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

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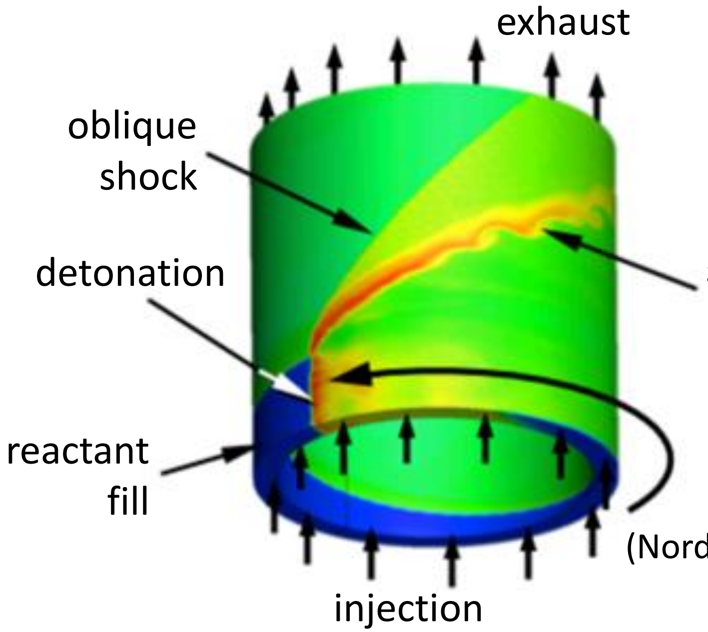
# Pressure-gain combustion appeal and rotary detonation engines

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)



(Nordeen, 2013)

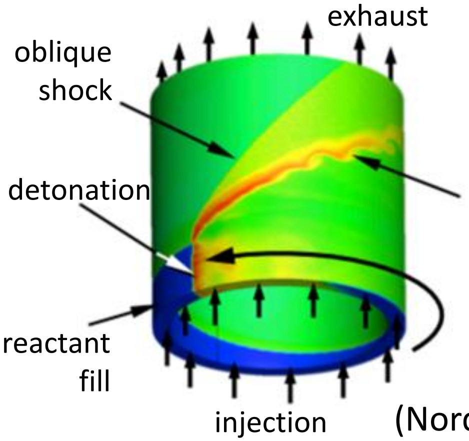
Rotary detonation engines are a particularly promising technology for integration in gas turbines for power generation. In a rotating detonation engine (RDE), the detonation propagates azimuthally around an annulus while fresh products are injected axially through the annulus .

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) Quantifing actual pressure gain
5) Fuel-oxidizer mixing
6) Detonation-mixture inhomogeneity interaction



(Nordeen, 2013)

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."

# Project Objectives

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:

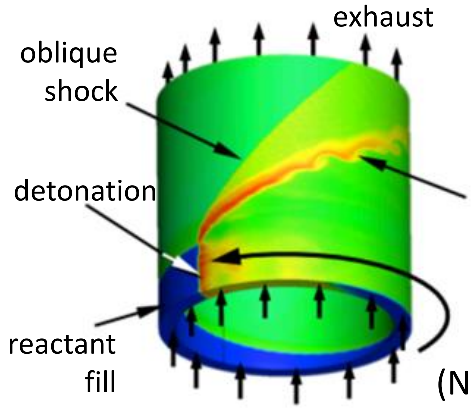
1) determine the degree of fuel-oxidizer mixture concentration inhomogeneity in a rotary detonation engine with a simple injector geometry widely used by the RDE experimental community fueled by hydrogen and hydrogen/natural gas blends with air

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

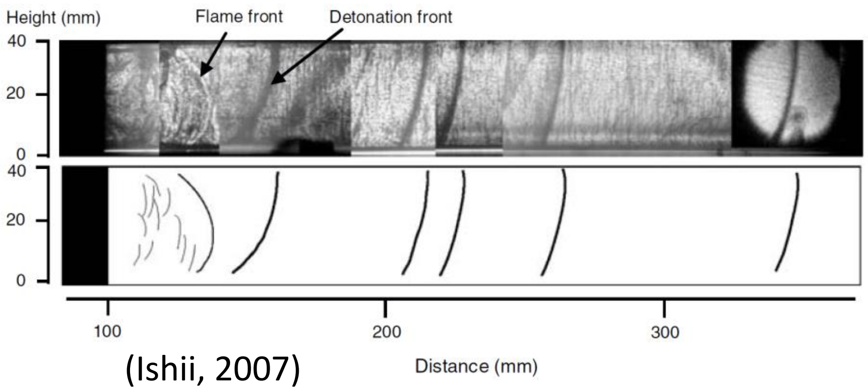
3) perform a parametric study to better understand the relationships between combustor geometries and fuel/oxidizer injection.

# Technical Background

Typical rotary detonation engine configurations



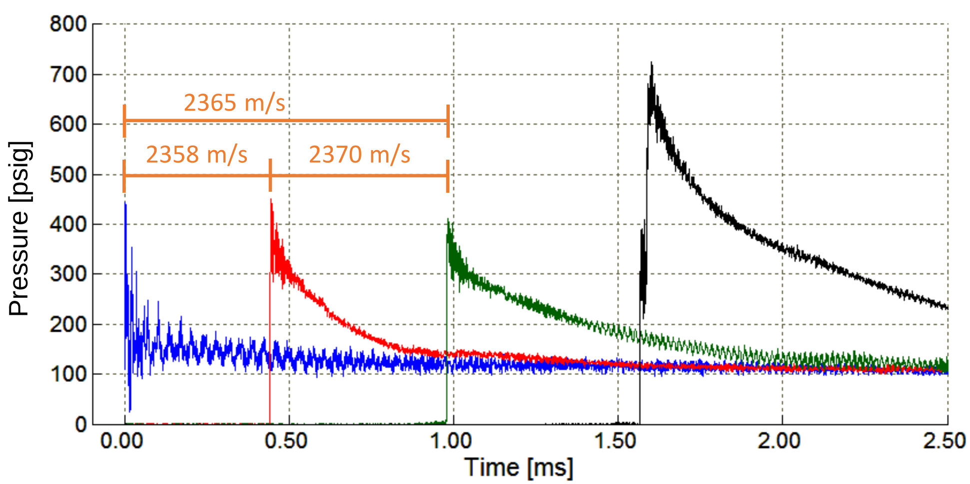

(Nordeen, 2013)




(Ishii, 2007)

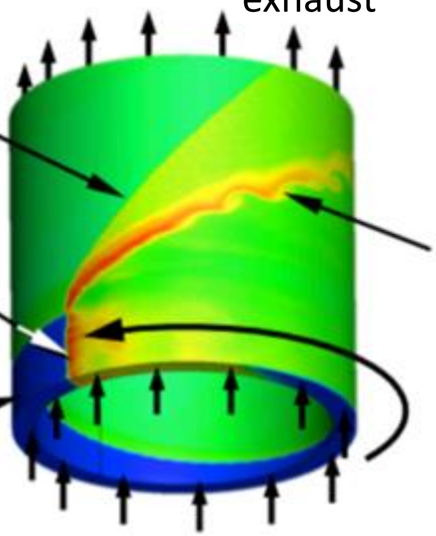
Previous studies of detonation-inhomogeneity interaction

