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COMBUSTION RESEARCH FACILITY

Bridging the Gap between Stoichiometric Knock Limits and Autoignition Reactivity for Lean Mixed-Mode Combustion

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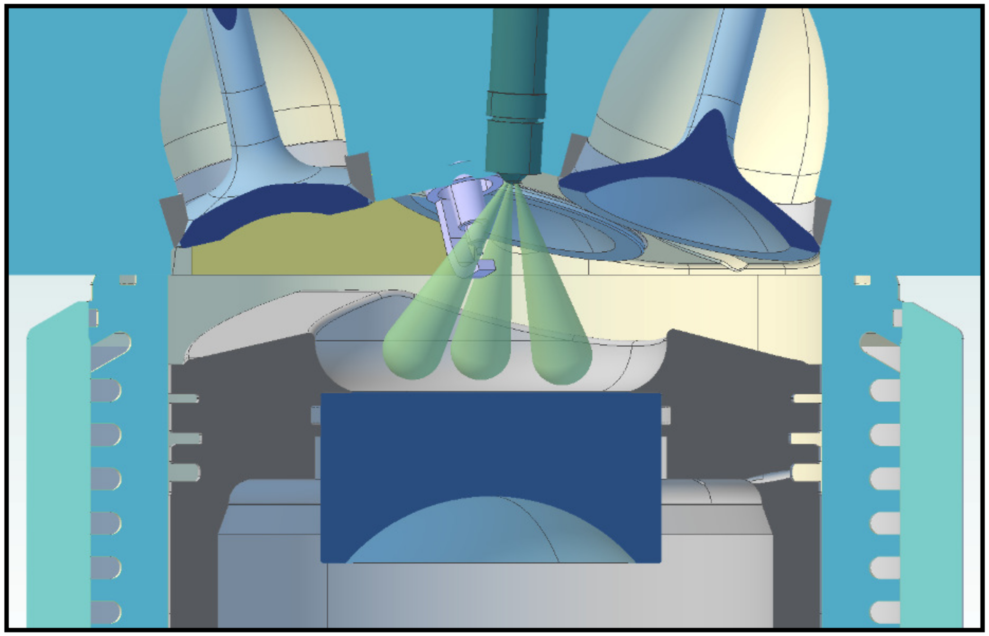
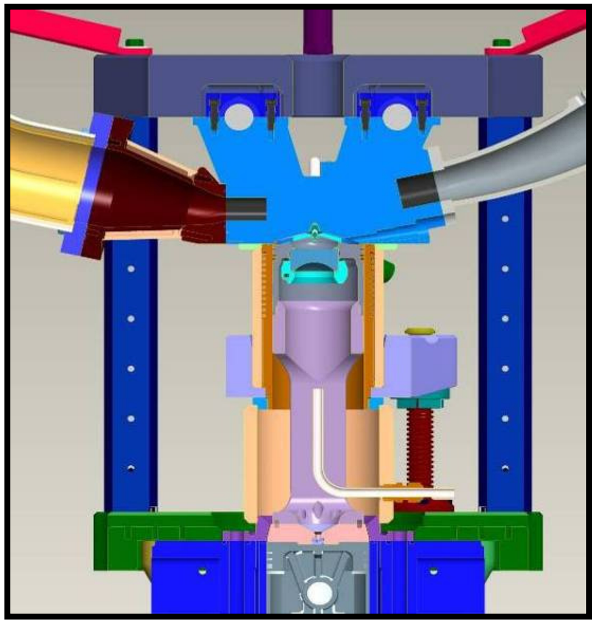
U.S. DEPARTMENT OF ENERGY

Co-Optimization of Fuels & Engines

Research Engine Characteristics

- DISI, CR = 12:1.
- 0.55 L displacement.
- High-swirl operation.
  - Single intake valve.
- Low residuals.
  - No valve overlap.
- Stoichiometric knock:
- KL-CA50 measured at 1400 rpm.
- Conventional High-Energy Ignition System used.
- Well-mixed charge operation.
  - 3- or 4- injection strategy for low PM emissions.
- New ultra-lean data:
  Partial Fuel Stratification.

