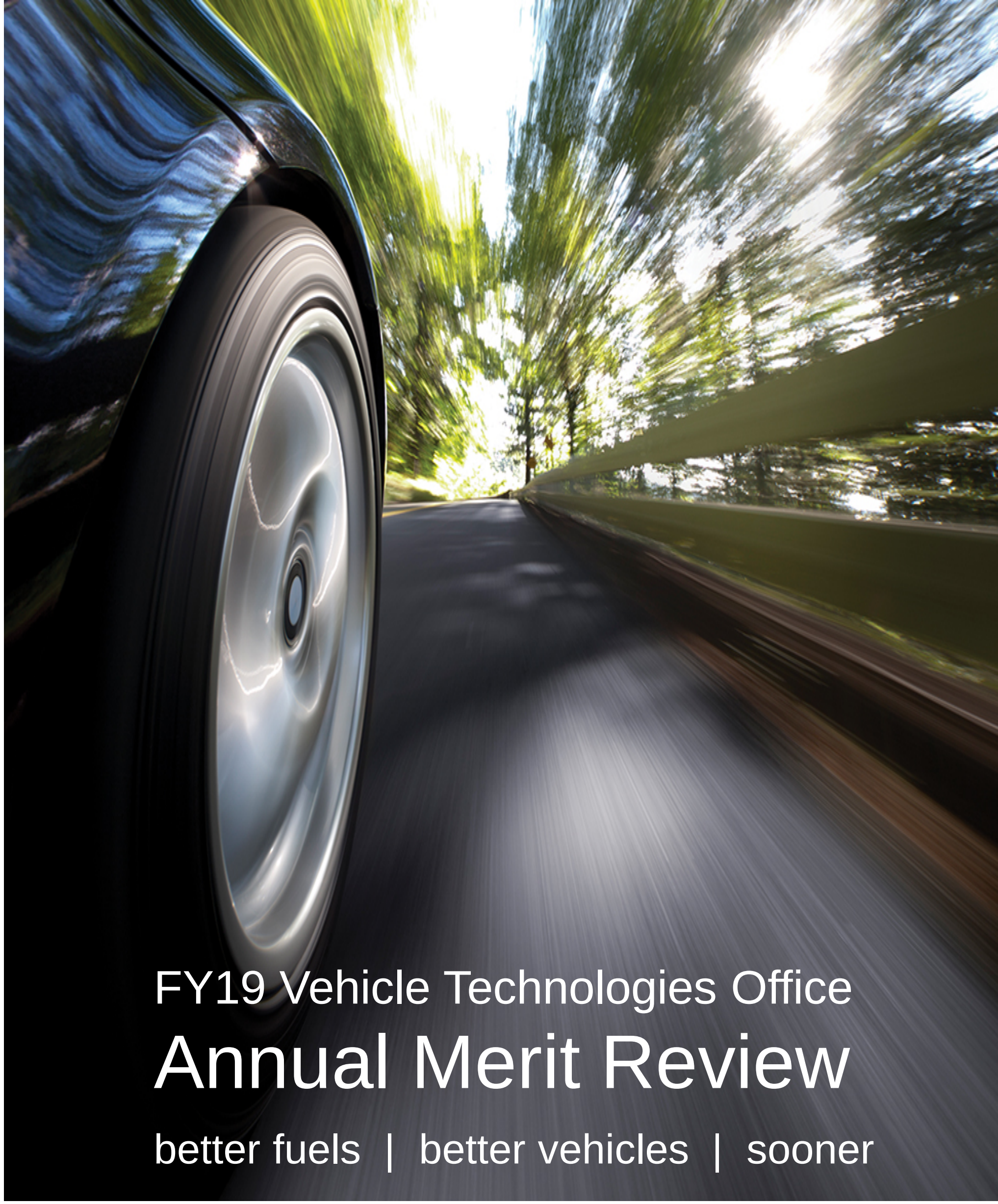
Co-Optimization of
Fuels & Engines

# MM: Autoignition in MM/ACI Combustion, Part 3

J. Dec, G. Gentz, R. Grout, A. Hoth, R. King, C. Kolodziej, D. Lopez Pintor, P. Pal, J. Pulpeiro Gonzalez, M. Ratcliff, T. Rockstroh, S. Schneider, A. Shah, S. Som

June 12, 2019

Project # FT072



FY19 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: 10/1/2018
- Project end date: *9/30/2021
- Percent complete: 16%

## Budget

- Total project funding
  - DOE share: $855k
  - Contractor share:
- Funding in FY 2018: $520k
- Funding for FY 2019: $1,083k

* Start and end dates refer to three-year life cycle of DOE lab-call projects

## Barriers

- Understand the impact of future fuels on Multi-Mode (MM) and Advanced Compression Ignition (ACI) combustion
- Determine whether ACI combustion can be more fully enabled by improved fuel specifications for ACI/MM engines
- Develop MM/ACI engine simulation tools to speed the development of ACI engines

## Partners

Partners include nine national labs, 20+ universities, external advisory board, and many stakeholders

# Overview

**Autoignition in MM/ACI Combustion, Part 3**

Deeper understanding of fuel property effects to enhance multi-mode and full-time ACI engine combustion, using simulations and engine experiments.

| Project | PI |
|---|---|
| E.2.1.2 - Low-Temperature Gasoline Combustion (LTGC) Engines – Fuel Effects ($240k) | Dec (SNL) |
| F.1.5.1 - Fuel Properties Effects on Auto-Ignition in Internal Combustion Engines ($243k) | Kolodziej (ANL) |
| G.1.5 - CFR Engine Simulations for ACI Combustion Analysis ($100k) | Pal (ANL) |
| F.2.6.1- Systematic Evaluation of RON, S, Phi Sensitivity, and Flame Speed Effects in ACI Combustion ($450k) | Ratcliff (NREL) |
| G.2.16.NREL(a) - Simulation support for NREL ACI experiments ($150k) | Grout (NREL) |

# Relevance

## Relevance of Co-Optima:

- Internal combustion engines and the use of liquid fuels will continue to dominate transportation for decades, and engine efficiency can be increased significantly.
- Research integrating fuels and engines is critical to accelerating progress towards our economic development, energy security, and emissions goals.

