The Importance of Intermediate-Temperature Reactions in HCCI and HCCI-like Engines

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Sponsors:

U.S. DOE, Office of Vehicle Technologies
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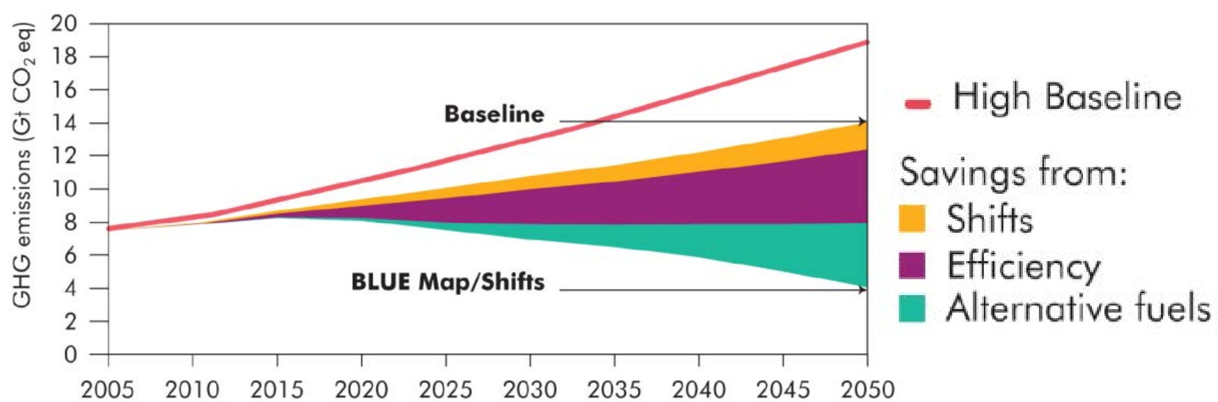
Motivation

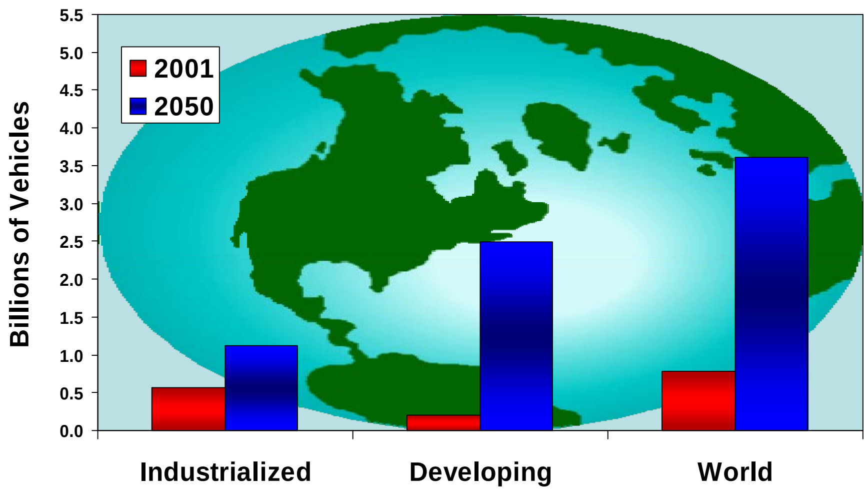
- Global demand for transportation fuels is increasing rapidly.
  - New discoveries of petroleum are not keeping pace.
- Global temperatures are rising.
  - CO_2 from transportation is a major contributor to GHG.
- Strong motivation to reduce petroleum consumption.
- Engine-efficiency improvements offer a huge potential !
  - Could be implemented in a relatively short time.
- Advanced biofuels or other renewable fuels ⇒ important part of solution.
  - Substantial discussion is beyond the scope of this presentation.



From: *Transport, Energy and CO_2: Moving Toward Sustainability*, International Energy Agency 2009.

Improving Vehicle-Fleet Efficiency

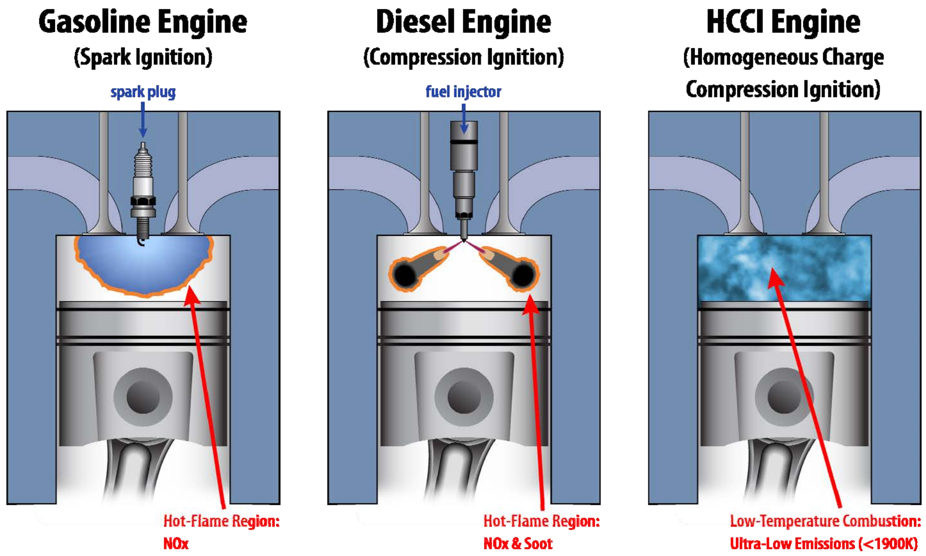
- Diesel engine is the most efficient transportation engine ever developed.
  - Potential fuel savings of ~30% over spark-ignition (SI) engines.
- Drawbacks to diesel engines:
  - Diesel emissions control is challenging ⇒ requires expensive aftertreatment.
  - Cost of a diesel is significantly higher than SI + expensive aftertreatment + demand is driving up fuel costs.
- Looking to the future, the vast majority of new vehicles added will be in the developing world.



- For high-efficiency vehicles to have a large impact, it is important that the technology be economical. ⇒ Particularly for the developing world.
- For full utilization of crude oil stocks ⇒ desirable to have a high-efficiency engine fueled with “light-end” distillates, *e.g.* gasoline.

Advanced High-Efficiency Engines

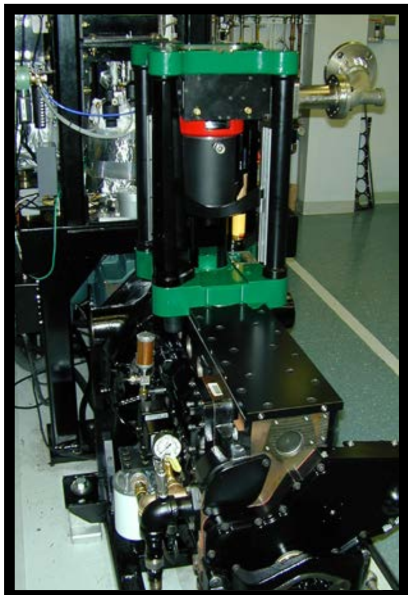
- Advanced engines using HCCI or HCCI-like combustion can provide both diesel-like or higher efficiencies and ultra-low emissions of NO_X and soot.
  - Potential for significantly lower cost than an emissions-compliant diesel.
  - More-volatile, light-end fuels are well suited for HCCI.
  - HCCI can also work well with biofuels and biofuel/gasoline blends.
- HCCI $\Rightarrow$ dilute premixed charge and compression ignition.
  - Volumetric flameless combustion.
  - Never truly homogeneous due to natural thermal stratification (TS).
  - Also advantages to adding limited mixture stratification at some conditions $\Rightarrow$ partial fuel stratification (PFS).
- Challenges for HCCI:
  - **Controlling start of combustion**
  - **Extending operation to higher loads**
- Fuel autoignition chemistry is critical for both.
- Other low-T, HCCI-like concepts also show promise (PCCI or RCCI).



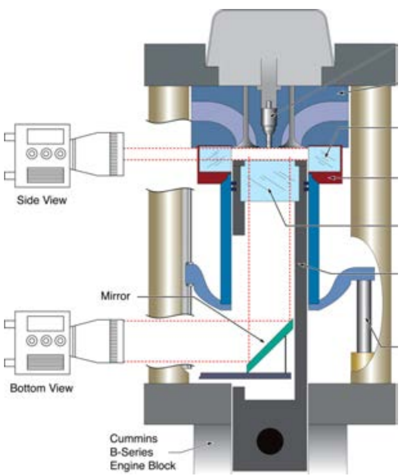
Low-Temperature Combustion Modes

- HCCI is the most fundamental low-temperature combustion process and the first to be widely investigated.
  - High Efficiencies ⇒ Relatively high CR = 12 – 16, no throttle, reduced heat losses due to low burned-gas temperatures, and higher γ (depends on EGR).
  - Ultra-low NOx ⇒ Lean or dilute with EGR so combustion temperatures < 1900 K
  - Ultra-low soot ⇒ Well mixed
- Other low-T combustion modes rely on these same principles.
  - PPC, PPCI or PCCI ⇒ originally developed to achieve HCCI-like combustion in diesel engines. DI fueling ~60° bTDC diesel fuel vap. & "premixed enough."
    - Still widely used with diesel fuel for low emissions at lower load ⇒ in production.
    - Recently adapted to gasoline fueling as in the Lund work ⇒ better for high loads, but difficulties ⇒ e.g. soot, and RON 70 gasoline = new fuel to the marketplace.
  - RCCI ⇒ new concept recently introduced by Reitz et al. ⇒ improves control and shows promise, but requires two fuels.
- HCCI is relatively well developed ⇒ GM has prototype cars operating in HCCI mode from idle → 70 mph, using regular pump gasoline (87 octane).
  - Controls ⇒ cam phasers, GDI fueling & Spark-Assist (SACI), significant strides.
  - Combustion efficiencies > 96%, typically 98 – 99% for higher loads.
- Active research on these low-T modes & autoig. chemistry important for all.

