Co-Optimization of Fuels & Engines

Heavy-Duty Advanced Compression Ignition

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Project # FT089

2020 DOE Vehicle Technologies Office

Annual Merit Review

better fuels | better vehicles | sooner

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

VTO Program Managers: Gurpreet Singh, Kevin Stork, & Michael Weismiller

Overview

Timeline

Project	Start Date	End Date*	% Complete
E.2.1.2	10/1/2018	9/30/2021	56%
E.2.1.1	10/1/2019	9/30/2021	33%
E.2.1.7	10/1/2019	9/30/2021	33%
G.2.22	10/1/2019	9/30/2021	33%
F.1.1.2-b	4/1/2020	9/30/2021	6%

* End dates based on three-year life cycle of DOE lab-call projects

Budget

Project	Lab, PI	FY19	FY20
E.2.1.2	SNL, Dec	$240k	$300k
E.2.1.1	ANL, Kolodziej	0	$160k
E.2.1.7	ORNL, Curran	0	$300k
G.2.22	ANL, Pal	0	$170k
F.1.1.2-b	NREL, Fioroni	0	$80k

Total funding for FY20: $1,010k

Barriers

- Improved understanding of fuel effects on Advanced Compression Ignition (ACI) Combustion
  - Including blends of conventional and biofuels
- Determine whether ACI can be better enabled by fuel specifications different from gasoline and diesel
- Improved low-load ACI combustion efficiency
- Reduced engine-out NOx emissions at low-loads where exhaust temperatures are low.
- Develop simulation tools to speed the development of ACI engines.

Partners

- **5 projects at 4 national laboratories** ⇒ next slide
- Partnering between these projects and with other national labs through the Co-Optima AED, FP, and HPF teams, 2 universities, Cummins and Caterpillar.

Overview

Heavy-Duty Advanced Compression Ignition (ACI)

Deeper understanding of fuel property effects to improve full-time and multi-mode ACI engine combustion for MD/HD applications, using engine experiments and simulations.

Project	Description	Lab, PI
E.2.1.2	Autoignition Metrics for Low-Temperature Gasoline Combustion (LTGC) and Fuel Blends to Improve LTGC Performance ($300k)	SNL, Dec
E.2.1.1	Fuel Properties that Enable HD GCI ($160k) ⇒ New project for FY20	ANL, Kolodziej
E.2.1.7	Fuel Properties Impacting MD/HD Multi-Mode ACI ($300k) ⇒ New project for FY20	ORNL, Curran
G.2.22	Numerical Study of Fuel Property Effects on HD GCI Using CFD ⇒ Simulating engine for E.2.1.1⇒ New project for FY20 ($170k)	ANL, Pal
F.1.1.2-b	Fuel Property Research and Screening for MD/HD ACI ($80k) ⇒ New project beginning Q3 FY20	NREL, Fioroni

Relevance

Overall Relevance

- For MD/HD applications, internal combustion engines using liquid fuels will continue to be the dominate power source for many years.
  - Engine efficiency can be increased significantly. $\Rightarrow$ ACI offers promising pathways to achieve this.
  - Advanced fuels can facilitate ACI engine development.
  - Increasing the renewable fraction of fuels can reduce the carbon footprint.
- Research integrating fuels and engines is critical to accelerate progress toward these goals.

Specific Projects Presented

- Studies reported here focus on understanding fuel properties and developing fuel compositions to improve the performance and emission of ACI combustion for MD/HD engines.
- Research includes three fuel and engine projects covering three methods for MD/HD ACI
  1) Kinetically controlled with moderate stratification $\Rightarrow$ **LTGC** (low-temperature gasoline combustion)
  2) Combined injection-timing and kinetically controlled $\Rightarrow$ **GCI** (gasoline compression ignition)
  3) Injection-timing controlled ACI for low loads as part of a multi-mode strategy with MCCI $\Rightarrow$ **low-load ACI**
- Advanced fuels can help: 1) improve combustion-phasing control, 2) improve low-load combustion efficiency and emissions, 3) extend the high-load limit, and 4) increase renewable fraction
- Research also involves autoignition metrics, chemical-kinetic analysis, and CFD engine simulations.

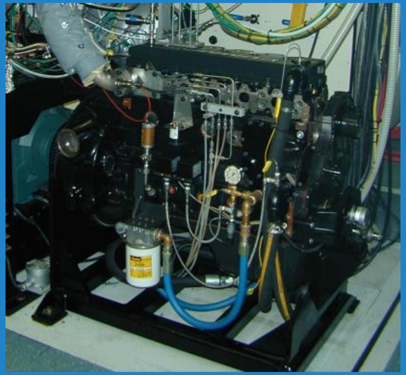
Milestones

Month / Year	Tracked Milestones	Status
6/30/20	E.2.1.2 - Complete testing of custom-tailored fuel blend for LTGC operation and comparison with regular-E10 gasoline. (Dec, SNL)	Completed
6/30/20	E.2.1.7 – Down-select ACI strategy for focused parametric sweeps. (Curran, ORNL)	On Track

Overarching Approach to MD/HD ACI

- **ACI with advanced fuels can increase efficiency and reduce emissions of MD/HD engines**
- **Co-Optima effort includes 3 engine projects covering 3 viable approaches to MD/HD-ACI**

