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HIGH-TEMPERATURE LOW-NO$_X$ COMBUSTOR CONCEPT DEVELOPMENT

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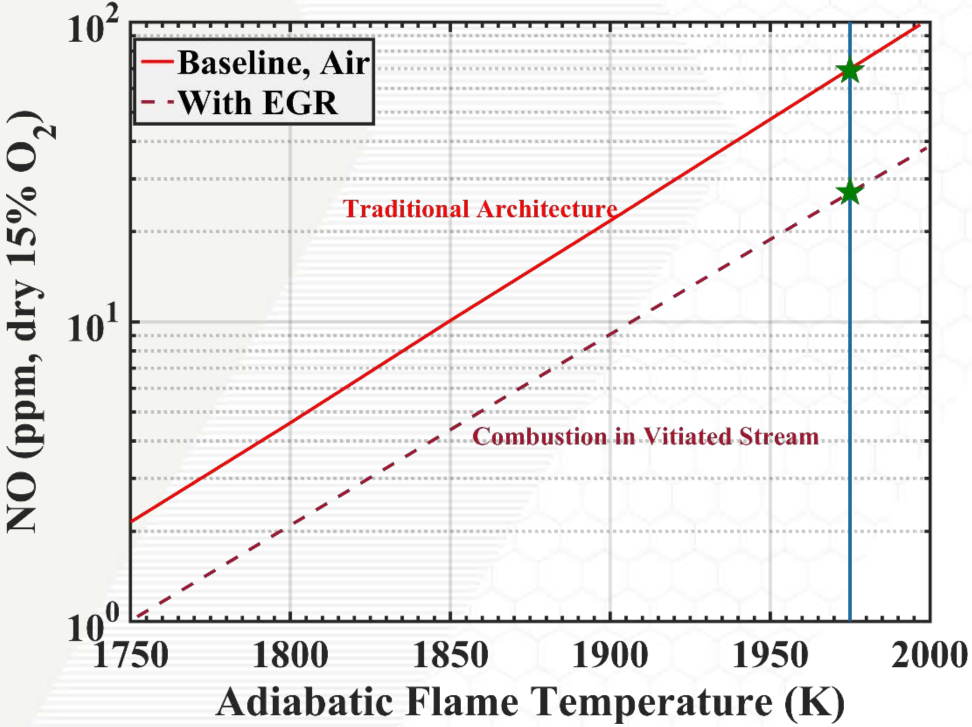
CREATING THE NEXT®

Need for Increased Firing T

- Combined cycle thermal efficiency has increased from 47% to 63% over the past 3 decades
  - driven by improvements in materials and cooling methods
  - advanced combustion technologies enabled simultaneous reduction in NOx emissions
- Further increases in $\eta_{thermal}$ will require higher firing temperatures
  - goal of $\eta_{thermal} = 65\%$ requires $T_{exit} = 1975\ K$

NOx Emissions Challenge

- At elevated temperatures, conventional architectures (DLN, EGR etc.) will fail to meet NO_x emissions standards
  - – main NO_x mechanism at high T: thermal NO_x



Thermal NO

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

$$O + N_2 \rightleftharpoons NO + N$$

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

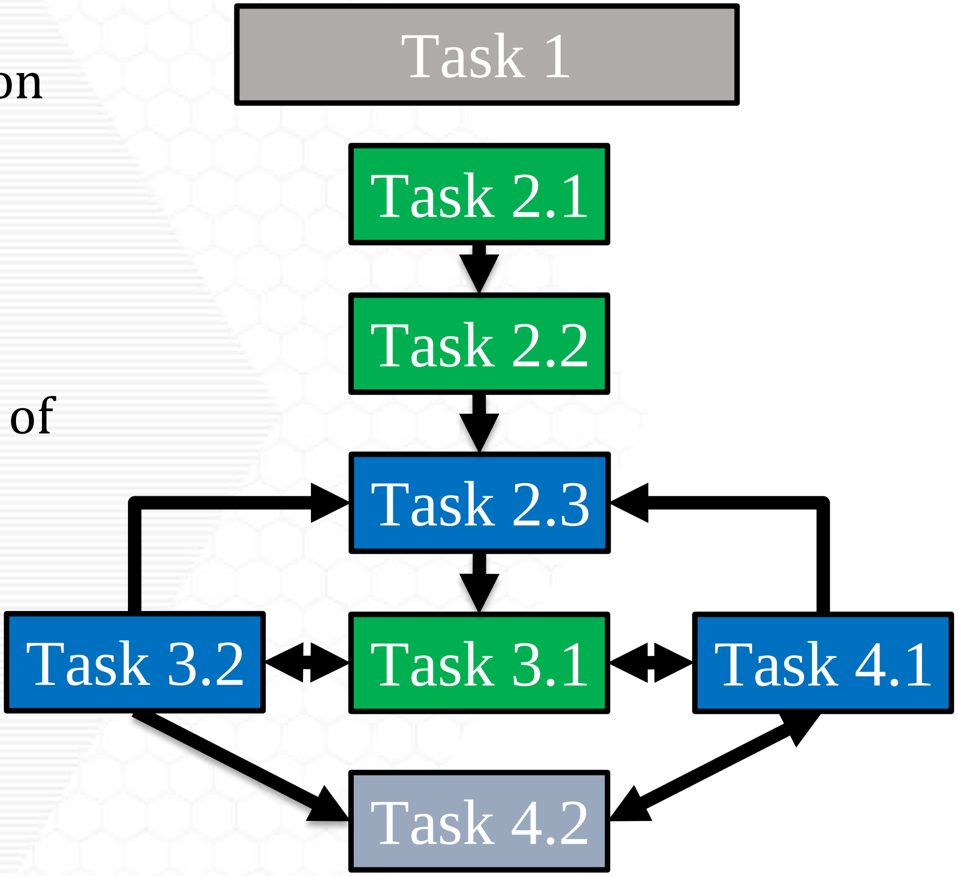
- To reduce $[NO]$,
  - $\tau_{res} \downarrow$
  - $T \downarrow$
  - $[O] \downarrow$
- Approaches:
  - dry, low-NO_x (DLN): reduces T_{max}
  - exhaust-gas recirculation (EGR): reduces [O] and T_{max}
  - **staged combustion: reduces [O] and τ_{res} at high T**

Overall Program Goals

- Combined modeling and experimental program to understand limits and sensitivities of NO_x emissions in gas turbine staged combustion
- Objectives - approach
  - determine **minimum theoretical NO_x limits** for a given firing temperature and residence time
    - reduced-order modeling
  - identify **fuel, air injection distributions** that can approach theoretical minimum NO_x levels
    - modeling and experiments
  - analyze **operational behaviors** of such a system
    - modeling and experiments

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

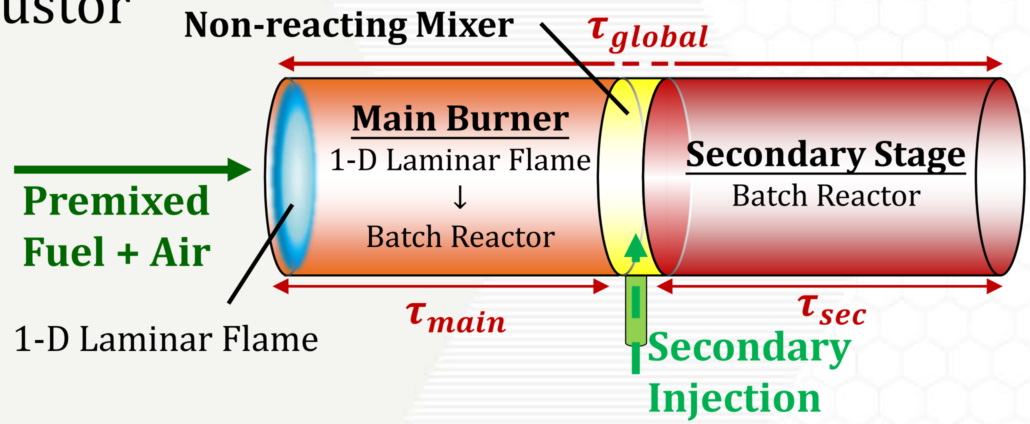
Tasks		Progress	Interdep.	Year	Quarter					Participants
Task-1				1	5	6	7	8	9	
1.1	Project Management and Planning	○		🟥	🟥	🟥	🟥	🟥	🟥	GTAE DOE Low-NOx Research Team
1.2	Reporting	○		🟥	🟥	🟥	🟥	🟥	🟥	
Task-2				1	5	6	7	8	9	
2.1	Fundamental Kinetic Studies	✓		🟧						Prof. Seitzman Prof. German Edwin Goh
2.2	Initial NO Optimization Studies	✓	2.1	🟧	🟧	🟧				
2.3	Constrained NO Optimization	○	2.2 4.1			🟧	🟧	🟧	🟧	
Task-3				1	5	6	7	8	9	
3.1	Experimental Facility Development	✓	2.2	🟩						Prof. Lieuwen Dr. Ben Emerson Matthew Sirignano Vedanth Nair
3.2	Initial Test Matrix & Facility Characteristics	✓	2.1, 2.2		🟩	🟩	🟩	🟩	🟩	
3.3	Refined Test Matrix & Facility Characteristics	○	2.3					🟩	🟩	
Task-4				1	5	6	7	8	9	
4.1	LES Studies for Subcomponent Geometry	○	2.3	🟦	🟦	🟦				Prof. Menon Prof. Lieuwen Dr. Andreas Hoffie
4.2	LES Studies for Experimental Rig	○	3.1, 3.2				🟦	🟦	🟦	
4.3	Experiments with High Speed Diagnostics	►	3.2, 3.2						🟦	

