SAND2018-3175PE

Co-Optimization of
Fuels & Engines

Light-duty Multimode: Current Status and Planning for the Future

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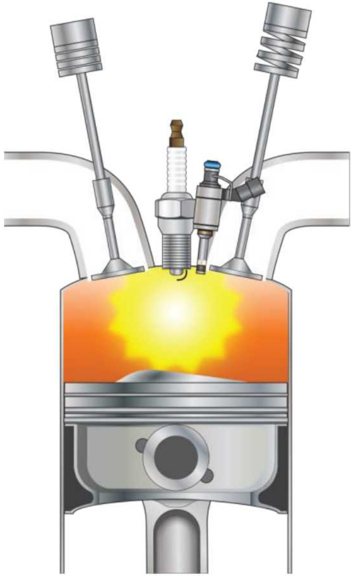
U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy

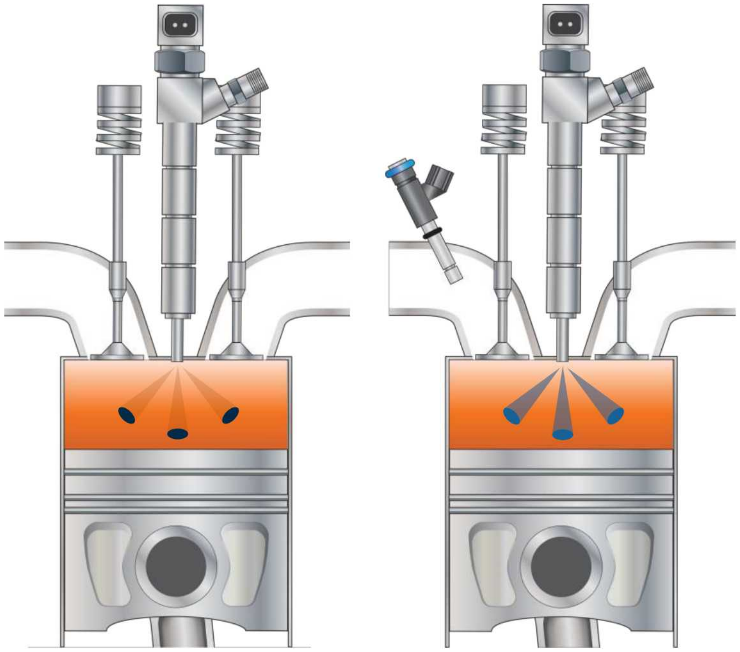
Multi-mode combustion involves use of two or more modes for full coverage of the speed-load map

Spark Ignition (SI)



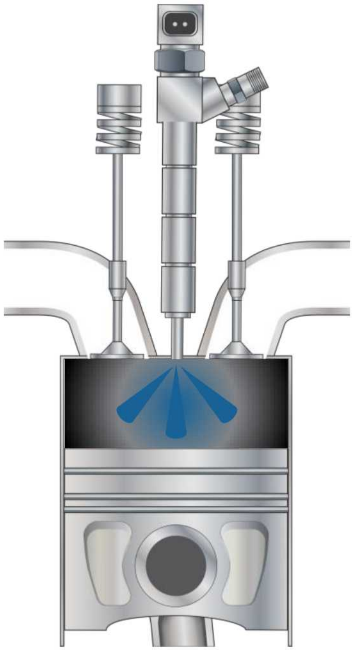
Low Reactivity Fuel

Advanced Compression Ignition (ACI)



Range of Fuel Properties TBD
(depends on combustion mode)

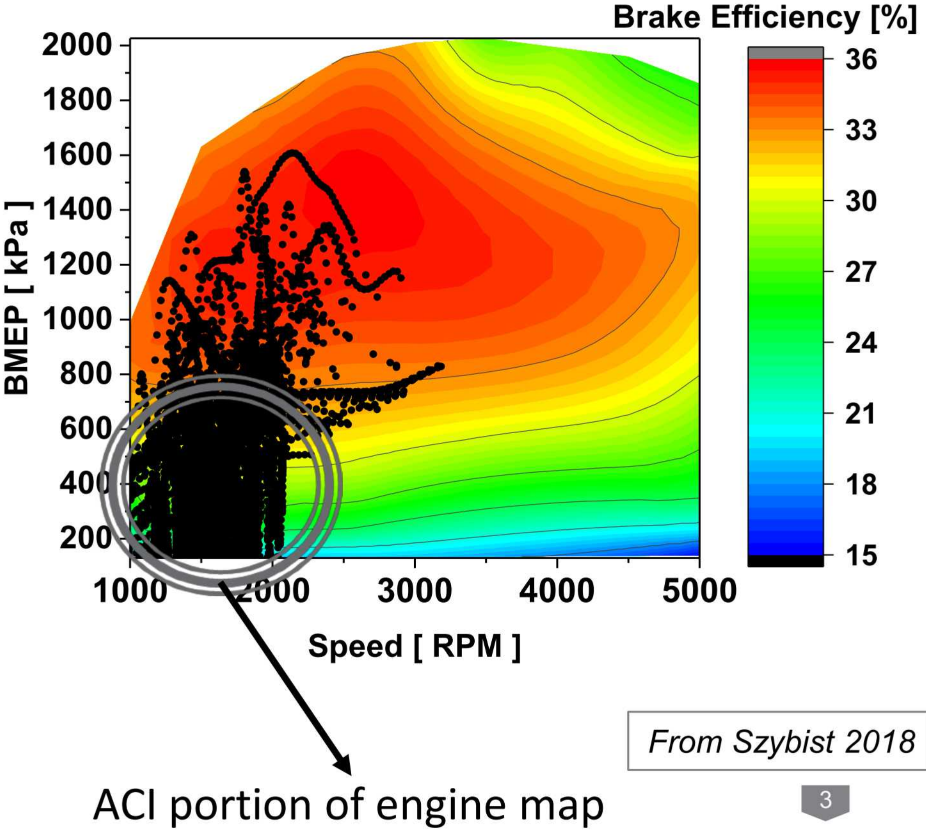
Mixing Controlled CI



High Reactivity Fuel

Co-Optima Shifting Emphasis of Light Duty (LD) Research from Standalone Boosted SI to Multi-Mode ACI

- Light duty multi-mode efforts combine SI and ACI combustion
  - ACI used at part-load for increased efficiency
  - SI used at high load/speed
- Approach maintains power density/ efficiency gains achieved through downsizing and downspeeding
- Full-time ACI addressed separately in Co-Optima heavy duty project
- Significant overlap, esp. in terms of autoignition research.



From Szybist 2018

Approach to Multimode Research

Many different part-load ACI approaches are candidates for multi-mode approach:

- NVO HCCI, exhaust re-breathe HCCI
- Spark-assisted CI (e.g, Mazda SPCCI)
- Gasoline compression ignition (GCI)
- Low temperature gasoline combustion (LTGC)

SPCCI = spark plug controlled compression ignition
NVO HCCI = Negative valve overlap homogeneous charge compression ignition

A multi-mode approach can include non-CI combustion modes:

- Lean well-mixed SI.
- Lean stratified-charge SI has high efficiency potential.

Avoid picking a winner has advantages.

Can we structure a research program that identifies fuel property and engine parameter impacts relevant to ALL part-load ACI approaches as well as competing approaches (variable CR engine, lean-burn SI, etc)?