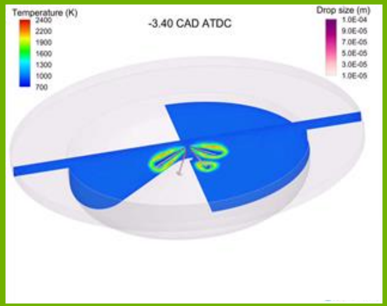
SNL, Dec – LTGC
MD: B x S = 102 x 120 mm
Gasoline-like – kinetic control with moderate stratification

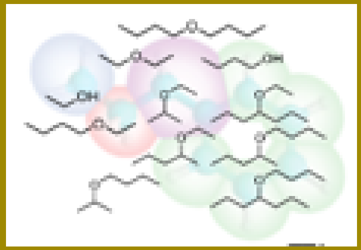


ANL, Kolodziej – GCI
HD: B x S = 137 x 165 mm
Gasoline-like – injection & kinetic control

ORNL, Curran – low-load ACI
MD: B x S = 107 x 124 mm
Diesel-like – injection control

ANL, Pal
CFD modeling
Supports ANL engine





NREL, Fioroni
Fuel Properties and Screening
Supports all engine projects

- **Approaches for specific projects are given on the Accomplishments slides**

Autoignition Metrics for LTGC – Understanding the Performance of OI in ACI/LTGC Engines from Beyond-MON to Beyond-RON

Objective #1 – Evaluate the performance of Octane Index (OI) as an autoignition metric for LTGC/ACI from Beyond-MON to Beyond-RON conditions. ⇒ OI = RON – K*(RON-MON)

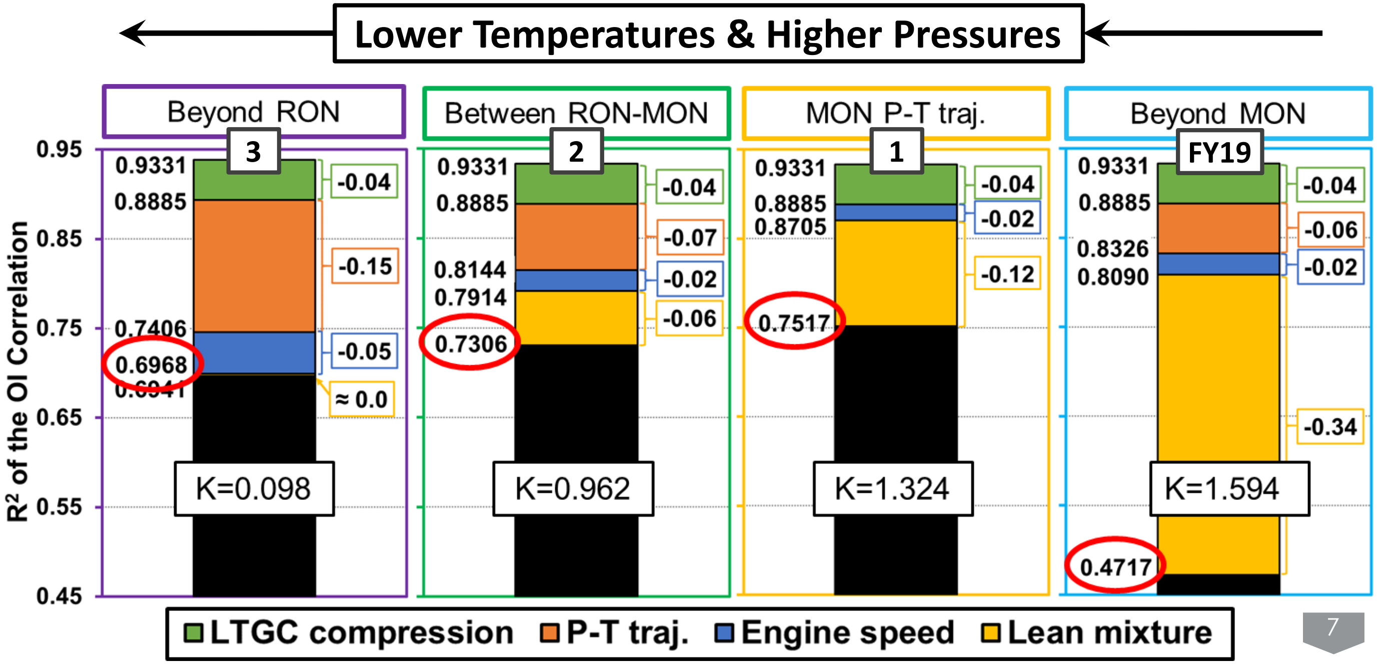
- In FY19: ⇒ Verified that OI works well for simulated MON test ⇒ **R^2 = 0.933**
  ⇒ Showed that OI does not work for P_{in} = 1 bar LTGC, Beyond-MON ⇒ **R^2 = 0.472**
- FY20 Objective: Extend analysis to evaluate OI as an autoignition metric for LTGC operation at **1)** MON P-T trajectory, **2)** between MON & RON, and **3)** Beyond-RON

Approach:

- CHEMKIN simulations with LLNL Co-Op mech. & validated fuel surrogates have been shown to match experiments well
- Apply to quantify effect of each difference from MON-test conditions to LTGC conditions **1**, **2**, and **3**

Results:

- The OI correlation does not perform well for any P-T trajectory tested when operating at realistic LTGC conditions
- Factors causing the poor performance of OI vary considerably with P-T trajectory
  - Lean mixture has large effect Beyond-MON
    ⇒ becomes smaller with ↘T & ↗P
    ⇒ Beyond-RON no effect, all fuels are ϕ-sensitive
  - Beyond RON ⇒ P-T trajectory has largest effect
- **OI not an adequate metric for LTGC autoignition**



