Single-Fuel Reactivity Controlled Compression Ignition (RCCI) Combustion Enabled by Onboard Fuel Reformation

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Project ID: FT060

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The City College of New York

Outline

- **Overview**
- **Relevance and Resources**
- **Approach and Milestones**
- **Technical Accomplishments and Progress**
- **Collaboration and Coordination**
- **Remaining Challenges and Barriers**
- **Proposed Future Research**
- **Summary**

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Overview

Timeline

- Start Date: October 1st, 2015
- End Date: September 30th, 2018
- Percent complete: 50%

Barriers

- Lack of fundamental knowledge of advanced engine combustion regimes
- Lack of actual emissions data on pre-commercial and future combustion engines
- Existing technologies are not capable of simultaneously high efficiency and low engine-out emissions

Budget

- Total Budget: $1.128M
- DOE Share: $1.014M
- Cost Share: $114k
- FY2016 DOE Share: $423k
- FY2017 DOE Share: $307k

Partners

Stony Brook University

- Lead – advanced combustion expertise

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- Subcontract – engineering firm with catalytic reformation expertise

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- Subcontract – analytical chemistry expertise

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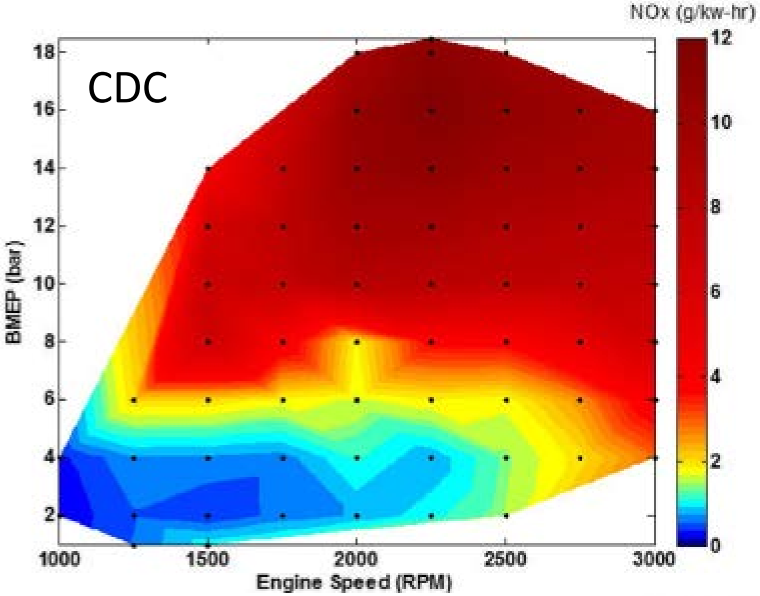
Relevance – Project Motivation

- Reactivity Controlled Compression Ignition (RCCI) combustion has demonstrated ultra-low NOx and soot emissions with efficiencies equal to, or higher than, conventional diesel combustion (CDC)
- RCCI also has significantly improved controllability compared to other LTC modes
- For these reasons, RCCI has the ability to meet the DOE VTO Program goals of developing high efficiency, low emissions combustion modes
- However, RCCI is limited in its commercial viability due to the requirement of two fuels



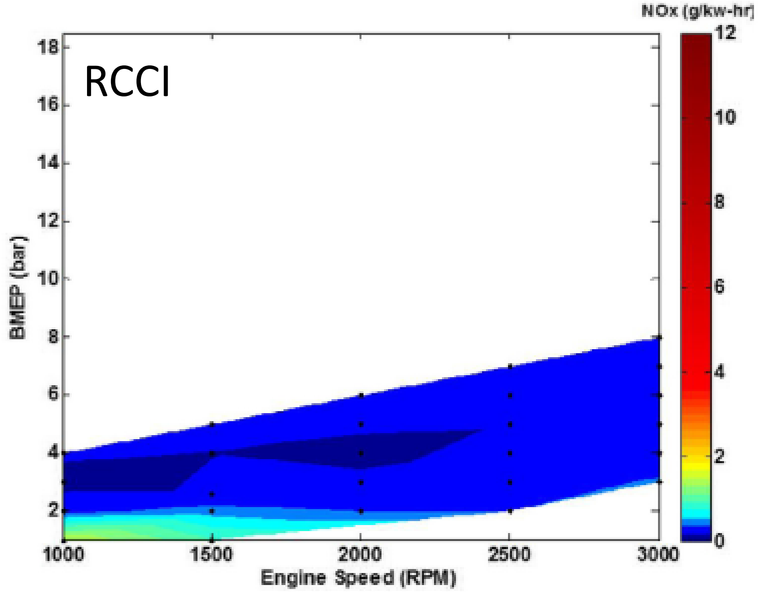


Figure Reference: Curran S, Hanson RM, Wagner RM, Reitz RD. Efficiency and emissions mapping of RCCI in a light-duty diesel engine. SAE Paper 2013; 2013-01-0289.