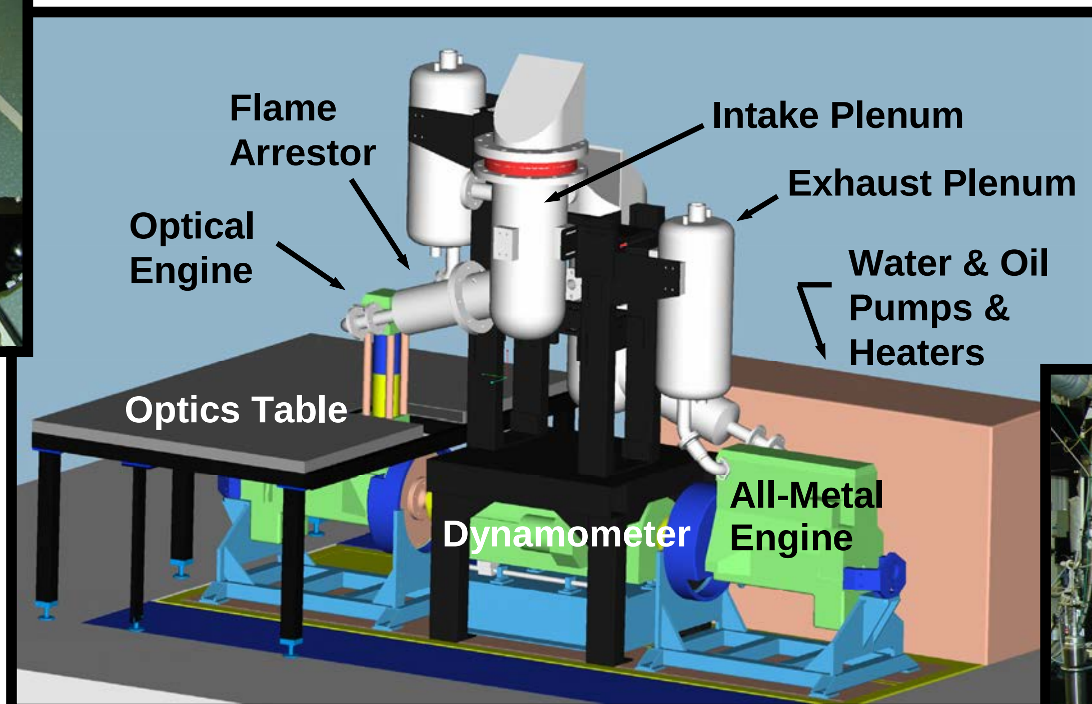
Sandia Dual-Engine HCCI Engine Laboratory



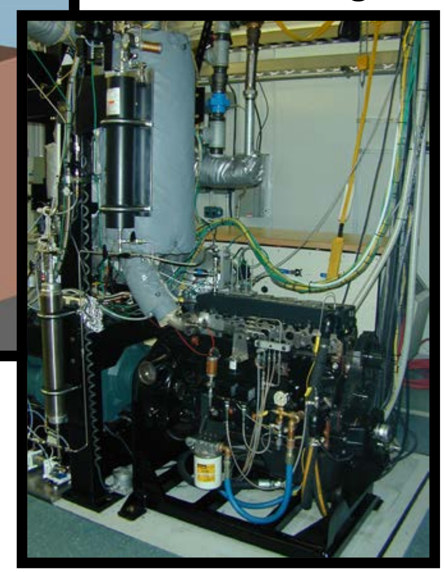
Optical Engine



- Matching all-metal & optical HCCI research engines.
  - Single-cylinder conversion from Cummins B-series diesel.
  - Open combustion chamber.



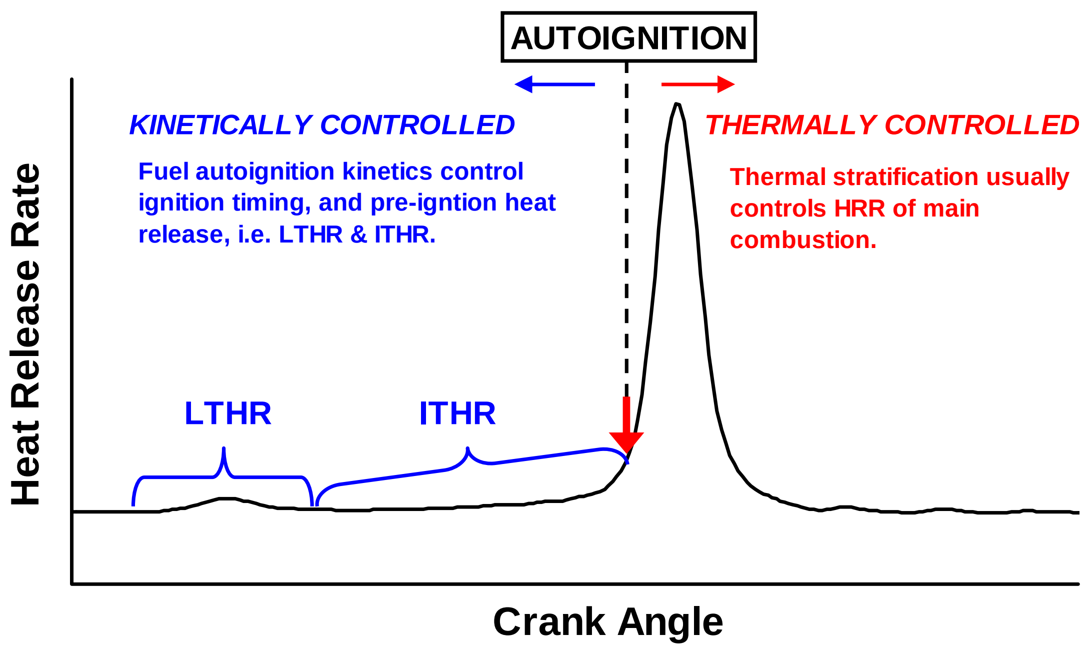
All-Metal Engine



- Bore x Stroke = 102 x 120 mm
- 0.98 liters, **CR=14**
  $P_{TDC\text{-}motored}$ = 30 – 100 bar

Nature of HCCI Combustion

- Ignition timing is mainly controlled by fuel autoignition chemistry.
  - Heat release prior to hot autoignition is kinetically controlled (LTHR, and ITHR).
  - Adjustment of operating parameters required to control ignition timing.
- Main combustion HRR is primarily controlled by thermal stratification.
  - TS occurs naturally due to heat transfer and imperfect mixing with hot residuals.
  - TS causes sequential autoignition & combustion of the in-cylinder charge.
    - > Crucial for controlling HCCI HRR for fully premixed combustion.
  - High-T combustion kinetics are rapid.

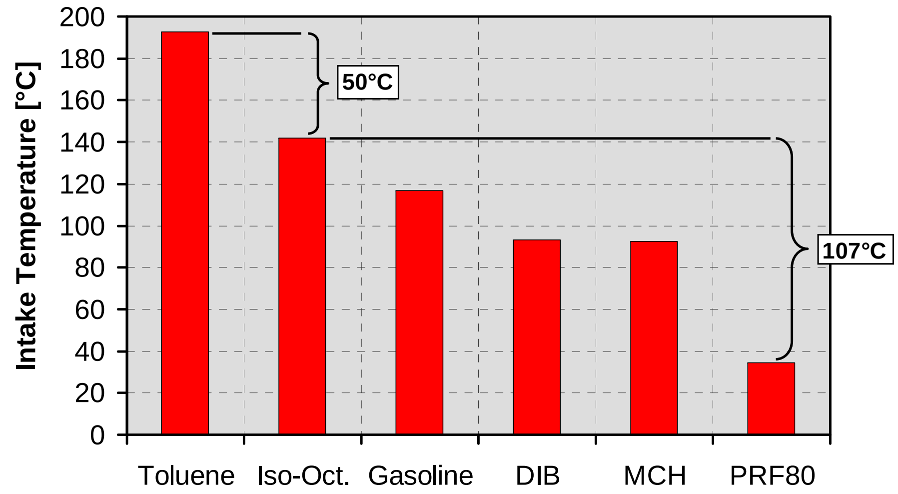


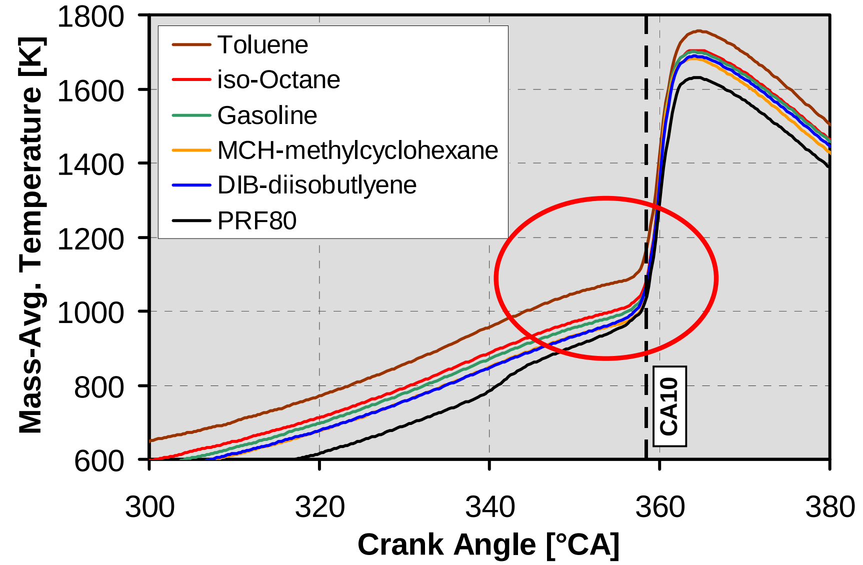
Chemiluminescence of HCCI
(iso-octane, ϕ = 0.24, fully premixed)

