Achieving High Efficiency Combustion by Controlling Fuel Reactivity

Sage Kokjohn

Acknowledgments

Direct-injection Engine Research Consortium (DERC)
US Department of Energy/Sandia National Labs
Rolf D. Reitz and Mark P.B. Musculus

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Outline

- Motivation for investigating internal combustion (IC) engine efficiency
- ICE background
- Requirements for high-efficiency combustion
- A pathway to high-efficiency clean combustion using in-cylinder blending of fuels with different auto-ignition characteristics
  - Conventional fuels
  - Details of combustion process
  - Alternative fuels
- Conclusions

Why research IC engine efficiency?

- Internal combustion engines are used in a variety of applications from transportation to power generation
- 70% of all crude oil consumed is used to fuel internal combustion engines
  - United States spends more than 3% of GDP on oil to fuel IC engines
- IC engines are expected to be the dominant (>90%) prime mover for transportation applications well into the future[1,2,3]
- Improvements in the efficiency of IC engines can have a major impact on fossil fuel consumption and green house gas (GHG) emissions on a global scale
  - A 1% improvement in efficiency equates to a fuel savings of ~$4 billion per year

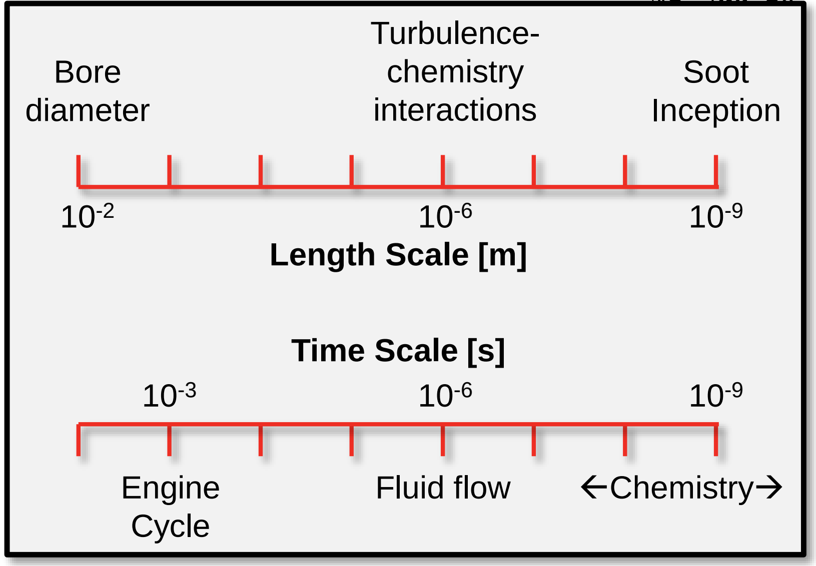
[1] Quadrennial Technology Review, DOE 2011

[2] *Review of the Research Program of the FreedomCAR and Fuel Partnership: 3rd Report,* NRC 2010

[3] Energy Information Agency, *Annual Energy Outlook 2012,* June 2012.

Engine Combustion Background

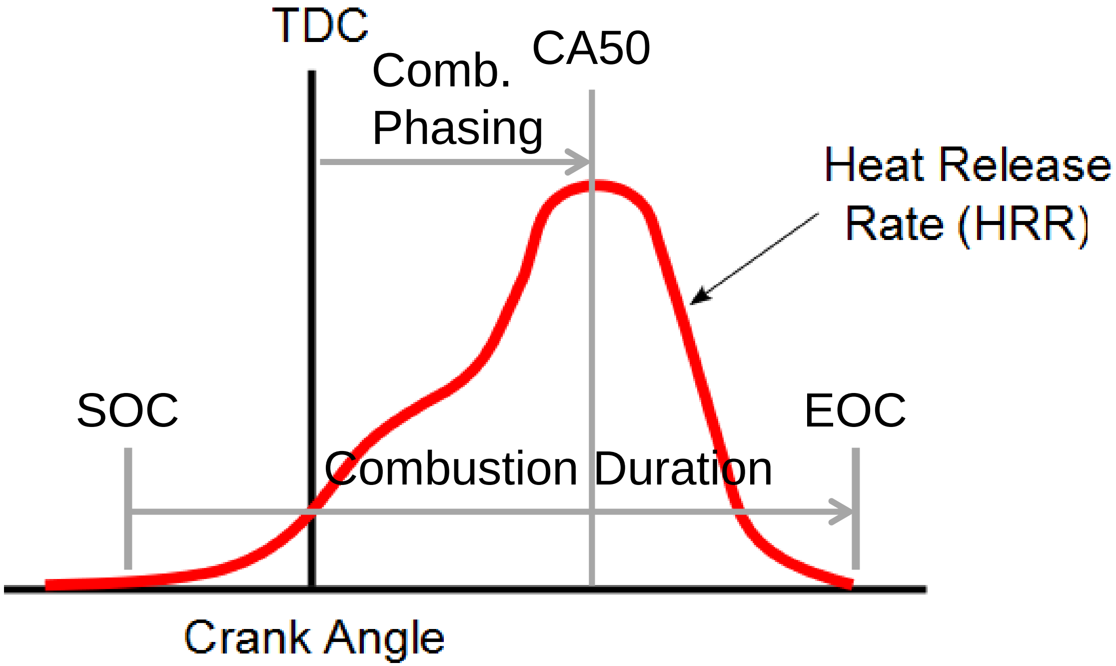
- Engine combustion involves physics that occur at a range of time and length scales
- Unique modeling challenge that includes every aspect of mechanical engineering
  - Turbulence
  - Combustion
  - Two-phase flow
- Chemistry of real fuels involves 100's of species and 1000's of reactions

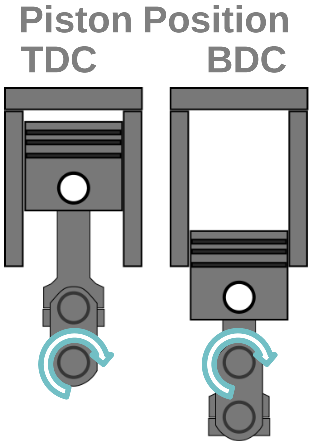


- Ideally all scales would be resolved considering all species and reactions → Direct Numerical Simulation with Detailed Chemistry → single engine cycle would take decades
- Engineering applications must model:
  - Small scales of turbulence (RANS or LES)
  - Turbulent combustion (average species production)
  - Chemical kinetics (reduced, but representative chemistry)
- In this work all scales of turbulence are modeled (Reynolds Averaged Navier-Stokes (RANS)) and combustion is modeled using direct-integration of a reduced chemical kinetics mechanism

Internal Combustion Engine Terminology

- **Heat release rate (HRR):** Rate at which the fuel energy is released due to combustion
- **CA50:** Crank angle (CA) when 50% of the fuel energy has been released
- **Combustion phasing:** Distances (in CA) between top-dead center (TDC) and CA50
- **Combustion duration:** Distances (in CA) between start-of-combustion (SOC) and end-of-combustion (EOC)





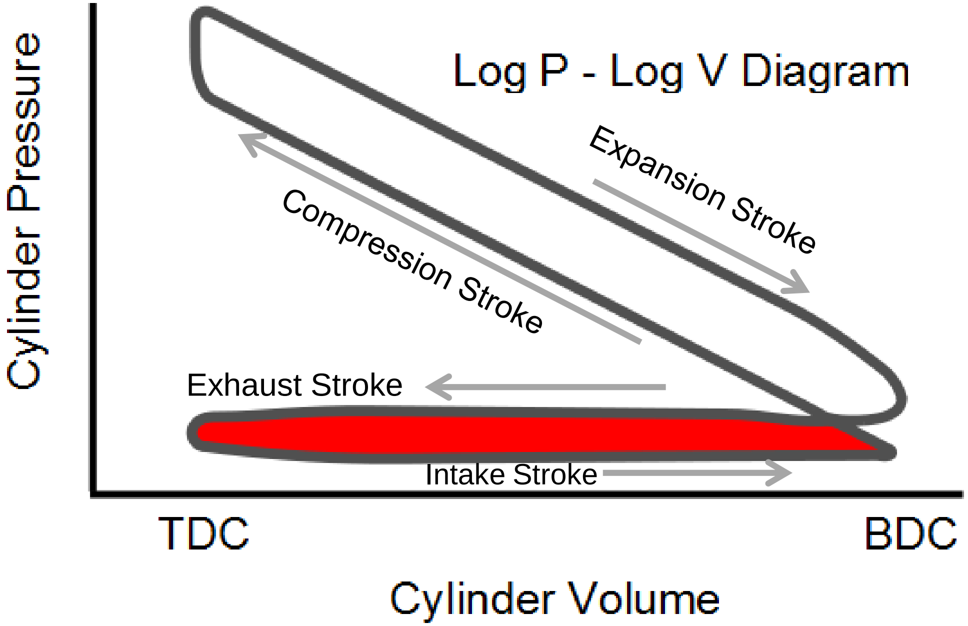
Internal Combustion Engine Terminology

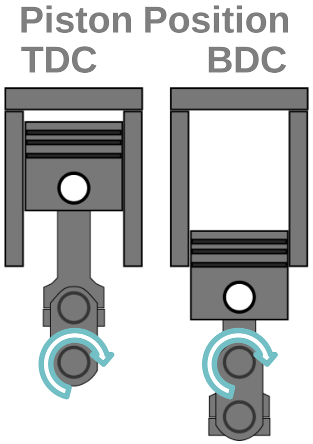
- **Gross Indicated Mean Effective Pressure (GIMEP):** PdV work from BDC of the compression stroke to BDC of the expansion stroke divided by the displacement volume
- **Gross Indicated Efficiency (GIE):** PdV work from BDC of the compression stroke to BDC of the expansion stroke divided by the fuel energy
- **Net Indicated Efficiency (NIE)**: PdV work over the full cycle divided by the fuel energy
- **Pumping Loss:** GIE - NIE

