Effect of Mixture Concentration Inhomogeneity on Detonation Properties in Pressure Gain Combustors

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Mechanical and Nuclear Engineering
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Pressure-gain combustion appeal and rotary detonation engines

Pressure gain combustion offers the potential of recovering and increasing the gas pressure lost in constant pressure combustion.

Gains in efficiency improvement have been estimated at potentially 5 to 10 percentage points, larger than most other single technological improvements (Idelchik, 2009)

Rotary detonation engines are a particularly promising technology for integration in gas turbines for power generation. In a rotating detonation engine (RDE), the detonation propagates azimuthally around an annulus while fresh reactants are injected axially through the annulus.

Advantages include continuous injection of reactants and quasi-steady exit flow profile.
Rotary detonation engine issues and the importance of inhomogeneity

Although a promising technology, several key issues must be addressed before rotary detonation engines can be implemented for power generation, including:

1) Measuring and controlling CO and NOx emissions
2) Reactant injection and reducing reverse flow
3) High local heat fluxes within the combustor
4) Quantifying actual pressure gain
5) Fuel-oxidizer mixing
6) Detonation-mixture inhomogeneity interaction

In a summary of the extensive RDE work completed at the Lavrent’ev Institute of Hydrodynamics, Bykovskii et al. (2006) concluded that “[t]he governing factor in obtaining an effective continuous detonation regime belongs to mixing in the region of transverse detonation wave propagation.”
• RDEs are especially prone to spatial variations in mixture concentration due to:
  – Short mixing times (0.05 to 1 msec), since the combustor mixture region must refill before the detonation wave passes the injector holes again
  – Time-varying reactant flow rates due to changes in pressure downstream of the injection holes as the detonation wave passes
In order to improve current rotary detonation engine designs to produce practical devices, the effect of concentration inhomogeneity on detonation properties will be determined.

The main objectives of this project are to:

1) determine the degree of fuel-oxidizer mixture concentration inhomogeneity in a rotary detonation engine

2) experimentally study the effects of inhomogeneity on detonation wave quality and stability (i.e., wave speed, planar vs non-planar, wave height, etc.)

3) perform a parametric study to better understand the relationships between combustor geometries and fuel/oxidizer injection.
Project Tasks and Accomplishments – Year 1

Year 1 focused on the design, construction, and assembly of the test facility and initial testing with hydrogen-air mixtures:

1) The parallel and perpendicular test channels were designed and the parallel channel was machined and assembled.

2) Measurement systems and other ancillary systems were assembled and tested.

3) Detonation measurements in several quiescent mixtures were completed as an initial test of the system.
Design and fabrication of the facility

Preliminary testing – parallel configuration

Future work
Overview of detonation facility

- Image shows all major components of the test facility
- Some components removed for clarity
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Detonation channel description

- Parallel test configuration shown
- Channel comprised of three main sections
- All sections bolted together to allow for geometry changes (no welds)
- Cross-section dimensions: 0.75” by 3.5”
- Overall length: ~10 ft.
- Sections are re-arranged to operate the test facility in different configurations
Detonation channel description

- Detonation initiated in DDT section
- Wave enters channel and expands along incline to prevent detonation wave failure
- Dilution air, water, and constrictions used to dampen detonation exiting combustor

- Location of fuel injection tubes is variable; allows for imagining of different parts of the fuel jet/air mixture without moving the optical window
- Channel can also be operated fully premixed
Channel wall sealing

- All channel walls sealed with silicone o-rings and o-ring cord stock
- “3D” o-ring design – silicone sealant used to connect o-rings at flanges
- Allows for relatively easy modification of the channel
Deflagration-to-detonation transition section

- O₂-H₂ mixture; spark plug (coil-on-plug type) ignition source
- 30” long DDT tube comprised of series of hollow cylinders (area reduction) and springs (hold spacing between cylinders)
- Pressure measured near tube exit
Optical access, schlieren, and PLIF systems

- Windows allow for complete optical access across the channel height
- Schlieren and PLIF optics aligned on single optics table
### Operating conditions / Measurement techniques

<table>
<thead>
<tr>
<th>Property</th>
<th>Range</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel composition</td>
<td>Hydrogen, blends of natural gas and hydrogen</td>
</tr>
<tr>
<td>Oxidizer composition</td>
<td>Air, oxygen, and oxygen-enriched air</td>
</tr>
<tr>
<td>Global equivalence ratio</td>
<td>Fuel lean through stoichiometric</td>
</tr>
<tr>
<td>Initial temperature</td>
<td>20 – 200°C</td>
</tr>
<tr>
<td>Initial pressure</td>
<td>1 – 4 atm</td>
</tr>
</tbody>
</table>