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Relevance – Project Objectives for Addressing Barriers

- **Overall Project Objectives**
  - Assess the feasibility of an on-board fuel reformer to enable RCCI combustion from a single parent fuel
  - Quantify the benefits and the losses of the system and benchmark the results against conventional diesel combustion (CDC) and dual-fuel RCCI
- **Objectives This Period**
  - Produce a matrix of reformate fuels from gasoline, diesel, and natural gas with varying degrees of reformation
  - Determine the composition of the reformate fuels
  - Determine an effective PRF# and an effective PRF separation between each parent fuel-reformate pair

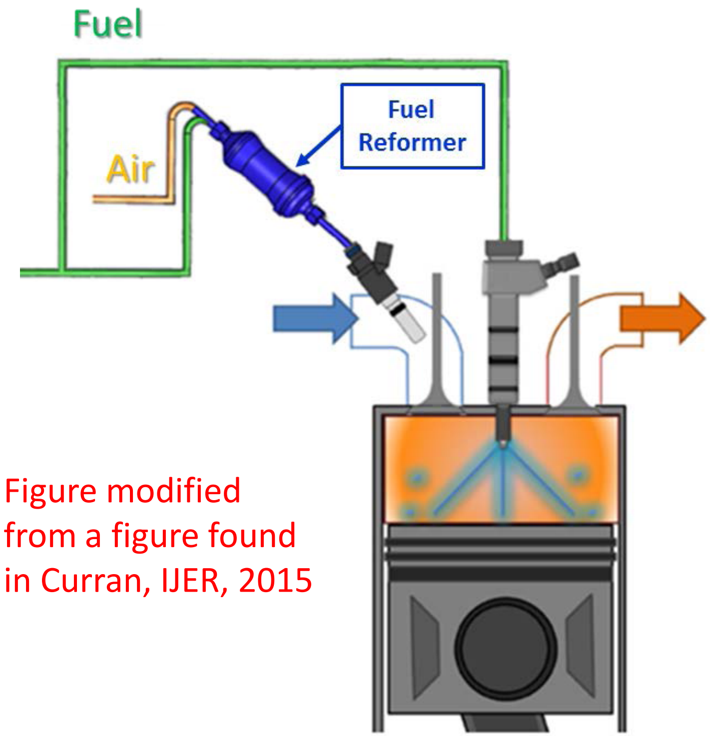


Figure modified from a figure found in Curran, IJER, 2015

- **Impact**
  - This project is aimed specifically at addressing some of the DOE VTO Program barriers by providing enhanced fundamental knowledge of advanced engine combustion regimes with actual emissions data on future combustion engines
  - Additionally, by alleviating the major drawback of dual-fuel RCCI, this research can bring RCCI closer to commercialization, enabling the previously reported efficiency and emissions benefits of RCCI

Approach

- Our approach to achieve the technical objectives is to systematically and fundamentally evaluate the proposed topic starting with the potential parent fuels
  - Gasoline, Diesel, and Natural Gas
- Divide the proposed work into three tasks:
  1. Reformate Production and Characterization
  2. Combustion and System-Level Modeling
  3. Experimental Concept Testing and Assessment

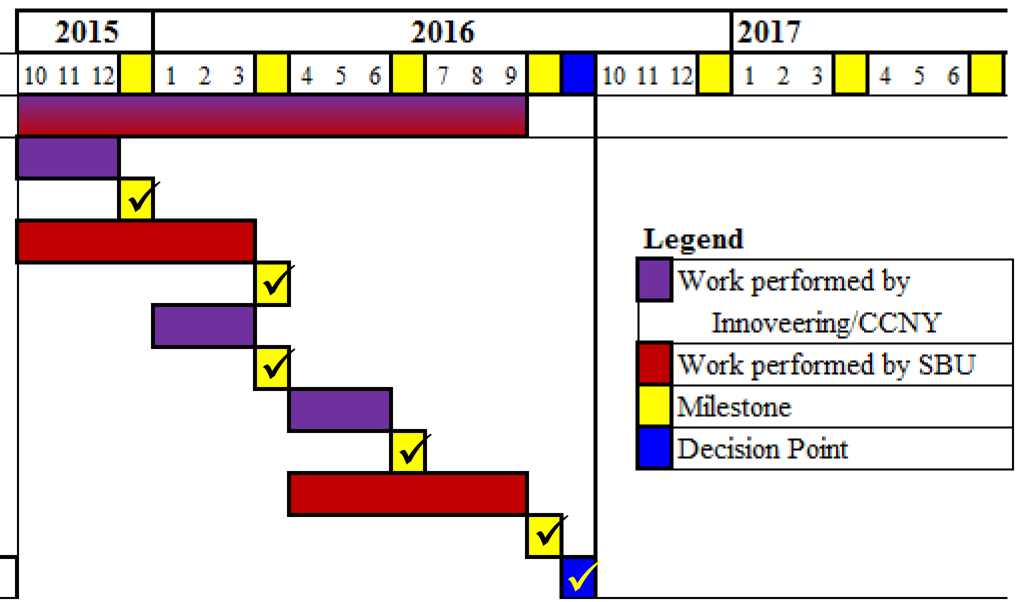
- This approach addresses the barriers of the project by thoroughly and methodically evaluating potential parent fuels with their respective reformate mixtures starting at the production of the reformate mixtures and continuing to engine testing of Reformate RCCI (i.e. RCCI with a fuel and its reformate)
- This research is well integrated with other research and development projects in the Vehicle Technologies Program such as conventional dual-fuel RCCI as well as NVO fuel reforming in HCCI

Approach / Milestones – (1) – First Budget Period

The first budget period focused on:

1. Experimental facilities development
2. Reforming the parent fuels and characterizing the reformate mixture
3. Determining the autoignition tendency of the reformate mixtures in comparison to the parent fuels

Task Number	Task Title
Task 1	**Reformate Characterization and Analysis**
Subtask 1.1	Modify facility to produce reformate matrix
Milestone 1.1	Completed facility to produce reformate matrix
Subtask 1.2	Modify CFR engine for experiments
Milestone 1.2	Completed modifications to CFR engine
Subtask 1.3	Produce the parent fuel-reformate matrix
Milestone 1.3	Completed production of reformate matrix
Subtask 1.4	Determine the properties of reformate matrix
Milestone 1.4	Determined properties of reformate matrix
Subtask 1.5	Determine effective PRF# of reformate matrix
Milestone 1.5	Determined effective PRF# of reformate matrix
Decision Point 1	Is there sufficient octane separation?