✓ : Done
○ : In Progress
► : Future

Optimization and Reduced-Order Modeling

Year 1: Minimum NO Modeling

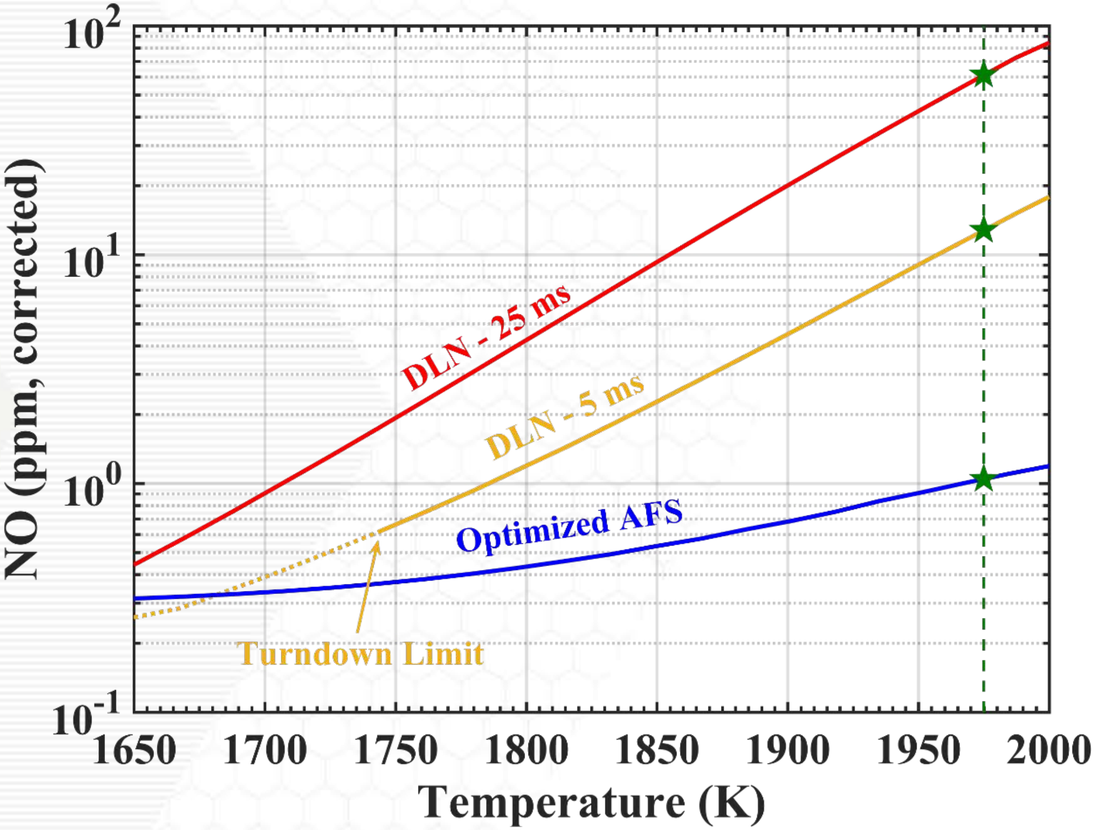
- Determine minimum NO emissions from axially-staged combustor under idealized flow conditions
  - developed reduced order (CRN) model of axially-staged combustor



  - assumes complete (ideal) mixing between fuel and vitiated products before reaction
  - for a fixed ϕ_{global} and τ_{global}, design parameters (for fuel injection) are:
    - main burner equivalence ratio ϕ_{main}
    - secondary injection location

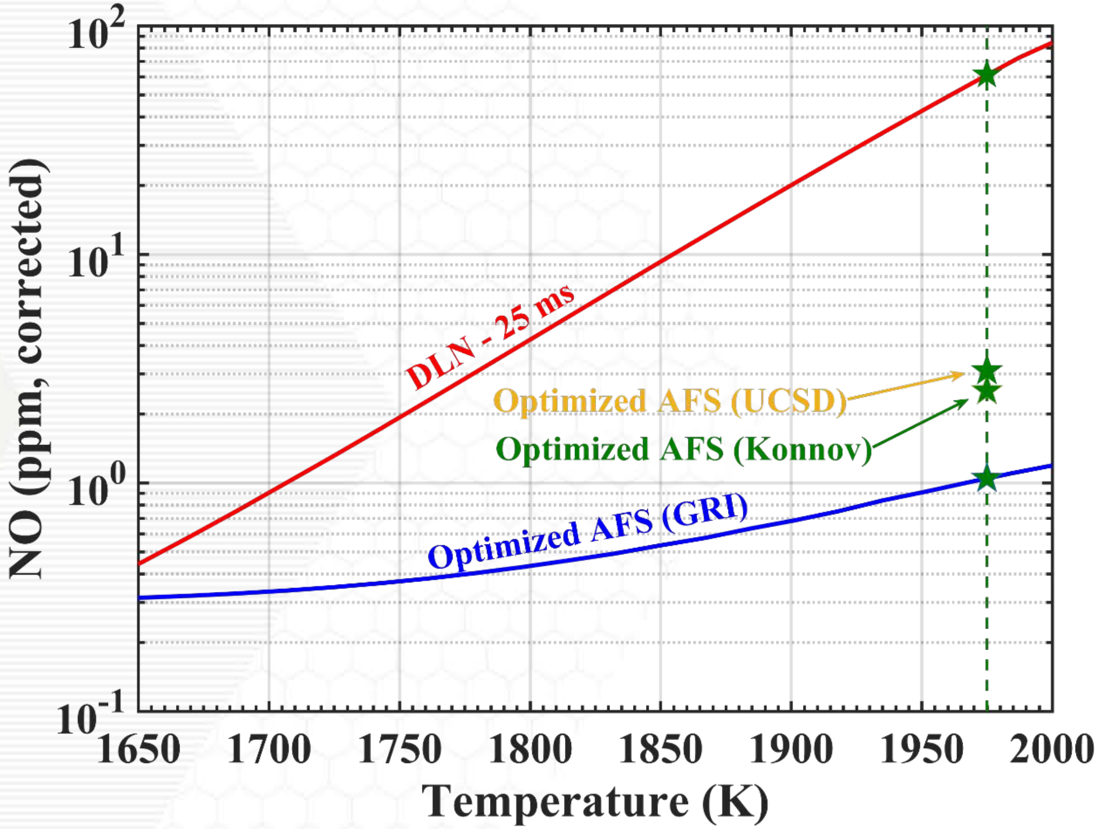
Year 1: Findings

- Performed parameter sweeps with constraint : $[CO] \leq 125\%$ of combustor $[CO]_{equilibrium}$
- Year 1 findings
  - **minimum NO~O(1ppm)**
  - **improvement increases with firing temperature**
  - **NO production is less dependent on T_{exit}**
  - **greater turndown compared to conventional DLN**
  - **head end (main burner) operating as lean as possible while still rapidly autoigniting secondary stage**
- Year 2: additional stages and fuel- dilution are detrimental under idealized conditions

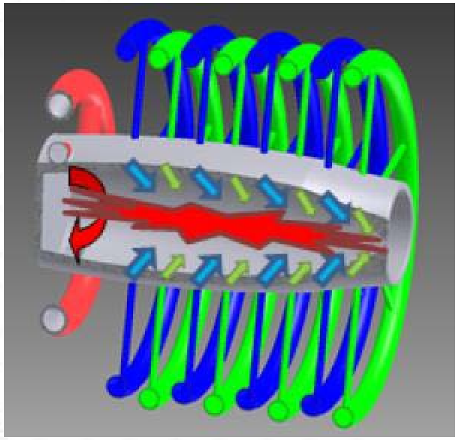


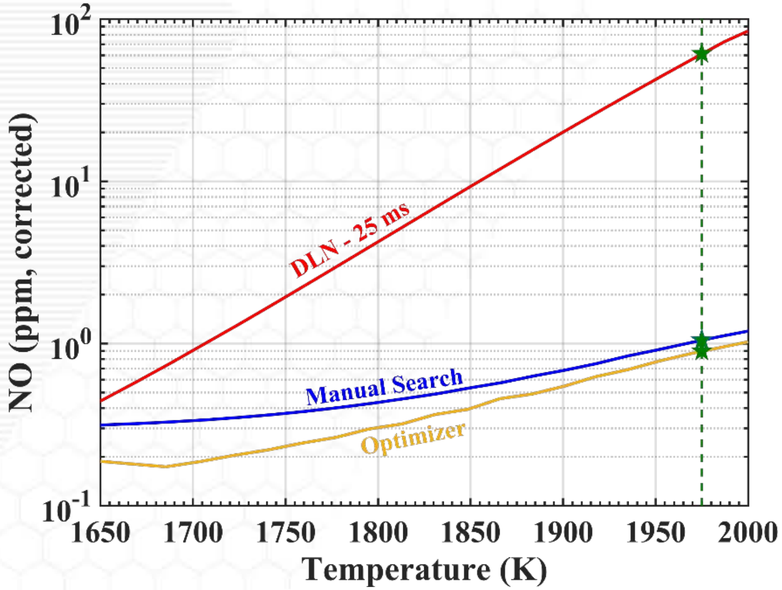
Chem. Mechanism Dependence

- Explored impact of uncertainty in rate parameters on minimum NO
- Konnov & UCSD mechanisms predict 2-3× higher NO than GRI
- Still O(1 ppm) - significant improvement over conventional approaches