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



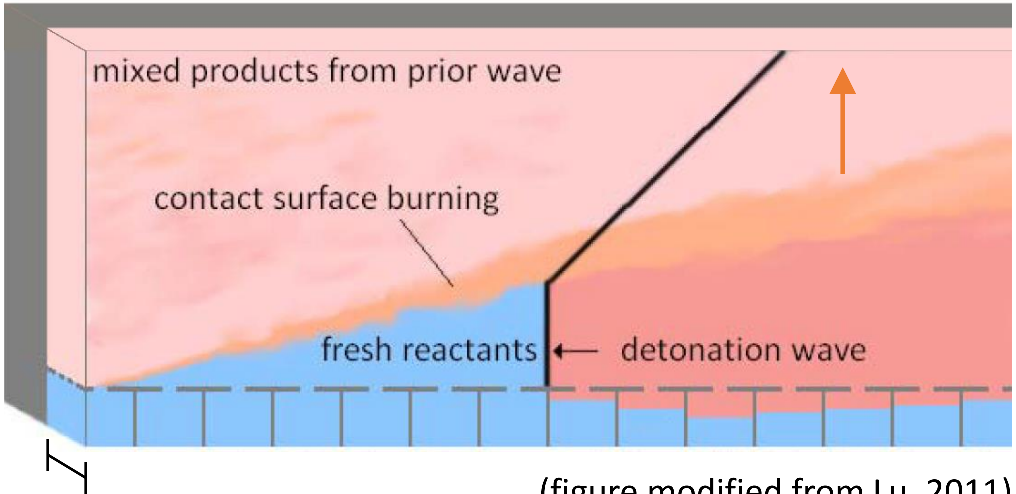
# RDE schematics and geometric influences on mixing

RDE illustration




(Nordeen, 2013)

RDE flow schematic




(figure modified from Lu, 2011)

- 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

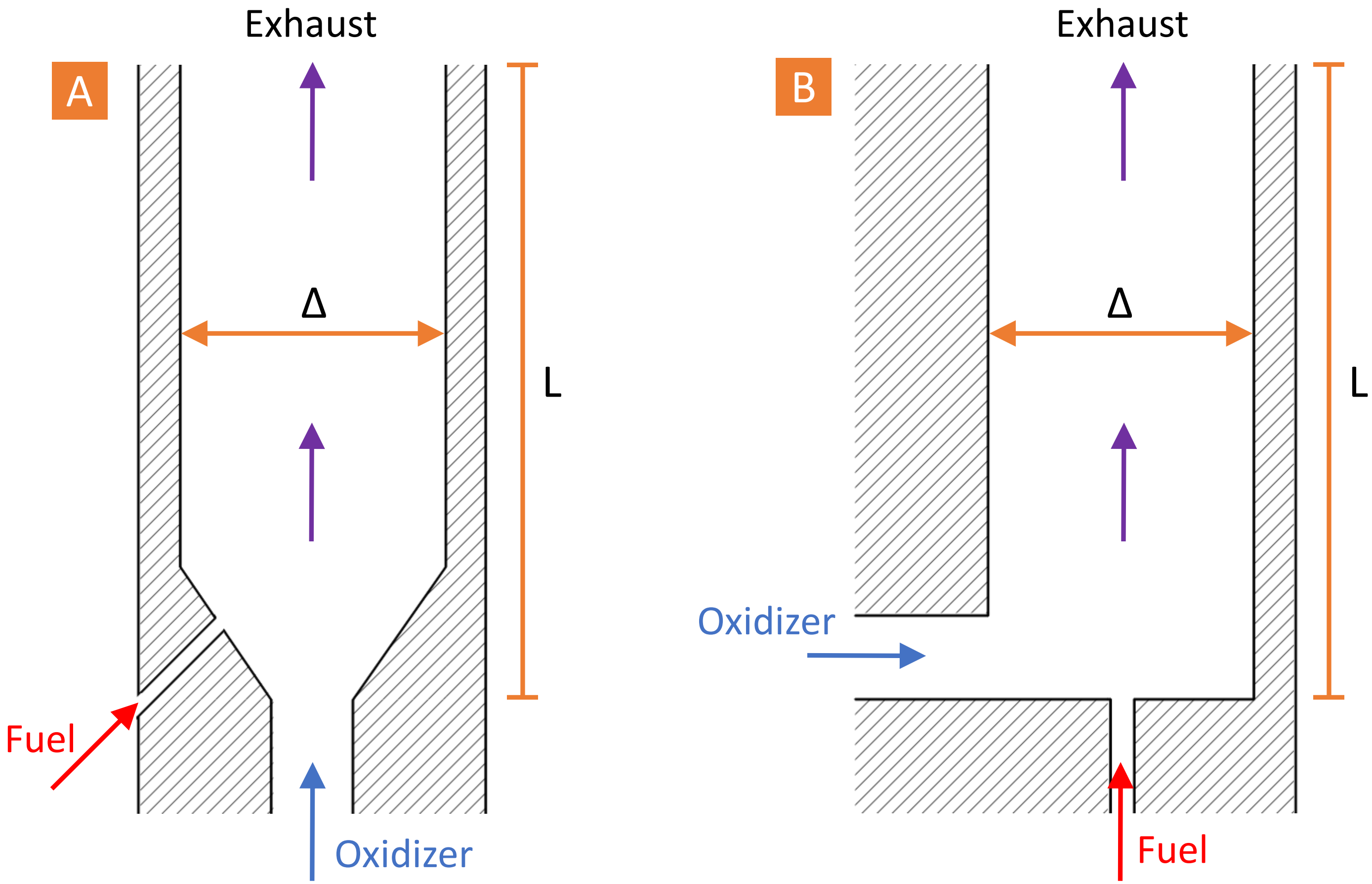
# Summary of RDE operating characteristics and dimensions

| Author | Location | Year | Mixture | Frequency [kHz] | Length (L) [mm] | Gap Width (Δ) [mm] | Cell Width* [mm] |
|---|---|---|---|---|---|---|---|
| Liu | Hunan, China | 2012 | $H_2$ – air | ~5.5 | 75 | 5 | 6 – 10 |
| Thomas | Wright-Patt | 2011 | $C_2H_4 - O_2$ | ~8 | 153 | 2, 6, 10 | 2 – 3 |
| Shank | Wright-Patt | 2012 | $H_2$ – air | 2.9 – 3.3 | 140 | 7.6 | 6 – 10 |
| Braun | UT Arlington | 2010 | $H_2 - O_2$<br>$C_3H_8 - O_2$ | 15.6<br>13.7 | 127 | 12.7 | 1 – 2<br>0.5 – 1 |
| Kindracki | Warsaw University of Technology | 2011 | $CH_4 - O_2$<br>$C_2H_6 - O_2$<br>$C_3H_8 - O_2$ | 13 – 14 | 30 mm + conic section | 4 | 2 – 4<br>1 – 2<br>0.5 – 1 |
| Bykovskii | Lavrent'ev Institute (Novosibirsk) | 1980<br>1980<br>2008<br>2011 | $CH_4 - O_2$<br>$C_2H_2 - O_2$<br>$H_2 - O_2$<br>$H_2$ – air | 13 – 14<br>13 – 17<br>~40<br>1.4 | 40 – 85<br>20 – 85<br>100<br>395 or 510 | 5<br>1.25 – 5<br>5<br>23 | 2 – 4<br>0.1 – 0.2<br>1 – 2<br>6 – 10 |

*Unconfined, stoichiometric mixture, atmospheric pressure

- Wide variety of mixtures and geometries have been tested
  - $H_2$ + Air or $O_2$ + hydrocarbon, due to narrow gap widths typical of RDEs
  - Combustor lengths (L) typically greater than 10× gap widths (Δ) – high aspect ratios
- The NETL RDE is based on the design used in Shank (2012), correct?

