Advanced Cost-effective Coal-Fired Rotating Detonation Combustor for High Efficiency Power Generation

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ISSI (Dr. John Hoke)
AFRL (Dr. Fred Schauer)
Siemens (Timothy Godfrey)

NETL CO\textsubscript{2} Capture Technology Project Review
August 14th, 2018
Outline

- Background
- Project Objectives
- Technical Approach
- Project Structure and Management
- Project Schedule
Deflagration-to-Detonation

Pressure Gain Combustion

**Detonation**
- Exploits pressure rise to augment high flow momentum
- Fundamental mechanism is turbulent flame acceleration
- High flow turbulence intensities and length scales
- Serious challenge for reliable, repeatable and efficient

**Deflagration-To-Detonation Transition Process**
1. Ignition of a deflagration flame
2. Turbulent flame acceleration due to turbulent mixing
3. Transition:
   - Reflected shock (*Oran et al.*)
   - Localized vortical explosion (*Zeldovich gradient mechanism*)
   - Boundary layer turbulence (*Oppenheimer*)
   - Turbulence-Driven DDT (*UCF-NRL*)
4. Formation of a self-sustaining detonation wave

**Thermodynamic Cycle**

![Thermodynamic Cycle Diagram](image)

**Deflagration-To-Detonation Process**

- Ignition and Flame Propagation with Compression Wave Formation
- Shock Formation
- Localized Explosions Leading to Detonation
- Detonation
Origin of Detonation:

- Detonation first discovered during disastrous explosions in coal mines, 19th century.
- Puzzling at first, how the slow subsonic combustion could produce strong mechanical effects. *Michael Faraday “Chemical History of a Candle”* 1848
- First detonation velocity measurement, Sir Frederic Abel 1869
- Coal particles and coal gas interaction, Pellet, Champion, Bloxam 1872
- Berthelot hypothesized shock wave reaction, detonation, 1870

Coal Mine Fast-Flame Deflagration Explosion

Coal Mine Detonation Explosion
Explore Advanced Cost-Effective Coal-Fired Rotating Detonation Combustor:
The proposed project aims to characterize the operability dynamics and performance of an advanced cost-effective coal-fired rotating detonation combustor for high efficiency power generation

- Development of an operability map for coal-fired RDC configuration
- Experimental investigation and characterization of coal-fired combustor detonation wave dynamics
- Computational investigation and characterization of coal-fired combustor detonation wave dynamics
- Measurement and demonstration of pressure gain throughout the coal-fired RDC operational envelope
- Measurement and demonstration of low emissions throughout the coal-fired RDC operational envelope
1. Operability Dynamics for Detonation Wave:
   a. Coal Injection: what is the coal particle size, effective volume fraction, and seeding technique? The focus here will be on effective refraction/burning rate and detonation-solid interaction.
   b. Initiation: is the reaction front that is formed a detonation or a deflagration flame that is acoustically coupled? The focus here will be on the mechanisms of deflagration-to-detonation transition and composition enrichment syngas and oxy-coal rotating detonation combustion.
   c. Directionality: which direction do the waves rotate and why? why and when do they change direction? The focus here will be on the conditions and mechanisms of detonation wave direction.
   d. Bifurcation: How many waves are generated and why? The focus here will be on the driving mechanisms of the form of detonation wave topology.

2. Performance:
   a. Pressure Gain: How much pressure gain is generated under steady and dynamic operability? The focus here will be on the direct measurement of pressure gain production.
   b. Emissions: what level of emissions coal RDC generate under steady and dynamic operability? The focus here will be on the direct measurement of emissions along with modeling.
Roles of Participants

DOE ACS Management

University of Central Florida (Prime Recipient)
Dr. Kareem Ahmed
Dr. Subith Vasu

Aerojet Rocketdyne (Industry Partner)
Dr. Scott Claflin

Georgia Institute of Technology (Sub-Recipient)
Dr. Suresh Menon

Innovative Scientific Solutions, AFRL (Industry Partner)
Dr. John Hoke
Dr. Fred Schauer
Detonation Propagation in a Premixed Supersonic Flow

Rotating Detonation Engine in Supersonic Flow


RDE Exhaust Velocimetry

Detonation wave velocimetry and structure conducted at Dr. Ahmed’s UCF lab

J. Chambers et al, ICDERS, 2017

Detonation Shock Particle Flame Flow

Aluminum Oxide Particles Flow

Detonation Turbulent Flame

Flame Velocity 1000 m/s

J. Chambers et al, ICDERS, 2017
Pressure Gain Combustion

Research focused on confined and free detonation
Simulations with inert and reactive (Al) particles
Condensed phase and gas phase detonation
Deflagration-to-Detonation Transition (DDT)
Code LESLIE in AFRL (Eglin) for detonation studies
http://www.ccl.gatech.edu