Ignition Chemistry Changes with Fuel-Type

- Intake temperature (T_{in}) required for a given combustion phasing varies substantially with fuel type.
  - Representative real-fuel constituents and gasoline.
- Hot-ignition temperature also varies, but proportionally less than T_{in}.
- One main reason is that low-temp. heat release (LTHR, or "cool flame") raises temperature for PRF80.
  - 80% iso-octane + 20% n-heptane
- However, for single-stage ignition fuels, early reactions also important.
  - Raise temperature to thermal runaway (hot-ignition point ≈ CA10).
  - "Intermediate temp. heat release" (ITHR) reactions.

CA50 = TDC, Fully Premixed, 1200 rpm

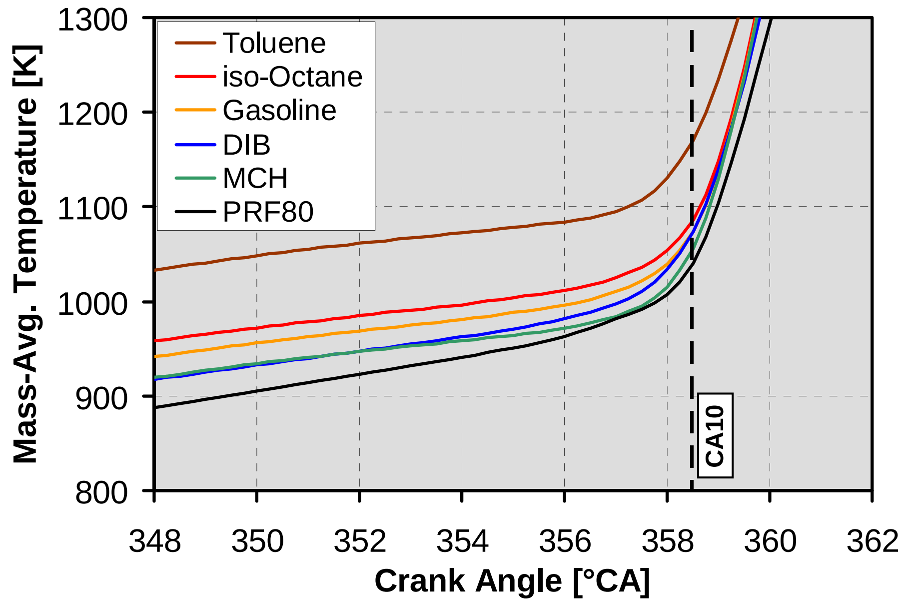




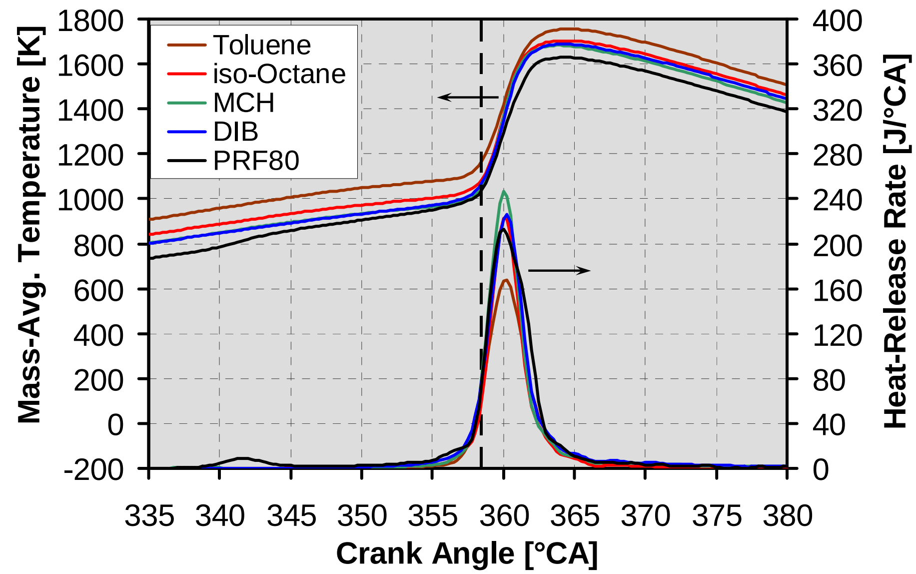
Hwang, Dec & Sjöberg, Combst. & Flame 154(3), 2008

Intermediate Temp. Heat Release (ITHR)

- For all fuels, slower ITHR reactions precede hot ignition (≈ CA10).
  - 900 < T < 1050 K
- For many single-stage fuels, trends are self-similar, $T_{ig.}$ varies with T_{in}.
  - T_{ig} varies significantly with fuel-type.
- However, DIB (diisobutylene) has more intense ITHR reactions.
- Also, for two-stage PRF80, ITHR reactions more intense after LTHR.
  - Note that HRR never goes to zero after LTHR ends.



- Examine the effects of ITHR in more detail for iso-octane (single-stage) and PRF80 (two-stage)



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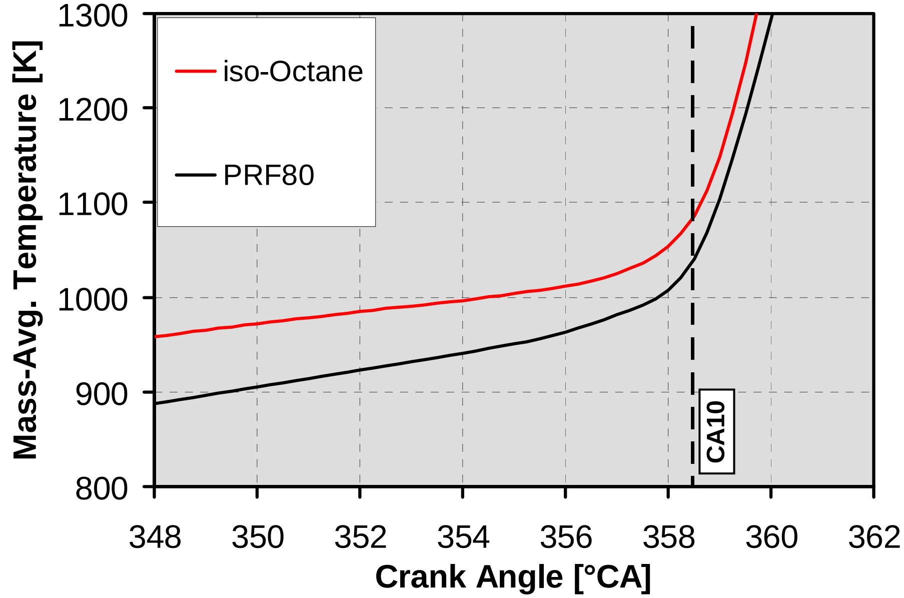
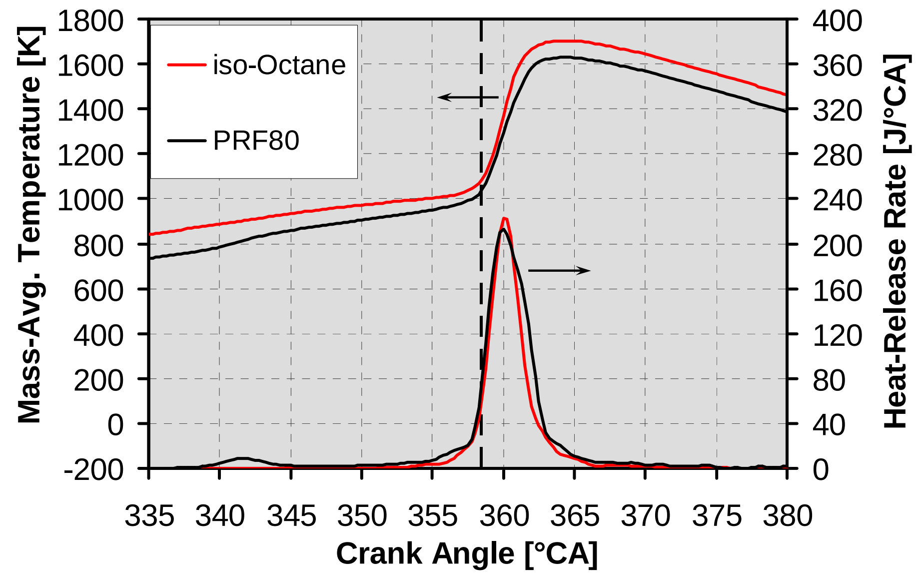