Constrained Optimization – Optimizer





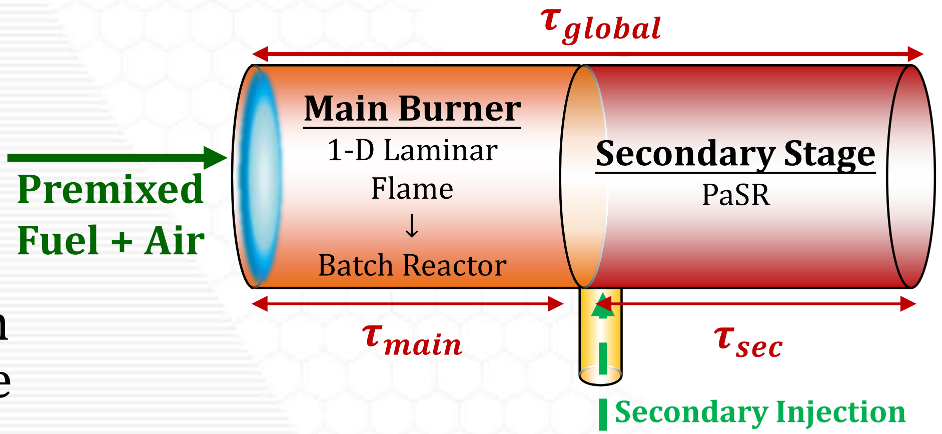
- Design space will grow with more complex configurations and constraints
  - too large for complete parameter sweeps to determine optimum configurations

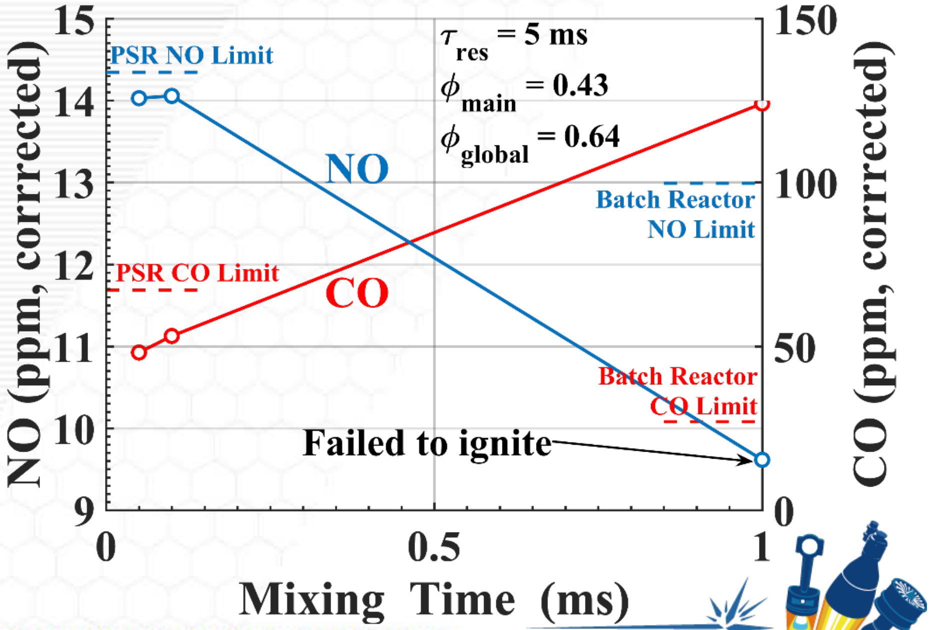
⇒ Need to automate process of exploring parameter space and finding minimums (optimum)

- Wrapped general optimizer around flexible CRN model
- Validated previous axial fuel-staged case with manually obtained minimums
  - significantly reduced runtime (weeks → days)

Constrained Optimization – Finite-Rate Mixing

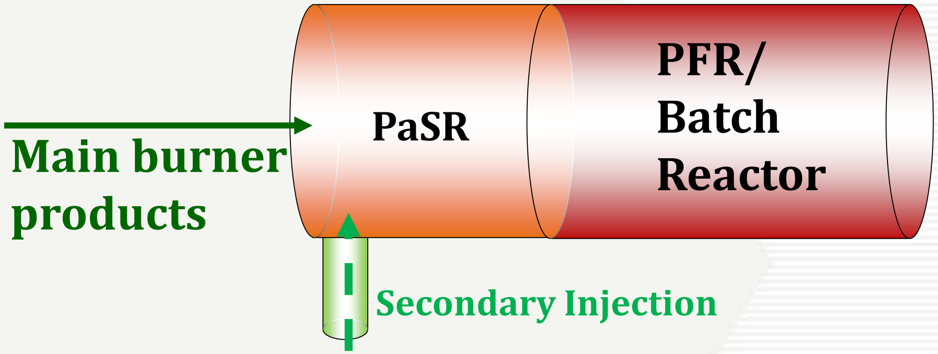
- In order to look at more practical design issues, should include effects of non-ideal flow conditions on chemical kinetics
- NO formation is highly dependent on degree of mixing in the reaction zone
  - identify/develop robust model to study effect of mixing rates on NO formation and inform combustor design
- Explored Partially-Stirred Reactor (PaSR) model:
  - 0-D reactor composed of particles (PSRs)
  - mixing model defines rules on mixing effect on particle composition
  - Chemkin implementation requires continuous injection of secondary fluid ⇒ does not properly model burnout





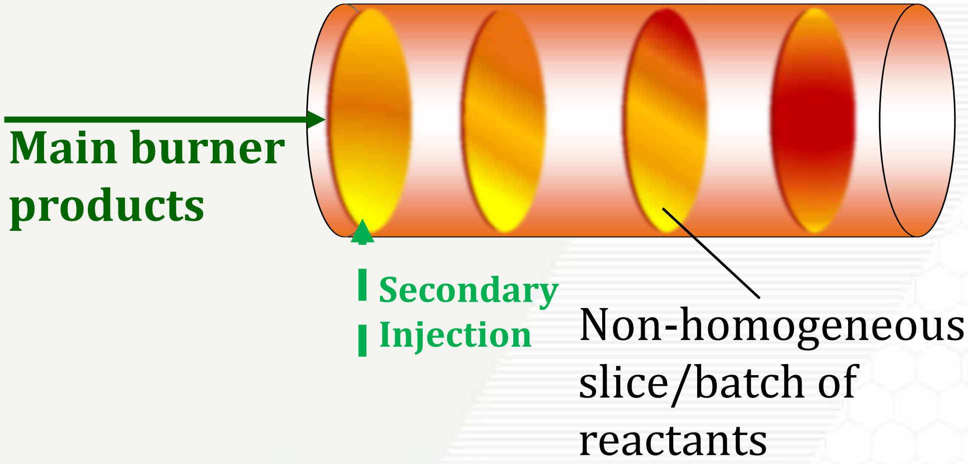
Modeling Finite-rate Mixing

- Two approaches to improve upon current PaSR model:



1. PaSR + Batch Reactor

- Burnout section after certain residence time in the PaSR



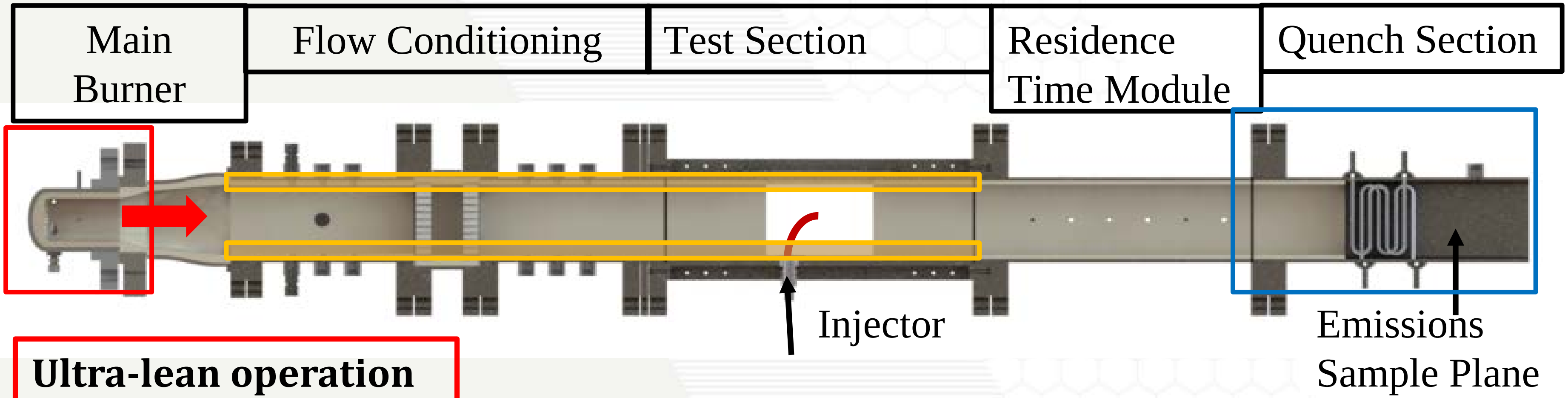
2. “Batch” PaSR

- Initially unmixed reactants
- Track non-homogeneous mixture as it evolves due to mixing and reaction
- Adaptable to model distributed fuel injection

Experimental Characterization

Facility Improvements

Experimental Facility



Main Burner

Flow Conditioning

Test Section

Residence Time Module

Quench Section

Injector

Emissions Sample Plane

Ultra-lean operation main burner

- tangential injection, high swirl concept
- hardware complete and tested

Ceramic heat shield for flow conditioning and test sections cast

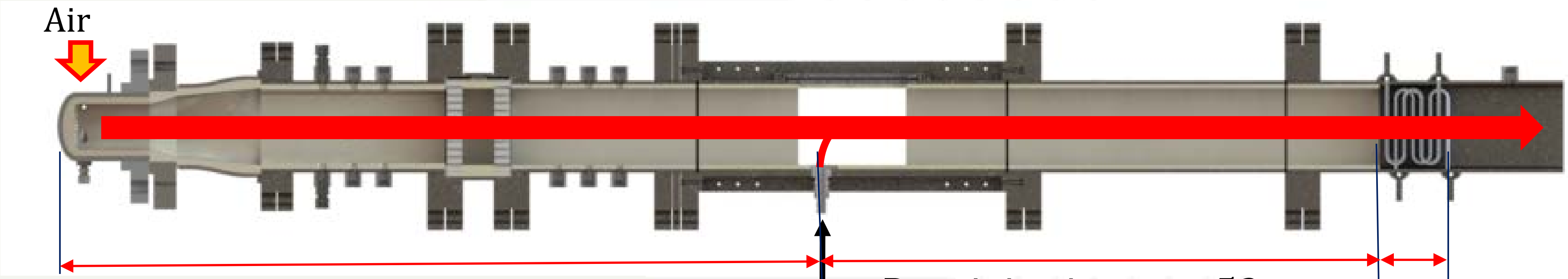
- to increase incoming crossflow temperature
- limited the temperature drop due to heat loss from 500K to 200K

