Low-Temperature Gasoline Combustion (LTGC) Engine Research

Project ID: ACS004

John E. Dec

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Sandia National Laboratories

June 19, 2018 – 9:00 a.m.

U.S. DOE, Office of Vehicle Technologies
Annual Merit Review and Peer Evaluation

Program Managers: Gurpreet Singh & Michael Weismiller

This presentation does not contain any proprietary, confidential, or otherwise restricted information.

Overview

Timeline

- Project provides fundamental research to support DOE/Industry advanced engine projects.
- Project directions and continuation are evaluated annually.

Budget

- Project funded by DOE/VT:
- FY17 – $690k
- FY18 – $675k

Barriers / Research Needs

- Rapid combustion-timing control for LTC engines ⇒ transient capable
- Fundamental understanding of fuel effects on the chemical-kinetics of autoignition and combustion
- Spark-Assisted LTC
- Improved cold-starting technologies for LTC.

Partners / Collaborators

- Project Lead: Sandia ⇒ John E. Dec
- Advanced Engine Combustion MOU: 15 industrial partners
- Cummins – Hardware
- GM – Hardware & Discussions
- LLNL – Kinetic Modeling
- LLNL – UQ Analysis
- Stony Brook Univ-SUNY – CFD Modeling

- Sandia LDRD – CA50-control project
- Co-Optima Fuels proj., separately funded
- Chevron, Funds-in – Adv. fuels for LTGC

Relevance/Objectives – 1

Relevance

- **Low-Temperature Gasoline Combustion (LTGC) engines can provide diesel-like or higher efficiencies with very low NOx & PM.**
- **Our LTGC method** ⇒ kinetically controlled compression ignition (CI) of a dilute charge with well-controlled moderate stratification that varies with operating condition.
- LTGC research is relevant to
  1) Multi-mode operation for LD, using LTGC up to ~10 bar IMEP for high efficiency, then switching to boosted SI for high loads
  2) Full-time LTGC for MD/HD ⇒ Loads up to 20 bar IMEPg achieved with ultra-low NOx and PM and no knock, max. $P_{cylinder}$ = 150 bar
- Several potential advantages for MD/HD:
  1) Efficiencies can modestly exceed those of diesel engines
  2) Lower cost fuel-injection equipment ⇒ GDI-type 300 – 600 bar
  3) Reduced aftertreatment costs for NOx and PM
  4) Would help balance demand for gasoline and diesel fuel ⇒ Potentially lower fuel costs for customer

Relevance/Objectives – 2

Project Objectives

1) **Provide the fundamental understanding (science-base) required for the development practical LTGC engines by industry.**
2) **Explore methods to exploit this understanding to overcome the technical barriers to LTGC.**

FY18 Objectives:

- Complete uncertainty quantification (UQ) analysis in collaboration w/ LLNL
- Initiate a collaborative CFD modeling project with SUNY–Stony Brook
- Collaborate with LLNL to improve kinetic models and gasoline surrogates

Combustion-Timing Control – Primary Effort

- Complete study of spark-assist (SA) for well-mixed LTGC (HCCI)
- Investigate the chemistry of ϕ-sensitivity & its relationship to Octane sens.
  $\Rightarrow$ ϕ-sensitivity & controlled stratification provide CA50 control & load extension
- Develop and demonstrate an advanced combustion-timing control system

Approach

Overall Technical Approach

- Combine metal- and optical-engine experiments, analysis and modeling to build a comprehensive understanding of LTGC fundamentals.
- Extend this understanding to develop and evaluate methods to overcome the technical barriers to LTGC.
  $\Rightarrow$ Example: combustion-timing control system
- Establish collaborations to leverage complementary capabilities and share expertise.
- Transfer results to industry.

Detailed approaches for selected studies

- CFD modeling needed to support and extend experiments.
  - Develop a collaboration w/ SUNY–Stony Brook to apply CONVERGE our engine.
- Investigate the chemistry causing ϕ-sensitivity & relation to octane sens.
  - Apply CHEMKIN with LLNL detailed mech. & develop improved surrogate blends
- New combustion-timing control technique
  - Developed a new concept that required expertise in micro-fluidics.
  - Wrote proposal for internal funds; developed device $\Rightarrow$ transfer to VTO program

Milestones and Project Goals

- ✓ **August 2017**
  Complete development of improved surrogate for Regular-E10 (RD5-87) gasoline and validation using LLNL chemical-kinetic mechanism.
- ✓ **October 2017**
  Transfer new combustion-timing control device to our VTO-funded project and begin shakedown testing.
- ✓ **January 2018**
  Determine the chemical-kinetic origins of ϕ-sensitivity and the potential for enhancing it while maintaining high RON and good octane sensitivity.
- ✓ **March 2018 – Formal Milestone**
  Complete mapping of the range of conditions for effective CA50 control with spark assist for premixed LTCG and submit SAE paper on results of this study.
- ✓ **May 2018**
  Finish initial studies of ability of the new device for controlling combustion timing through changes in fueling rate, boost pressure and speed.
- **August 2018**
  Determine potential of the new control device to extend the low-load limit and for cold start. Give AEC presentation on combined studies with new control device.

Response to Reviewer Comments

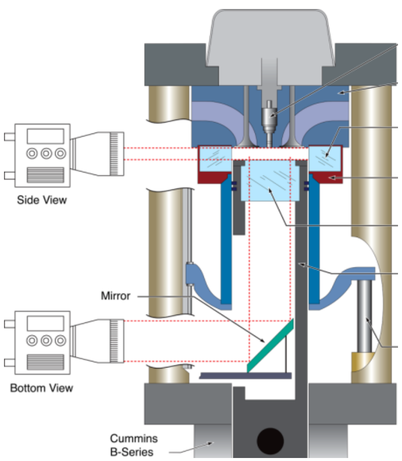
- **Studies [of double-injection strategies] are well done & valuable, but aren't there similar results in literature? Reviewer would like to see a transition to optical engine studies.**
  - Some previous works have reported the use of double or multiple direct injections to stratify the charge to control CA50, but they report few details about what was done and studies are not sufficiently well-characterized to provide the fundamental understanding needed to determine limits or to advance the capabilities of this technique.
  - Thus, additional well-characterized studies were required, such as those we have conducted.
  - Optical studies are planned to provide additional detail for optimizing injection strategies, but metal-engine tests are needed first to determine conditions that merit optical studies, since they can be time consuming.
  - CFD studies are also planned to improve the fuel stratification for this control technique.
- **A reviewer expressed concern that current proposed future research would not sufficiently move barriers to LTC, suggested we use an increased variety of hardware.**