$$GIMEP = \frac{\int_{CA=-180}^{CA=180} PdV}{V_d}$$

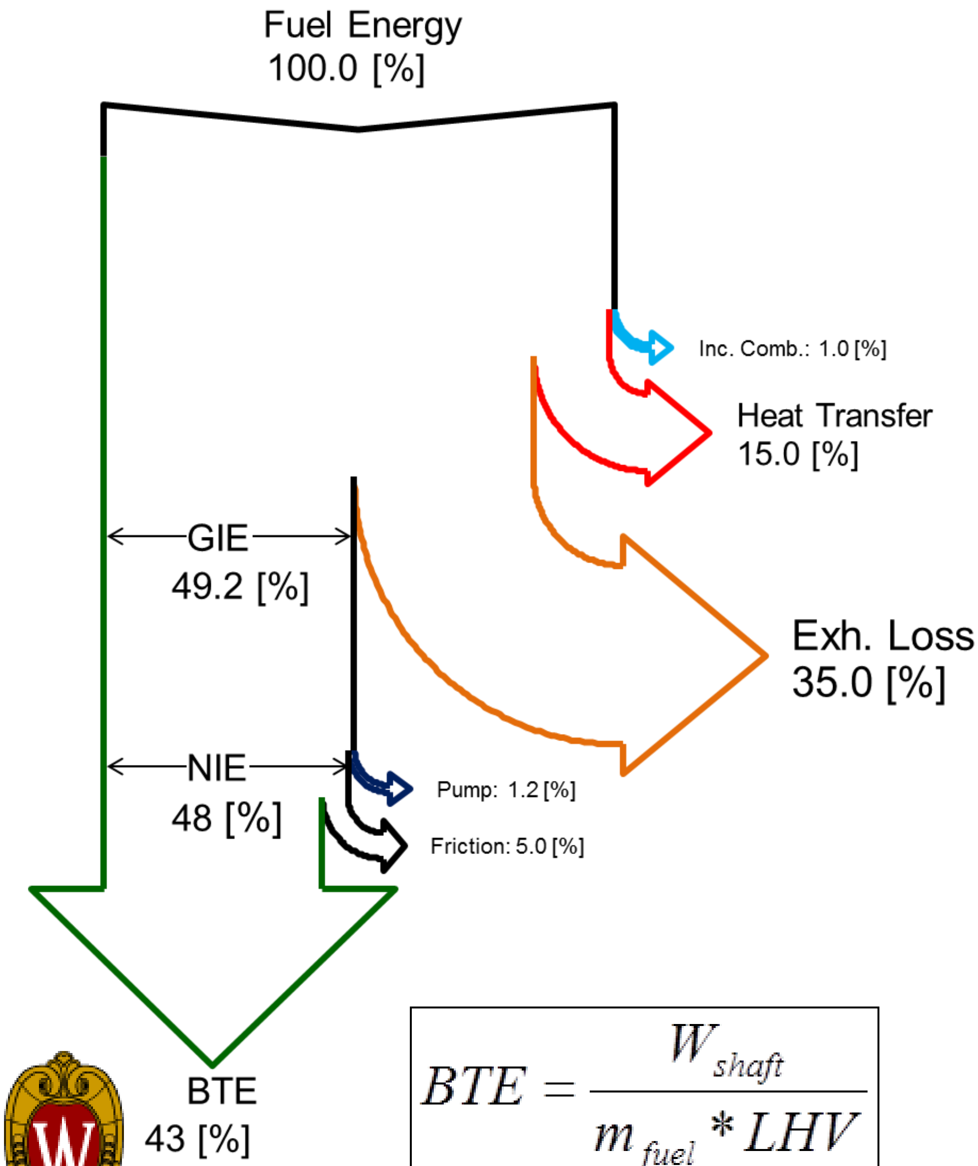
$$GIE = \frac{\int_{CA=-180}^{CA=180} PdV}{m_{fuel} * LHV}$$

$$NIE = \frac{\int_{CA=-360}^{CA=360} PdV}{m_{fuel} * LHV}$$





Maximizing Engine Efficiency



$$BTE = \frac{W_{shaft}}{m_{fuel} * LHV}$$

- Fuel energy is wasted due to:
  - Incomplete combustion (i.e., combustible material flowing out the exhaust)
  - Heat transfer losses to the coolant, oil, and air
  - Unrecovered exhaust energy
  - Pumping losses
  - Friction losses
- Research goal is to maximize the BTE by developing a fundamental understanding of pathways leading to high efficiency energy conversion and proposing techniques to achieve this goal

Maximizing Engine Efficiency

- Maximize combustion efficiency
  - In-cylinder temperatures must exceed ~1500 K to convert CO to CO_2
- Minimize fuel (or fluid) consumption penalties of aftertreatment → avoid forming NOx and soot emissions
  - Peak combustion temperatures must be below ~2000 K to avoid forming NOx
  - Fuel and air must be sufficiently mixed to avoid soot
- Minimize heat transfer losses
  - Keep combustion temperatures low and avoid high levels of charge motion (minimize convection losses)
- Maximize expansion work (i.e., operate with a high expansion ratio)
  - Begin with high geometric compression ratio
  - Combustion phasing must be well controlled and near TDC
  - Combustion duration must be short, but controlled

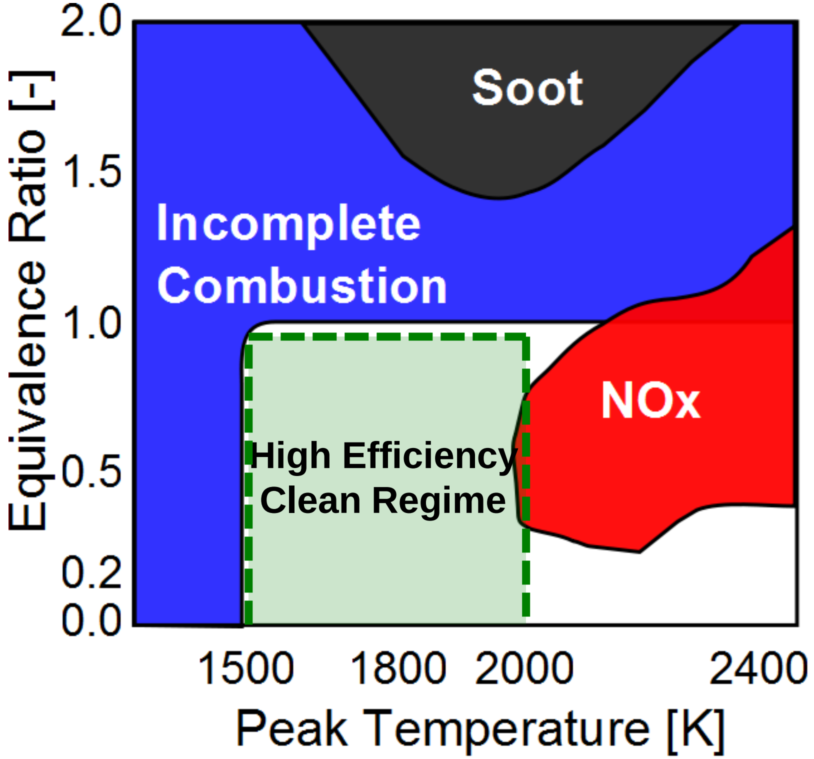
Equivalence ratio (ϕ): the stoichiometric air-fuel-ratio (AFR) divided by the actual air-fuel-ratio.