Quench section designed & fabricated

- freeze NO_X chemistry
- mix exhaust to facilitate emissions measurement

Operational Capabilities

Cross flow speeds taken as ~ 17m/s for τ_{res} estimates



NG + Air

Pre-injection τ_{res} ~60 ms

CH_4 + Air

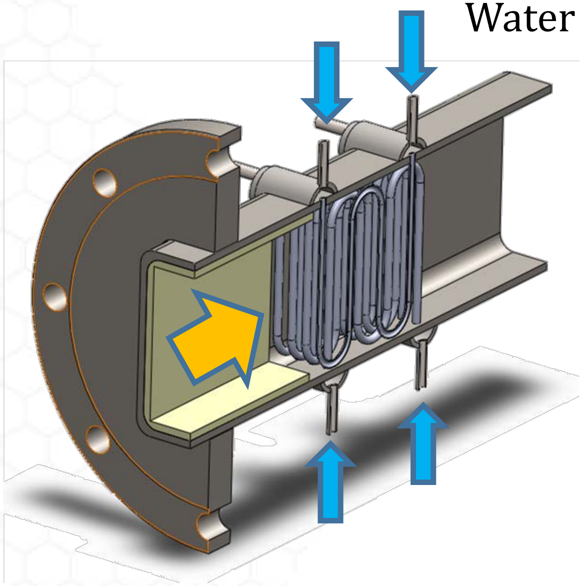
Post-injection τ_{res} ~52 ms

Quenching τ_{res} ~8.67 ms

- Main burner provides lean, combustion products
  - equivalence ratios ranging from 0.5 to 0.65 at a constant velocity of 17 m/s
  - test section temperatures ranged from 1650 – 1810K
- 12 mm premixed methane/air jet
  - straight for 40 diameter prior to exit; premixed 100 diameters prior to exit
  - preheated to temperatures ranging from 420 to 460K
- Facility operated at P = 1atm
  - large residence times used to match NO_x production values at pressure

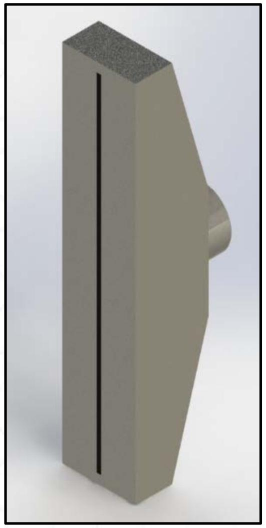
Quench Section and Gas Analyzer

- Emissions measurements require rapid quenching, spatial mixing before sampling
  - using air-to-water heat-exchanger to quench chemistry at sampling location
  - achieved T_{exit}=700 – 800 K
- Measure NO_x, CO with Horiba PG-350 gas analyzer



Shakedown Testing - Emissions Measurements

- Tested variety of jet equivalence (Φ_{jet}) and momentum (J) ratios to determine effectiveness of quench section at creating uniform sample plane
- Unacceptable NO_x variation in vertical direction (jet penetration)



12-point grid results for single operating condition

[NO] (ppm15%O2)

4.14	4.37	4.50
4.01	4.26	4.08
3.13	3.00	3.63
3.33	3.49	3.70

5”

3”

Temperature (K)

727	731	701
735	733	727
716	728	733
710	717	712

3”

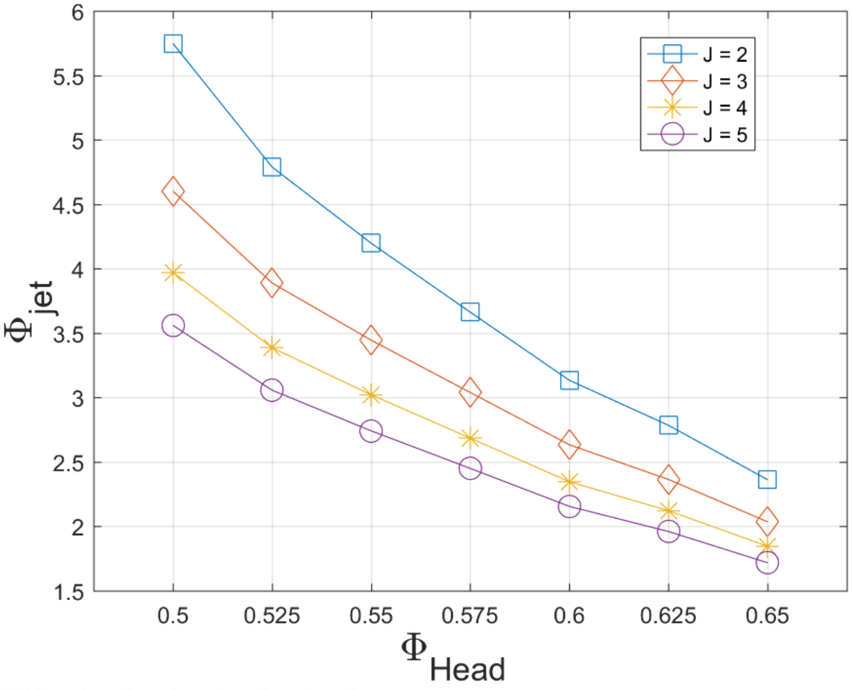
- Slotted probe designed to sample gas in a vertical line
- Sampling plane $(NO_x)_{AV}$ =3.83 ppm
  $(NO_x)_{SLOT}$ =3.9 ppm
- Slotted probe overcomes changes in vertical NO_x distribution due to changing jet penetration

Year 2 Testing

- Premixed jets were used in the axial stage to validate the operability and to take preliminary NO_X measurements
  - removes influence of fuel-air mixing
  - industry relevant configuration
- Goal: for fixed turbine inlet temperature (T_{exit}), impact of staging configuration on ΔNO_X, which is the NO_X contribution from the axial stage
- Configuration changed by varying:
  - air split between the main burner and axial stage
  - jet momentum flux ratio (J) and
  - jet equivalence ratio (ϕ_{jet})

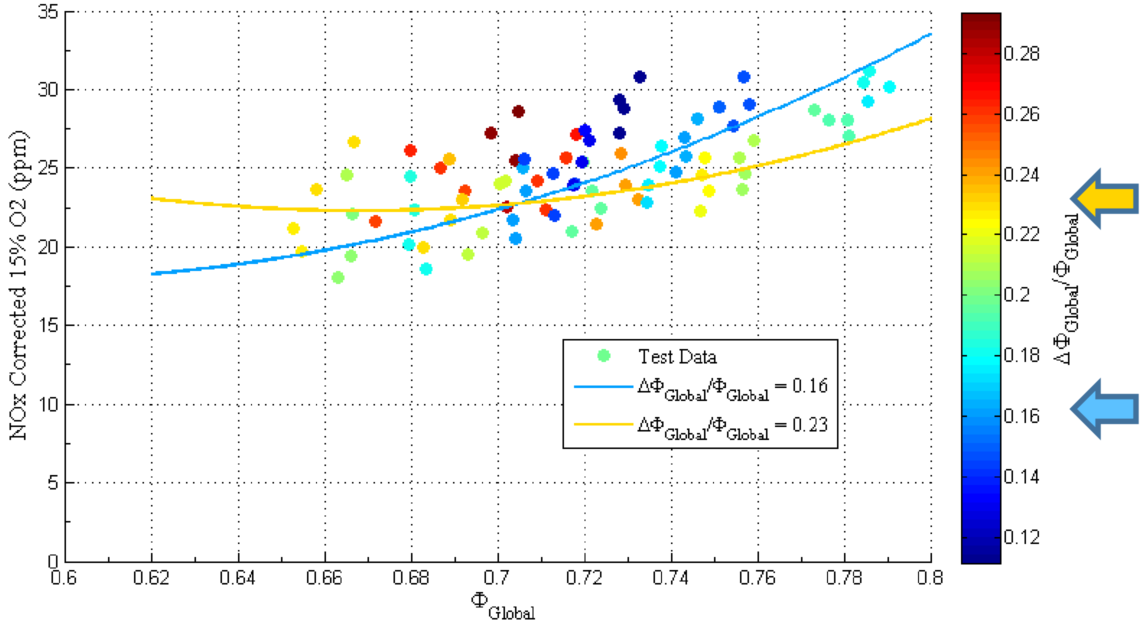
Test Matrix

- Three T_{exit} targets
  - 1873, 1915, 1956 K
  - also determines ϕ_{global} based on estimate of heat loss prior to the test section
- Main burner equivalence ratio range (ϕ_{head})= 0.5 – 0.65 (7 points)
- J sweep from 2 → 5 (4 points)
- ϕ_{jet} fixed for T_{exit}, ϕ_{head} and J
  - for current configuration, constraints lead to rich staged injection