# RDE configuration illustrations (cross sections through combustor)




Δ: 2 – 23 mm
L: 20 – 510 mm

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

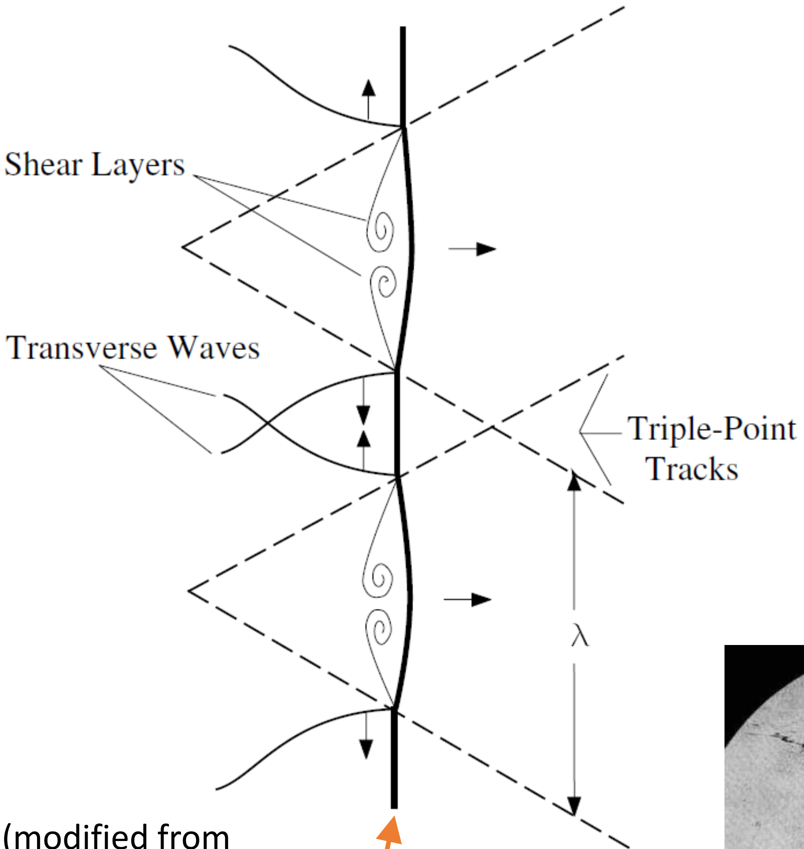
<u>NETL RDE?</u>
Type B
Δ = 7.6 mm
L = 140 mm

# Previous studies on detonation-inhomogeneity interaction

| Author | Year | Experimental or Numerical | Perpendicular or Parallel | Mixture | Description |
|---|---|---|---|---|---|
| Mikhalkin | 1996 | N | N/A | $C_2H_4$-$O_2$<br>$CH_4$-$O_2$ | Regions of poorly mixed gases have a similar effect as inert diluents on detonation properties |
| Kuznetsov | 1998 | E | = | $H_2$-Air | Strong mixture concentration gradients dampen detonation propagation |
| Brophy | 2006 | E | ⊥ | $C_2H_4$-Air | Fuel distribution effects in a PDE |
| Bykovskii | 2006 | E | ⊥ | Various mixtures | Summary of RDE experiments highlighted the effects of poor mixing on operation |
| Ishii | 2007 | E | ⊥ | $H_2$-$O_2$<br>$H_2$-$O_2$-$N_2$ | Deflection of detonation wave, skewing of cell structure and changes in detonation velocity |
| Kessler | 2012 | N | = | $CH_4$-Air | Shock wave-combustion zone decoupling led to turbulent deflagration |
| Ettner | 2013 | N | ⊥ | $H_2$-$O_2$ | Concentration gradient effected on detonation cell shape, instability, and pressure distribution |
| Nordeen | 2013 | N | ⊥ | $H_2$-Air | Simulation of an RDE with variable mixedness |
| Driscoll | 2015 | N | N/A | $H_2$-Air | Simulation of mixing in a RDE |

- Studies highlighted in red are discussed in further detail in later slides

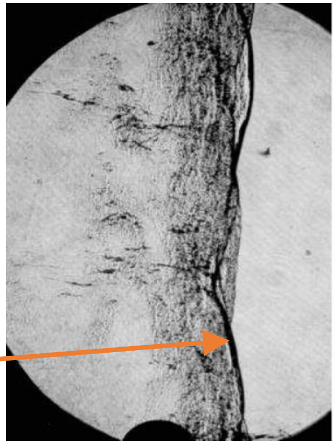
# Detonation propagation and cell structure



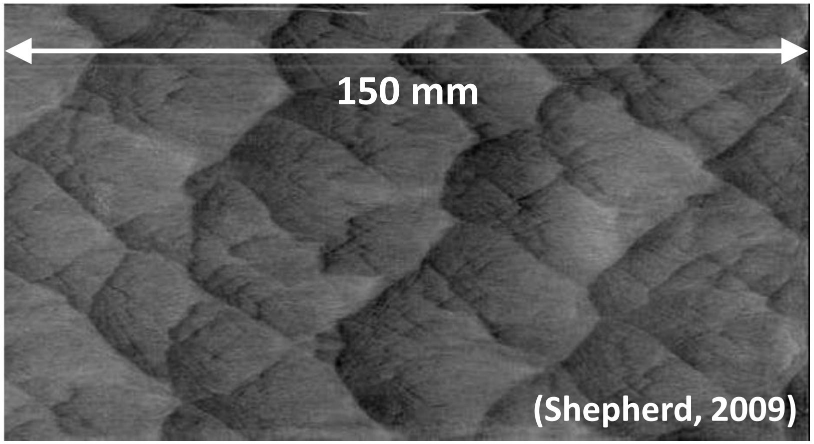

(modified from Austin, 2003)