E.2.1.2
Dec, SNL

Fuel Blends to Improve Low-Temperature Gasoline Combustion (LTGC) Performance

Objective #2 – Expand testing of improved fuel blend for LTGC and boosted SI introduced in FY19 – CB#1

- CB#1 ⇒ **iso-butanol (HPF fuel) blend** designed to be a better LTGC fuel than Reg. E10 (RD5-87). Also higher RON & S for boosted SI (see FT070) ⇒ FY20 Goals:
  1) Quantify ϕ-sensitivity improvement, P_{in}=1.0 - 1.6 bar
  2) Determine potential for high-load LTGC with CB#1

Approach:

ϕ-sens. ⇒ phasing control, extend load range

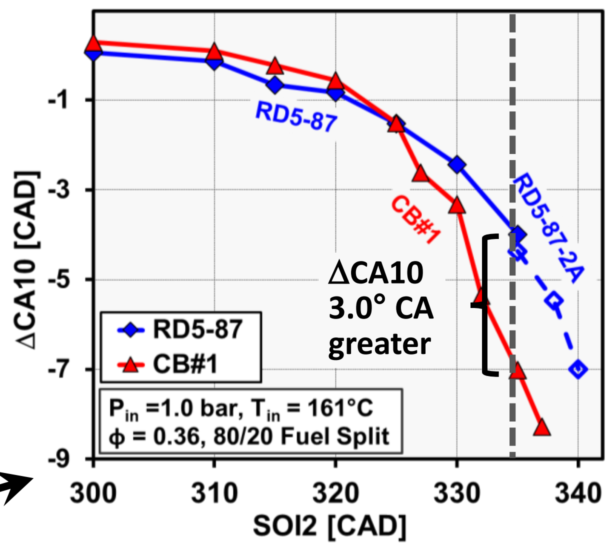
- Develop two metrics to quantify ϕ-sensitivity
  - Metric-1: CA10 advance for a given stratification (SOI2)
  - Metric-2: Spread in HR for given stratification (back-up slide)
- Determine max. load at P_{in} = 2.4 bar (representative high-load point)

Results:

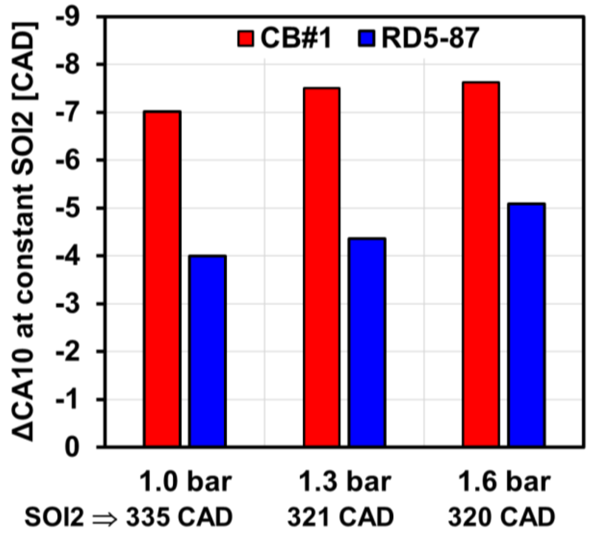
- **Both Metric-1 & Metric-2 show CB#1 has significantly higher ϕ-sensitivity** for P_{in} = 1.0 – 1.6 bar vs. RD5-87
- **High-load LTGC capability for CB#1 ~same as RD5-87**
- Previous results showed CB#1 has ~same reactivity at P_{in} = 1, higher RON & higher Octane-Sens. (S) vs. RD5-87

- **Shows both ϕ-sensitivity & S can be increased simultaneously**
- **CB#1 is a promising fuel for MD/HD ACI & ACI/SI multi-mode**

