A Joint Experimental/Computational Study of Non-idealities in Practical Rotating Detonation Engines

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UTSR/NETL
Summary

• Title:
  – A Joint Experimental/Computational Study of Non-idealities in Practical Rotating Detonation Engines

• Funding agency:
  – University Turbine Systems Research/NETL
  – Funding Opportunity Number: DE-FOA-0001248
  – Topic Area 2: Pressure Gain Combustion R&D
  – Project manager: David Lyons

• Personnel:
  – PI: Mirko Gamba, University of Michigan
  – Co-I: Venkat Raman, University of Michigan
  – Students currently involved:
    • Fabian Chacon
    • Yasin Abul-Huda
    • TBD
  – Key external collaborators:
    • Dr. John Hoke, Innovative Scientific Solution, Inc. (ISSI)
    • Drs. Adam Holley and Peter Cocks, United Technology Research Center (UTRC)
    • Dr. K. Kailasnath, Navy Research Labs (NRL)
Outline

- Programmatic overview
- Introduction to the problem and general approach
- Experimental activities
- Computational activities
- Interactions and collaborations
Outline

• Programmatic overview

• Introduction to the problem and general approach

• Experimental activities

• Computational activities

• Interactions and collaborations
Overarching objectives

• **Objective 1:**
  Develop canonical and operational RDE configurations, as well as imaging-based laser diagnostics for understanding fuel stratification, leakage, parasitic combustion and detonation structure under non-ideal conditions in RDEs.

• **Objective 2:**
  Develop a comprehensive picture of the fundamental physics governing non-idealities and how they impact RDE performance and operability from both experiments and simulations.

• **Objective 3:**
  Develop detailed computational tools (DNS & LES) for studying detonation wave propagation processes in RDEs.
Expected outcomes

• **Outcome 1:**
  Identify the sources and properties of non-idealities in RDEs, their contribution to loss in pressure gain, and potential design limitations

• **Outcome 2:**
  Detailed experimental tools and measurements (databases) about fundamental aspects of RDEs will become available to the RDE design community.
  – e.g., transfer of techniques and data to UTRC, ISSI, NRL

• **Outcome 3:**
  Detailed computational tools (DNS/LES) as well as combustion models with detailed chemistry for pressure gain combustion will be made available to the RDE design community.
  – e.g., openFoam development of RDE modeling
  – e.g., transfer of detonation computational models to UTRC, ISSI, NRL
Objectives and tasks

A Joint Experimental/Computational Study of Non-idealities in Practical Rotating Detonation Engines

**Objective 1**
Develop canonical RDE flowfield for laser-diagnostic study of non-idealities in RDE

- **Task 2.1** Investigate degree of unmixedness due to injection and how it affects shock propagation and leakage
- **Task 2.2** Investigate the structure of the detonation wave under non-uniformly mixed, turbulent mixtures

**Objective 2**
Understand the physics of non-idealities in RDEs and how they impact performance and operability

- **Task 3.1** Investigate and determine how non-idealities affect RDE performance and operability
- **Task 3.2** Investigate how fuel reactivity in non-uniform mixtures affect RDE performance and operability

**Objective 3**
Develop DNS/LES combustion models for prediction of detonation wave propagation

- **Task 4.1** Develop DNS capability for turbulent detonation of fuel/air mixtures
- **Task 4.2** Conduct DNS of configurations replicating the linearized RDE analogue
- **Task 4.3** Develop LES models for turbulence generation and combustion in the presence of detonation waves
- **Task 4.3** Conduct LES analysis of RDEs to understand the effect of non-idealities on performance and operability
Objectives and tasks

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**RDE physics**
- Non-idealities
- Performance
- Operability

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Experimental tools

Computational tools
## Timeline of the project

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<th>Task</th>
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Outline

• Programmatic overview

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• Interactions and collaborations
Overview of RDE operation and Pressure Gain (PG)

From:
Schwer D. A. and Kailasanath K., AIAA 2010-6880
RDE flowfield (unwrapped)

