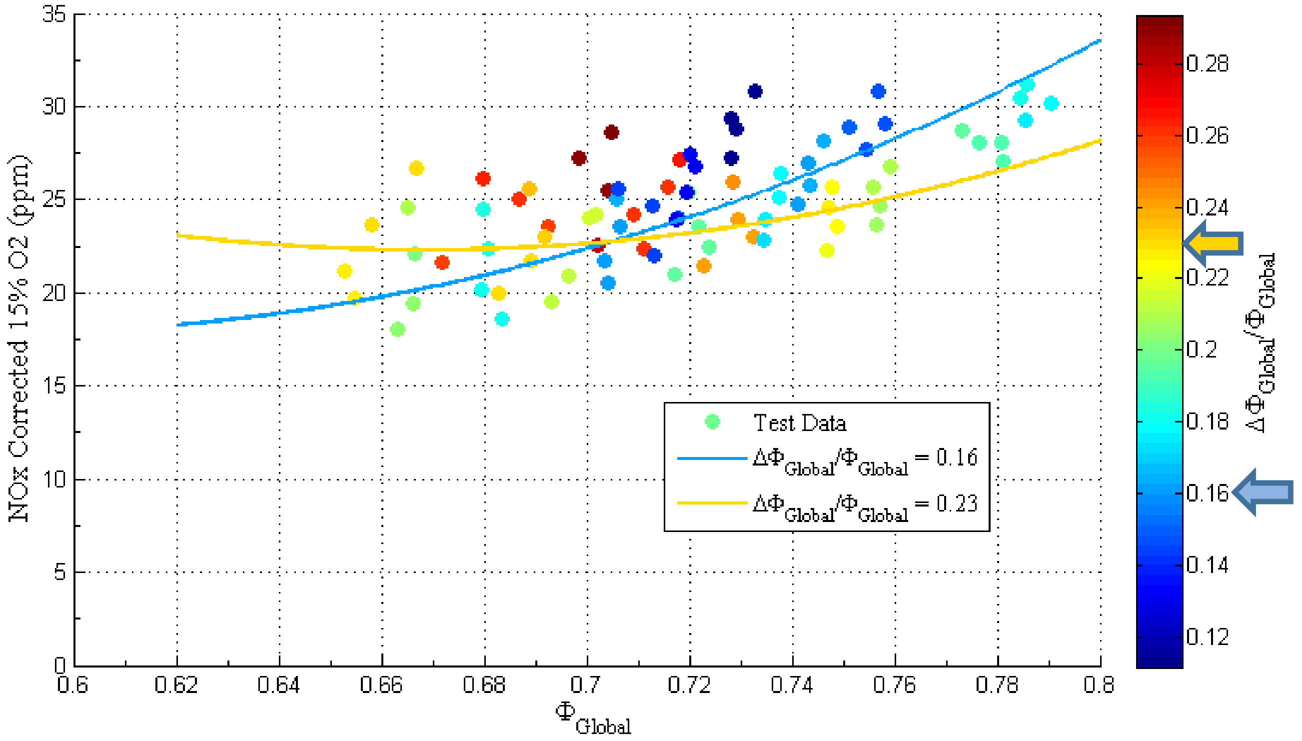


# PROJECT TIMELINE

| Tasks | | Progress | Interdep. | Year | | Quarter | | | | | Participants |
|---|---|---|---|---|---|---|---|---|---|---|---|
| **Task-1** | | | | 1 | 2 | 9 | 10 | 11 | 12 | 13 | |
| 1.1 | Project Management and Planning | ○ | | | | | | | | | GTAE DOE Low-NOx Research Team |
| 1.2 | Reporting | ○ | | | | | | | | | |
| **Task-2** | | | | 1 | | 9 | 10 | 11 | 12 | 13 | |
| 2.1 | Fundamental Kinetic Studies | ✓ | | | | | | | | | Prof. Seitzman |
| 2.2 | Initial NO Optimization Studies | ✓ | 2.1 | | | | | | | | Prof. German |
| 2.3 | Constrained NO Optimization | ○ | 2.2 4.1 | | | | | | | | Edwin Goh |
| **Task-3** | | | | 1 | | 9 | 10 | 11 | 12 | 13 | |
| 3.1 | Experimental Facility Development | ✓ | 2.2 | | | | | | | | Prof. Lieuwen |
| 3.2 | Initial Test Matrix & Facility Characteristics | ✓ | 2.1, 2.2 | | | | | | | | Dr. Ben Emerson |
| 3.3 | Refined Test Matrix & Facility Characteristics | ○ | 2.3 | | | | | | | | Matthew Sirignano<br>Vedanth Nair |
| **Task-4** | | | | 1 | | 9 | 10 | 11 | 12 | 13 | |
| 4.1 | LES Studies for Subcomponent Geometry | ○ | 2.3 | | | | | | | | Prof. Menon |
| 4.2 | LES Studies for Experimental Rig | ○ | 3.1, 3.2 | | | | | | | | Prof. Lieuwen |
| 4.3 | Experiments with High Speed Diagnostics | ▶ | 3.2, 3.2 | | | | | | | | Dr. Andreas Hoffie |