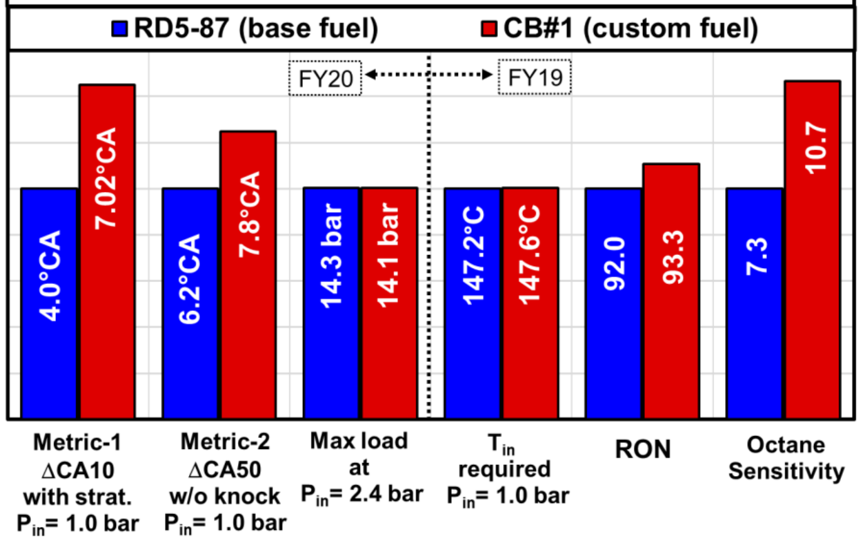
Metric-1: ΔCA10 with SOI2



Metric-1: P_{in} = 1.0, 1.3 & 1.6 bar

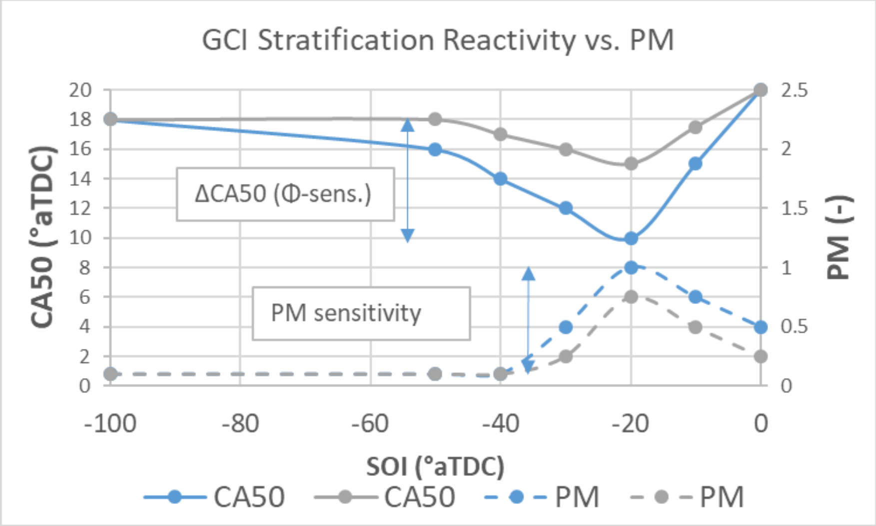


CB#1 ⇒ 18.3% 1-hexene + 27.4% n-pentane + 11% iso-octane + 30.9% p-xylene + 12.4% iso-butanol (Liquid vol. fractions)



E.2.1.1. Fuel Properties that Enable HD GCI (ANL) – 1

- **Objective:** Experimentally identify gasoline-range fuel properties that improve the trade-off between increased combustion phasing control with fuel stratification (phi-sensitivity) vs. increased emissions in Heavy-Duty (HD) ACI combustion.
- **Approach:** Measure combustion phasing advance vs. particulate emissions (ΔCA50/PM) while conducting start of injection (SOI) timing sweeps.
- Use a large bore (137 mm) HD single-cylinder engine (SCE) with narrow injector inclusion angle (130°) to minimize spray impingement effects.
- Blend candidate biofuels into varied base BOBs for constant CFR HCCI Number reactivity and varying chemical composition and physical properties.
- Use 3D CFD (G.2.22, Pal) to characterize cylinder temperature and mixture stratification.



Conceptual Model (hypothetical)

Base Engine	Caterpillar SCE
Injection System	PFI, DI Common Rail
Bore x Stroke	137 × 165 mm
Displacement	2.44 liters
Compression Ratio	16.2:1

Project Status:

- **CFR HCCI fuel blending to occur once lab re-opens**
- **March 30th engine re-commissioning delayed (COVID-19)**
- **Scoping 1D spray impingement simulations underway**

E.2.1.1. Fuel Properties that Enable HD GCI (ANL) – 2

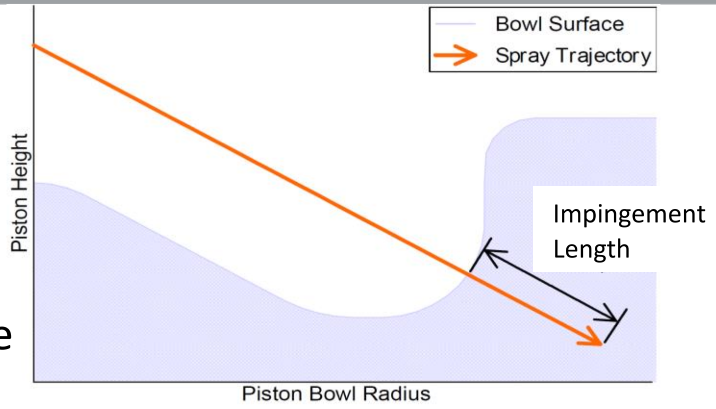
Objective: Prior to conducting engine experiments, determine the test conditions which will avoid fuel liquid impingement

Approach:

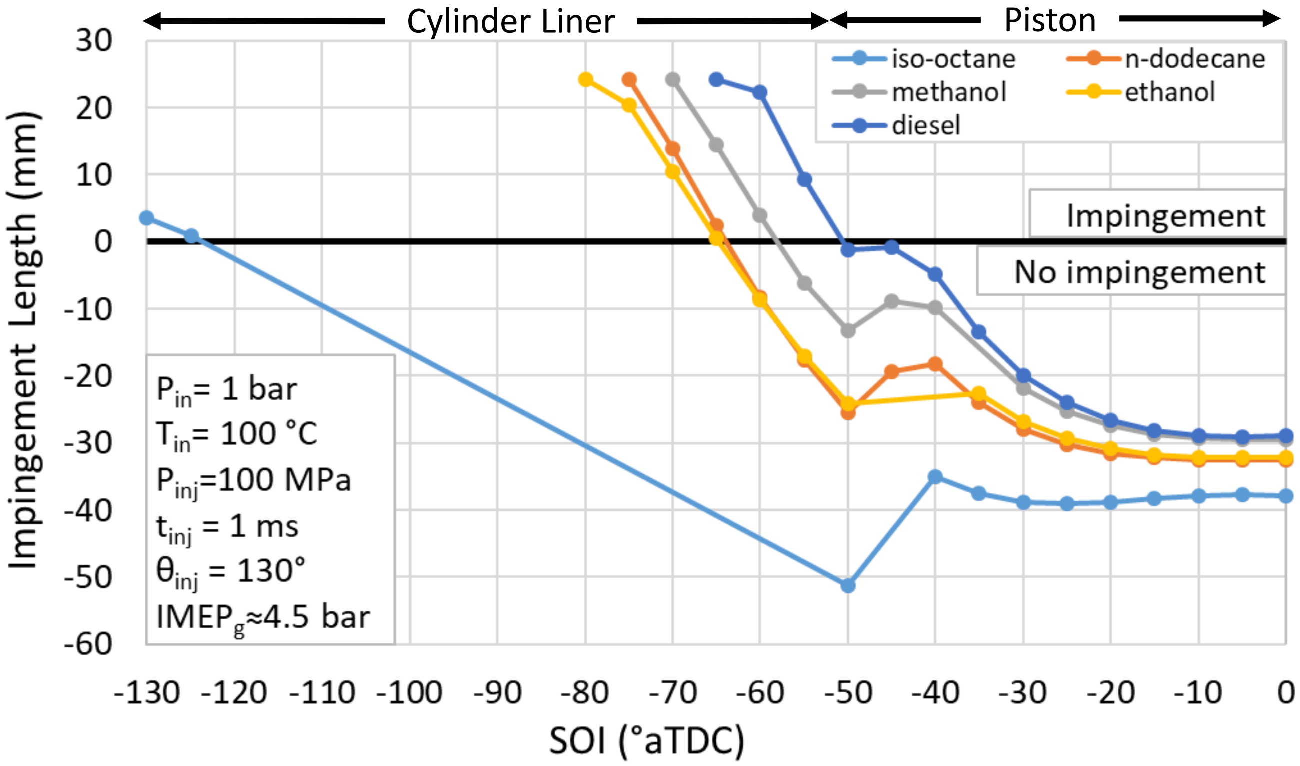
- Simulate spray liquid length of a wide range of injection timings and fuel properties using a 1D spray simulation (DICOM)
- Compare to length available in the combustion chamber (piston and cylinder)

Results:

- **Isooctane (gasoline surrogate) allowed ≈2x wider range of injection timings than diesel and n-dodecane (diesel surrogate)**
- **Pure alcohols (ethanol & methanol) can have similar impingement as diesel fuel**



Impingement Length
= Liquid Length - Length Available



DICOM 1D spray model, by CMT-Motores Térmicos: https://www.cmt.upv.es/ECN11.aspx

E.2.1.7
Curran/Sluder, ORNL

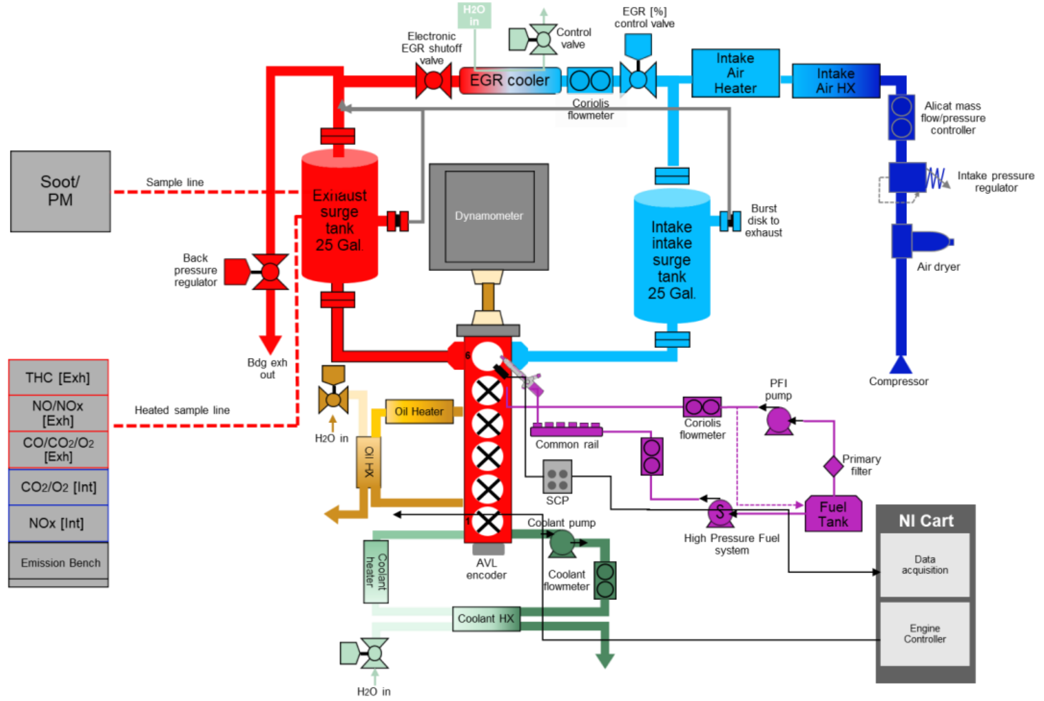
Single-cylinder diesel-range fuel properties experiments to explore ability for LTC for MD/HD ACI multi-mode