## Presentation Specific Relevance:

- This presentation is focused on SI/ACI multi-mode and full-time ACI combustion.
- Improved understanding of fuel property effects on autoignition allow for improved SI knock mitigation and ACI combustion phasing control.
- The work presented used engine experiments, fuels rating metrics, and 3D CFD simulations.

ACI: advanced compression ignition
SI: spark ignition

# Milestones

| Month / Year | Description of Milestone or Go/No-Go Decision | Status |
|---|---|---|
| 12/31/18 | Measure three RON 90 fuels (PRF90, Toluene/n-heptane, Ethanol/n-heptane) in HCCI combustion conditions on the CFR engine to map reactivity in expanded temperature/pressure operating space (Kolodziej, ANL). | Completed |
| 12/31/18 | Develop a CFR engine model for HCCI conditions and validate with available experimental data. (Pal, ANL) | Completed |
| 6/30/19 | MCCI Operation of Single Cylinder Engine. (Ratcliff, NREL) | On Track |
| 6/30/19 | Identify the causes of the poor performance of the octane index as an autoignition metric for LTGC and quantify the magnitude of these various causes for naturally aspirated operation. (Dec, SNL) | On track |
| 9/30/19 | Multi-dimensional CFD model of single cylinder engine. (Grout, NREL) | On track |

# Low-Temperature Gasoline Combustion (LTGC) Engines – Fuel Effects

## Objective #1 – Autoignition Metrics

- Identify the causes for the failure of Octane Index (OI) as an autoignition metric for LTGC Engines
  - ➢ OI = RON – K*(RON-MON) gives a poor correlation, $R^2 = 0.447$

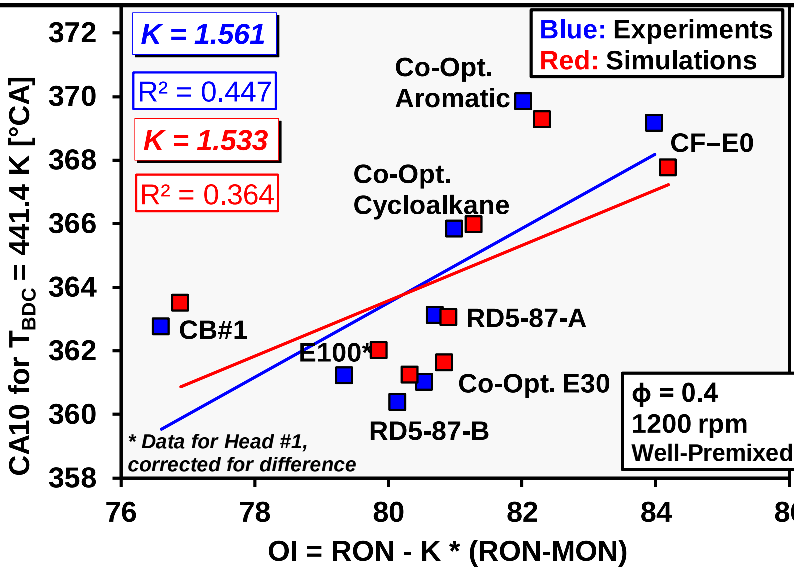
## Approach:

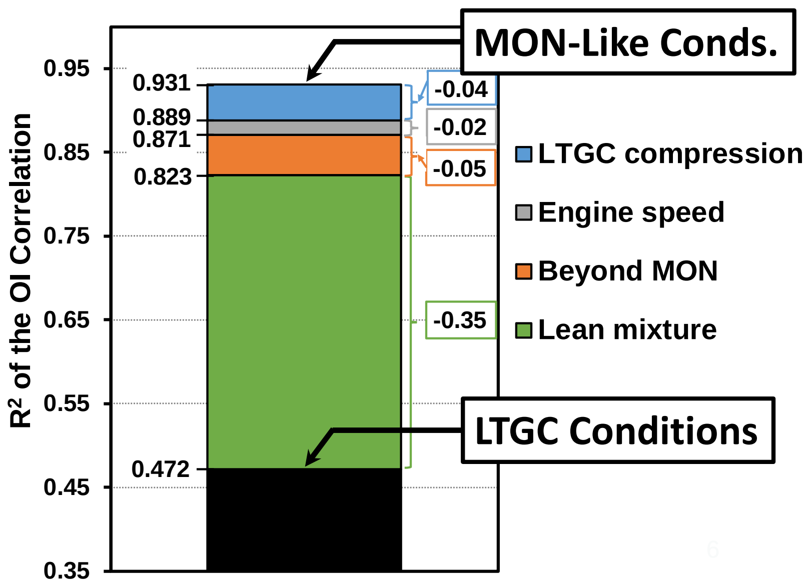
- Apply CHEMKIN with LLNL Co-Op mech. and validated surrogates to simulate exper. data
  - ➢ **CHEMKIN matches experiments very well, K-factor and $R^2$ are both similar**
- Evaluate effect of each difference from MON-test conditions ⇒ Data are beyond MON

## Results:

- For simulated MON-type test, OI performs well, K = 1.07 and $R^2$ = 0.931
- Evaluate: 1) compression by piston + flame (MON) to piston-only (LTGC), 2) engine speed, 3) beyond MON conds., and 4) reduced equiv. ratio (ϕ) from ~1.0 (MON) to 0.4 (LTGC)
- **<u>Lower ϕ of LTGC is the biggest factor</u>** ⇒ due to differences in ϕ-sensitivity between fuels

