High Temperature, Low NOx Combustor Concept

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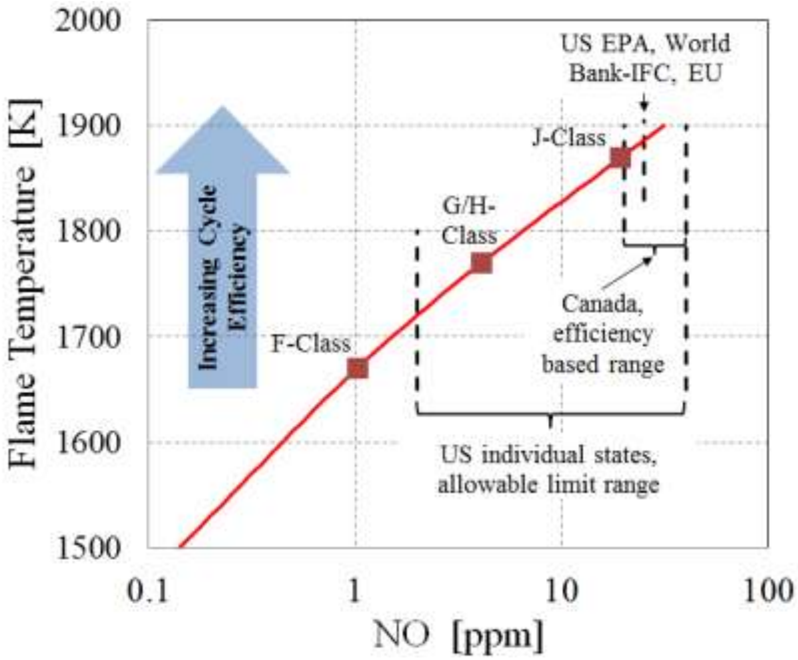
MOTIVATION

- Thermal efficiency has steadily increased from 47% to 62% over the past 3 decades
  - Driven by improvements in materials and cooling methods
  - Advanced combustion technologies enabled simultaneous reduction in NOx emissions
- Goal: combined cycle thermal efficiency of 65% (or 67%!!)
  - New challenge: low NOx at elevated temperatures
- Current architectures can't meet current emissions standards at elevated $T_{\text{Turb Inlet}}$ (thermal NOx challenge)



New combustor paradigm is required to meet goal

PROPOSED APPROACH

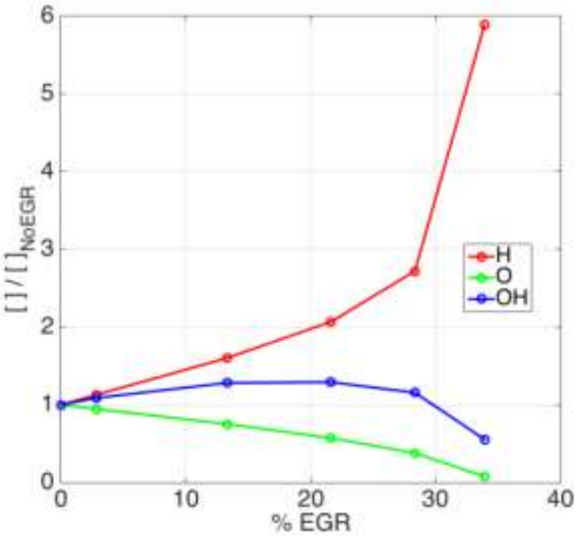
- Thermal NO formation dependent temperature, residence time, and O radical concentration

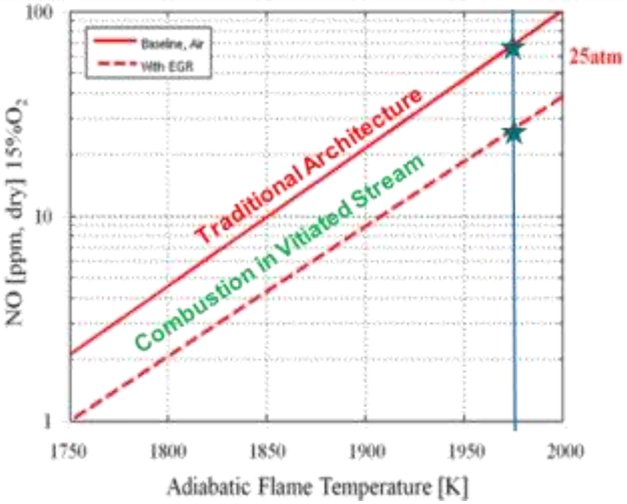
  $O + N_2 \Leftrightarrow NO + N$

  $[NO] \propto [O][N_2]e^{-38{,}379/T}\tau_{res}$

- Approach
  - Reduce residence time @ high temperatures
  - Incorporate advantages of EGR (reduce [O])

$\Rightarrow$ Optimization of staged injection





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?

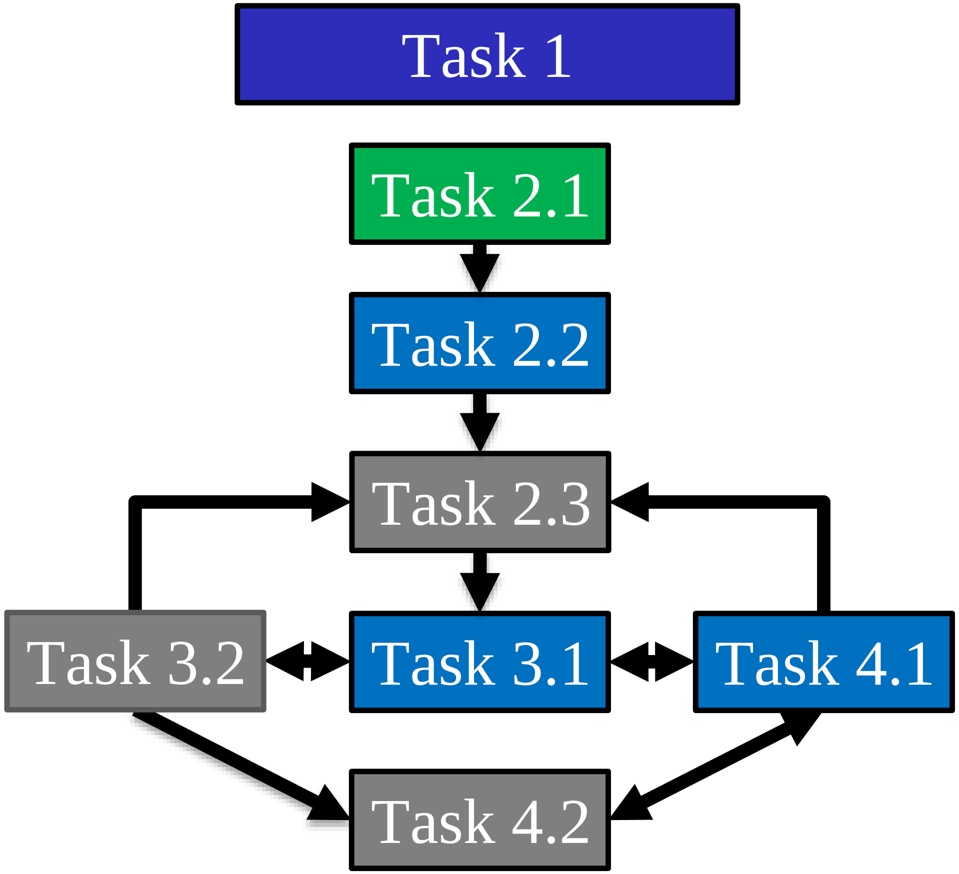
(2) What do the actual fuel and air distribution patterns look like that attempt to achieve these theoretical values?

- 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?

PROPOSED WORK

- 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		Interdep.	Quarter					Participants
Task-1			1	2	3	4	5	
1.1	Project Management and Planning		🟥	🟥	🟥	🟥	🟥	GTAE DOE Low-NOx Research Team
1.2	Reporting		🟥	🟥	🟥	🟥	🟥	
Milestones								
1 - 6	Semi-Annual Report			X		X		
7 - 9	Annual Report					X		
10	Final Report							
Task-2			1	2	3	4	5	
2.1	Fundamental Kinetic Studies		🟧	🟧				Prof. Seitzman Prof. German Edwin Goh
2.2	Initial NO Optimization Studies	2.1			🟧	🟧	🟧	
2.3	Constrained NO Optimization						🟧	
Milestones								
11	Reactor Model Readiness Review				X			
12	Theoretical NOx Limits							
Task-3			1	2	3	4	5	
3.1	Experimental Facility Development	2.2	🟩	🟩	🟩	🟩		Prof. Lieuwen Dr. Benjamin Emerson Matthew Sirignano Vedanth Nair
3.2	Initial Test Matrix & Facility Characteristics	2.1, 2.2					🟩	
Milestones								
14	Facility Design Review				X			
15	Test Article Preliminary Design Review			X				
16	Test Article Critical/Manufacturing Design Review				X			
17	Test Readiness Review					X		
Task-4			1	2	3	4	5	
4.1	LES studies for subcomponent geometry	2.3			🟦	🟦	🟦	Prof. Menon Dr. Benjamin Farcy Anant Girdhar
Milestones								
19	Prelim LES Results Review							

TASK 2: KINETIC AND OPTIMIZATION STUDIES

TASK 2: NOX OPTIMIZATION STUDIES

- Primary focus of first year optimization effort has been aimed at answering the first key research question:
  - 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?

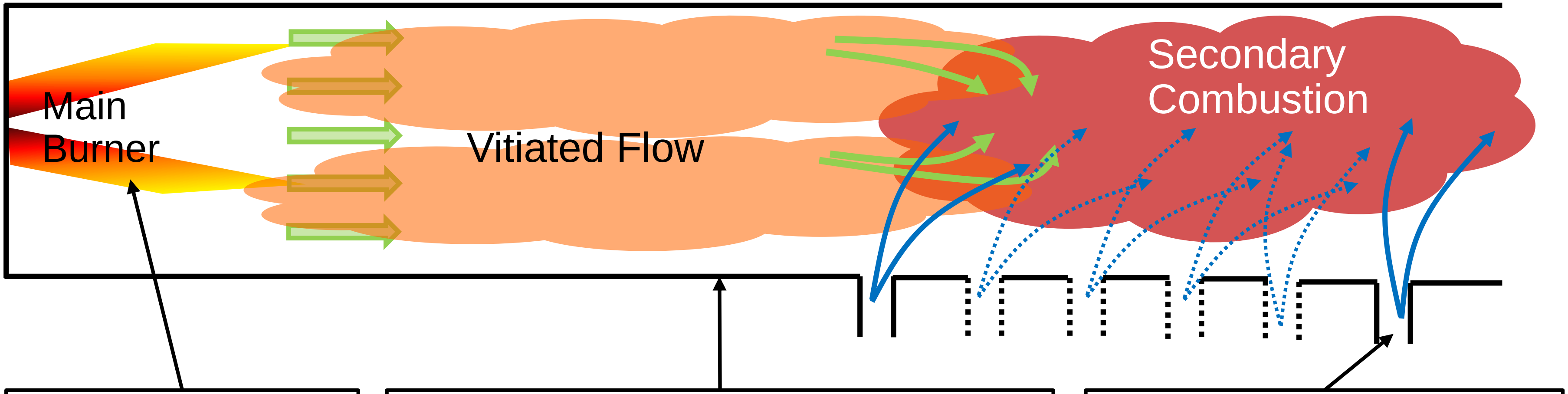
OPTIMIZATION TOOLKIT

- Developed optimizer-compatible software in MATLAB to expedite simulations and facilitate optimization
  - MATLAB chosen due to availability of optimization libraries (both built-in and in-house)

1. Enables users to easily construct various combustor configurations
2. Provides optimizers with a function to perform optimization studies
3. Utilizes batch reactors to provide precise temporal control of injection
4. Native parallel computing: allows for large parameter sweeps—helps with parameter space exploration
   - ➢More than 20,000 runs since development