$$\phi = \frac{AFR_{stoich}}{AFR}$$

Fuel Rich

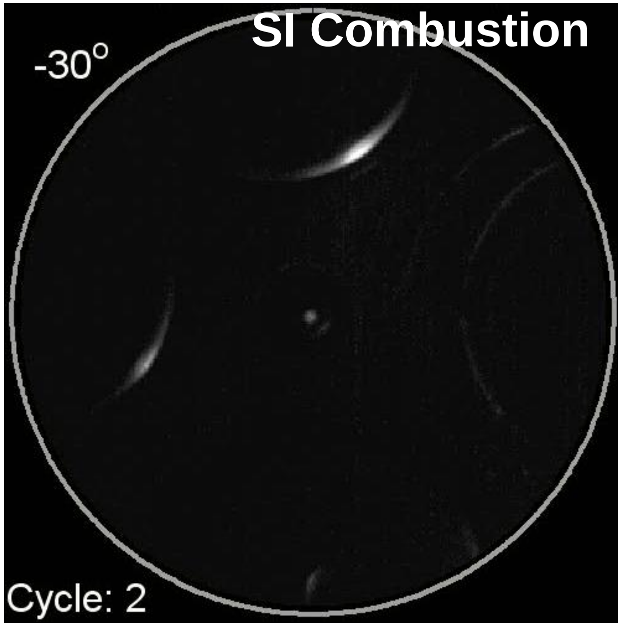
Stoichiometric

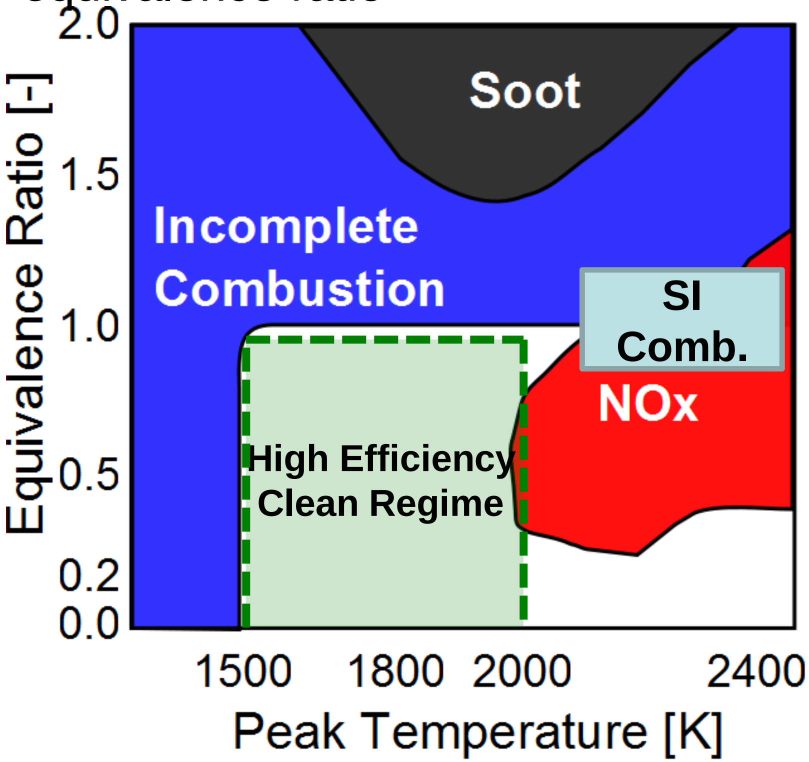
Fuel Lean



Conventional Combustion Modes

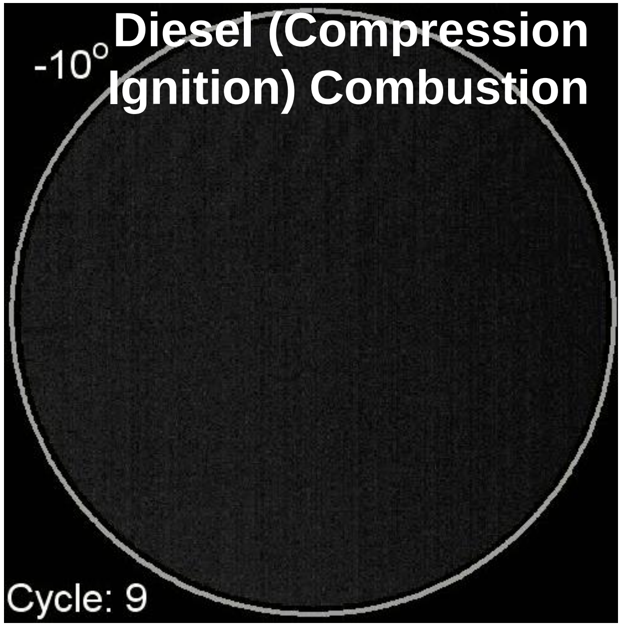
- **Spark Ignited Combustion**
  - Premixed fuel and air
  - Combustion phasing controlled by spark timing
  - Heat release rate controlled by flame propagation (equivalence ratio is typically near stoichiometric to maintain high flame speed)
  - Low cost aftertreatment using three-way catalyst (TWC)
  - Efficiency is poor due to low compression ratio (knock limited combustion) and requirement to operate near stoichiometric equivalence ratio

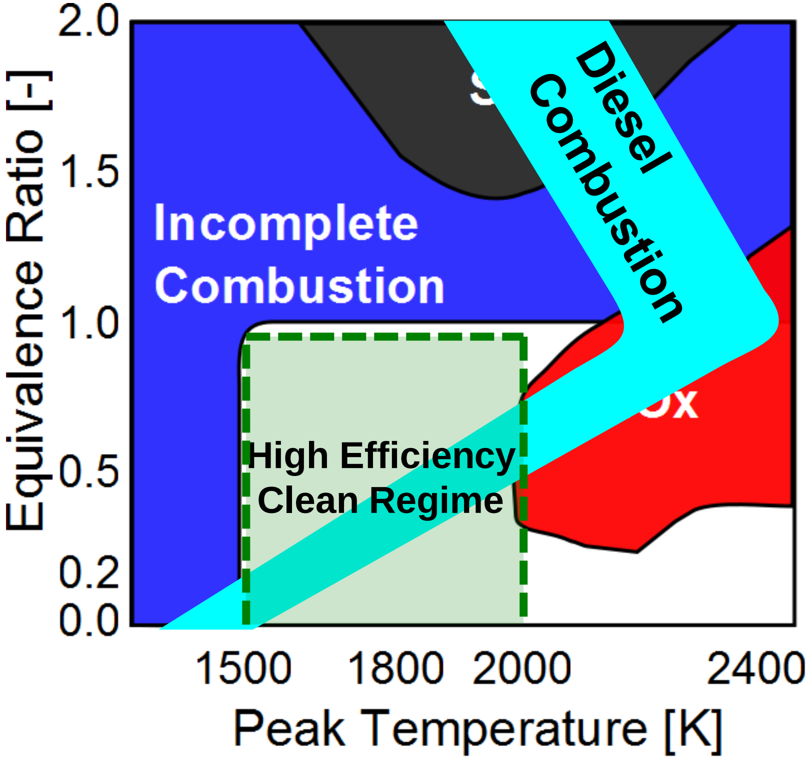




Conventional Combustion Modes

- **Diesel Combustion**
  - Fuel and air are mixed during the combustion process
  - Mixing controlled combustion results in soot and NOx formation
  - High compression ratio and lean operation results in higher efficiency than spark ignited combustion
  - Lean operation does not allow the use of a three-way catalyst → NOx aftertreatment is costly and increases fuel (fluid) consumption
  - High temperature regions increase heat transfer losses



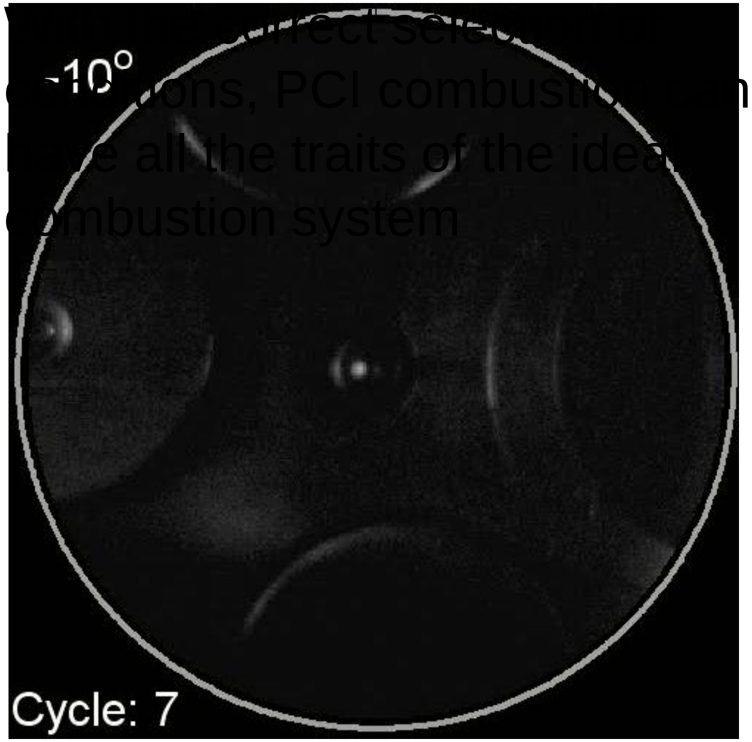


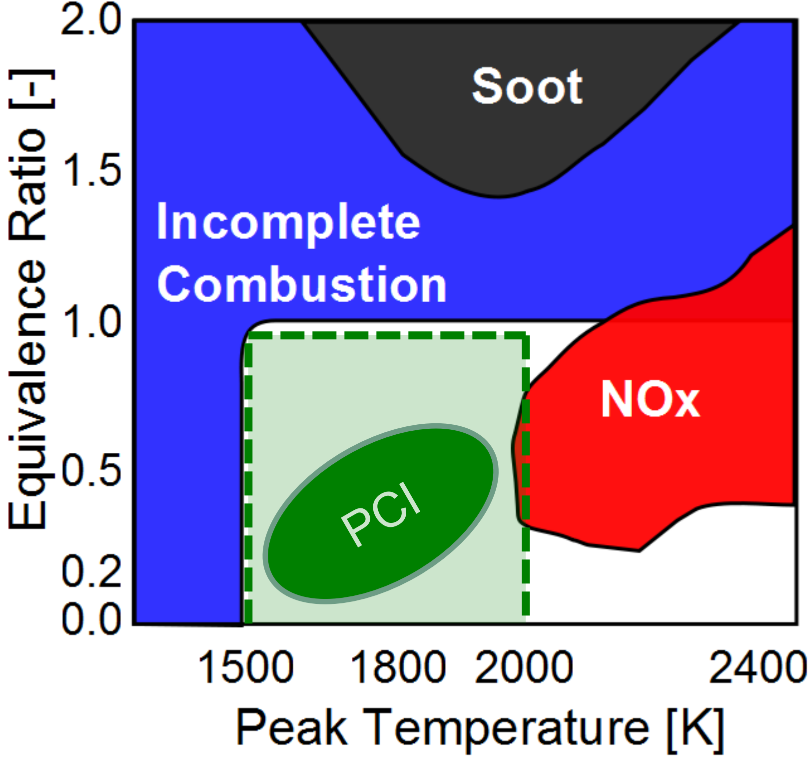
Advanced Combustion Modes

Combustion controlled by chemistry →No direct-control over the combustion phasing or rate of heat release

Injection and combustion events are decoupled (comb. control is a challenge)

- **Premixed Compression Ignition (PCI)**
  - Ideal combustion system has a high compression ratio using a lean, well-mixed charge, resulting in a short burn duration near TDC with temperatures between 1500 K and 2000 K
- With the correct selection of [illegible] conditions, PCI combustion can have all the traits of the ideal combustion system



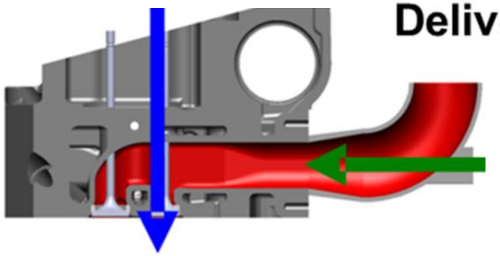


Advanced Combustion Modes

- Highly-premixed compression ignition (PCI) strategies offer attractive emissions and performance characteristics; however, in practice PCI strategies are generally confined to low-load operation due to
  - lack of adequate combustion phasing control
  - difficulties controlling the rate-of-heat release (combustion noise)
- Common fuels (e.g., gasoline and diesel fuel) have different auto-ignition characteristics
  - Diesel fuel is easy to ignite (high reactivity) – good for low load/low temp.
  - Gasoline is difficult to ignite (low reactivity) – good for high load/high temp
- This work proposes in-cylinder fuel blending of two fuels with different auto-ignition characteristics to simultaneously control combustion phasing and rate-of-heat release
- Alternative combustion mode controlled by fuel reactivity → **Reactivity Controlled Compression Ignition (RCCI) combustion**

Fuel Delivery Strategy

High Reactivity Fuel (Diesel fuel, bio-diesel, DME, etc..)