$\Rightarrow$ **Total number of data points = 3x7x4 = 84 points**

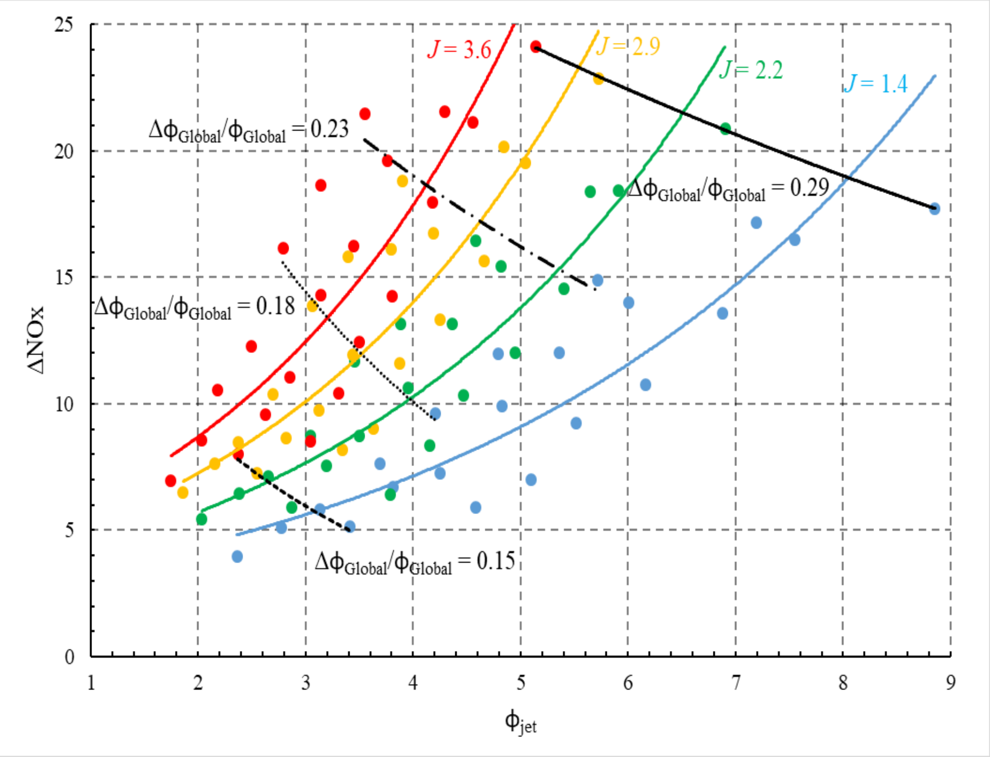
NO_X vs Global Equivalence Ratio



- Total NO_X increases with increasing ϕ_{global}
- $\Delta\phi_{global}$ defined as $\phi_{global} - \phi_{head}$ which is a measure of the axial stage contribution

- For low $\Delta\phi_{global}$, low axial stage utilization
  - NO_X increases with higher ϕ_{global}
  - benefit at low Φ_{global} limited by finite mixing
- For higher $\Delta\phi_{global}$
  - NO_X increase relatively flatter
  - axial stage benefit at higher Φ_{global}

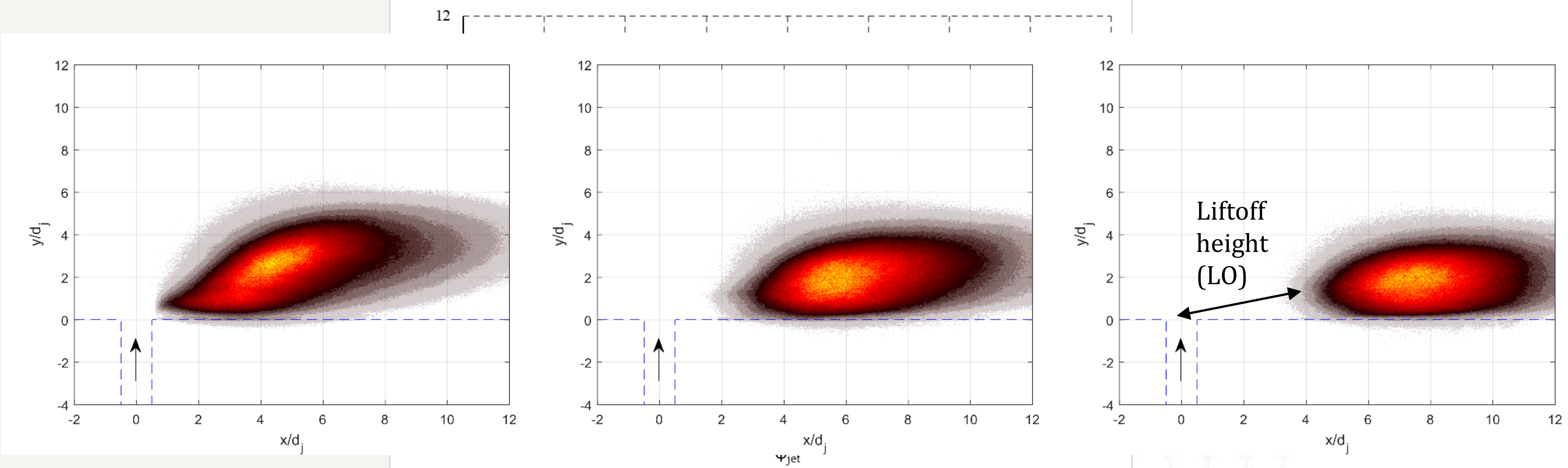
NO_X Contribution from Staging



- ΔNO_X is defined as the NO_X contribution from the axial stage
- If we hold J fixed and increase ϕ_{jet}, we increase stage contribution ($\Delta\phi_{global}$)
  - higher stage NO_X as might be expected
- For a fixed axial stage contribution, the ΔNO_X decreases with increase in ϕ_{jet}
  - **Why does richer jet produce lower NO_x (in stage and overall)?**

Flame Lift Off

Time averaged CH* flame images; $\Phi_{Head} = 0.6$

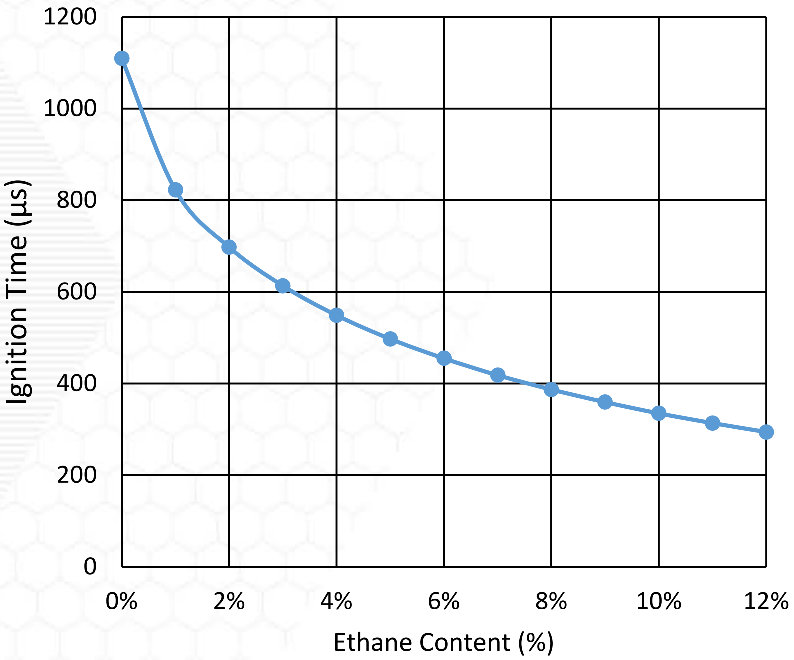


$\Phi_{jet} = 2.2$ $\Phi_{jet} = 2.65$ $\Phi_{jet} = 3.15$

- For $\phi_{jet} > 3$, significant lifting of the flame was observed
- Lift-off distance increases as jet becomes richer (increasing ϕ_{jet})
- Hypothesis: increased liftoff allows for more mixing with hot crossflow – allows for more burning at lean conditions than for less rich jets

Planned Work

- Focus on expanded jet parameter space at constant ΔT
  - less head end and target temperature conditions
  - Φ_{jet}: both rich and lean jets
  - J: high (> 10) and low (< 10) cases
  - requires reducing flow cross-section
    - high J cases will also explore confinement
- Isolate liftoff impact
  - dope methane with 0-12% ethane to reduce ignition times
  - can control degree of lifting
- Diagnostic techniques
  - emissions sampling: NOx levels
  - OH* & CH* chemiluminescence, Mie scattering: jet fluid mixture fraction, equivalence ratio of combustion, & jet trajectory
  - high-speed PIV and PLIF (detailed flow/flame interaction)



LES Studies

Previous Work – Current Status

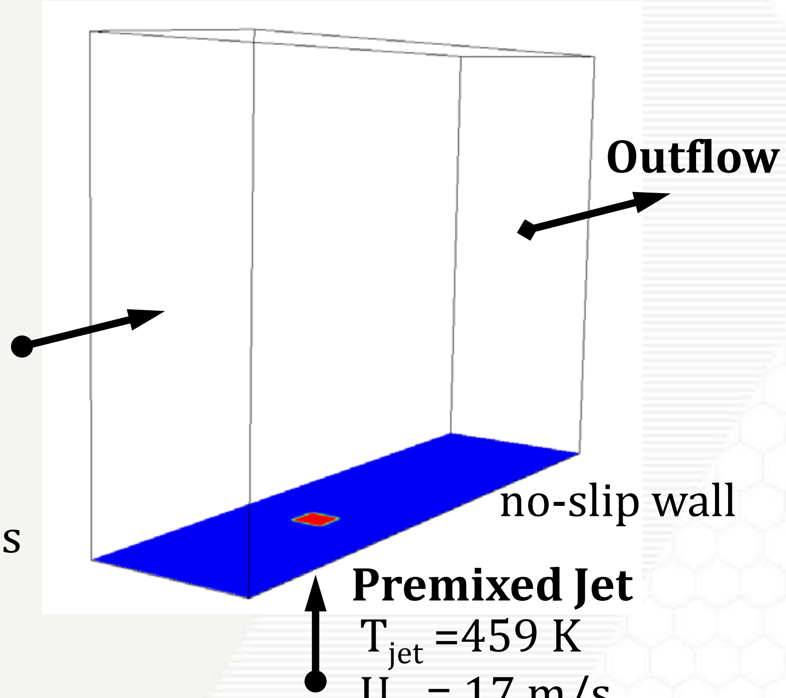
- Previous Work
  - adaptive mesh refinement (AMR) approach was validated by comparison to experimental results for hydrogen JICF flames[1]
  - preliminary non-premixed, reacting CH_4 baseline case without AMR was examined
- Current Status
  - premixed JICF studies with AMR – motivated by GT experiments
  - non-reacting JICF study of planned GT configuration