OPTIMIZATION TOOLKIT—FEATURES

5. Allows for dynamic variation of combustor parameters for a given configuration. e.g.:



Main burner parameters:

- ϕ_{main} (⇔ main-secondary mass split)
- $T_{air,main}$
- $T_{fuel,main}$

Global configuration/parameters:

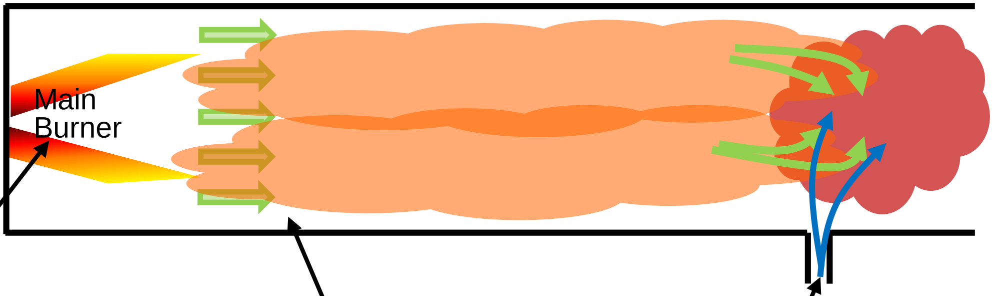
- $\phi_{global} \Leftrightarrow T_{exit}$
- τ_{global}
- P
- n (number of secondary injectors)
- Mass split between main burner and secondary injectors

For each injector:

- $\chi_{(fuel,air,steam,etc.)}$
- T_{inlet}
- τ_{sec} → residence time post-injection

2. OPTIMIZATION STUDY—SETUP

- Goal: For a given architecture, find minimum achievable NOx and corresponding configuration
- Architecture being studied:
  - Two-stage
  - Pure-fuel secondary injection
- Constants:
  - Fuel: CH_4
  - $T_{fuel} = 300K$
  - $T_{air} = 650K$
  - $\tau_{global} = 20\ ms$
  - $P = 25\ atm$
- Parameters varied:
  - ϕ_{global}
  - ϕ_{main}
  - τ_{sec}



Main burner parameters:

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Global configuration/parameters:

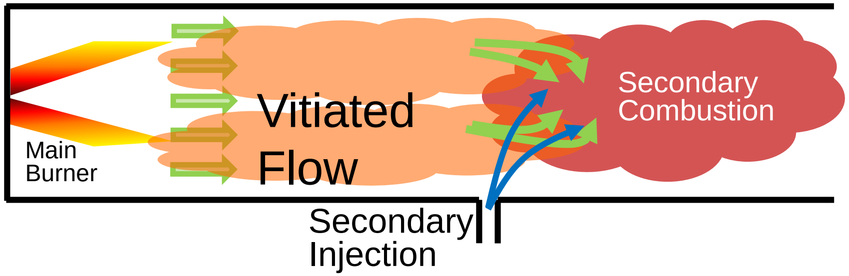
- $\phi_{global} \Leftrightarrow T_{exit}$
- τ_{global}
- P
- n(number of secondary injectors)
- Mass split between main burner and secondary injectors

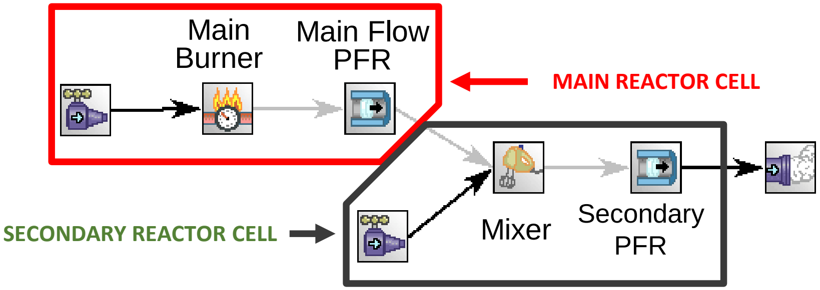
Secondary injector:

- $\chi(fuel)$
- T_{inlet}
- τ_{sec}

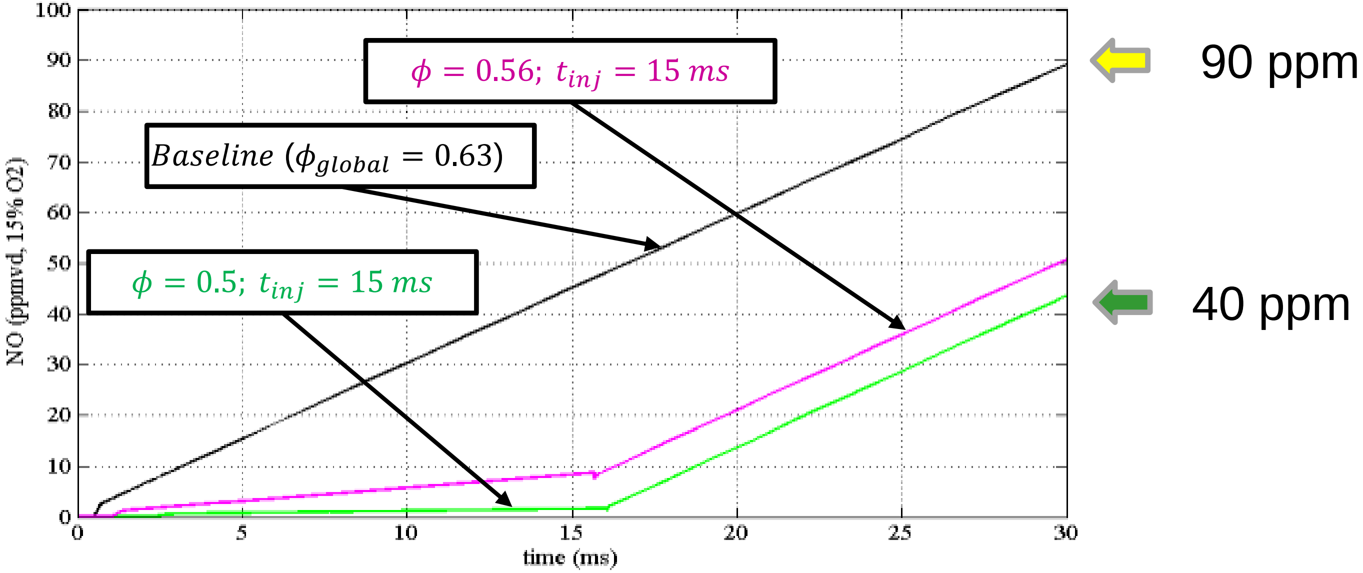
PRELIMINARY CALCULATIONS: STAGING IMPACT

- Initial calculations utilized reactor model for two-stage combustor architecture with pure-fuel injection at the secondary inlet



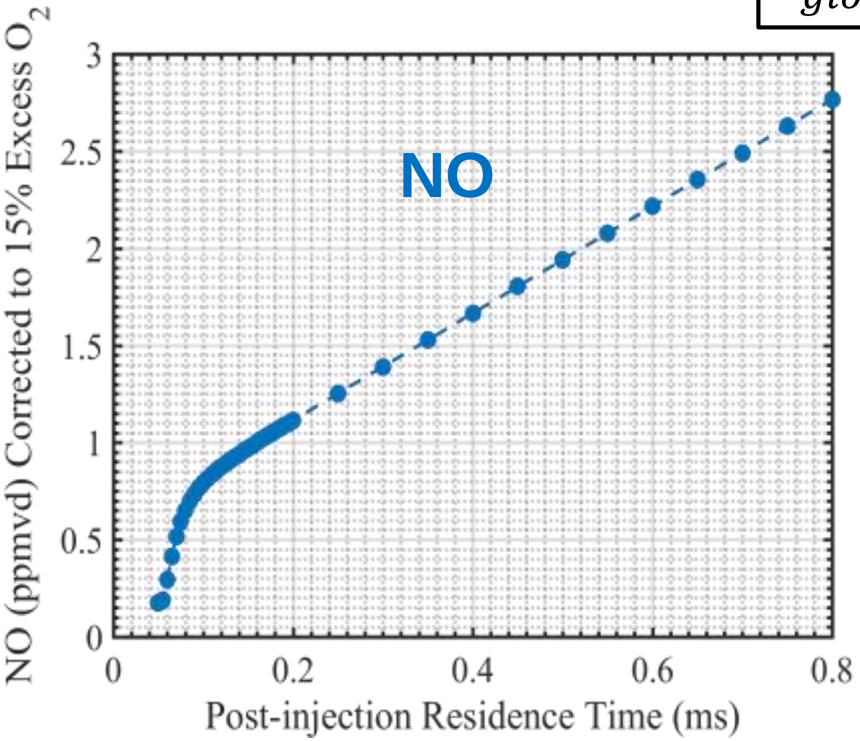


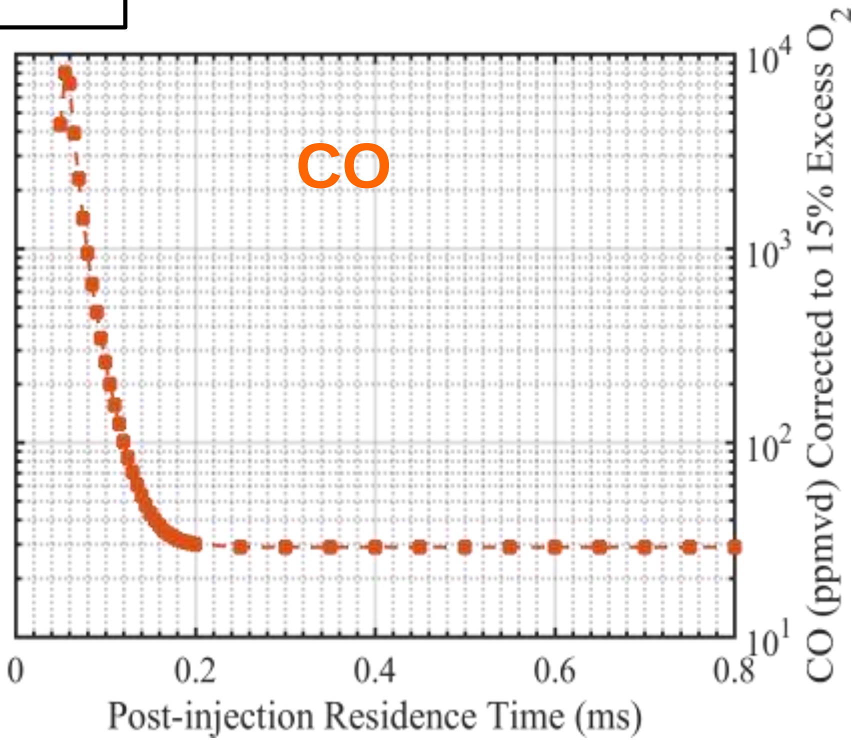
- Preliminary results showed that staging provided potential for significant NOx reduction vs. conventional architectures