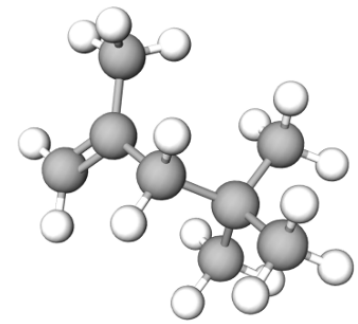




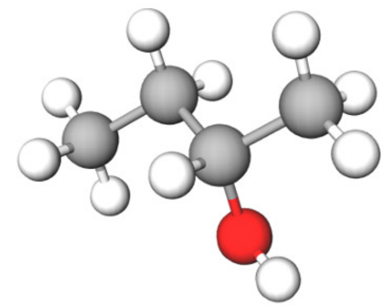
Tier III Blendstocks

- Isobutanol, 2-butanol, and diisobutylene chosen for blendstock evaluation in the DISI engine
  - Based on information available at 2017 Jan, Co-Optima All Hands meeting
- NREL 4-component surrogate used as “gasoline” blendstock
- 98 RON level targeted by varying blendstock volume fraction – via interpolation of NREL RON data
  - Interpolation worked well, with all blends coming in on-target

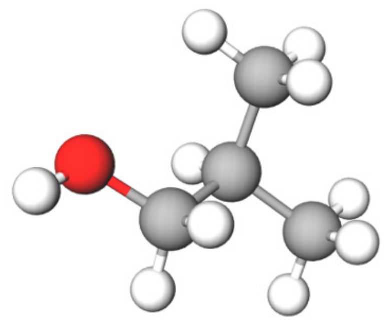
2,4,4-trimethyl-1-pentene



2-butanol



iso-butanol



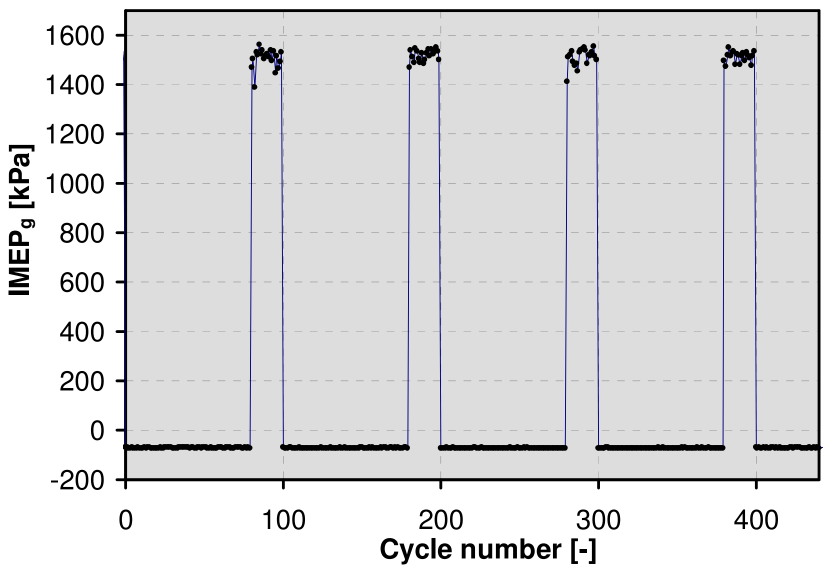
	Volume Percentages [%]						
	Tier III Blendstock	NREL BOB	RON	MON	S	RON Target	MON Target
2-Butanol Blend	28.4	71.6	98.2	89.1	9.1	98	89.4
Diisobutylene Blend	19.6	80.4	98.3	88.5	9.8	98	87.9
Isobutanol Blend	24.1	75.9	98.1	88.0	10.1	98	87.8