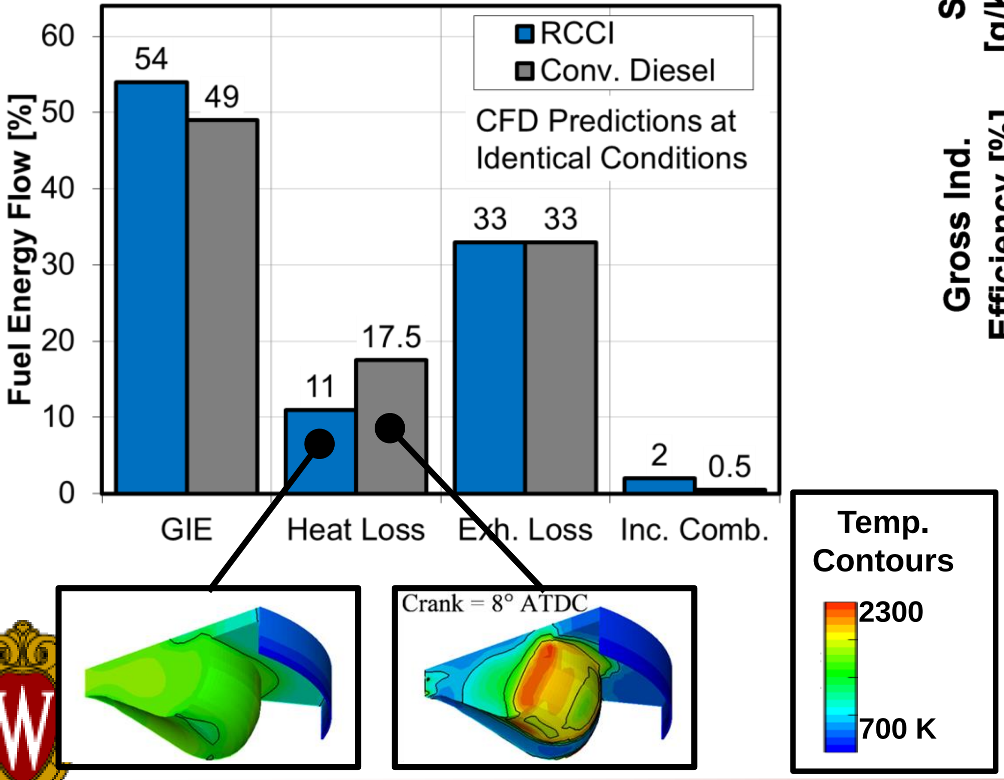


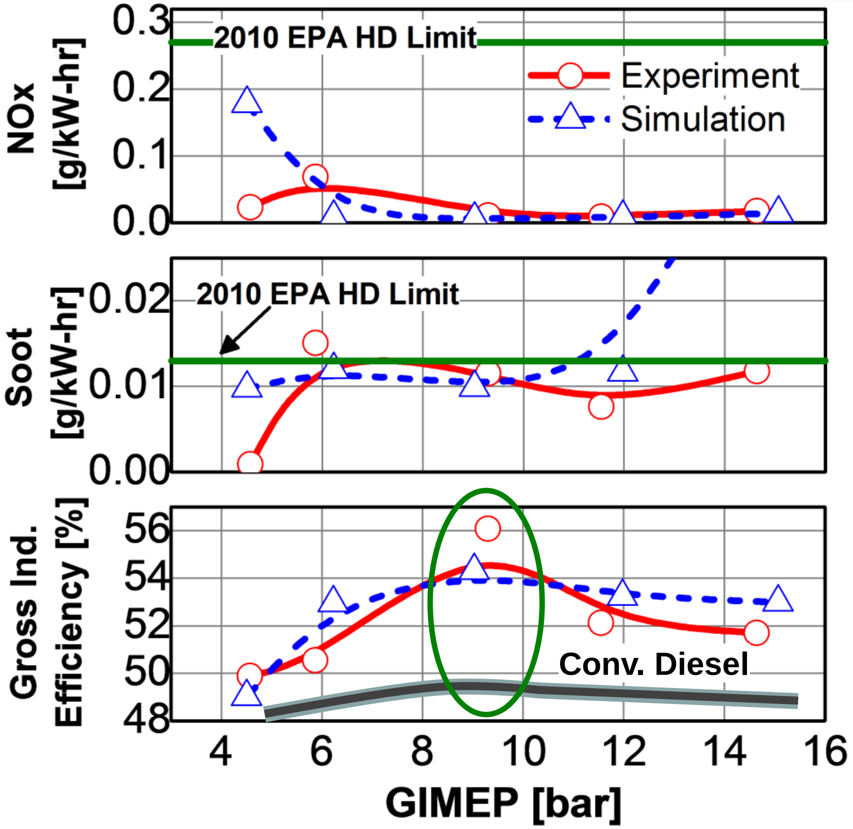
Low Reactivity Fuel (Gasoline, ethanol, natural gas etc…)

Demonstration of RCCI Performance

Kokjohn et al. IJER 2011
Hanson et al. SAE 2010-01-0864

- Heavy-duty RCCI has demonstrated near zero NOx and soot and a **peak gross indicated efficiency of 56%**
- Conventional diesel shows 49% GIE at identical conditions with an order of magnitude higher NOx and soot

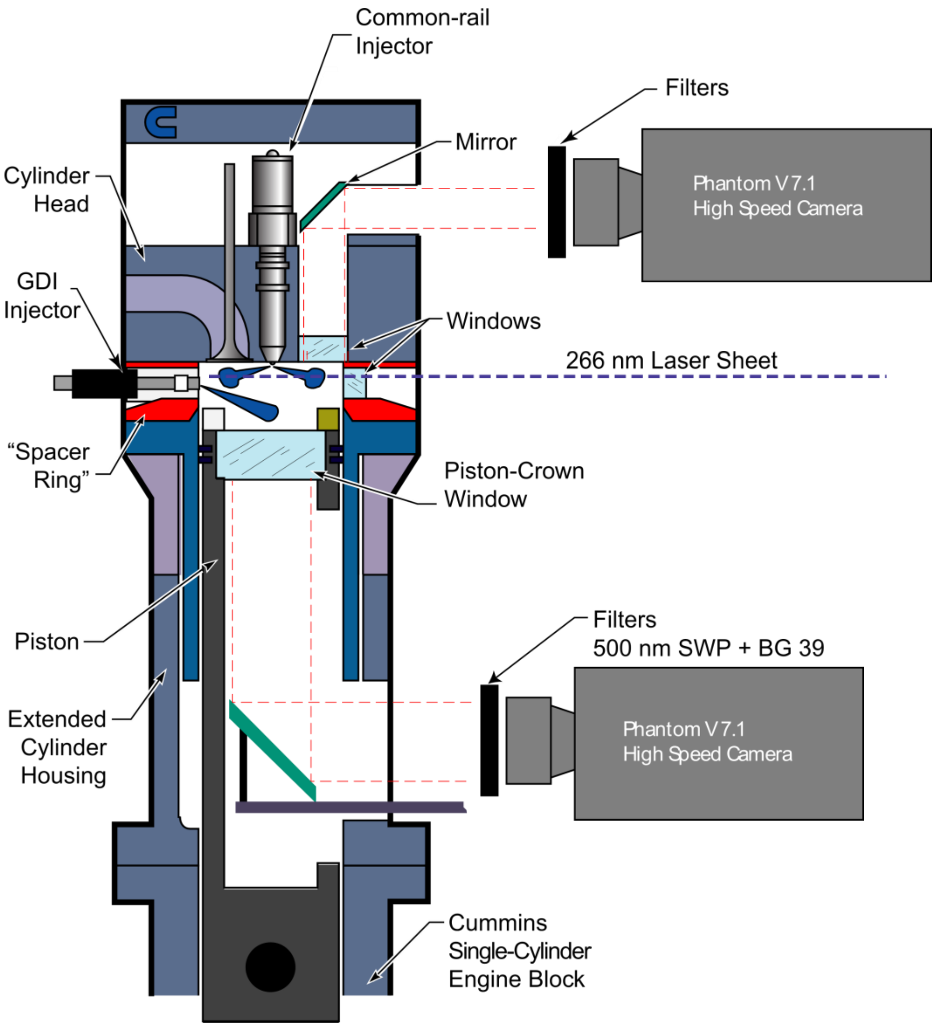




- GIE improvement is primarily explained by reduced heat transfer
  - Lower temperatures by avoiding near stoichiometric regions
  - High temperature regions are away from surfaces

What are the dominant mechanisms controlling RCCI combustion?