- **Objective:** Experimentally investigate diesel-range fuel property effects on LTC in a LTC/diesel multimode - enabling ACI in low-load MD/HD engines to allow for low-NOx operation via multi-mode strategy when conditions are too cold inject urea for SCR systems
- **Approach:** Single-cylinder MD/HD multi-mode engine experiments investigating the fundamental effects of fuel properties such as boilng range, reactivity and HOV enabling low-load ACI for MCCI engines. Focus on distillation impact on mixing processes and in-cylinder phenomenon + effect on ACI operation

Fuel	Property Targets
#2 base fuel	Cetane = 44, T90 = 338°C
# 1 base fuel	Cetane = 44, T90 = 288°C
“#0*” base fuel	Cetane = 44, T90 = 238°C
* #0 diesel fuel does not exist but this new fuel represents	

- **Project status:** The build of the new MD single cylinder engine platform is underway and on track for completion of FY 20 milestones (even with current work from home protocols)

ORNL Single-Cylinder MD Single Cylinder Engine Platform



Specification	(-)
Base engine	2019 ISB 6.7 250
Bore x stroke:	107×124mm
Base CR	20:1
Firing cylinder	Cyl 6 (SCE config)

G.2.22
Pal, ANL

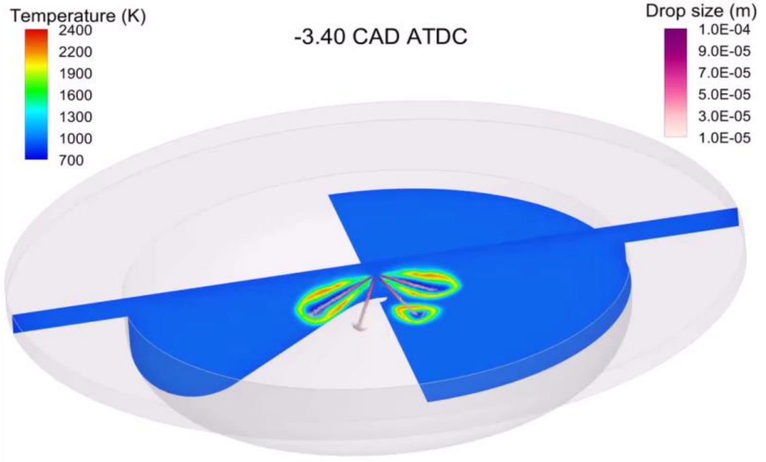
Numerical Study of Fuel Property Effects on HD GCI Using CFD

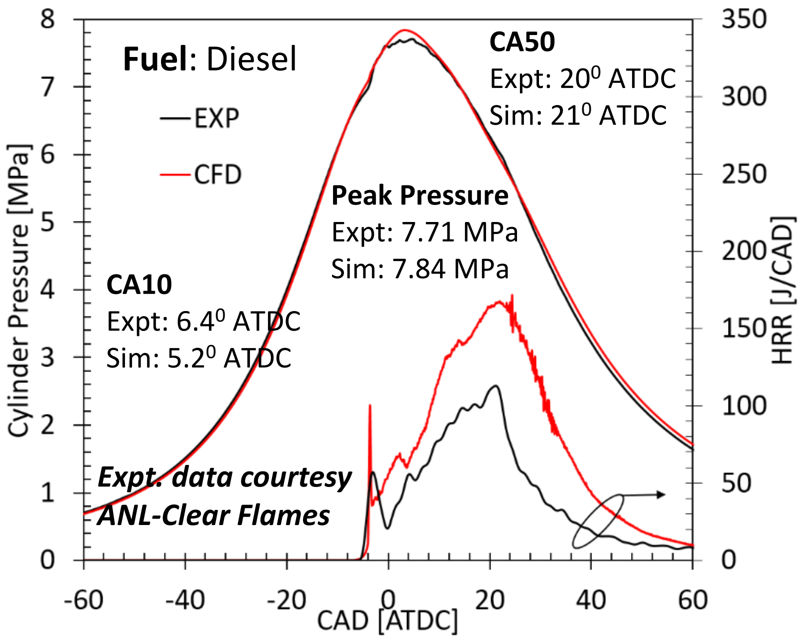
- **Objective:** Investigate fuel property effects that can improve the trade-off between engine efficiency and PM emissions under HD GCI conditions with fuel stratification

- **Approach:** Develop and validate CFD model for ANL HD GCI engine, perform injection timing sweeps for gasoline-biofuel blend surrogates, investigate sensitivity of CA50 and PM emissions

- **Project status:**

1) A CFD model was developed incorporating accurate description of the piston bowl
2) Tabulated flamelet model with detailed chemistry based lookup table [*Magnotti & Kundu @ACE135*] was employed to speed up CFD simulations by 3-5x compared to well-stirred reactor approach
3) Preliminary comparison of closed-cycle simulations was performed against available diesel experimental data (received in Feb 2020) with good agreement





Responses to Previous Year Reviewers' Comments

- **Many of projects presented are new tasks for FY20**
  - E.2.1.7 Curran, ORNL and F.1.1.2-b Fioroni, NREL are completely new tasks for FY20.
  - E.2.1.1 Kolodziej, ANL presents a new HD-ACI task, but presented work on a MM/ACI project last year.
  - G.2.22 Pal, ANL presents CFD results on a new engine, but presented CFD work on a MM/ACI project last year.
  - E.2.1.2 Dec, SNL continues work initiated last year.