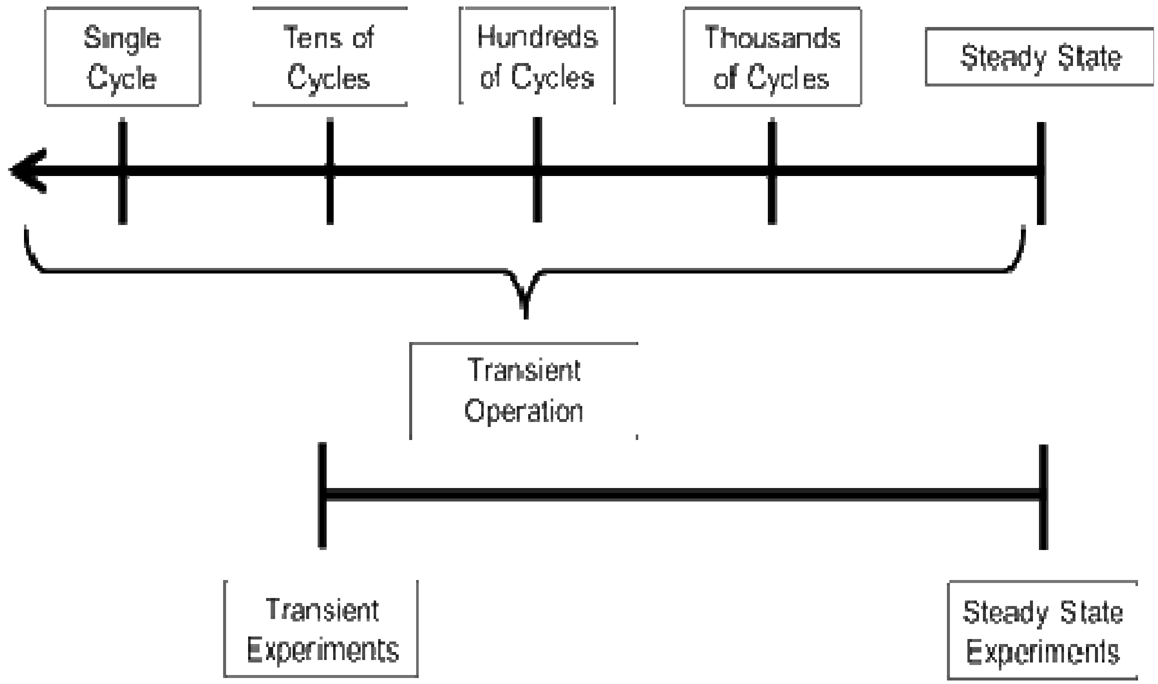
Co-Optima Core Fuels Matrix + RD5-87

- Customer selects fuel based on AKI or RON.
- However, RON and MON are both important.
- Here, study five RON = 98 fuels, and one regular E10 gasoline.
- S = RON – MON.
- Octane sensitivity and composition vary greatly.

	E10 RD5-87	Alkylate	E30	High Aromatic	High Olefin	High Cycloalkanes
S	7	1	10	11	10	11
RON	92	98	98	98	98	98
MON	85	97	88	87	88	87
Ethanol [vol.%]	11	0	31	0	0	0
Aromatics [vol.%]	21	1	8	31	13	33
Alkanes [vol. %]	49	98	41	46	56	41
Cycloalkanes [%]	11	0	7	8	3	24
Olefins [vol. %]	6	0	6	5	27	2
T90 [℃]	156	106	155	158	136	143

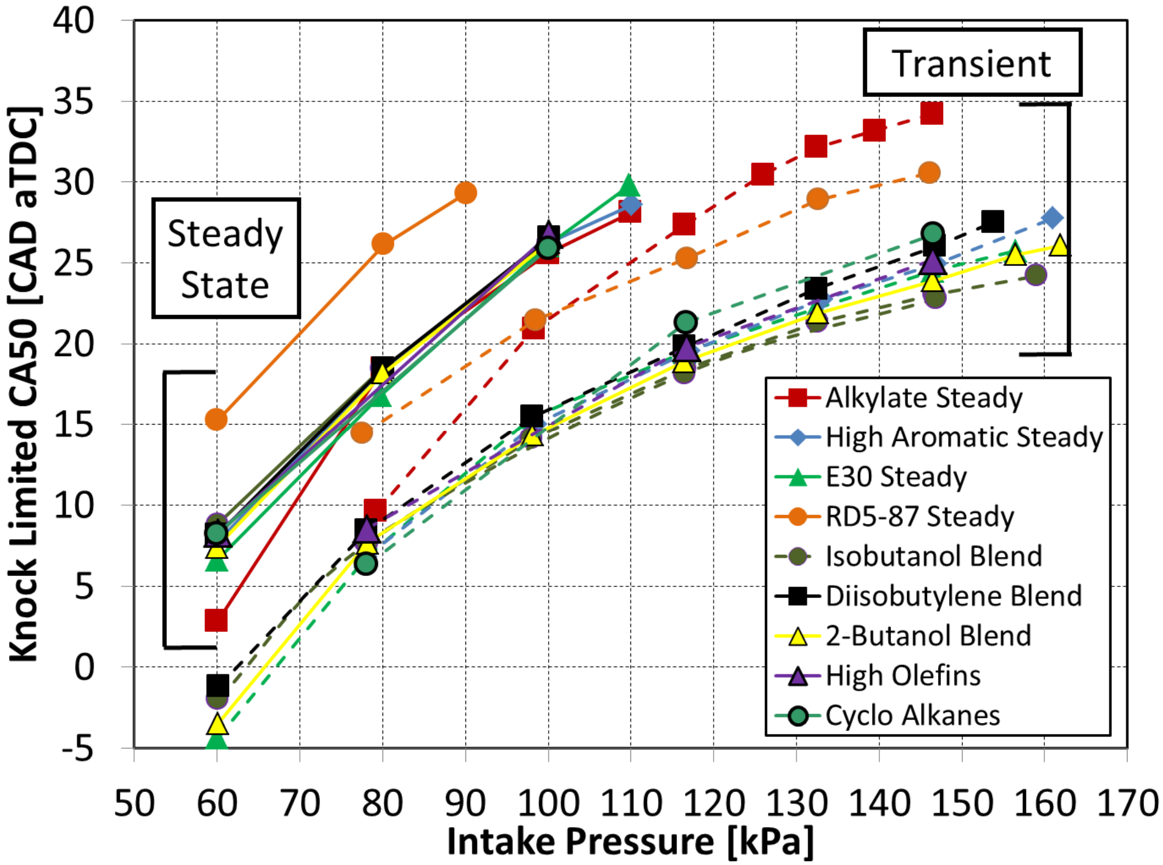
Stoichiometric Test Regimes: Steady State and Transient