✓ : Done
○ : In Progress
▶ : Future

# EXPERIMENTAL: SYSTEM EMISSIONS



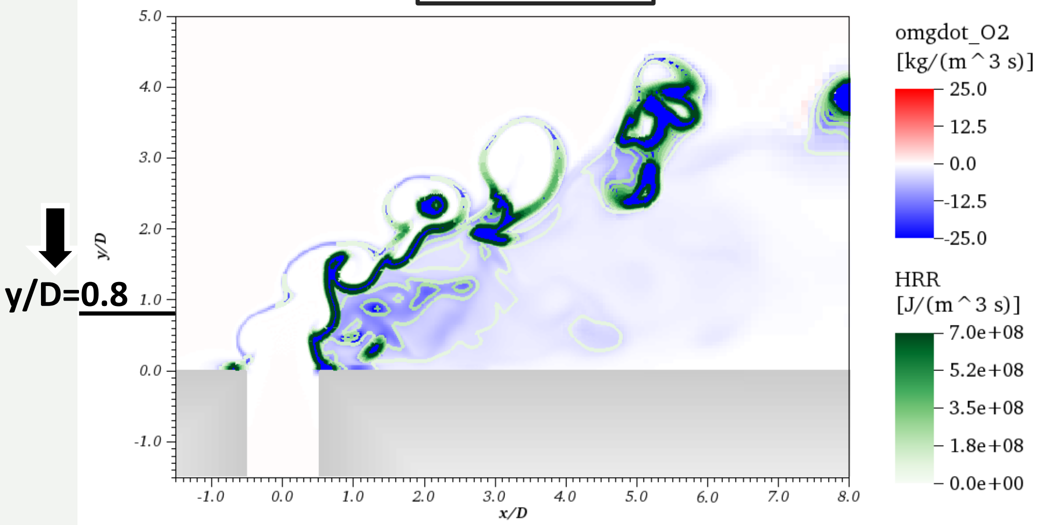

- Total $NO_X$ increases with increasing $\phi_{global}$
- $\Delta\phi_{global} \equiv \phi_{global} - \phi_{head}$ which is a measure of the axial stage contribution
- For low $\phi_{global}$: low $\Delta\phi_{global}$ → lower NOx
- For high $\phi_{global}$: high $\Delta\phi_{global}$ → lower NOx

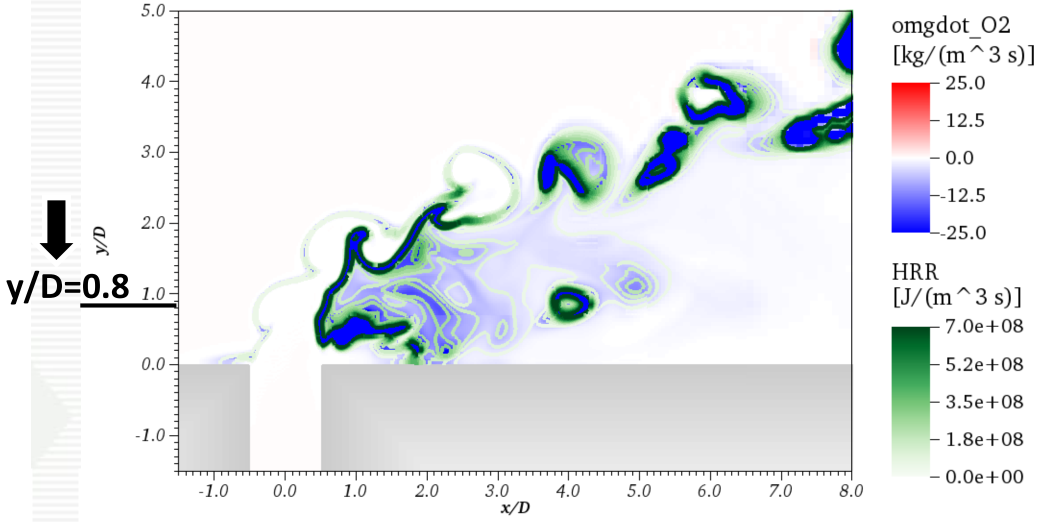
**NOx benefit from RJICF observed for high $\phi_{global}$**