**$P_{in}$ = 1.0 bar, $T_{in}$ = 154°C ⇒ Beyond MON Condition**



# Low-Temperature Gasoline Combustion (LTGC) Engines – Fuel Effects

## Objective #2 – Develop an Improved Fuel Blend

- Investigate the potential of using a Co-Optima HPF fuel species to blend a fuel that improves LTGC perform. vs. Reg. E10 (RD5-87) ⇒ Goals:
  1) Increase ϕ-sensitivity at $P_{in}$ = 1.0 – 1.6 bar
  2) Similar reactivity at $P_{in}$ = 1 bar
  3 & 4) Increase octane-sensitivity (O-S) and RON

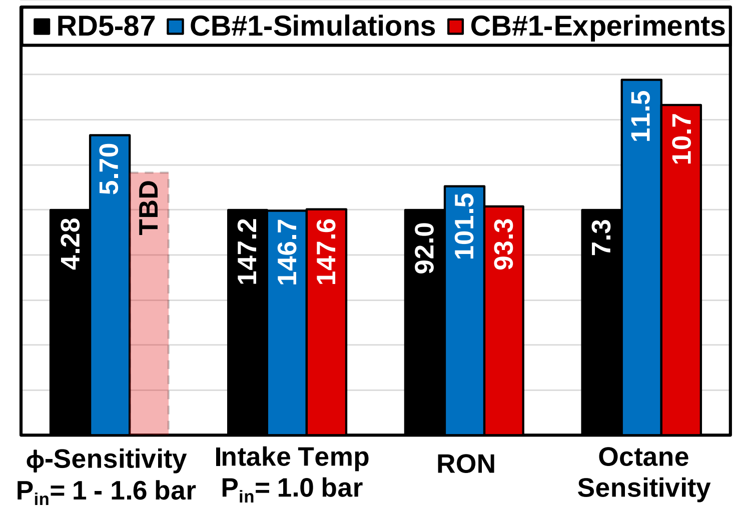
## Approach:

- Apply CHEMKIN with LLNL mech. to screen many gasoline components, HPF fuels, and binary blends for ϕ-sensitivity & reactivity
- Use findings to make multi-compon't blends

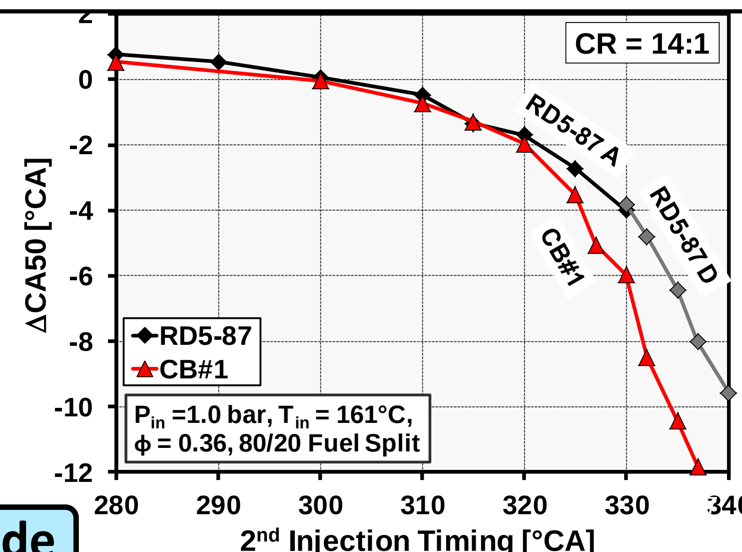
## Results:

- Best blend, **CB#1**, is shown in bar graph
  - ➢ CHEMKIN ⇒ predicts desired improvements
  - ➢ **Experiments ⇒ match simulations for higher O-S and similar $T_{in}$ ⇒ modestly higher RON ⇒ indicate higher ϕ-sensitivity**
- Increased fuel stratification with later 2nd-inj. advances CA50 more with CB#1 vs. RD5-87 ⇒ **indicates ↗ ϕ-sens.** (add'l data planned)
- **CB#1 is a promising fuel for ACI & SI multi-mode**

CB#1 ⇒ 17.5% 1-hexene + 28.5% n-pentane + 8% iso-octane + 30% p-xylene + 16% iso-butanol




### CA50 Advance with Increased Stratification



# Fuel Properties Effects on Auto-Ignition in Internal Combustion Engines

**Objective #1:**

- Measure the effects of lambda and cylinder pressure transducer based knock intensity on RON