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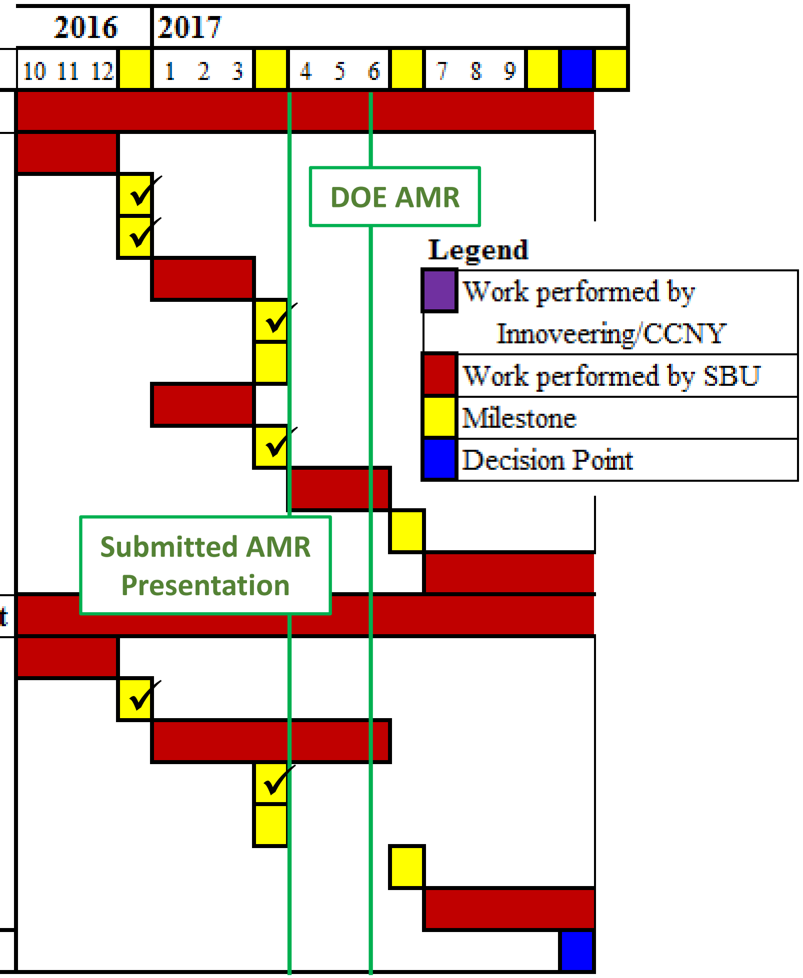
Approach / Milestones – (2) – Second Budget Period

Task Number	Task Title
Task 2	**Combustion and System-Level Modeling**
Subtask 2.1	Construct GTS models
Milestone 2.1	Completed GTS model of CFR engine
Milestone 2.2	Completed GTS model of Ricardo Hydra
Subtask 2.2	Validate GTS models
Milestone 2.3	Calibrated CFR GTS engine model
Milestone 2.4	Calibrated Ricardo Hydra GTS engine model
Subtask 2.3	Construct CFD model of Hydra engine
Milestone 2.5	Completed CFD model of Hydra engine
Subtask 2.4	Validate CFD model of Hydra engine
Milestone 2.6	Validated ConvergeCFD Hydra engine model
Subtask 2.5	Simulate Ref. RCCI with ConvergeCFD
Task 3	**Experimental concept testing and assessment**
Subtask 3.1	Modify the Hydra engine to run RCCI
Milestone 3.1	Completed modifications to Ricardo Hydra engine
Subtask 3.2	Supply model validation data for engine models
Milestone 3.2	Supplied validation data to CFR GTS model
Milestone 3.3	Supplied validation data to Hydra GTS model
Milestone 3.4	Supplied validation data to Converge model
Subtask 3.3	Collect data on eff., emissions, and BC
Decision Point 2	Does prelim. data show successful Ref. RCCI?