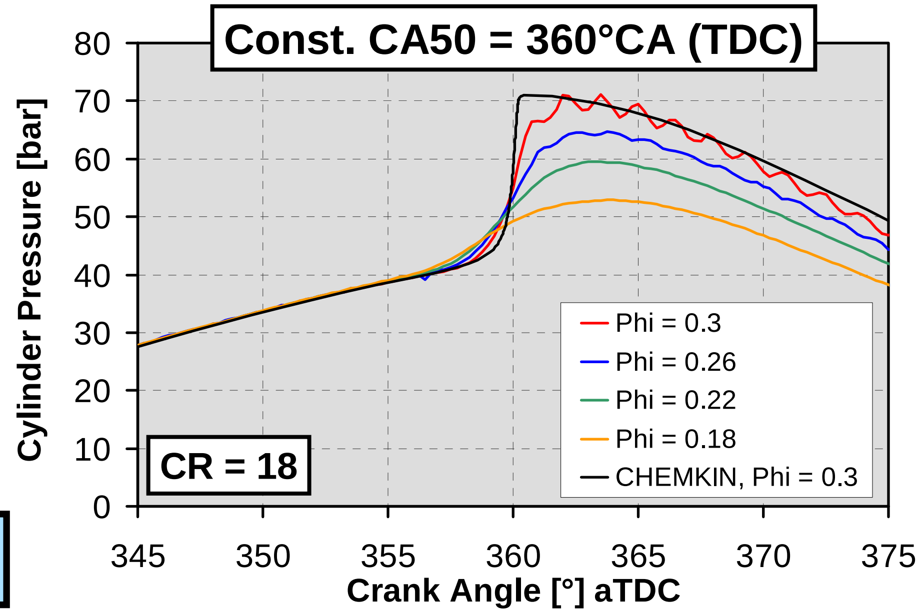


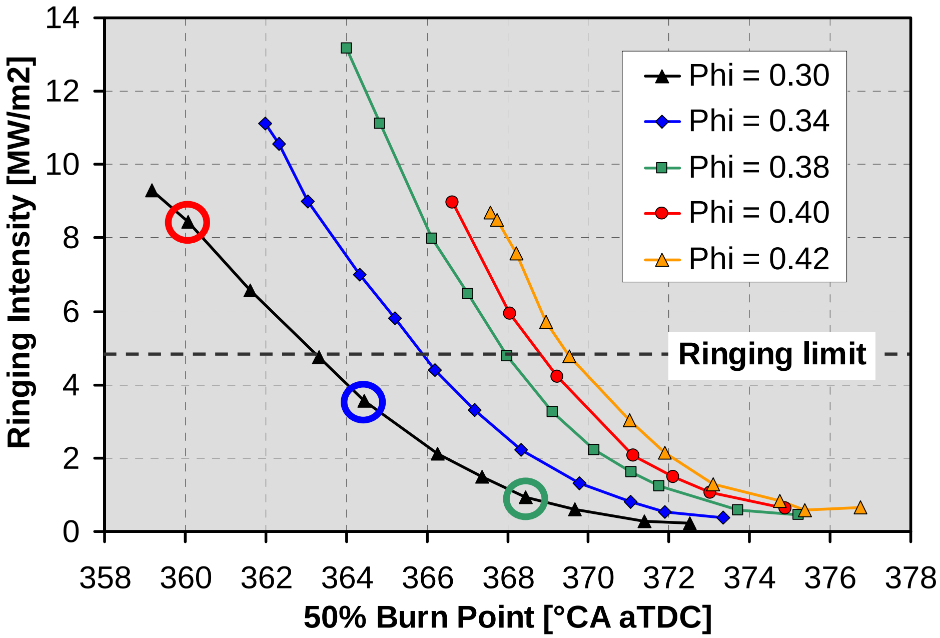
Hwang, Dec & Sjöberg, Combst. & Flame 154(3), 2008

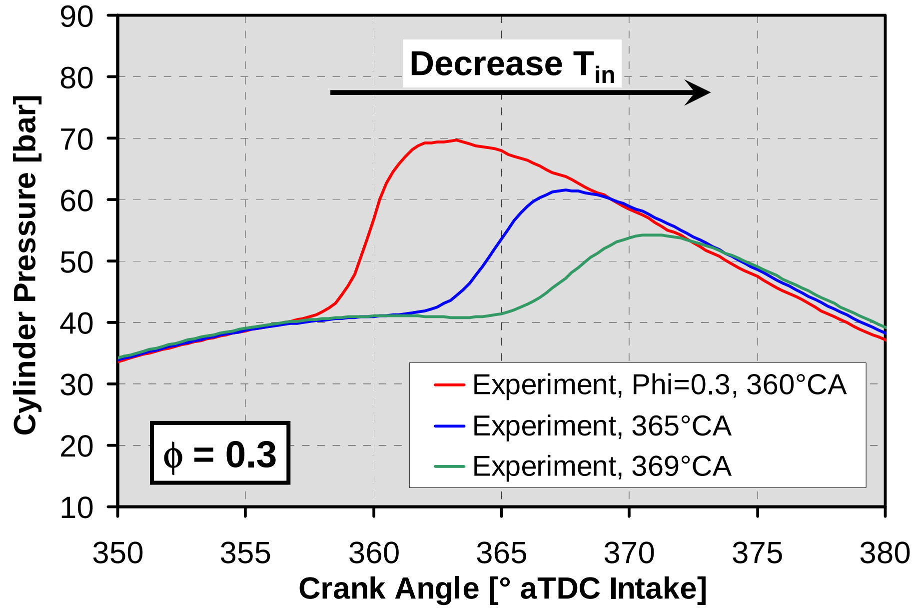
Retarded Combustion Allows Higher Loads

- Nat. TS in the bulk gas significantly slows the combustion rate.
- High-load op. still limited by knock.
- Retarding combustion phasing reduces PRR & ringing intensity.
- Allows higher fueling.

- **Why does timing retard slow PRR?**



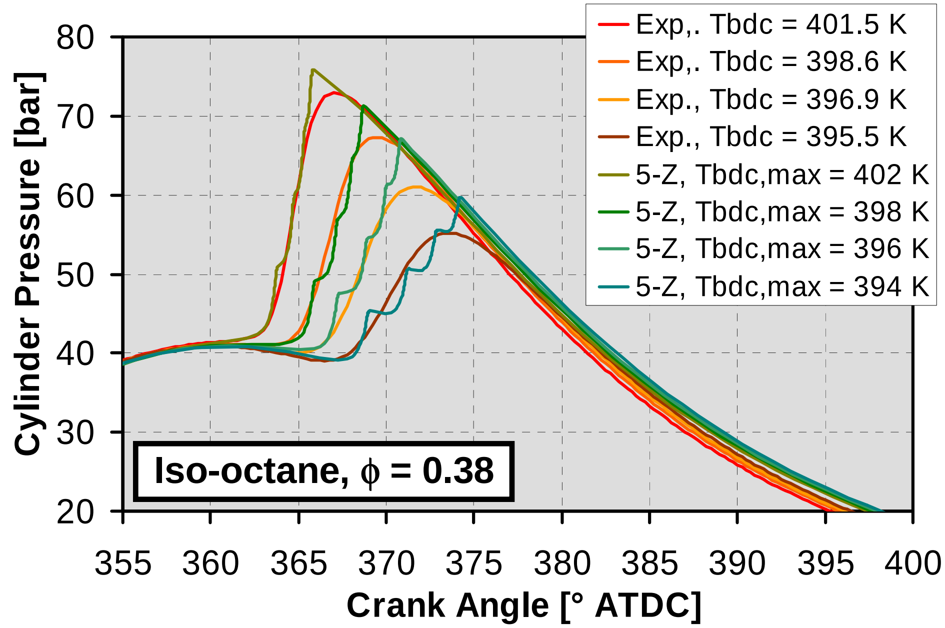


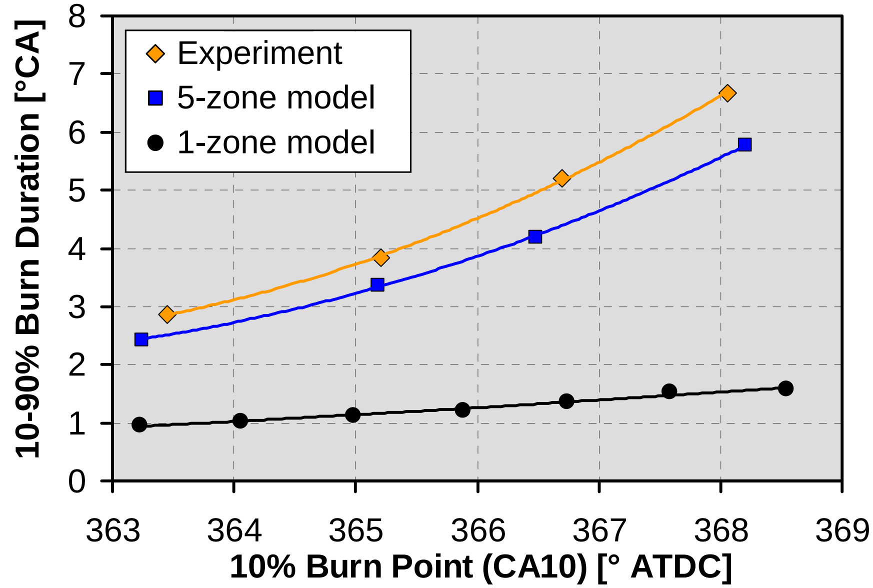


Benefit of CA50 Retard is Related to Thermal Strat.