Compare “best-in-class” Vehicles with Advanced Combustion

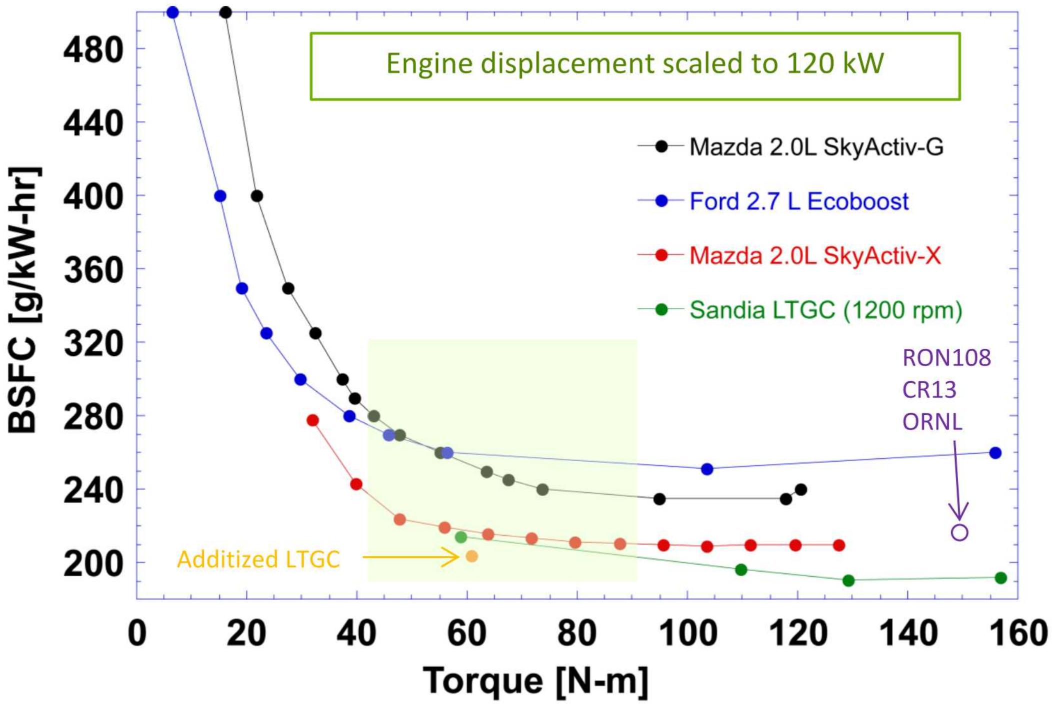
Introduction of...

and

Load Expansion of...

advanced combustion modes can provide substantial fuel-economy benefits.

What fuel properties and market scenarios promote this?



AED / FP Poll Results for Barriers

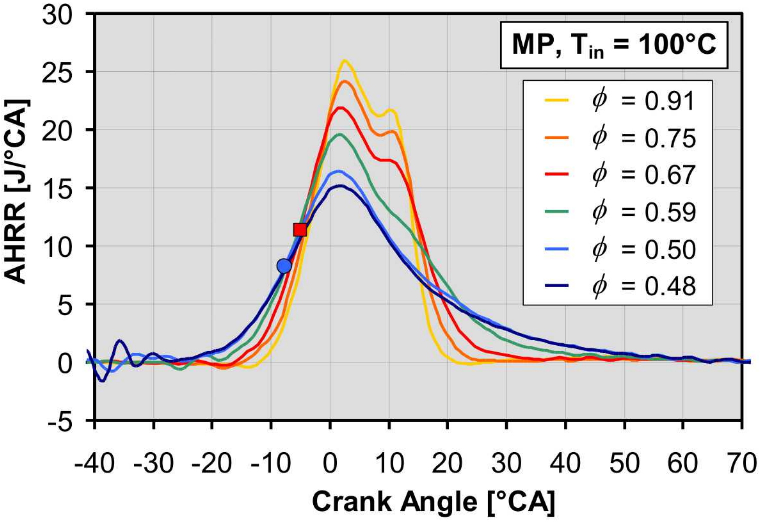
Support AOP Planning

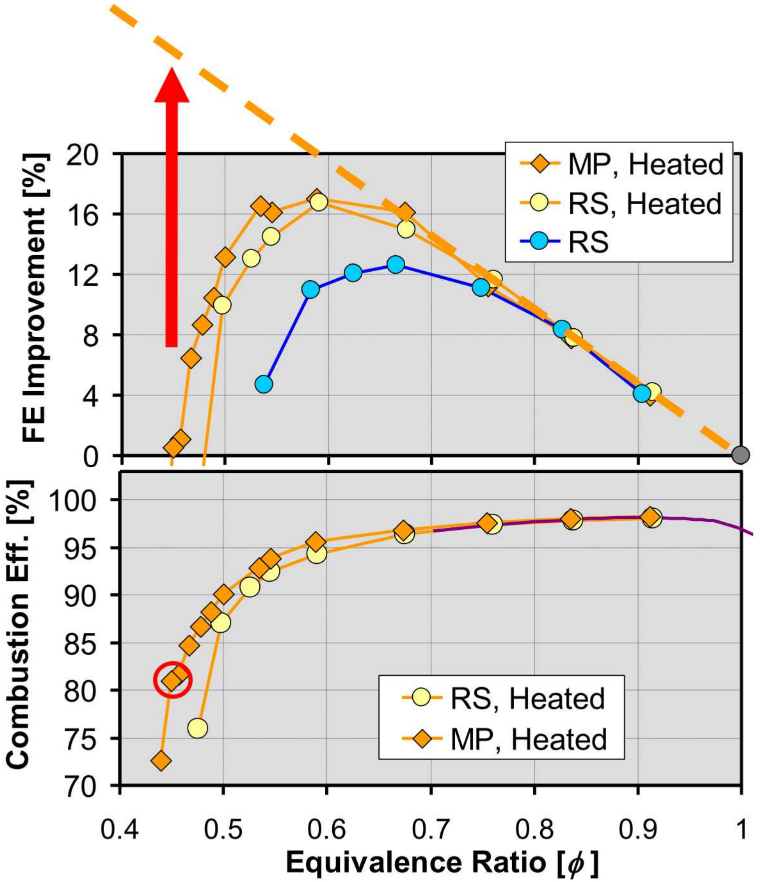
Lean homogeneous SI deflagration:

- Excessive burn duration. **Fuel property (FP) - Flame Speed.**
- Low-load instability. **FP - Flame Speed.**
- Increased HC and CO emissions.
- Excessive engine-out NO_x emission and aftertreatment burden.

Sandia: Lean Homogeneous SI Deflagration

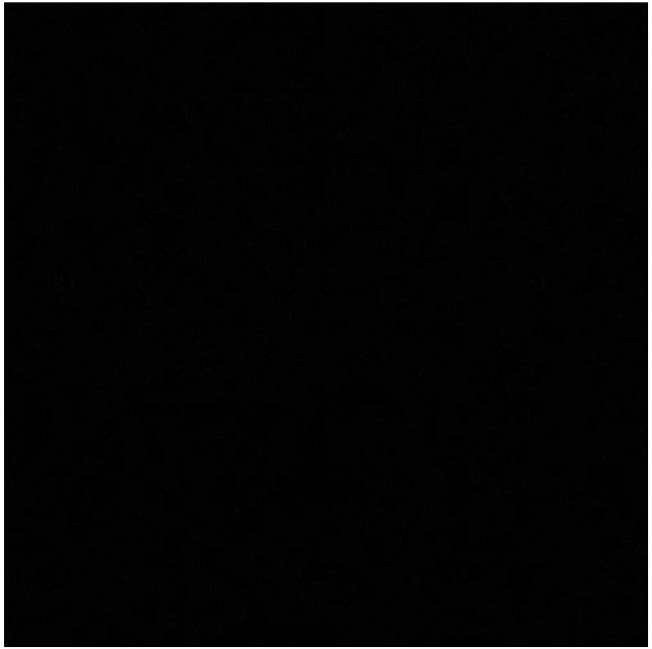
- Reduced peak AHRR, longer burn.
- Dropping combustion efficiency.
- Limits efficiency gain.