Acronyms:
GTS: GT-Suite

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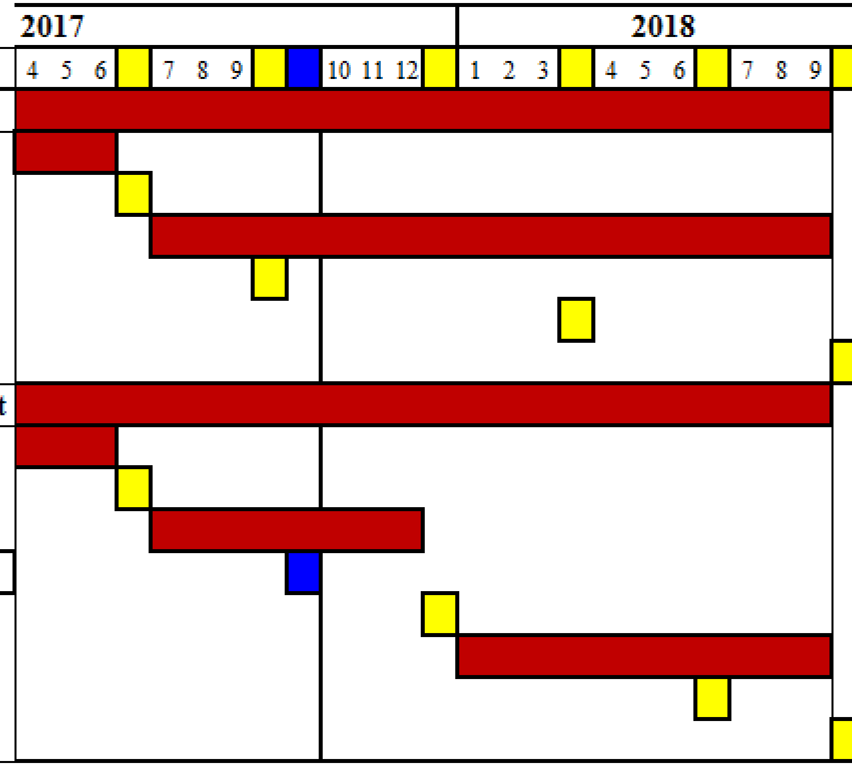
Approach / Milestones – (3) – April 2017 – September 2018

Task Number	Task Title
Task 2	**Combustion and System-Level Modeling**
Subtask 2.4	Validate CFD model of Hydra engine
Milestone 2.6	Validated ConvergeCFD Hydra engine model
Subtask 2.5	Simulate Ref. RCCI with ConvergeCFD
Milestone 2.7	Sim. results of eff. and emissions of Ref. RCCI
Milestone 2.8	Sim. results comparing Ref. RCCI to literature
Milestone 2.9	Final report of all sim. results of Ref. RCCI
Task 3	**Experimental concept testing and assessment**
Subtask 3.2	Supply model validation data for engine models
Milestone 3.4	Supplied validation data to Converge model
Subtask 3.3	Collect data on eff., emissions, and BC
Decision Point 2	Does prelim. data show successful Ref. RCCI?
Milestone 3.5	Data of eff., emissions, and BC of Ref. RCCI
Subtask 3.4	Experimentally determine OR of Ref. RCCI
Milestone 3.6	Data comparing OR of Ref. RCCI to literature
Milestone 3.7	Final report of all experimental data of Ref. RCCI



Milestone Summary:

All previous milestones and decision points have been met with the exception of the most recent experimental milestones related to the Hydra engine, which is about 1 month behind schedule

Acronyms:
BC: Burn Characteristics
OR: Operating Range
Ref. RCCI: Reformate RCCI

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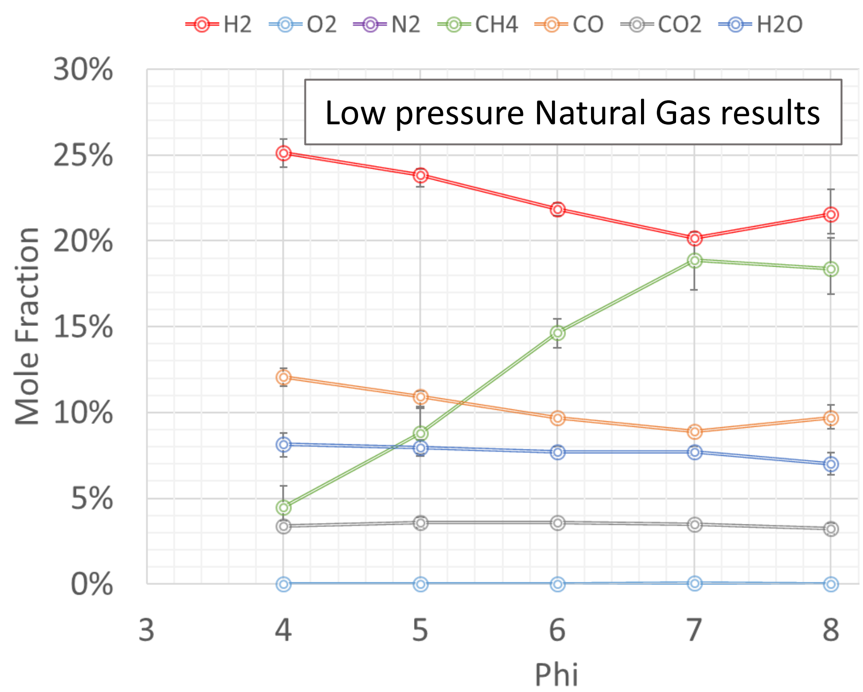
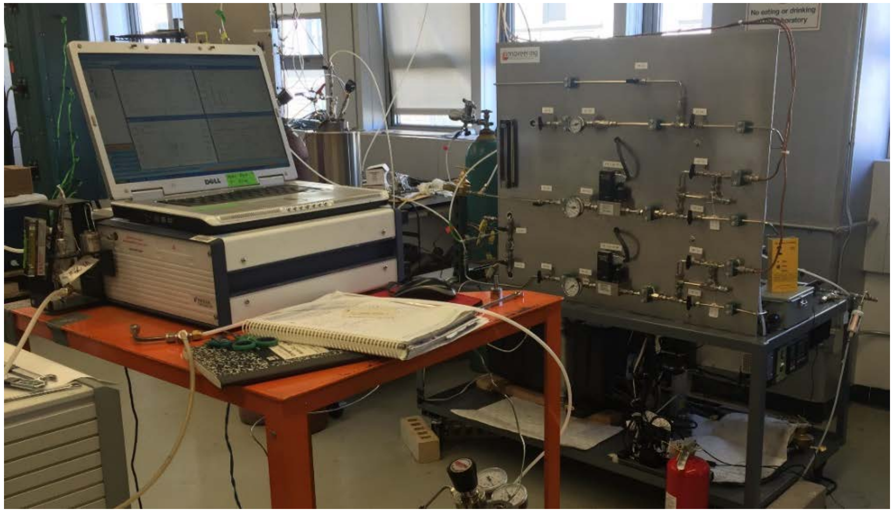
Technical Accomplishments: Fuel Reforming and Characterization