- Initially thought that colder temperatures slow kinetic rates.
  - Does not explain experimental data.
- Add simulation of TS with multi-zone Senkin.
  - Zones independent except for compression heating.
  - Adjust “thermal-width” to match the experimental maximum PRR.
- Changes in PRR with phasing are reproduced well by model.
  - Greater time delay between sequentially cooler zones.
  - Due to larger combustion-chamber volume and faster expansion rate.

- Retarded timing amplifies the benefit of a given stratification.

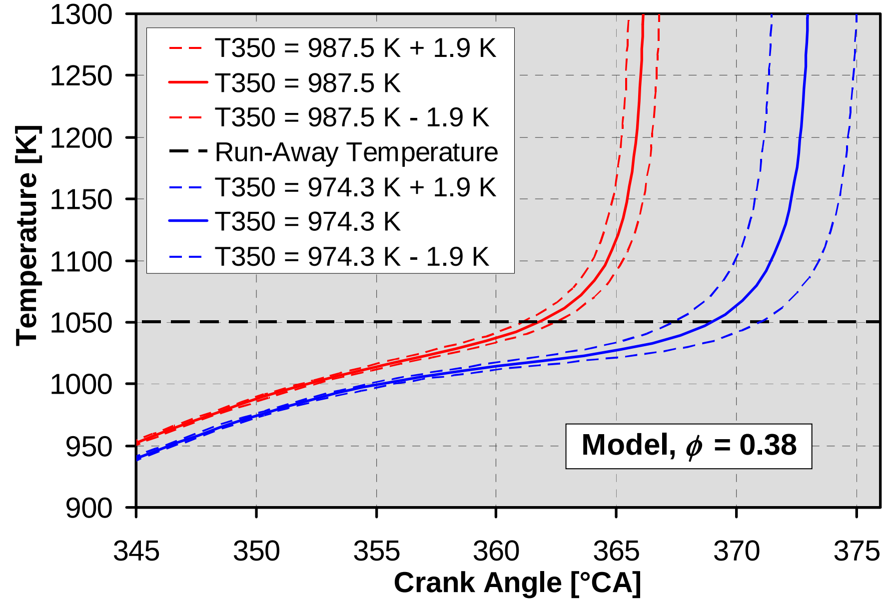


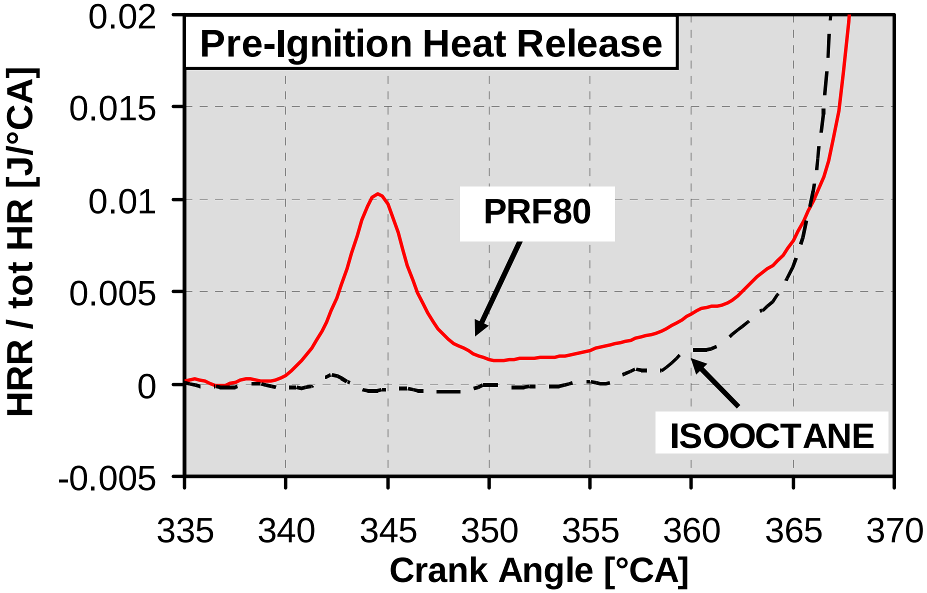


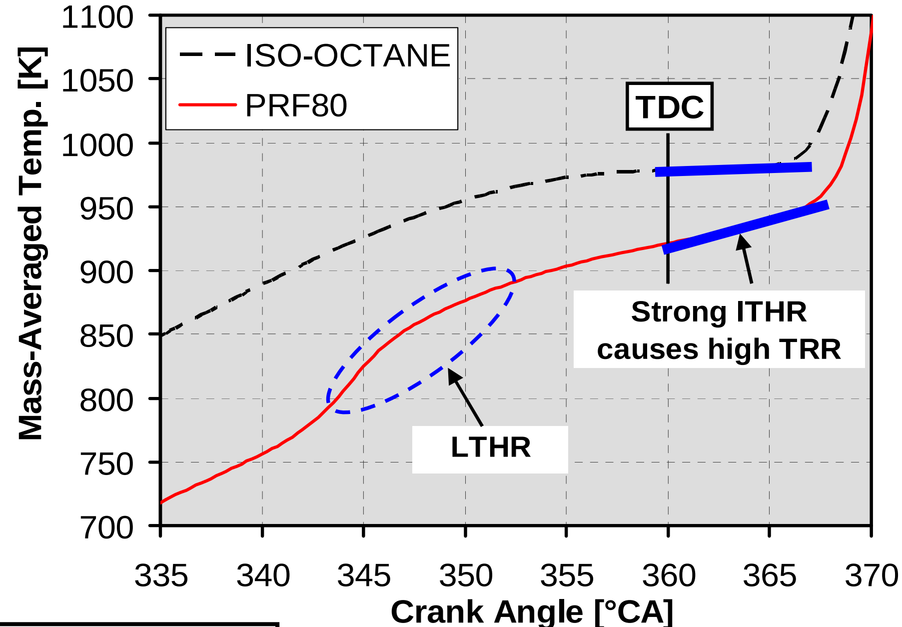
Sjöberg *et al.*, SAE 2005-01-0113

Combustion Retard Relies on ITHR

- Allowable CA50 retard limited by combustion stability.
  - Must maintain positive temperature rise rate (TRR) before hot ignition.
  - Lack of sufficient TRR causes combustion to become unstable and eventually misfire.
- Fuels with stronger ITHR, e.g. PRF80, produce higher TRR.
  - Can sustain more CA50 retard.







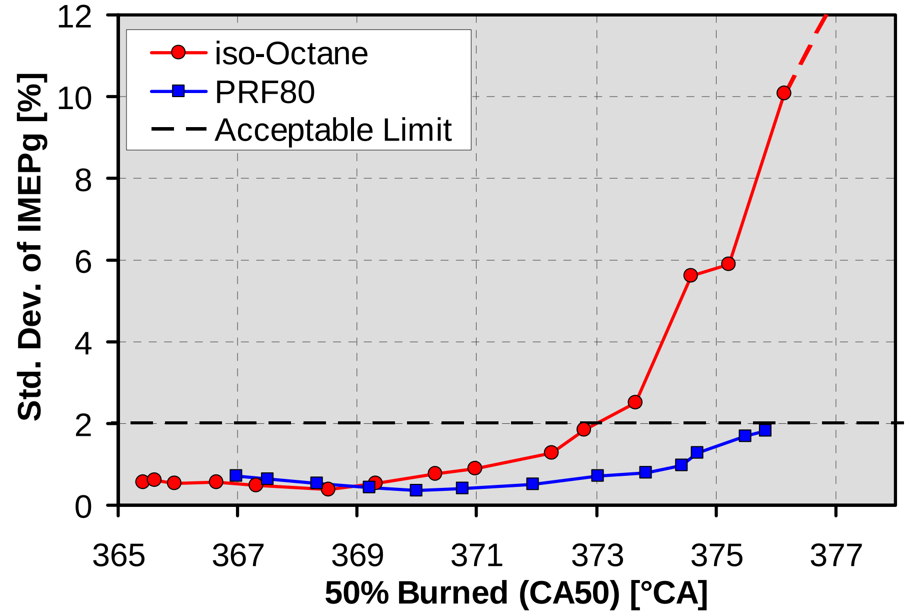
Sjöberg *and Dec*, Proc. Combst. Inst. 2007