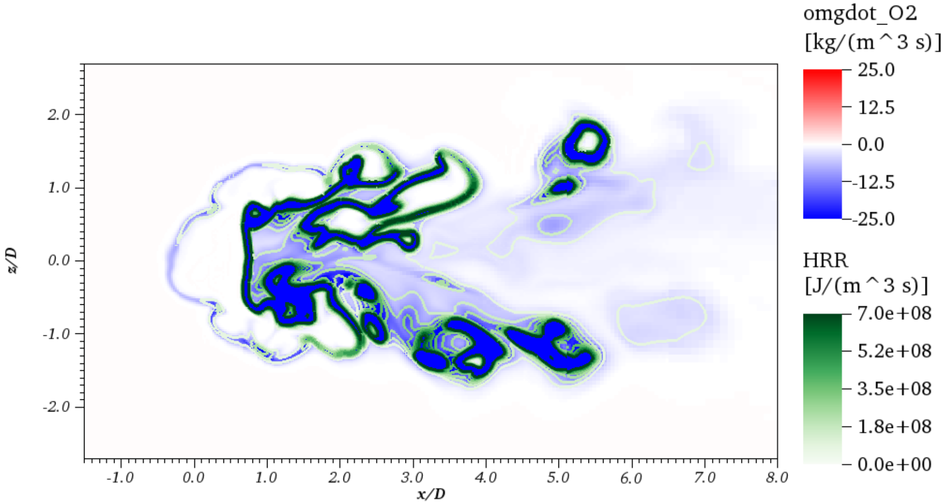
# SIMULATION: ATTACHED VS LEE-STABILIZED