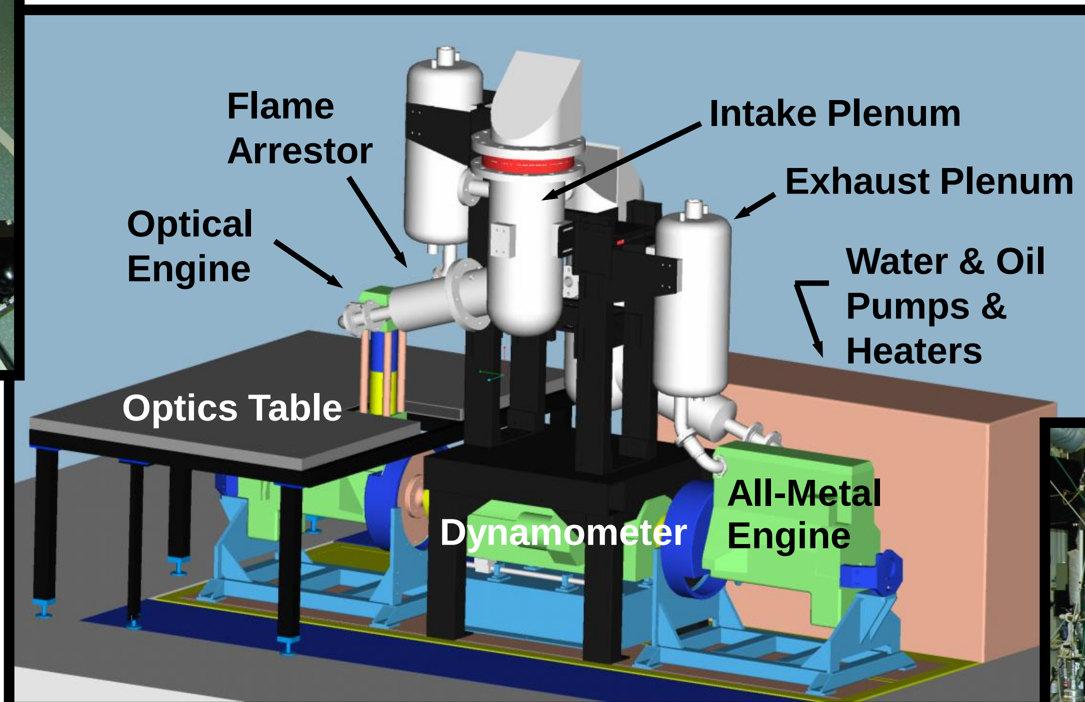
  Another reviewer also suggested the project needs more variety of hardware.
  - The main barrier to LTC is combustion-timing control ⇒ still unresolved after nearly two decades.
  - Adding new hardware could be useful, but it is unclear if new hardware for any of the existing techniques would be sufficient to overcome the barriers.
  - To be effective, adding new hardware must be done in a way that goes beyond previous studies.
  - Since all known approaches to LTC control had serious limitations, I started developing a completely new approach under internal funding more than 3 years ago.
  - This new control method has recently been transferred to our VTO program, and the hardware has been installed on our research engine. ⇒ Results are very promising, as will be shown.

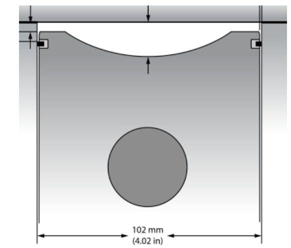
Sandia LTGC Engine Laboratory

- Matching all-metal & optical LTGC research engines.
  - Single-cylinder conversion from Cummins B-series Medium-Duty diesel.

Optical Engine

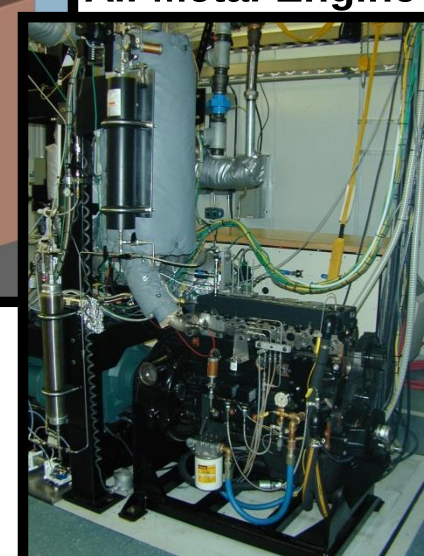






Open-chamber LTGC piston CR = 14:1

All-Metal Engine



- Bore x Stroke = 102 x 120 mm
- 0.98 liters, CR = 14:1 (adjustable)
- GDI fuel injector & fully premixed fuel system
- Spark-plug capable
- Independent control of most engine parameters

Overview of Accomplishments

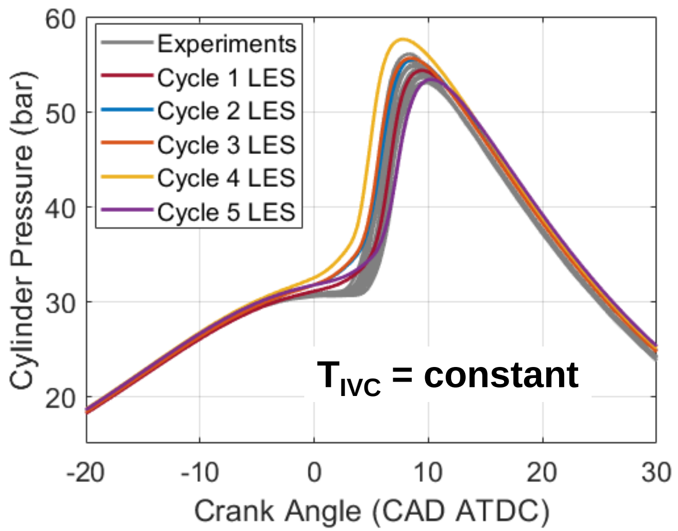
- Established a collaborative CFD modeling project with SUNY–Stony Brook
  ⇒ Applied LES to understand sources of thermal stratification.
- Collaborated with LLNL to test their kinetic mechanisms for gasoline.
  ⇒ Developed an improved surrogate for Regular E10 gasoline (RD5-87).
- Investigated the chemistry causing ϕ-sensitivity and its relationship to Octane sensitivity (S).
  ⇒ Extended this understanding to develop fuel blends that have strong ϕ-sensitivity and high RON with high octane sensitivity.
- **Developed and demonstrated a new rapid and robust combustion-timing control system.**

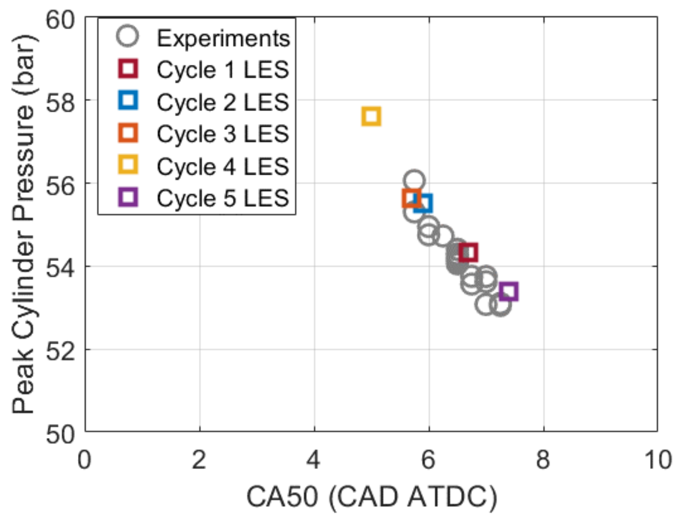
Also completed two studies started in FY17
⇒ Not presented due to time limitations

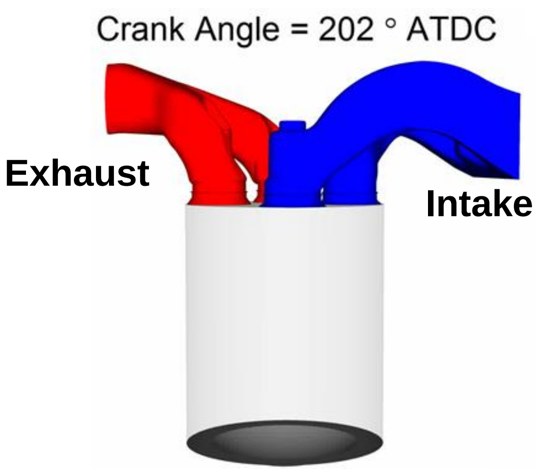
- Completed a study of spark-assist for well-mixed LTGC (HCCI) published in SAE 2018-01-1252.
- Completed uncertainty quantification (UQ) analysis in collaboration with LLNL, and published in SAE 2018-01-1248.

