Co-Optimization of
Fuels & Engines

Multi-Mode: Desired Fuel Properties for Advanced Compression-Ignition and Spark-Ignition Engine Performance

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June 3, 2020

Project # FT072

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

Overview

Timeline

- Project start date: 10/1/18
- Project end date: 9/30/2021
- Percent complete: Approx. 58%

Task	FY19	FY20
F.1.5.1 Fuel Properties Effects on Auto-Ignition in Internal Combustion Engines (ANL – Kolodziej, Waqas, Hoth, Song, Rockstroh, Goldsborough)	$263k	$290k
F.2.6.1 Systematic Evaluation of RON, S, Phi Sensitivity, and Flame Speed Effects in ACI Combustion (NREL – Ratcliff, Martin)	$450k	$450k
G.2.16 Simulation support for NREL ACI experiments (NREL – Grout, Yellapantula)	$150k	$200K
G.2.16(b) Simulation support for NREL ACI experiments (NREL – Grout)	$110k	$0k
Total	**$973k**	**$940**

Barriers

- Determine factors limiting low temperature combustion (LTC) and develop methods to extend limits
- Understanding impact of likely future fuels on LTC and whether LTC can be more fully enabled by fuel specifications different from gasoline

Partners

- Partners include nine national laboratories, 20+ universities, external advisory board, and many stakeholders
- Task specific partners:
  - ANL: CFR Engines, Inc.
  - ANL: Prof. Bengt Johansson – KAUST
  - NREL: Ford Motor Co.
  - NREL: Bosch

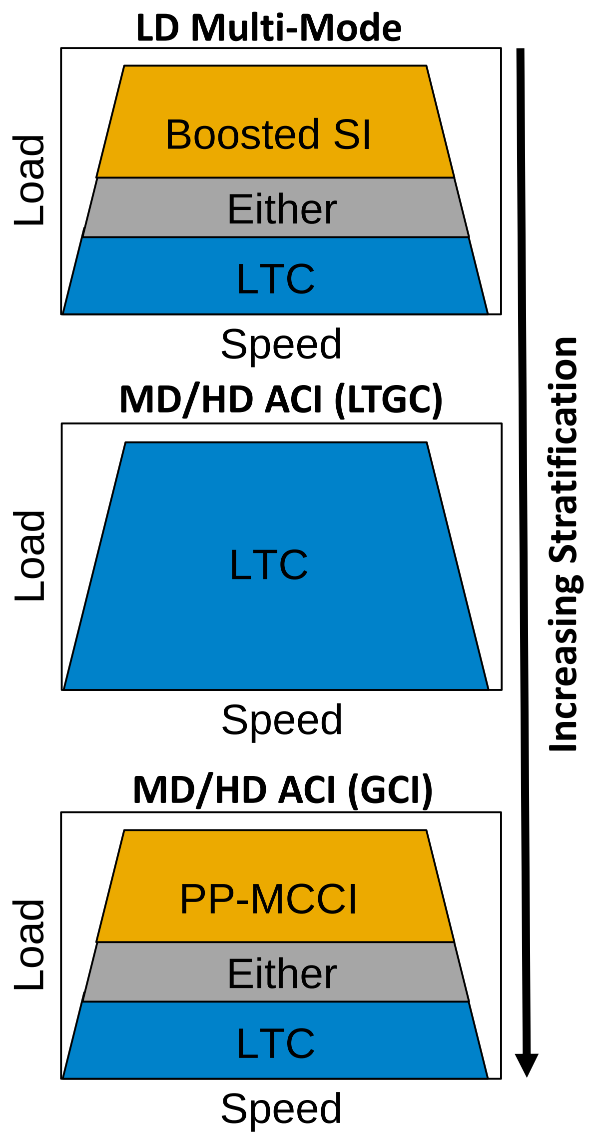
Relevance

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:

- Improved understanding of fuel property effects on autoignition allow for improved SI knock mitigation and ACI combustion phasing control.
- Better suited fuel properties for a given engine design can reduce engine emissions.



SI: spark ignition
LTC: low temperature combustion
PP-MCCI: partially premixed-mixing controlled compression ignition

Tracked Milestones

Month / Year	Description of Milestone or Go/No-Go Decision	Status
6/30/20 ANL, F.1.5.1	Test BOB aromatic content effects on HCCI # blending behavior (Kolodziej).	**On Track**
6/30/20 NREL, F.2.6.1	Demonstrate ACI combustion in single cylinder engine (Ratcliff).	**Delayed to FY21**

F.1.5.1 Kolodziej, ANL — Fuel Properties Effects on Auto-Ignition in Internal Combustion Engines