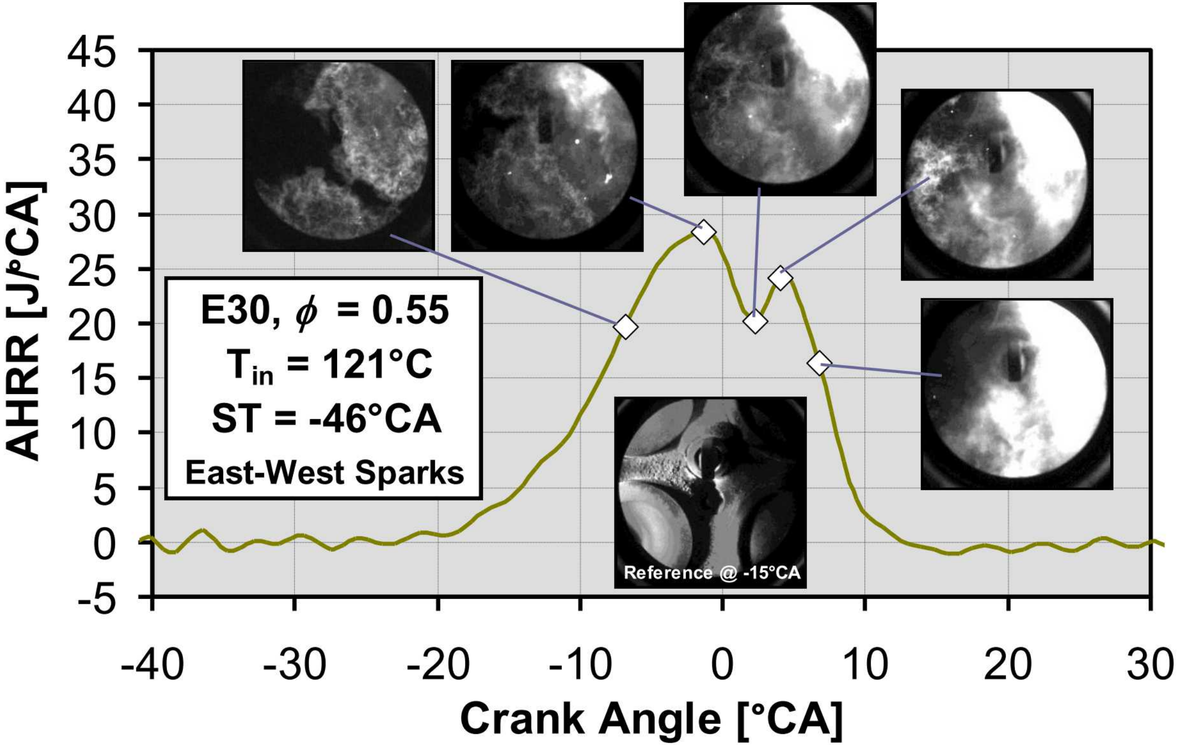




Sandia: Mixed-Mode Combustion (SACI)

- End-gas autoignition shortens combustion.



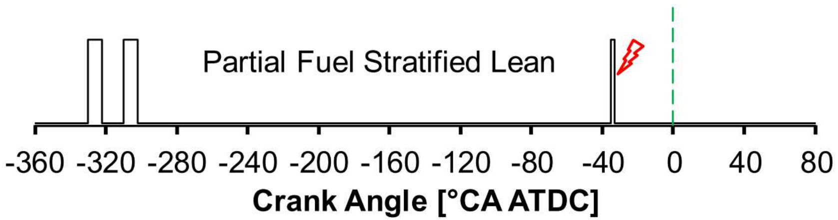


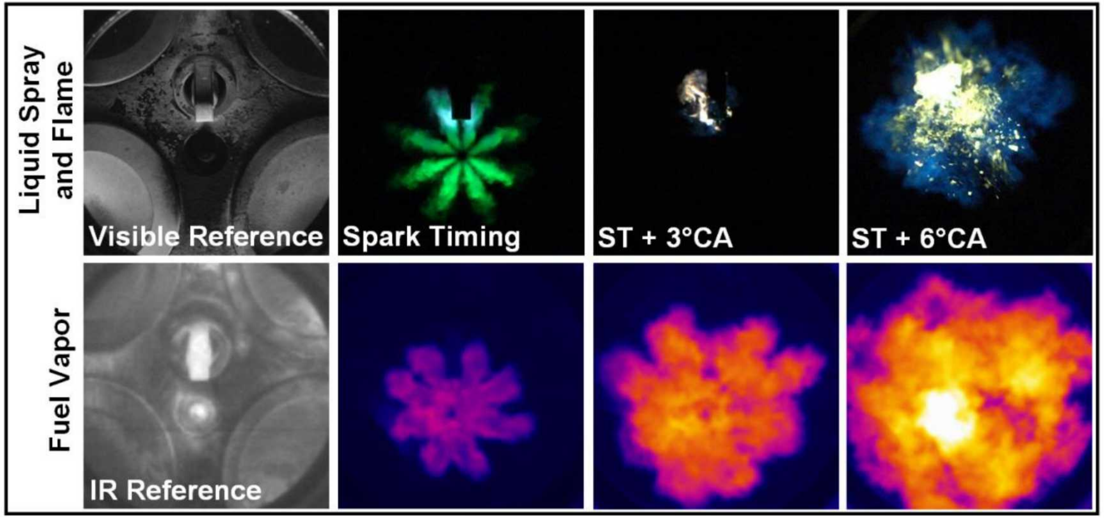
Poll - Barriers: SACI (SPCCI)

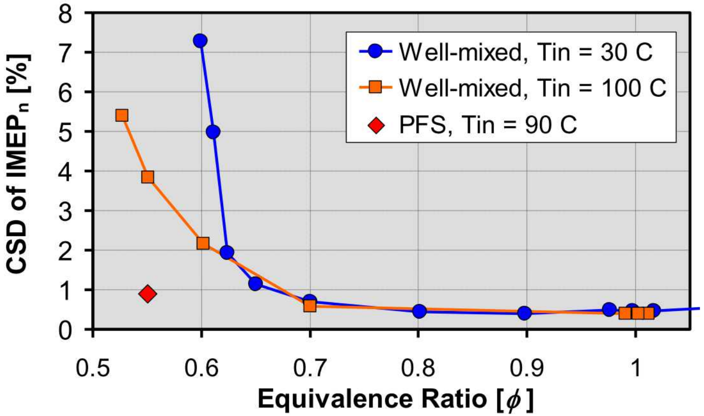
- Excessive pressure rise rates and combustion noise limit upper load. **FP - Autoignition reactivity.**
- High cycle-to-cycle variability in noise.
- Cycle-to-cycle instability (due to slow flame kernel development with high dilution). **FP - Flame Speed.**
- Transient control.
- High NO_x emissions due to initial flame propagation.

Mazda SKYACTIV-X: Commercial Multimode Engine

Sandia DISI: SPCCI



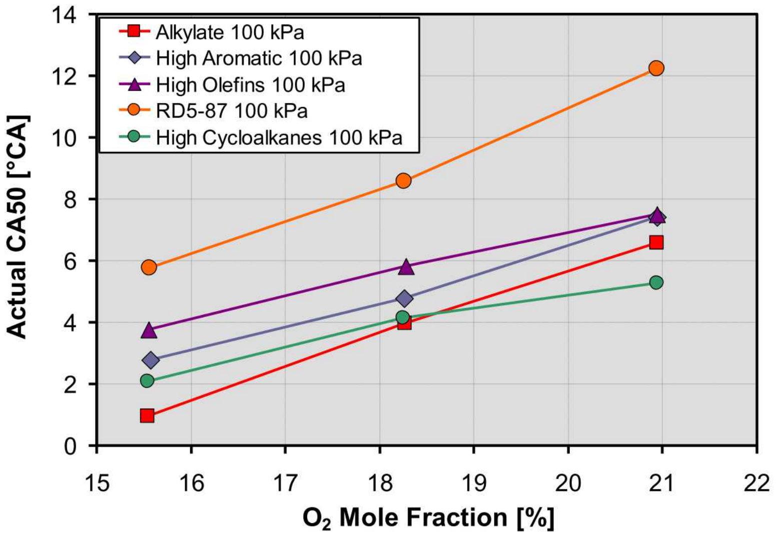


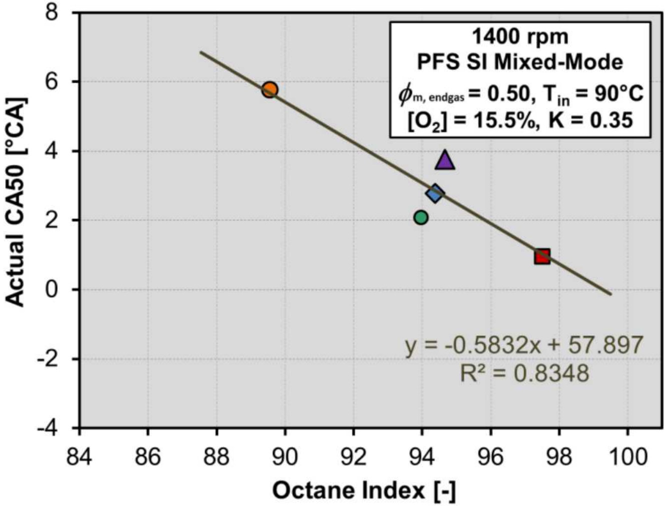


- Stratification can stabilize ultra-lean combustion.