Steady 3D Detonation in a channel

DDT in two-phase channel with obstacles

Detonation charge surrounded by inert steel particles
Vision

The goal is to measure stagnation pressure for fundamental understanding of pressure gain within a rotating detonation engine. This will allow for proper understanding of flow field effects.

\[
\left( \frac{P_{d,ex}^0}{P_M^0} \right) = \left( \frac{P_{c,ex}^0}{P_{c,in}^0} \right) \left( \frac{P_M^0}{P_{c,in}^0} \right) \left( \frac{P_{c,ex}^0}{P_{d,ex}^0} \right)
\]

\(1\) - Combustion Chamber

\(2\) - Injector/Isolator

\(3\) - Diffuser

Aerojet Rocketdyne RDE cutout

PIV on exit plane of nozzle of the Aerojet RDE

Entire CAD of Aerojet RDE cutout sitting on static test fire stand

Computed pressure gain through engine

J Speed: 1919 m/s
Coal Rotating Detonation Combustor: Modeled After the AFRL RDE and the NETL (Dr. Don Ferguson)

Russia: Bykovskii et al. 2013

Deflagration-to-Detonation Facility

Standing Detonation Facility
**Characterization of Materials**

<table>
<thead>
<tr>
<th>Dust</th>
<th>Size</th>
<th>$K_{ST}$</th>
<th>$d_{min}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>U.S. W. Sub-Bituminous coal$^a$</td>
<td>$\leq 100$</td>
<td>59$^b$</td>
<td>0.6</td>
</tr>
<tr>
<td>Cornstarch</td>
<td>10</td>
<td>160</td>
<td>0.3</td>
</tr>
<tr>
<td>Anthraquinone</td>
<td>$22 \times 6 \times 6$</td>
<td>274</td>
<td>0.14</td>
</tr>
<tr>
<td>Aluminum</td>
<td>$36 \times 36 \times 1$</td>
<td>359</td>
<td>0.12</td>
</tr>
</tbody>
</table>

Note: $a$ - Gardner et al. (1986); $b$ - Fangrat et al. (1987).

F. Zhang et al., *Journal of Shock Waves*, 2001

**Potential:**

- Carbon Black (very fine)
- Cannal Coal (Russians coal of choice)
- Aluminum Iodate Hexahydrate (for doping)
- Liquid Isopropyl nitrate (for doping, need a new injection scheme)

Bituminous Coal, Anthracite Coal, Carbon Black

*(All coal sizes as low at 75 micrometers with the exception of carbon black. Carbon black can be found as low as 18 nanometers)*

Anthraquinone Powder, Aluminum Nanoparticles, Liquid Isopropyl nitrate
Bit Coal

Asbury provides LOW SULFUR Bituminous Coal commonly known as Bit Coal. This material is ground and screened to specifications commonly used for foundry sand and addition, brake linings and other industrial applications.

Chemistry

<table>
<thead>
<tr>
<th></th>
<th>TARGET MIN</th>
<th>TARGET MAX</th>
<th>C3 TYPICAL</th>
<th>D4 TYPICAL</th>
</tr>
</thead>
<tbody>
<tr>
<td>% SULFUR</td>
<td>0</td>
<td>1</td>
<td>0.71</td>
<td>0.74</td>
</tr>
<tr>
<td>% VOLATILE</td>
<td>34</td>
<td>44</td>
<td>87.4</td>
<td>88.6</td>
</tr>
<tr>
<td>% MOISTURE</td>
<td>0</td>
<td>7</td>
<td>5.2</td>
<td>3.4</td>
</tr>
<tr>
<td>% ASH</td>
<td>0</td>
<td>10</td>
<td>8</td>
<td>7.1</td>
</tr>
<tr>
<td>% FIXED CARBON</td>
<td>50</td>
<td>60</td>
<td>54.6</td>
<td>54.3</td>
</tr>
</tbody>
</table>

The percentages above/below are “Targets” and not meant to be a guarantee.

Sizing

<table>
<thead>
<tr>
<th></th>
<th>+15 (&lt;1.18mm)</th>
<th>+20 (350 Microns)</th>
<th>+50 (630 Microns)</th>
<th>+60 (25 Microns)</th>
<th>+106 (150 Microns)</th>
<th>+200 (75 Microns)</th>
<th>+200 (75 Microns)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C3 Target</td>
<td>0</td>
<td>2.9</td>
<td>6.18</td>
<td>8.15</td>
<td>27.35</td>
<td>max 27.5</td>
<td></td>
</tr>
<tr>
<td>C3 Typical</td>
<td>0</td>
<td>2.6</td>
<td>6.14</td>
<td>8.15</td>
<td>27.35</td>
<td>max 27.5</td>
<td></td>
</tr>
<tr>
<td>D4 Target</td>
<td>0</td>
<td>2.6</td>
<td>6.14</td>
<td>8.15</td>
<td>27.35</td>
<td>max 27.5</td>
<td></td>
</tr>
<tr>
<td>D4 Typical</td>
<td>0</td>
<td>2.6</td>
<td>6.14</td>
<td>8.15</td>
<td>27.35</td>
<td>max 27.5</td>
<td></td>
</tr>
</tbody>
</table>

- Packaging includes 50 lb bags or 2000 lb super sacks.
- Export Packaging and containerization available.
- Shipping to any port destination.