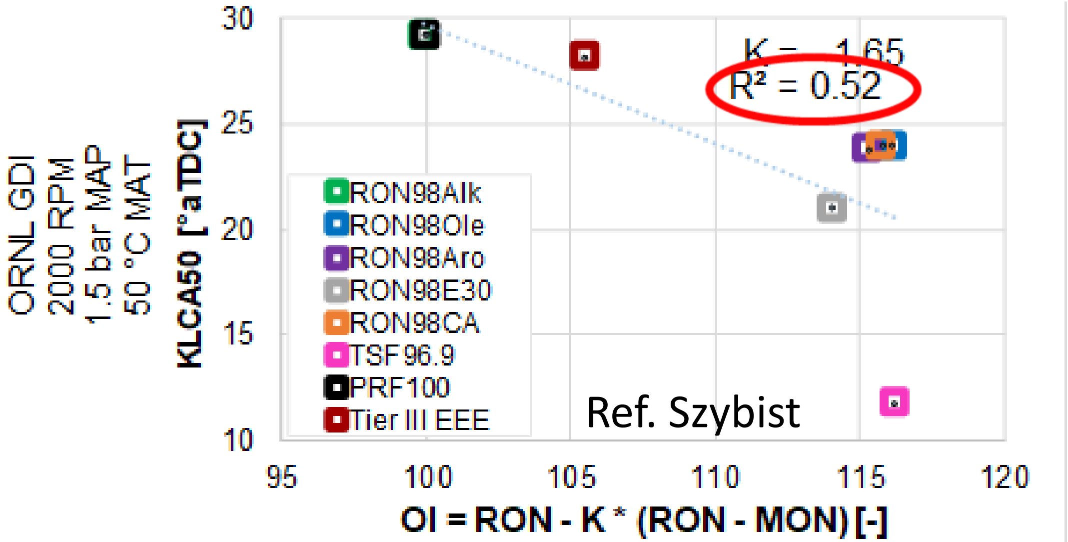
Objective: Use a Supercharged Octane Number (SON) test to improve Octane Index under Boosted SI

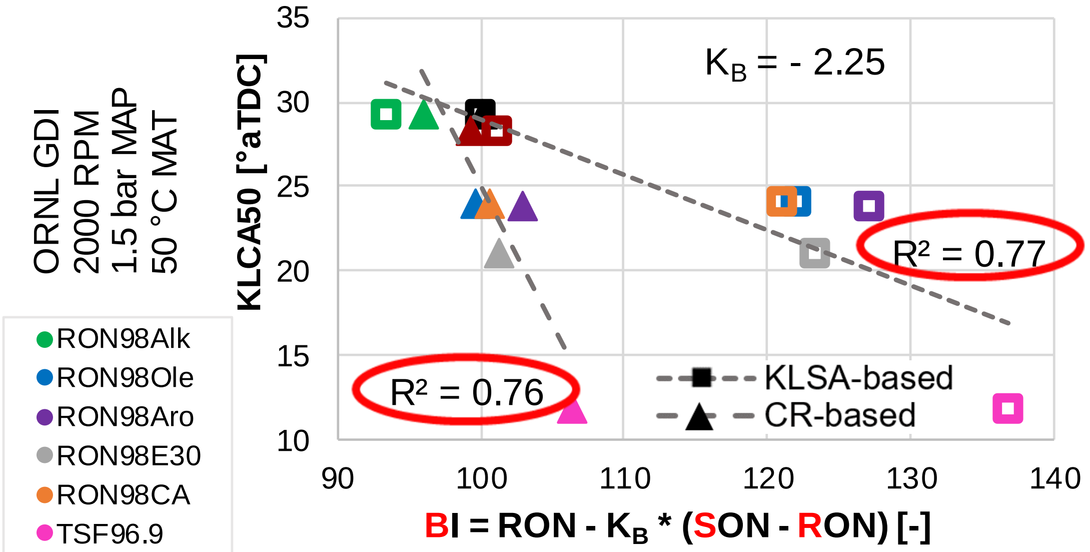
Approach:

- Rate fuels on a supercharged CFR octane engine at 1.5 bar intake pressure and constant knock intensity by adjusting spark advance or a critical compression ratio (CR)
- Extend Octane Index to use "SON" and RON for "beyond RON" conditions instead of RON and MON

Results:

- **Boosted Octane Index (BI) improves the correlation with Boosted SI KLCA50 data from R^2 = 0.52 with OI to R^2 = 0.76-0.77 with "BI"**
- **A negative K_B value is needed for BI to correlate with Boosted SI engine data, indicating the "SON" test still requires higher intake pressure**





ANL CFR 1.5 bar MAP at 600 RPM
52°C intake temperature and 0.6 bar MAPO threshold

F.1.5.1
Kolodziej, ANL

Fuel Properties Effects on Auto-Ignition in Internal Combustion Engines

Objective: Detect LTHR experimentally and using chemical kinetics for stoichiometric (λ = 1) and lean (λ = 3) combustion

Approach:

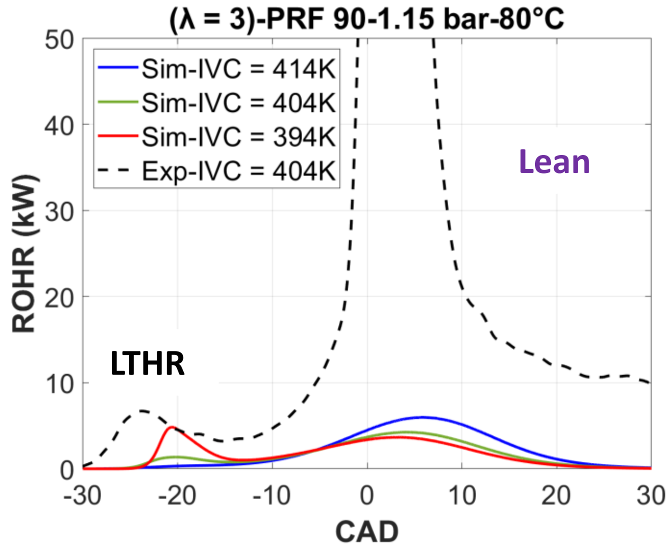
- A standard Cooperative Fuel Research (CFR) engine was operated at 600 rpm at lean (λ = 3) and stoichiometric (λ = 1) conditions for three RON 90 binary blends
- Zero-D modelling was used to qualitatively mimic the LTHR in both lean and stoichiometric combustion

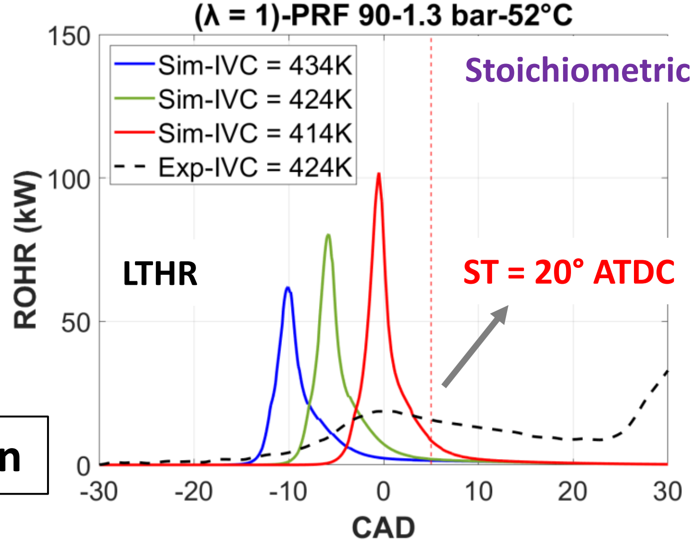
Results:

- **LTHR was quantified in both lean and stoichiometric combustion for both experiments and simulations**
- **Despite the same RON, difference exists in LTHR in both lean and stoichiometric conditions, and between fuels**

Accepted for presentation at the 38th Int'l Symposium on Combustion

Three fuel blends : PRF 90 : Iso-octane (90% Vol.)/ n-heptane (10%Vol.), TRF 90 : Toluene (70.5% Vol.)/ n-heptane (29.5% Vol.), ERF 90 : Ethanol (55% Vol.)/ n-heptane (45 % Vol.)





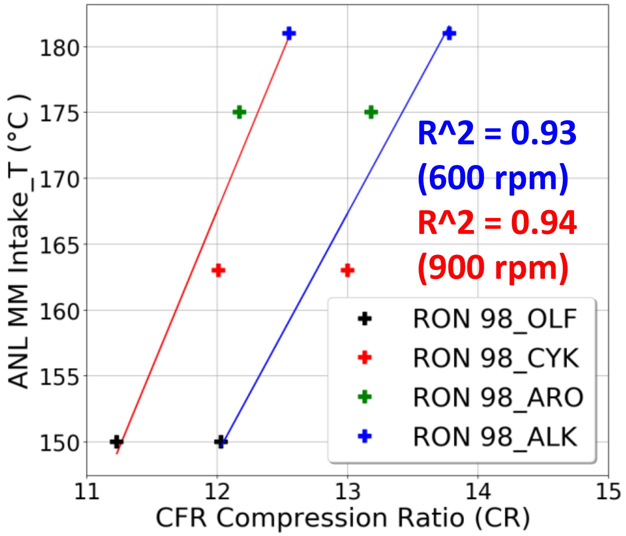
- **Lean : Based on the compression ratios required to achieve a CA50 of 3°aTDC**
- **The intake valve closure (IVC) is critical in linking lean and stoichiometric combustion**
- **Similarly LTHR was detected for TRF 90 and ERF 90**
- **Stoichiometric : compression ratio was increased until the maximum LTHR occurred at TDC, while spark timing was set to 20°aTDC**