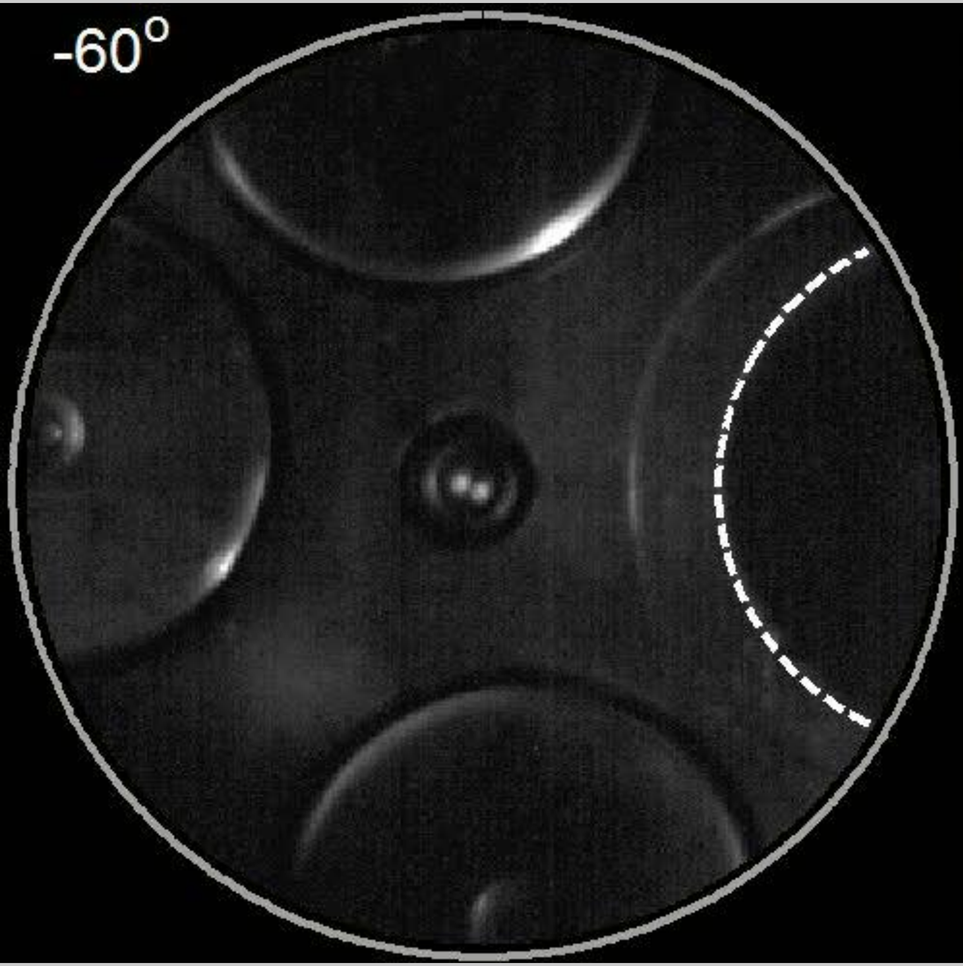
- Answer this question using optical engine experiments.
- Optical engine has several windows allowing imaging of the spray, mixing, and combustion process
- High speed chemiluminescence imaging
  - Evaluate overall reaction zone growth
- Fuel tracer fluorescence imaging
  - Relate the fuel distribution prior to ignition to the reaction zone progression
  - Evaluate heat release rate control using spatial stratification of fuel reactivity



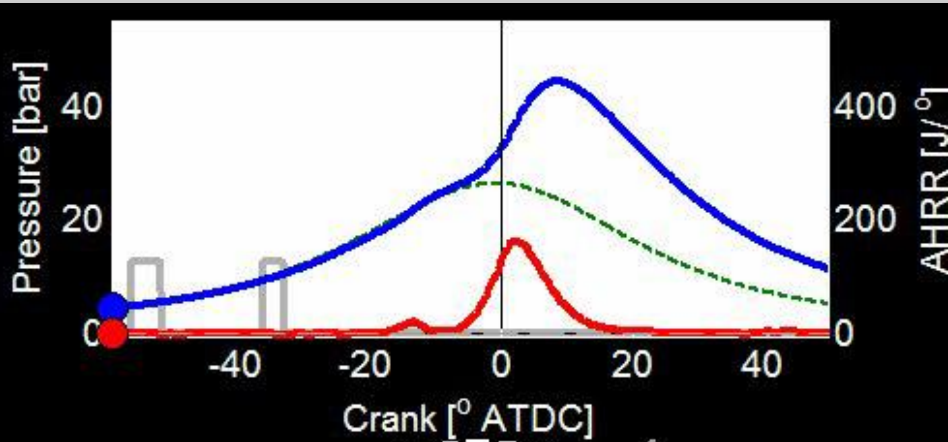
High Speed Combustion Luminosity Imaging

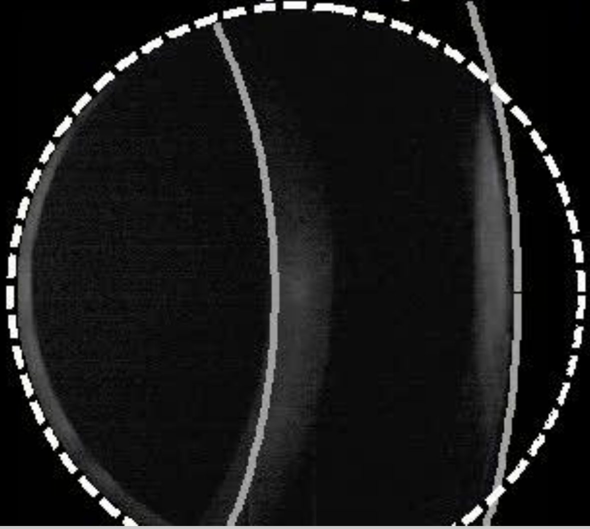
Load: 4.2 bar IMEP
Speed: 1200 rpm
Intake Temperature: 90° C
Intake Pressure: 1.1 bar abs.

GDI SOI: -240°ATDC
n-heptane SOI: -57°/-37° ATDC
Iso-octane mass %: 64
Effective gain: 500



Bowl Window





Cylinder Head Window

Kokjohn et al. ILASS 2011

Toluene Fuel Tracer PLIF

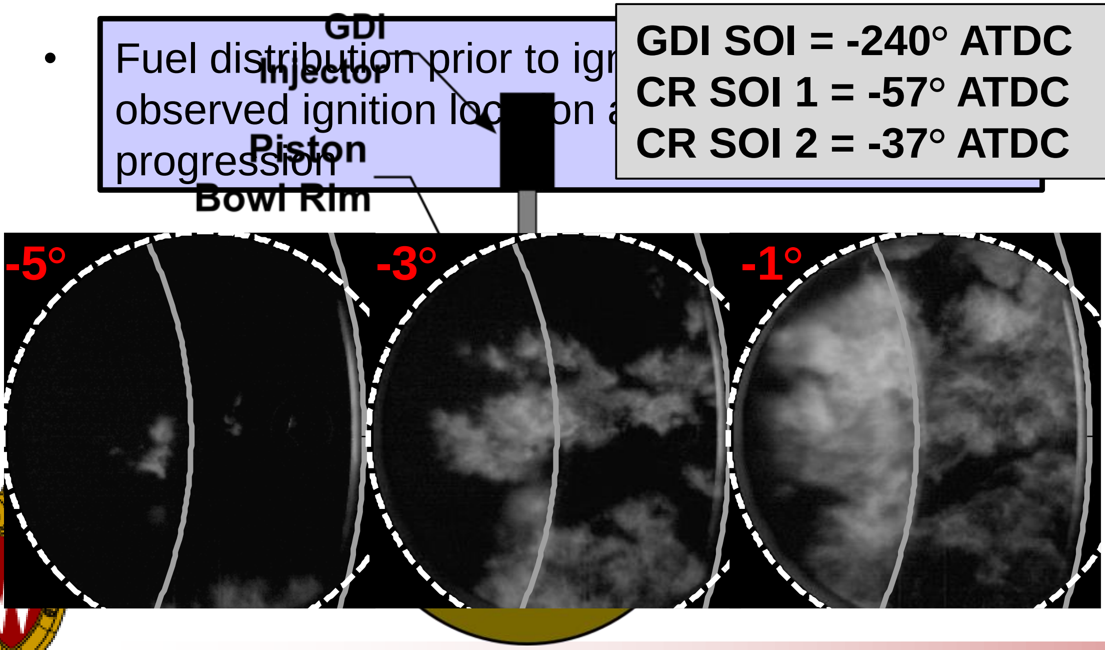
- In-cylinder fuel distribution measurements using fuel tracer fluorescence imaging
- Image shortly before low-temperature heat release shows a stratified local octane # (PRF) distribution resulting from the direct-injection event
- Most reactive region (minimum octane #) is located near the center of the piston bowl rim
- Reactivity decreases (octane # increases) toward the center of the combustion chamber

Diagnostic Overview

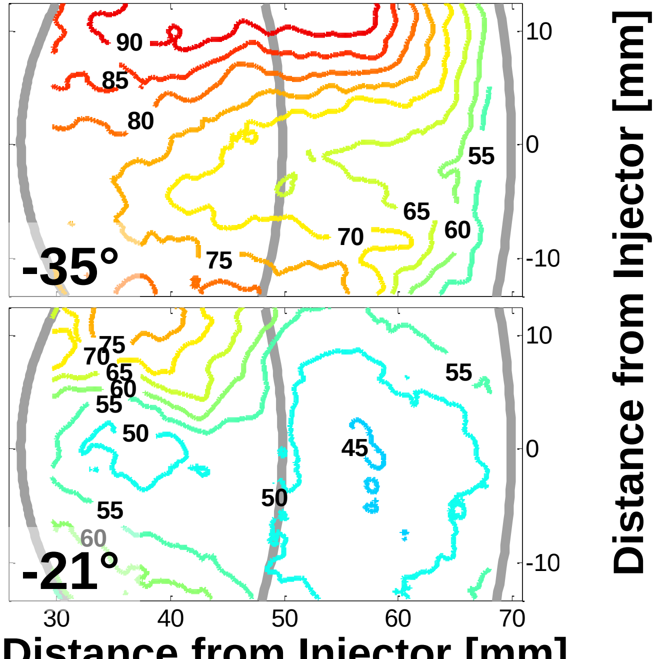
1. Fuels doped with 1% toluene
2. Toluene fluorescence excited by 266 nm (UV) laser sheet
3. Fluorescence images processed to show fuel distribution

- Fuel distribution prior to igr observed ignition loc on a progression

GDI SOI = -240° ATDC
CR SOI 1 = -57° ATDC
CR SOI 2 = -37° ATDC



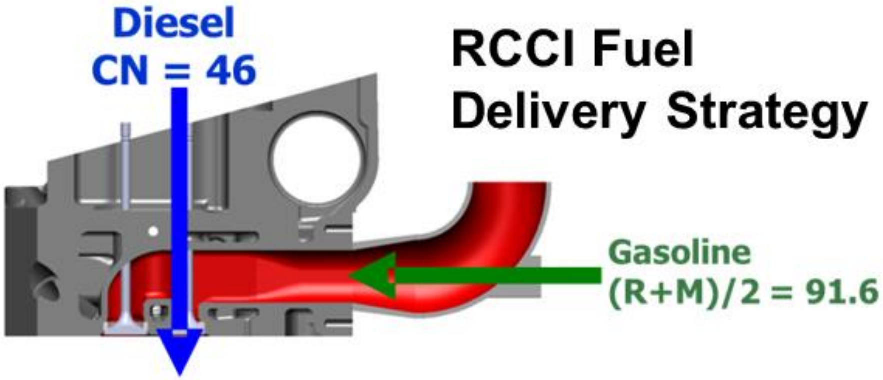
Local Octane # (PRF) Distribution



Kokjohn et al. ILASS 2011

RCCI Combustion Summary

- Combustion phasing is controlled by the overall fuel blend (i.e., ratio of gasoline-to-diesel fuel – or fuel reactivity)