Fuel effects in LTGC Engines (Dec), Fuel effects on autoignition (Kolodziej), and ACI CFD simulations (Pal)

Comment: "the approach to this work is extremely thorough and scientific. There is substantial technical detail in the work at SNL and ANL."

Response – We thank the reviewer for these comments.

Comment: A reviewer indicated that this project may have the best future opportunities because team members covered the entire space from very fundamental to applied with simulation support. Also, it focuses on compression ignition in all regimes, which is of primary importance to the non-automotive community (MD/HD).

Response – Thank you, we also think that compression ignition approaches have the most potential for MD/HD applications and are going forward in this manner for our FY20 and FY21 tasks.

Comment: "A reviewer liked the simulation work, but expressed concern as to whether the kinetic mechanisms used are sufficiently robust to capture the synergistic and antagonistic behaviors between fuels relevant to Co-Optima."

Response – This work used the LLNL Co-Optima mechanism which was found to match experimental data quite well across a wide range of conditions for RD5-87 and the co-optima core fuels **when well-developed fuel surrogates were used**, as shown in our FY18 AMR presentation. However, if the mechanism is applied to new fuels and/or applied to significantly different conditions it must be validated. Overall, although the mechanism is imperfect, it work sufficiently well to give good guidance for fuel development as demonstrated by our CB#1 results.

Collaboration and Coordination with Other Institutions

- **Co-Optimization of Fuels and Engines**
  - Collaboration across nine national laboratories and two DOE offices (+8 Universities)
  - 145 stakeholders from 86 organizations
- **Autoignition Metrics for LTGC/ACI and Fuel Blends to Improve LTGC Performance (Dec, SNL)**
  - LLNL (Pitz and Wagnon) – detailed chemical-kinetic mechanism and mechanism evaluation
  - SNL (Sjöberg and Kim) – evaluation of CB#1 for spark-ignition (SI) and boosted-SI combustion
  - PACE fuel surrogate team, LLNL, SNL, ANL (led by McNenly) – development of improved surrogate for RD5-87
  - Univ. of Connecticut – development of a skeletal mechanism for CFD
- **Fuel Properties that Enable HD GCI (Kolodziej, ANL)**
  - Caterpillar – supplied engine and common-rail injection system upgrade
  - ANL (Pal) – CFD simulations of HD GCI
- **Fuel Properties Impacting MD/HD Multi-Mode ACI (Curran, ORNL)**
  - AED, FP and HPF teams – coordination of tasks, MD/HD multi-mode research directions, and fuel properties
  - SNL (Busch) – coordination on fuels
  - ORNL (Wissink & DeBusk) shared platform and coordination of experiments
  - Cummins – supplied engine and technical input on directions for research
- **Numerical Study of Fuel Property Effects on HD GCI Using CFD (Pal, ANL)**
  - ANL (Kolodziej) – experimental data for model validation
  - Univ. of Illinois at Chicago (UIC) – CFD simulations
  - LLNL (Pitz et al.) – detailed chemical-kinetic mechanism

Remaining Challenges and Barriers

- An accurate autoignition metric is needed for LTGC-ACI for operation at all conditions from Beyond-MON to Beyond-RON. Need is particularly significant at the Beyond-MON conditions used for naturally aspirated LTGC-ACI. Metric could potentially also be applied to other MD/HD ACI operating modes.
- New fuel blends that improve ACI performance and use a higher HPF (renewable-fuel) fraction are needed for all three MD/HD ACI combustion modes.
- Identify desired fuel properties for HD GCI engines.
- Overcome longstanding barriers for enabling LTC with fuels having diesel-range properties.
- Improved spray models for both GDI and diesel-type injectors that are applicable to both early injections (low-density in-cylinder gases) and late injection near TDC (high-density in-cylinder gases).

Proposed Future Work

Any proposed future work is subject to change based on funding levels.

- **Autoignition Metrics for LTGC/ACI and Fuel Blends to Improve LTGC Performance (Dec, SNL)**
  - Develop new fuel blends for LTGC-ACI with high HPF content up to 30% or more. These new blends must also improve LTGC performance compared to Regular E10 gasoline (RD5-87) in terms improved combustion-phasing control and increased load range.
  - Develop new fuel blends based on selected HPF components combined with real distillate BOBs.
- **Fuel Properties that Enable HD GCI (Kolodziej, ANL)**
  - Formulate fuel blends with constant HCCI number on the CFR engine
  - Test fuels under non-impinging SOI sweeps to quantify the effects of stratification on combustion-phasing advance and PM and NOx emissions.
- **Fuel Properties Impacting MD/HD Multi-Mode ACI (Curran, ORNL)**
  - Commission new MD/HD SCE platform – on track to support milestone "Down-select ACI strategy for focused parametric sweeps."
  - Complete initial experiments on distillation-curve effects on ACI for low-NOx multi-mode (with MCCI) strategy.
- **Numerical Study of Fuel Property Effects on HD GCI Using CFD (Pal, ANL)**
  - Validate combustion model coupled with Method of Moments approach for soot emissions.
  - Investigate soot-efficiency trade-off for gasoline-HPF blends under GCI conditions.
- **Fuel Property Research and Screening (Fioroni, NREL)**
  - Work with the AED and FP teams to define key fuel properties for MD/HD ACI engines. Based on these properties, screen the fuel-property database to produce a list of promising candidate HPF components for blending.
  - Provide fuel property data to Co-Optima team members and maintain fuel property database.

Summary

Relevance

- Better integration of fuels and engines research is critical to accelerating progress toward higher-efficiency engines with lower emissions and less costly aftertreatment.