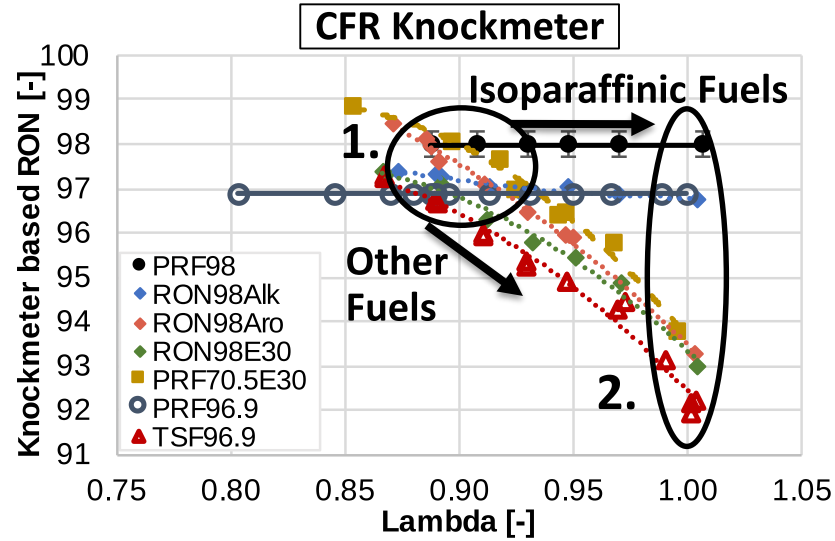
**Approach:**

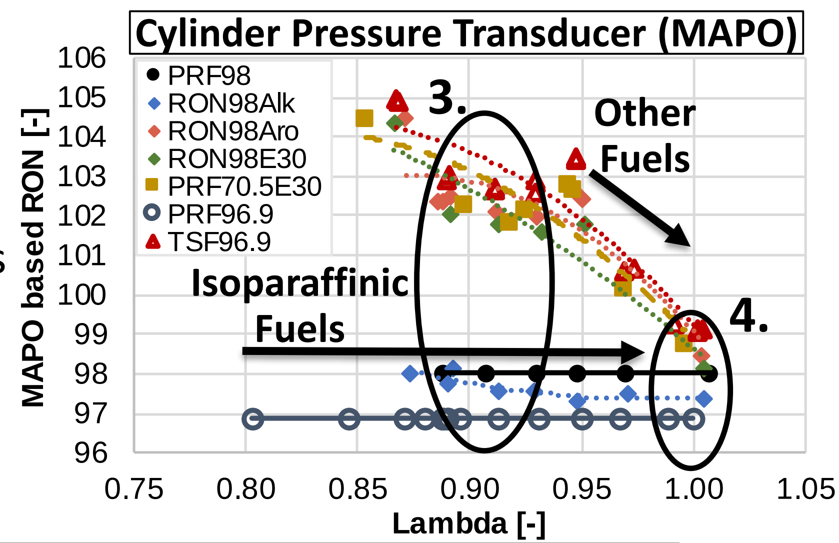
- Re-rate the RON of several RON 98 test fuels by:
  a) CFR knockmeter vs. Max. Amplitude of Pressure Oscillations (MAPO) knock intensities
  b) Sweep lambda from peak knock (rich) to λ=1

**Results:**

1. Peak knocking lambda with CFR knockmeter
   - All RON 98 fuels rated ≈98 RON
2. λ=1 with CFR knockmeter
   - Non-isoparaffinic fuels rate lower than PRFs
3. Peak knocking lambda based on MAPO
   - Non-isoparaffinic fuels rate higher than PRFs
4. λ=1 based on MAPO
   - RON values coincidentally converge.

**Highly isoparaffinic fuels, such as Primary Reference Fuels (PRFs), react differently to lambda changes than other fuels tested.**




Raw knock intensity data (knockmeter & MAPO) in Technical Back-Up Slides.

# Fuel Properties Effects on Auto-Ignition in Internal Combustion Engines

**Objective #2:**

- Evaluate ability of HCCI# testing on the CFR engine to correlate with modern HCCI engines.

**Approach:**

a) Test all fuels under HCCI at 900 RPM and λ=3

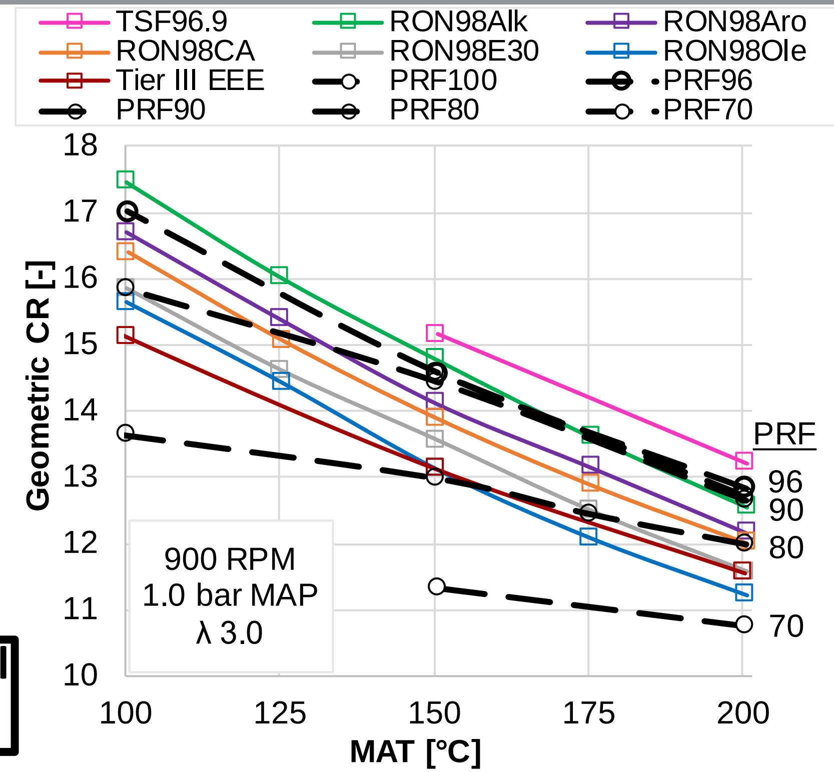
b) Sweep intake air temperature and pressure

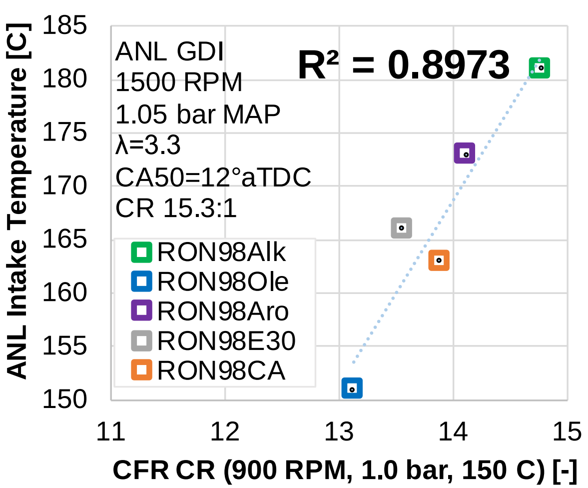
c) Adjust CFR compression ratio to maintain constant combustion phasing (CA50=3°aTDC)

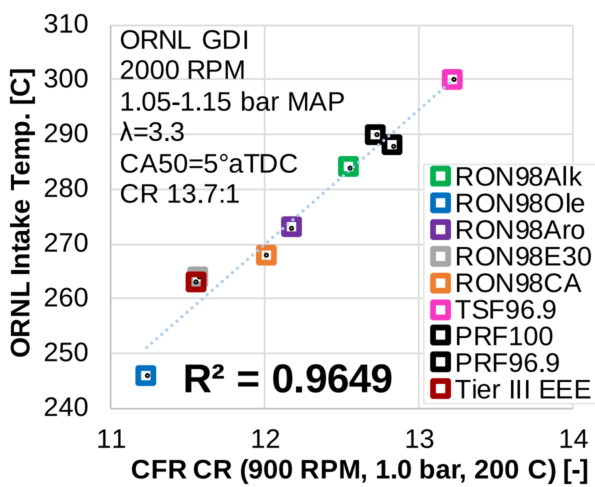
d) Identify HCCI# intake conditions with best correlation to fuel reactivity on modern engines.