Leading shock

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



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

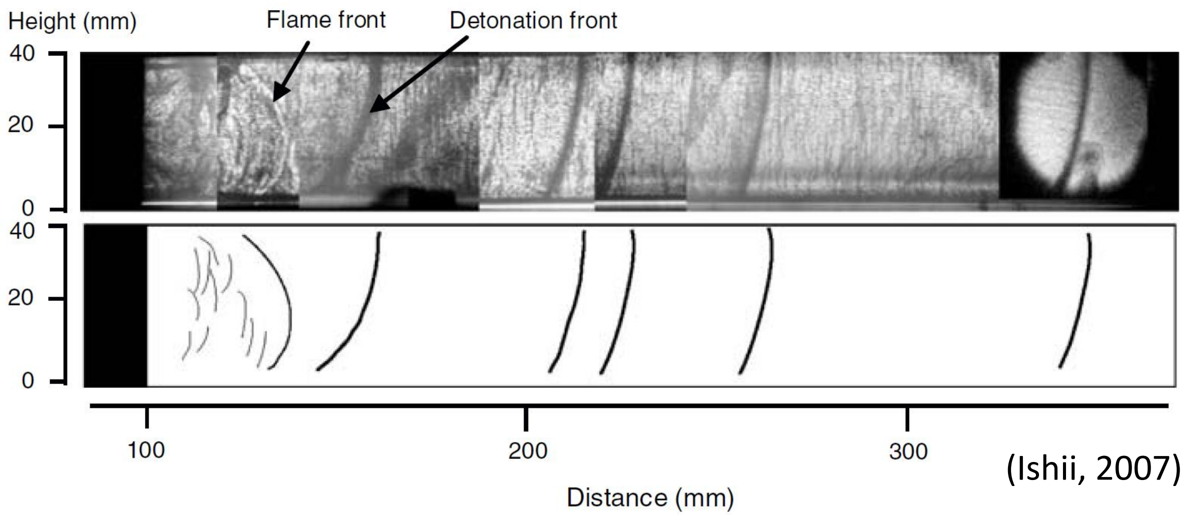



Smoke foil record of triple-point tracks ($2H_2$-$O_2$-$2N_2$)

# Previous studies on detonation-inhomogeneity interaction

- Majority of experimental studies relied on diffusion to produce concentration gradients
- However, these experiments and simulations yield some insight to the importance of detonation-inhomogeneity interaction in RDEs

direction of detonation propagation




direction of $O_2$ diffusion

(Ishii, 2007)

- 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

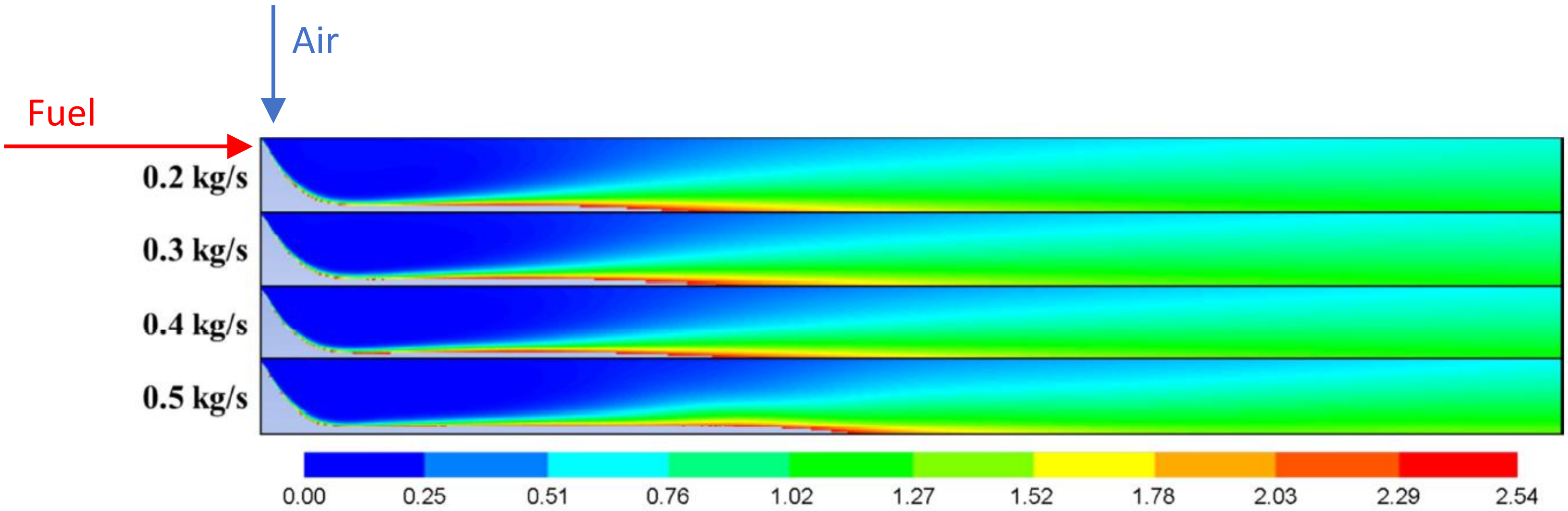
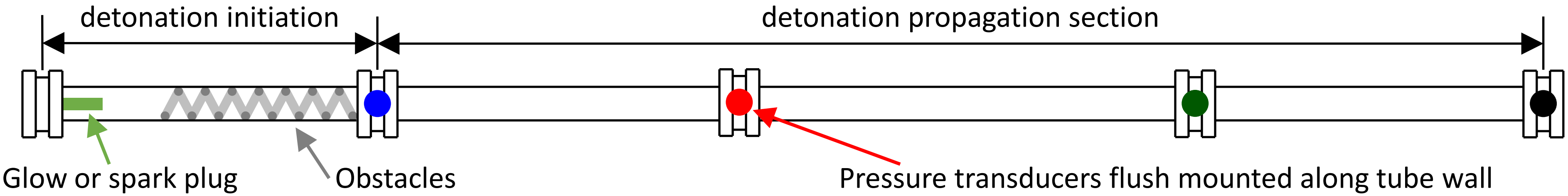