Approach

- Conduct research on three viable methods for MD/HD ACI engines using advanced fuels to improve performance and emissions.
- For each method, develop understanding of required fuel properties & formulate appropriate fuel blends using Co-Optima blendstocks.
- Combine engine experiments with CFD simulations and chemical-kinetic analysis.

Accomplishments

- Evaluated the Octane Index (OI) as an autoignition metric for LTGC-ACI from Beyond-MON to Beyond-RON. Showed that OI was not an adequate metric for LTGC-ACI and quantified the key factors limiting the accuracy of OI as an autoignition metric.
- Showed that CB#1, a new HPF fuel blend, has increased ϕ-sensitivity for improved MD LTGC performance over reg. E10 gasoline (RD5-87).
- A new HD engine lab has been established at ANL to investigate fuel properties that can enable HD GCI-ACI.
  $\Rightarrow$ Simulations were conducted to determine potential for liquid wall impingement with various fuel types.
- A new MD/HD engine lab is under development at ORNL to investigate fuels for low-load ACI for a multi-mode ACI/MCCI operation.
- CFD modeling capability of new HD engine at ANL has been established and validated against existing MCCI combustion data.

Collaborations

- These projects are supported by multiple collaborations among national lab partners in Co-Optima, ANL, NREL, LLNL, ORNL, and SNL.
- External collaborations include: Univ. of Connecticut, Univ. of Illinois at Chicago, Caterpillar, and Cummins.

Future Work

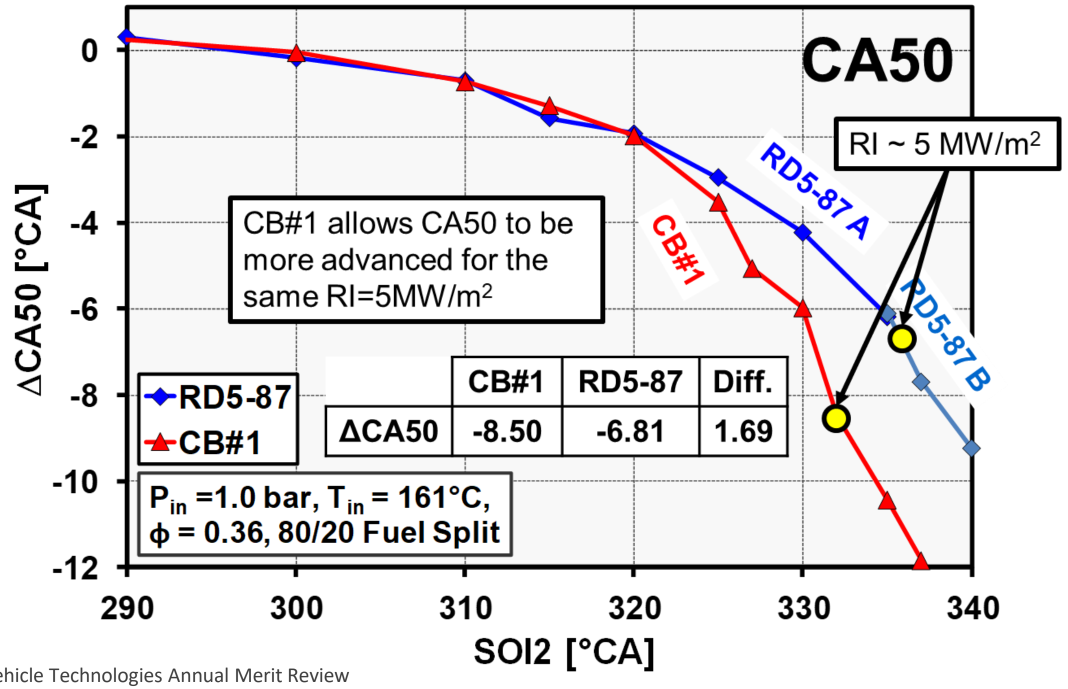
- Develop and test new fuel blends for MD/HD LTGC-ACI that have high HPF content up to 30% and improve engine performance.
- Formulate new fuel blends for GCI-ACI fuels & test under non-impinging conditions to quantify the effects on performance & emissions.
- Commission new MD/HD engine and conduct initial experiments of distillation-curve effects on ACI for low-NOx in multi-mode ACI/MCCI.
- Validate combustion model for GCI-ACI and investigate soot-efficiency trade-off for gasoline-HPF blends under GCI condition.
- Define key fuel properties for MD/HD ACI engines and screen the fuel-property database for promising HPF blending components.

Technical Back-Up Slides

Metric-2 for ϕ-Sensitivity

- **Metric-2: Higher ϕ-sensitivity fuels have a slower heat release for a given fuel stratification.**
  - Results in a lower peak HRR and thus, a lower PRR and lower Ringing Intensity (RI) for the same stratification.
  - When SOI2 retard is used to produce the fuel stratification, this effect allows CA50 to be more advanced for the same RI = 5 MW/m² when the fuel is more ϕ-sensitive. ⇒ Shown in left-hand plot.
- **The greater CA50 advance for RI = 5 MW/m² shows that CB#1 has a higher ϕ-sensitivity than RD5-87.**

CA50 advance with SOI_2 for CB#1 & RD5-87



Difference in CA50 advance with SOI_2 for RI = 5 MW/m² at P_{in} = 1.0, 1.3, and 1.6 bar for CB#1 and RD5-87