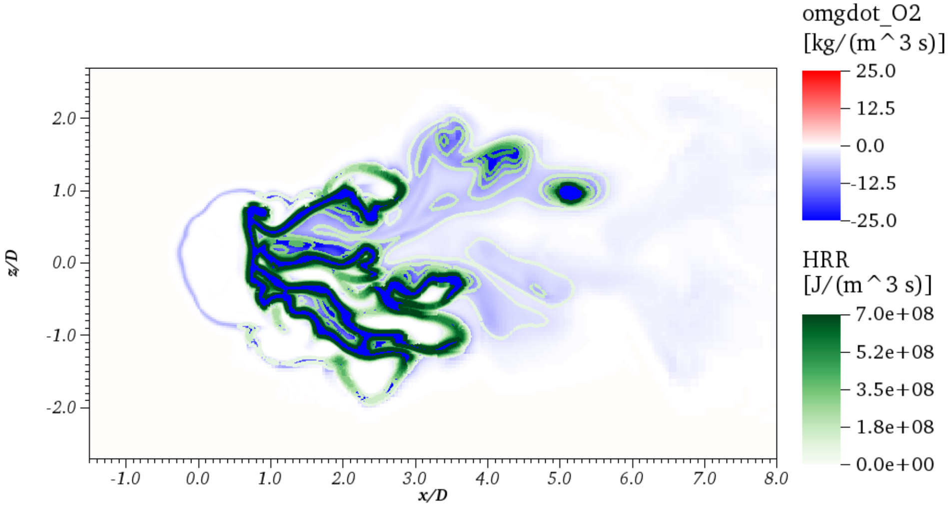
Attached

Lee-Stabilized



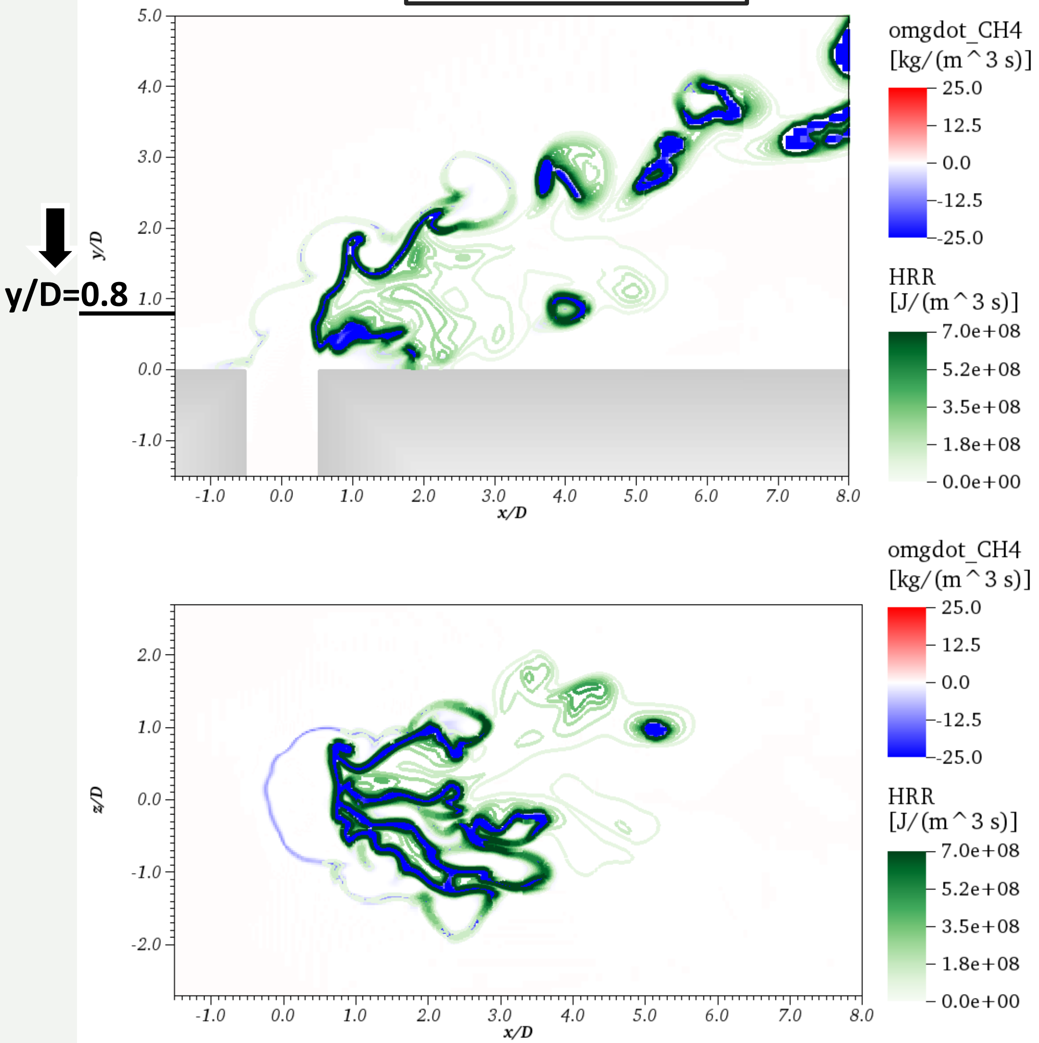