2. OPTIMIZATION STUDY RESULTS—τ_{res} DEPENDENCE

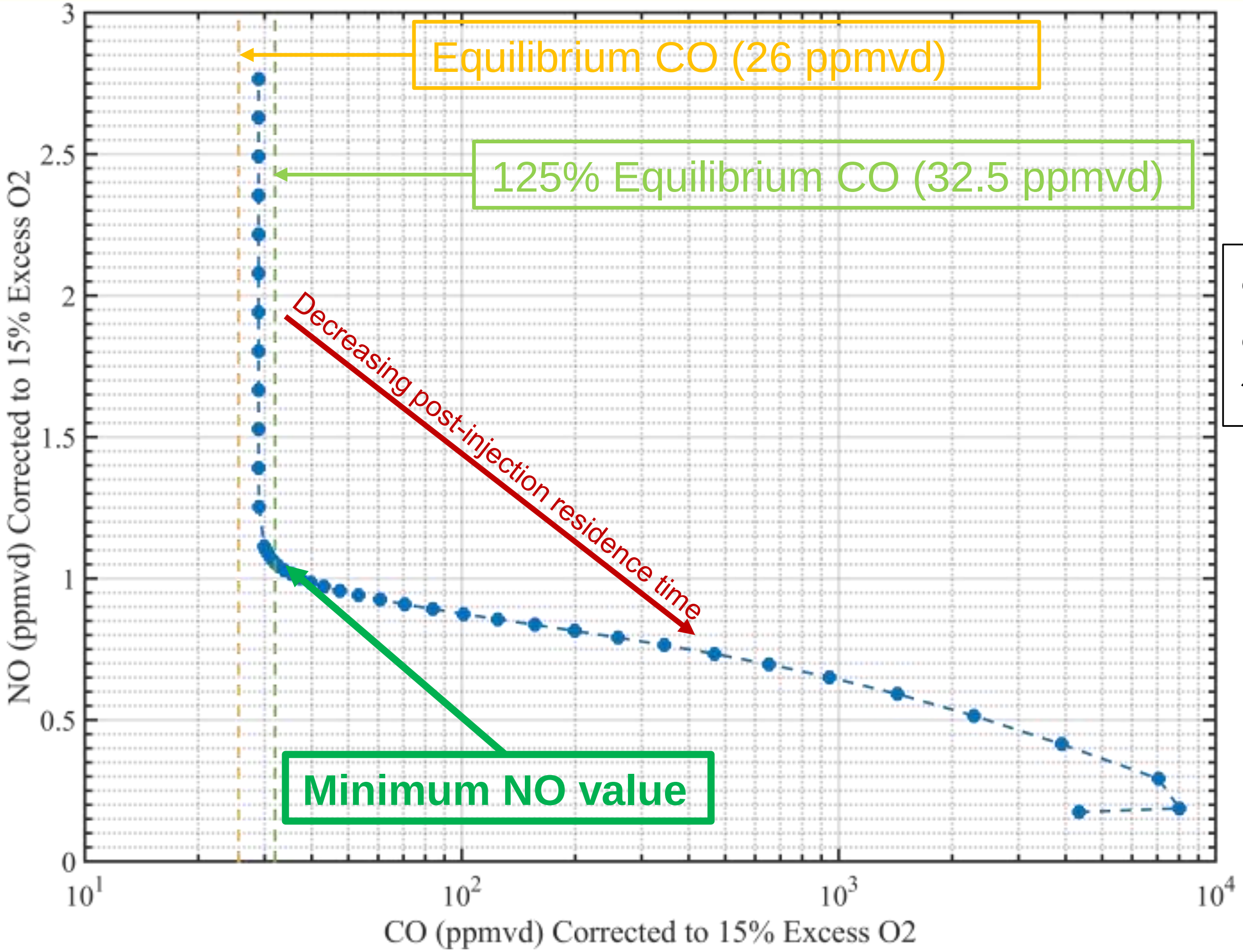
$$\phi_{global} = 0.64$$
$$\phi_{main} = 0.43$$
$$\tau_{global} = 20\ ms$$





Shorter secondary injection residence times ⇒ lower NO but limited by CO burnout

2. OPTIMIZATION STUDY RESULTS—τ_{res} DEPENDENCE



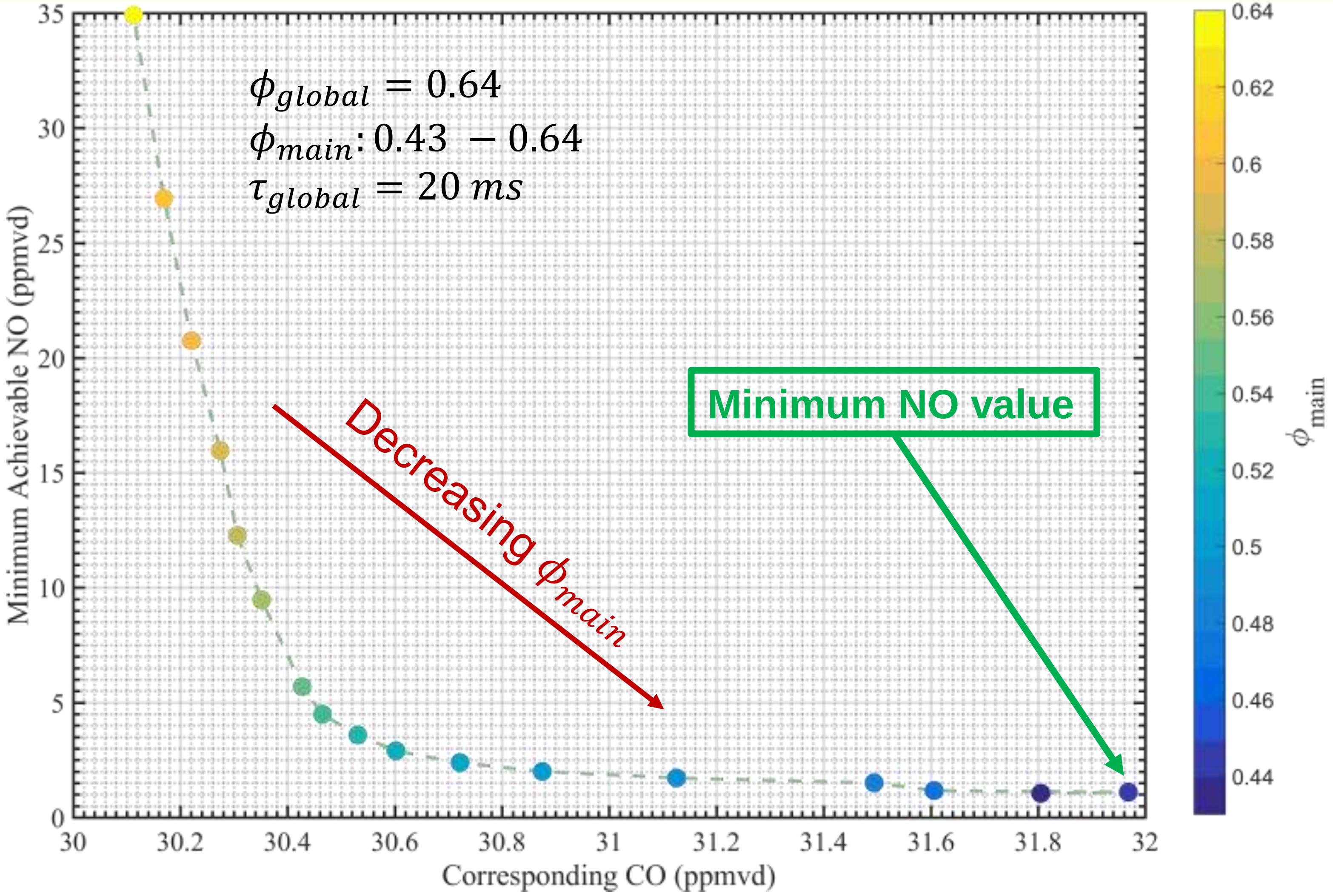
$\phi_{global} = 0.64$
$\phi_{main} = 0.43$
$\tau_{global} = 20ms$

Establish "optimum" secondary injection time O(100 μs) for minimum NO within CO constraint