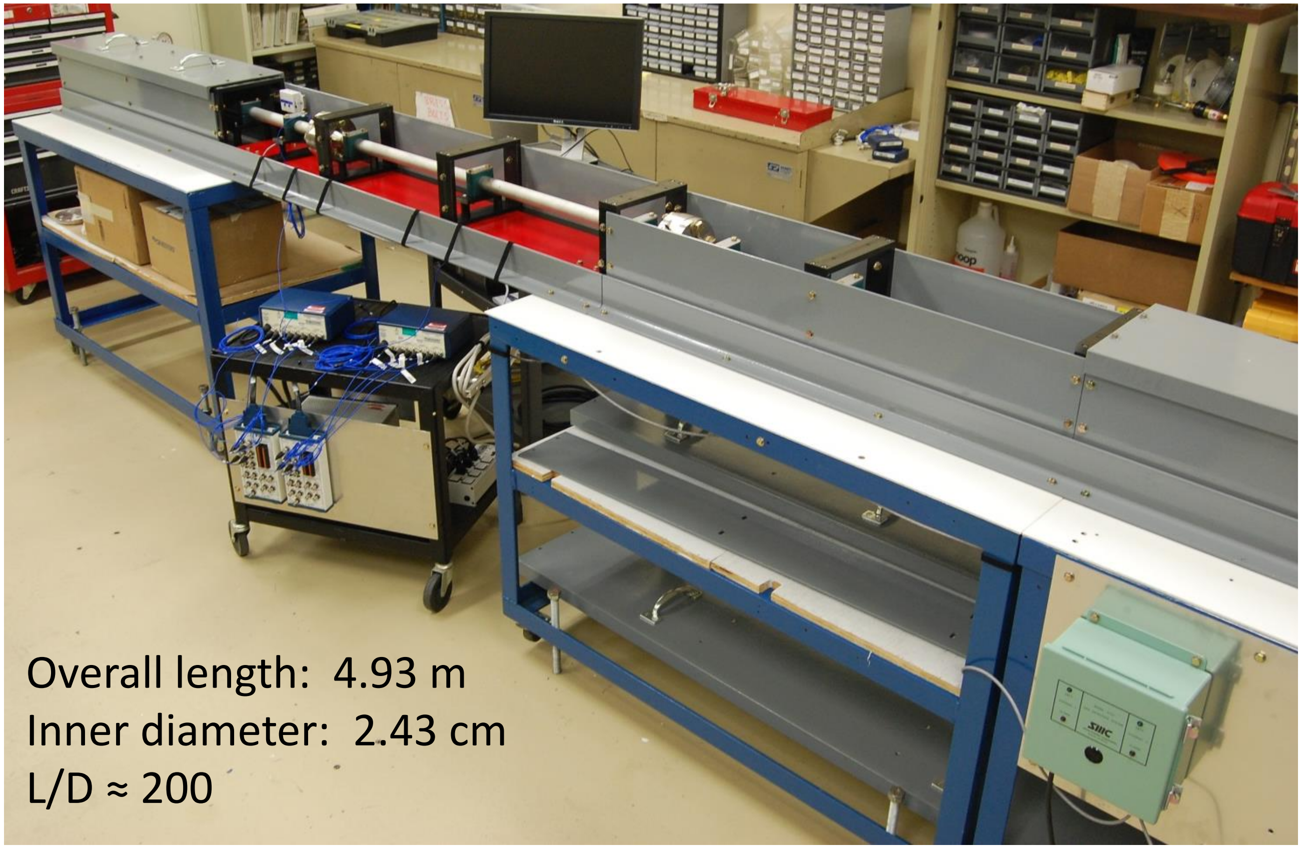

**Figure 5: Contours of Equivalence Ratio for Case 1.00_1.0**

(Driscoll, 2015)

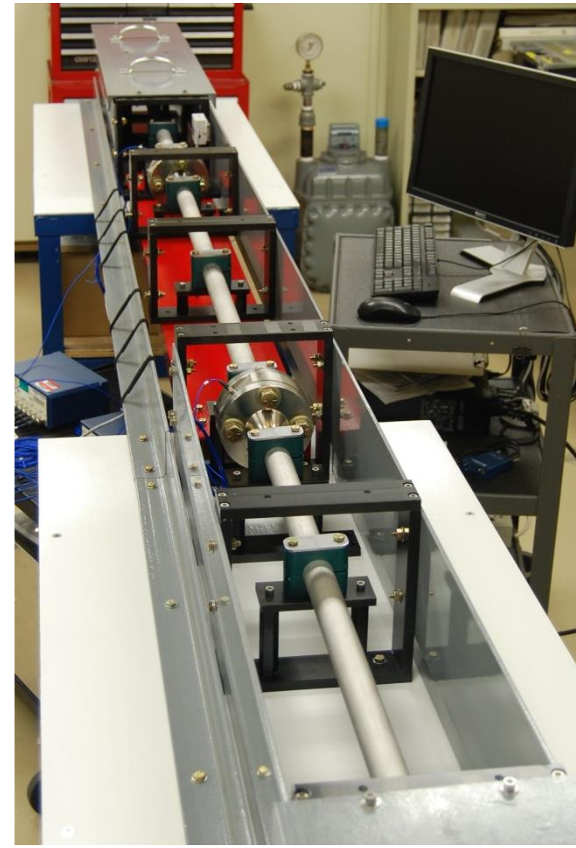
- Simulation of $H_2$-air mixing in the Shank (2012) rotary detonation engine
- Authors found low fuel penetration into the air cross-flow near the injection location at baseline condition
- Air mass flux, fuel mass flux, and fuel injection location were varied

# Confined channel – detonation interaction study facility



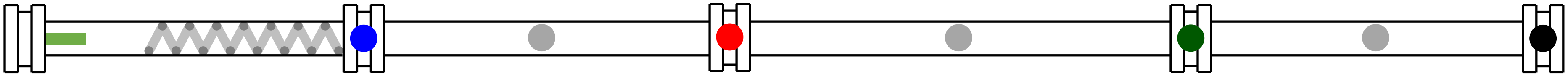



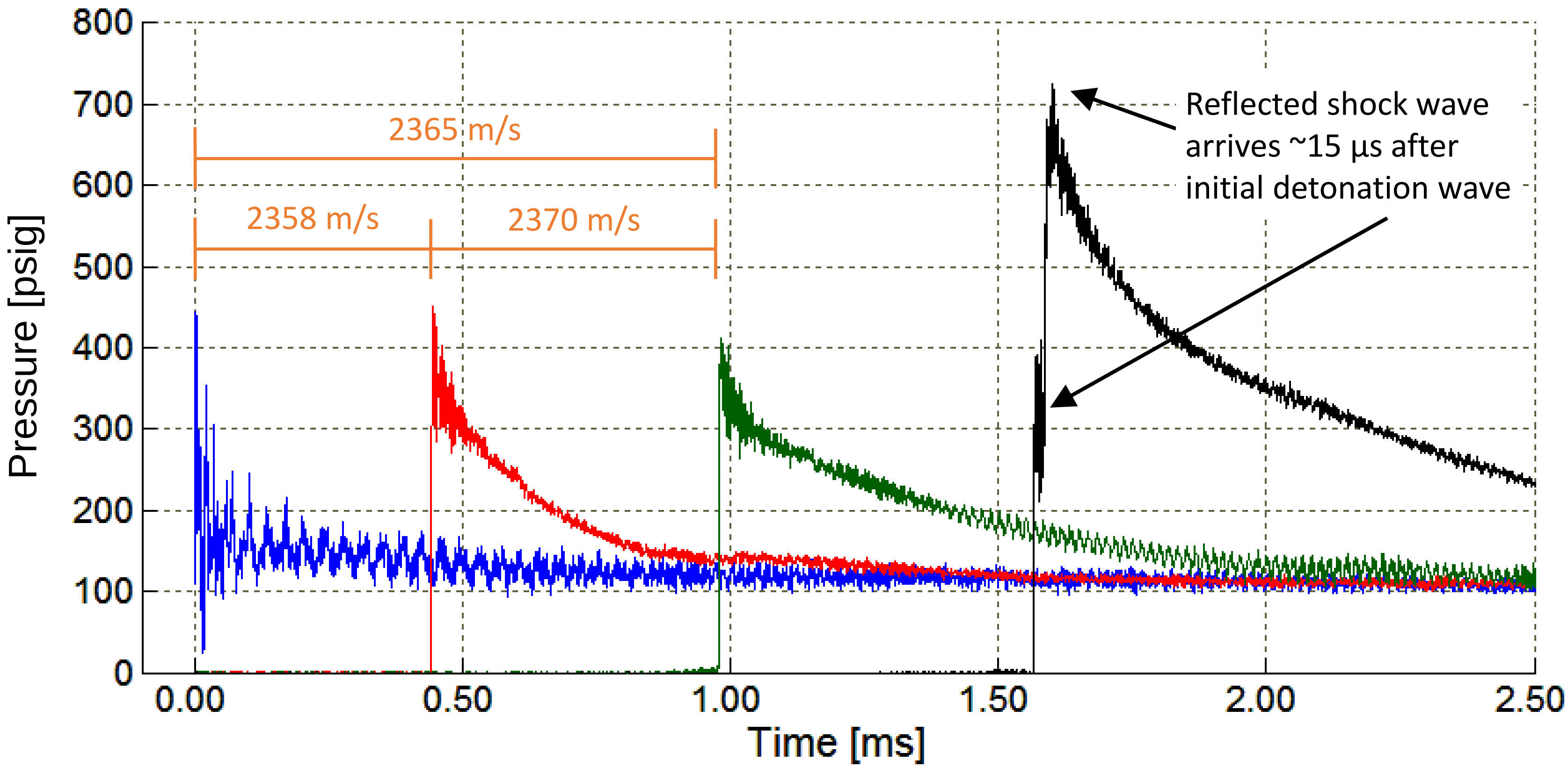
Overall length: 4.93 m
Inner diameter: 2.43 cm
L/D ≈ 200