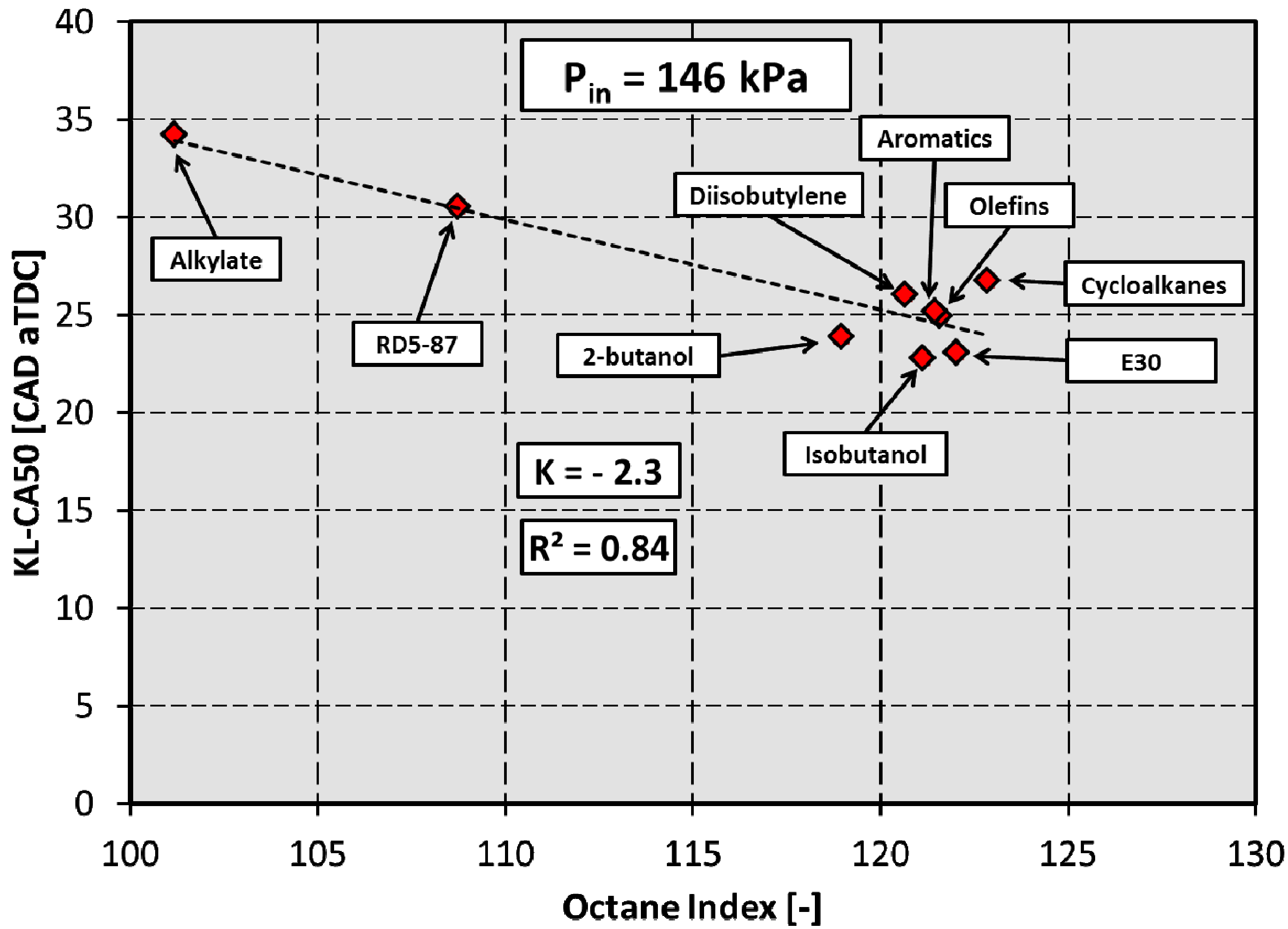
- Steady-state operation reflects knock-limited operation at throttled and naturally aspirated conditions.
- 20/80 load-transient operation allows testing of knock-limited boosted "beyond RON" conditions.
  - Reduced wall temperatures move conditions farther "beyond RON" than steady-state operation at the same intake conditions and engine speed.