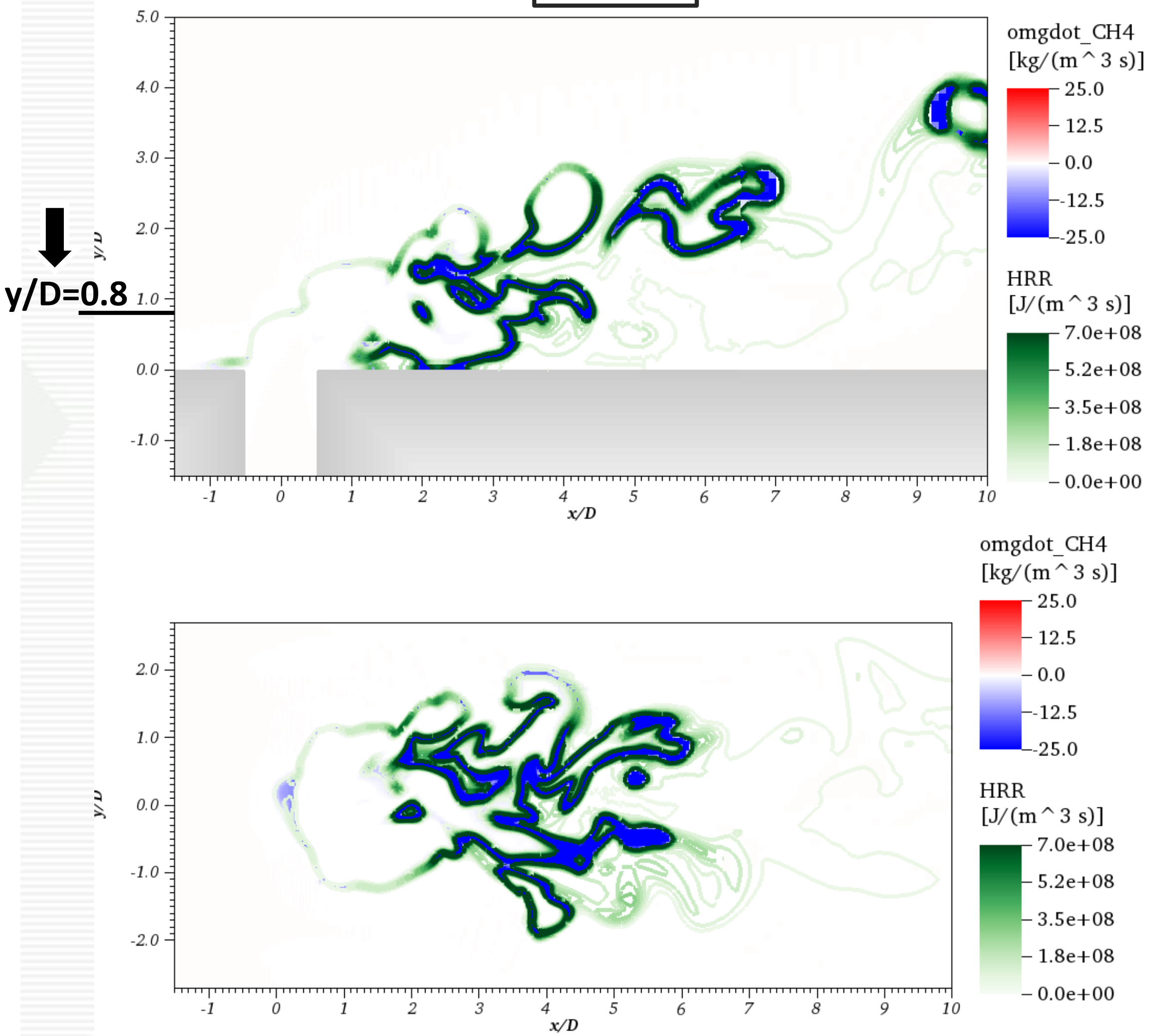



# SIMULATION: LEE-STABILIZED VS LIFTED

**Lee-Stabilized**




**Lifted**