- This work was conducted by Innoveering, LLC with City College of New York (CCNY)
- A flow cart was assembled to control the flow rates of air and fuel into the reformer, as well as control the temperatures and pressures
- The resulting reformate was then directed into gas chromatography equipment to determine the speciation of the mixture





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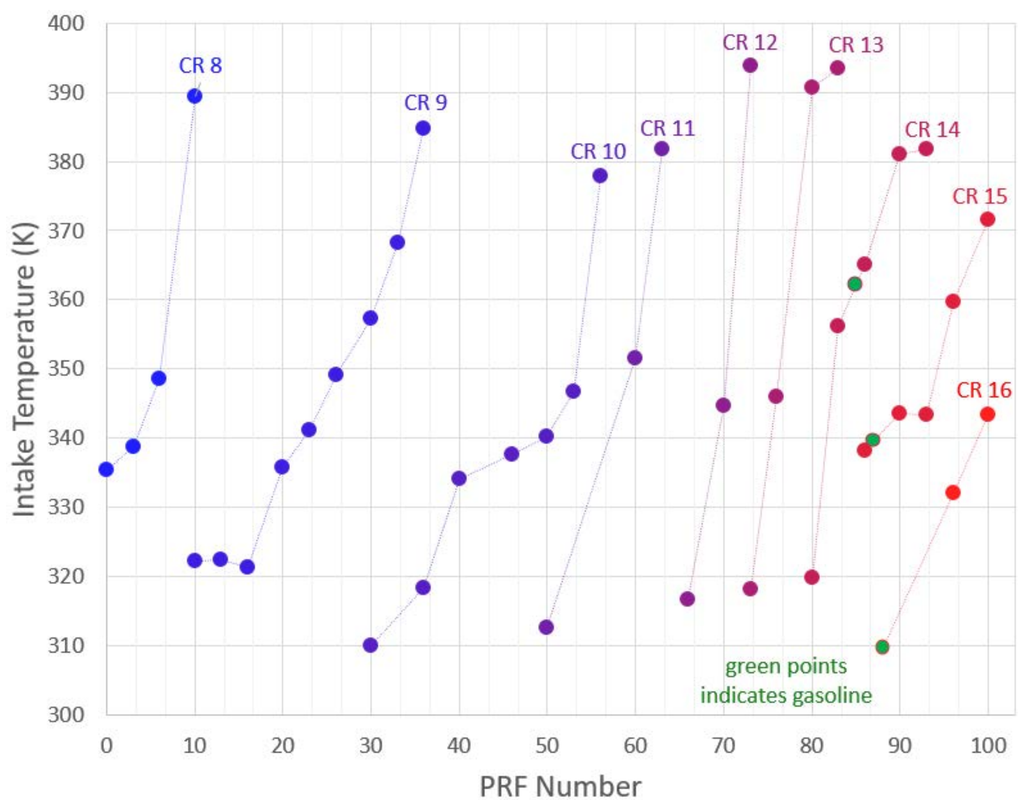
Technical Accomplishments: PRF Mapping to Characterize Reformate

- A CFR engine was used to autoignite various primary reference fuel (PRF) blends in HCCI at different compression ratios and intake temperatures
  - The engine speed, equivalence ratio ($\Phi = 0.3$), CA50, intake pressure, and exhaust pressure were all kept constant while the compression ratio, PRF #, and intake temperature varied
- Once the map was created, it can be used to determine an effective PRF # for any fuel by autoigniting it under the same conditions to determine the required intake temperature at a given compression ratio
- Gasoline is shown as an example in the green data points
  - Interpolated or extrapolated to determine its effective PRF # of 87, which agrees well with its octane
- This methodology uses HCCI as a diagnostic to determine the autoignition tendency of any fuel