Collaborative CFD Modeling w/ SUNY–Stony Brook

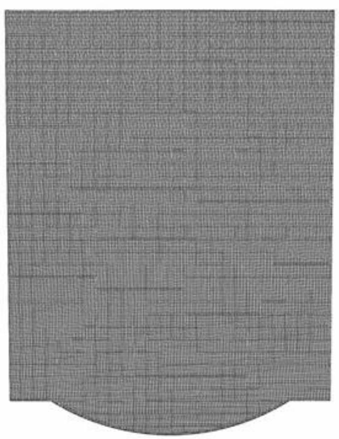
- Strong need exists for CFD modeling to supplement/extend our experimental work.
- We have established a new collaboration with SUNY–Stony Brook.
  - Led by Profs. Lawler and Mamalis
- Use CONVERGE CFD software
  - Large Eddy Simulations (LES) ⇒ Grid 0.5 mm
- Initial validation with premixed fueling.
  - Five LES cycles show random variation in combust. timing ⇒ turbulence & heat transfer
  - Spread similar to experiment, one outlier.







Engine Model



800 k cells at TDC

8.8 M cells at IVC

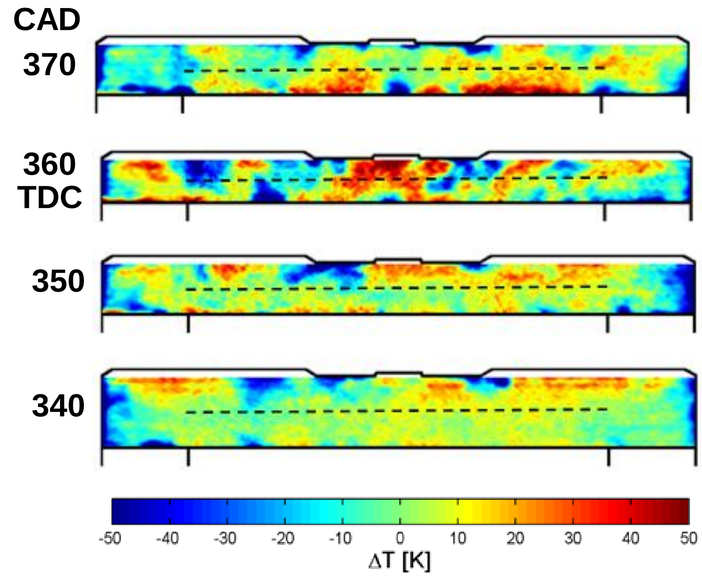
Grid

- CONVERGE CFD appears to be working well. ⇒ Apply to studies of LTGC.

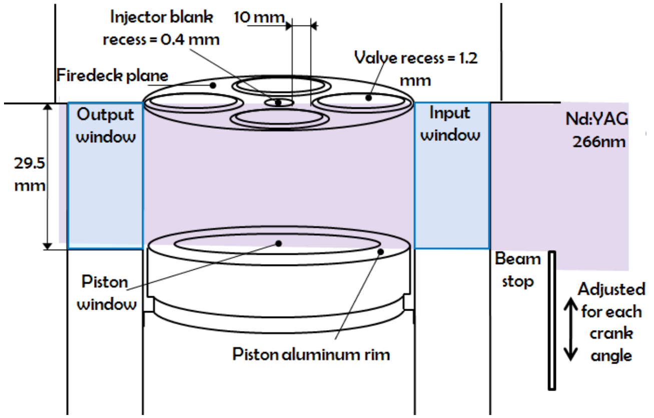
LES Shows Development of Thermal Stratification

- Understanding the mechanism that produces Thermal Stratification (TS) is important for LTGC/HCCI ⇒ Allows higher loads w/o knock.
  - **Enhancing TS could extend load range**
- Our laser-imaging studies showed that TS results from large-scale turbulent structures.
- Need to understand source of this turbulence & its relationship to engine geometry.

Experimental Temperature-Maps
Derived from toluene PLIF images
SAE 2012-01-1111



Vertical laser-sheet for T-Maps – Optical Engine



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  - **Enhancing TS could extend load range**
- Our laser-imaging studies showed that TS results from large-scale turbulent structures.
- CONVERGE with LES provides a means of investigating the source of this turbulence.
- LES indicates that TS results from large-scale turbulence, already present early in the compression stroke, combined w/ heat transfer.
  - Suggests that turbulence may persist from intake flows ⇒ additional analysis needed.

CONVERGE LES Simulations
Temperature-Maps on Vertical Cut Plane
Metal Engine

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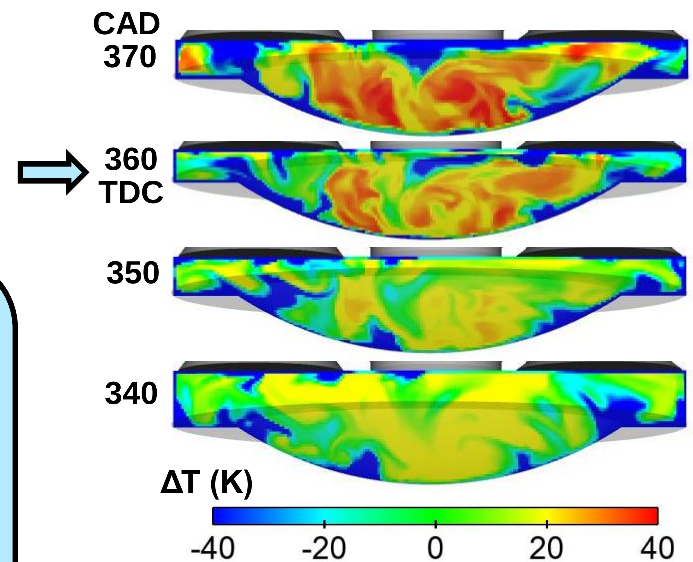
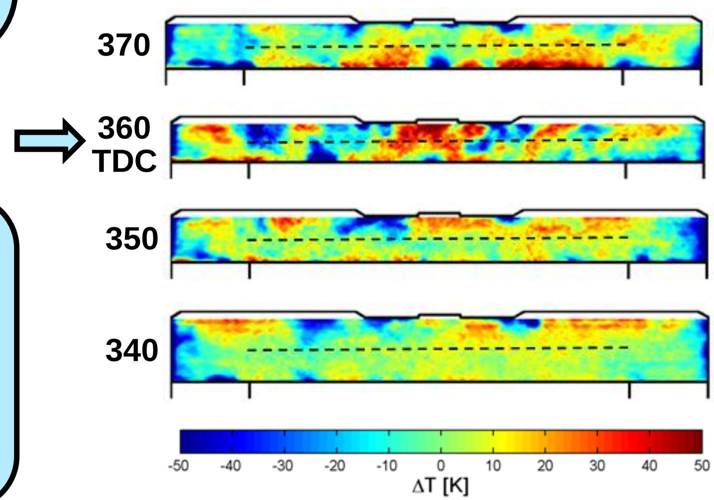
- LES indicates that TS results from large-scale turbulence, already present early in the compression stroke, combined w/ heat transfer.
  - Suggests that turbulence may persist from intake flows ⇒ additional analysis needed.
- TS is similar to experiment despite differences in metal and optical engine geometry & ports.
- Future CFD studies:
  1) Verify the source of large-scale turbulence ⇒ investigate methods for enhancing TS.
  2) Effects of these flows on heat transfer losses
  3) Injection strategies for improved fuel strat.