[1] Muralidaran and Menon, AIAA SciTech, 2014

Premixed Study

Reacting, premixed methane jet in vitiated cross flow

- configuration based on GT experimental conditions
- **simplified geometry,** square jet with D = 12mm, J=3.7
- **1 step-5 species** Westbrook-Dryer[1] mechanism – unrealistic but fast



Vitiated Cross Flow

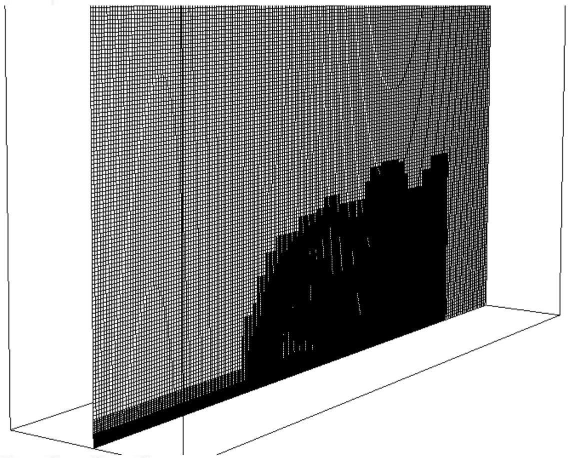
T_∞ =1782 K
U_∞= 17.3 m/s
ϕ_{Head} = 0.6

Outflow

no-slip wall

Premixed Jet

T_{jet} =459 K
U_{jet}= 17 m/s
ϕ_{jet} = 1.1

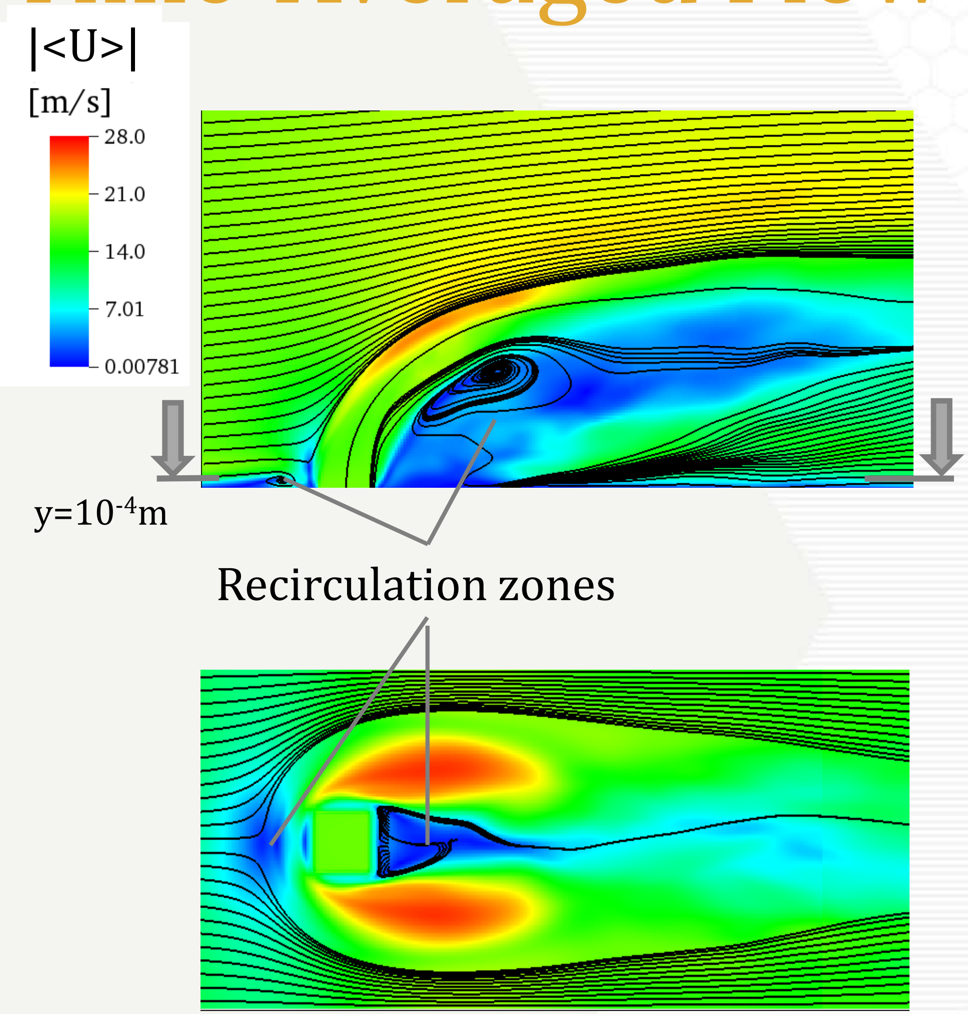


- AMR LESLIE[2] grid, mid plane
- Domain size 5.5D x 15D x 20D

[1] Westbrook, C.K., Dryer, F.L. Comb.Sci.Tech., (27), 1981, pp.31-43

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

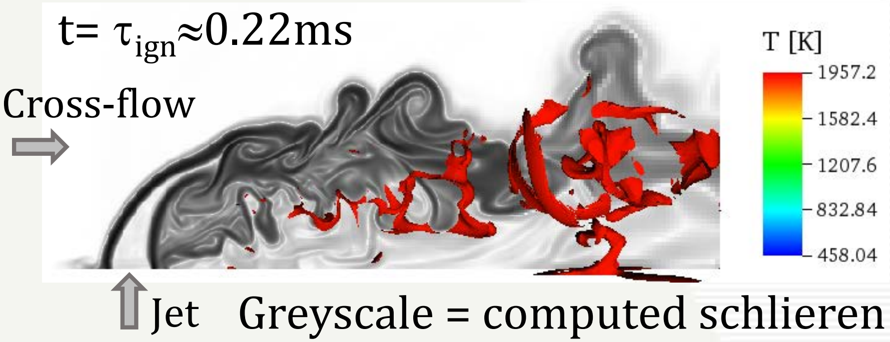
Time-Averaged Flow Field



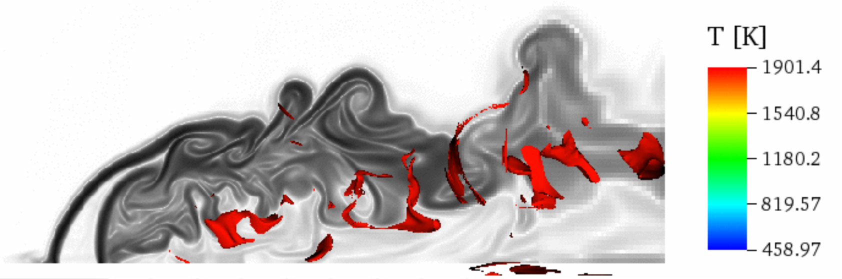
- Simulation predicts flame anchoring on the windward and leeward-side
  - – experiment, leeward-side only
- Discrepancy due to
  - **1-step chemistry**
  - thinner upstream boundary layer
  - square, plug flow jet BC

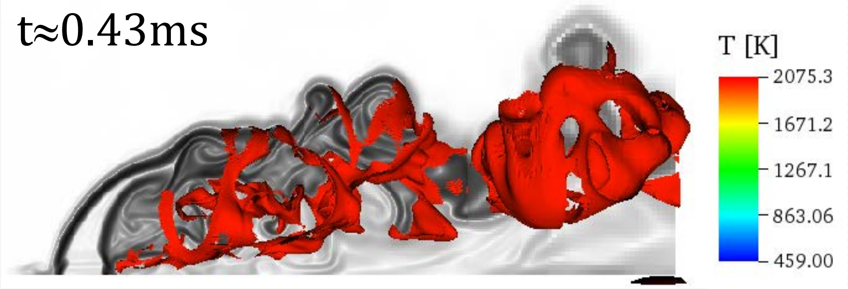
- Time averaged velocity magnitude overlaid with streamlines
- Leading boundary layer separation and recirculation zones can form potential regions for flame anchoring