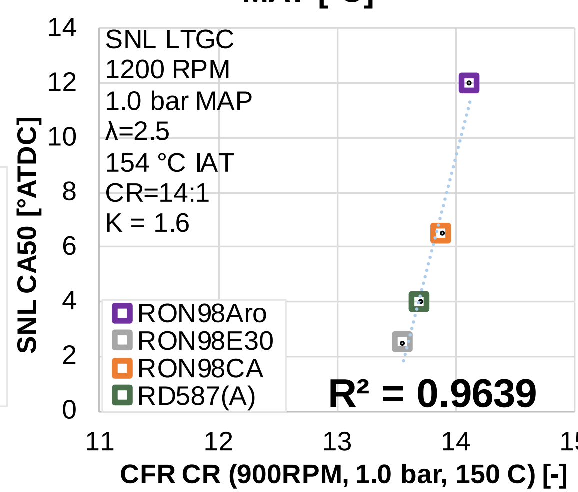
**Results:**

**Strong ($R^2$≥0.9) correlation between CFR HCCI critical compression ratio and modern engine HCCI results.**



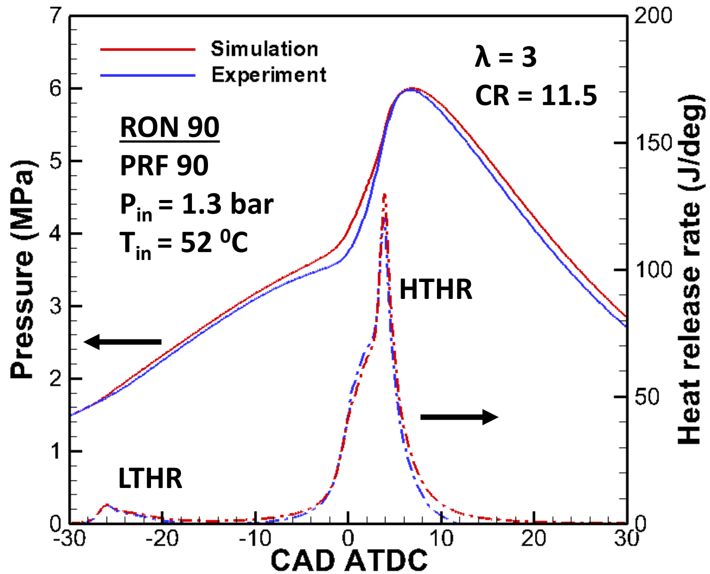



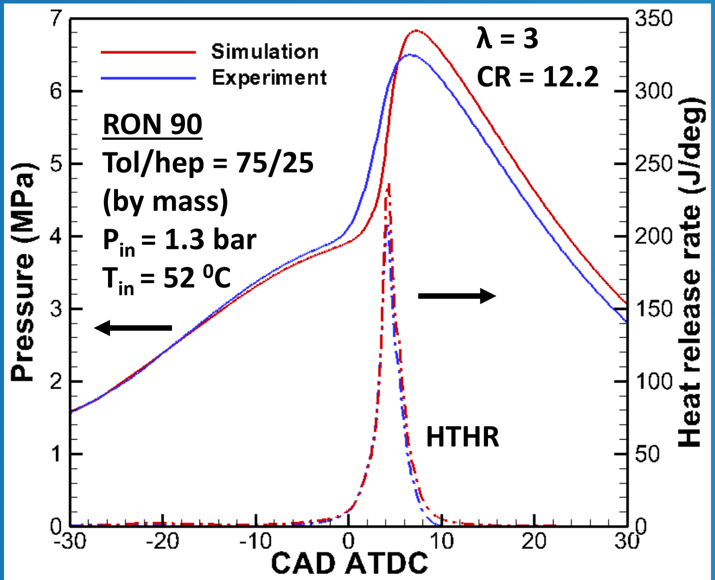



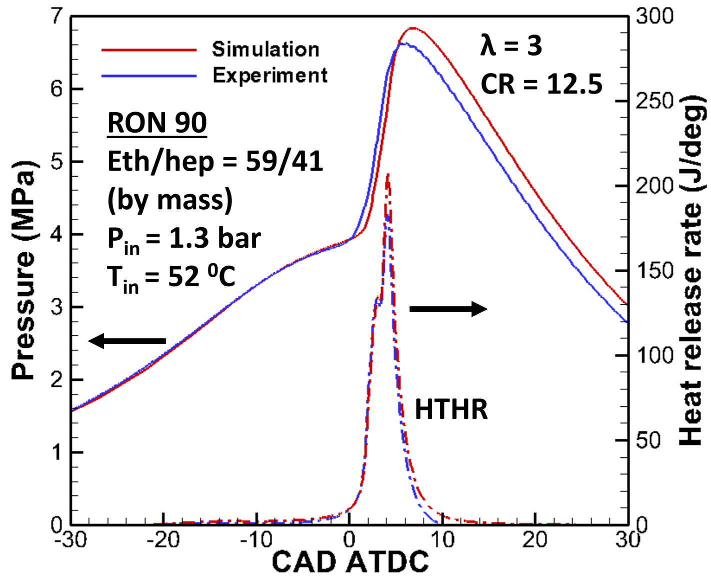



# CFR Engine Simulations for ACI Combustion Analysis

- **Objective:** Numerically investigate fuel property effects on ACI/HCCI combustion using virtual CFR engine model
- **Approach:** Validate URANS CFD model under HCCI conditions, investigate the impact of fuel composition on CA50, test central fuel property hypothesis
- **Project status:** The CFD model was validated against experiments for a variety of fuel blends showing good accuracy