CONVERGE LES Simulations
Temperature-Maps on Vertical Cut Plane

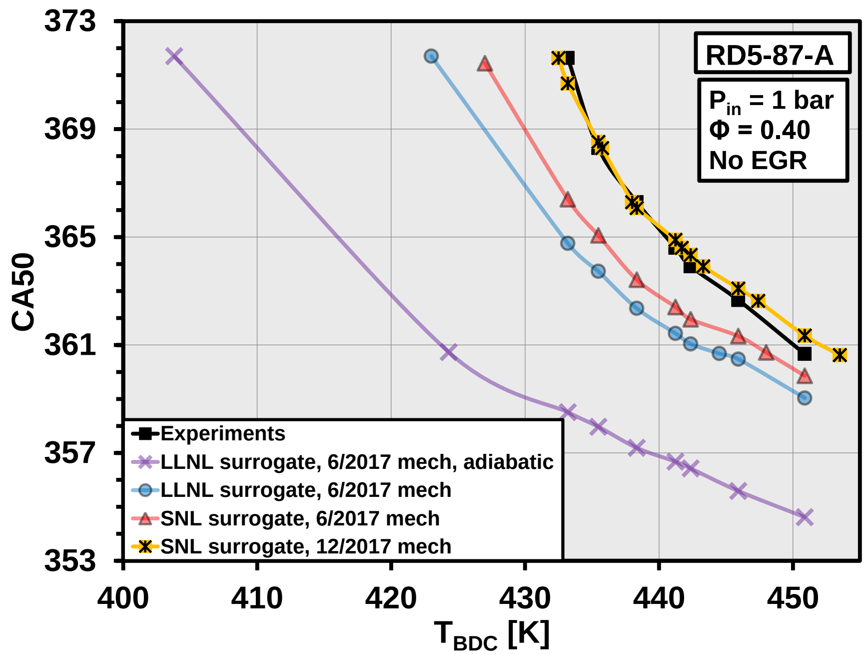


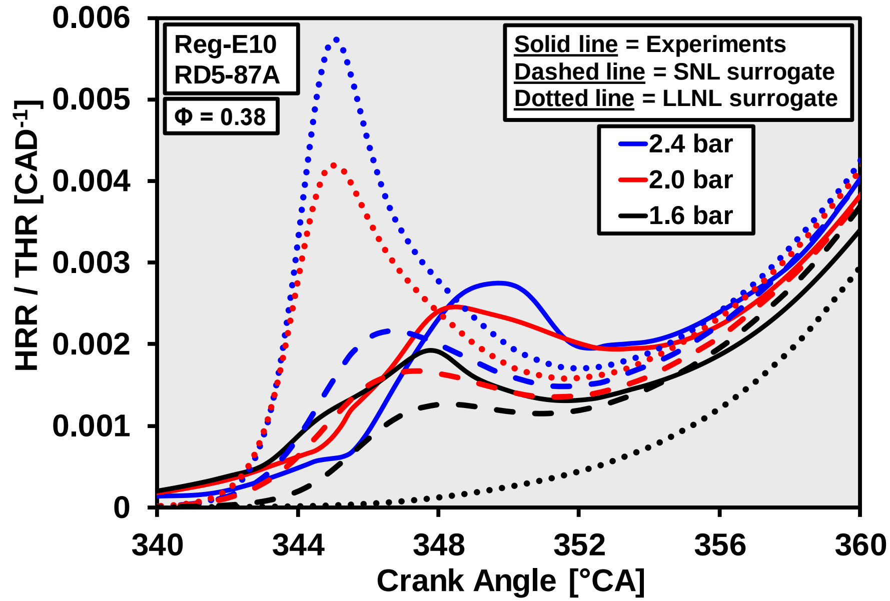
Experimental T-Maps



Improved Kinetic Modeling of Reg-E10 Gasoline

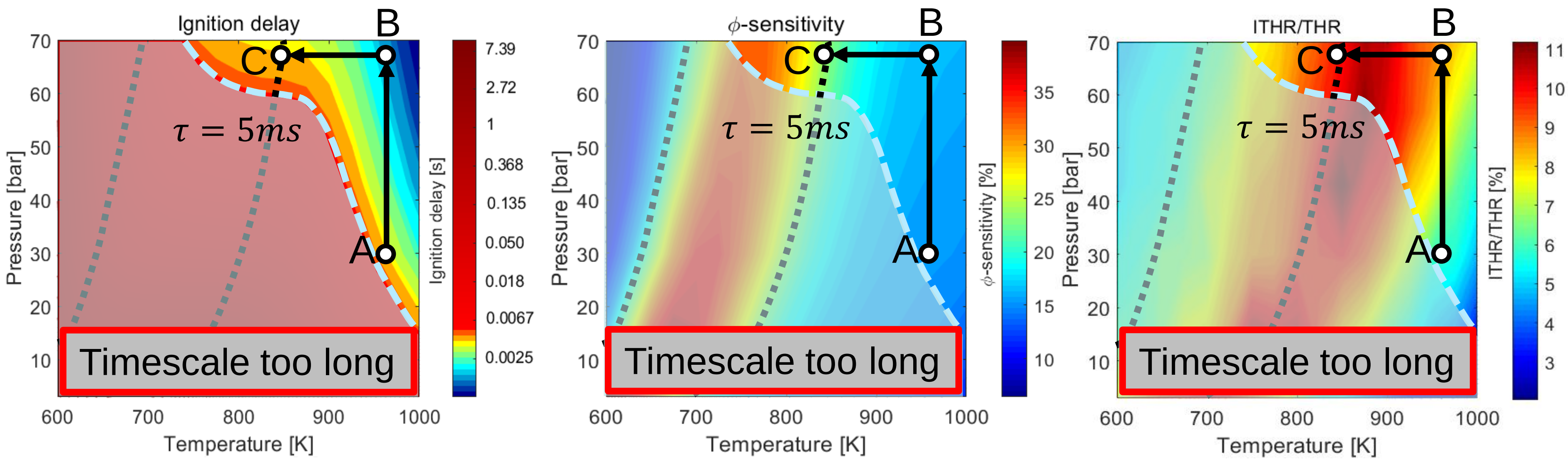
- Collaborated with LLNL to evaluate their kinetic mech. & surrogate for Regular-E10 ⇒ Compare with premixed engine data.
- CHEMKIN 1-zone & detailed LLNL mech.
  1) Typical adiabatic-core assmpt ⇒poor match
  2) Corrected for mass-averaged heat transfer
  3) Developed new surrogate w/ 7 components **based on fuel composition**, vs. 5 for LLNL
  4) Obtain new Kinetic Mechanism from LLNL
- Final match of combustion timing (CA50) at P_{in} = 1.0 bar is very good.
- For boosted operation, the new SNL surrogate also gives better results. ⇒ Much closer match for the low-temperature heat release (LTHR).
- Developing surrogates by selecting component types and quantities to match the DHA significantly improves results.
- New LLNL kinetic mechanism works well.





Investigate Φ-Sensitivity & ITHR, and their Relationship to Octane Sensitivity

- Φ-Sensitive fuels allow controlled charge stratification to provide CA50 control, load extension, and noise reduction ⇒ Chemical-kinetics of Φ-sensitivity not understood.
- Applied CHEMKIN with detailed mechanism
  - Select iso-octane as a representative fuel with NTC behavior (Φ_m = 0.4, 21% O2).