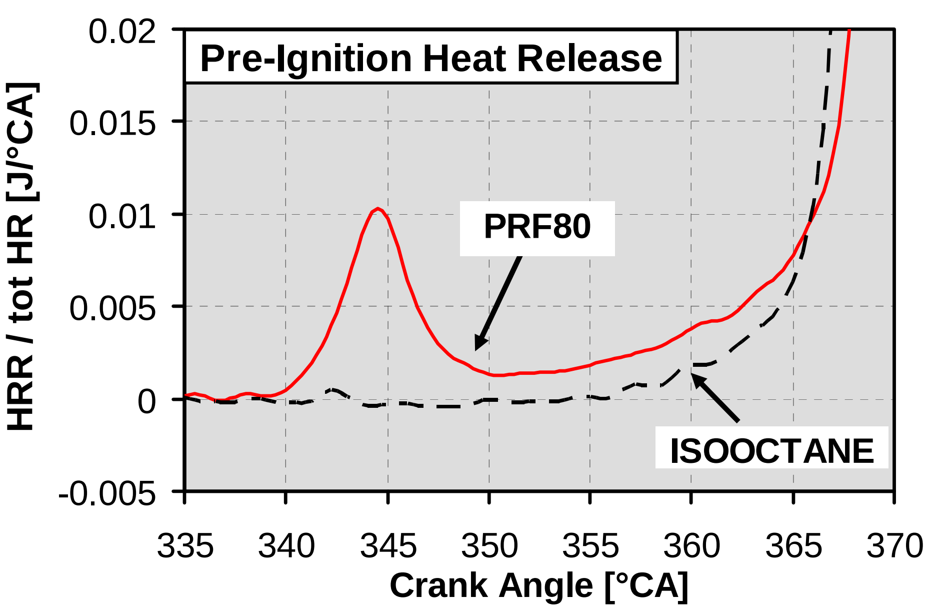
Combustion Retard Relies on ITHR

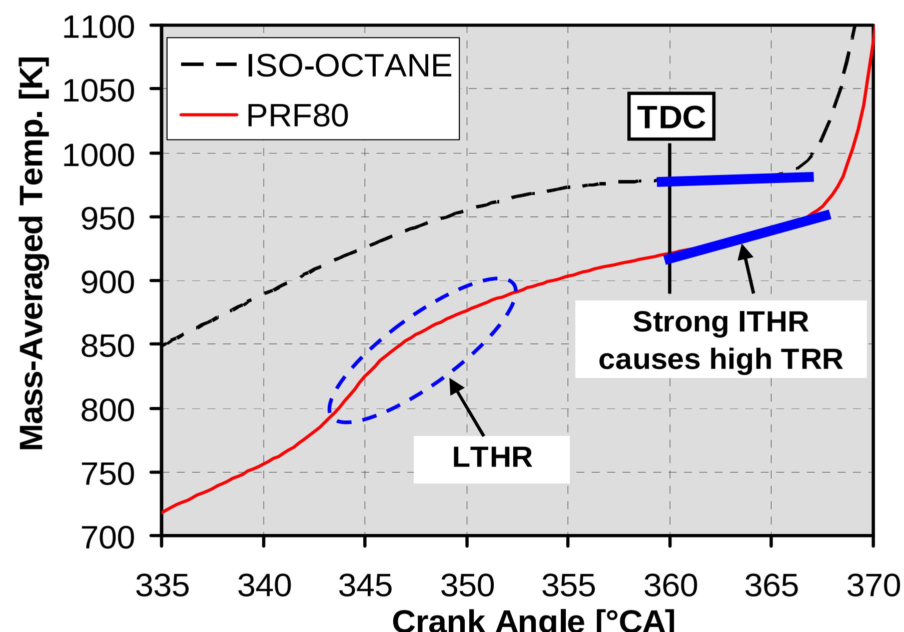
- Allowable CA50 retard limited by

<u>Strong ITHR</u>
⇨ **High TRR**
⇨ **More retarded CA50 with Good Stability**
⇨ **Reduced HRR**
⇨ **Higher loads without knock**

- PRF80, produce higher TRR.
  - Can sustain more CA50 retard.





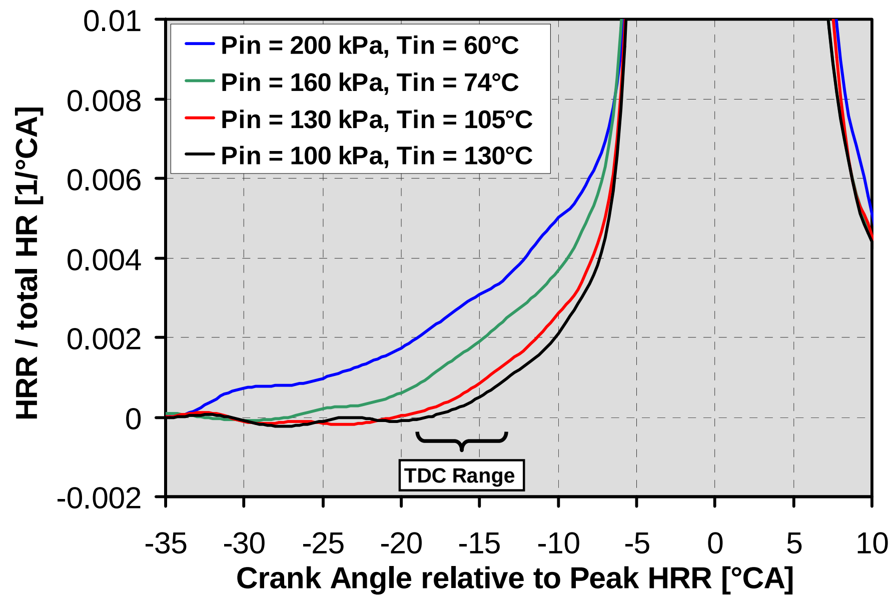


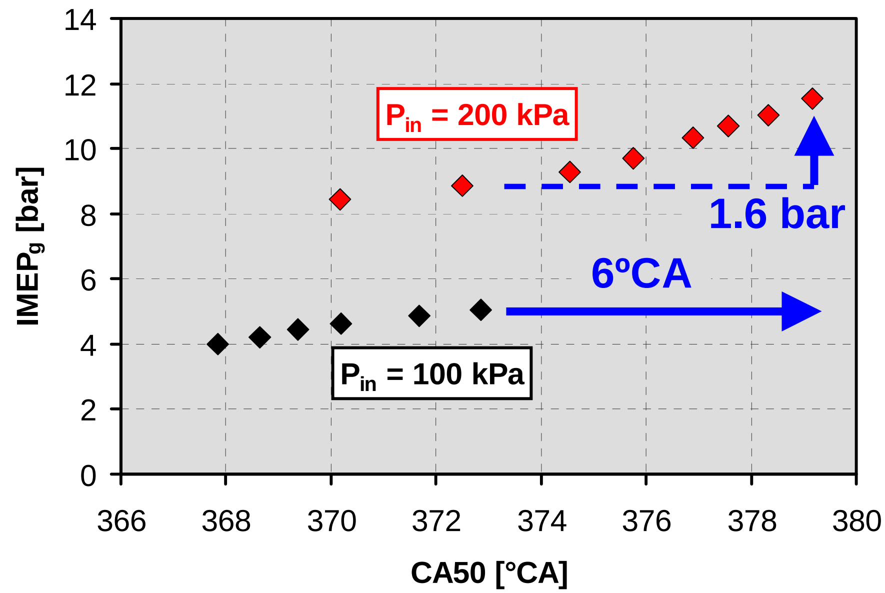
Sjöberg *and Dec*, Proc. Combst. Inst. 2007

Intake Boosting Enhances ITHR of Gasoline

- Intake-pressure boosting enhances the ITHR of gasoline.
  - Remains as single-stage ignition.
  - Allows considerable CA50 retard with good stability.
- For P_{in} = 200 kPa, CA50 retard can be > 379°CA.
  - 6°CA more than for P_{in} = 100 kPa.
  - Allows significantly higher $IMEP_g$.
- As a result, very high loads can be reached with boosted gasoline HCCI.
  - $IMEP_g$ = 16.3 bar at P_{in} = 325 kPa.
  - Limited by cylinder head ~160 bar.
  - Approaching loads of conventional diesel engines.

- Enhanced ITHR with boost is the key to high-load operation with premixed fueling, using gasoline.



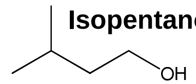


Dec and Yang, SAE 2010-01-1086

Can Biofuels Give Similar Performance?