2. OPTIMIZATION STUDY RESULTS—ϕ_{main} DEPENDENCE

For the same T_{exit}, repeat over multiple ϕ_{main} values…

2. OPTIMIZATION STUDY RESULTS—ϕ_{main} DEPENDENCE



$\phi_{global} = 0.64$
ϕ_{main}: 0.43 – 0.64
$\tau_{global} = 20\ ms$

Decreasing ϕ_{main}

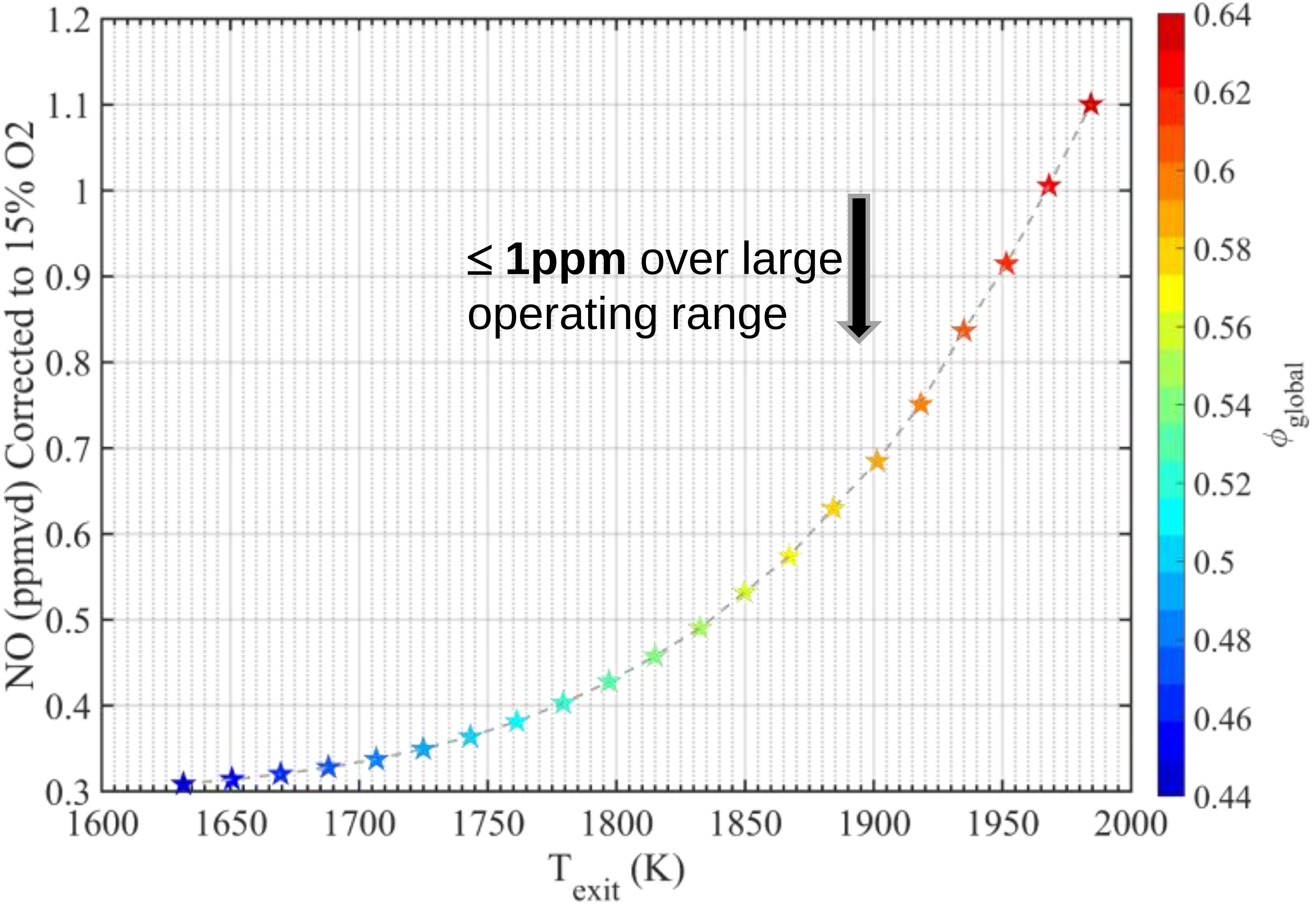
Minimum NO value

Lower ϕ_{main} improves NOx performance in staged combustion architecture

2. OPTIMIZATION STUDY RESULTS—ϕ_{main} DEPENDENCE

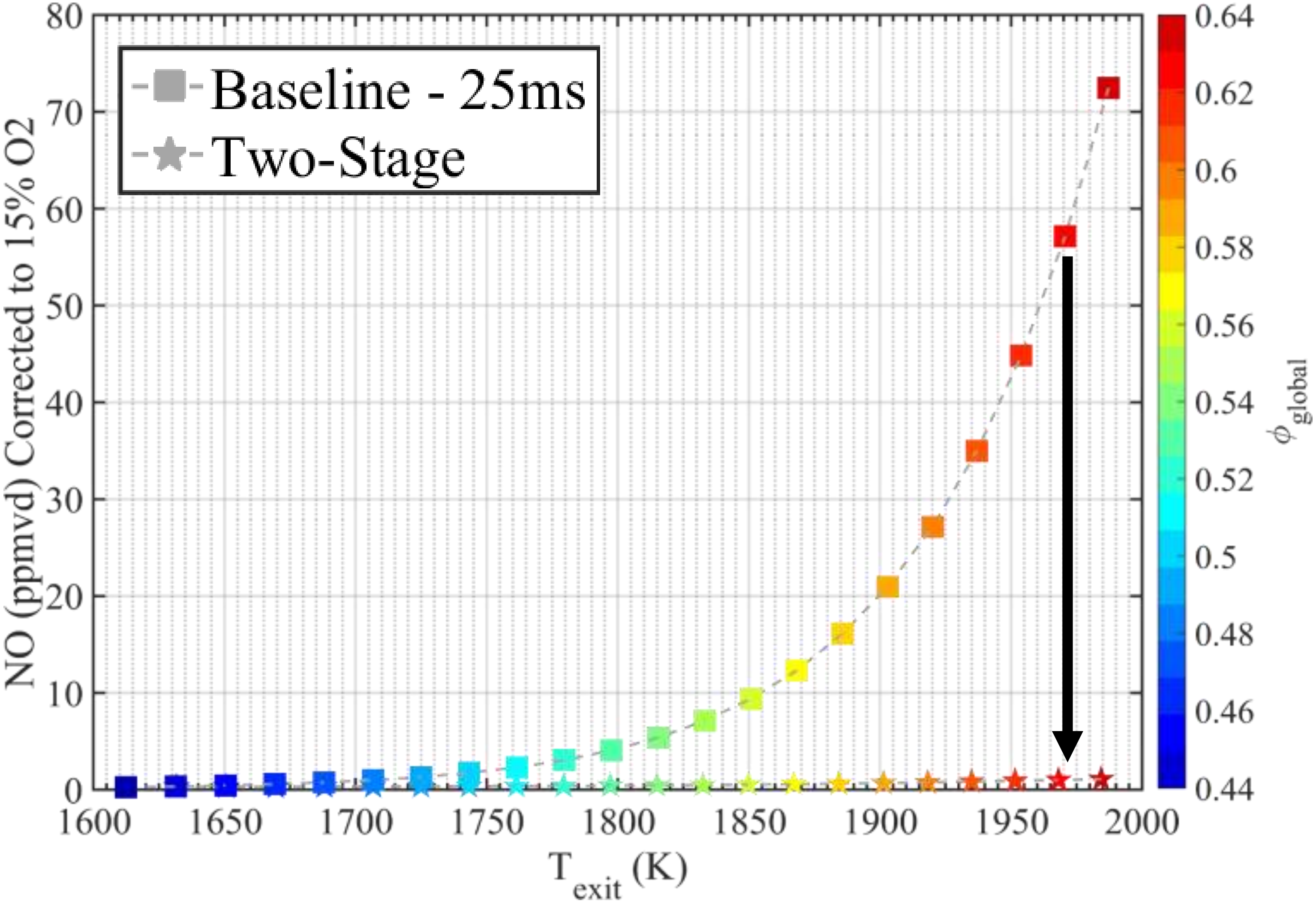
Repeat for multiple T_{exit}…

2. OPTIMIZATION STUDY RESULTS—STAGED VS. CONVENTIONAL



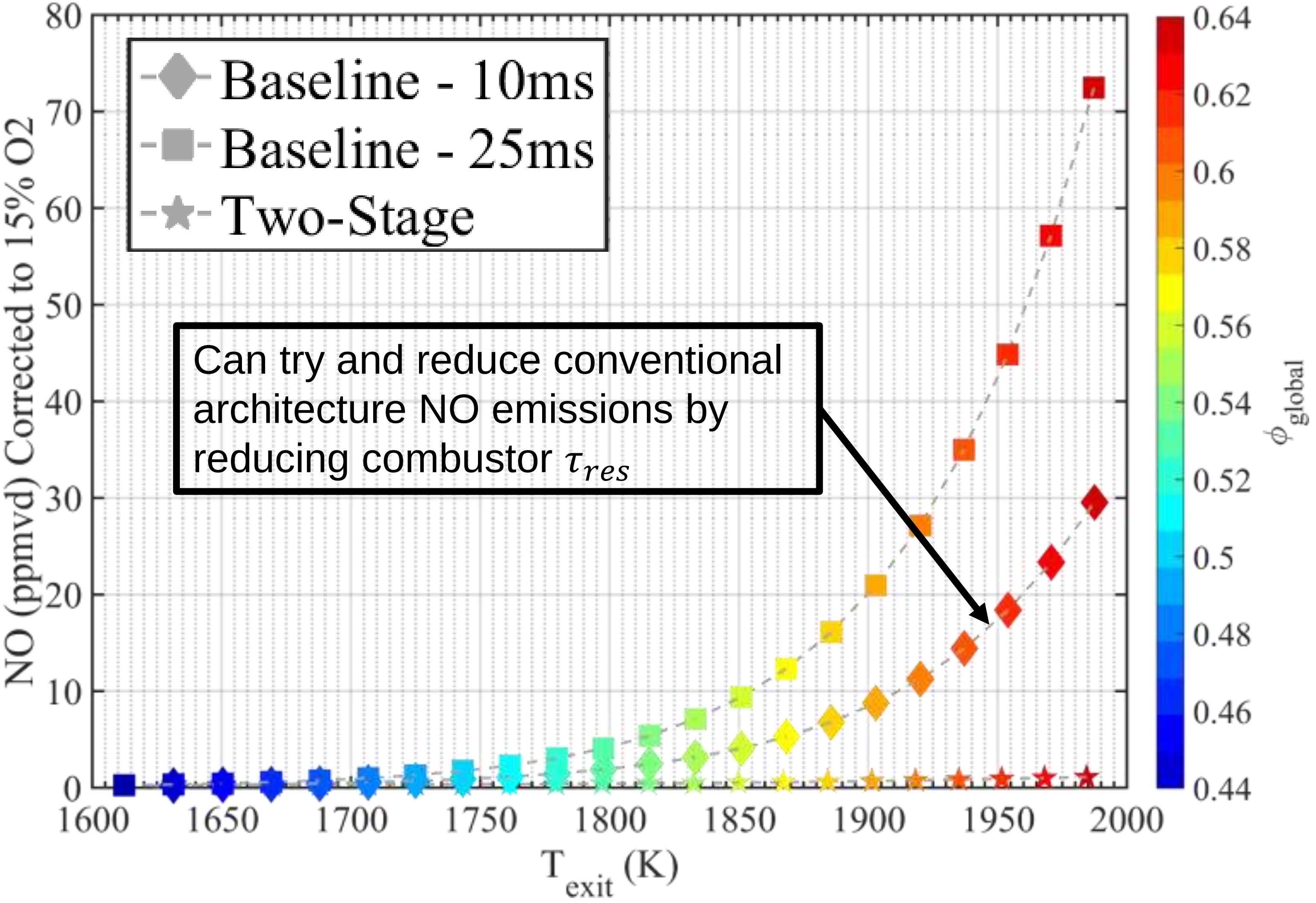
≤ **1ppm** over large operating range

2. OPTIMIZATION STUDY RESULTS—STAGED VS. CONVENTIONAL



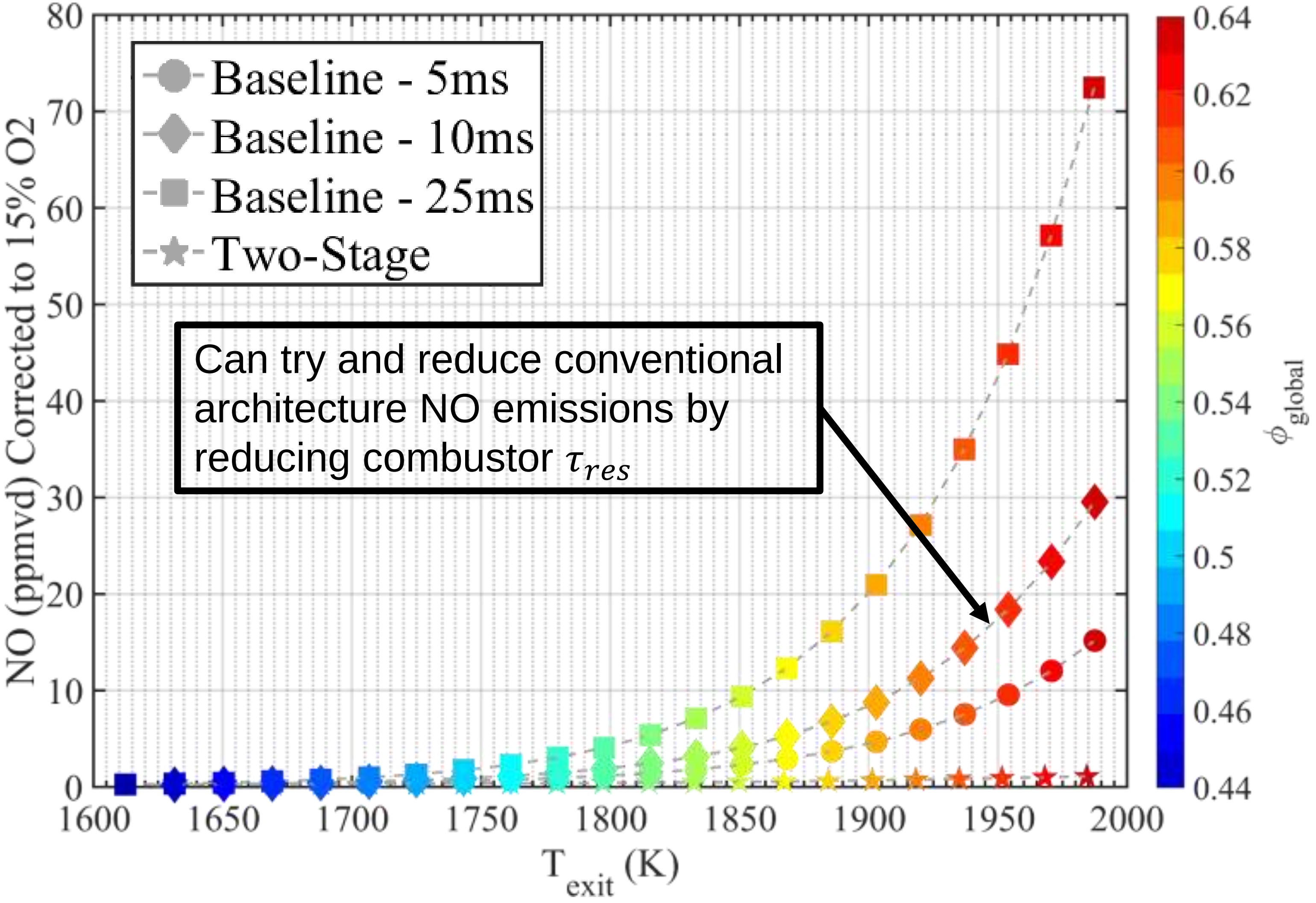
Under ideal conditions, staged combustion drastically reduces NO emissions at target $T_{exit} = 1975K$

2. OPTIMIZATION STUDY RESULTS—STAGED VS. CONVENTIONAL



Can try and reduce conventional architecture NO emissions by reducing combustor τ_{res}