Vacuum system, gas mixing/delivery system, etc. not shown

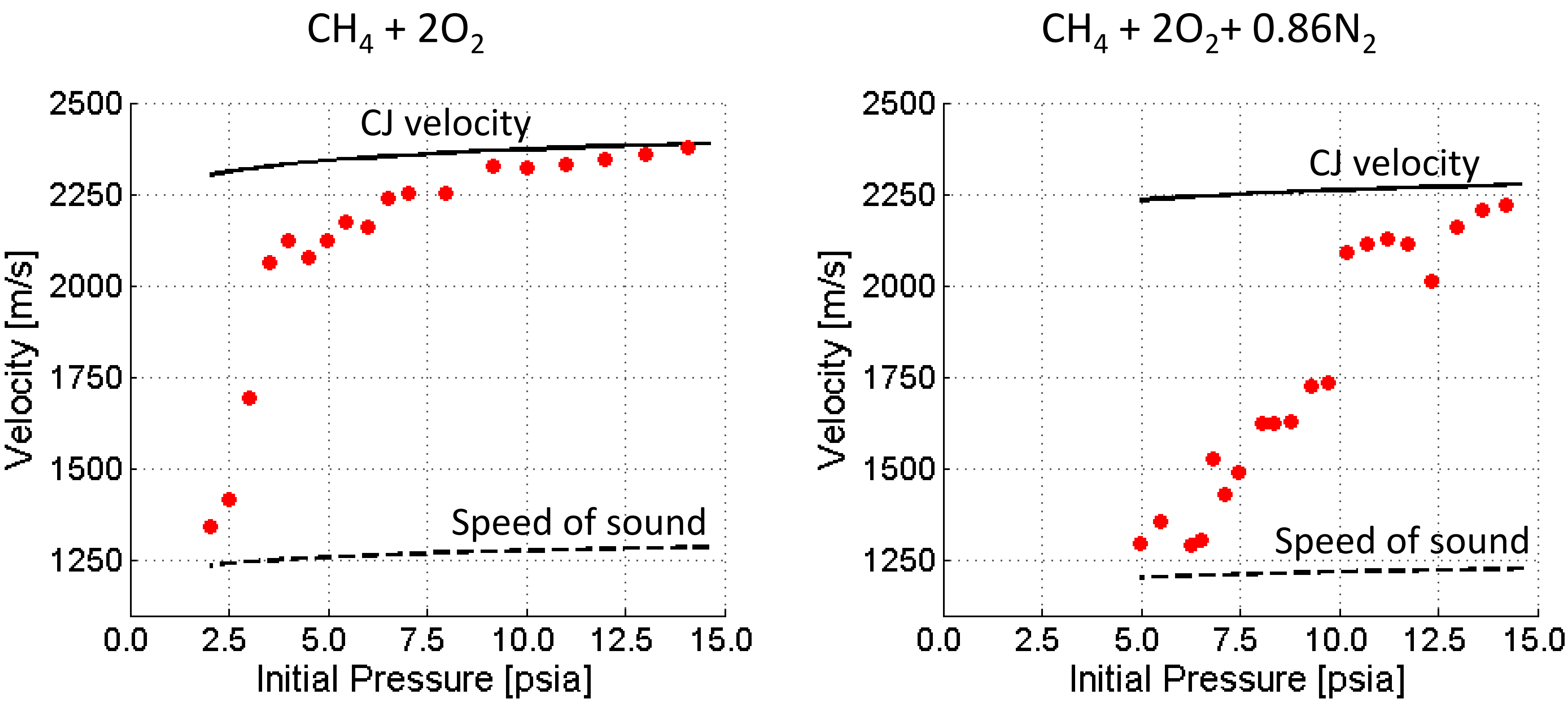
# Example pressure profiles and detonation velocity calculation






- $C_3H_8$-$O_2$ 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

# Detonation velocity v. initial pressure

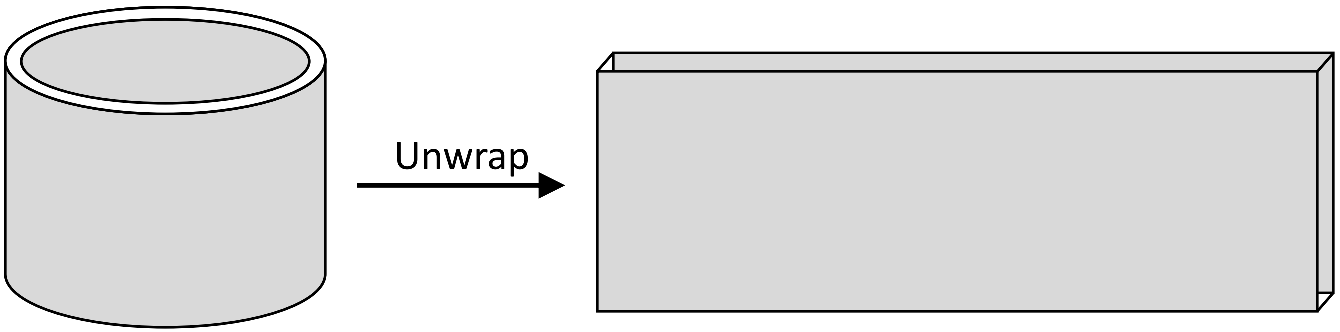



- $CH_4$–$O_2$–$N_2$ mixtures tested with nitrogen concentration between 0% and 30%
- Increasing the nitrogen concentration increased the initial pressure where the measured velocity began to significantly deviate from the predicted velocity