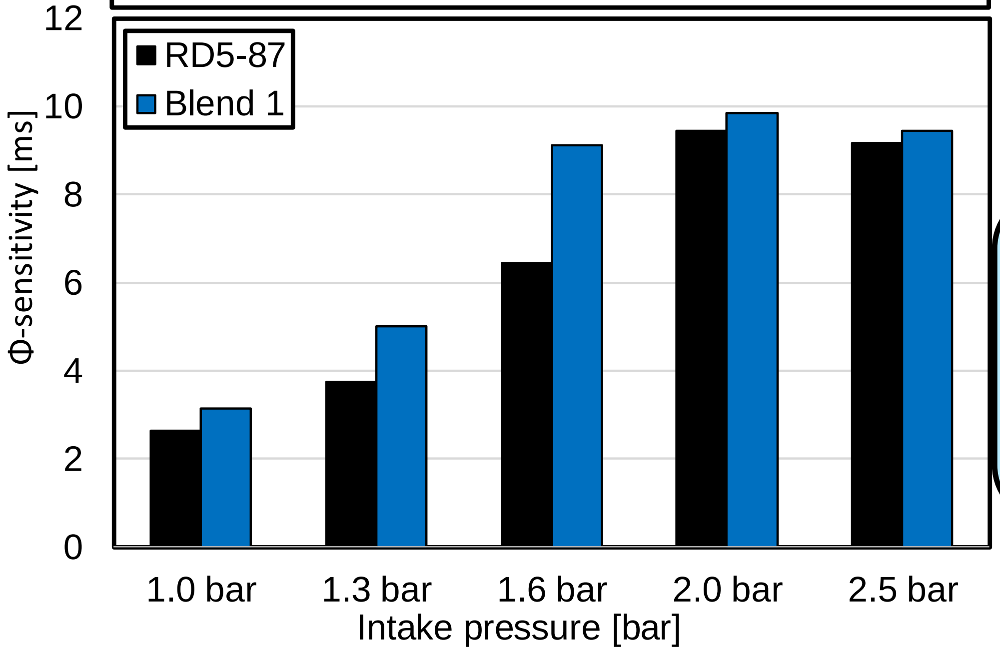


- Φ-Sensitivity is greatest in the **NTC zone ⇒ but still significant on the edges.**
- Intermediate temp. heat release (ITHR) has same trend, but offset to higher Temps. **⇒ The ITHR chain branching reactions control the Φ-sensitivity.**
- For gasoline-like fuels at P_{in} = 1.0 bar, usually T > NTC zone ⇒ With boost, T must be reduced, both P↗ & T↘ shift operation toward NTC zone, increasing ϕ-sensitivity.
- Is it possible to have a fuel w/ increased Φ-sens. at low P_{in} and high RON & high S?

Explore the Potential to Increase Both Φ-Sensitivity & Octane Sensitivity Above Reg-E10 (RD5-87)

- CHEMKIN simulations with detailed mechanism ⇒ Φ-sensitivity = $\frac{d\tau}{d\Phi}[ms]$
- Multiple fuel blends tested using a systematic methodology.
- <u>Best blend without legal limitations:</u>

76.5% 1-hexene + 23.5% p-xylene



EPA limits: Olefins ≤ 17.5%
Aromatics ≤ 30.4%

- All fuels show high Φ-sensitivity at high pressures (P_{in} >1.6 bar)
- Achieved a significant Φ-sensitivity improvement at low & medium press. (P_{in} ≤ 1.6 bar)
- RONs are high, and Ss are good. ⇒ Good for boosted-SI or multi-mode
- 2-butanol is a promising HPF species.

	RON	MON	S	T_{BCD} (1bar)	H/C ratio	O/C ratio
RD5-87	92.1	84.8	7.3	408K	2.025	0.0335
Blend 1	108.4	94	14.4	401.5K	1.782	0

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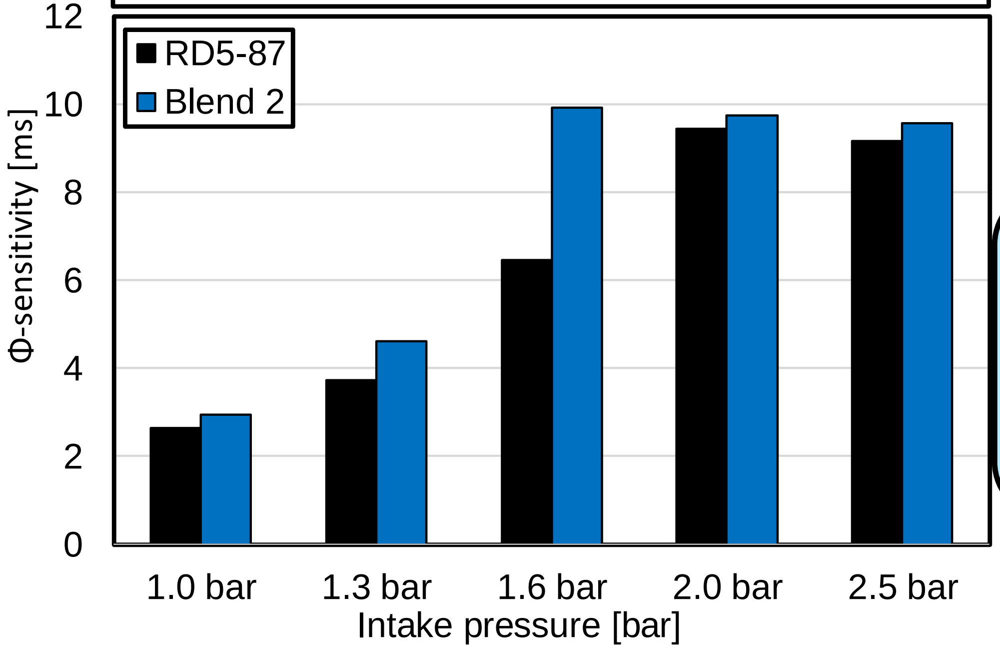
- Multiple fuel blends tested using a systematic methodology.
- Best blend that meets EPA regulations:

17.5% 1-hexene + 21% 2-methyl-hexane + + 30% p-xylene + 31.5% iso-octane



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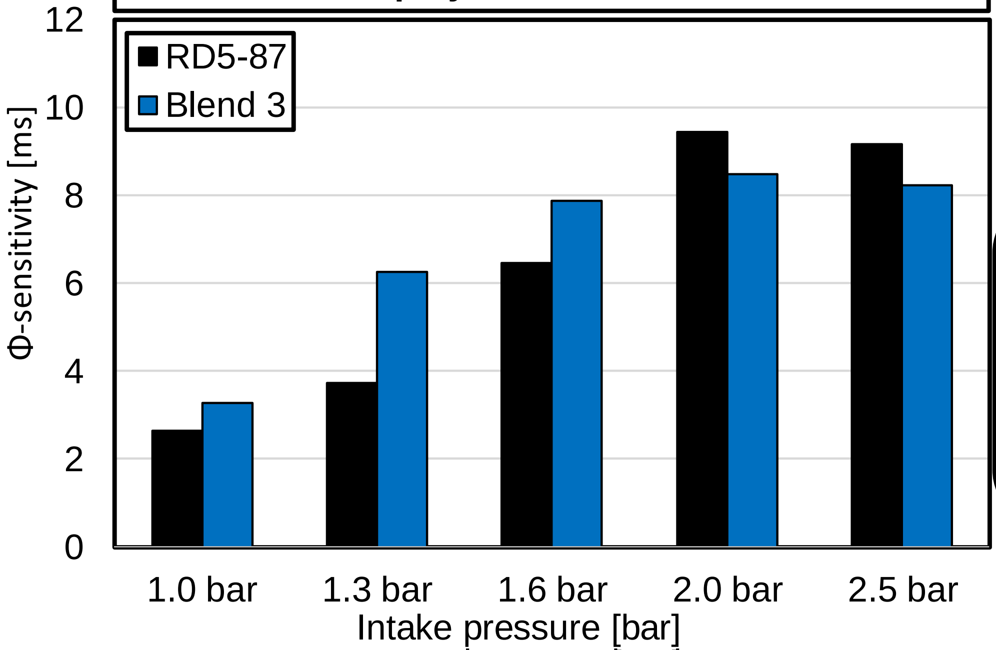
	RON	MON	S	T_{BCD} (1bar)	H/C ratio	O/C ratio
RD5-87	92.1	84.8	7.3	408K	2.025	0.0335
Blend 2	98.5	92.2	6.3	414K	1.899	0

Explore the Potential to Increase Both Φ-Sensitivity & Octane Sensitivity Above Reg-E10 (RD5-87)