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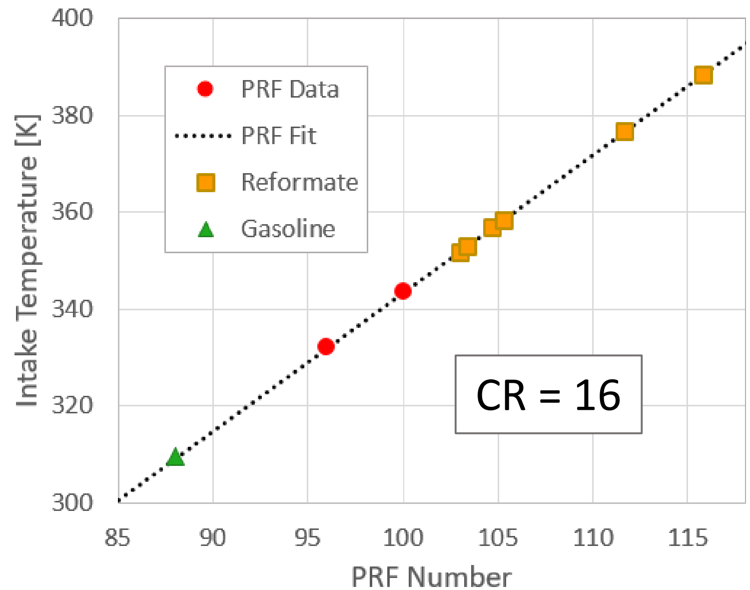
Technical Accomplishments: Autoignition Tendency of the Reformate

- The reformate mixtures were then autoignited in HCCI under the same conditions as the PRF blends to determine their effective PRF numbers
- Although the reformate mixtures were slightly outside of the range of PRF blends and therefore required extrapolation to determine their effective PRF number, the extrapolated distance is small, especially in comparison to the separation between the parent fuel and reformate
- The effective PRF number of each reformate mixture is shown in the table in the bottom right
- Based on the octane separation between the parent fuel and its reformate, Diesel seems to be the best candidate for Reformate RCCI (i.e. single fuel RCCI with onboard fuel reformation)
- The octane separation between natural gas and its reformate or gasoline and its reformate might not be sufficient to enable RCCI combustion



		Effective PRF # or Octane Rating	Parent Fuel	Octane Separation
Natural Gas		130	NA	NA
Gasoline		87	NA	NA
Diesel		0	NA	NA
Reformate Mixture	1	103.0	Gasoline	16.0
	2	103.4	Gasoline	16.4
	3	104.7	Natural Gas	25.3
	4	105.3	Natural Gas	24.7
	5	111.6	Diesel	111.6
	6	115.8	Diesel	115.8

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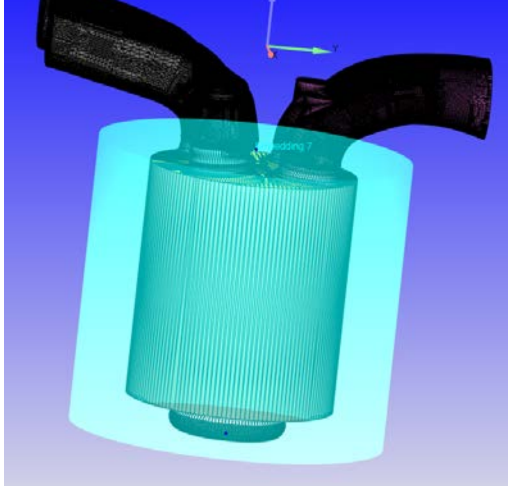
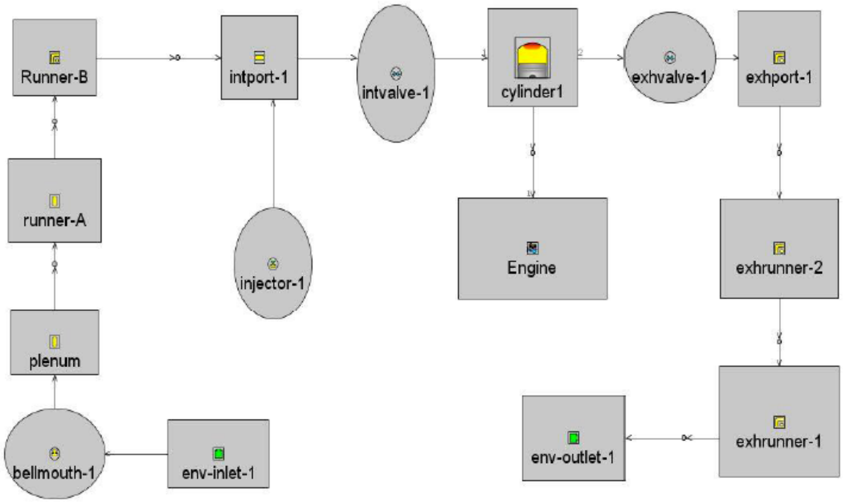
Technical Accomplishments: Combustion and System-Level Modeling

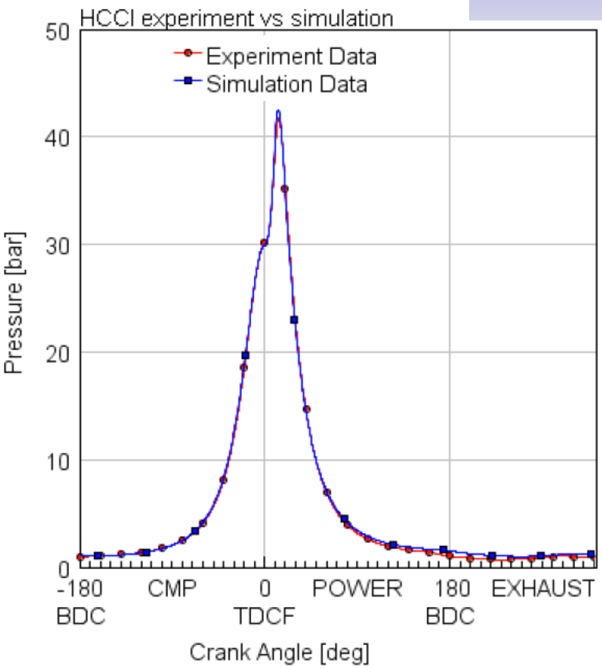
- In addition to the experimental efforts, system-level and detailed 3D CFD modeling efforts will be used throughout the project to provide further insight and complement the experimental data
- A GT-Power model has been constructed, validated against experimental data, and is currently being used to study the efficiencies and energy flows of the system
- A CFD model has also been constructed of the geometry that will be used to experimentally test Reformate RCCI