2. OPTIMIZATION STUDY RESULTS—STAGED VS. CONVENTIONAL



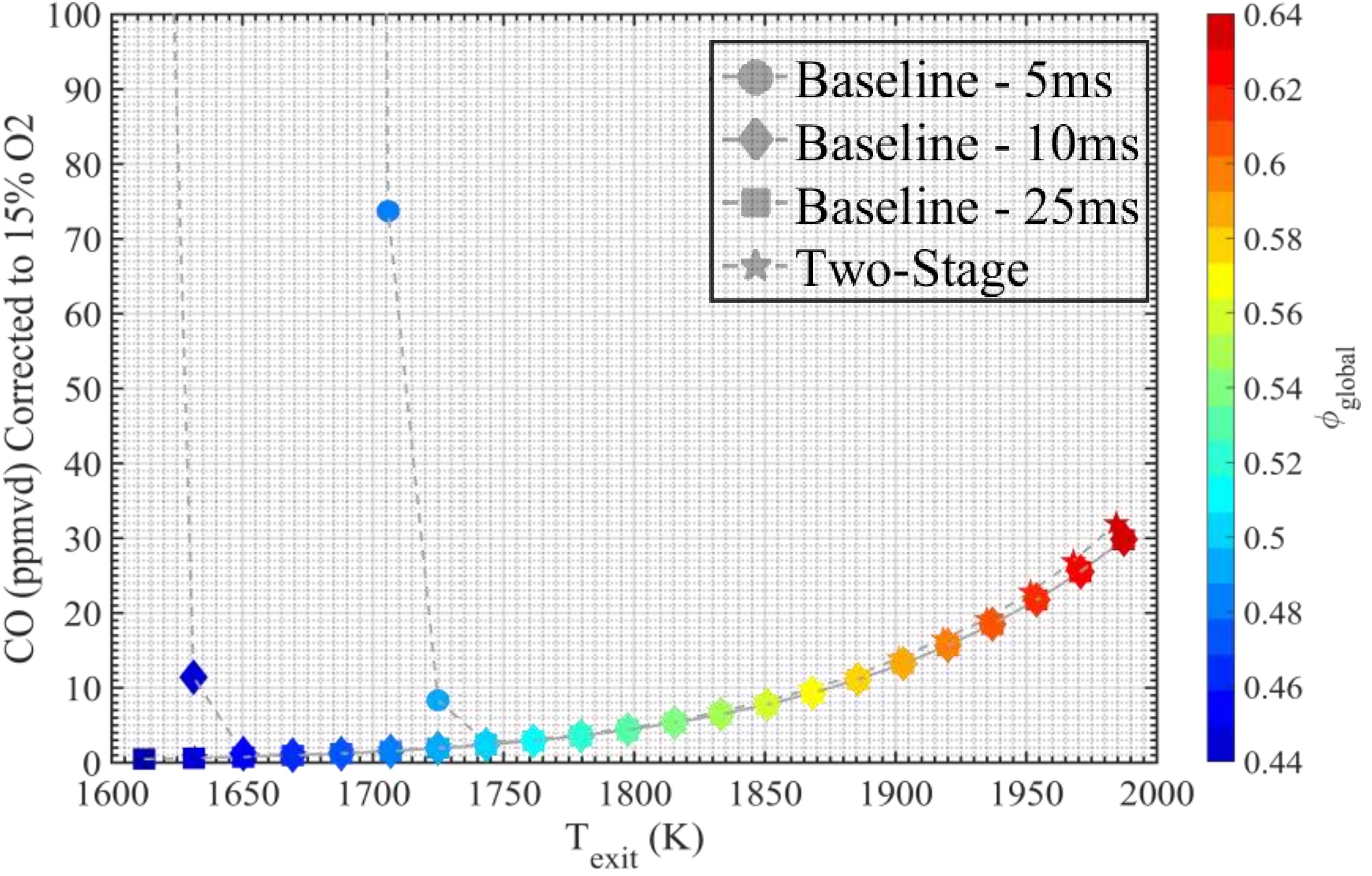
Can try and reduce conventional architecture NO emissions by reducing combustor τ_{res}

2. OPTIMIZATION STUDY RESULTS—STAGED VS. CONVENTIONAL

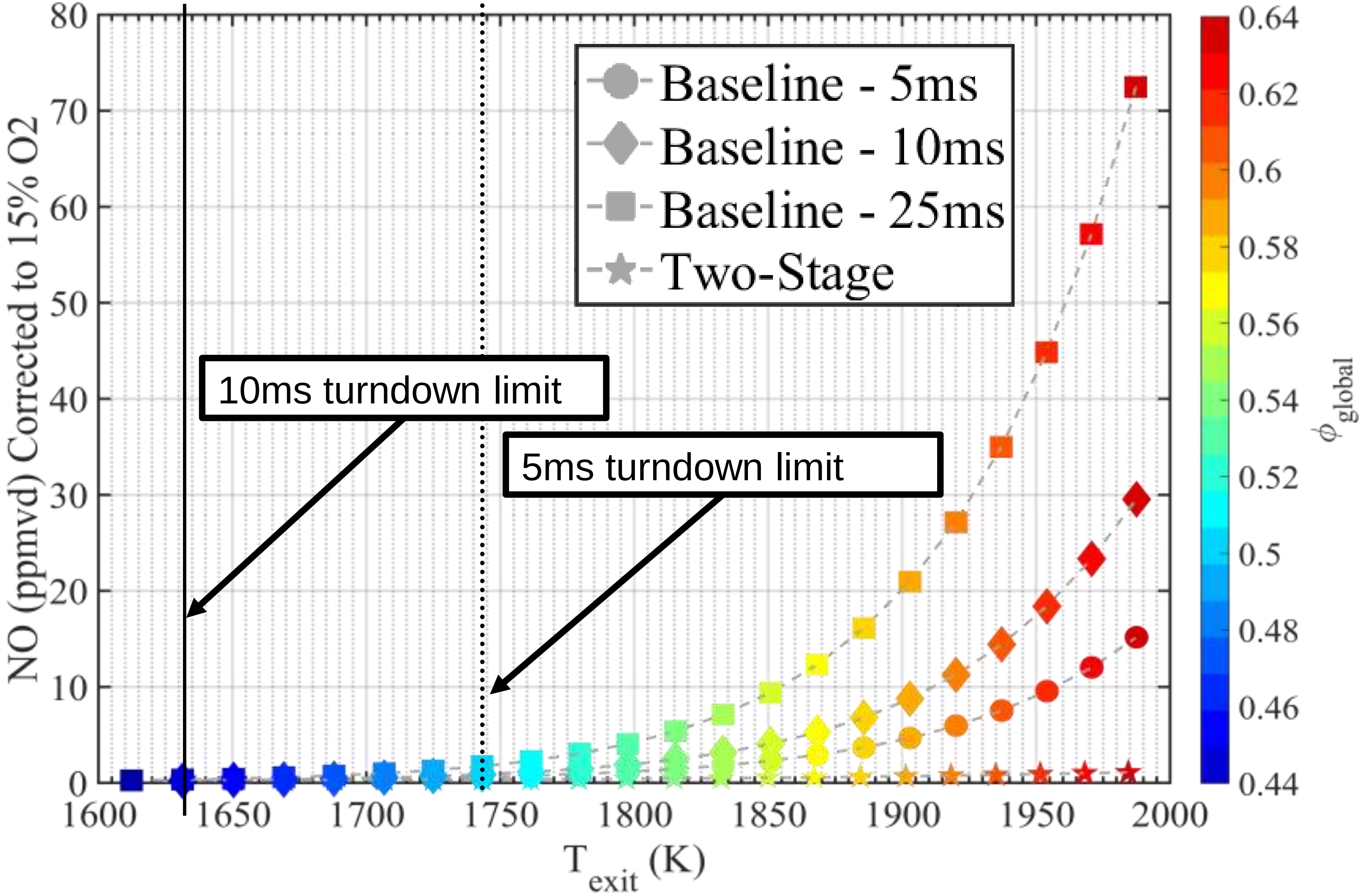
HOWEVER!

Observe variation in CO emissions levels with turndown…

2. OPTIMIZATION STUDY RESULTS—STAGED VS. CONVENTIONAL



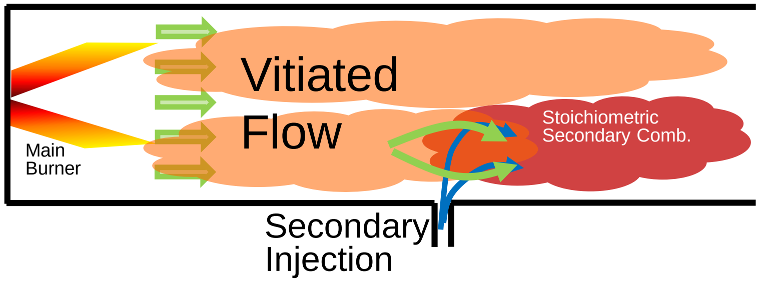
2. OPTIMIZATION STUDY RESULTS—STAGED VS. CONVENTIONAL



Based on CO constraints, staging provides better NOx AND turndown vs. reduced τ_{res}

PRELIMINARY CALCULATIONS: MIXING IMPACT

- Impact of non-infinite mixing was then investigated

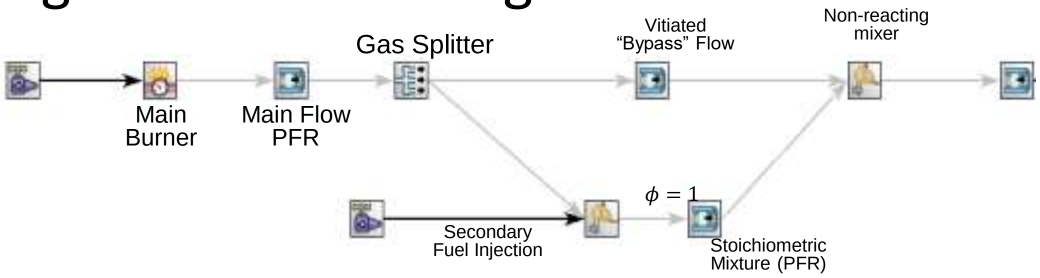


Vitiated Flow

Stoichiometric Secondary Comb.

Main Burner

Secondary Injection



Gas Splitter

Vitiated “Bypass” Flow

Non-reacting mixer

Main Burner

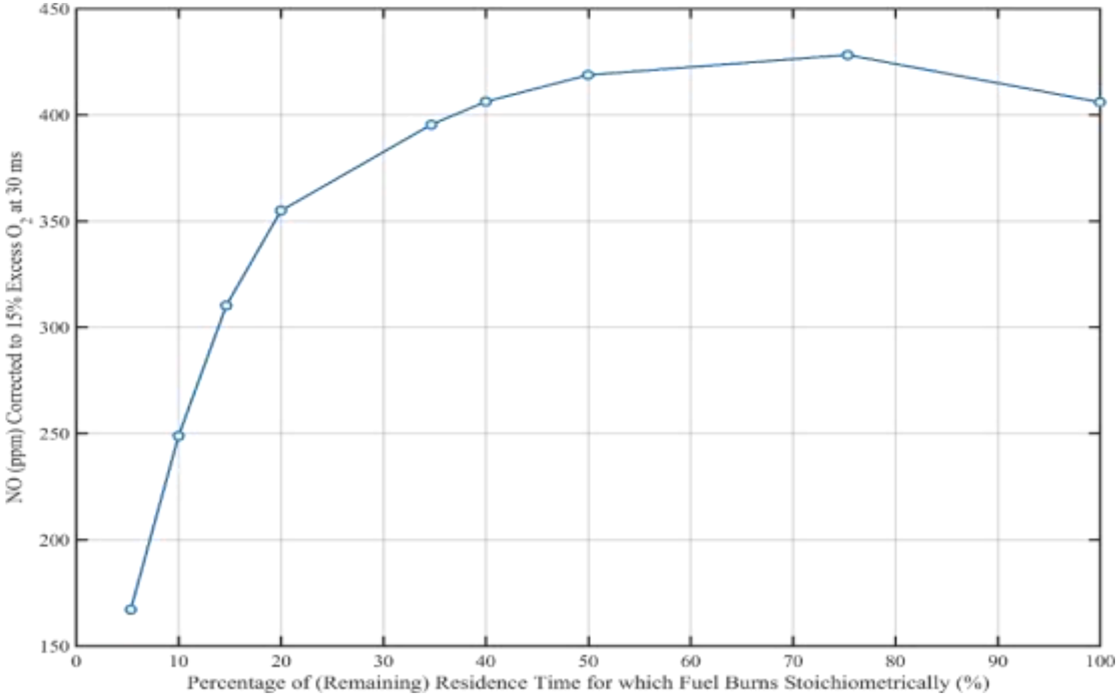
Main Flow PFR

$\phi = 1$

Secondary Fuel Injection

Stoichiometric Mixture (PFR)