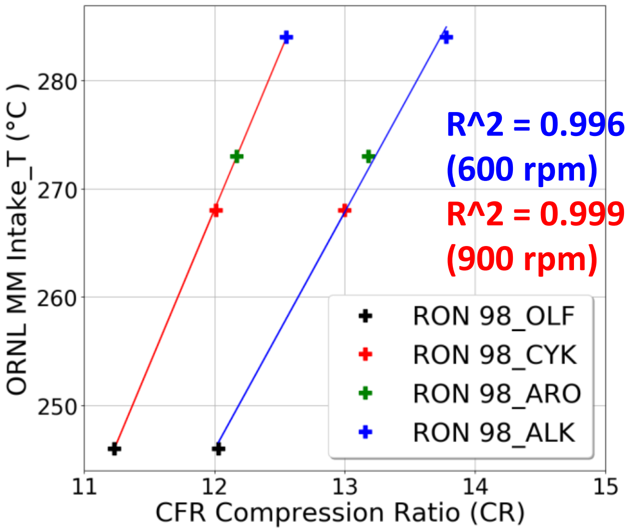
F.1.5.1 Kolodziej, ANL — Fuel Properties Effects on Auto-Ignition in Internal Combustion Engines

Objective: Investigate the effects of engine speed on a Beyond-MON CFR HCCI # to correlate with MM engines

Approach:

- A CFR engine was operated at 600/900 RPM, while two LD MM engines were operated at 1500/2000 RPM.
- Test RON 98 gasolines and Primary Reference Fuels (PRFs)

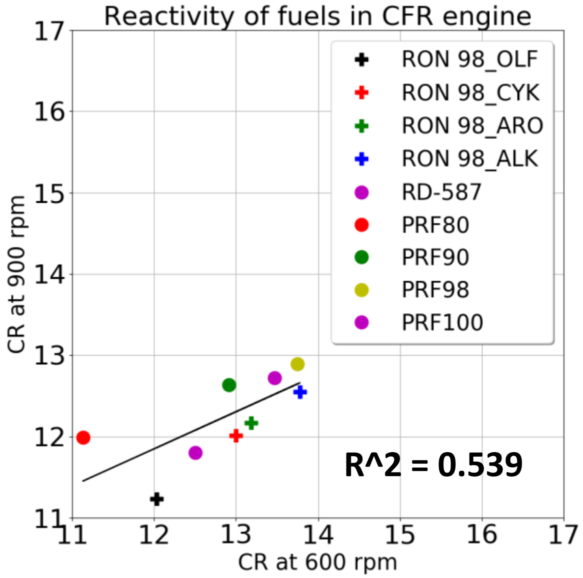




Results:

- **With four RON 98 gasoline fuels, ACI reactivity can be tested on the CFR engine at MON-like and Beyond-MON conditions at 600 or 900 RPM to correlate with ACI reactivity at higher speeds**
- **Additional gasoline-range fuels need to be tested**

CFR : Compression Ratio (CR)
Engine speed = 600/900 rpm
Lambda = 3
CA50 = 3°ATDC
Ford engine : Intake Temperature
Engine speed = 1500 rpm
Lambda = 3
CA50 = 12°ATDC
ORNL engine : Intake Temperature
Engine speed = 2000 rpm
Lambda = 3.3
CA50 = 5°ATDC