Sandia DISI: Mixed-Mode Comb. / SACI / SPCCI

- Trapped hot residuals can be used achieve higher reactant temperature and facilitate mixed-mode combustion.
  - Reactant $[O_2]$ would be affected.
- The fuels show different sensitivities to $[O_2]$.





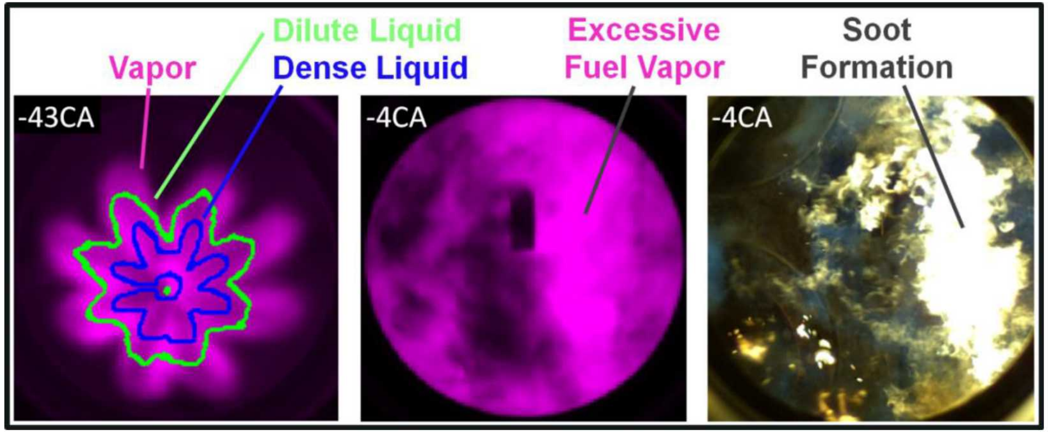
- Octane Index appears applicable for rank ordering fuels.

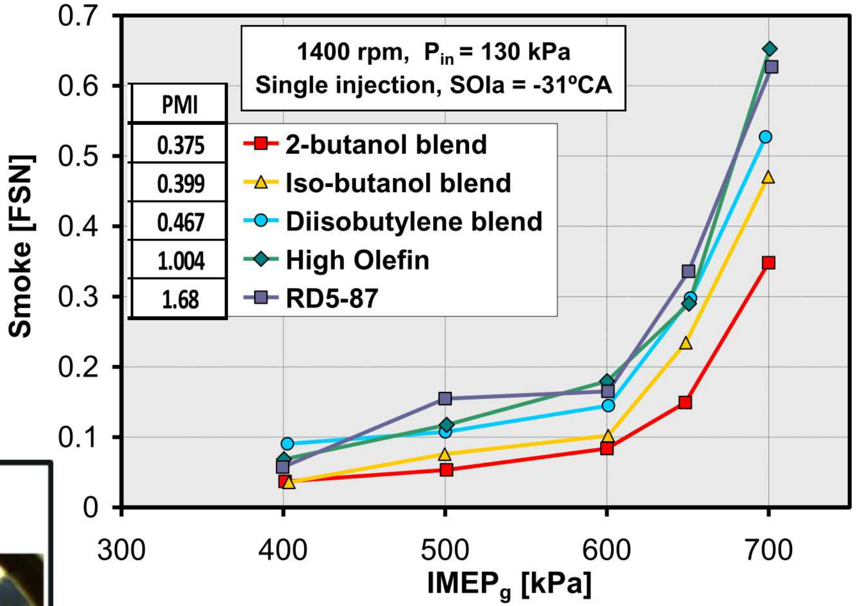
Poll - Barriers: Stratified Lean SI

- Excessive engine-out PM/PN limits upper load. **FP - Sooting tendency**.
- Combustion instability. **FP - Flame Speed.**
- Fuel-lean zone can result in high unburned emissions.
- High lean HC and NO_x concentrations and low exhaust temperatures.

Sandia DISI: Stratified Lean

- Excessive engine-out smoke limits upper load.
- Assessing applicability of fuel metrics.
- Optical diagnostics of soot-production pathways.





ACEC LTC Research Priorities

Highest priorities for low-temperature combustion:

a. Expanded speed and load range

b. Reduced engine out HC and CO emissions

c. Lower combustion noise

d. Simpler transient control/combustion mode switching

e. Improved cold operation

f. Increase tolerance to changes in ambient temperature and humidity, and **market fuel variability**

g. Reduce cost of lean-NOx aftertreatment system

h. Research that reduces the content, complexity, and cost of engines while increasing efficiency to enable a higher penetration of hybrid electric vehicles

AED / FP Poll Results for Barriers: HCCI

- Low-load stability. **FP - Autoignition reactivity**.
- Transient control.
- High sensitivity to thermal boundary conditions.
- High input temperature or fuel reactivity requirements. **FP - Autoignition reactivity.**
- CR required for HCCI may be too high for SI.
- Excessive pressure rise rates and combustion noise. **FP - Autoignition reactivity.**
- High HC and CO emissions combined with low exhaust temperature may make emissions control challenge insurmountable.
- Some form of low temperature lean NOx control likely needed.
- Low combustion efficiency may exacerbate LSPI in SI mode.
- Cylinder-to-cylinder breathing differences.

Poll - Barriers: NVO for Low-load HCCI

- High heat losses during NVO.
- High sensitivity to thermal boundary conditions.
- May be incompatible with multi-mode (compression ratio too high).
- Combustion noise is excessive and/or doesn't follow the noise trends with conventional SI engines (noise vs. load).
- High HC and CO emissions combined with low exhaust temperature may make emissions control challenge insurmountable.
- Some form of low temperature lean NOx control likely needed.
- Low combustion efficiency may exacerbate LSPI in SI mode.
- Cylinder-to-cylinder breathing differences.

Poll - Barriers: Partially-Stratified LTGC

- Stratification greatly improves low-load stability and combustion efficiency over HCCI. However, increased charge temperature, spark assist, or increased fuel reactivity are still required for low loads down to idle. **FP - Autoignition reactivity.**
- Need for improved transient control methods.
- Full load can be difficult with true LTC.
- Excessive noise and/or pressure rise rate. **FP - Autoignition reactivity.**
- Low load and cold-start performance issues.
- High sensitivity to thermal boundary conditions.
- High HC and CO emissions and low exhaust temperatures, esp. after turbocharger.
- Some form of low temperature lean NOx control likely needed.