Stoichiometric Knock Limits: Steady and Transient



- Hotter Steady-state: All RON98 fuels provide knock suppression benefits, compared to RON92.
- Load Transient: All fuels benefit from the cooler state, but benefit is greater for high-S fuels.
  - RON98 low-S Alkylate fuel is outperformed by RON92 RD5-87 fuel.
  - High-Cycloalkanes fuel underperforms expectations based on RON and S.

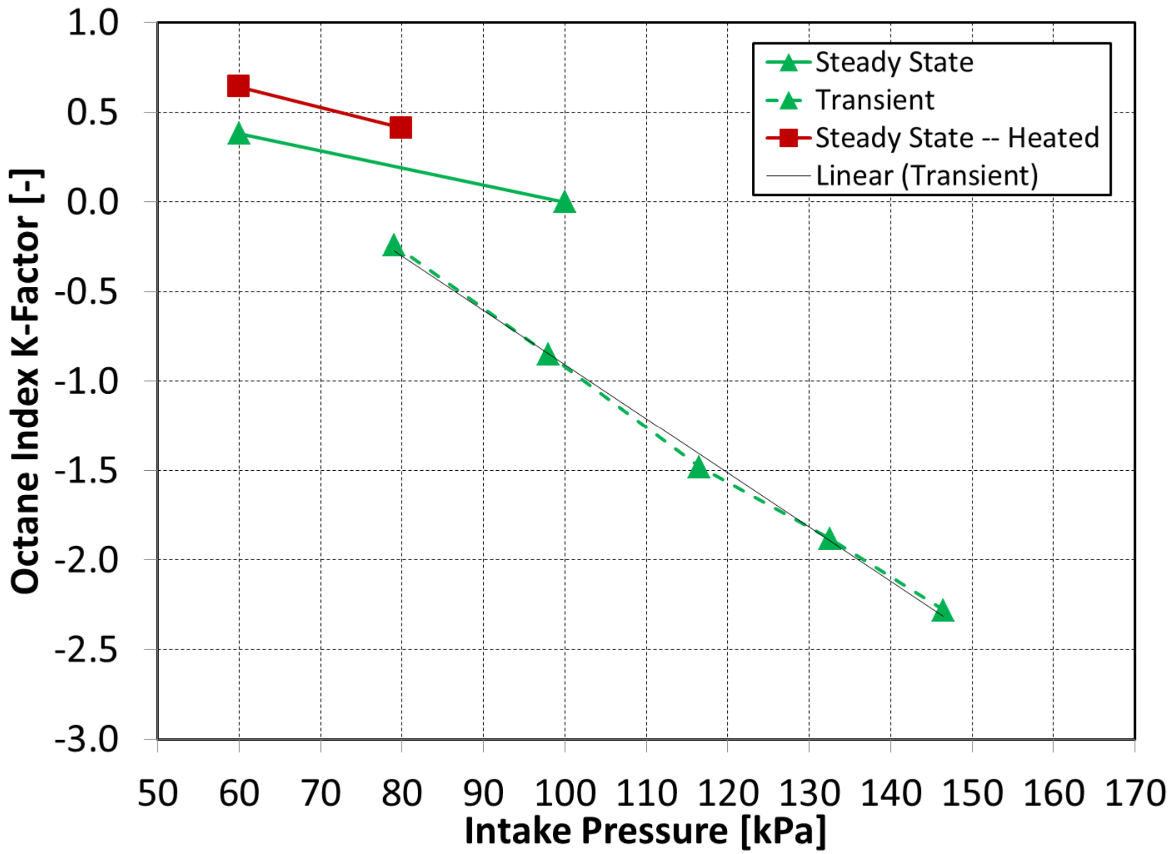
Deviations from OI-based Ranking



- Alcohol blends outperform OI predictions.
- Diisobutylene (iso-octene) and High-Cycloalkanes underperform.