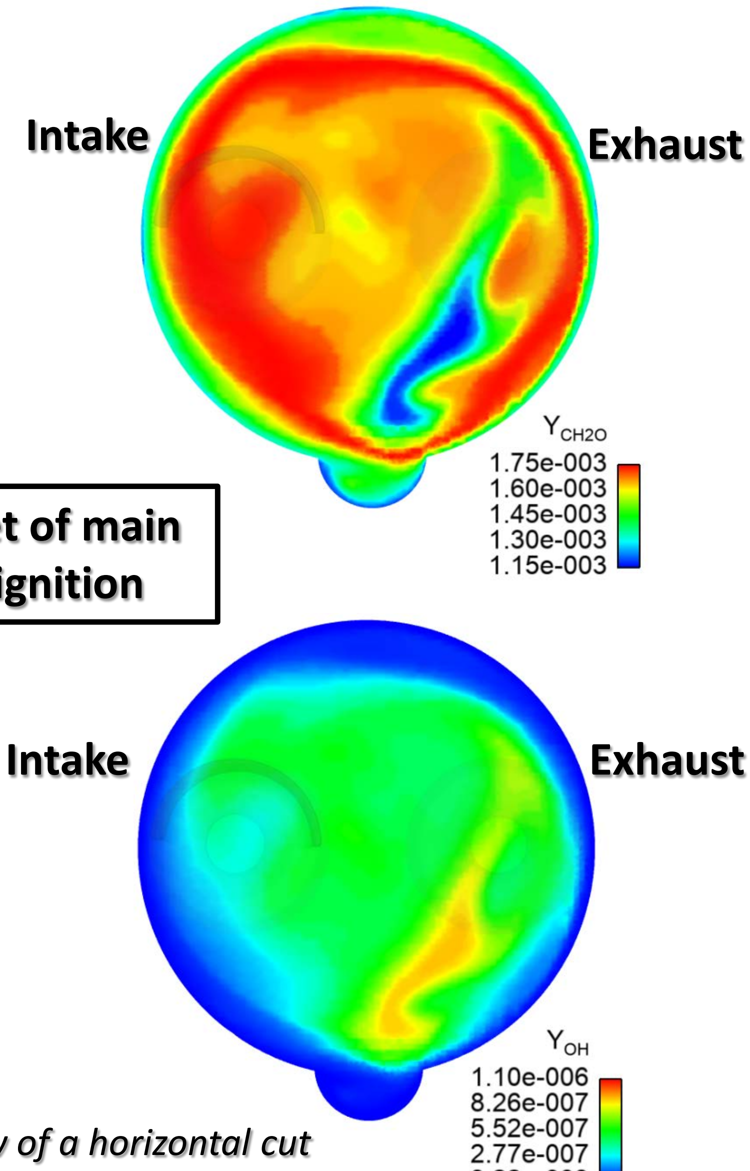


G.1.5
Pal, ANL

# CFR Engine Simulations for ACI Combustion Analysis

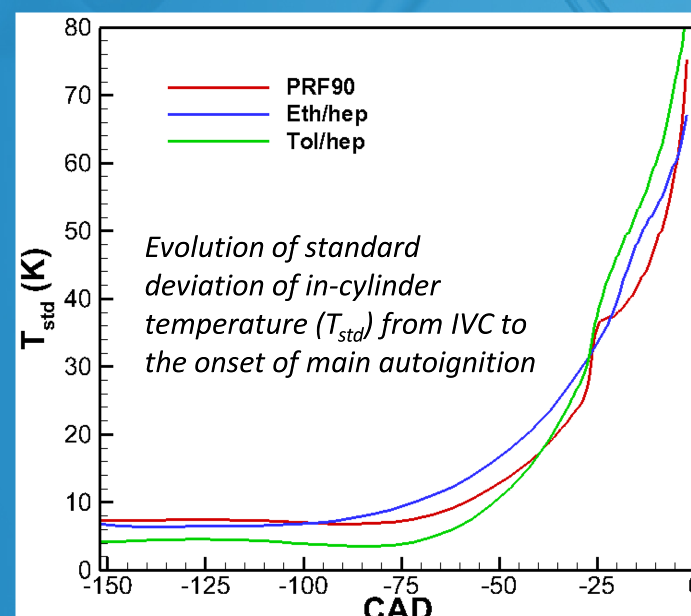



**Onset of main autoignition**

*Top view of a horizontal cut plane (PRF90 boosted case)*

## Thermal stratification:

- The CFD simulation data was analyzed to investigate the autoignition phenomena and thermal stratification in the engine
- Inhomogeneous autoignition was observed, initially triggered close to the exhaust side
- Significant in-cylinder thermal stratification was observed; the level of stratification was similar among all the fuel blends tested




*Evolution of standard deviation of in-cylinder temperature ($T_{std}$) from IVC to the onset of main autoignition*

F.2.6.1
Ratcliff, NREL

# Systematic Evaluation of RON, S, Phi Sensitivity, and Flame Speed Effects in ACI Combustion

**Objective**

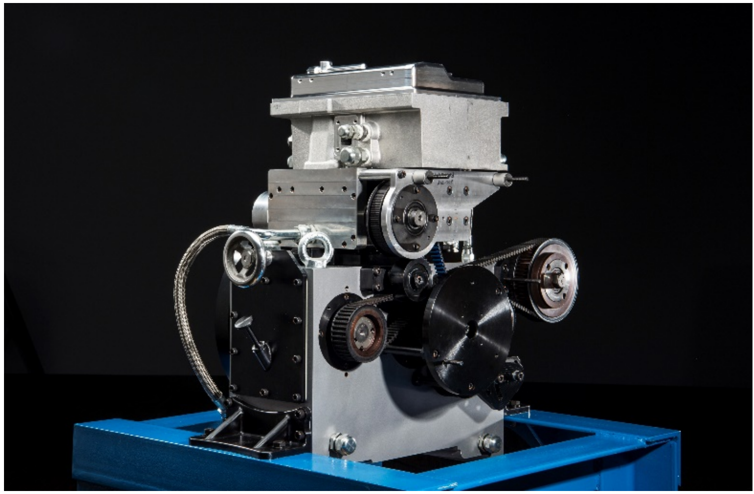
Develop matrix of ACI control strategies (degree of stratification) and quantified fuel property impacts