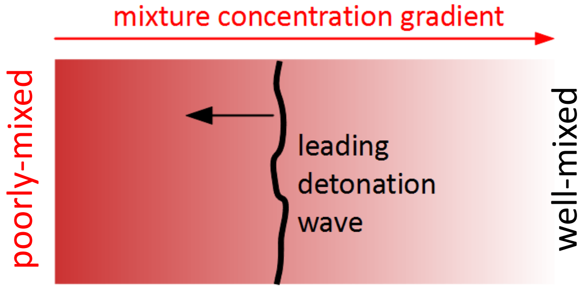
# Technical Approach

# Previous studies on detonation-inhomogeneity interaction

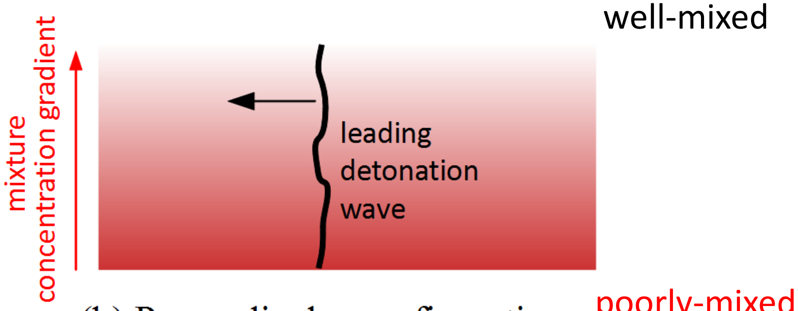
- In order to increase measurement access, an “unwrapped” RDE will be tested in this study:




- Two configurations (parallel and perpendicular) will also be tested

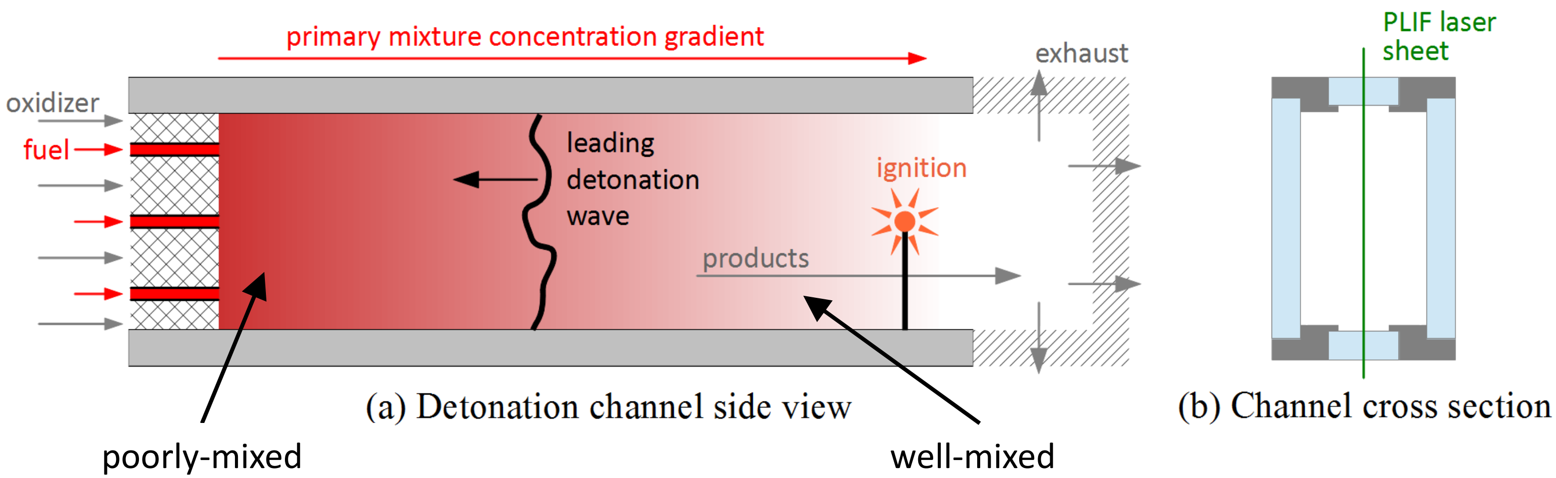



(a) Parallel configuration




(b) Perpendicular configuration

# Parallel configuration illustration

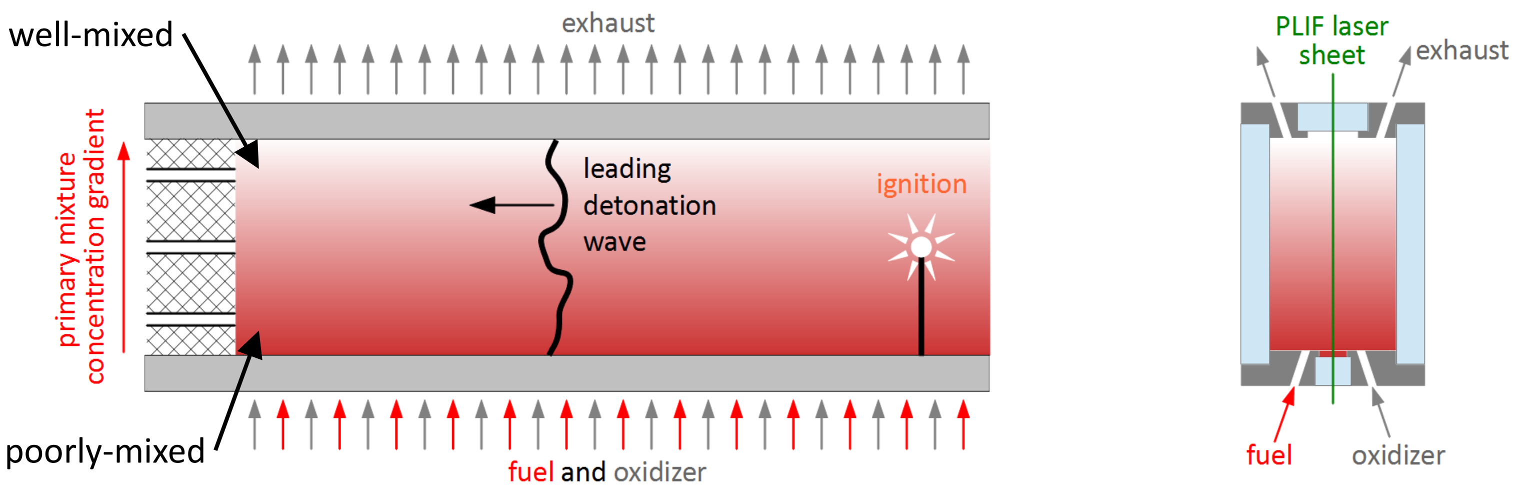



(a) Detonation channel side view

(b) Channel cross section

- 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




(a) Detonation channel side view

(b) Channel cross section

- 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

# Design operating condition range

| Property | Range |
|---|---|
| Fuel composition | Hydrogen, Blends of natural gas and hydrogen |
| Oxidizer composition | Air, oxygen, and oxygen-enriched air |
| Global equivalence ratio | Fuel lean through stoichiometric |
| Initial temperature | 20 – 300°C |
| Initial pressure | 1 – 4 atm |