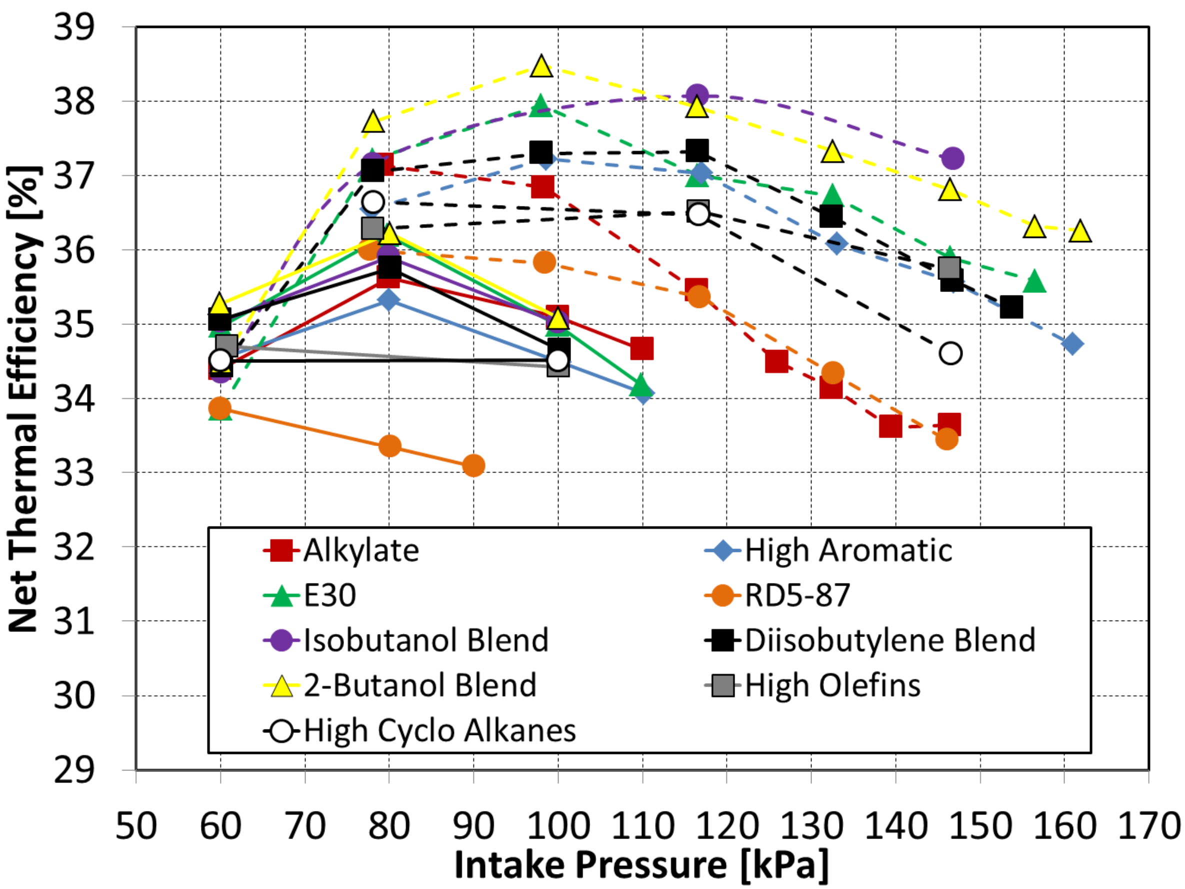
Octane-Index K Factor

- Steady-state operation falls between K = 0 and K = 0.5.
  - T_{in} = 30°C or 90°C
    (90°C data not discussed here, but used to bridge to lean operation.)
- Transient operation result in
  K < 0, "beyond RON" conditions.