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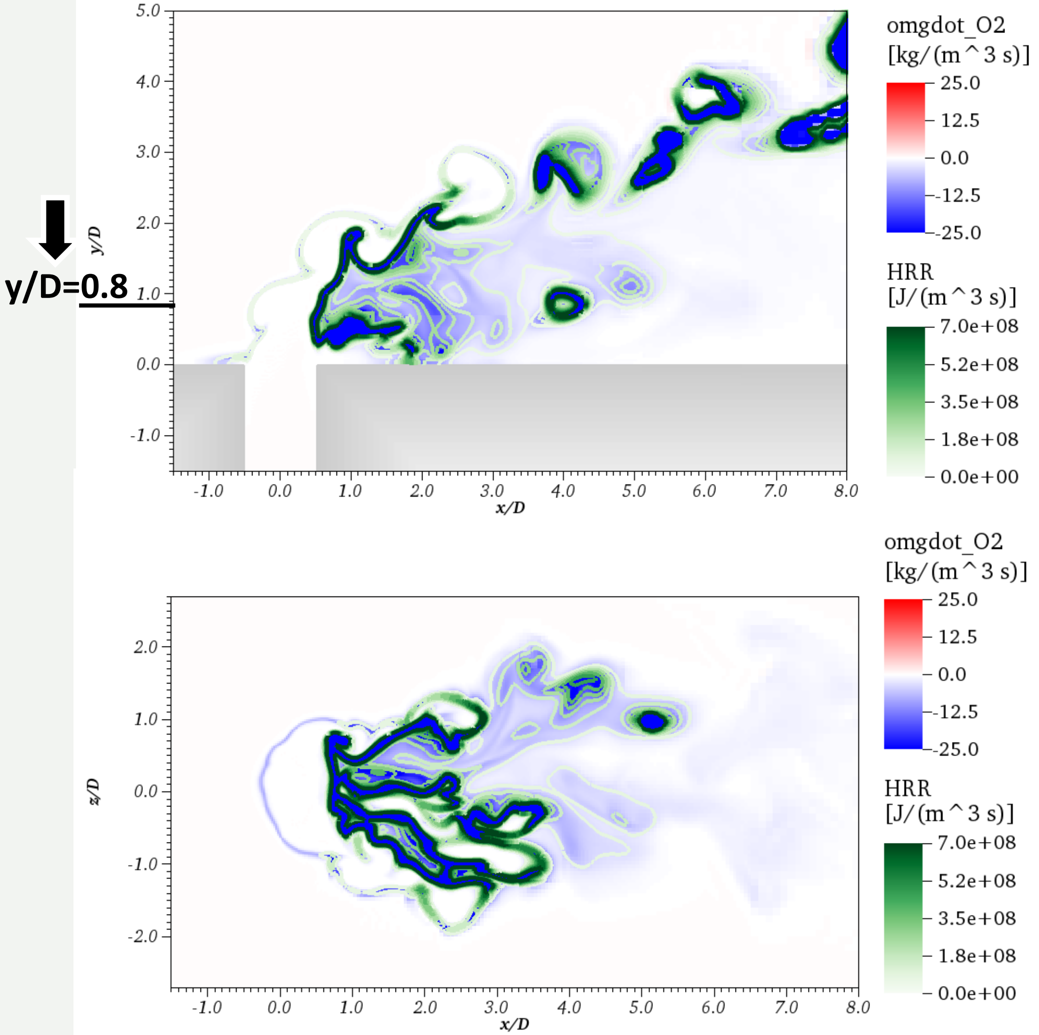
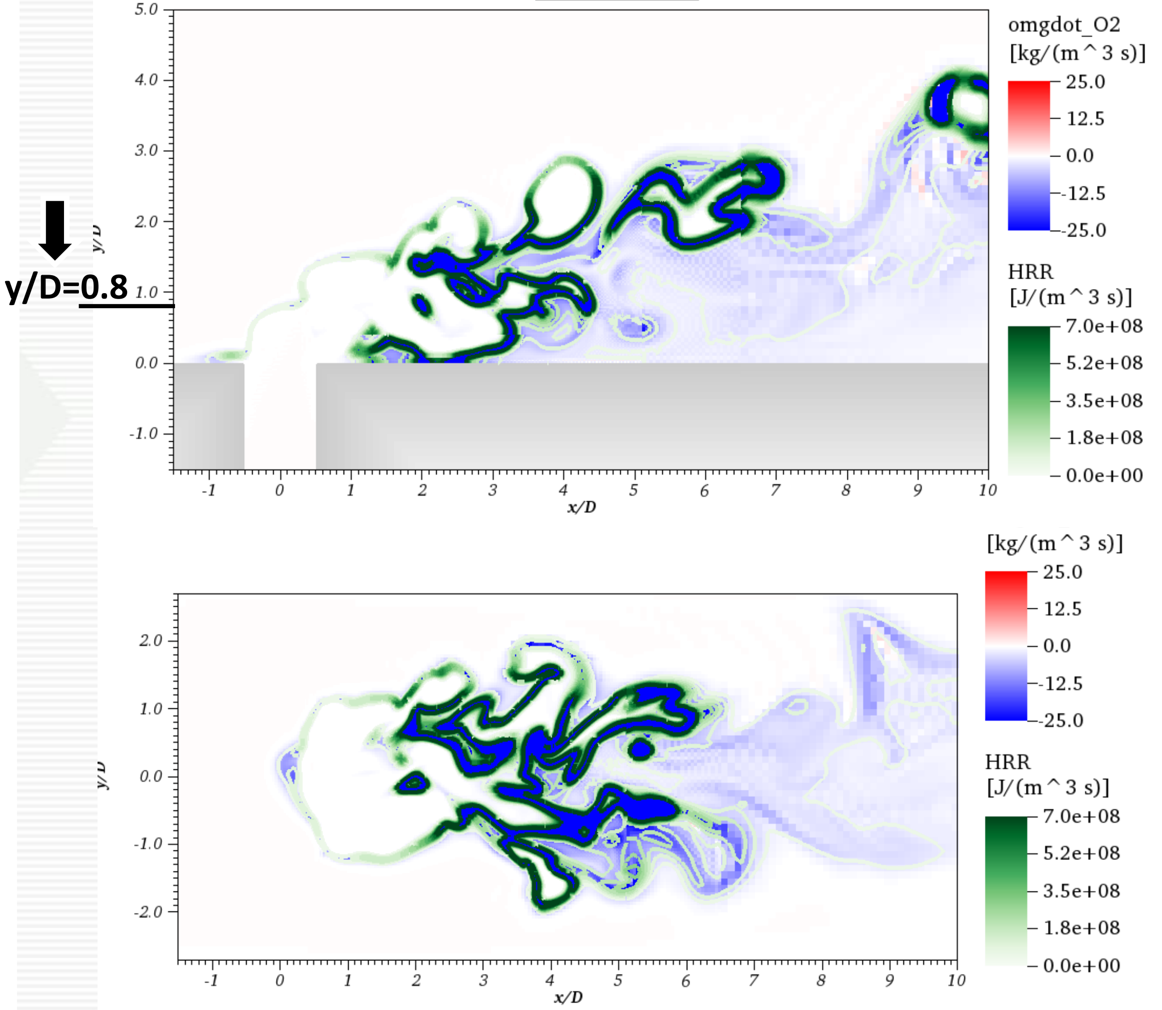
Lee-Stabilized