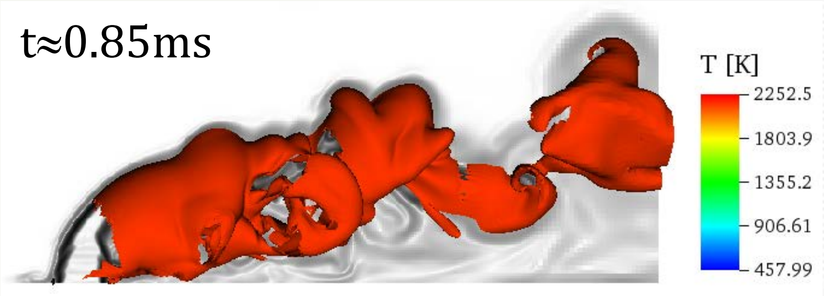
Autoignition Sequence


$t = \tau_{ign} \approx 0.22$ms

Greyscale = computed schlieren



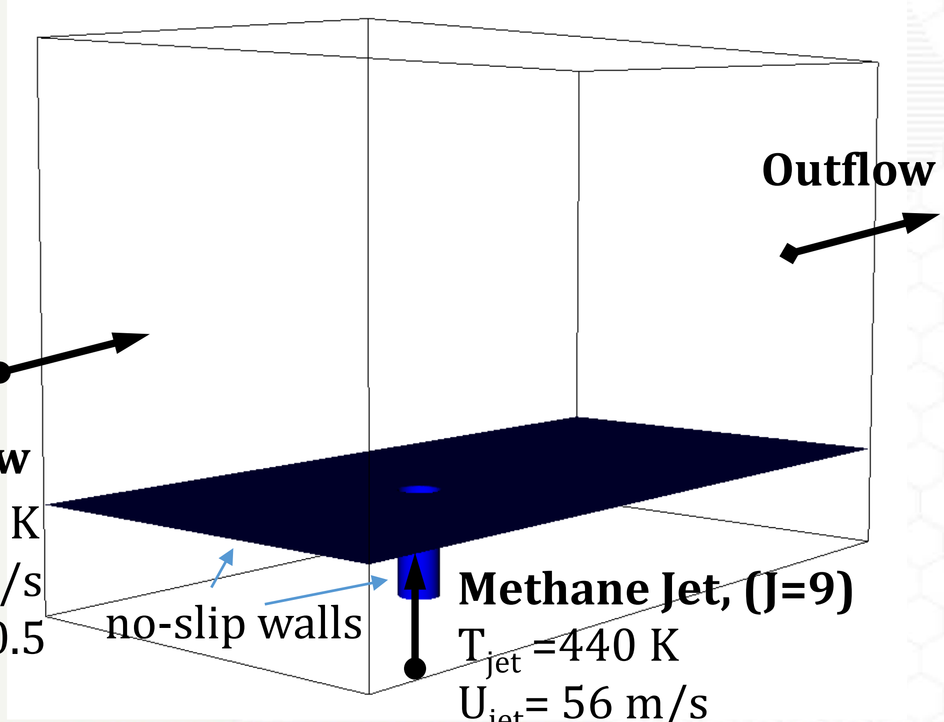

$t \approx 0.43$ms


$t \approx 0.85$ms

- Auto-ignition starts downstream in leeward-side recirculation
- Flame moves upstream at apparent speed of O(100 m/s) $>> S_{L,jet}$=O(1 m/s)
- Flame eventually propagates toward windward shear layer and envelopes entire jet

Moving Toward Experimental Geometry

- Geometry and conditions based on planned GT experimental configuration
  - includes finite length (2.5D) round injector tube and upstream BC, utilizing the novel AMR Cutcell[1] method
- Equilibrium products for vitiated cross-flow
- Non-reacting study to investigate flow field and mixing



Outflow

Vitiated Cross Flow

T_∞ =1650 K

U_∞= 27 m/s

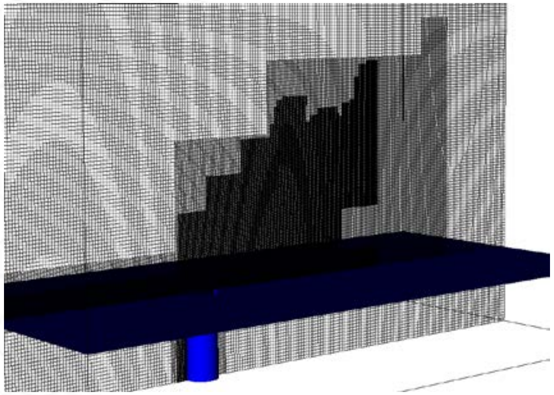
$\phi_{\text{Head}} = 0.5$

no-slip walls

Methane Jet, (J=9)

T_{jet} =440 K

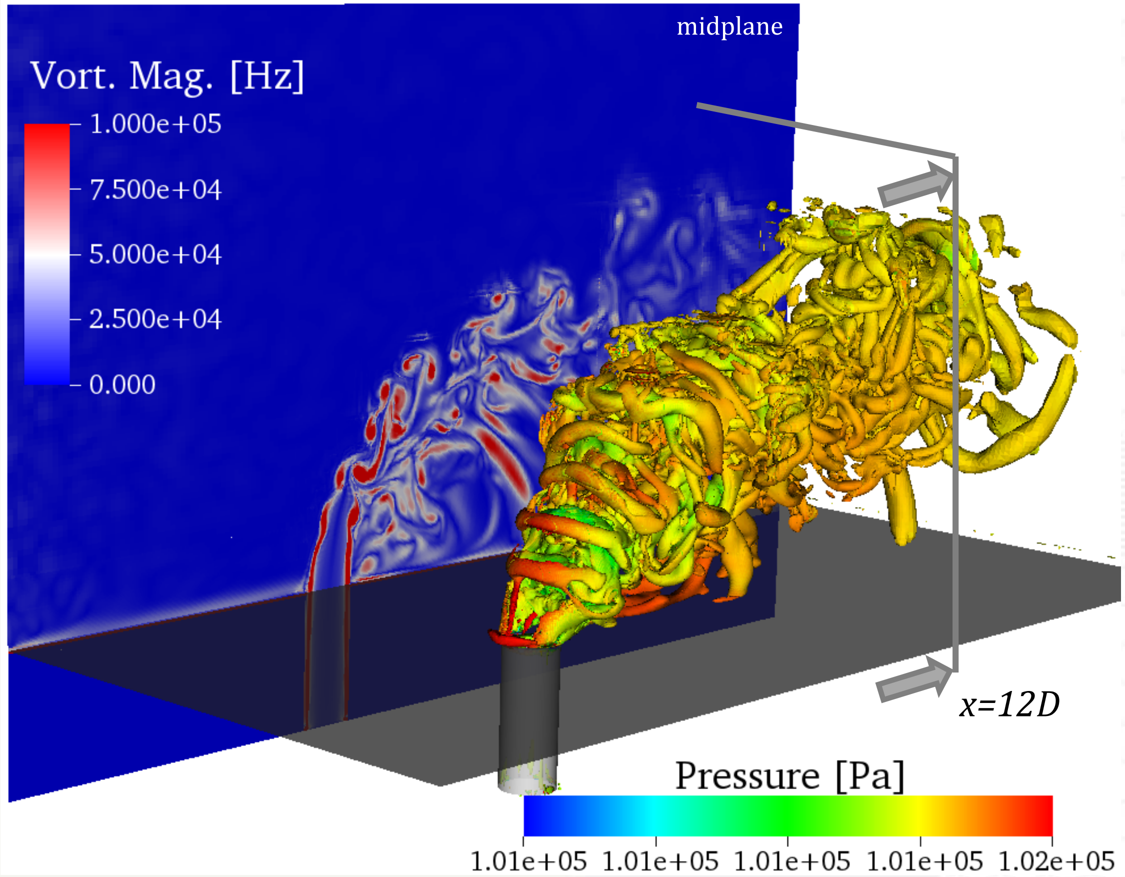
U_{jet}= 56 m/s



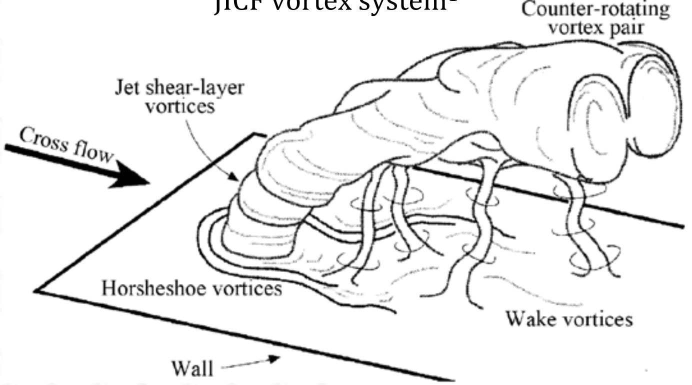
- Adaptive LESLIE grid, mid plane
- Channel size 10D x 10.5D x 20D

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

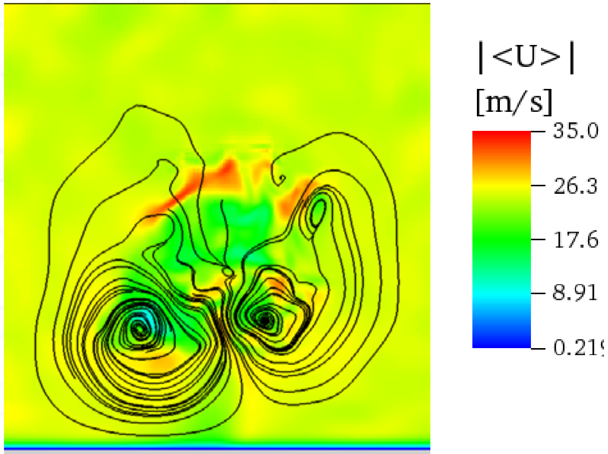
JICF Vortex System



JICF vortex system[1]