From: Nordeen et al., AIAA 2011-0803
Thermodynamics of RDE and Pressure Gain

Detonation pressure gain (constant volume) heat release

Constant pressure heat release based cycle

From: Schwer D. A. and Kailasanath K., AIAA 2010-6880
(Some) Practical challenges

- Detonation initiation
- Detonation sustainment
- Produce and maintain pressure gain
- Injector design
  - Mixing, minimize pressure drop, prevent back-flow
- Integration with turbomachinery (compressor/turbine)
  - Unsteady operation
- (High-frequency) unsteady loads (mechanical/thermal)
Non-idealities and loss of pressure gain

- **Detonation non-idealities**
  - Incomplete fuel/air mixing
  - Fuel/air charge stratification
  - Mixture leakage (incomplete heat release)
  - Parasitic combustion:
    - Premature ignition (e.g., burnt/unburnt interface)
    - Stabilization of deflagration (flame)
  - Detonation-induced flow instabilities
    - Richtmyer-Meshkov (R-M) instability
    - Kelvin-Helmholtz (K-H) instability
- **They lead to loss in pressure gain**
  - Linked to loss of detonation propagation
- **Additional losses exist during flow expansion**
  - Secondary shock and (multiple) oblique shock
  - Flow instabilities (e.g., K-H instability)
  - Mixture leakage through burn/unburnt interface
Past/current analysis/investigation approach

- Past/current approach is based on **global performance assessment**

- Experimentally:
  - Global performance assessment
  - Low-fidelity and/or global metrics
    - Pressure measurements
    - Luminosity-based analysis (optical access is a challenge!)
  - Parametric study
    - Variation with flow rate, (global) equivalence ratio, fuel, pressure
    - Injector design / annulus / exhaust flowpath testing

- Prediction/computation
  - Euler solver or **limited viscous** effects modeling
  - One-dimension, perfect mixture
  - Single-step reaction
  - Induction-time based combustion models
  - Neglect mixing, three-dimensional **viscous effects and turbulence**
Our approach: a multi-level physics study

Practical RDE

Unit-physics decomposition

Diagnostics
- Laser-based imaging
- Mixing measurement
- Detonation structure
- Temperature and species imaging

Injection & mixing
- Free single injector
- Free multiple injection
- Confined multiple injection
- Shock-induced mixing
- DNS/LES modeling
- Experiments

Turbulence & detonations
- Linear analogue
- Detonations in stratified mixtures
- DNS/LES modeling
- Experiments

Detailed modeling
- Variable mixture ignition model
- Homogeneous reactor model with tabulated ignition times
- Non-equilibrium
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Experimental multi-level approach

RDE full system:
- Link between mixing and performance
- Design from ISSI/AFRL

Linearized analogue:
- Detonation structure
- Detonation/turbulence interaction
- Detonation in stratified mixtures
- Design from ISSI/AFRL

Single or multiple injectors:
- Mixing studies
- Shock-induced mixing
- Our starting point
Shock-induced mixing: detonation/shock analogy

Detonation

Shock analogy

From: Schwer D. A. and Kailasanath K., AIAA 2010-6880
Scaling of detonation/shock analogy

![Diagram showing the scaling of detonation/shock analogy]

- **Density Ratio Ambient/Crossflow** vs **Wave Speed (km/s)**
  - Normal Shock
  - Det H$_2$/Air ($\phi = 1$)
  - Det CH$_4$/Air ($\phi = 1$)

- **Induced Speed (km/s)** vs **Wave Speed (km/s)**
  - Normal Shock
  - Det H$_2$/Air ($\phi = 1$)
  - Det CH$_4$/Air ($\phi = 1$)
Scaling of detonation/shock analogy

Typical RDE operation

Normal shock

Wave Speed (km/s)

Momentum Flux Ratio

Wave Speed (km/s)
Shock-induced mixing in turbulent jets

• Flexible configuration
  – Single isolated injector
  – Multiple isolated injectors
  – Confined multiple injectors
  – Different injector configurations can be tested conveniently