- In addition to the optical measurements described on the previous slide, the channel is instrumented with pressure transducers
  - 11 locations for pressure measurements
  - Velocities calculated from pressure measurements
  - Flush mounted with the inner channel wall
  - Used to trigger camera in schlieren system

- DAQ: 12 simultaneously sampled channels (2 to 4 MS/s/channel)
Perpendicular configuration (RDE simulation)

- Perpendicular test section is attached to part of the test channel to simulate an RDE
- Slow flow of fully premixed fuel/oxidizer used to establish planar detonation wave prior to interaction with the high velocity, perpendicular flow in the end section
- Gap width variable between 0.20 and 0.75 in. (discrete increments)
Presentation Outline

Design and fabrication of the facility

Future work

Preliminary testing – parallel configuration
Deflagration-to-detonation section example pressure curve

- Initial testing was completed with quiescent fully premixed H₂-air mixture in the channel
  - Premixed mixture produced using partial pressures
- Predetonator operated normally – stoichiometric mixture of H₂/O₂, 21°C, ~16.5 psia
- Figure demonstrates successful firing of predetonator device
  - Spark duration, spark gap width, and valve timing varied to achieve detonation
Example pressure profiles and detonation velocity calculation

- H₂-air stoichiometric mixture, 16.5 psia initial pressure, 21°C initial temperature
- Time delays calculated using a cross-correlation of the pressure signals
- Calculated velocity: 1921 m/s, ~2.5% below CJ velocity (1971 m/s)
Uniformity of detonation wave at exit of initiation section

- Three PTs installed at same axial location to measure uniformity of detonation wave
- Leading detonation wave is uniform heading into window test section (~4 μs difference, approximately equal to the travel time across each PT face)
Presentation Outline

Design and fabrication of the facility

Preliminary testing – parallel configuration

Future work
Next steps

- The channel is fully assembled and has been tested with quiescent mixtures of H₂ and air

- Move the channel to a reinforced test cell by mid-November
  - Additional safety precaution for inhomogeneous mixture tests

- Start detonation measurements of inhomogeneous mixtures in the parallel test configuration
  - Measure mixture concentration variations with PLIF system
  - Schlieren imaging of detonation structures

- In addition, fully premixed detonation testing will be performed for comparison with mixtures with concentration variations
Additional tasks to be completed in Year 2

• In addition to parallel configuration detonation testing, measurements of the concentration variation in simulated RDE configurations is expected to begin next spring

• Will start with configuration shown on right
  – H₂ jets: round holes
  – Air jet: slot

• Variable gap width, H₂ hole diameter, air slot width

• Perpendicular test section can be swapped out for testing of different geometries (H₂-air coflow configuration, for example)
Future work / project goals

- Mixing conditions that result in leading wave separation from the reaction zone

- Effect of mixedness on detonation cell structure and propagation mode (stable, spinning, galloping waves)
  - affects detonation velocity and peak local pressures

- Measure leading wave front angle and detonation wave lift-off height above injection plane in a simulated RDE channel
Thank you!

Questions?
## Project tasks – Year One

<table>
<thead>
<tr>
<th>Task</th>
<th>Quarter</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0 Project Management and Planning</td>
<td>● ● ● ● ● ● ● ● ● ●</td>
</tr>
<tr>
<td>2.0 Design detonation channel and safety enclosure modifications</td>
<td>● ● ● ● ● ● ● ● ● ●</td>
</tr>
<tr>
<td>3.0 Machining and setup of facility</td>
<td>● ● ● ● ● ● ● ● ● ●</td>
</tr>
<tr>
<td>4.0 Determine the nature of detonation-inhomogeneity interaction in the <em>parallel</em> interaction configuration</td>
<td>● ● ● ● ● ● ● ● ● ●</td>
</tr>
<tr>
<td>5.0 Determine the nature of detonation-inhomogeneity interaction in the <em>perpendicular</em> interaction configuration</td>
<td>● ● ● ● ● ● ● ● ● ●</td>
</tr>
<tr>
<td>6.0 Development of design guidelines and rules for detonation-inhomogeneity interaction</td>
<td>● ● ● ● ● ● ● ● ● ●</td>
</tr>
<tr>
<td>7.0 Reporting</td>
<td>● ● ● ● ● ● ● ● ● ●</td>
</tr>
</tbody>
</table>