Poll - Barriers: GCI late injection

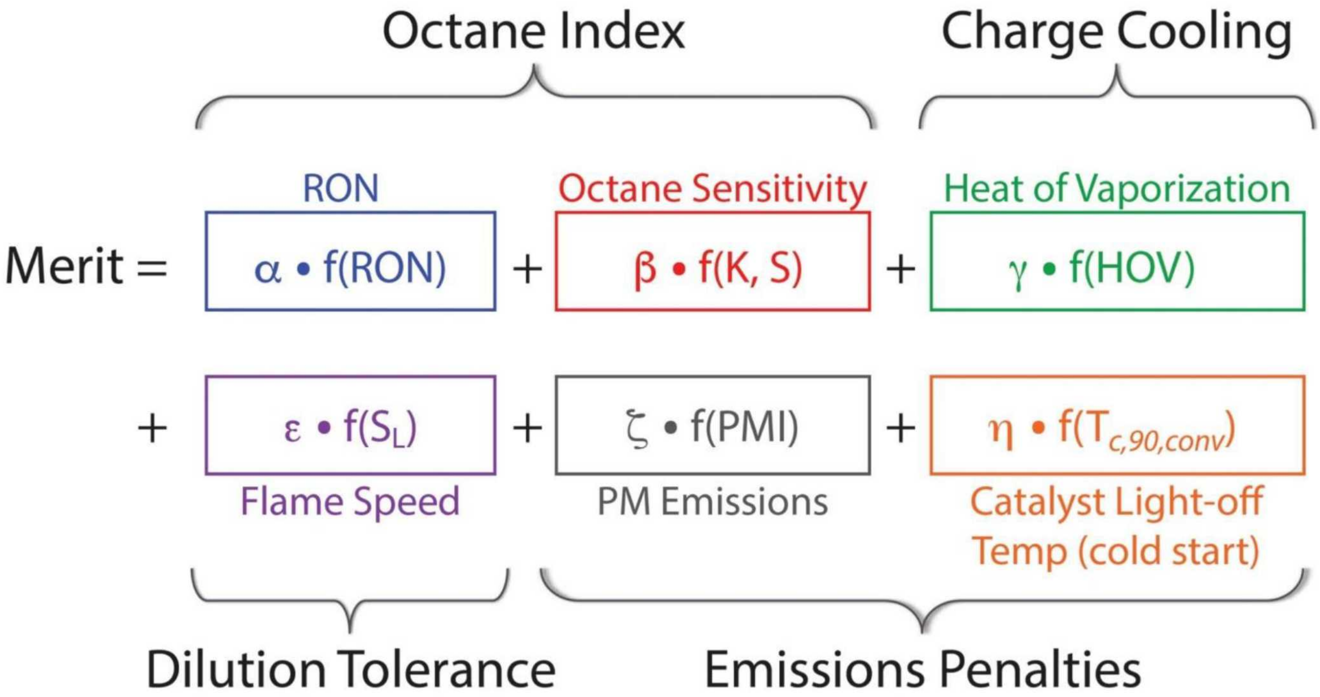
- Low-load stability. **FP - Autoignition reactivity.**
- Risk of misfires. **FP - Autoignition reactivity.**
- Increased combustion noise.
- Could require a lower octane gasoline like fuel (could be a benefit as well). **FP - Autoignition reactivity.**
- High EGR requried to achieve simultaneous ultra-low engine out NOx and soot.
- Excessive NOx, soot, HC and CO emissions under some operating conditions.
- Low exhaust temperatures at low loads.
- Some form of low temperature lean NOx control likely needed.

Common Barriers for Multimode Operation

- Performance is linked to autoignition ⇒ Study autoignition reactivity.
- Unstable combustion and misfires linked to flame developement ⇒ Study flame speed.
- Stratification is linked to soot emissions ⇒ Study sprays and sooting propensity.
- Combustion often forms high CO, HC and NO_x , and low exhaust temperatures are expected ⇒ Study lean aftertreatment.

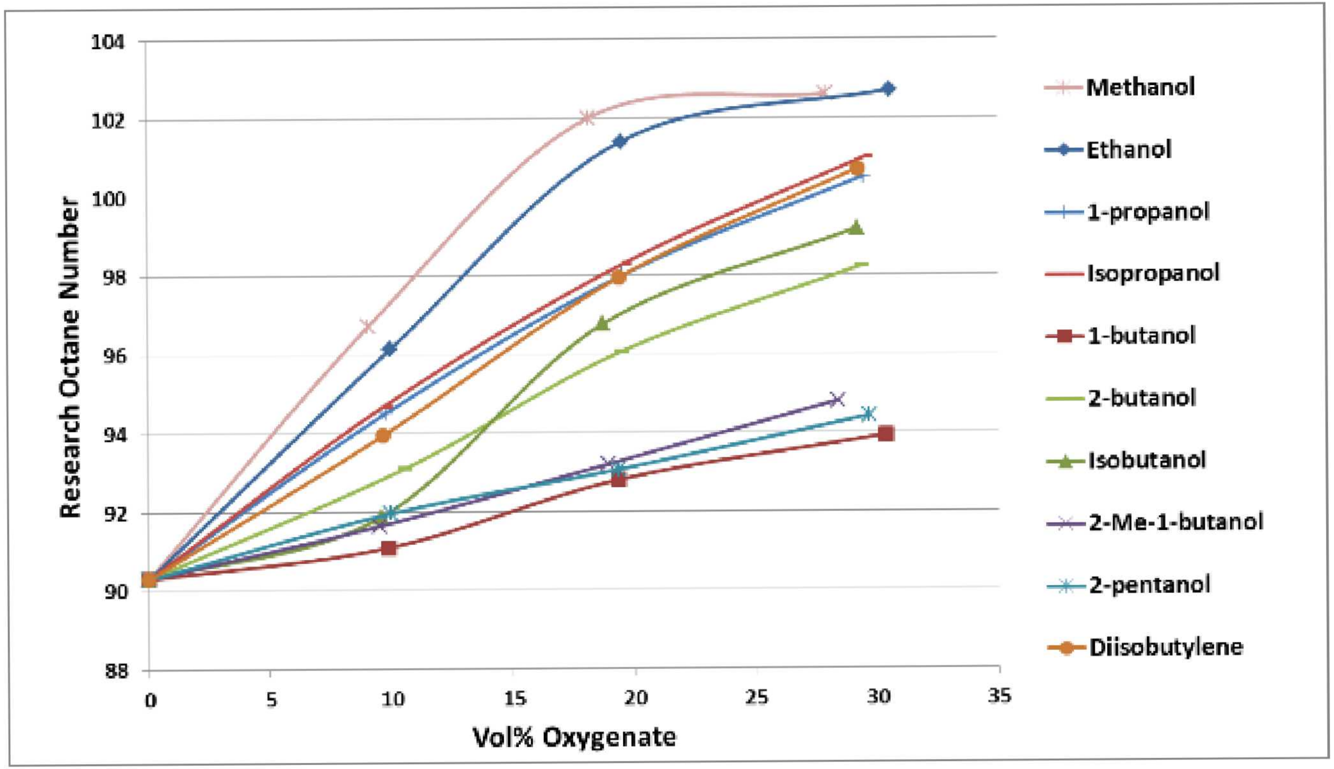
- Seems like wide-open research space.
- Inconsistent with DOE request for impactful results within 30 months.
- Defining fuels scenarios can aid in formulating objectives.

Boosted SI Effort was Guided by Merit Function



- Merit function quantifies impact of fuel properties on engine efficiency

Blending Octane Data



Merit Function Scores – modeled (K = - 1.25)