ConvergeCFD Model



GT-Power Model





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Response to Previous Year Reviewers' Comments

- This project is a new start.

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Collaboration with Other Institutions

Stony Brook University Relationship: Prime - Type: University

- The Advanced Combustion Laboratory has several fully instrumented, single cylinder, research engines including the CFR and a Ricardo Hydra used for this project, state-of-the-art DAQ systems, and two Horiba MEXA emissions analyzers. The group has expertise in experimental and modelling engine research of advanced combustion concepts.

innoveering innovative engineering solutions Relationship: Sub - Type: Industry

- Innoveering LLC, is an engineering firm with catalysis and fuel reforming experience. They designed and built the test cart to control the flow rates of air and fuel through their proprietary SynTec™ fuel reformer.

The City College of New York Relationship: Sub - Type: University

- The Combustion and Catalysis Laboratory at CCNY has gas chromatography equipment as well as the necessary expertise to characterize the reformate mixtures exiting the fuel reformer.

Remaining Challenges and Barriers

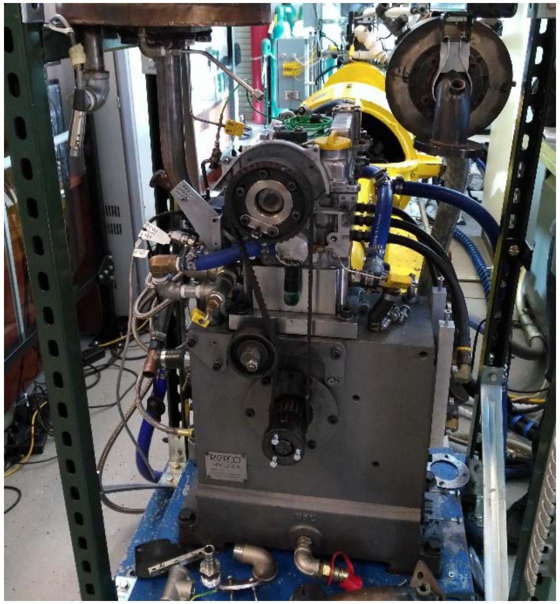
Project challenges:

- Experimental: Manage any experimental setbacks or delays
- CFD modeling: choice of a kinetics mechanism that can accurately capture the effects of the reformate mixture in addition to the parent fuel

Barriers of the technology are:

- Energy lost in the reformer
  - Some energy is lost in the reformer due to this particular exothermic CPOX reaction
  - Need to keep track of this energy and count it against the system efficiency
- Introduction of the gaseous fuel
  - If the gaseous reformate mixture is more reactive than the parent fuel (as is the case for the natural gas parent fuel), then it will need to be direct injected, which will be a challenge
  - Introducing the reformate mixture in the port would not be an issue (which is the case for Diesel and Gasoline parent fuels)
- Production concerns of reliability, cost, and transient response
  - These issues are valid concerns for the technology, but beyond the scope of this preliminary investigation of this early/low TRL technology

Proposed Future Work



Key Upcoming Milestones:

- Validate the CFD model against experimental data of CDC and dual-fuel RCCI
- Use the CFD model, along with the system-level model, to simulate Reformate RCCI over various operating conditions
- A Ricardo Hydra engine will be used to conduct experiments on Reformate RCCI to determine the efficiency, burn characteristics, and emissions in comparison CDC and dual-fuel RCCI

Next Decision Point:

- Does the preliminary data show successful RCCI combustion with a parent fuel and its reformate?
- Specifically, can Reformate RCCI achieve the same efficiency or higher than CDC with greater than 50% reductions in soot and NOx emissions?
- Any proposed future work is subject to change based on funding levels.

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Summary

- In summary, this project is aimed at evaluating the potential of an onboard fuel reformer to provide the necessary octane separation to enable RCCI combustion from a single fuel
- The project includes a close collaboration with Innoveering, LLC, whose expertise lie in catalytic fuel reformation, and with City College of New York, who has experience with gas chromatography and the necessary equipment to characterize the reformate mixtures
- The first task involved reforming the potential parent fuels (gasoline, diesel, and natural gas) to varying levels and characterizing the reformate mixture, including the speciation, as well as determining an effective PRF number for each reformate mixture
- The following tasks, which are ongoing, include CFD and system-level modeling of Reformate RCCI and experimental testing to determine the burn characteristics, efficiency, emissions, and operating range of Reformate RCCI

Thank you

Questions?