- Poor mixing can negate the potential benefit of staged-combustion



MULTI-POINT INJECTION IMPACT

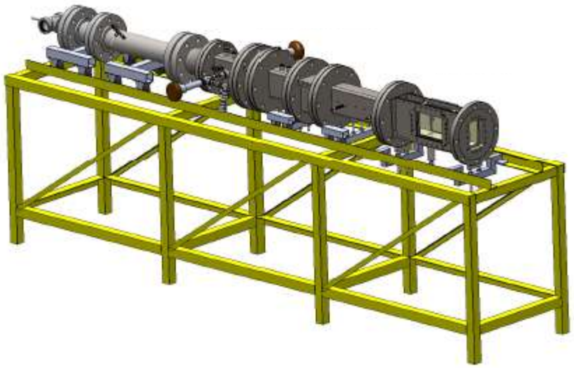
- Increased secondary injection points to two
- Investigated nine perturbations about base case
  - Base case: 1975K theoretical minimum configuration
  - Temporal displacement: 0.025, 0.05, & 0.1 ms about original secondary injector location
  - Secondary mass flow split: 75%-25%, 50%-50%, and 25%-75% between secondary injectors
- Results indicated that lower NOx could not be achieved over base case without increasing CO
  - Optimized base case ↔ max allowable CO

Single secondary stage gives theoretical NOx minimum

TASK 3: EXPERIMENTAL CHARACTERIZATION

TASK 3.1: FACILITY DEVELOPMENT

- Developed ulta-lean operation main burner
  - Tangential injection, high swirl concept
  - hardware complete and tested
- Highly modular test section injection system designed
  - Allow future testing of multi-point injection or novel injection configurations
- Exhaust quench section designed & fabricated
  - Freeze NOx chemistry and mix exhaust to facilitate emissions measurement
- Test rig installed
  - Air/fuel flow delivery and control system modified to meet program experimental needs



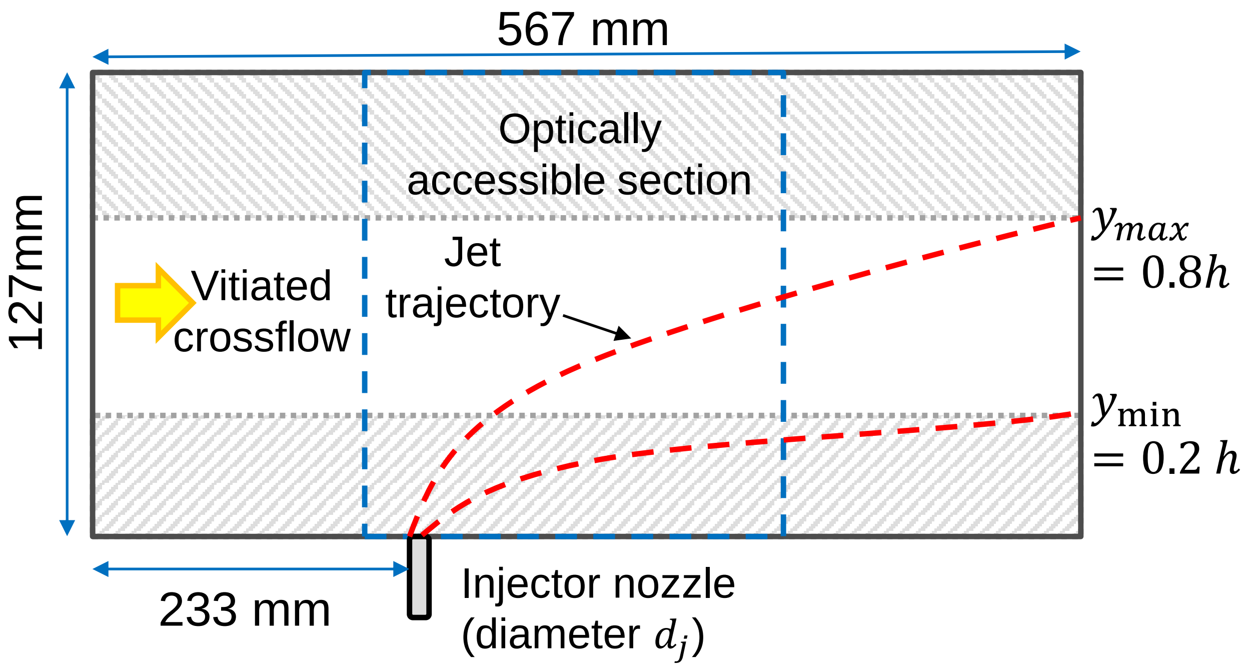
Facility characterization testing currently underway

TASK 3.2: INITIAL TEST MATRIX & FACILITY CHARACTERIZATION

TASK 3.2: INITIAL TEST MATRIX OBJECTIVE

- Initial test matrix to be single-point injection
- Goal of single-point test matrix is to establish relationship between ΔT & ΔNOx across test section
  - Want to decouple/investigate impact of specific jet trajectories → multiple injection diameters for ΔT
- Establish a performance baseline with which to compare impact of multi-point injection

TASK 3.2: TEST SECTION CONSTRAINTS



- Fuel split (ΔT) is constrained by jet trajectory
  - Set by height at end of test section
- Constraint lead to range of accessible momentum flux (J) ratios for each jet diameter (d_j) considered
- J & d_j -> range of achievable fuel splits -> ΔT's

TASK 3.2: FUEL ONLY TEST SPACE

	d_j= 1.5mm	d_j = 3mm	d_j = 4.5mm	d_j = 6 mm
J_{min}	18.6	4.6	2.07	1.16
J_{max}	193.97	48.49	21.55	12.12
$\phi_{global,min}$	0.52	0.55	0.58	0.60
$\phi_{global,max}$	0.58	0.66	0.74	0.82
ΔT_{min} (K)	10	37	121	174
ΔT_{max} (K)	136	277	400	510

Overlapping ranges of ΔT achievable

TASK 3.2: PREMIXED TEST SPACE

	d_j= 6mm	d_j = 9mm	d_j = 12mm
J_{min}	1	1	1
J_{max}	23.73	10.55	5.93
ΔT_{min} (K)	7	15	25
ΔT_{max} (K)	20	30	42

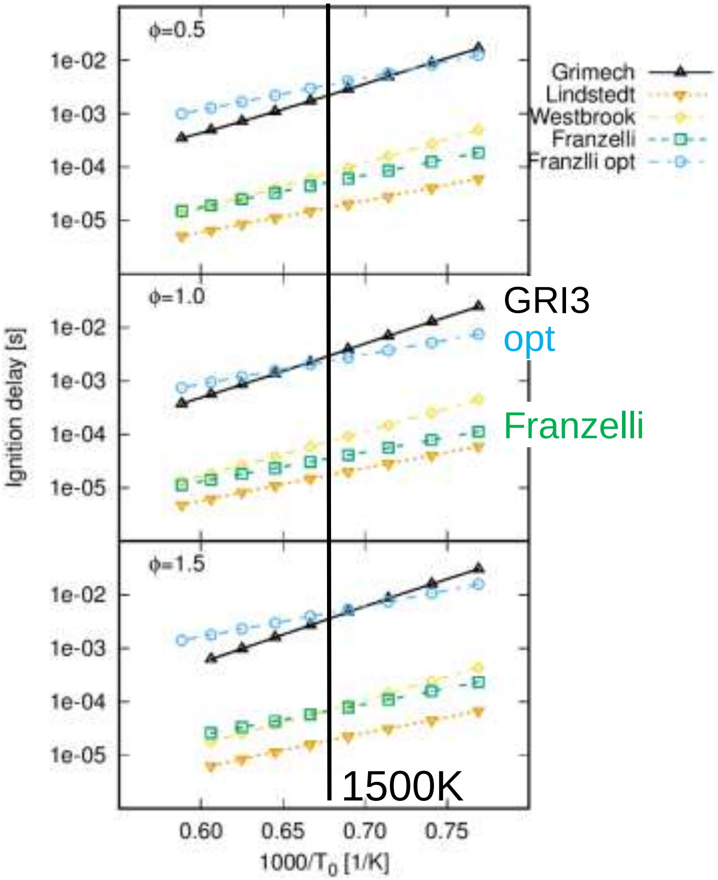
ΔT values based on secondary injection Φ = 0.95

- Maintain identical head end operation
- Secondary injection equivalence ratio to be varied to simulate degree of pre-ignition entrainment
- Lower achievable ΔT due to addition of air

TASK 4.1 LES STUDIES FOR SUBCOMPONENT GEOMETRY

LARGE EDDY SIMULATION PROGRESS

- Computational procedure has been validated using LES for reacting (Hydrogen) Jet In Cross Flow (JICF) configuration
  - LES of single reacting JICF [1] [2] using the Adaptive Mesh Refinement (AMR) [3] demonstrates cost effectiveness and accuracy.
- Developing adequate chemistry modeling to predict:
  - Flame characteristics (Ignition delay – Flame speed – Flame thickness)
  - Pollutant emissions (Thermal NOx – Prompt NOx)
  - Constrained to under 10 species & 5 reactions to enable parametric studies
- Modified Franzelli [4] two-step CH_4 mechanism to better match auto-igniton predicted by GRI 3.0



[1] W. L. Chan and M. Ihme, Large-Eddy Simulation of a Turbulent Reacting Jet in Crossflow, 8th US National Combustion Meeting (2013)
[2] A. M. Steinberg et al., Structure and stabilization of hydrogen jet flames in cross-flows, Proceedings of the Combustion Institute 34 (2013)
[3] B. Muralidaran and S. Menon. A conservative cutcell method with adaptive mesh refinement for large eddy simulation of compressible flows. 53rd AIAA Aerospace Sciences Meeting. (2015)
[4] Franzelli, B, et al. "Large eddy simulation of combustion instabilities in a lean partially premixed swirled flame." *Combustion and flame* 159.2 (2012): 621-637.

NOX CHEMICAL KINETICS

- Thermal NOx mechanism

$$\text{Extended Zeldovich mech} \left\{ \begin{array}{l} \text{Zeldovich mech} \left\{ \begin{array}{l} N_2 + O \rightarrow NO + N \\ N + O_2 \rightarrow NO + O \end{array} \right. \\ N + OH \rightarrow NO + H \end{array} \right.$$

  - Either by integrating it to an existing reduced methane chemistry that includes the O radical (and OH for extended mechanism).
  - Or by post processing a solution with a quasi steady state assumption for N and an equilibrium approach to determine the O radical concentration from O2.

- Prompt NOx are the result of reactions between N2 and the radicals within the flame (C, CH, CH2 ..). Its modeling implies the use of a detailed mechanism and might not be possible to integrate in design and parametric studies.