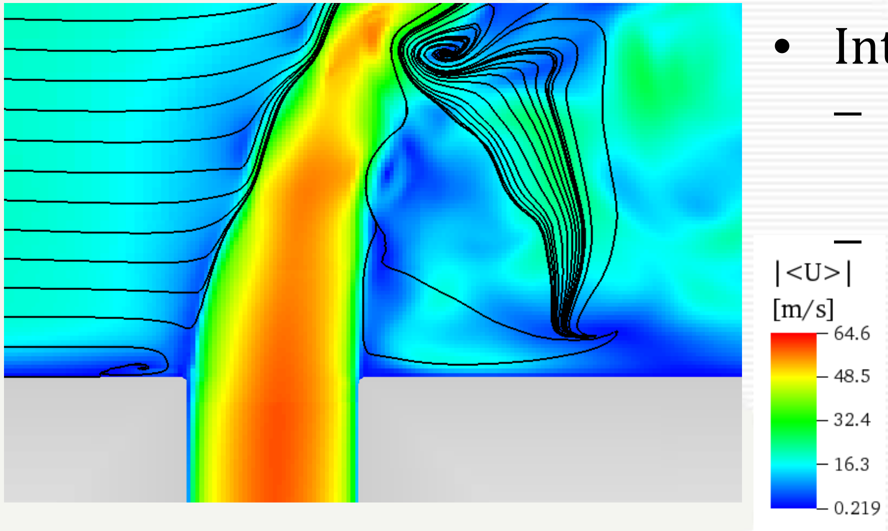
[1] Fric, T. F. and Roshko, A., JFM., 279, 1-47, 1994



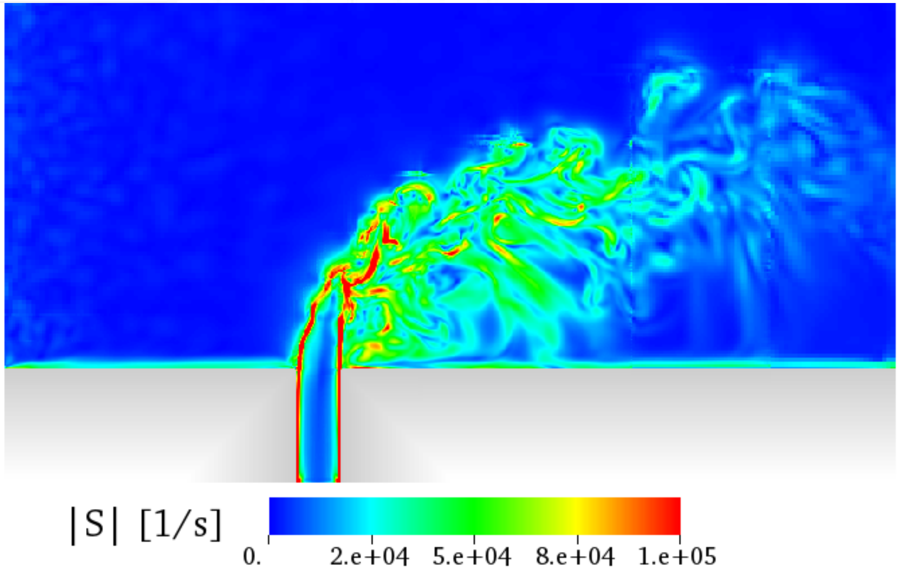
Average from 2 to 2.5 flow through times

- Iso-surface of Q-criterion shows vortical structures
- Vorticity magnitude illustrates vortex roll-up
- Counter-rotating vortices forming toward outlet

Flow Field



- Interaction of cross flow with jet conditions
  - influence of windward side pressure rise on fuel tube: reduced velocity
  - BL separation and recirculation on windward side of fuel tube



- Flame-anchoring is expected to take place outside high strain rate regions

$$S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right); \quad |S| = \sqrt{2S_{ij}S_{ij}};$$

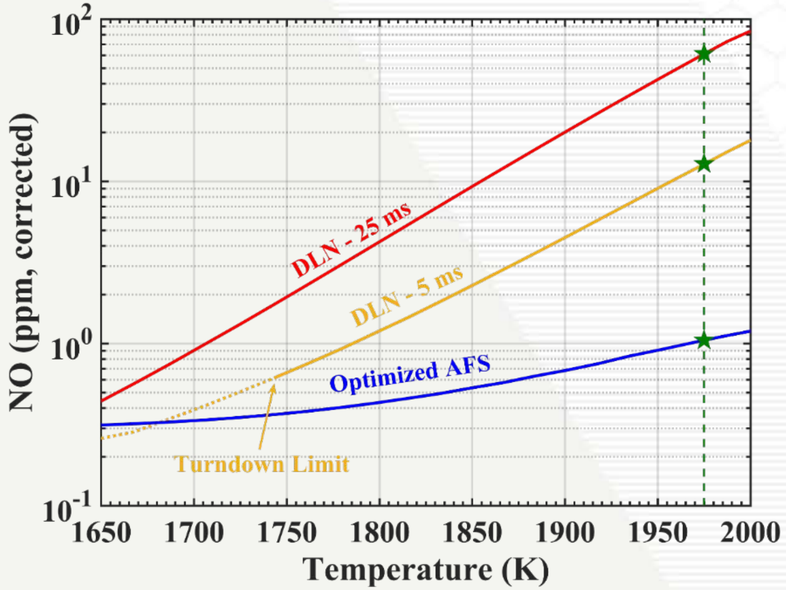
- Auto-ignition studies needed with accurate, multistep mechanism

Future plans

- Focus on premixed JICF studies
  - pick 2-3 cases with range of flame dynamics/stabilization
- Detailed plan
  - auto-ignition to be revisited using more detailed kinetics (e.g., 13 specie CH_4-air mechanism)
  - inflow turbulence and resolution sensitivity will be assessed by increasing levels of near-wall refinement
  - Zeldovich and "prompt" NO kinetics model to be included once flame anchoring and auto-ignition issues are resolved
  - number of simulation cases limited by resources available within GT; therefore, choice of cases will be down selected after more assessment of experimental cases

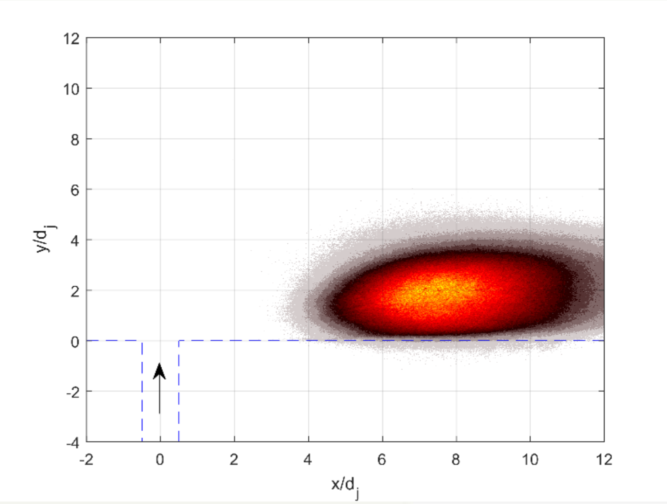
Brief Year 2 Summary

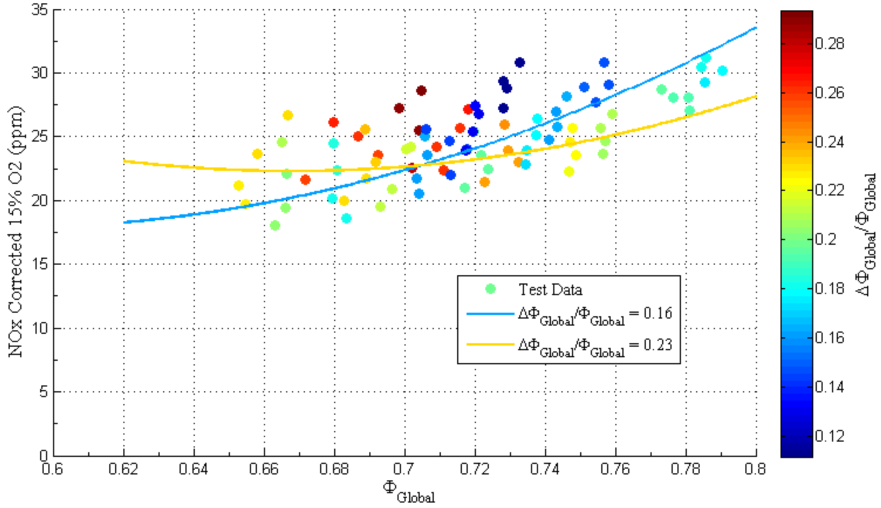
- Reduced-order modeling
  - minimum (ideal) NOx for staging: O (1 ppm) and similar for different chemical mechanisms and jet mixtures
  - automated optimizer with new PaSR models to explore impact of finite mixing – can use inputs from LES studies
- Experiments
  - demonstrated axial staging improvements in total NO_X for premixed cases
  - NOx advantages of staging improve with firing temperature as expected from ROM results
  - NO_x production in JICF staging dependent on mixing, strongly coupled to flame lifting – new experiments planned to focus on mixing limitations
- LES studies
  - initial LES examination of experimental conditions show expected flow features and suggest importance of near-field strain and "autoignition" type behavior
  - including more appropriate kinetics for detailed studies


NO (ppm, corrected)
10^2
10^1
10^0
10^{-1}
DLN - 25 ms
DLN - 5 ms
Optimized AFS
Turndown Limit
1650
1700
1750
1800
1850
1900
1950
2000
Temperature (K)


T [K]
1957.2
1582.4
1207.6
832.84
458.04

Questions?


12
10
8
6
4
2
0
-2
-4
y/d$_j$
-2
0
2
4
6
8
10
12
x/d$_j$


NOx Corrected 15% O2 (ppm)
35
30
25
20
15
10
5
0
0.6
0.62
0.64
0.66
0.68
0.7
0.72
0.74
0.76
0.78
0.8
Φ_{Global}
Test Data
$\Delta\Phi_{Global}/\Phi_{Global} = 0.16$
$\Delta\Phi_{Global}/\Phi_{Global} = 0.23$
0.28
0.26
0.24
0.22
0.2
0.18
0.16
0.14
0.12
$\Delta\Phi_{Global}/\Phi_{Global}$