- Testing will commence with stoichiometric hydrogen-air mixtures at atmospheric pressure and room temperature

# Project Tasks, Risk Management, Milestones

# Project tasks

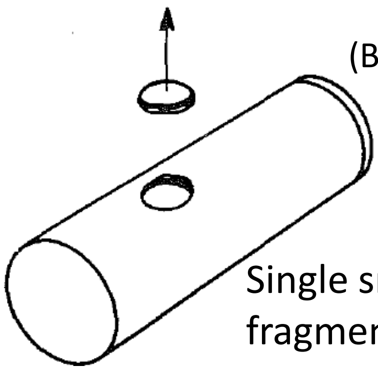
| Task | | Quarter | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
| 1.0 | Project Management and Planning | ● | | ● | | ● | | ● | | ● | | ● | |
| 2.0 | Design detonation channel and safety enclosure modifications | ● | | | | | | | | | | | |
| 3.0 | Machining and setup of facility | ● | ● | ● | | | | | | | | | |
| 4.0 | Determine the nature of detonation-inhomogeneity interaction in the *parallel* interaction configuration | | | ● | ● | ● | ● | | | ● | ● | | |
| 5.0 | Determine the nature of detonation-inhomogeneity interaction in the *perpendicular* interaction configuration | | | | | | ● | ● | ● | ● | ● | ● | ● |
| 6.0 | Development of design guidelines and rules for detonation-inhomogeneity interaction | | | | | | | | | | ● | ● | ● |
| 7.0 | Reporting | ● | ● | ● | ● | ● | ● | ● | ● | ● | ● | ● | ● |

# 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



(Baum, 1988)

Single small fragment ejection

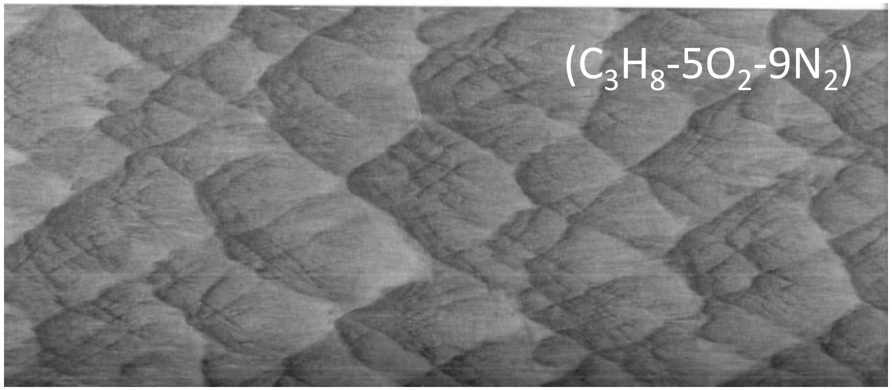
2. Acetone-PLIF measurement of local fuel concentration

- For $H_2$-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, schileren 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

# Project Milestones

| | |
|---|---|
| Q3 | Design, construction, and assembly of the detonation channel facility |
| Q4 | Local fuel concentration measurements in the parallel test configuration |
| Q4 | Initial detonation property measurements in the parallel test configuration |
| Q6 | Local fuel concentration measurements in the perpendicular test configuration |
| Q7 | Initial detonation property measurements in the perpendicular test configuration |
| Q9 | Successful operation of the test facility at elevated initial pressure and temperature |
| Q12 | Detonation structure characterization for property normalization across all conditions |

- 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.

Questions, Comments, and Discussion

# Extra Slides

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# Project tasks

| Task | | Quarter | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
| 1.0 | Project Management and Planning | | | | | | | | | | | | |
| 1.1 | Revise PMP after contract is negotiated (30 days after award). | ● | | | | | | | | | | | |
| 1.2 | Update PMP as project progresses. | | | ● | | ● | | ● | | ● | | ● | |
| 2.0 | Design detonation channel and safety enclosure modifications | | | | | | | | | | | | |
| 2.1 | Design detonation channel modifications for inhomogeneity study | ● | | | | | | | | | | | |
| 2.2 | Design safety enclosure modifications | ● | | | | | | | | | | | |
| 3.0 | Machining and setup of facility | | | | | | | | | | | | |
| 3.1 | Machine the detonation channel, safety enclosure and assemble | ● | ● | ● | | | | | | | | | |
| 3.2 | Setup measurement equipment | | ● | ● | | | | | | | | | |
| 3.3 | Overall system and measurement equipment test | | | ● | | | | | | | | | |

# Project tasks

| Task | | Quarter | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
| 4.0 | Determine the nature of detonation-inhomogeneity interaction in the parallel interaction configuration | | | | | | | | | | | | |
| 4.1 | Quantify mixture concentration inhomogeneity using acetone-PLIF | | | ● | ● | ● | | | | ● | ● | | |
| 4.2 | Perform detonation-inhomogeneity measurements (1 atm., 20°C initial condition) | | | ● | ● | ● | | | | | | | |
| 4.3 | Quantify inhomogeneity effects on detonation pressure, velocity, and failure limits | | | | ● | ● | ● | | | | | | |
| 4.4 | Determine inhomogeneity effects on leading wave and detonation cell structure | | | | ● | ● | ● | | | | | | |
| 4.5 | Determine the effect of increased initial pressure and temperature on detonation-inhomogeneity interaction | | | | | | | | | ● | ● | | |

# Project tasks

| Task | | Quarter | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
| 5.0 | Determine the nature of detonation-inhomogeneity interaction in the perpendicular interaction configuration | | | | | | | | | | | | |
| 5.1 | Quantify mixture concentration inhomogeneity using acetone-PLIF | | | | | | ● | ● | | | ● | ● | ● |
| 5.2 | Perform detonation-inhomogeneity measurements (1 atm., 20°C initial condition) | | | | | | ● | ● | | | | | |
| 5.3 | Quantify inhomogeneity effects on detonation pressure, velocity, and failure limits | | | | | | ● | ● | | | | | |
| 5.4 | Determine inhomogeneity effects on leading wave and detonation cell structure | | | | | | | ● | ● | ● | | | |
| 5.5 | Determine the effect of increased initial pressure and temperature on detonation-inhomogeneity interaction | | | | | | | | | | ● | ● | ● |

# Project tasks

| Task | | Quarter | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
| 6.0 | Development of design guidelines and rules for detonation-inhomogeneity interaction | | | | | | | | | | ● | ● | ● |
| 7.0 | Reporting | | | | | | | | | | | | |
| 7.1 | Quarterly progress reports | ● | | ● | | ● | | ● | | ● | | ● | |
| 7.2 | Semi-annual reports | | ● | | | | ● | | | | ● | | |
| 7.3 | Annual Report | | | | ● | | | | ● | | | | |
| 7.4 | Final Report | | | | | | | | | | | | ● |