• Well-suited for controlled unit-physics experiments
  – Quantitative mixing measurements
  – Flexibility in range of conditions
    • Shock strength
    • Injection details (speed, configuration, molecular weight)
  – What learnt here can be extended to the linearized RDE
Shock-induced mixing in turbulent jets

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Shock-induced mixing in turbulent jets

- Shock wave from shock tube
- Laser sheet forming optics
- Camera
Interaction of shock wave with turbulent jet

- Detonation-induced mixing analogue
- Visualization data
  - 100 kHz movie with 300 ns exposure (shock smears by 0.13 pixel)
  - Injection of H₂ into still air subject to a Mach 1.39 shock wave
  - Played back at 5 frames/second
  - Elapsed time 0.5 ms (50 frames)
Interaction of shock wave with turbulent jet

$M = 1.39$

Planar shock

$u = 194 \text{ m/s}$

$\rho_j/\rho_1 = 1.7$

$u_j/D \sim 1/12$

$u_j/u \sim 1/5$

$\rho_j/\rho_2 \sim 1/24$

$H_2$

$u_j \sim 40 \text{ m/s}$

Density-driven instability (e.g., R-M instability)
Experimental multi-level approach

RDE full system:
• Link between mixing and performance
• Design from ISSI/AFRL

Linearized analogue:
• Detonation structure
• Detonation/turbulence interaction
• Detonation in stratified mixtures
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Single or multiple injectors:
• Mixing studies
• Shock-induced mixing
• Our starting point
Suite of diagnostic techniques for the study of RDE physics

- **Traditional techniques:**
  - Pressure, heat flux, flame chemiluminescence
  - Schlieren imaging

- **Laser-based imaging diagnostics:**
  - Planar laser-induced fluorescence (PLIF) mixing and flame marker
  - Two-color toluene PLIF thermometry and mixing (non-reacting) imaging
  - OH/CH$_2$O/CH/NO PLIF imaging
    - e.g., Simultaneous OH/CH$_2$O PLIF imaging for flame structure and heat release distribution study in premixed combustion
  - Rayleigh scattering imaging (thermometry in reacting flows)

- **Some examples follow**

  ![Simultaneous OH/CH$_2$O PLIF imaging in inverted oxy-fuel coaxial non-premixed CH$_4$ flames](image-url)
Mixing and combustion measurements in compressible turbulence

Study of transverse jets in supersonic crossflow - reacting

Distribution of OH radical (flame marker)

Side-view centerplane

Plan-view 1mm off the wall
Mixing and combustion measurements in compressible turbulence

Study of transverse jets in supersonic crossflow – non-reacting mixing using toluene PLIF thermometry

$$J = \frac{\rho U}{\rho U'} = \frac{\gamma_{CS}}{\gamma_{CF}} \frac{1}{M_s^2}$$

$$M \approx 2.3 \quad T \approx 500 \text{ K} \quad p \approx 1 \text{ atm}$$

Seeded N₂

Bow shock

Mixing layer

Acoustic waves

LIF signal

Pure jet fuel

Jet entrainment

Wake

H₂ injection

H₂ (MW=2)

He (MW=4)

He/Ar (MW=9)

N₂ (MW=28)

Ar (MW=40)

$J$, $s$ and $r$ are coupled

MW: molecular weight

Momentum flux ratio: $J = \frac{\rho U^2}{\rho U'^2} = \frac{\gamma_{CS}}{\gamma_{CF}} \frac{1}{M_s^2}$

MW: molecular weight

$T_0 = 29$ K

$\rho_s$ constant (±10%)

W variable

$r_s \approx 200,000$ (He) – 600,000 (N₂)

$M \approx 2.3$

$T \approx 500$ K

$p \approx 1$ atm

Seeded N₂

$M \approx 2.3$

Observations:

- $T \approx 500$ K
- $p \approx 1$ atm
- Seed N₂

Steady State

Mach Number

Temperature

H₂ injection

N₂ injection

Plume

Wake
Flame structure in scramjet model, (H2/air at $\phi = 0.23$)
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Computational issues in RDEs