**Approach**

- Screen fuel property database for ACI fuels:
  1. Select high S fuels with RON ranging 70 - 100
  2. Select subset spanning range of phi-sensitivities using LLNL values
  3. Select subset spanning range of flame speeds using literature data / published models
- Prepare / fully characterize 30 vol% blends in a gasoline BOB (RON of 90-91)
- Test blends in new SCE (based on Ford 6.7L Scorpion) in lean, dilute ACI modes
  - Control fuel stratification with direct injection
  - Load and phi sweeps at select stratification and EGR levels. Measure fuel property effects on:
    - Combustion phasing
    - Thermal efficiency
    - Exhaust emissions

**Project Status**

- New SCE installed, in shakedown
- On track to meet milestone demonstrating MCCI in Q3
- Screen fuel property database in Q3
- Start ACI experiments in Q4



# Simulation support for NREL ACI experiments

**Objective**

Simulation support for design and operation of NREL engine platform.

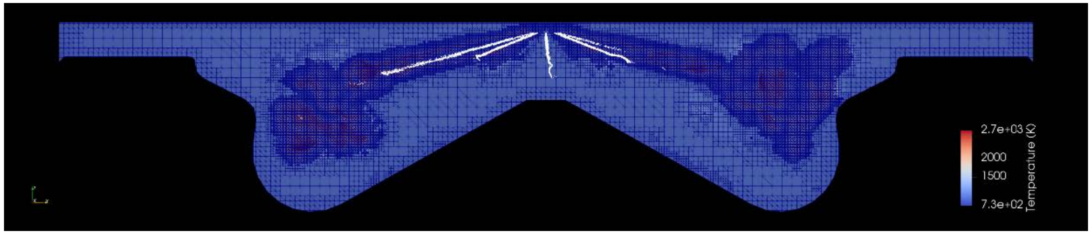
**Approach**

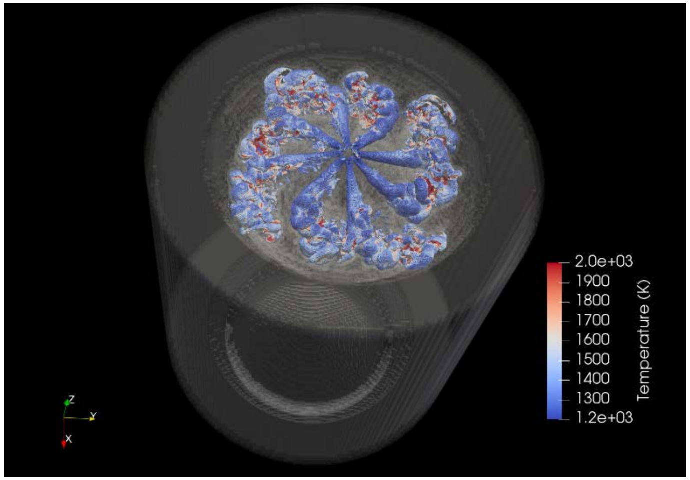
Multi-dimensional CFD of NREL SCE research platform (previous slides), validate against experimental measurements of pressure rate rise under baseline MC operation. Refine combustion subgrid mode and validate against lean, dilute ACI mode operation. Conduct sensitivity studies to assist in design of experimental test matrix.

**Project Status**

Baseline CONVERGE simulation executed; awaiting validation data.

- OEM piston bowl geometry, injector flow rates, spray angles, nozzle position, etc
- Dyn. Smag. LES and k-e RANS, CTC combustion w/ shell ignition, diesel spray model
- 3 level AMR on velocity and temp gradients




$\nabla T$ isovolume colored by temperature showing piston at BDC and 14 deg past TDC

# Responses to 2018 AMR Reviewer Comments

**Low-Temperature Gasoline Combustion (LTGC) Engines – Fuel Effects (Dec-SNL)**

Comment: "This project seemed to be on task and doing well. The work seems very detailed and thorough."

Response – We thank the reviewer for these comments.

Comment: "It appeared to one reviewer that the same results were presented as both Co-Optima results and Advanced Combustion Engine (ACE) activity results."

Response – A fraction (<10%) of our ACE work involved development of a methodology for formulating and validating an accurate computational surrogate for a regular-E10 gasoline. For Co-Optima, we leveraged this methodology to formulate and validate new surrogates for three Co-Optima core fuels.

The development of these surrogates is valuable to the whole Co-Optima team because previously available surrogates for the core fuels were not sufficiently accurate – as was shown in our presentation.

Comment: "It was unclear to one reviewer how this work was unique compared to mixed-mode work."

Response – The LTGC facility is uniquely capable of providing fundamental autoignition data for well-controlled near-homogeneous conditions at Ts and Ps relevant to the LTGC-ACI combustion in mixed-mode engines, not possible using typical partially stratified, spark-assisted mixed-mode engines. Examples:

- Understanding how fuel composition affects autoignition for fuels with the same RON and MON is central to selecting appropriate fuels for mixed-mode engines & for developing improved autoig. metrics.
- The new surrogates for the Co-Optima core fuels have been shared with the Co-Optima team and are allowing more accurate modeling of mixed-mode combustion.

# Responses to 2018 AMR Reviewer Comments

**CFR Engine Simulations for ACI Combustion Analysis (Pal-ANL)**

Comment: "…CFD model validations and understanding knock in boosted SI operation are the major accomplishment of this project."

Response: The researchers thank the reviewer for those comments.