Technical Backup

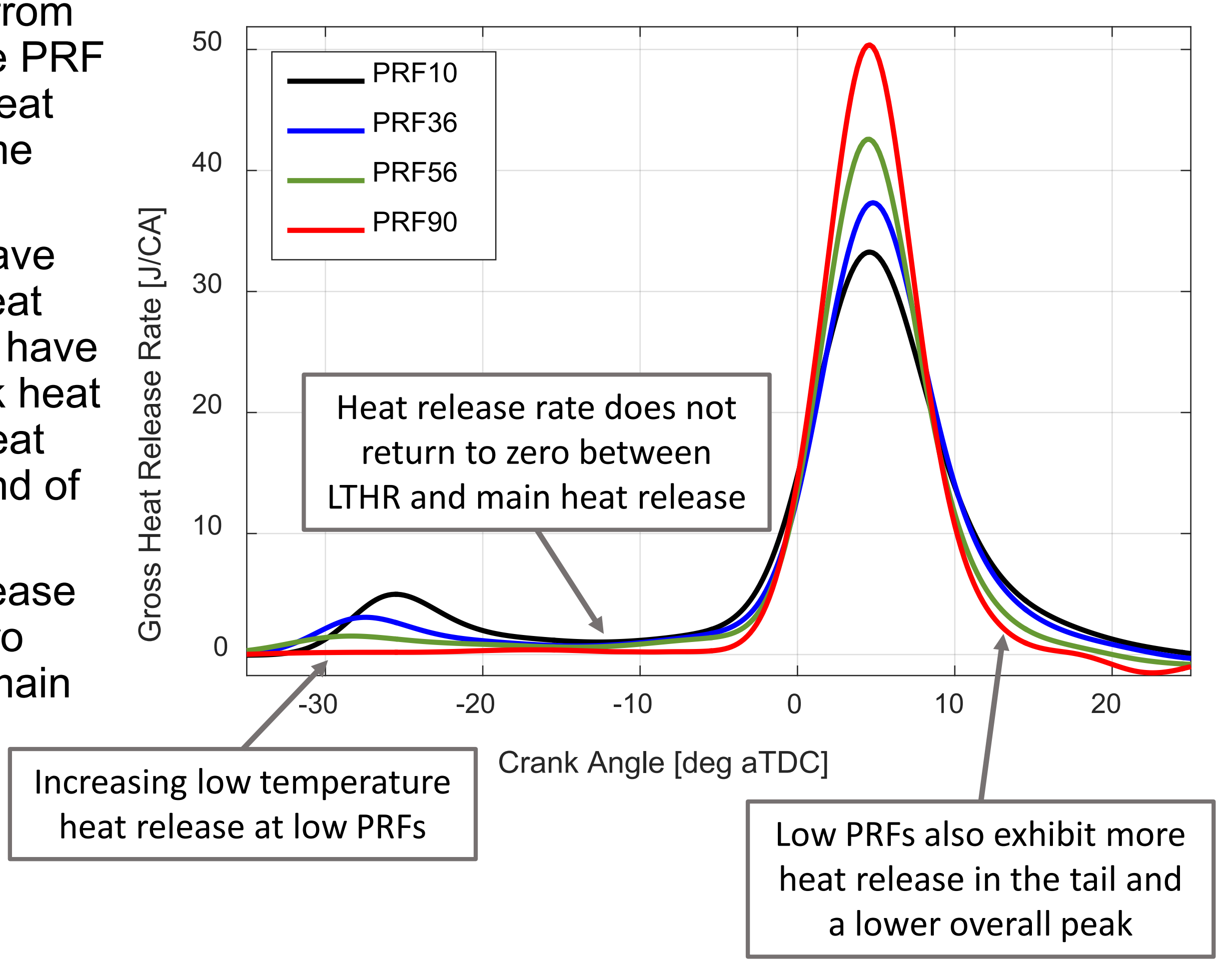
Slides

Technical Accomplishments: Engine Setup Modifications

- As part of this project, a large number of modifications were made to an existing CFR engine test setup to enable the required experimentation and data collection
- These modifications included the addition of a high accuracy National Instruments data acquisition system to collect both the high and low speed data
  - This also required writing custom, in-house LabView code to do the data collection, real-time heat release calculations, and controls
- Additionally, an intake heater was required to heat the intake charge to the desired temperature and enable HCCI
- The Horiba MEXA7100DEGR needed to be commissioned, configured, and calibrated
- The engine needed to be modified to accept the gaseous fuels including a gaseous fuel flow meter and an appropriate port in the intake plenum to allow sufficient mixing
- Our Ricardo Hydra also needed significant modifications that have been completed in the first year of the project

Technical Accomplishments: PRF Heat Release Results

- In addition to the effective PRF number that was determined from the experimental testing of the PRF and reformate mixtures, the heat release shapes illuminate some interesting features
  - The lower PRF values have more low temperature heat release (LTHR), but also have a significantly lower peak heat release rate and more heat release toward the tail end of the combustion
  - Additionally, the heat release rates do not return to zero between the LTHR and main heat release



Technical Accomplishments: Example Reformate Heat Release

- Two examples heat release rates from the reformate mixture testing are shown on the right

- Although the reformate mixtures constitute a mixture of various species including CO, H_2, CH_4, unreacted fuel, and other hydrocarbon species, the reformate mixtures all exhibited single-stage heat release with no low temperature heat release (LTHR)

- The heat release characteristics resembled isooctane or other single-stage fuels