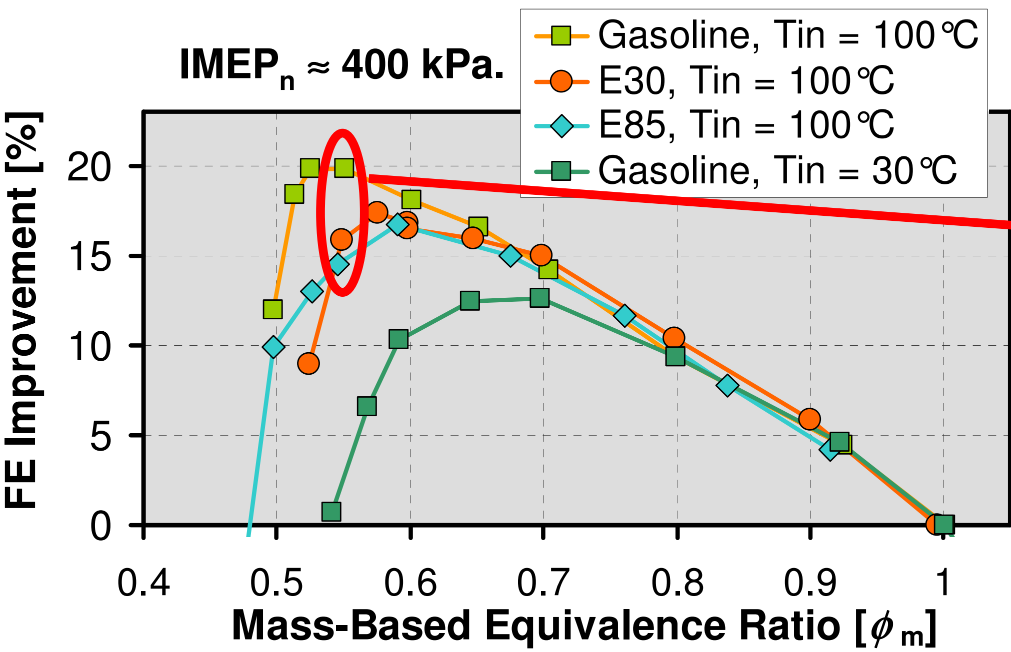
Thermal Efficiency

- For higher loads, thermal efficiency is governed by knock resistance (KL-CA50).
- Higher efficiency is an important benefit for (some) high-S fuels, and justifies further fuels research.
- Focus will now shift to ultra-lean SI operation, for highly efficient operation.



Lean Operation with E85, E30 and Gasoline

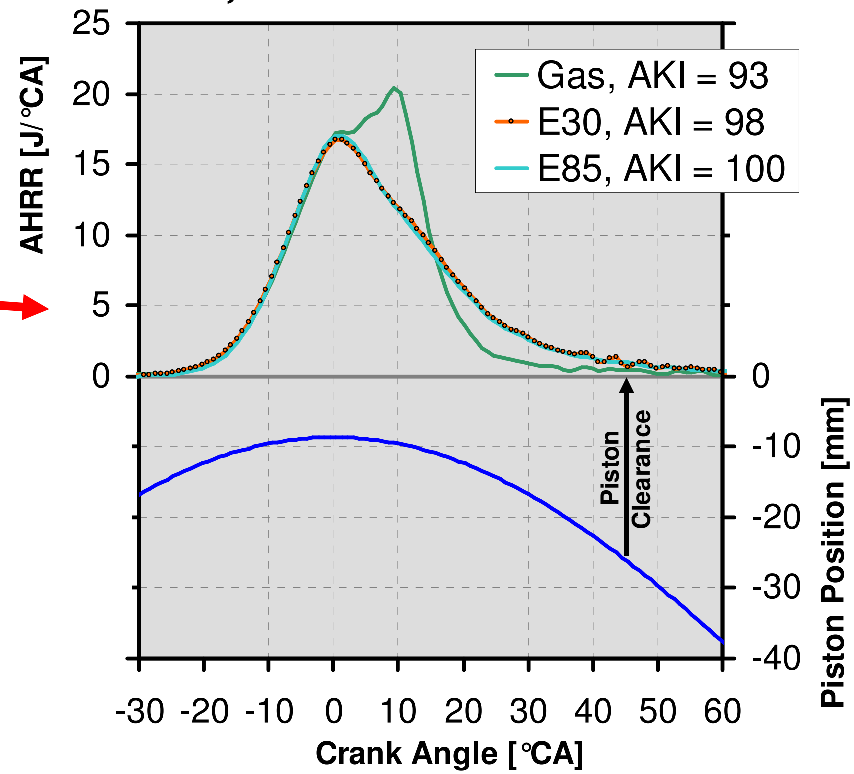
- Lean operation provides efficiency benefits.
- Intake air heating improves lean operation for all fuels.
  - Higher temperature stabilizes early flame development.
  - FE gain is less for E30 and E85. High octane number suppresses beneficial end-gas autoignition.
  - With current hardware, mixed-mode combustion is required for 10-90% duration < 30°CA at ultra-low ϕ.



ϕ = 0.55

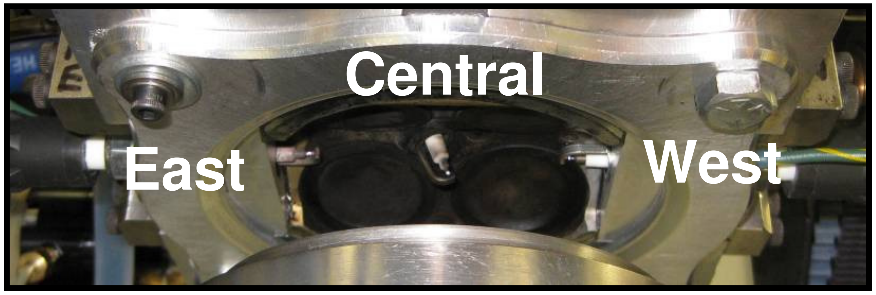
Gasoline: 10-90% = 23°CA.