	10%			20%			30%			10%			20%			30%				
Blendstock	cBOB	CARBOB	sBOB	cBOB	CARBOB	sBOB	cBOB	CARBOB	sBOB	F1 BOB	F2 BOB	F3 BOB	F1 BOB	F2 BOB	F3 BOB	F1 BOB	F2 BOB	F3 BOB	Green	Yellow
Furan Mixture	8.6	1.9	5.1	12.8	6.8	9.6	12.9	7.7	10.2	1.1	5.1	9.0	6.1	9.6	13.1	7.1	10.2	13.2	14	2
Methanol	7.1	0.3	3.6	15.0	9.0	11.9	15.6	10.4	12.9	(0.4)	3.5	7.4	8.4	11.9	15.3	9.8	12.9	15.9	14	0
Ethanol	5.7	(1.1)	2.2	12.2	6.2	9.1	12.7	7.5	10.0	(1.8)	2.1	6.0	5.6	9.1	12.5	6.9	10.0	13.0	13	1
n-propanol	4.4	(2.3)	0.9	8.5	2.6	5.4	11.6	6.4	8.9	(3.0)	0.9	4.8	1.9	5.4	8.8	5.8	8.9	11.9	8	3
Diisobutylene	2.9	(3.8)	(0.6)	7.7	1.7	4.5	11.0	5.7	8.3	(4.5)	(0.6)	3.3	1.0	4.5	8.0	5.2	8.2	11.2	7	1
Isobutanol	1.0	(5.8)	(2.6)	7.3	1.3	4.2	10.2	4.9	7.4	(6.5)	(2.6)	1.3	0.6	4.1	7.6	4.4	7.4	10.4	6	1
Cyclopentanone	2.8	(3.9)	(0.7)	6.5	0.6	3.4	10.4	5.1	7.6	(4.6)	(0.7)	3.2	(0.1)	3.4	6.8	4.6	7.6	10.6	6	1
iso-propanol	4.0	(2.7)	0.5	7.2	1.2	4.1	9.8	4.6	7.1	(3.4)	0.5	4.4	0.6	4.1	7.5	4.0	7.1	10.1	6	0
2-butanol	2.2	(4.5)	(1.3)	5.4	(0.5)	2.3	7.5	2.3	4.8	(5.2)	(1.3)	2.6	(1.2)	2.3	5.7	1.7	4.8	7.8	3	3
Anisole	1.9	(4.8)	(2.6)	4.8	(1.2)	1.7	7.9	2.7	5.2	(5.6)	(1.6)	2.2	(1.8)	1.7	5.1	2.1	5.2	8.2	2	4
2-butanone (MEK)	1.1	(5.6)	(2.4)	4.0	(2.0)	0.9	6.0	0.8	3.3	(6.4)	(2.4)	1.4	(2.6)	0.9	4.3	0.2	3.3	6.3	2	0
Methyl acetate	0.8	(5.9)	(2.7)	3.7	(2.3)	0.6	6.2	1.0	3.5	(6.7)	(2.7)	1.1	(2.9)	0.6	4.0	0.4	3.5	6.5	2	0
Ethyl butanoate	0.8	(5.9)	(2.7)	2.7	(3.3)	(0.5)	5.5	0.2	2.8	(6.6)	(2.7)	1.2	(4.0)	(0.5)	3.0	(0.3)	2.7	5.8	1	1
2-Me-1-butanol	1.1	(5.6)	(2.4)	3.3	(2.7)	0.2	5.2	(0.1)	2.5	(6.3)	(2.4)	1.5	(3.4)	0.1	3.6	(0.6)	2.4	5.4	0	2
Ethyl acetate	0.5	(6.3)	(3.0)	2.9	(3.1)	(0.2)	4.9	(0.4)	2.1	(7.0)	(3.1)	0.8	(3.7)	(0.2)	3.2	(1.0)	2.1	5.1	0	2
1-butanol	(0.1)	(6.9)	(3.6)	3.4	(2.6)	0.3	4.6	(0.7)	1.9	(7.6)	(3.7)	0.2	(3.2)	0.3	3.7	(1.2)	1.8	4.8	0	1
3-Me-1-butanol	(0.0)	(6.7)	(3.5)	1.4	(4.6)	(1.7)	2.9	(2.4)	0.2	(7.5)	(3.5)	0.3	(5.2)	(1.7)	1.7	(2.9)	0.1	3.2	0	0
Butyl acetate	(0.2)	(6.9)	(3.7)	0.9	(5.1)	(2.2)	1.1	(4.2)	(1.6)	(7.7)	(3.7)	0.1	(5.7)	(2.2)	1.2	(4.7)	(1.7)	1.3	0	0
2.4 dimethyl-3- pentanone	(2.3)	(9.0)	(5.8)	(0.3)	(6.3)	(3.4)	0.7	(4.5)	(2.0)	(9.7)	(5.8)	(1.9)	(7.0)	(3.5)	(0.0)	(5.1)	(2.1)	1.0	0	0
2-pentanone	1.2	(5.5)	(2.3)	2.8	(3.1)	(0.3)	3.4	(1.8)	0.7	(6.2)	(2.3)	1.6	(3.8)	(0.3)	3.1	(2.4)	0.6	3.7	0	0
2-pentanol	1.3	(5.5)	(2.2)	1.9	(4.1)	(1.3)	3.1	(2.1)	0.4	(6.2)	(2.3)	1.6	(4.8)	(1.3)	2.2	(2.7)	0.4	3.4	0	0
Ketone Mixture	(0.9)	(7.6)	(4.4)	(1.2)	(7.2)	(4.4)	(0.7)	(6.0)	(3.4)	(8.3)	(4.4)	(0.5)	(7.9)	(4.4)	(0.9)	(6.5)	(3.5)	(0.5)	0	0
Triptane	(0.2)	(6.9)	(3.7)	(0.3)	(6.3)	(3.4)	2.1	(3.2)	(0.7)	(7.7)	(3.7)	0.2	(6.9)	(3.4)	0.0	(3.8)	(0.7)	2.3	0	0

cBOB: conventional blendstock for oxygenated blending (premium)

CARBOB: California Reformulated Gasoline BOB

sBOB: Summer BOB

F1 BOB: 86 RON (S = 2)

F2 BOB: 86 RON (S = 8)

F3 BOB: 86 RON (S = 13)

Understanding stakeholder value propositions is essential to Co-Optima

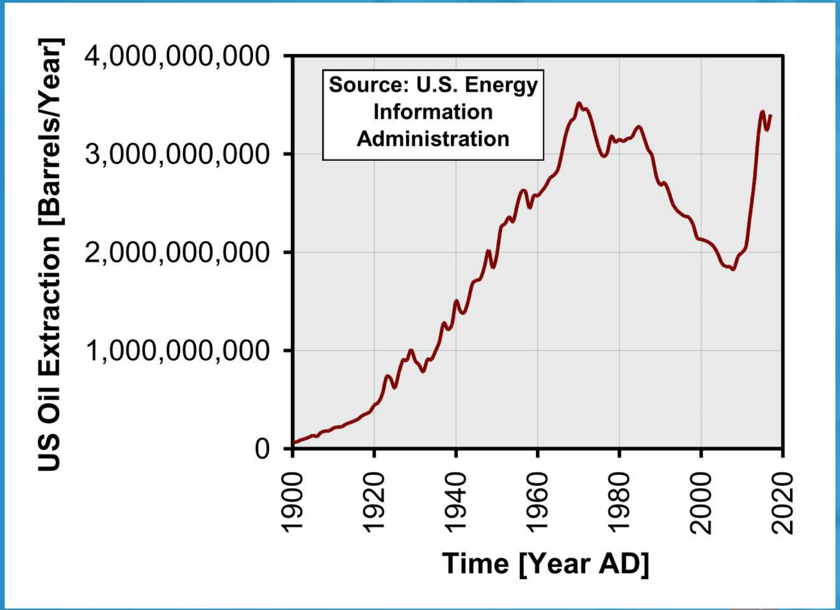
Achieving a
win-win-win
means (ideally) that all stakeholders make money

From a research perspective, this means that we’re working on the right problems

The Inconvenient Truth - is still just that

60 Years Ago, Edward Teller warned the American Petroleum Institute (API) about global warming.

Market analysis shows no evidence that conservation is prioritized.



Fuels Scenarios

Ideal for high efficiency of boosted SI engine:

RON > 98

S > 10

$\Rightarrow$ AKI > 93

Hard to convince consumer to buy more costly fuel.

So energy companies are reluctant to invest.

Lower ambition for boosted SI, but perhaps more ideal for multimode operation.