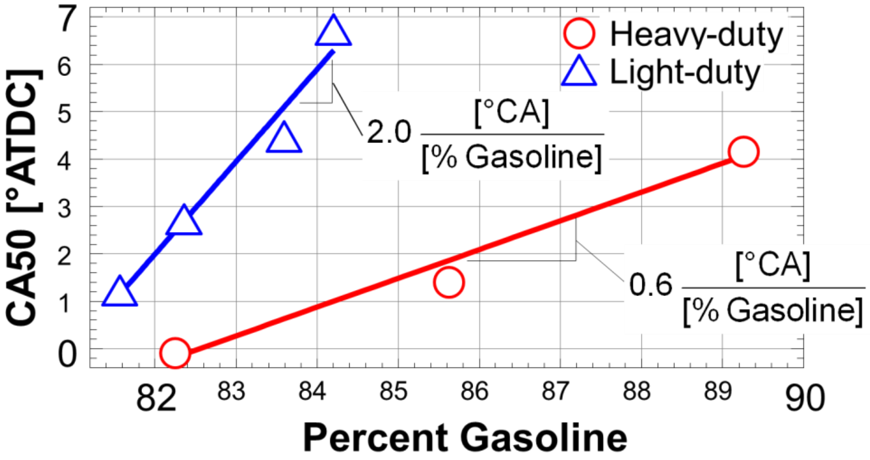


RCCI Fuel Delivery Strategy

- The combustion duration is controlled by spatial stratification in the fuel reactivity

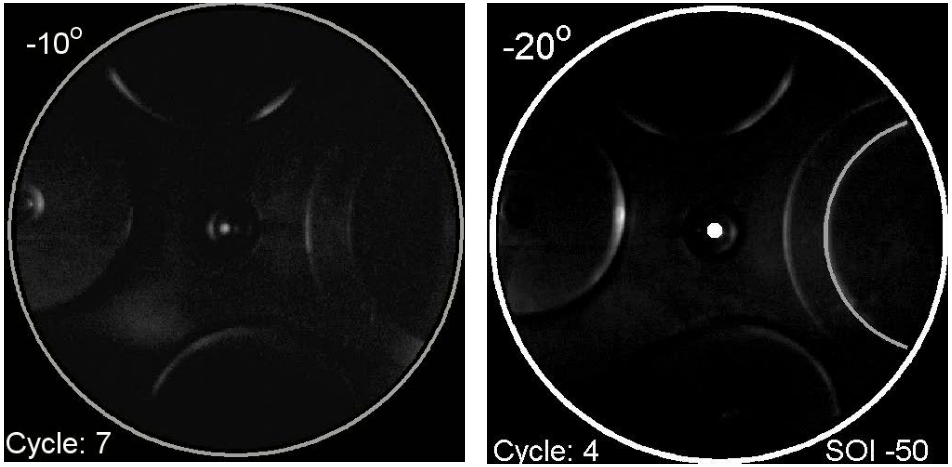
- **RCCI combustion address the two primary issues of PCI combustion**

Kokjohn et al. SAE 2011-01-0357



Uniform Reactivity

Stratified Reactivity

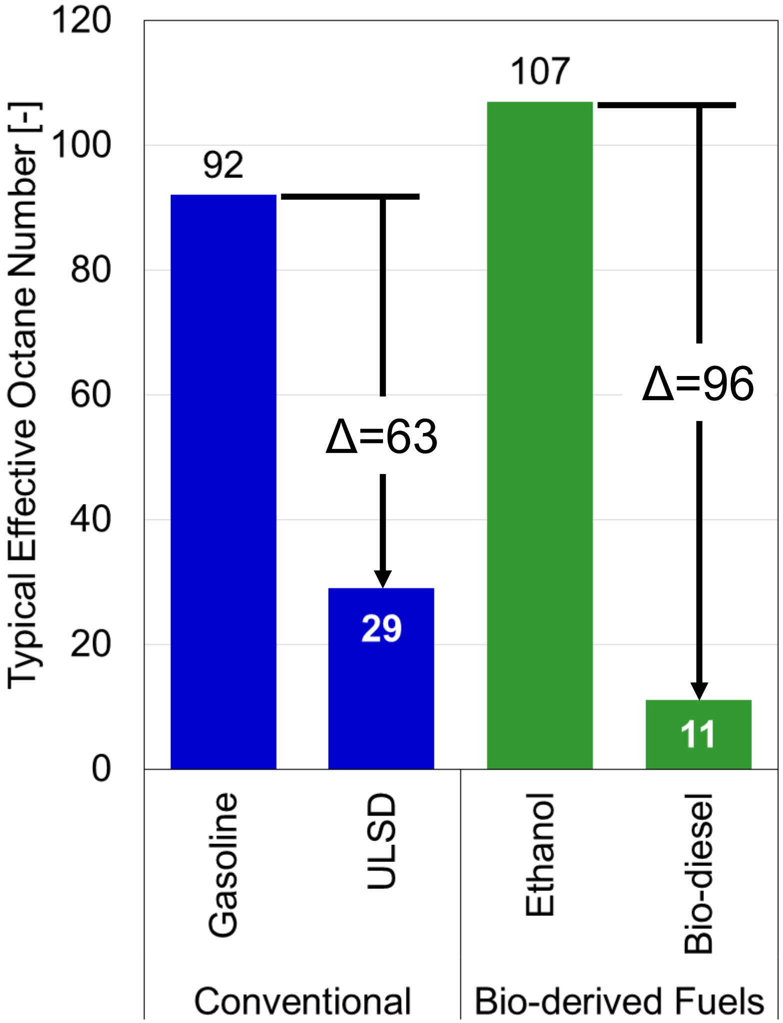


Kokjohn et al. SAE Int. J. of Engines 2012

Can bio-derived fuels be used for RCCI?

- RCCI depends on auto-ignition characteristics of the charge → controlled by in-cylinder blending
- RCCI is inherently fuel flexible (with two fuels with different auto-ignition characteristics)

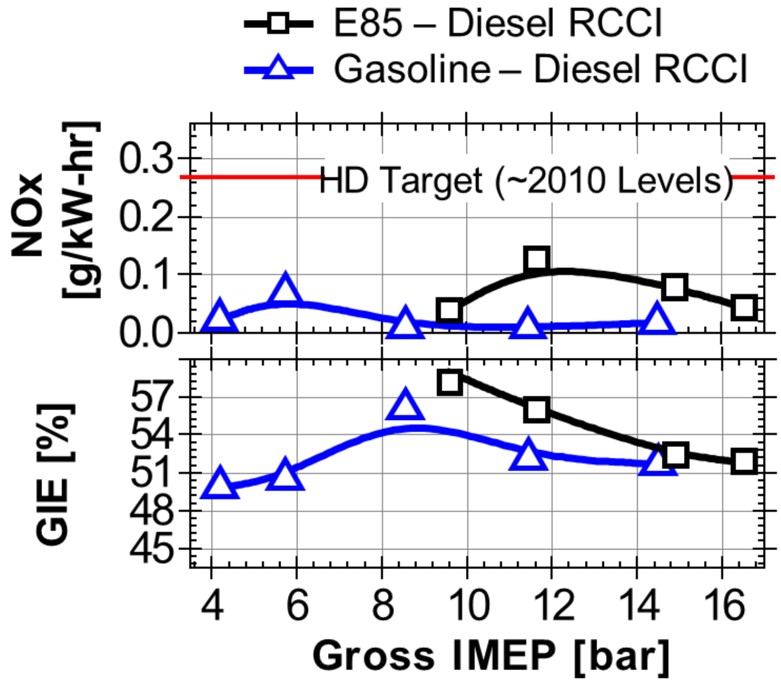
- Example, ethanol is less reactive than gasoline and bio-diesel is (typically) more reactive than diesel fuel → larger differences in auto-ignition characteristics → great fuels for RCCI combustion!

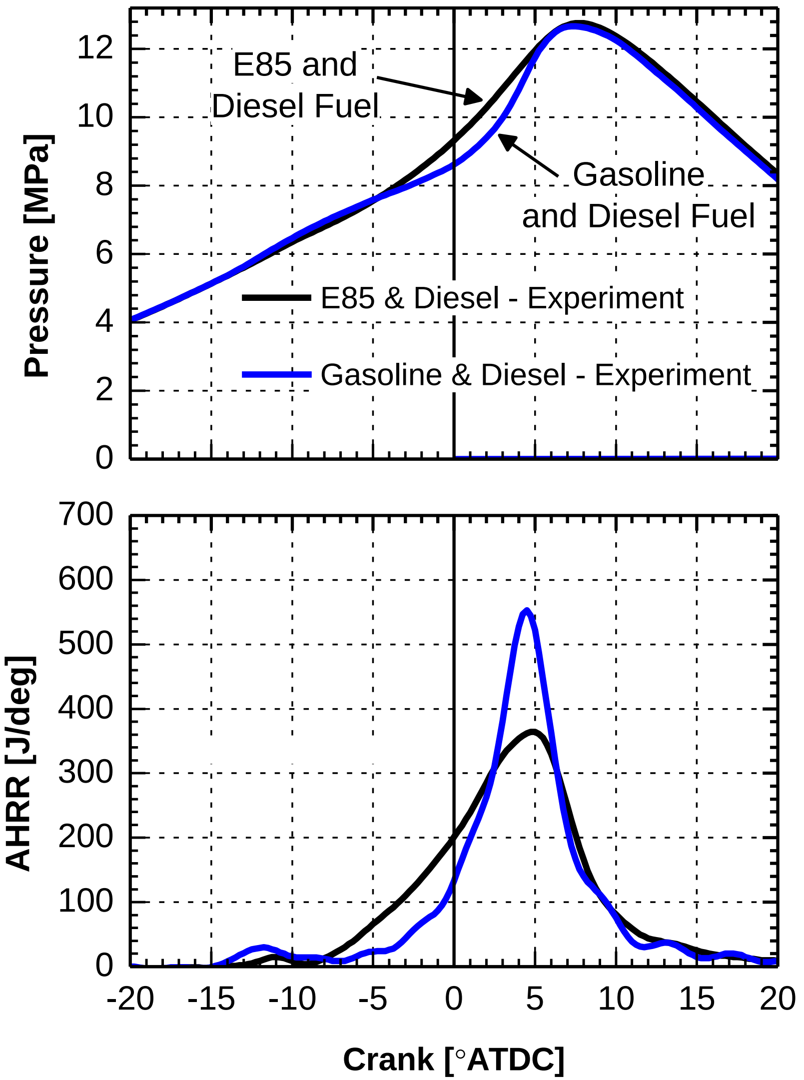


Can bio-derived fuels be used for RCCI?