- **Year 1:** Design and build detonation channel modifications
  Test mixtures in the parallel configuration
### Project tasks – Years 2 and 3

<table>
<thead>
<tr>
<th>Task</th>
<th>Quarter</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.0 Project Management and Planning</td>
<td>● ● ● ● ● ● ● ● ● ●</td>
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<tr>
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</tr>
<tr>
<td>3.0 Machining and setup of facility</td>
<td>● ● ● ● ● ● ● ● ● ●</td>
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</tr>
<tr>
<td>7.0 Reporting</td>
<td>● ● ● ● ● ● ● ● ● ●</td>
</tr>
</tbody>
</table>

- **Year 2:** Finish testing in the parallel configuration  
  Test mixtures in the perpendicular configuration  

- **Year 3:** Finish testing in the perpendicular configuration  
  Elevated pressure and temperature testing  
  Develop design guidelines and rules for detonation-inhomogeneity interaction
Thank you!

Project Objectives:

1) determine the degree of fuel-oxidizer mixture concentration inhomogeneity in a rotary detonation engine with a simple injector geometry widely used by the RDE experimental community fueled by hydrogen and hydrogen/natural gas blends with air

2) experimentally study the effects of inhomogeneity on detonation wave quality and stability (i.e., wave speed, planar vs non-planar, wave height, etc.)

3) perform a parametric study of combustor geometries and fuel/oxidizer injection.
Extra slides
### Previous studies on detonation-inhomogeneity interaction

<table>
<thead>
<tr>
<th>Author</th>
<th>Year</th>
<th>Experimental or Numerical</th>
<th>Perpendicular or Parallel</th>
<th>Mixture</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mikhalkin</td>
<td>1996</td>
<td>N</td>
<td>N/A</td>
<td>C₂H₄-O₂, CH₄-O₂</td>
<td>Regions of poorly mixed gases have a similar effect as inert diluents on detonation properties</td>
</tr>
<tr>
<td>Kuznetsov</td>
<td>1998</td>
<td>E</td>
<td>=</td>
<td>H₂-Air</td>
<td>Strong mixture concentration gradients dampen detonation propagation</td>
</tr>
<tr>
<td>Brophy</td>
<td>2006</td>
<td>E</td>
<td>⊥</td>
<td>C₂H₄-Air</td>
<td>Fuel distribution effects in a PDE</td>
</tr>
<tr>
<td>Bykovskii</td>
<td>2006</td>
<td>E</td>
<td>⊥</td>
<td>Various mixtures</td>
<td>Summary of RDE experiments highlighted the effects of poor mixing on operation</td>
</tr>
<tr>
<td>Ishii</td>
<td>2007</td>
<td>E</td>
<td>⊥</td>
<td>H₂-O₂, H₂-O₂-N₂</td>
<td>Deflection of detonation wave, skewing of cell structure and changes in detonation velocity</td>
</tr>
<tr>
<td>Kessler</td>
<td>2012</td>
<td>N</td>
<td>=</td>
<td>CH₄-Air</td>
<td>Shock wave-combustion zone decoupling led to turbulent deflagration</td>
</tr>
<tr>
<td>Ettner</td>
<td>2013</td>
<td>N</td>
<td>⊥</td>
<td>H₂-O₂</td>
<td>Concentration gradient effected on detonation cell shape, instability, and pressure distribution</td>
</tr>
<tr>
<td>Nordeen</td>
<td>2013</td>
<td>N</td>
<td>⊥</td>
<td>H₂-Air</td>
<td>Simulation of an RDE with variable mixedness</td>
</tr>
<tr>
<td>Driscoll</td>
<td>2015</td>
<td>N</td>
<td>N/A</td>
<td>H₂-Air</td>
<td>Simulation of mixing in a RDE</td>
</tr>
</tbody>
</table>

- Studies highlighted in red are discussed in further detail in later slides
Detonation propagation and cell structure

1. Transverse shock waves travelling in opposite directions periodically collide, producing regions of high temperature and pressure.

2. The leading shock is initially accelerated at the triple-point track interaction location, and then decelerates and weakens as the gas expands.