- CHEMKIN simulations with detailed mechanism ⇒ Φ-sensitivity = $\frac{d\tau}{d\Phi}[ms]$
- Multiple fuel blends tested using a systematic methodology.
- Best blend that meets EPA regulations and includes a high-performance fuel (HPF):

17.5% 1-hexene + 22.5% 2-methyl-hexane + + 30% p-xylene + 30% 2-butanol



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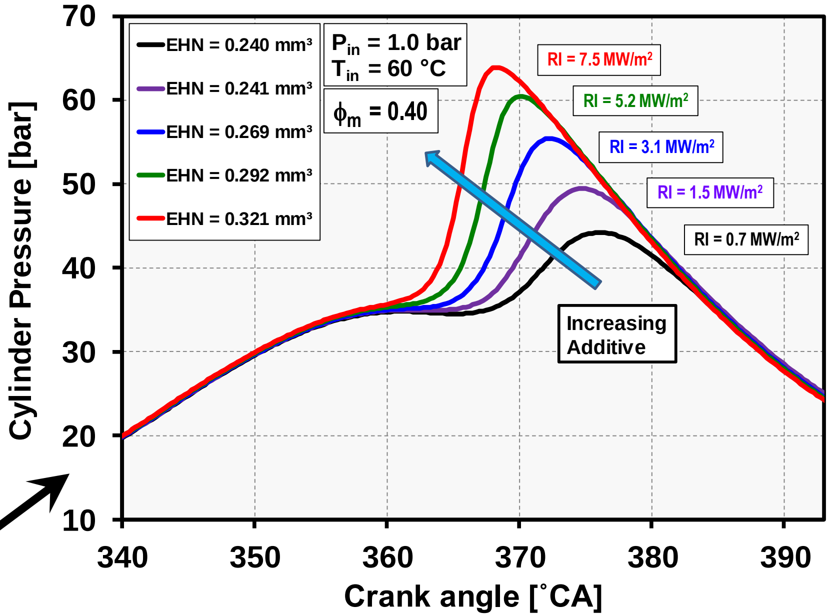
RD5-87	92.1	84.8	7.3	408K	2.025	0.0335
Blend 3	98.7	88.1	10.6	408K	1.880	0.0482

Advanced Combustion-Timing (CA50) Control

- Combustion-timing control is perhaps the most challenging barrier to practical LTC (LTGC, HCCI, GCI, etc.) engines.
- Current methods are complex, typically involving a combination of control mechanisms, and they have difficulties at various conditions.
- <u>Desired</u>: “single-knob” direct control of combustion-timing that is robust and sufficiently fast to handle rapid transients.
  - Also desirable to reduce the heating/hot-residuals required for autoignition.
- We have developed a such a system.
  - Works by metering and mixing a controlled amount of ignition enhancing additive each engine cycle ⇒ fast response.
  - Additive amounts are tiny (~tenths of mm^3) with precision ~hundredths of mm^3.
- Currently using 2-ethylhexyl nitrate (EHN), but others are available, such as di-tert-butyl-peroxide (DTBP), which has the advantage of no increase in NOx.
  - Estimate ~gallon-sized reservoir replenished at service intervals ~7000 miles for LD applications. Not expensive < $20/gallon in 2016.
  - Less additive needed at higher loads, so amount required is expected to be proportionally less for MD/HD applications.
- First presentation of this **Additive-Mixing Fuel Injection (AMFI)** system ⇒ Results are very promising, but many details & capabilities not yet investigated.

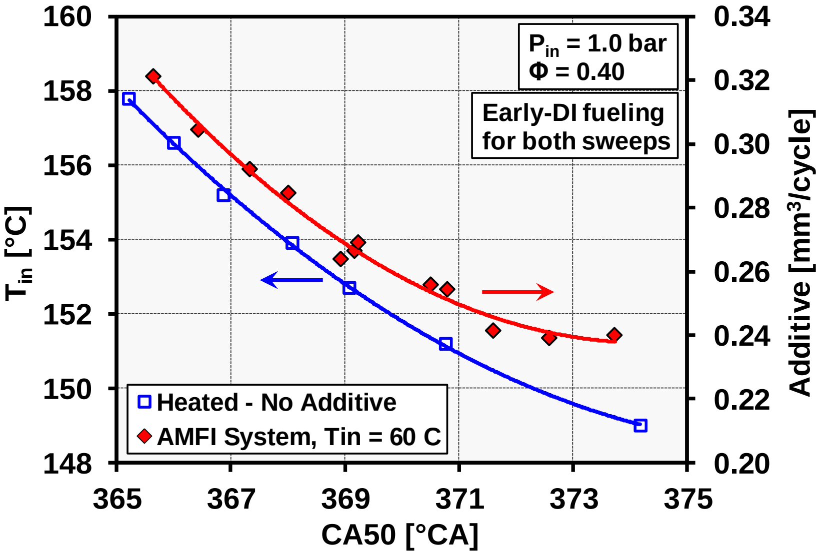
AMFI System Provides Rapid CA50 Control

- Regular E10 gasoline (RD5-87) requires heated T_{in} ~ 150°C for compression ignition (CI) at P_{in} = 1.0 bar, with early-DI fueling.
- Additive enhances autoignition, reducing or eliminating need for intake heat or hot-residuals. **Selected T_{in} = 60°C for studies.**
- Adjusting the additive easily shifts the 50% burn point (CA50) from very retarded (near misfire) to overly advanced (knocking), **in a few seconds.**
- W/o additive adjust T_{in} from 149 – 158°C for same CA50 variation ⇒ very slow
- Demonstration of the transient response is given in a technical back-up slide.



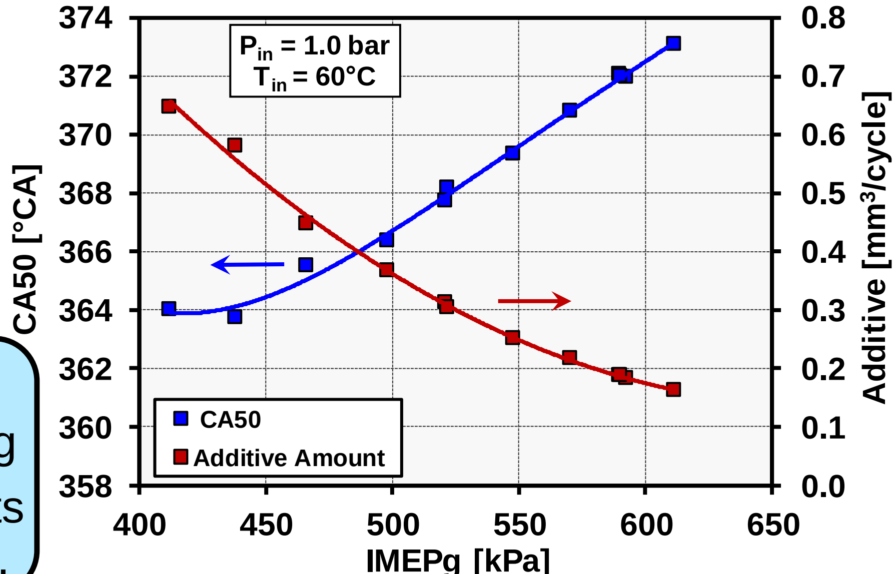
Ringing Intensity (RI) indicates knock propensity.
RI ≤ 5 MW/m² no knock ⇒ Eng, SAE 2002-01-2859