AKI > 87

S > 11

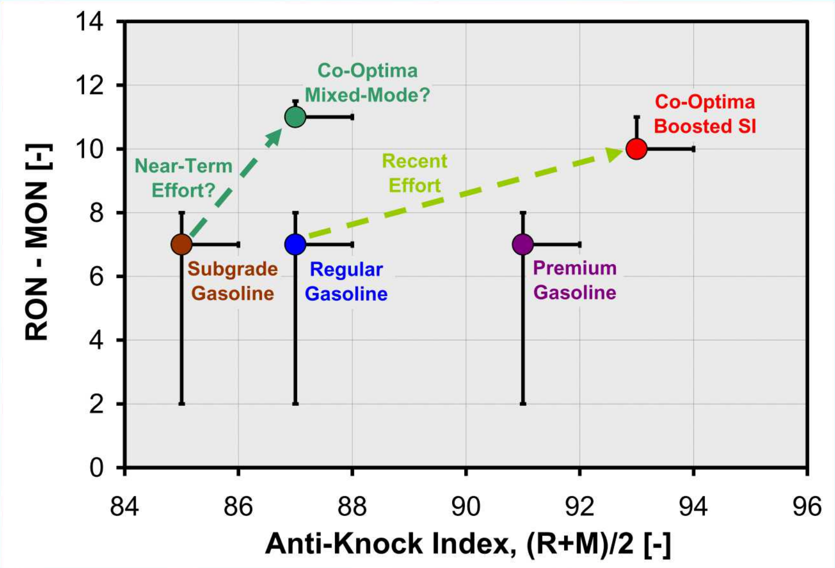
$\Rightarrow$ RON > 92.5

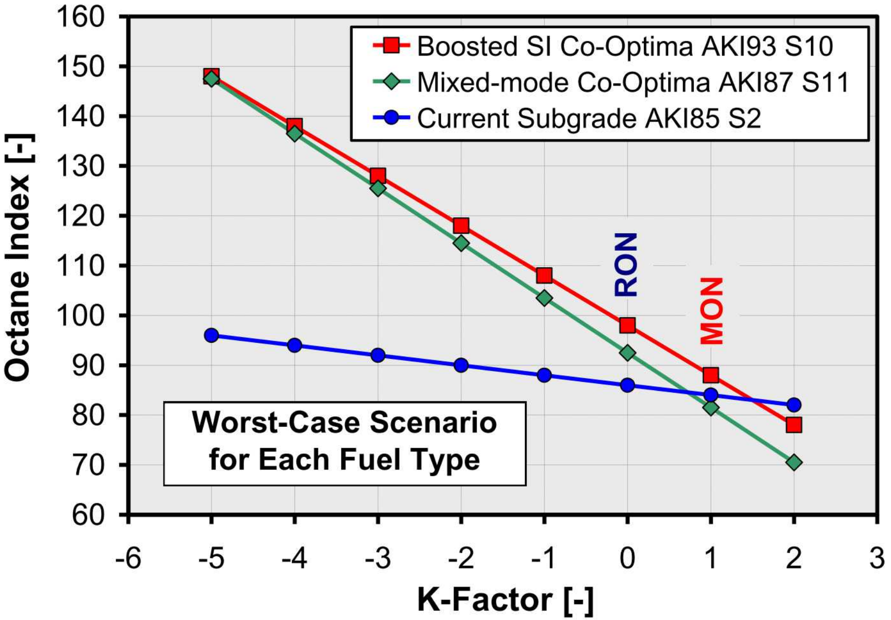
Cheaper BOB, use renewables to increase S.

Consumer can select lowest AKI, which tends to be their preference.

Fuels Scenarios with New AKI87+

- Ban low-S fuels for use in newer vehicles.
- New high-S AKI87+ fuel looks attractive.





RON95 - New US Gasoline Baseline?

Reasonable for higher efficiency of boosted SI engine:

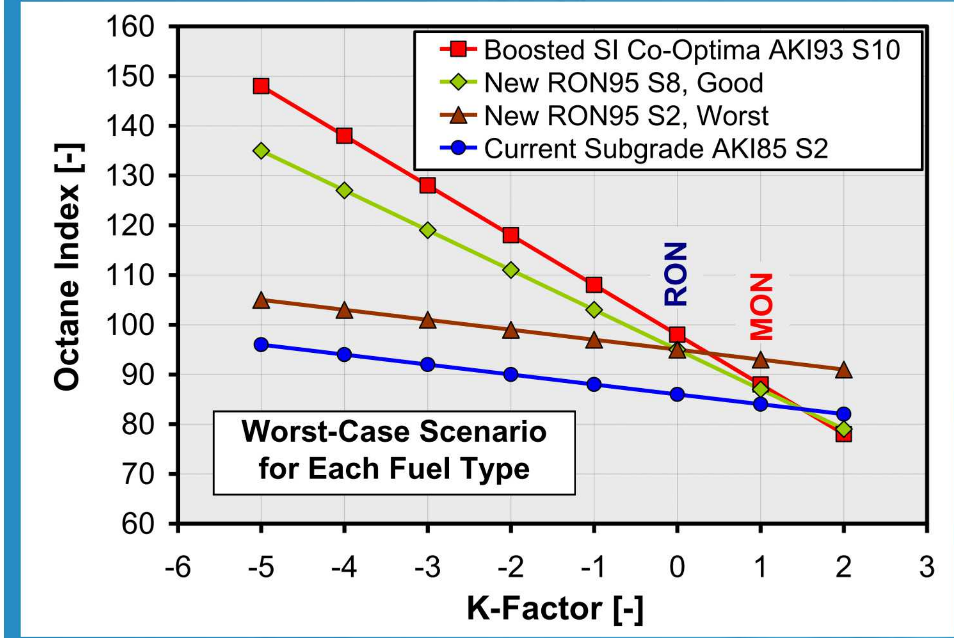
RON > 95

S = ?

⇒ AKI ?

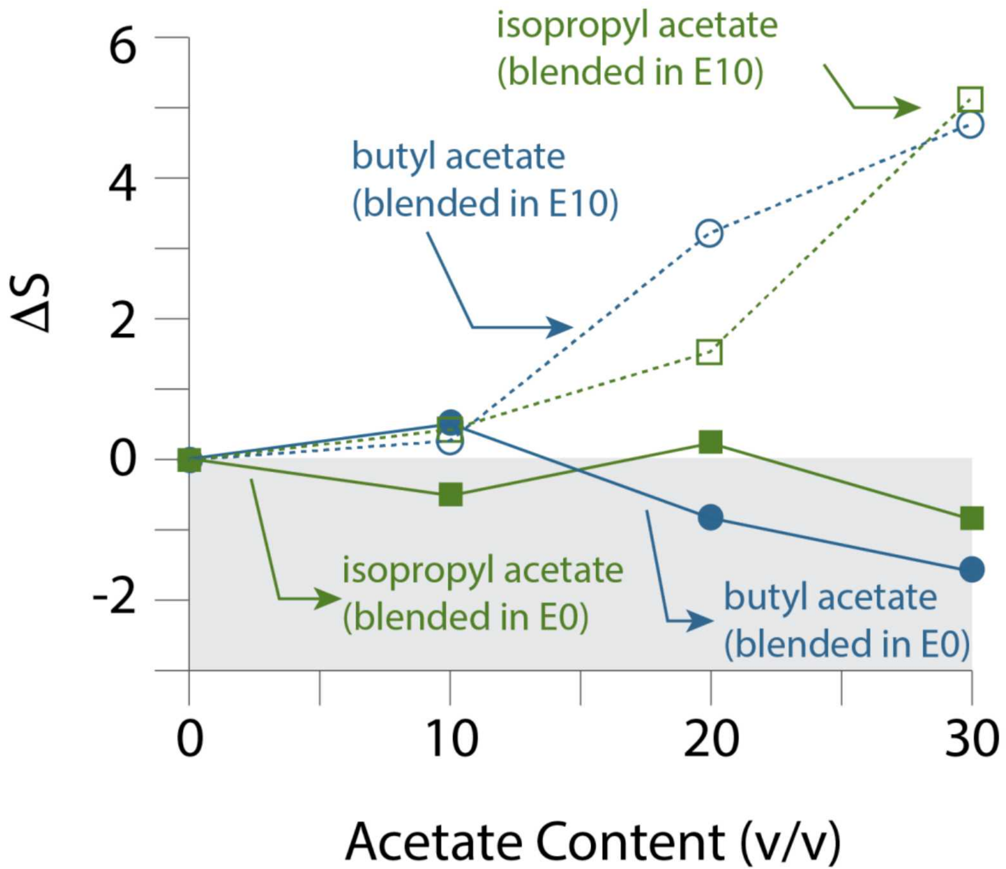
Controlling S can be a big deal. Co-Optima can inform stakeholders.