Lifted



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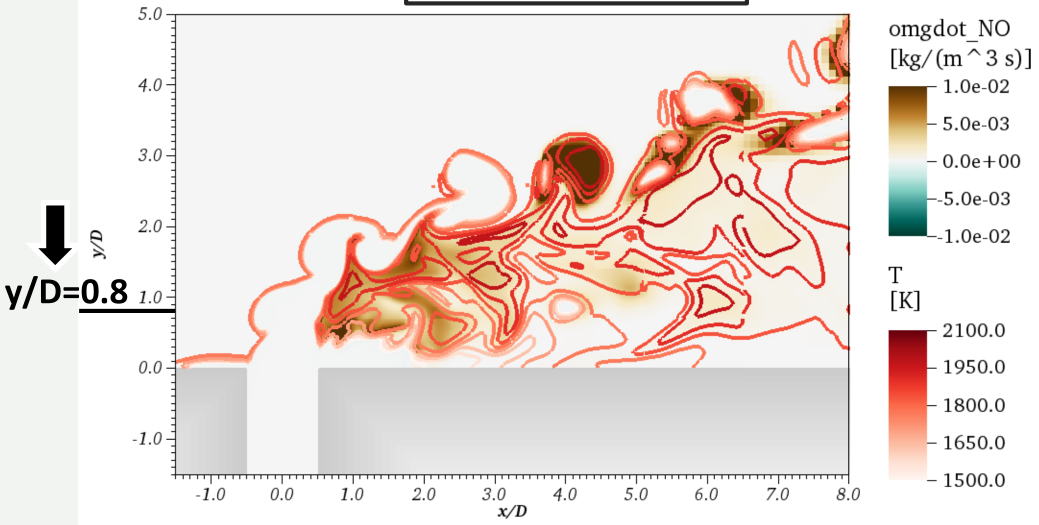
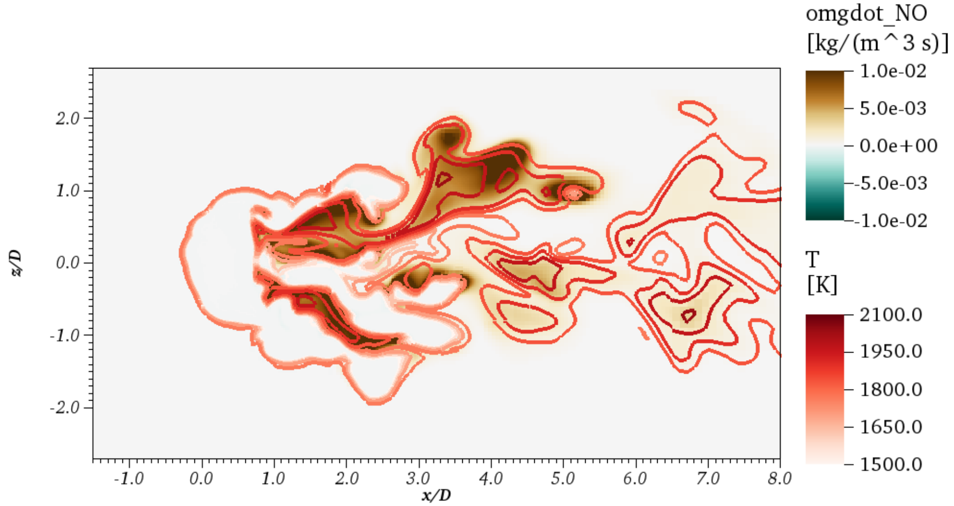
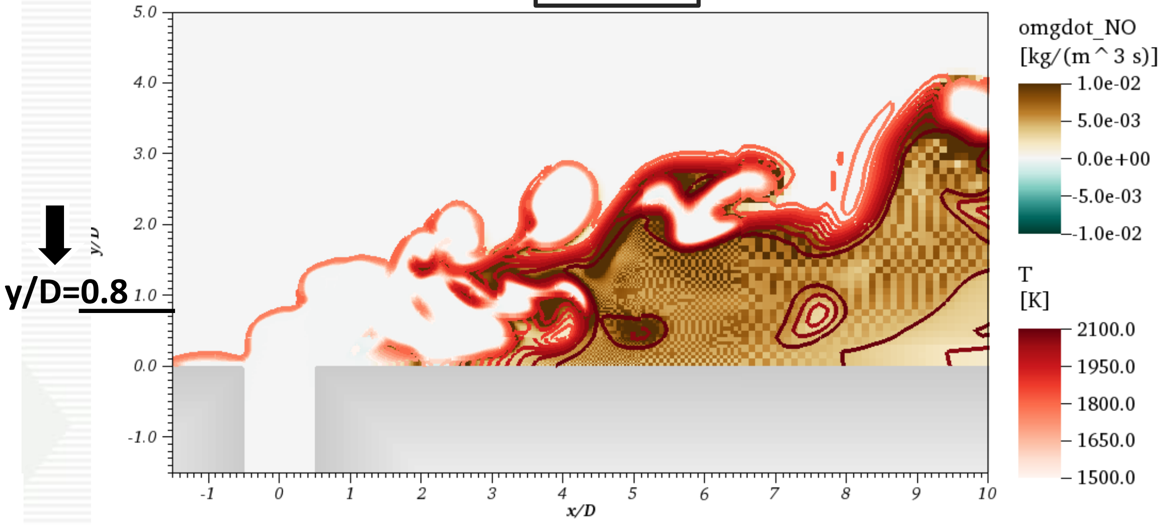
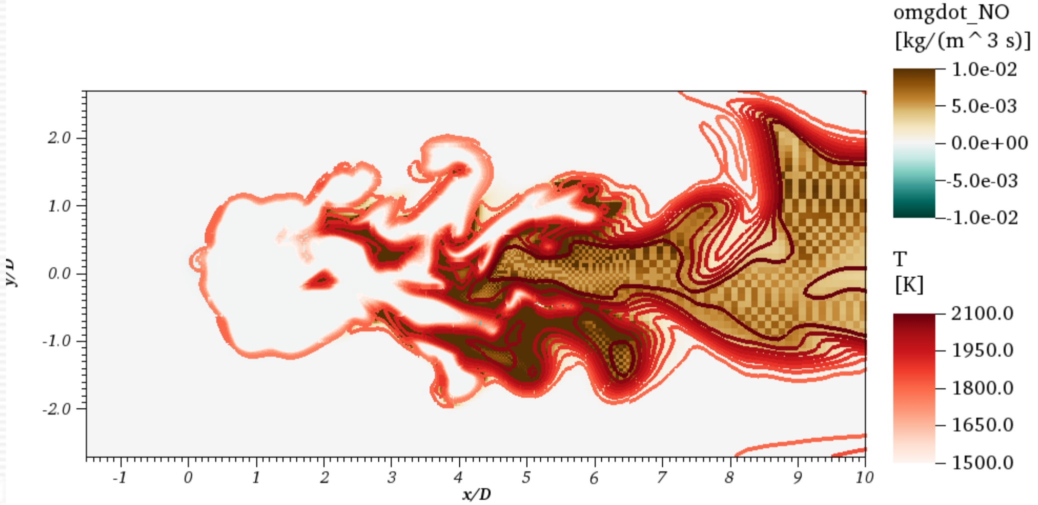
Lee-Stabilized