EXPLORATORY TEST CASE

Parameters of the current exploratory test case:

- The domain is a channel of section 127x74 mm and length 300 mm
- The vitiated co-flow from the equilibrium of methane/air mix at an equivalence ratio of 0.5 using GRI 3.0:

Vitiated co-flow

P [atm]	T unburnt [K]	Phi [-]	Tburnt [K]	U [m/s]
1	300	0.5	1478	10

- To design the jet injection the following constraints are considered:
  - Target equilibrium temperature is ~ 1975K
  - Jet momentum ratio keeping the trajectory of the jet between 25 and 75% of the channel height 300mm downstream

Jet parameters

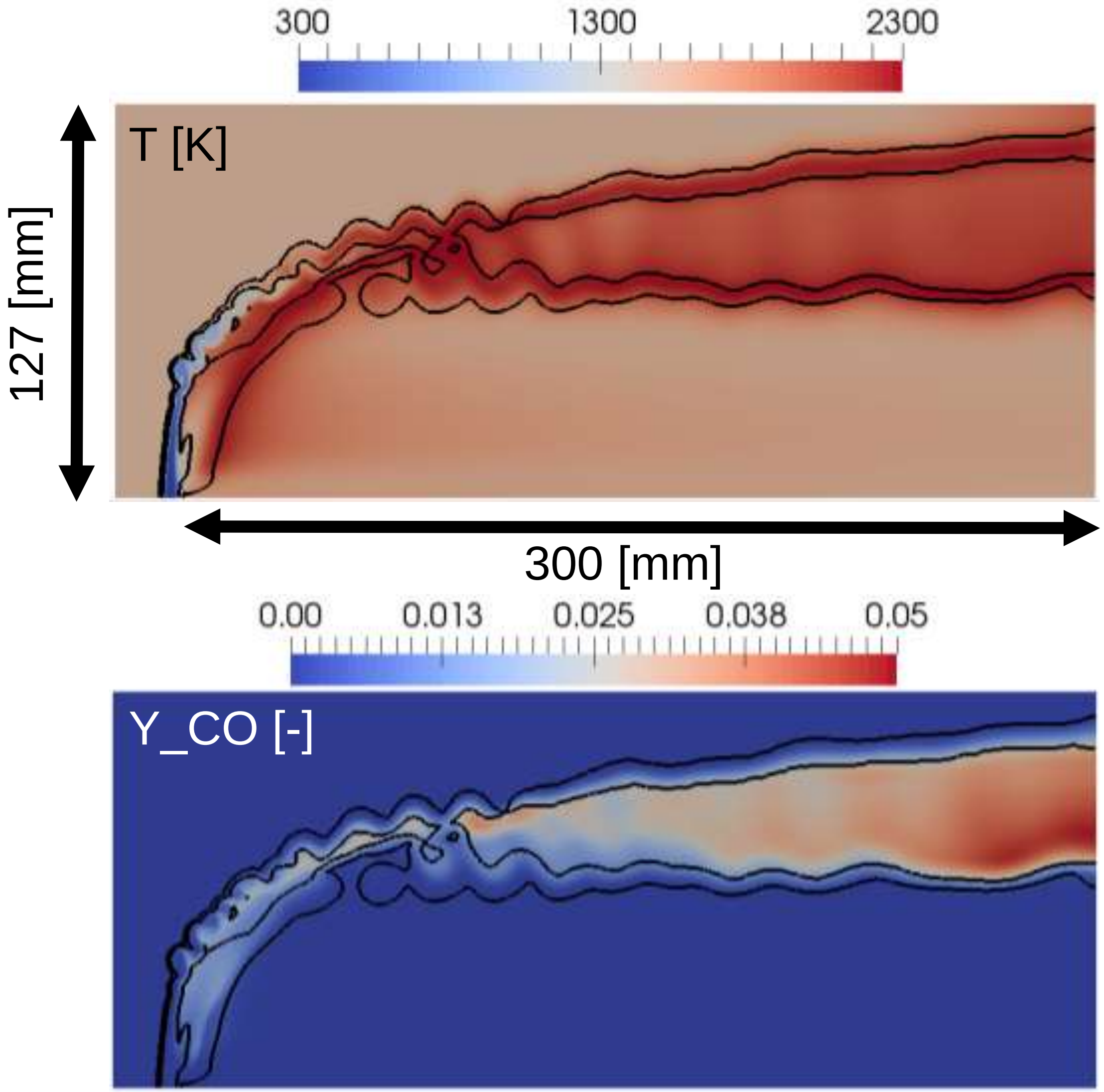
D_{jet} [mm]	T_{jet} [K]	U_{jet} [m/s]	Jet ratio	Projected height at 300 [mm]	Final T [K]
4	300	32.93	30	99	1904 [K]

EXPLORATORY TEST CASE

Current case:

- Baseline case without AMR.
  - 16 millions grid points
  - 12 points in the diameter and stretched grid in other directions.
- Isoline of CH4 consumption rate on a temperature and CO mass fraction field
- The jet evolves toward 75% of the channel height as expected.

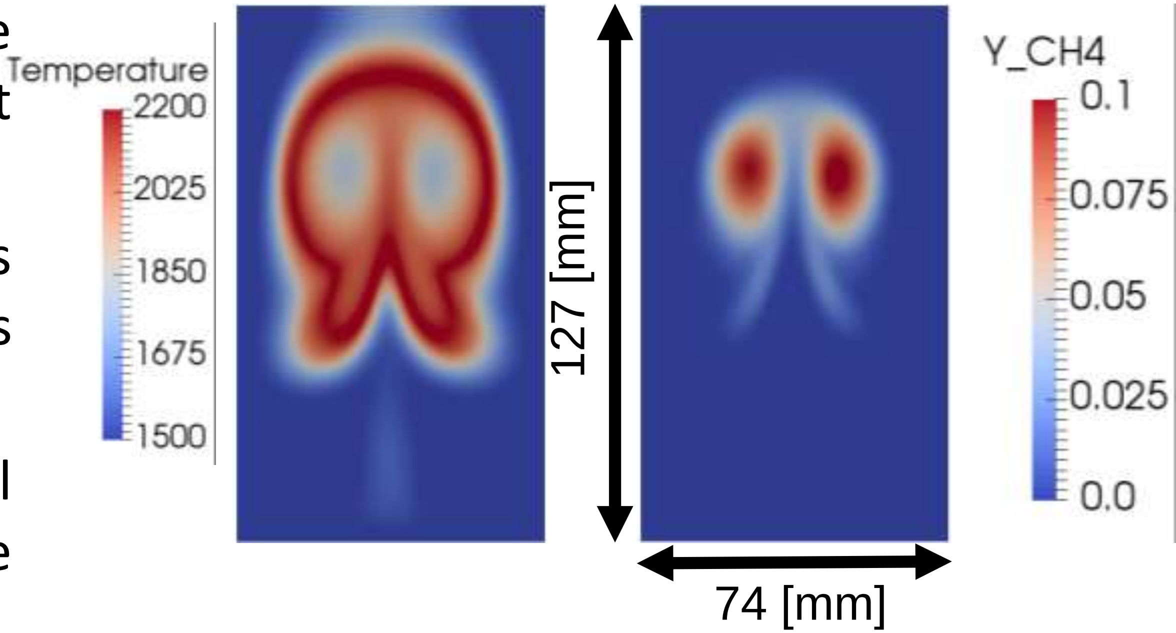
Instantaneous 2D snapshots



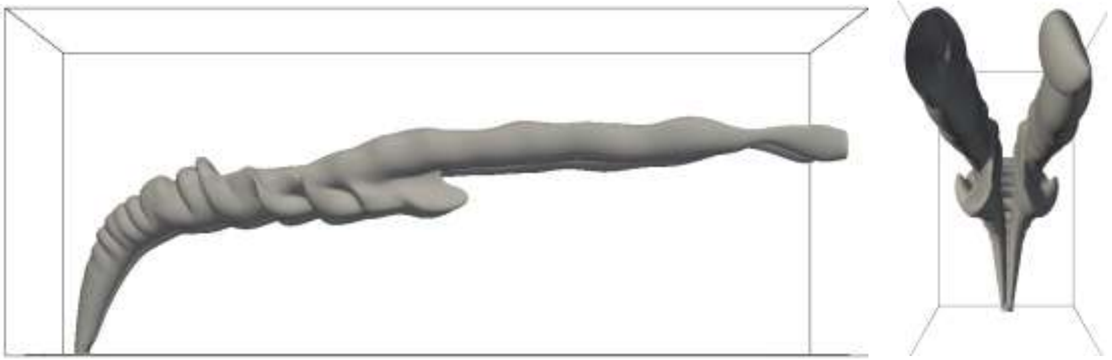
EXPLORATORY TEST CASE

- The outflow is roughly 30ms of residence time downstream of the jet injection
- Time averaged outflow cuts show an heterogeneous field of temperature.
- In this case, 40% of the fuel is left unburnt at the outflow plane.
- The current configuration is not turbulent enough to provide efficient mixing.
- The fuel trapped in the counter rotation vortex pair of the JICF is left unburnt.