Splitter et al., SAE 2011-01-0363

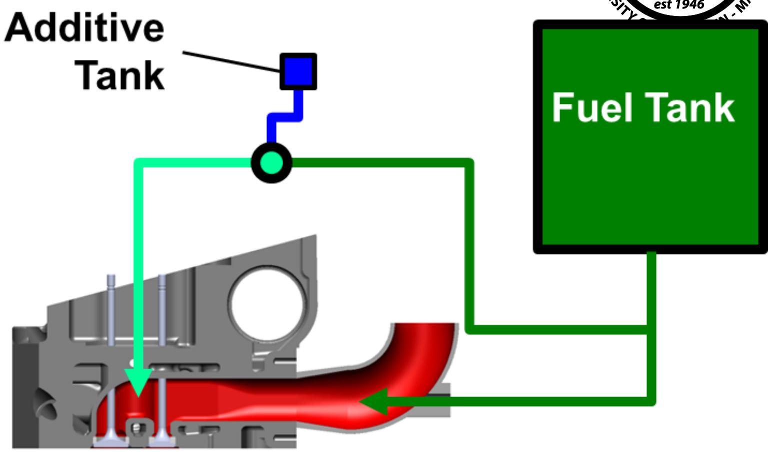
- Gasoline-diesel RCCI is compared to E85-diesel RCCI combustion
- E85-diesel DF RCCI exhibits significantly reduced HRR compared to gasoline-diesel RCCI → quieter operation and extended load range
- Both show near zero levels of NOx and GIE significantly above state of the art diesel engines (diesel GIE ~49% at peak)

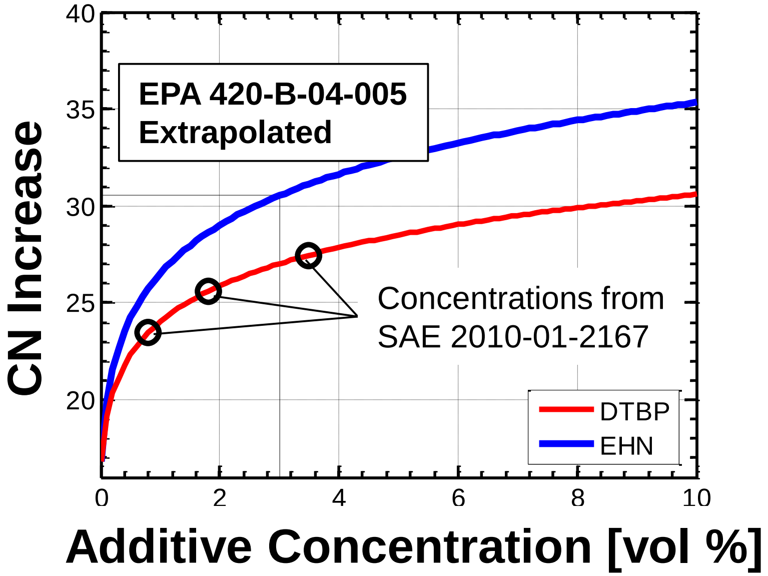




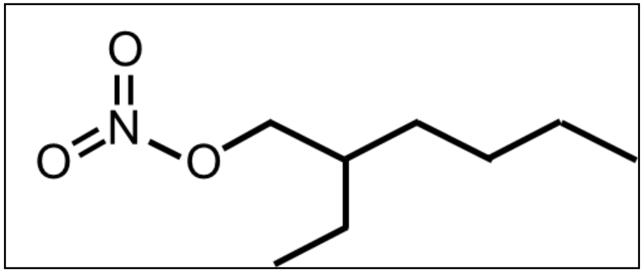
Are two fuels required?

- Dual-fuel RCCI is a promising method to control PCI combustion. Can similar results be achieved with a single fuel and an additive?
- Chemicals exist to increase the cetane number (CN) of commercial fuels
- Approach: Use a single fuel + a small amount of a cetane improver to achieve RCCI combustion



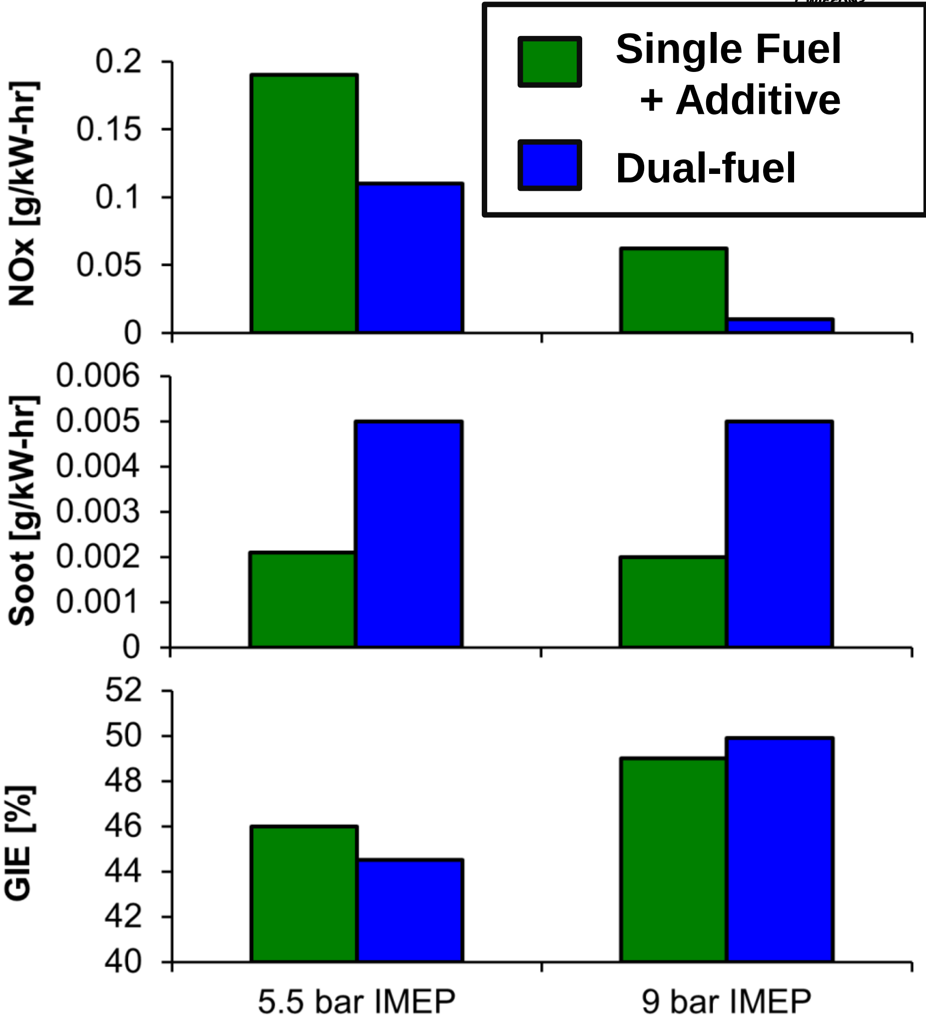


- 2-Ethylhexyl Nitrate (EHN) is a common cetane improver used to condition diesel fuel → focus of this investigation



Performance of E10 and E10+EHN RCCI

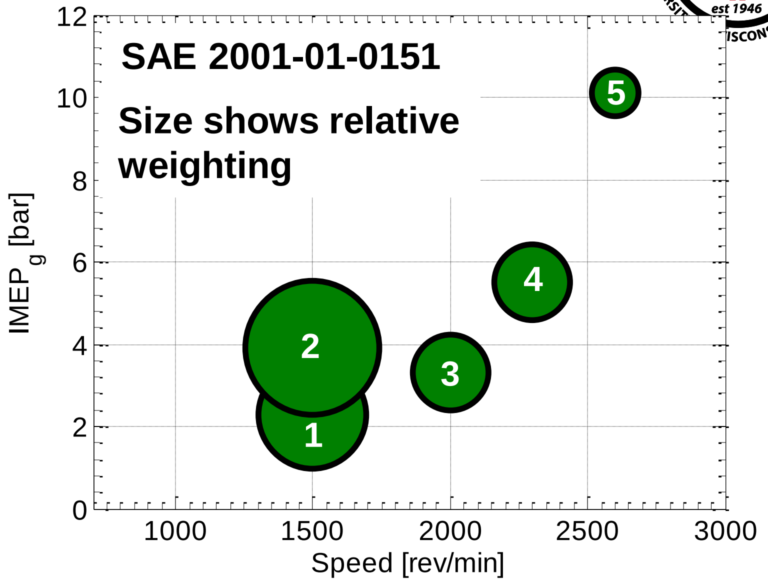
- Parametric studies were performed to optimize the efficiency of single-fuel RCCI at 5.5 and 9 bar IMEP
- Performance characteristics of single-fuel + additive RCCI are similar to those of dual-fuel RCCI
  - Peak efficiency data for E10/E10+EHN shows higher, but acceptable NOx emissions → due to fuel bound NOx
  - Soot is very low for all cases
  - GIE is similar for single fuel + additive and true dual-fuel modes