3. This process repeats cyclically after another transverse wave interaction.

(modified from Austin, 2003)

Shear Layers

Transverse Waves

Triple-Point Tracks

Leading shock

Shadowgraph
\(2H_2-O_2-3N_2\)

Smoke foil record of triple-point tracks
\(2H_2-O_2-2N_2\)

(Shepherd, 2009)
Previous studies on detonation-inhomogeneity interaction

- Majority of experimental studies relied on diffusion to produce concentration gradients

- For example, Ishii (2007) showed that concentration gradients can “skew” the leading detonation wave, resulting in irregular cell structures and a reduction in wave velocity

- Other studies have shown that inhomogeneity can result in shock waves decoupling from the combustion zone (resulting in turbulent deflagrations), a reduction or an increase in peak detonation pressure, and changes in mixture failure limits
Fuel-oxidizer mixing in an example RDE

- Simulation of H₂-air mixing in the Shank (2012) rotary detonation engine

- Authors found low fuel penetration into the air cross-flow near the injection location at baseline condition

- Air mass flux, fuel mass flux, and fuel injection location were varied

Figure 5: Contours of Equivalence Ratio for Case 1.00_1.0

(Driscoll, 2015)
Typical rotary detonation engine configurations

Previous studies of detonation-inhomogeneity interaction

Penn State’s detonation tube facility and other gaseous detonation work

Pressure [psig] vs. Time [ms]

- 2365 m/s
- 2358 m/s
- 2370 m/s

Technical Background
Confined channel – detonation interaction study facility

Overall length: 4.93 m
Inner diameter: 2.43 cm
L/D ≈ 200

Vacuum system, gas mixing/delivery system, etc. not shown
Example pressure profiles and detonation velocity calculation

- $\text{C}_3\text{H}_8$-$\text{O}_2$ stoichiometric mixture, 13.5 psia initial pressure, 21°C initial temperature
- Time delay calculated using a cross-correlation of the pressure signals
- Detonation velocity calculated from time delay and distance between transducer pairs

Reflected shock wave arrives ~15 μs after initial detonation wave

Pressure [psig]

2358 m/s 2370 m/s 2365 m/s
Detonation velocity v. initial pressure

\[
\text{CH}_4 + 2\text{O}_2
\]

\[
\text{CH}_4 + 2\text{O}_2 + 0.86\text{N}_2
\]

- \text{CH}_4–\text{O}_2–\text{N}_2 mixtures tested with nitrogen concentration between 0\% and 30\%
- Increasing the nitrogen concentration increased the initial pressure where the measured velocity began to significantly deviate from the predicted velocity
General technical approach

• In order to increase measurement access, an “unwrapped” RDE will be tested in this study:

• Two configurations (parallel and perpendicular) will also be tested
• Configuration will provide fundamental data on the role of concentration inhomogeneity on detonation propagation

• Spatial variations in fuel concentration measured using acetone-PLIF

• Measurements: pressure fluctuations, chemiluminescence intensity images, smoke foil records, and schlieren images

• The effect of inhomogeneity on detonation pressure, velocity, failure limits, propagation mode (planar or non-planar) will be determined
Perpendicular configuration illustration

- Representative of a rotary detonation engine configuration
- Variable gap widths, combustor lengths, and reactant injection geometries will be tested to better understand the relationship between geometry and detonation propagation
- Same measurements as parallel configuration, plus:
  - concentration inhomogeneity present in a rotary detonation engine
  - leading detonation wave front angle
  - detonation lift-off height above the injector plane
Project Tasks
Risk management

Several technical risks have been identified:

1. Failure of the detonation channel during testing
   - Due to the unstable nature of the mixtures in this study, pressure piling is possible, leading to equivalent pressures that may cause wall failure
   - Mitigated by previous experience in designing enclosed detonation facilities, porous boundaries/dilution gases in exhaust, high energy “prompt” ignition sources, and protective shield surrounding entire experiment

2. Acetone-PLIF measurement of local fuel concentration
   - For H₂-air test mixtures, acetone-PLIF images may not provide an accurate measurement of local fuel concentration due to the difference in diffusive properties between acetone and hydrogen
   - Due to the high injection velocities and turbulence levels typically found in RDEs, mixing may be dominated by turbulence
   - If analysis shows that acetone cannot be used a marker for the local fuel concentration, another appropriate method will be used.
Risk management

3. Smoke-foil records (soot deposited on thin sheet of metal)
   • Used in detonation studies since the 1940s; however, mixture is typically quiescent
   • High velocity flow may remove soot from foil
   • Fixative can be added to soot, or another technique for measuring cell structure will be used (open shutter photography, schlieren imaging)

