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 on temperature, residence time, and O radical concentration

\[ O + N_2 \leftrightarrow NO + N \]

\[ [NO] \propto [O][N_2]e^{-38.379/T\tau_{res}} \]

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

⇒ Optimization of staged injection
(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

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

**Main burner parameters:**
- $\phi_{\text{main}}$ (⇔ main-secondary mass split)
- $T_{\text{air,main}}$
- $T_{\text{fuel,main}}$

**Global configuration/parameters:**
- $\phi_{\text{global}} \Leftrightarrow T_{\text{exit}}$
- $\tau_{\text{global}}$
- $P$
- $n$ (number of secondary injectors)
- Mass split between main burner and secondary injectors

**For each injector:**
- $\chi(\text{fuel,air,steam,etc.})$
- $T_{\text{inlet}}$
- $\tau_{\text{sec}} \rightarrow$ 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:**
  - $\phi_{global}$
  - $\phi_{main}$
  - $\tau_{sec}$

**Main burner parameters:**
- $\phi_{main}$
- $T_{air,main}$
- $T_{fuel,main}$

**Global configuration/parameters:**
- $\phi_{global} \leftrightarrow T_{exit}$
- $\tau_{global}$
- $P$
- $n$ (number of secondary injectors)
- Mass split between main burner and secondary injectors

**Secondary injector:**
- $\chi(fuel)$
- $T_{inlet}$
- $\tau_{sec}$
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.

\[
\phi = 0.56; \ t_{inj} = 15 \ ms
\]

\[
\phi = 0.5; \ t_{inj} = 15 \ ms
\]

Baseline (\(\phi_{global} = 0.63\))

- 90 ppm
- 40 ppm
2. OPTIMIZATION STUDY RESULTS—$\tau_{res}$ DEPENDENCE

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

Shorter secondary injection residence times $\Rightarrow$ lower NO but limited by CO burnout
2. OPTIMIZATION STUDY RESULTS—$\tau_{res}$ DEPENDENCE

Establish “optimum” secondary injection time $O(100 \ \mu s)$ for minimum NO within CO constraint
For the same $T_{exit}$, repeat over multiple $\phi_{main}$ values...
2. OPTIMIZATION STUDY RESULTS—$\phi_{main}$ DEPENDENCE

Lower $\phi_{main}$ improves NOx performance in staged combustion architecture

$\phi_{global} = 0.64$

$\phi_{main}: 0.43 - 0.64$

$\tau_{global} = 20\text{ ms}$
Repeat for multiple $T_{exit}$...
2. OPTIMIZATION STUDY RESULTS—STAGED VS. CONVENTIONAL

$\leq 1\text{ppm}$ over large operating range
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 $\tau_{res}$
Can try and reduce conventional architecture NO emissions by reducing combustor $\tau_{res}$.
2. OPTIMIZATION STUDY RESULTS—STAGED VS. CONVENTIONAL

HOWEVER!
Observe variation in CO emissions levels with turndown…
2. OPTIMIZATION STUDY RESULTS—STAGED VS. CONVENTIONAL
Based on CO constraints, staging provides better NOx AND turndown vs. reduced $\tau_{res}$.
PRELIMINARY CALCULATIONS: MIXING IMPACT

- Impact of non-infinite mixing was then investigated

- 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
• Initial test matrix to be single-point injection
• Goal of single-point test matrix is to establish relationship between $\Delta T$ & $\Delta NOx$ across test section
  – Want to decouple/investigate impact of specific jet trajectories $\rightarrow$ multiple injection diameters for $\Delta T$
• Establish a performance baseline with which to compare impact of multi-point injection
**Task 3.2: Test Section Constraints**

- Fuel split ($\Delta T$) 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 -> $\Delta T$’s
### TASK 3.2: FUEL ONLY TEST SPACE

<table>
<thead>
<tr>
<th></th>
<th>$d_j = 1.5\text{mm}$</th>
<th>$d_j = 3\text{mm}$</th>
<th>$d_j = 4.5\text{mm}$</th>
<th>$d_j = 6\text{mm}$</th>
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<tbody>
<tr>
<td>$J_{\text{min}}$</td>
<td>18.6</td>
<td>4.6</td>
<td>2.07</td>
<td>1.16</td>
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<tr>
<td>$J_{\text{max}}$</td>
<td>193.97</td>
<td>48.49</td>
<td>21.55</td>
<td>12.12</td>
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<tr>
<td>$\phi_{\text{global,min}}$</td>
<td>0.52</td>
<td>0.55</td>
<td>0.58</td>
<td>0.60</td>
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<tr>
<td>$\phi_{\text{global,max}}$</td>
<td>0.58</td>
<td>0.66</td>
<td>0.74</td>
<td>0.82</td>
</tr>
<tr>
<td>$\Delta T_{\text{min}} (\text{K})$</td>
<td>10</td>
<td>37</td>
<td>121</td>
<td>174</td>
</tr>
<tr>
<td>$\Delta T_{\text{max}} (\text{K})$</td>
<td>136</td>
<td>277</td>
<td>400</td>
<td>510</td>
</tr>
</tbody>
</table>

Overlapping ranges of $\Delta T$ achievable
**TASK 3.2: PREMIXED TEST SPACE**

<table>
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<tr>
<th></th>
<th>$d_j = 6\text{mm}$</th>
<th>$d_j = 9\text{mm}$</th>
<th>$d_j = 12\text{mm}$</th>
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</thead>
<tbody>
<tr>
<td>$J_{\text{min}}$</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$J_{\text{max}}$</td>
<td>23.73</td>
<td>10.55</td>
<td>5.93</td>
</tr>
<tr>
<td>$\Delta T_{\text{min}} (\text{K})$</td>
<td>7</td>
<td>15</td>
<td>25</td>
</tr>
<tr>
<td>$\Delta T_{\text{max}} (\text{K})$</td>
<td>20</td>
<td>30</td>
<td>42</td>
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$\Delta T$ values based on secondary injection $\Phi = 0.95$

- Maintain identical head end operation
- Secondary injection equivalence ratio to be varied to simulate degree of pre-ignition entrainment
- Lower achievable $\Delta T$ due to addition of air
TASK 4.1 LES STUDIES FOR SUBCOMPONENT GEOMETRY
• Computational procedure has been validated using LES for reacting (Hydrogen) Jet In Cross Flow (JICF) configuration
• 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 CH₄ mechanism to better match auto-ignition predicted by GRI 3.0

• Thermal NOx mechanism

\[
\text{Extended Zeldovich mech} \quad \left\{ \begin{array}{l}
\text{Zeldovich mech} \quad \begin{align*}
N_2 + O & \rightarrow NO + N \\
N + O_2 & \rightarrow NO + O \\
N + OH & \rightarrow NO + H
\end{align*}
\end{array} \right.
\]

• 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:

<table>
<thead>
<tr>
<th>Vitiated co-flow</th>
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<tbody>
<tr>
<td>P [atm]</td>
</tr>
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<td>1</td>
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</table>

- 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

<table>
<thead>
<tr>
<th>Jet parameters</th>
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<tr>
<td>$D_{jet}$ [mm]</td>
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<tr>
<td>4</td>
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</tbody>
</table>
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.
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
Mie scattering images of reacting JICF (sPIV)  
Simultaneous OH-PLIF image
VORETEX 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

Windward vortex growth

Normalized Circulation

Centerline coordinate

Leeward vortex growth

Normalized Circulation

Centerline coordinate

Reacting
Non-Reacting

Georgia Tech
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