Kaddatz SAE 2012-01-1110

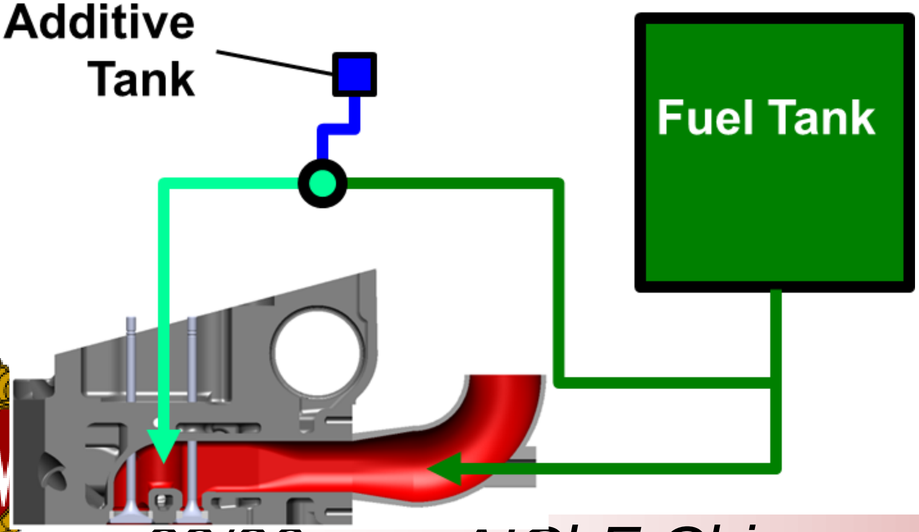
Additive Consumption Estimate

- Light-duty drive cycle average is 55% PFI fuel (i.e., 45% additized fuel) [Kokjohn IJER 2013]
- 3% additive level → EHN volume is ~1.4% of the total fuel volume
  - Similar to DEF levels
- Assuming 50 mpg and 10,000 mile oil change intervals, additive tank must be ~2.7 gallons



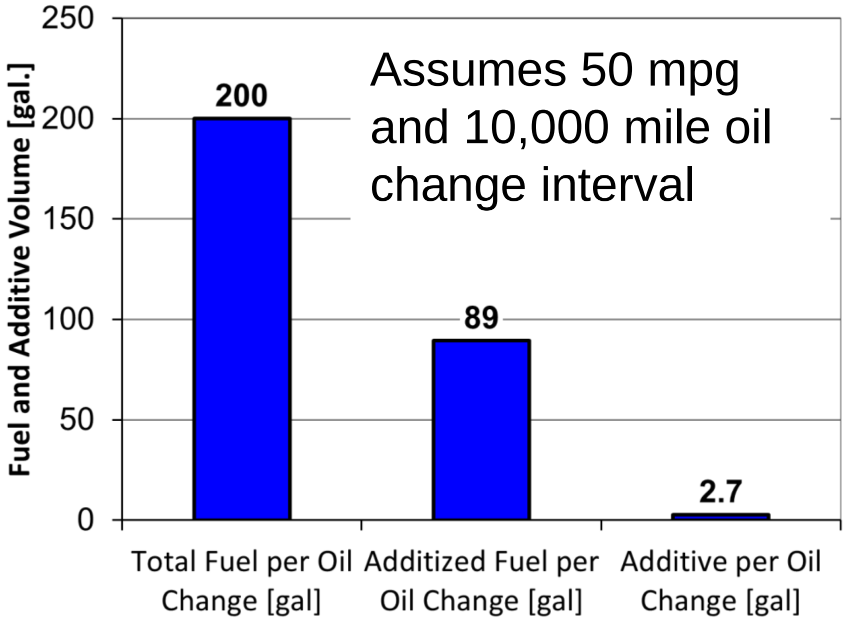
SAE 2001-01-0151

Size shows relative weighting



Additive Tank

Fuel Tank

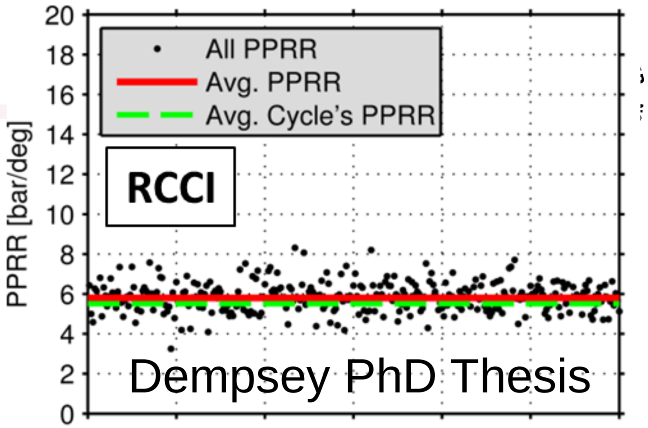


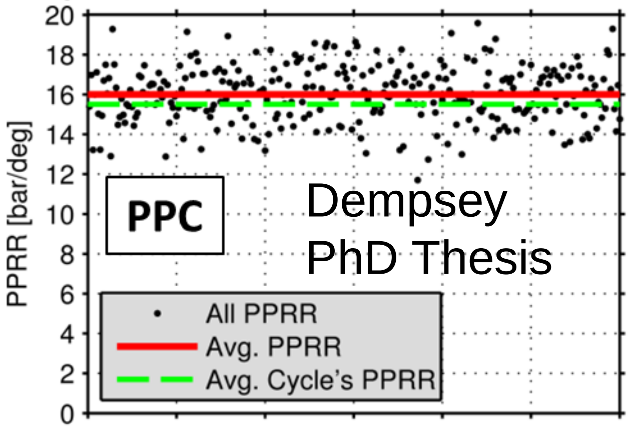
Assumes 50 mpg and 10,000 mile oil change interval

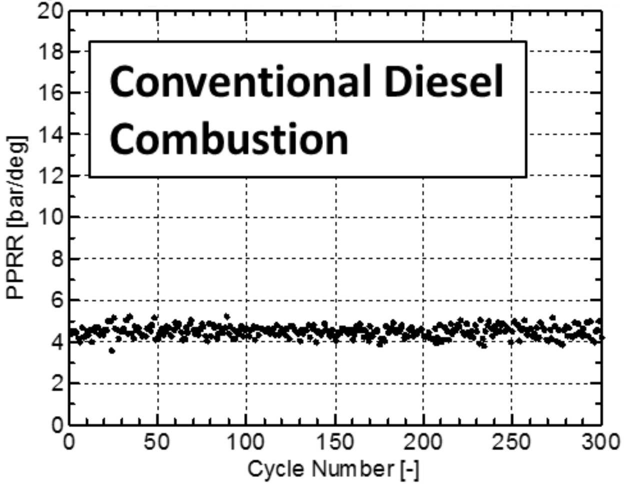
What’s Next?

- RCCI is a promising technique to control the average combustion phasing and duration → the next challenge comes in controlling cycle-to-cycle variations
- All advanced combustion modes are sensitive to charge conditions and show significant cycle-to-cycle fluctuations

- Fundamental work is focused on the mechanisms controlling the cycle-to-cycle variability
- Applied work is focused on identifying injection and combustion strategies to minimize instability







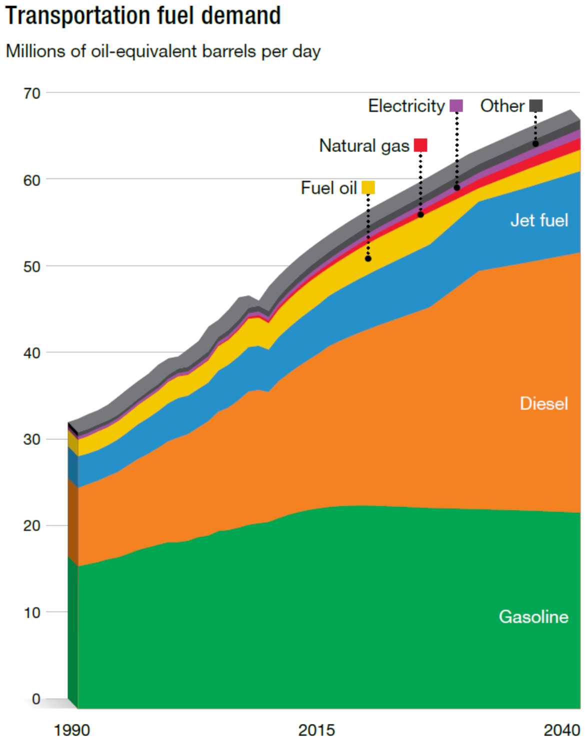
What's Next?

- Fuels will continue to be of interest
- Projections show diverging transportation fuel demand → diesel usage increases while light fuels (e.g., gasoline) remains flat
  - Largest growth is driven by mid-range and heavy-duty application in emerging markets
- There is a need to develop combustion modes to utilize light-fuels and natural gas in mid-range and heavy-duty applications
  - RCCI is a start, but single fuel techniques are also of interest

Development of future engines requires

1) improvements in the understanding of combustion physics

2) implementation of this knowledge into engineering design tools (improved analysis)



ExxonMobil: The Outlook for Energy: A View to 2040

Conclusions

- A dual-fuel PCI concept is proposed using in-cylinder blending of two fuels with different auto-ignition characteristics
- Controlled PCI operation demonstrated with very high efficiency and near zero NOx and soot emissions over a range of loads
- New combustion concept addresses the two primary issues limiting acceptance of PCI combustion
  - Combustion phasing is easily controlled by adjusting the overall fuel reactivity (e.g., gasoline-to-diesel ratio)
  - Combustion duration is controlled by introducing spatial stratification into the auto-ignition characteristics of the charge
- RCCI combustion is inherently fuel flexible and well-suited for use with bio-derived fuels → engine adapts to fuel ignition characteristics on-the-fly to maintain peak efficiency
- Single-fuel + additive operation can achieve similar performance to a dual-fuel strategy with an additive tank that needs to be filled at oil change intervals.

Questions???

Contact Info

Sage Kokjohn
kokjohn@wisc.edu
(608) 263-1610

More Information

- "Engine Combustion Control via Fuel Reactivity Stratification" - P100054US01, Nov. 2013
- Kokjohn et al. IJER 2011
- Kokjohn et al. IJER 2013