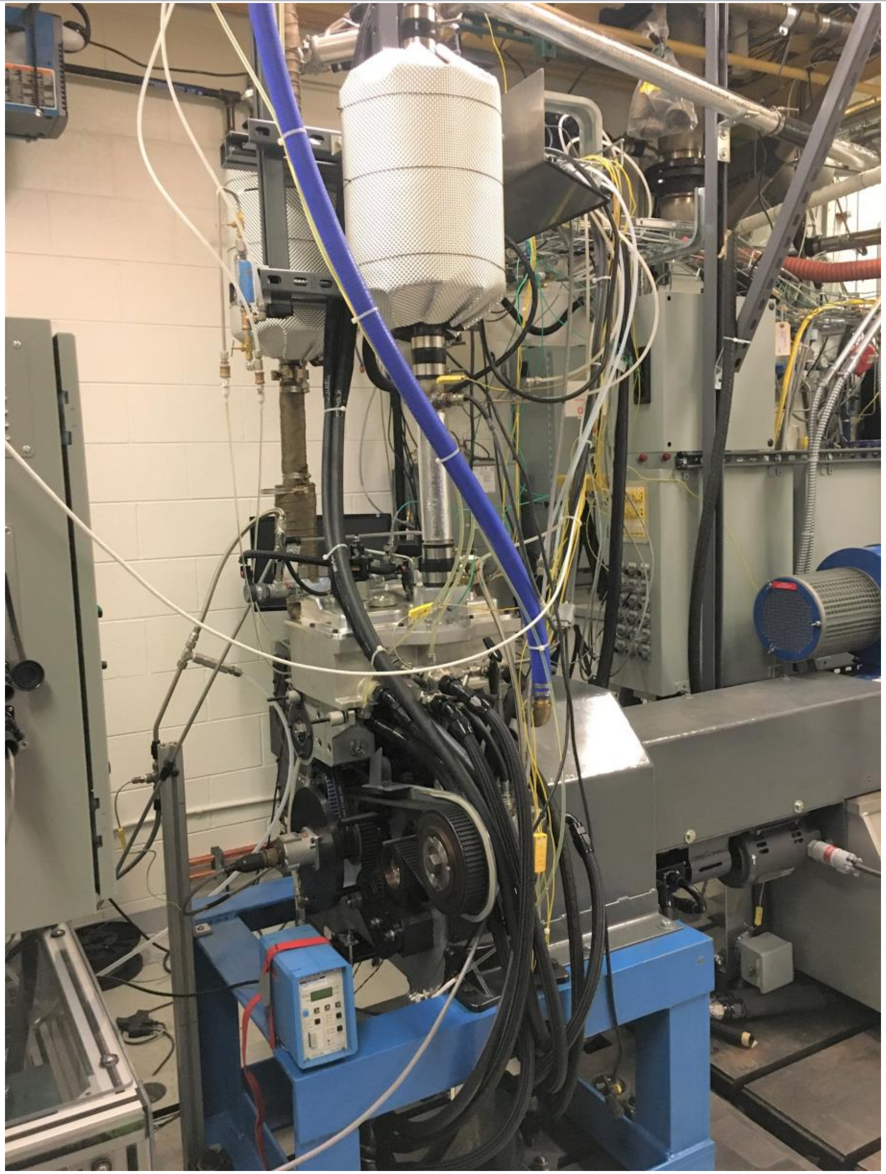
Systematic Evaluation of RON, S, Phi Sensitivity, and Flame Speed Effects in ACI Combustion

Objective

Develop a matrix of ACI control strategies and quantified fuel property impacts

Approach

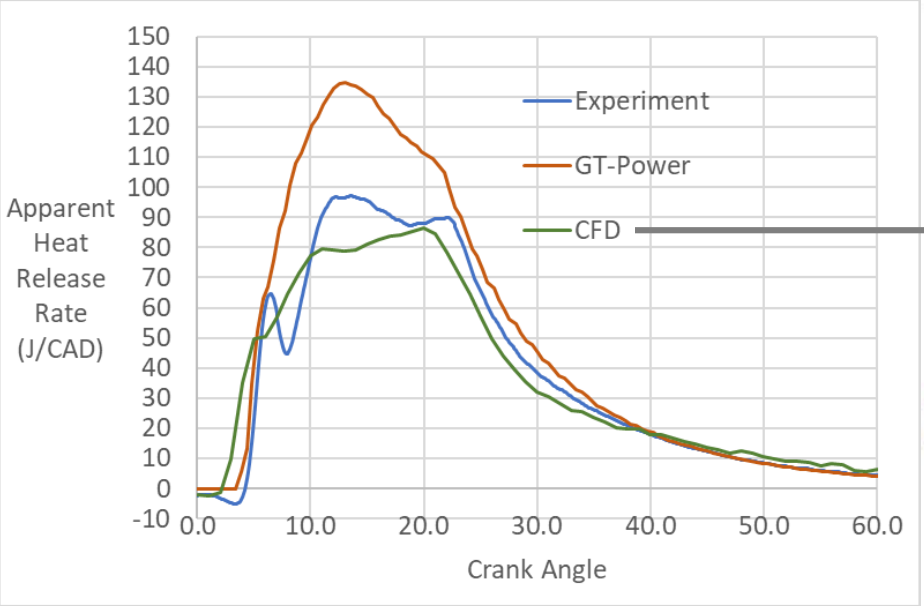
- Screen fuel property database for ACI enabling fuels:
  1. Select high S fuels in RON range 70 - 110
  2. Identify subset with range of phi-sensitivity
  3. Identify subset with range of flame speeds
- Prepare / characterize 30 vol% blends in a gasoline surrogate BOB w/ RON ≈ 90, S ≈ 6
- Run blends in new SCE (Ford 6.7L Scorpion based) in ACI mode
  1. Control fuel stratification with DI timing
  2. Perform load and phi sweeps at select stratification / EGR levels, measuring fuel property effects on
     a. Load range and pressure rise rates
     b. Combustion phasing control
     c. PM, NOx and other emissions
     d. Thermal efficiency