In the US or abroad...

Let Asbury handle your Bit Coal requirements

Asbury Graphite Mills, Inc.
405 Old Main Street • PO Box 143 • Asbury, New Jersey 08802
Phone: 908.537.2155 • Fax: 908.537.2908
www.asbury.com
Seeder Design

$\frac{1}{2}''$ Coiled Tube with 32 Sonic Orifices at a diameter of $\frac{3}{32}''$

Seeder inline with air, downstream of Sonic Orifice

Ball Valve for Seed Insertion

Pressure Transducer

Air Out

Air In

3.068” ID

15.663” Inner Length
RDE

Manifold Connections
Red: Hydrogen, 6 in total
Blue: Air

Flat for LAS
Simplified outer body to easily of create an operational map

Pre-Det
First Fire!

2 lbm, two detonation waves
Both PIV and LAS are traversable axially
Advanced Optical Diagnostics

- High-speed PIV system (20kHz, 40kHz, 60kHz, 100kHz)
- High speed cameras 21,000-2,100,000 frames per second
- High-speed chemiluminescence CH*, OH* (40 kHz, 80kHz, 100kHz)
- Light-field focusing system for flow measurements and visualization
- LabVIEW control hardware and software
- Dynamic pressure transducers (PCB)
- Codes: DMD, POD, PIV, Physics-Based Models (Matlab/Fortran)
Tunable Diode Laser Absorption Spectroscopy (TDLAS)

Two sub-systems:

The pitch (left):
Contains four lasers at different wavelengths.

2.55\(\mu\)m and 2.48\(\mu\)m for water concentration and temperature.

4.2\(\mu\)m for CO\(_2\) concentration.

4.7\(\mu\)m for CO concentration.

Each wavelength is multiplexed into a single beam and focused into a fiber cable.

The catch (right):
After passing through RDE combustion channel.

The four wavelengths are demultiplexed through diffraction gratings.

Signals measured with highly sensitive photovoltaic detectors.
TD: LAS

• Beer-Lambert Law

\[- \ln \left( \frac{I}{I_0} \right) = \sum_i \sum_j S_{ij}(T) X_j P L \phi_{ij} (\nu - \nu_{0ij}) \]

- \(I\) = Transmitted Intensity \(\frac{W}{cm^2 sr Hz}\)
- \(I_0\) = Incident Intensity \(\frac{W}{cm^2 sr Hz}\)
- \(S_{ij}\) = Linestrength \(\frac{cm^{-2} atm}{W}\)
- \(T\) = Static Temperature (K)
- \(X_j\) = Mole Fraction
- \(P\) = Static Pressure (atm)
- \(L\) = Path Length (cm)
- \(\phi_{ij}\) = Lineshape Function (cm)
- \(\nu\) = Optical Frequency (Hz)
- \(\nu_{0ij}\) = Line Center Optical Frequency (Hz)
- Subscripts:
  - \(i\) = Quantum Transition
  - \(j\) = Atomic/Molecular Species

Off-Axis Parabolic Mirror

Fiber Port

Process

Diode Laser
Numerical Model and Challenges

- LESLIE code - compressible LES solver with hybrid O(2)-O(3) central-HLLC scheme
  - Well established for detonation modeling under DTRA and AFRL effort
  - Time-accurate and parallel with two-phase capability operational
  - Initial grid ignores injectors: 3D grid 2160 x 500 x 40 cells used for simulations
  - Effusion BC in 2D (right) showed promise in 2D but failed in 3D to maintain mixture
  - Characteristic inflow BC implemented using inflow fixed stagnation temperature and pressure that allows inflow to shut down and restart based on local conditions

Successful sustained detonation in 2D setup

Successful sustained detonation for 1 cycle but failed in second cycles since mixture penetration was incorrect using the effusion BC.
To evaluate the RDE inlet system a linear model based on NETL design is being modeled. Full resolution of the injection assembly is being used here to understand the mixing process. Such resolution in full 3D LES is impractical so assessment will be designed to modify the characteristic based BC to account for mixture variation. This study will be non-reacting and focus only on mixing and assessing impedance based BC.

Summary and Future Plans

- Coal-RDE Facility has been setup and testing with seeded coal particles are under way
- 3D NETL/UCF rig has now been setup for simulations using LESLIE
  - Studies have been conducted to ensure grid quality and parallel performance
- Characterization of coal particle seeding: flowrate and stoichiometry
- Laser diagnostics implementation for pressure grain combustion and emissions measurements
- Evaluate mixing between air and fuel in an array of injectors as in the NETL/UCF rig focusing on non-premixed system to obtain impedance type BCs for 3D LES
- Two-phase LES is now being set up to study flames with coal mixtures