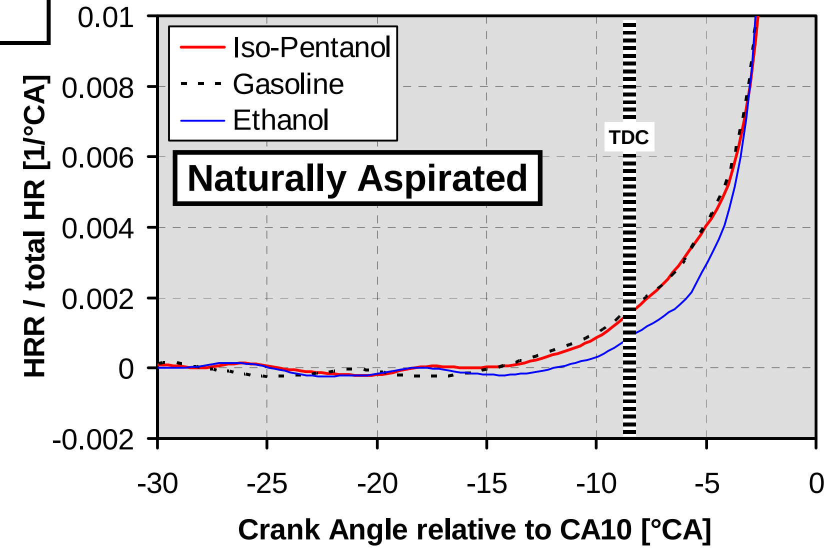
Iso-Pentanol and Ethanol

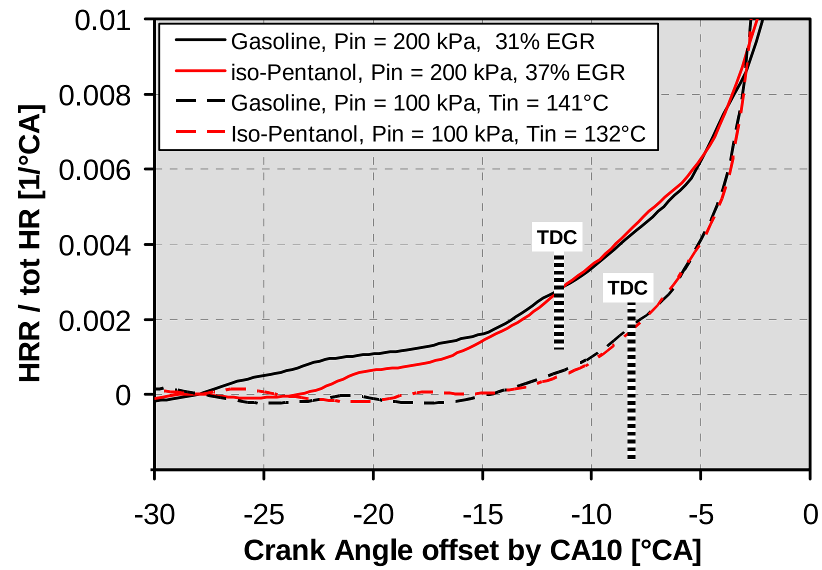
Isopentanol



- Iso-pentanol is a next-generation biofuel ⇒ process developed by JBEI.
- Iso-pentanol shows gasoline-like ITHR, naturally aspirated.
  – Greater than ethanol.
- ITHR of iso-pentanol is significantly enhanced by boost, similar to gasoline.
  – Provides good stability with significant timing retard.
- Allows a substantial increase in load with boost ⇒ like gasoline.

Yang *et al.* SAE 2010-01-2164

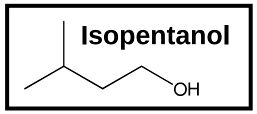




- Iso-pentanol closely matches gasoline performance ⇒ good compatibility.

Can Biofuels Give Similar Performance?

Iso-Pentanol and Ethanol



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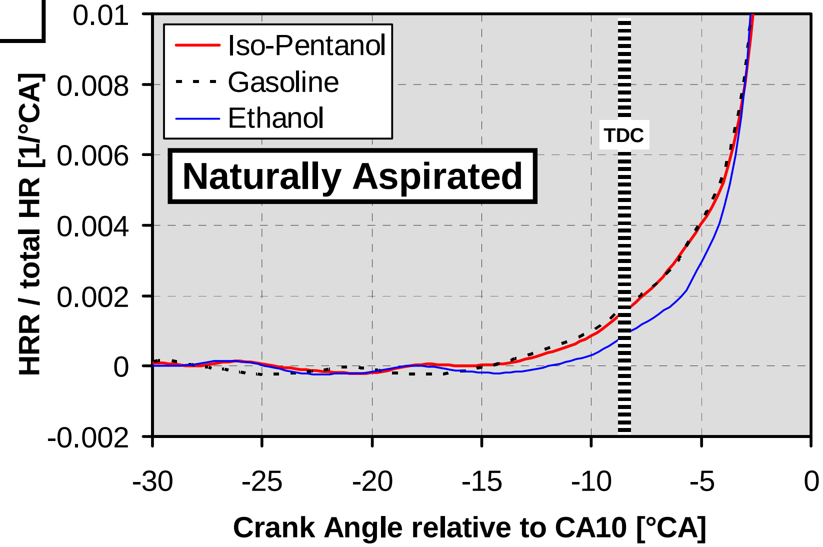
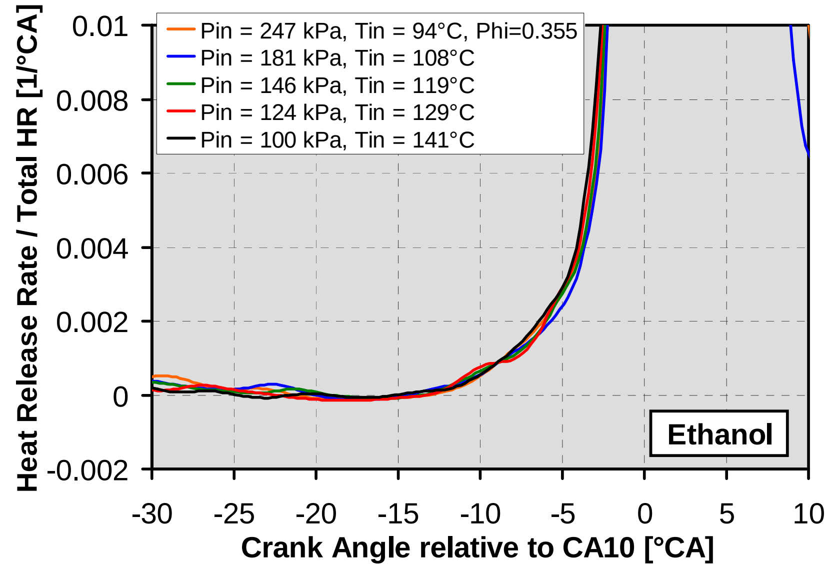
  - Greater than ethanol.
- ITHR of iso-pentanol is significantly enhanced by boost, similar to gasoline.
  - Provides good stability with significant timing retard.
- Allows a substantial increase in load with boost ⇒ like gasoline.
- Ethanol shows no enhancement in ITHR with boost.
  - Not as good for high-load HCCI.
  - Likely more knock resistance for boosted SI operation.

Yang *et al.* SAE 2010-01-2164

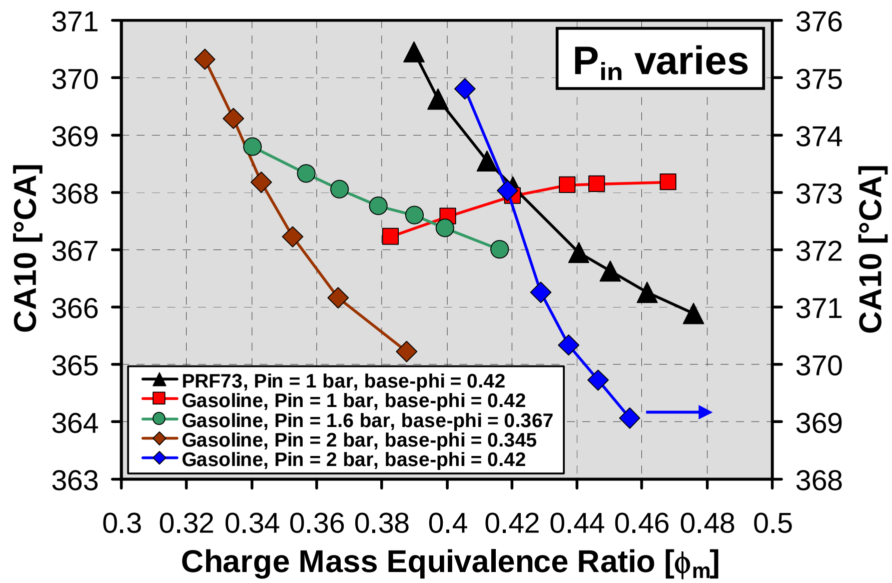


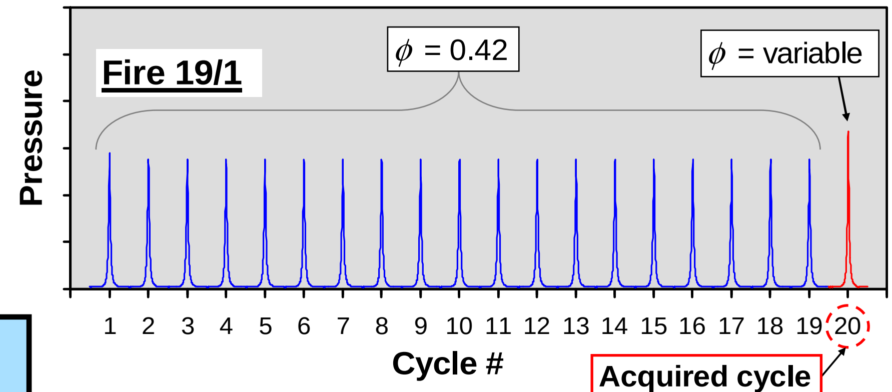


- Engine compatibility must be considered in developing new biofuels/blends.

Φ-Sensitivity of Gasoline and ITHR

- Use Fire19/1 technique to isolate fuel-chemistry effects from thermal effects.
  - Dec & Sjöberg *SAE 2004-01-0557*.
- PRF73 ⇒ strong ϕ-sensitivity
  - Autoignition timing significantly advanced by higher ϕ.
  - Chemical reaction rates promoted by higher fuel concentration.
- P_{in} = 1 bar ⇒ gasoline not ϕ-sensitive.
  - Retards due to cooling effect of γ .
- ϕ-Sensitivity of gasoline increases greatly from P_{in} = 1 to 2 bar.
  - Correlates with the increase in ITHR.