• RDEs driven by strong discontinuities
  – Shocks, pressure jumps, strong velocity gradients
  – Numerically challenging

• Coupling to turbulence and inhomogeneities
  – Small-scale gradients in concentration, temperature etc.
  – Ability to capture strong jumps and small-scale features
    • Low dispersion and dissipation in numerical tools

• Combustion modeling
  – How to describe combustion in detonation-based devices?
Numerical capabilities

• Prior work in high-speed shock-containing flows
  – Low dispersion numerics
  – Near-shock resolution using specialized non-oscillatory schemes
  – Central schemes to preserve turbulent kinetic energy away from shock
  – Shock region determined using numerical “sensors”
    • Strain rates and pressure gradients used as sensors
Current focus

• Need to use complex geometries to model injectors
  – Need unstructured and complex mesh capabilities

• Current work
  – Move solvers to open source framework
  – Ability to directly import CAD files
  – Easily portable across machines
  – Most importantly, can be easily shared with researchers
    • No IP issues on code transfer
    • Preliminary solvers developed using NETL-funded work
OpenFOAM capabilities

- Used for low-speed reacting flows
  - Multiple combustion models implemented
  - Ability to handle detailed chemical kinetics
  - Tested for Euler-type high-speed flows
  - Currently being ported to Siemens Inc.; Collaborations with GE and Rolls Royce
Combustion modeling

• If detonation is uniform, only time-lag model is needed
  – Only valid under ideal conditions
  – Injection leads to spatially non-uniform mixing
  – Variations in fuel/air composition
    • Leads to non-uniform detonation
    • Generation of baroclinic torque and vorticity generation
    • Enhances the effect of non-uniform mixtures

• Combustion modeling focus
  – Develop a variable mixture ignition model
Combustion modeling focus

• Low-speed models are not accurate
  – Turbulent mixing dominated ignition

• RDEs
  – Pressure-driven detonation
    • Induction time dependent on pressure response of fuel
  – Response of variable equivalence ratio mixing
    • Non-uniformity in fuel-air ratio can lead to variable delays in ignition
    • Formation of cellular shock structures
    • Loss of efficiency and fuel leakage

• First approach
  – A local mixture dependent ignition time
  – Use homogeneous reactor configuration to tabulate ignition times
Additional issues

• Strong detonation waves can introduce internal energy nonequilibrium
  – Internal modes cannot be described by Boltzmann distribution
  – Strongly affects ignition and combustion processes

• Our group has been working on nonequilibrium effects through a simultaneous AFOSR-funded effort
  – Use ab-initio computational chemistry to understand effect of nonequilibrium
  – This effort will be leveraged here
  – Strong interest from NRL (Dr. Kailasnath)
External collaborations

• Initiating collaboration with NRL
  – Get input on code development
  – Provide information on nonequilibrium and combustion modeling

• University of Maryland (Prof. Yu)
  – Use existing experimental data for initial validation
  – Provides stop-gap validation data until UM experiments come online

• UTRC and ISSI/AFRL
  – Develop and transfer code and modeling expertise
  – Interact to work on injector modeling
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Interactions, collaborations and synergies

• Strong coupling between experiments and computations
  – Model development and validation
  – Experiment design and understanding
  – Combined investigation of the physics of detonations under turbulent mixing, incomplete fuel/air mixing, stratification

• Key external collaborations
  – ISSI/AFRL (Dr. John Hoke) on RDE and linearized RDE analogue operation, performance and modeling
  – UTRC (Drs. Adam Holley and Peter Cocks) on modeling and non-ideal behavior
  – Initiating collaboration with NRL (Dr. Kailasnath) on code and combustion model development

• Other collaborations/interactions
  – University of Maryland (Prof. Yu) on initial use of existing experimental data for initial validation
  – Interested in establishing interaction with NETL (Dr. Ferguson)
Questions?