**Fuel Properties Effects on Auto-Ignition in Internal Combustion Engines (Kolodziej-ANL)**

Comment: "…work on RON and HOV is providing new knowledge and increased understanding of how these fuel properties affect engine performance. Knock-correlation work with various knock metrics has also provided new information that industry can use."

Response: The researchers appreciate that the work is relevant and useful.

Comment: "…the project shows limited accomplishments in the areas of robust lean-burn and EGR-diluted combustion control and determining factors limiting LTC and method to extend limits for the barriers identified as the program objectives."

Response: Work on the CFR engine at Argonne has expanded to now include fuel characterization under lean HCCI conditions to help reduce the fuel-related limitations of LTC and research in the past year have shown strong correlations with modern engine test results.

# Collaborations

**Co-Optimization of Fuels and Engines**

- Collaboration across nine national laboratories and two DOE offices (+8 Universities)
- 145 stakeholders from 86 organizations

**Low-Temperature Gasoline Combustion (LTGC) Engines – Fuel Effects (Dec-SNL)**

- LLNL – Validation of LLNL kinetic mechanism & discussions on formulating surrogates
- GM – Fuel-injector support and technical discussions on the use of OI for LTGC vs SI
- NREL – Shared information on the fundamentals of phi-sensitivity

**Fuel Properties Effects on Auto-Ignition in ICEs (Kolodziej-ANL)**

- CFR Engines, Inc. – Hardware support and technical guidance
- Marathon Petroleum – Hardware support and technical guidance
- KAUST – Ongoing discussions with Prof. Bengt Johansson and hosted PhD student

**CFR Engine Simulations for ACI Combustion Analysis (Pal-ANL)**

- Univ. of Connecticut - Mechanism reduction
- Convergent Science – CFD code guidance
- Univ. of Illinois at Chicago (UIC) – CFD simulations

**Systematic Evaluation of RON, S, Phi Sensitivity, and Flame Speed… (Ratcliff-NREL)**

- Ford – Engineering support for single-cylinder engine based on Scorpion 6.4L diesel
- Bosch – Piezo diesel and GDI injector support

# Remaining Challenges and Barriers

- For operation at Beyond-RON and between RON and MON conditions, the performance of RON, MON, and OI as autoignition metrics for LTGC-ACI needs to be evaluated.
- An accurate autoignition metric is needed for LTGC-ACI at the Beyond-MON conditions commonly used for LTGC-ACI as part of a mixed mode-operating strategy. (Also could be used for low loads of a full time LTGC-ACI engine).
- Initial HCCI # testing on a variable compression ratio CFR engine shows strong correlation with limited fuels and engine tests, but comparisons with more fuels and modern engine operating conditions are needed.
- Develop and test additional fuel blends containing HPF blendstocks that simultaneously increase φ-sensitivity, RON, and octane-sensitivity compared to regular-E10, thus improving both the LTGC-ACI and SI parts of mixed-mode operation. → Initial efforts (slide 7) show that it is possible to blend a fuel that simultaneously increases all three of these properties.

# Future Work

**Low-Temperature Gasoline Combustion (LTGC) Engines – Fuel Effects (Dec-SNL)**

- Expand testing our new HPF-based fuel blend to evaluate its ability to improve LTGC-ACI & boosted-SI performance vs. regular-E10 over a wider range of conditions, including boosted, beyond RON conditions.

**Fuel Properties Effects on Auto-Ignition in ICEs (Kolodziej-ANL)**

- Test interactions between BOB composition and blending component on fuel HCCI # ratings across pressure, temperature, and phi space

**CFR Engine Simulations for ACI Combustion Analysis (Pal-ANL)**

- Investigate the impact of fuel composition on ACI efficiency and test the validity of central fuel property hypothesis under beyond-MON conditions

**Systematic Evaluation of RON, S, Phi Sensitivity, and Flame Speed Effects in ACI Combustion (Ratcliff-NREL)**

- Perform load and phi sweeps, additionally varying fuel stratification while measuring the effects on combustion phasing, thermal efficiency and exhaust emissions

**Simulation support for NREL ACI experiments (Grout-NREL)**

- Experimentally validate SCE simulations and subgrid models using pressure trace and firing data, undertake sensitivity study to develop experimental test matrix

Any proposed future work is subject to change based on funding level

# Summary

## Relevance:

- Better integration of fuels and engines research critical to accelerating progress towards economic development, energy security, and emissions goals

## Approach:

- Engine experiments and simulations provide detailed analysis on how fuel properties affect engine combustion in SI/ACI multimode and full-time ACI combustion

## Accomplishments:

- The lower φ of LTGC-ACI is the biggest factor causing the discrepancy in the performance of OI as an autoignition metric between SI and LTGC operation, due to differences in φ-sensitivity of various fuels.
- CHEMKIN simulations were used to successfully formulate a fuel blend containing an HPF component that gives improved LTGC-ACI/SI multi-mode performance over regular-E10 gasoline (RD5-87).
- Fuels with the same RON, but different chemical composition can rate very differently when changing the RON test to stoichiometry or to a cylinder pressure transducer based knock intensity.
- HCCI testing on a standard ASTM CFR engine showed a strong ($R^2 \geq 0.9$) correlation between CFR HCCI critical compression ratio (for constant CA50) and modern engine HCCI results.
- The virtual CFR engine model was validated against experiments under ACI/HCCI conditions and the thermal stratification in the engine was analyzed.

# Technical Back-Up Slides

F.1.5.1
Kolodziej, ANL

# Fuel Properties Effects on Auto-Ignition in Internal Combustion Engines

**Knock intensities used to calculate new RON values on Slide 8**

- CFR knockmeter
- Cylinder pressure transducer based Maximum Amplitude of Pressure Oscillations (MAPO)
- Both knock intensity metrics decrease more at stoichiometry with isoparaffinic fuels

**Highly isoparaffinic fuels, such as Primary Reference Fuels (PRFs), are more sensitive to lambda than other fuels tested.**