Dec and Yang SAE 2011-01-0897

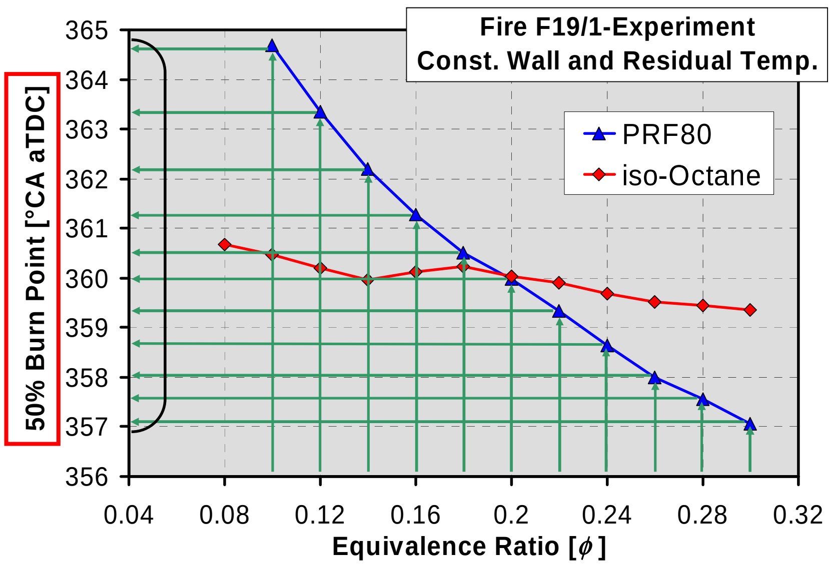
- ITHR correlates with ϕ-sensitivity over a range of fuels and op. conditions

- High ϕ-sensitivity of gasoline with boost offers the possibility of using mixture stratification to reduce the HRR and allow higher loads.

Controlling the HRR with Mixture Stratification

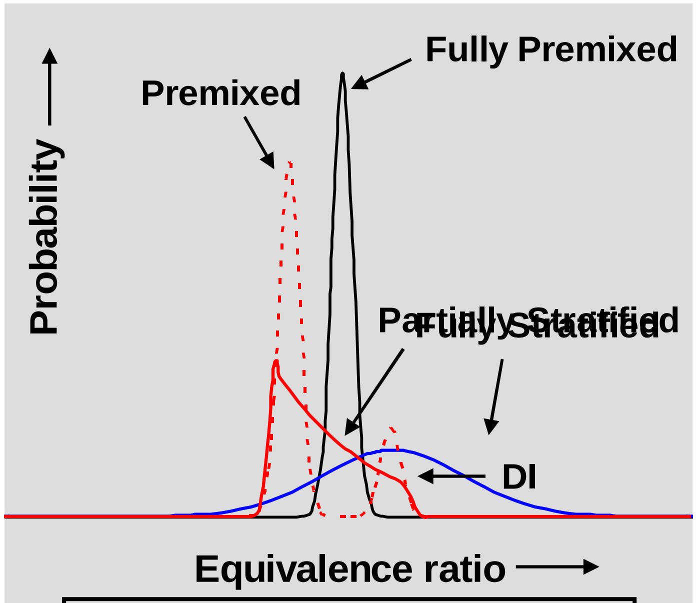
- Potential to reduce HRR beyond TS ⇒ Higher loads & Higher efficiency.
- Two requirements must be met for mixture stratification to be effective:

1) ϕ-Sensitive Fuel



Dec and Sjöberg, SAE 2004-01-0557

2) Appropriate ϕ-Distribution

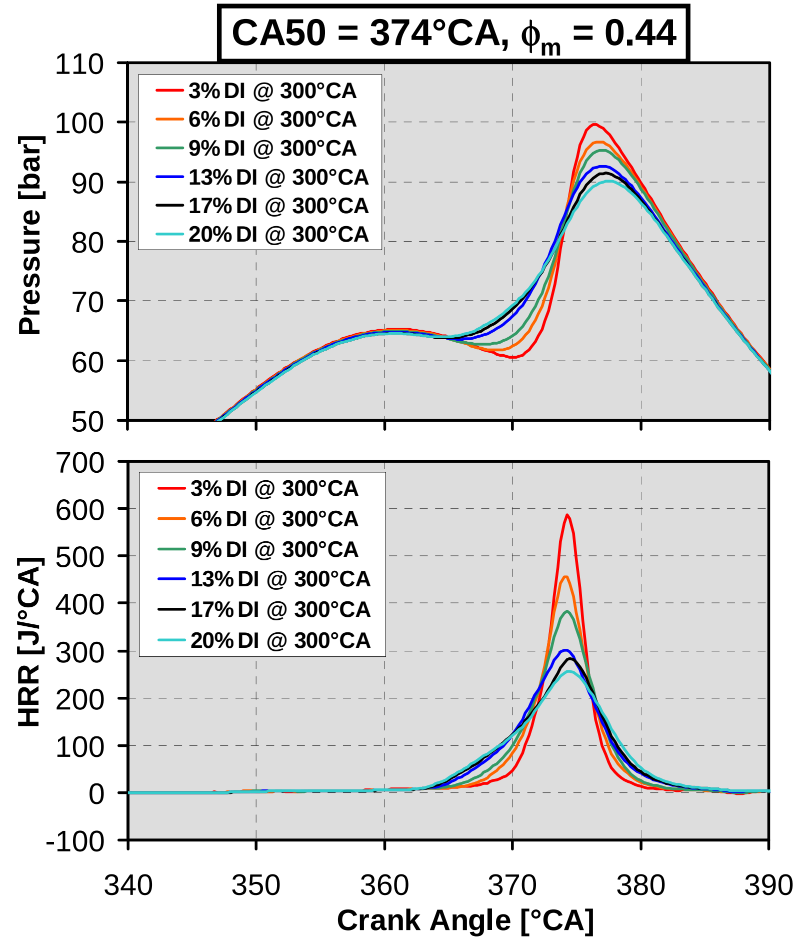


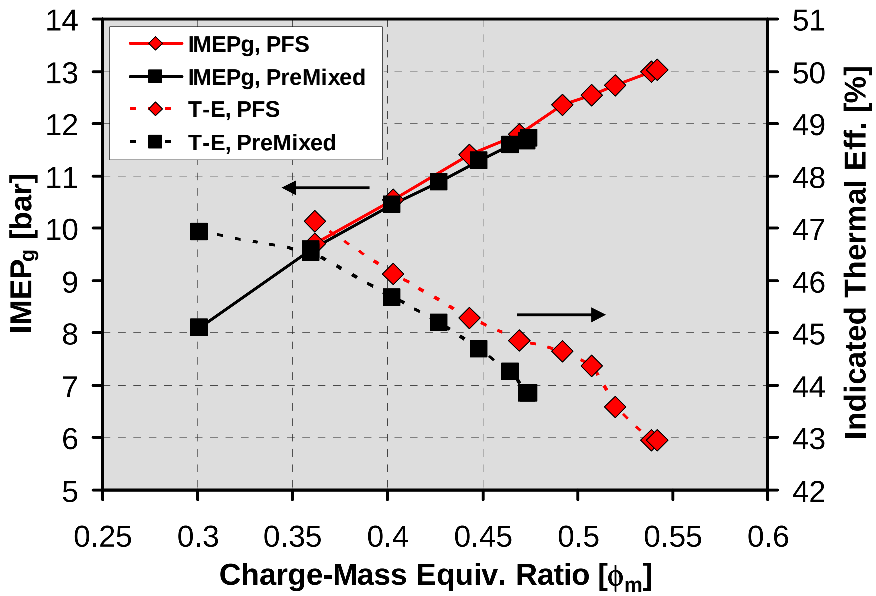
Sjöberg and Dec, SAE 2006-01-0629

- PRF80 is strongly ϕ-sensitive (high ITHR), iso-octane is not (weak ITHR)
- Partial fuel stratification (PFS) ⇒ most fuel premixed, up to 20% late DI.
  1. Provides sufficient stratification.
  2. Good air utilization with leanest regions burning hot enough for good comb.

Advantages of PFS for Boosted Gasoline, P_{in} = 2 bar

- Increase PFS by increasing the DI%.
  - Greatly reduces HRR, PRR and ringing.
- PFS allows significantly higher loads.
  - PFS ⇒ $IMEP_g$ = 13.0 bar, ϕ_m = 0.54
  - Premixed ⇒ $IMEP_g$ = 11.7 bar, ϕ_m = 0.47
  - Approaching O_2 availability limit (0.9%).
- Thermal Eff. is higher for the same load.
  - More advanced CA50.
  - Lower ringing ⇒ less heat loss (& quieter).





Dec and Yang SAE 2011-01-0897

- Ultra-low NOx and soot.

- Using PFS to exploit ϕ-sensitivity provides substantial advantages.
- Important to understand chemistry responsible for this behavior.

Summary and Conclusions

- Advanced low-temperature compression-ignition engines such as HCCI offer substantial advantages for high-efficiency, low emiss. & moderate cost.
- Early autoignition chemistry is critical for the operation of these engines.
  - LTHR $\Rightarrow$ 760 < T < 870 K
  - ITHR $\Rightarrow$ 900 < T < 1050 K
- ITHR varies significantly with fuel type even when no LTHR is present.
- Magnitude of the ITHR is critical for allowing sufficient combustion-phasing retard to prevent engine knock $\Rightarrow$ retard amplifies the benefit of natural TS.
  - ITHR must be sufficient to keep a positive TRR during the early expansion.
- Intake boosting greatly increases the ITHR of gasoline allowing very high loads without knock and with good stability $\Rightarrow$ up to $IMEP_g$ = 16.3 bar.
  - Enhanced ITHR also found with the biofuel iso-pentanol, but not with ethanol.
- Amount of ITHR also appears to correlate with the ϕ-sensitivity of the fuel.
  - ϕ-Sensitivity allows the use of PFS to significantly reduce the HRR & PRR.
  - Provides higher loads and higher efficiencies.
- A more complete understanding of I-T chemistry at engine conds. is needed