Including multi-mode engines



Ester Sensitivity Enhanced with Ethanol

- Esters are high-RON, low S blendstocks
- Esters blended into E0 impart no octane sensitivity
- Blending into E10 “turns on” S
- Value proposition:
  - Identify mechanism behind ethanol enhancement
  - Identify bioblendstocks that synergistically blend with ethanol to yield high S

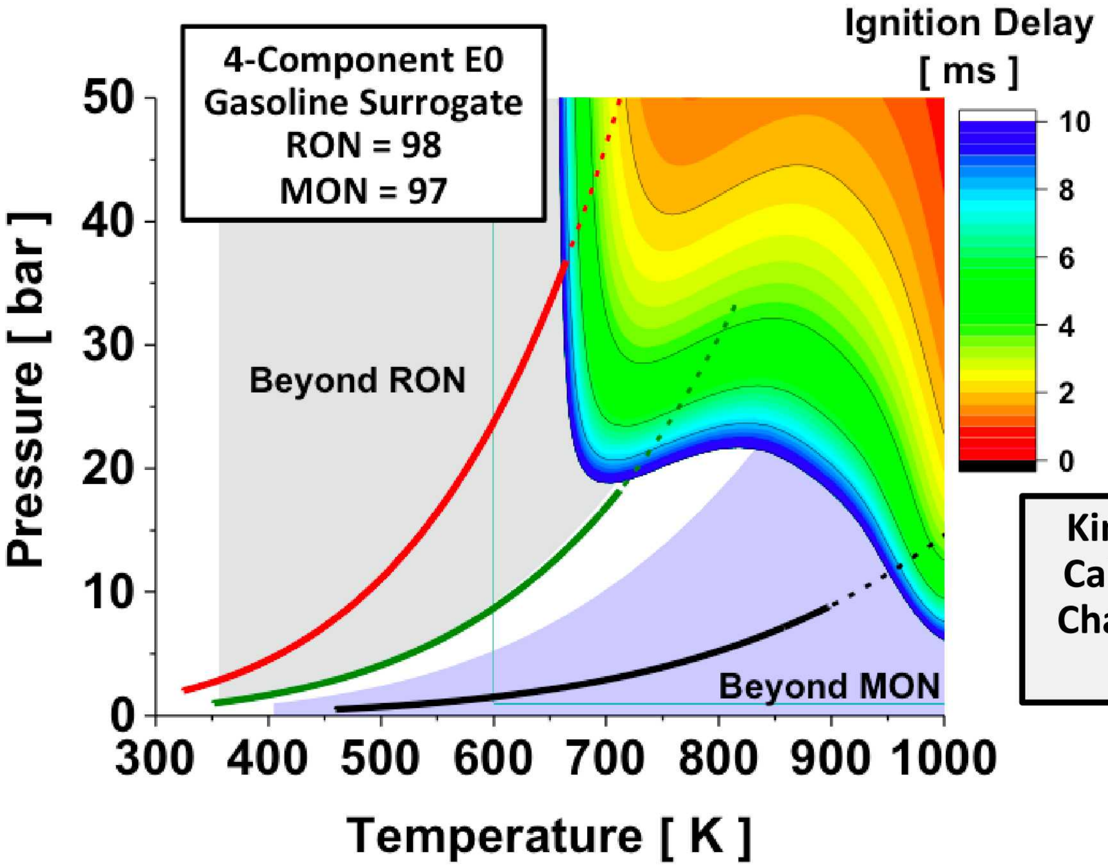


Merit Function Assessment for Mixed-mode Operation

$$Merit = \frac{(RON_{mix} - 91)}{1.6} - K\frac{(S_{mix} - 8)}{1.6}$$
$$+ \frac{0.085[ON / kJ / kg_{mix}] \cdot ((HoV_{fuel} / (AFR_{mix} + 1)) - (415[kJ / kg] / (14.0[-] + 1)))}{1.6}$$
$$+ \frac{((HoV_{mix} / (AFR_{mix} + 1)) - (415[kJ / kg] / (14.0[-] + 1)))}{15.2} + \frac{(S_{L,mix} - 46[cm / s])}{5.4}$$
$$- H(PMI_{mix} - 1.6)[0.7 + 0.5(PMI_{mix} - 1.4)] + 0.008\,^{\circ}C^{-1}\left(T_{c,90,conv} - T_{c,90,mix}\right)$$

- Re-assess Merit Function.
- What is considered a benefit for boosted SI, could be a detriment for mixed-mode operation.

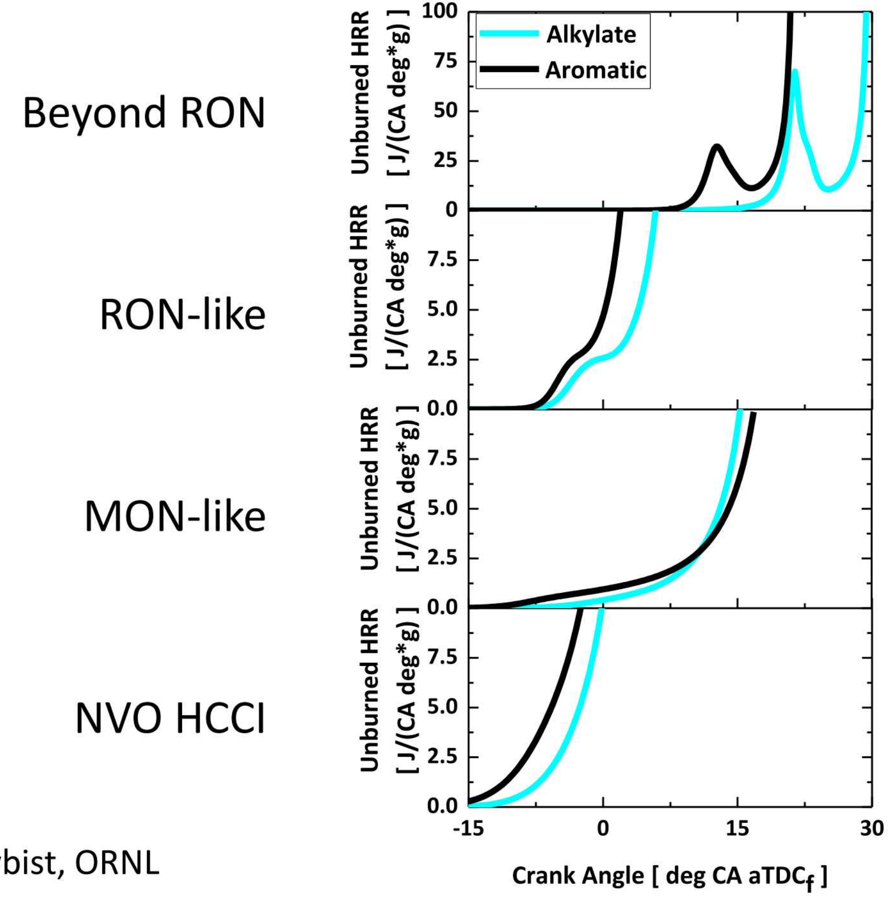
ORNL / LLNL: Initial In-Cylinder Conditions Determine P-T Trajectory; Autoignition Chemistry is Dependent on Trajectory



Kinetic Ignition Delay Calculations Illustrate Changing Autoignition Chemistry

Szybist, ORNL

ORNL / LLNL: Heat Release Prior to Main Ignition Varies Significantly Between Conditions



- Importance of low-temperature heat release varies greatly.
- Suggests that a holistic chemical-kinetics model approach should be used.

Szybist, ORNL

Possible Efforts for FY19 - 20 (1)

- Re-assess Merit Function.
  - Identify areas of conflict between boosted SI and multimode SI.
- Assess SI multimode oppertunities for various fuels scenarios.
- Perform blendstock search to identify fuels that provide:

– Correct RON and MON to ensure knock-free stoichiometric SI operation.

– Correct lean autoignition reactivity.

  - Including sensitivities to ϕ, pressure, and EGR - [O_2].

– High flame speed for lean conditions.

– Low sooting propensity.

– High compatibility with lean aftertreatment.

Possible Efforts for FY19 - 20 (2)

- Perform multimode engine and spray experiments.
  - Quantify thermal efficiency benefits.
  - Determine fuel-property impacts.
  - Provide CFD and chemical-kinetics validation data.
- Perform fundamental studies of lean autoignition.
- Literature review of fuel effects for mixed-mode combustion.
  - Identify requirements for additional fuel property metrics.
- Literature review of proposed lean fuel autoignition metrics.
  - Assess viability.
  - Propose enhanced metrics/methods.
- Inform stakeholders before RON95 plans have been finalized.

Possible Discussion Points

- Importance of having clear fuel scenarios?
- Exclude any advanced combustion strategies mentioned here?
- What aspects of Boosted SI efforts should be duplicated here?
- Tiered screening of blendstocks?

What does DOE consider high impact?

Informing RON95 effort?

Additions to Merit Function?

Demonstrating high MPG?

Finding viable blendstocks?

Recommendations for new fuel property metrics?

Predictive modeling of lean SI operation?