Smoke-foil record example of an unstable mixture (irregular detonation cell structure)

(Austin, 2003)

4. Effects of turbulence on detonation properties
   • To separate out the effects of mixture inhomogeneity and turbulence, additional measurements will be completed with fully premixed, turbulent mixtures
   • Results still relevant since test geometry will match RDE geometry
References


### Project Milestones

<table>
<thead>
<tr>
<th>Q3</th>
<th>Design, construction, and assembly of the detonation channel facility</th>
</tr>
</thead>
<tbody>
<tr>
<td>Q4</td>
<td>Local fuel concentration measurements in the parallel test configuration</td>
</tr>
<tr>
<td>Q4</td>
<td>Initial detonation property measurements in the parallel test configuration</td>
</tr>
<tr>
<td>Q6</td>
<td>Local fuel concentration measurements in the perpendicular test configuration</td>
</tr>
<tr>
<td>Q7</td>
<td>Initial detonation property measurements in the perpendicular test configuration</td>
</tr>
<tr>
<td>Q9</td>
<td>Successful operation of the test facility at elevated initial pressure and temperature</td>
</tr>
<tr>
<td>Q12</td>
<td>Detonation structure characterization for property normalization across all conditions</td>
</tr>
</tbody>
</table>

- Seven milestones were chosen for the three year project. These milestones are all necessary to achieve the goals of the project and completion of these milestones will indicate progress towards the overall project goals and objectives.
Summary of RDE operating characteristics and dimensions

<table>
<thead>
<tr>
<th>Author</th>
<th>Location</th>
<th>Year</th>
<th>Mixture</th>
<th>Frequency [kHz]</th>
<th>Length (L) [mm]</th>
<th>Gap Width (Δ) [mm]</th>
<th>Cell Width* [mm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Liu</td>
<td>Hunan, China</td>
<td>2012</td>
<td>H₂ – air</td>
<td>~5.5</td>
<td>75</td>
<td>5</td>
<td>6 – 10</td>
</tr>
<tr>
<td>Thomas</td>
<td>Wright-Patt</td>
<td>2011</td>
<td>C₂H₄ – O₂</td>
<td>~8</td>
<td>153</td>
<td>2, 6, 10</td>
<td>2 – 3</td>
</tr>
<tr>
<td>Shank</td>
<td>Wright-Patt</td>
<td>2012</td>
<td>H₂ – air</td>
<td>2.9 – 3.3</td>
<td>140</td>
<td>7.6</td>
<td>6 – 10</td>
</tr>
<tr>
<td>Braun</td>
<td>UT Arlington</td>
<td>2010</td>
<td>H₂ – O₂, C₃H₈ – O₂</td>
<td>15.6, 13.7</td>
<td>127</td>
<td>12.7</td>
<td>1 – 2, 0.5 – 1</td>
</tr>
<tr>
<td>Kindracki</td>
<td>Warsaw University of Technology</td>
<td>2011</td>
<td>CH₄ – O₂, C₂H₆ – O₂, C₃H₈ – O₂</td>
<td>13 – 14</td>
<td>30 mm + conic section</td>
<td>4</td>
<td>2 – 4, 1 – 2, 0.5 – 1</td>
</tr>
<tr>
<td>Bykovskii</td>
<td>Lavrent’ev Institute (Novosibirsk)</td>
<td>1980, 2008, 2011</td>
<td>CH₄ – O₂, C₂H₂ – O₂, H₂ – O₂, H₂ – air</td>
<td>13 – 14, 13 – 17, ~40</td>
<td>40 – 85, 20 – 85, 395 or 510</td>
<td>5, 1.25 – 5, 23</td>
<td>2 – 4, 0.1 – 0.2, 1 – 2, 6 – 10</td>
</tr>
</tbody>
</table>

*Unconfined, stoichiometric mixture, atmospheric pressure

- Wide variety of mixtures and geometries have been tested
  - H₂ + Air or O₂ + hydrocarbon, due to narrow gap widths typical of RDEs
  - Combustor lengths (L) typically greater than 10× gap widths (Δ) – high aspect ratios

- Frequency of wave propagation determines reactant refill time
RDE configuration illustrations (cross sections through combustor)

- Two typical RDE configurations are shown above
  - Fuel is typically injected through holes
  - Oxidizer is injected through either a slot or holes

Δ: 2 – 23 mm
L: 20 – 510 mm