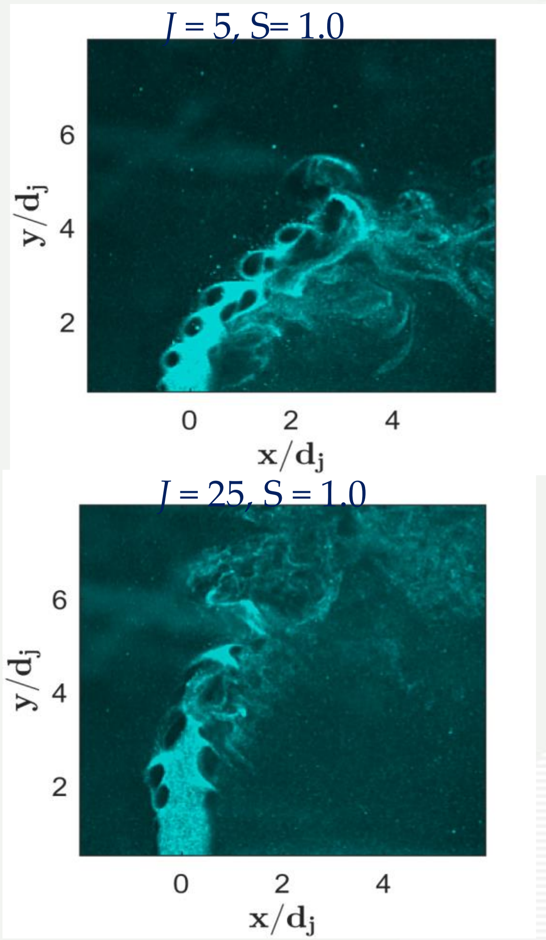

Lifted



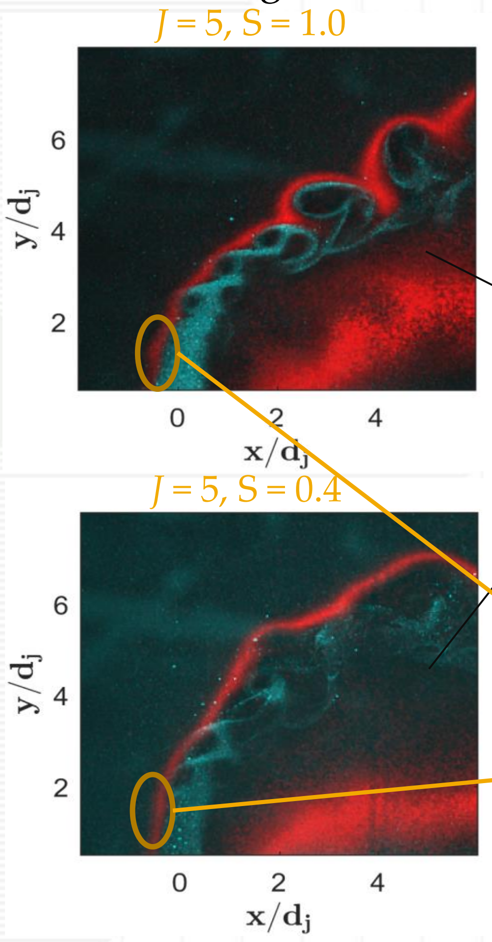



# FLAME IMPACT ON SHEAR-LAYER VORTICES

Non-reacting cases




Reacting cases




Reacting cases which should show globally unstable behavior based on *S* and *J* show convectively unstable SLV structure

Suppressed SLV behavior

# FLAME IMPACT ON SHEAR-LAYER VORTICES

- Cases arranged according to decreasingly globally unstable behavior
- Between the non-reacting cases the convectively unstable case has a decreased growth rate
- Reacting cases show consistently suppressed SLV growth rate compared to non-reacting cases