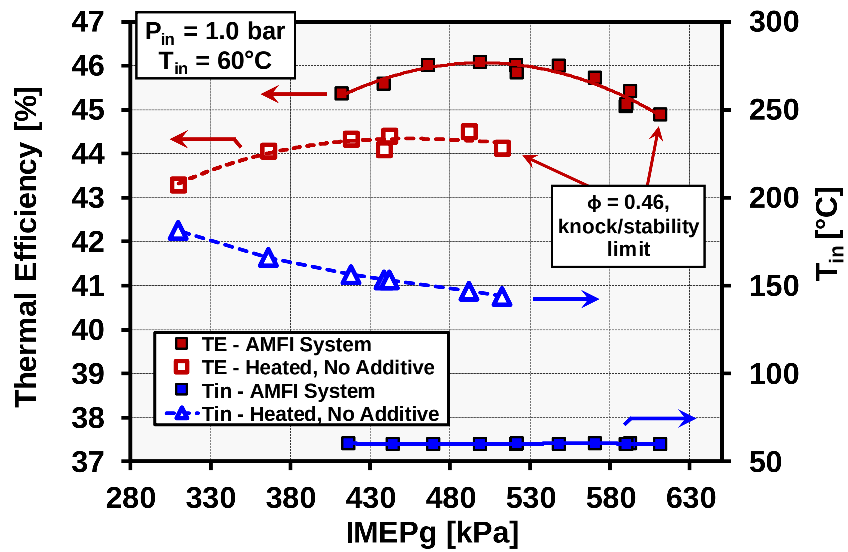
$$RI = \frac{1}{2\gamma} \cdot \frac{\left(0.05 \cdot \left(\frac{dP}{dt}\right)_{max}\right)^2}{P_{max}} \cdot \sqrt{\gamma R T_{max}}$$



CA50 Control Through a Load Sweep

- Sweep fueling rate ($0.3 \le \phi \le 0.46$) with AMFI control, constant T_{in} = 60°C.
- AMFI can quickly adjust CA50 as req'd. ⇒ Currently limited by manual controls.
- Without additive, must adjust T_{in} by 37°C
- The lower T_{in} with the AMFI system also:
  - Increases charge density ⇒ higher IMEPg
  - Increases Thermal Eff. (TE) by 1.6 %-units due to higher γ and reduced heat transfer.





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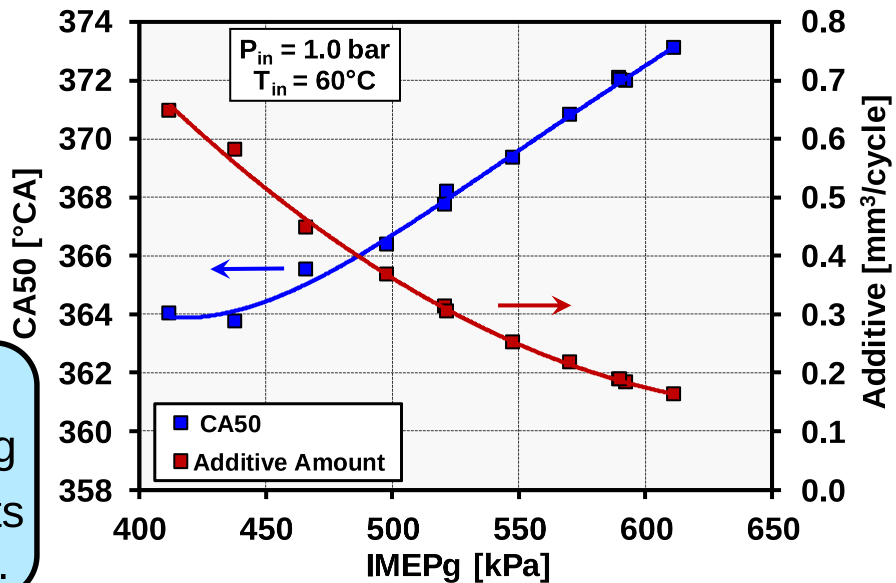
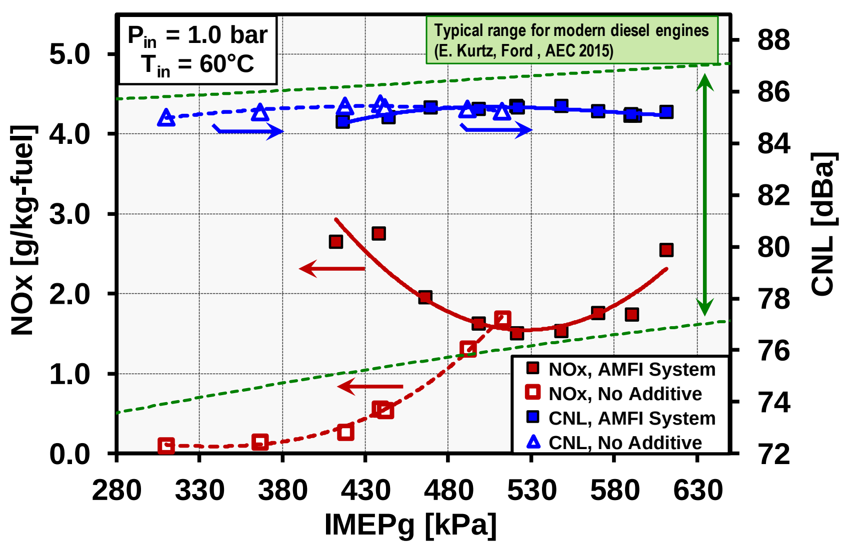
- The lower T_{in} with the AMFI system also:
  - Increases charge density ⇒ higher IMEPg
  - Increases Thermal Eff. (TE) by 1.6 %-units due to higher γ and reduced heat transfer.
- NOx emissions are a little higher than w/o additive due to EHN but < 3 g/kg-fuel.
  - Lower T_{in} partially compensates for EHN.
  - Switching from EHN to DTBP would result in much lower NOx than w/o additive.
- Combustion Noise (CNL), 85 – 86 dBA is below limit from Ford, ~same as no-additive.
  - Greater potential to reduce CNL w/ additive ⇒ allows > CA50 retard with good stability.