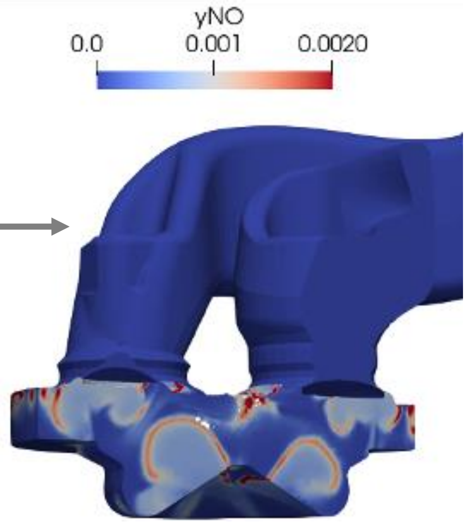


F.2.6.1
Ratcliff, NREL

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

- **Project Status**
  - New SCE in service on MCCI project (until lab closure)
  - First ACI experiments expected at completion of MCCI project (est. 2 months after lab reopens)
  - Determined cylinder head can be adapted to fit a production-based GDI injector
- **GT-Power model being tuned**
  - Currently with MCCI / diesel fuel data
  - Sufficient to tune gas exchange, residual trapping, some HT, etc.
- **CFD model developed for comparison/validation/prediction**
  - Predict phi/T distribution with ACI DI timings (-100° to -40° aTDC)





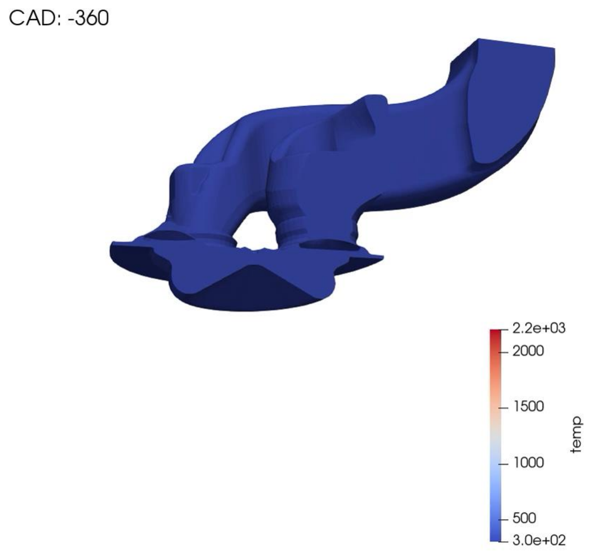
Advanced Fuels Research Single Cylinder Engine (AFR-SCE) features:

- Fully independent control of-
  - Intake P, T, ṁ
  - Exhaust P
  - Injection P, timing
- Cooled EGR loop-
  - ṁ control limited at some operating conditions

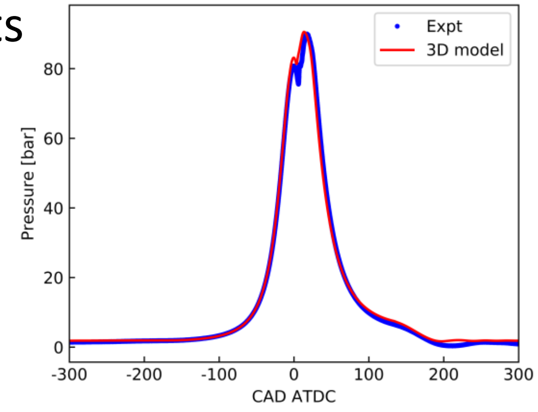
Simulation support for NREL ACI experiments

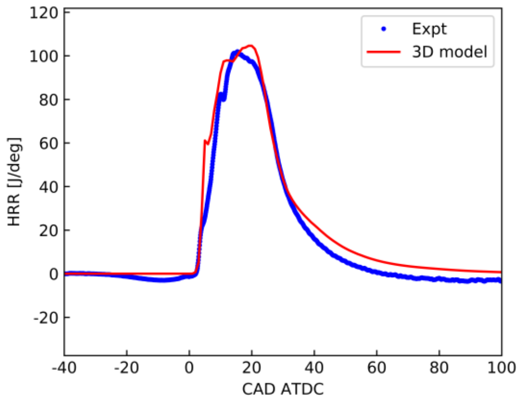
Objective: Simulation support for design and operation of NREL engine platform.

Approach:
- Cleaned up AFR-SCE geometry and mesh all input & output manifolds
- Perform multi-dimensional CFD with gas exchange of AFR SCE for modeling MCCI and ACI combustion



Results:
- CFD model with gas exchange validated against MCCI experiments





Future work:
- Study gasoline surrogate BOB spray behavior and compare against Diesel spray
- Further investigate ignition kinetics of surrogate BOB to study impact of boost, EGR, equivalence ratio under highly stratified conditions

Responses to Previous Year Reviewers' Comments

- **"…the approach to this work is extremely thorough and scientific. [*These projects have*] a basis in compression ignition engines, which should lead very well into the changing Co-Optima focus for larger engines in the HD space.**
- **"…the value proposition of utilizing a modified CFR engine for HCCI-like fuel characterization is appealing."**
- **"The technical detail that was presented is exactly the type of work this DOE program should be producing. The reviewer said that the very thorough, very extensive data and modeling correlation leads to much better understanding of how MM combustion systems link to one another and how fuel properties can enable this opportunity."**
- **"…limited interaction between the sub-groups that comprise this project team."**
  - The gasoline ACI projects are trying to better coordinate some of their test fuels for better inter-connectivity.