Time averaged 2D cuts at the outlet

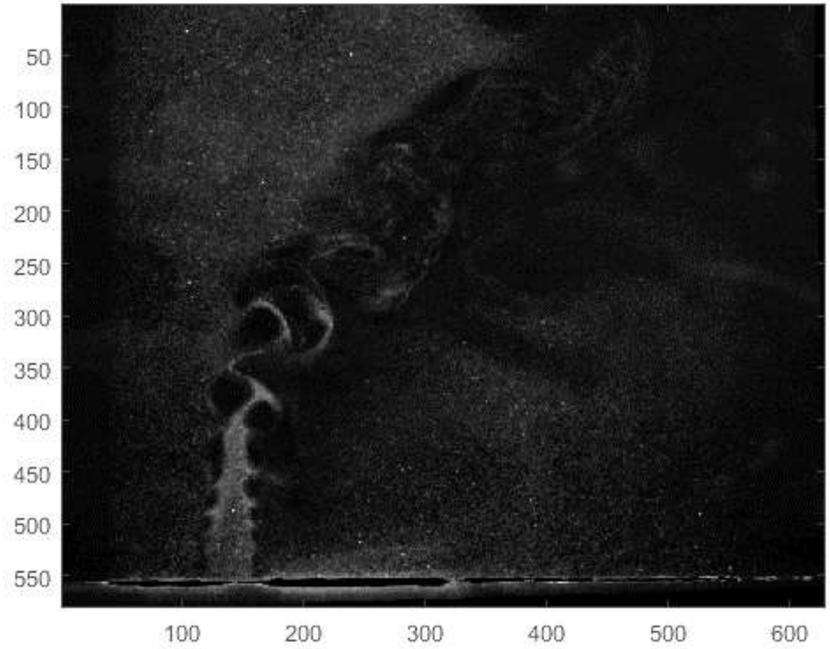


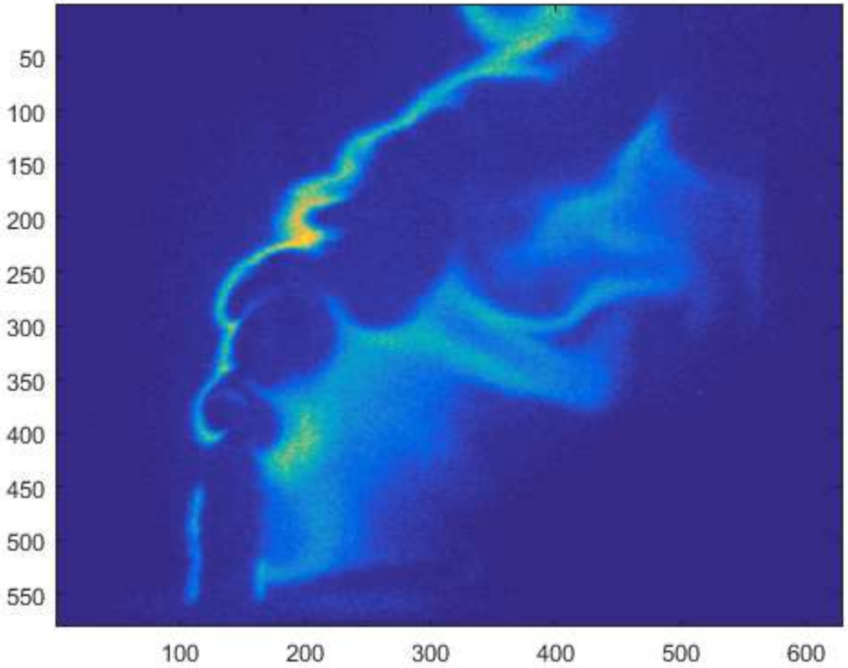
Instantaneous 3D isocontour of CH4



TASK 4.2 EXPERIMENTAL CHARACTERIZATION USING HIGH-SPEED LASER DIAGNOSTICS

JICF OPTICAL DIAGNOSTICS



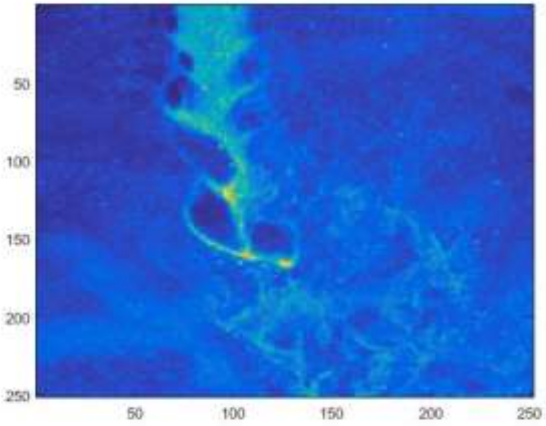


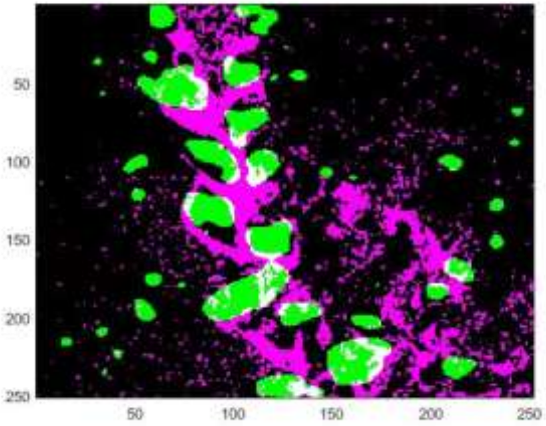
Mie scattering images of reacting JICF (sPIV)

Simultaneous OH-PLIF image

VORTEX TRACKING

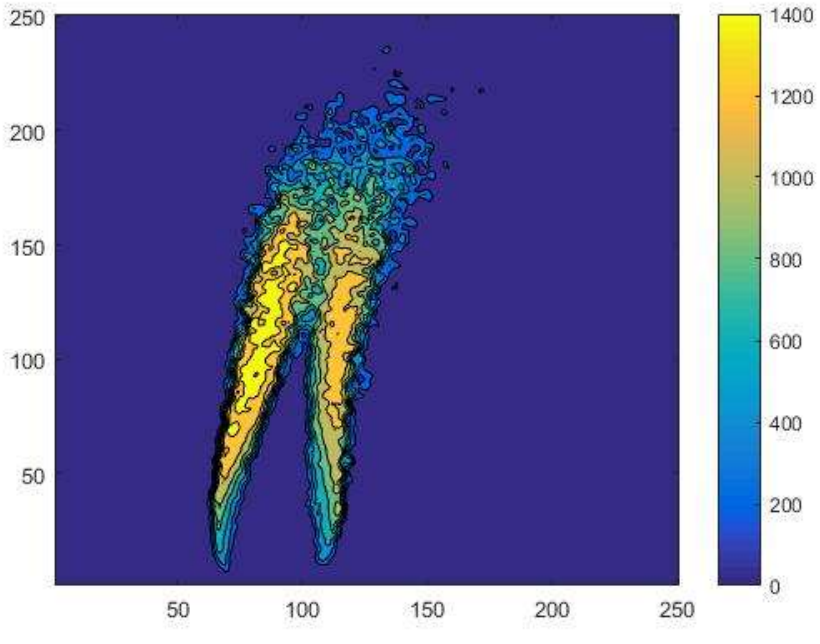
- Using data collected on previous incarnation of current test rig to develop analysis techniques
- Vortex tracking of reacting and non-reacting jets in crossflow
  - Vortex identified via swirling strength criteria
  - Decompose velocity gradient to obtain part of eigenvalues
  - Complex eigenvalue indicative of fluid rotation



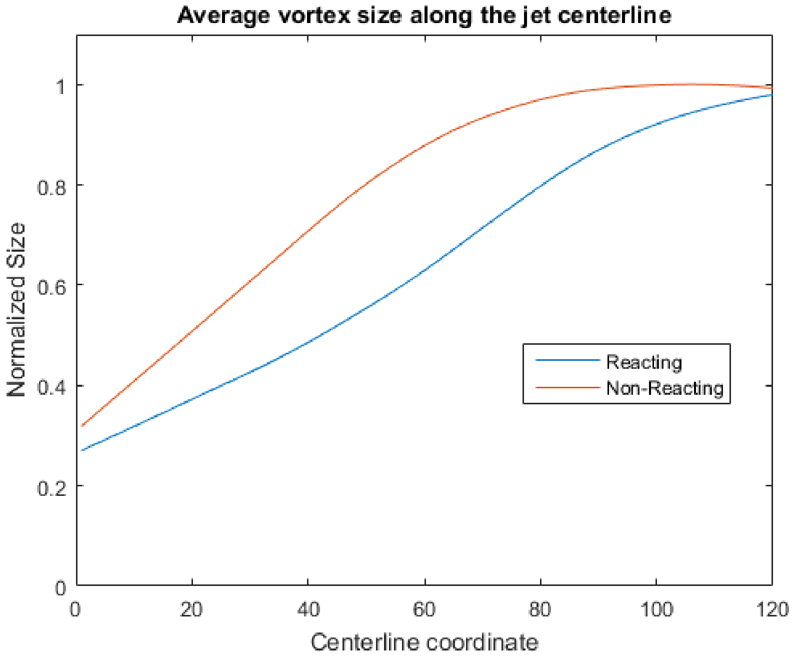


VORTEX TRACKING RESULTS

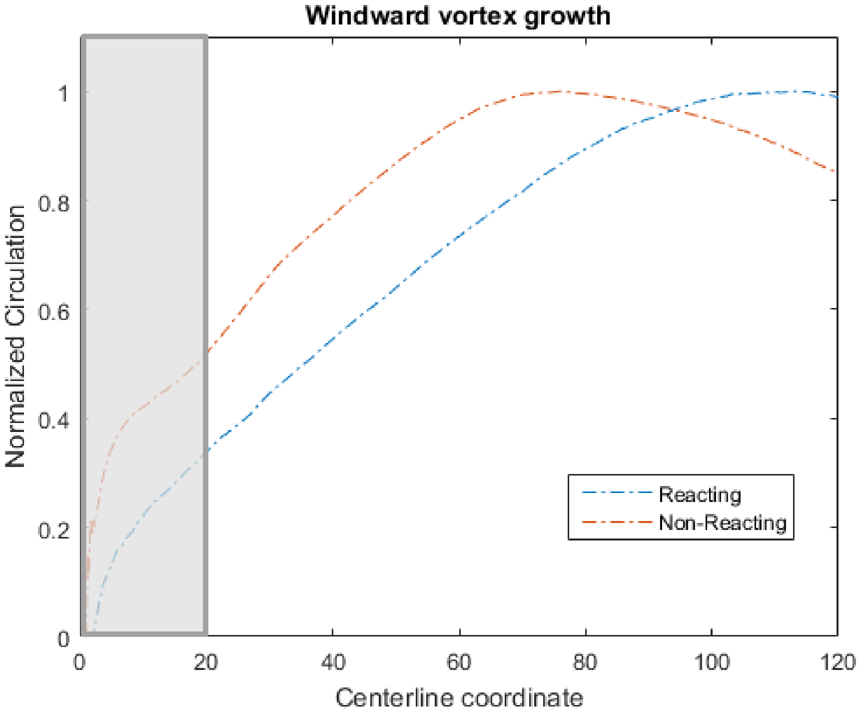
- The spatial vortex growth can be analyzed by tracking the change in vortex size and/or circulation long the jet centerline.
- The influence of the reacting jet on the hydrodynamics can be observed by comparing the growth rate between the reacting and non-reacting cases.

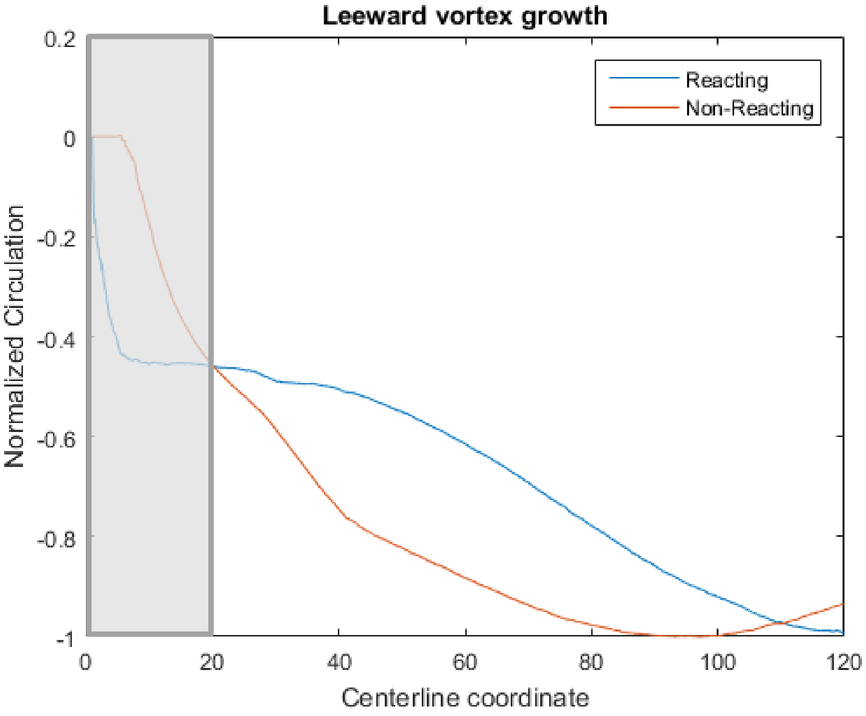


Results from 10,000 shots- vortex location



WINDWARD AND LEEWARD GROWTH RATES





SUMMARY

- Task 2
  - Developed software to perform optimization studies in MATLAB
  - Performed optimization study on two-stage pure-fuel combustor architecture
    - Showed: stage combustion theoretically enables better NOx and turndown performance
    - Substantial reductions in NOx possible relative to current architectures- achieving these minima will require significant work
- Task 3
  - Facility Development Complete
  - Facility Characterization testing underway
  - Initial test matrix established
- Task 4.1
  - Validated computational procedure using AMR
  - Developed two step CH_4 reaction mechanism
  - Conducted exploratory test simulation
- Task 4.2
  - Reacting JICF analysis tools developed

FUTURE WORK

- Task 2:
  - Incorporate physically limited mixing into reactor model
  - Optimizer integration
  - Automate process of finding optimum configuration for each combustor architecture
  - Eventually determine combustor architecture that minimizes NOx for target $T_{exit} = 1975K$
- Task 3:
  - Complete shakedown testing
  - Axial Stage Testing
    - Begin with single-point injection
- Task 4.1:
  - Add NOx mechanism to the reduced CH4 mechanism
  - Complete analysis of the current simulations to provide information to other project tasks:
    - Rig design: Comparison of the analytical JICF trajectory to the simulation reactive JICF predicted trajectory
    - Reactor modeling: Provide mixing times, combustion efficiency.
  - Extend to more detailed kinetics with subgrid closure issues
    - Multiple closures in code: EDC, PaSR, LEMLES but optimal approach is needed
  - Simulate experimental test cases
- Task 4.2:
  - Complete analysis of current data
  - Prepare current rig for laser diagnostic campaign