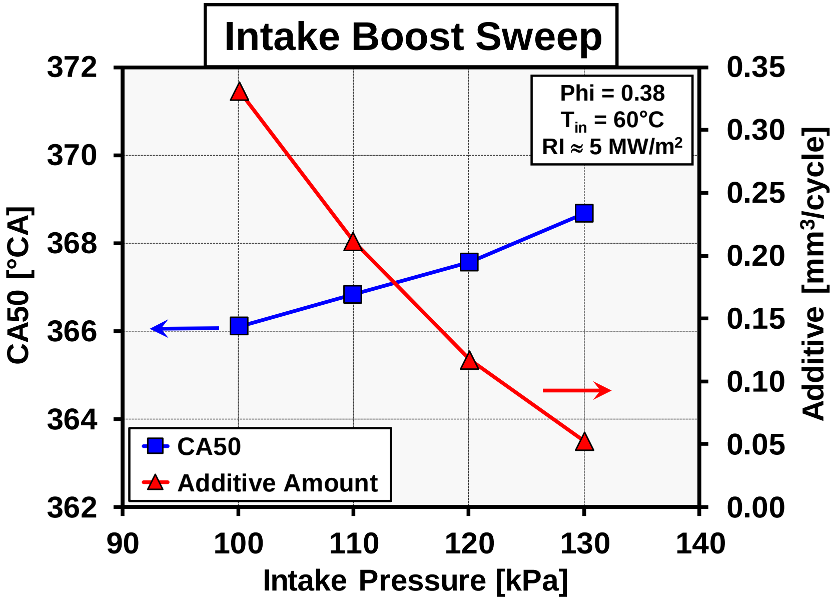


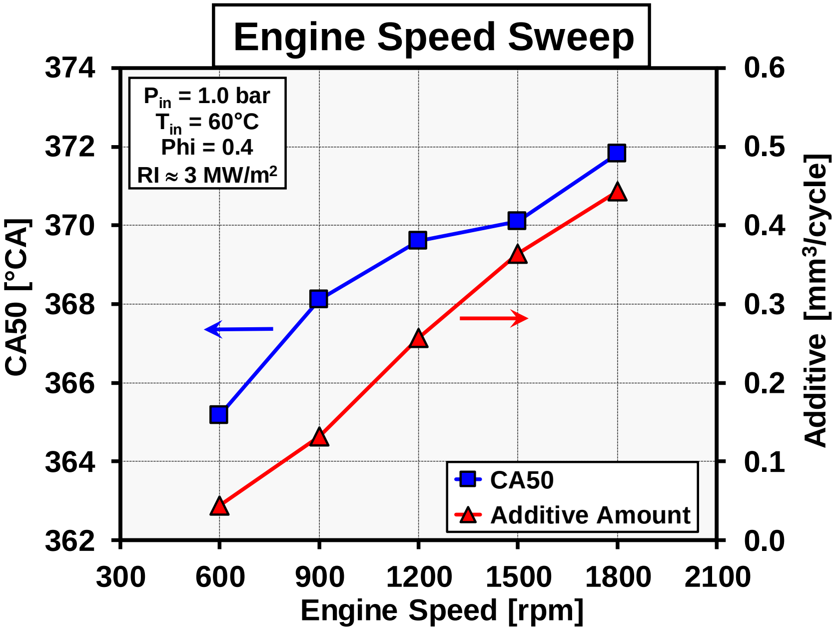


- **AMFI system has sufficient control authority for a large change in load.**

AMFI System Provides Sufficient Control Authority for Boost and Speed Sweeps

- AMFI system also controls CA50 well through boost and speed sweeps.
  - Constant T_{in} = 60°C for both sweeps.
- With increased P_{in}, fuel becomes more reactive, and CA50 must be retarded to maintain constant RI = 5 MW/m^2.
  $\Rightarrow$ Additive reduced
- With increased speed, less time for autoignition $\Rightarrow$ Additive increased
  - Additive increase is mitigated by need to retard CA50 to maintain RI = 3MW/m^2
- At 600 rpm, amount of additive is very small $\Rightarrow$ low-speed allows more time for the slower low-temperature reactions.
  - Indicates AMFI may allow Cold Start without excessive additive.





Collaborations

- Project is conducted in close cooperation with U.S. Industry through the **Advanced Engine Combustion (AEC) Working Group**, under a memorandum of understanding (MOU).
  - Twelve OEMs, Three energy companies, Six national labs, & Several universities.
- **General Motors:** Bimonthly internet meetings ⇒ presentations and in-depth discussions of recent research. Support for GDI injectors & spark ig. system.
- **Cummins:** Engine hardware support
- **SUNY- Stony Brook Univ.:** New collaboration for CFD modeling of our LTGC engine using LES.
- **LLNL:** Completed UQ analysis w/ Whitesides & Petitpas.
- **LLNL:** Validated LLNL's chemical-kinetic mechanisms for gasoline. Collaborated to improve surrogate blends for Regular E10 & other gasolines, with Pitz et al.

DOE-OVT Project is also leveraged through 3 con-current research efforts

- **Sandia LDRD:** Developed the AMFI combustion-timing control system.
- **Co-Optima Fuels Project:** Separately funded project on advanced fuels LTGC engines, and evaluation of new fuels for boosted-SI engines.
- **Chevron:** Funds-in project on improved petroleum-based fuels for LTGC.

Remaining Challenges and Barriers

- Combustion-timing control remains a key barrier that still lacks sufficient understanding.
  ⇒ Our LTGC facility has good potential for advancing two methods.
  1) Double or Multiple-DI strategies to vary charge stratification to change autoignition timing.
  2) **New AMFI system can control combst. timing over wide range of conds.**
     ⇒ Many additional studies are needed to understand its full capabilities.
- Development of methods for achieving robust autoignition at low loads.
- Improved understanding of how intake flows produce the large-scale turbulence responsible for thermal stratification and how these flows might be beneficially altered.
- Determine the cause of increased cycle-to-cycle variability at higher fueling rates for mid-range intake boost pressures
  - Apply this knowledge to develop methods that overcome the problem.
- Improved understanding of fuel effects on the above processes.

Future Research

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

- **AMFI Control System:** Additional studies are needed to understand its capabilities for combustion-timing (CA50) control and other benefits.
  - Effect of changes in intake temperature
  - Compatibility with EGR for control at high boost levels
  - Benefits of combining AMFI with partial fuel stratification (PFS)
  - Potential to extend low-load limit for robust autoignition
  - Potential to enable cold starting
- **Double or multiple-injection PFS** for CA50 control $\Rightarrow$ Optimize injection strategies to increase CA50 control authority & minimize NOx emissions.
- CFD Modeling of fuel sprays & resulting vapor-fuel distributions to improve charge stratification techniques – in collaboration with SUNY-Stony Brook
- Infra-Red (IR) imaging of fuel distributions to guide improvements in charge stratification.
- Develop a closed-loop feedback control system do allow CA50 control through rapid transients.
- Investigate fuel effects as related to combustion-timing control methods.

Summary

Relevance

- LTGC can provide efficiencies at or above diesel engines with low NOx & soot
  - Multi-mode for LD, use LTGC up to ~10 bar IMEPg, then switch to boosted SI for high loads.
  - Full-time for MD/HD, loads to 20+ bar IMEPg; lower-cost fuel system, aftertreatment, & potentially fuel
- A rapid CA50 control system is required. Fuel effects & thermal stratification also important.

Approach

- Combine metal- and optical-engine experiments with CHEMKIN and CFD modeling.
- Develop a collaboration w/ SUNY–Stony Brook to apply CONVERGE CFD to our engine.
- Apply CHEMKIN with LLNL detailed mech. & develop improved surrogate blends.
- Develop a new rapid combustion-timing control system under internal funds; transfer to VTO

Accomplishments

- Developed and demonstrated a new rapid, robust combustion-timing control system for LTCG. Showed that it can easily control CA50 over a range of loads, intake pressures, and engine speeds, with a response time sufficient for rapid transients.
- Determined the cause of ϕ-sensitivity in gasoline autoignition, and showed that it is possible for a fuel with RON = 98.7 and octane sensitivity = 10.6 to also have strong ϕ-sensitivity.
- Developed a significantly improved chemical-kinetic surrogate for Reg-E10 (RD5-87) gasoline.
- Conducted a CFD-LES investigation of thermal stratification (TS) with SUNY-Stony Brook.
  - Showed that model results correlate with optical-engine data, and that TS is caused by large-scale turbulence, already present early in the compression stroke, possibly produced by the intake flows.
- Completed initial study of spark-assist; showed limits correlate w/ laminar flame spd. ⇒ publish
- Completed UQ study with LLNL, including connecting rod compression ⇒ published results

Collaborations: Multiple collaborations as listed on Collaborations slide

Future Research: Future Research slide lists several studies, mostly related to CA50 control.

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

Acknowledgement

- This work was performed at the Combustion Research Facility, Sandia National Laboratories, Livermore, CA.

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Technical Backup Slides

Transient Response of the AMFI System

- With constant T_{in} = 60°C, start with CA50 retarded to near misfire limit.
  1) First, a step increase in additive to advance CA50 ~6° CA, to near onset of knock.
  2) Second, a step decrease additive to retard CA50 ~2° CA.
- Time response ~ 6 seconds due to:
  - Fuel dead-volume effect, estimate ~2 seconds at this condition.
  - Wall temperature (T_{wall}) effect, estimate ~4 secs.
- Dead-volume could be reduced by careful engineering.
- Could also combine with double-inj. PFS for near-instantaneous response.
- T_{wall} effect is fundamental ⇒ Can overdrive AMFI system to compensate
- Speed of AMFI system can provide a means of studying T_{wall} effect ⇒ listed as a barrier in 2018 ACEC roadmap.