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

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

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

- **An accurate auto-ignition metric is needed for low load ACI at the Beyond-MON conditions (LD MM) and from Beyond-MON to Beyond-RON (MD/HD ACI)**
- **Beyond-MON 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.**
- **Better understanding of how candidate blendstocks and base fuel chemical composition affect ACI reactivity and emissions**
- **Define optimum fuel property targets for MM ACI/SI and MD/HD ACI engines**
- **Demonstrate how alternative HPF blendstocks can be used to tailor a gasoline-range fuel that provides enhanced combustion-phasing control in MD/HD ACI engines while maintaining low NOx and PM.**

Proposed Future Research

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

- Test interactions between BOB composition and blending component on CFR HCCI # ratings across speed, pressure, temperature, and phi space
- Correlate CFR HCCI #(s) to additional ACI test conditions

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

- Run ACI simulations with surrogate BOB blends during engine lab shutdown (Yellapantula-NREL)
- A revised combustion system based on a GDI injector (already identified) will be developed and installed to allow a wider range of fuel stratification / injection timing

Simulation support for NREL ACI experiments (Grout/Yellapantula-NREL)

- Study gasoline surrogate BOB spray behavior and compare against Diesel spray
- Further investigate ignition kinetics of surrogate BOB to study impact of boost, EGR, equivalence ratio under highly stratified conditions

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

Summary

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

- Boosted Octane Index (BI) improves the correlation with Boosted SI KLCA50 data from $R^2 = 0.52$ with OI to $R^2 = 0.76$-0.77 with "BI"
- An experimental engine-based methodology was developed to characterize fuel low temperature heat release under lean and stoichiometric conditions
- Initial data indicates that engine speed may not be an important factor when correlating MON-like and Beyond-MON ACI reactivity

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

- New single-cylinder research engine in service, currently performing MCCI testing
- Determined cylinder head can be adapted to fit a production-based GDI injector
- GT-Power and CFD models are being tuned with current MCCI data

Simulation support for NREL ACI experiments (Grout-NREL)

- CFD model with gas exchange validated against MCCI experiments

Technical Back-Up Slides

(Include this “divider” slide if you are including back-up technical slides **[maximum of five]**. These back-up technical slides will be available for your presentation and will be included in the USB drive and Web PDF files released to the public.)

E.2.1.1. Fuel properties which enable HD GCI (ANL)

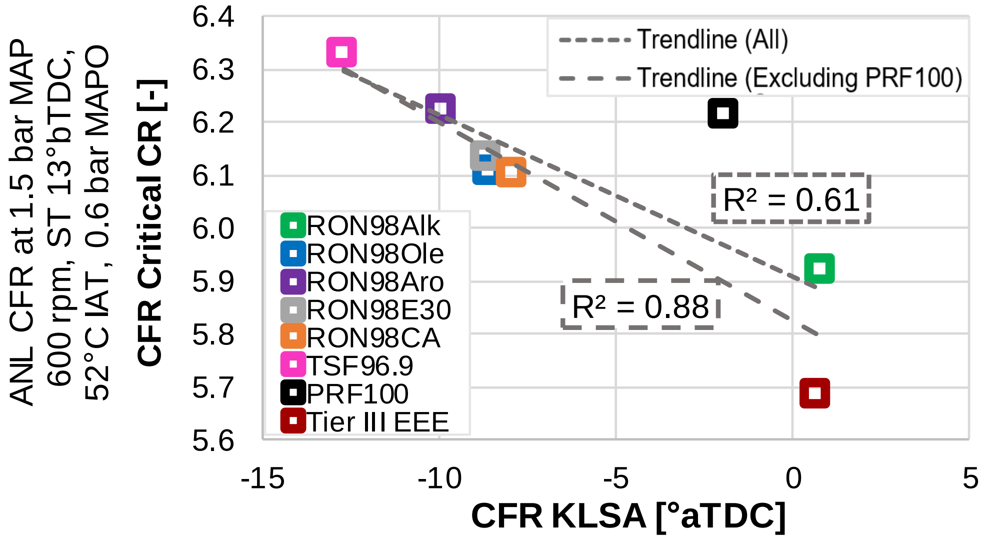
Objective: Development of a Supercharged Octane Number (SON) and a Boosted Index (BI)

Approach:

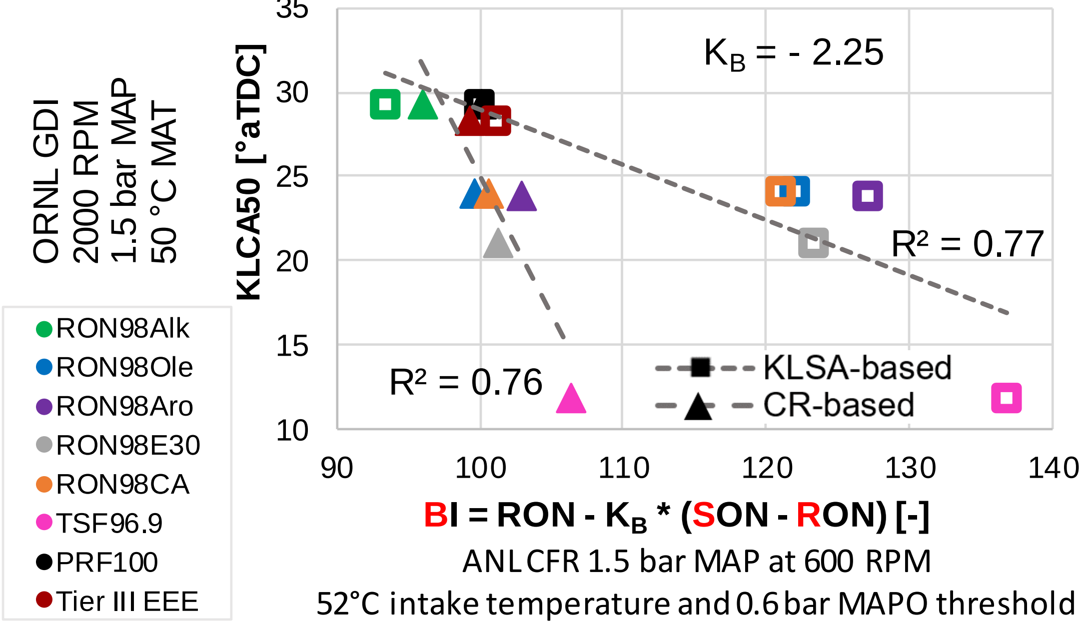
- **Creation of a knock limited spark advance (KLSA) - and compression ratio (CR) - based SON at stoichiometry and 1.5 bar intake pressure**
- **Advancement of Kalghatgi's octane index to boosted index (BI) for beyond RON conditions (K<0)**

Results:

- **Critical CR and KLSA-methodology match with exception of PRF, presumably affected by combustion phasing (WIP)**
- **BI improves correlation over octane index (R^2 = 0.52) when at beyond RON conditions but higher intake pressure recommended**



ANL CFR at 1.5 bar MAP, 600 rpm
CR 6.40, 52°C IAT, and 0.6 bar MAPO



ANL CFR 1.5 bar MAP at 600 RPM
52°C intake temperature and 0.6 bar MAPO threshold

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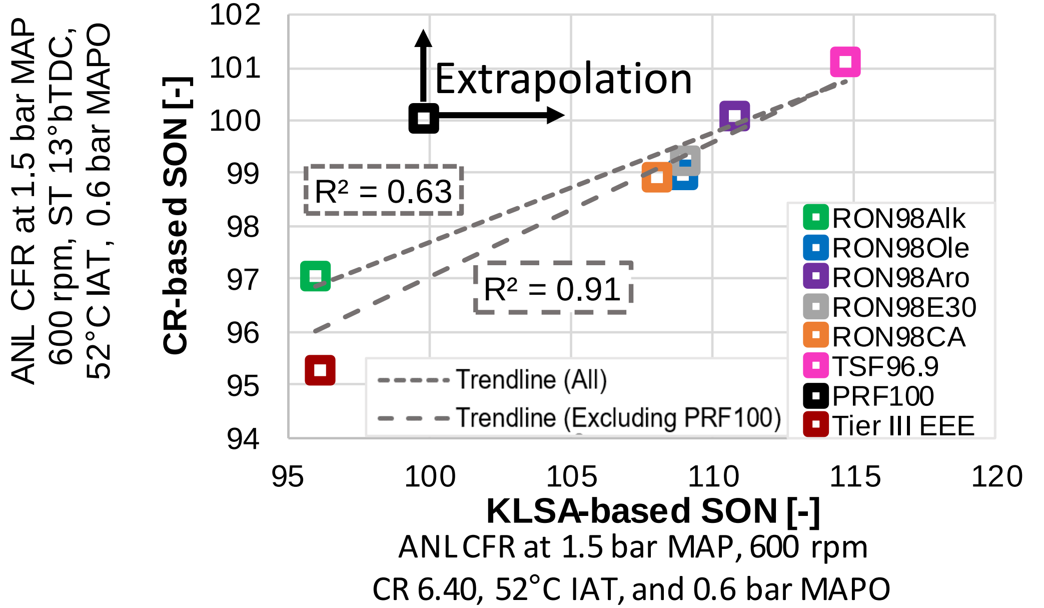

Results:

- **SON dependent on the knock limit evaluation methodology, presumably affected by combustion phasing (WIP)**
- **BI improves correlation over octane index (R^2 = 0.52) when at beyond RON conditions but higher intake pressure recommended**