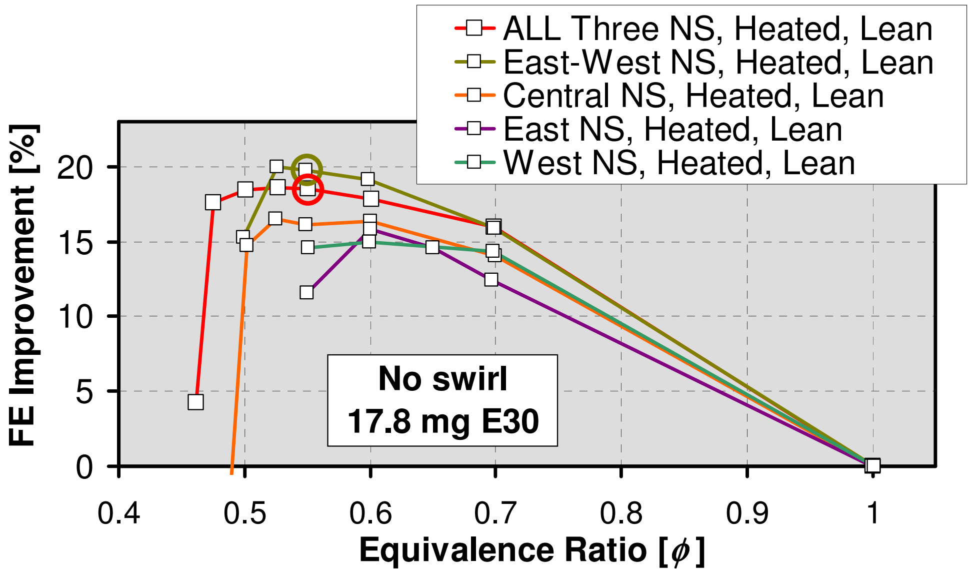
E30, E85: 10-90% = 32°CA.



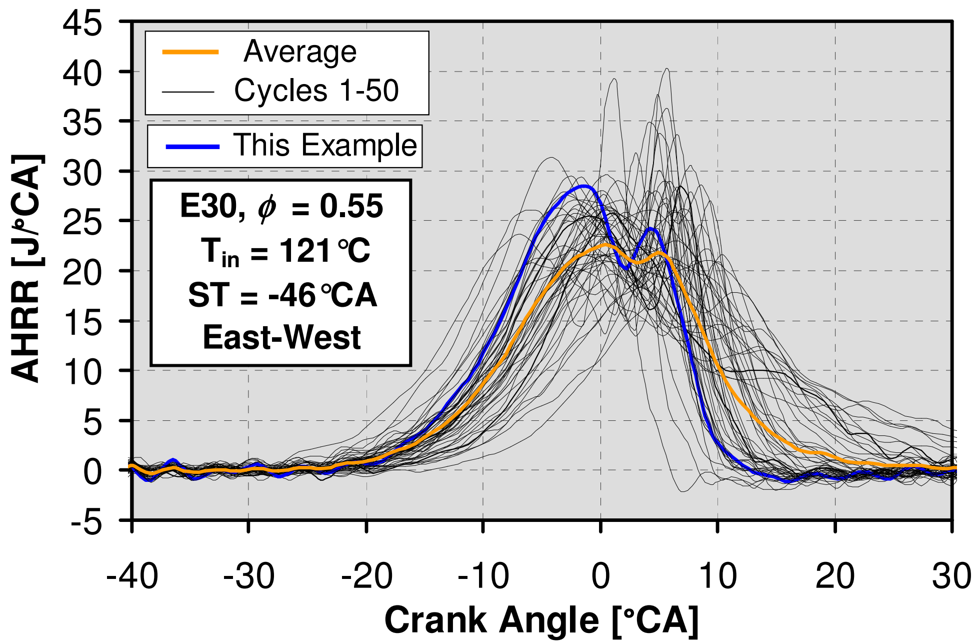
Triple-Spark Setup for Imaging of End-gas Autoignition

- E30 fuel used here was mixed from certification gasoline.
  - RON = 105, MON = 91.
- East-West and ALL scenarios have best TE improvement. Provide sufficient control authority to induce mixed-mode combustion, despite high RON.

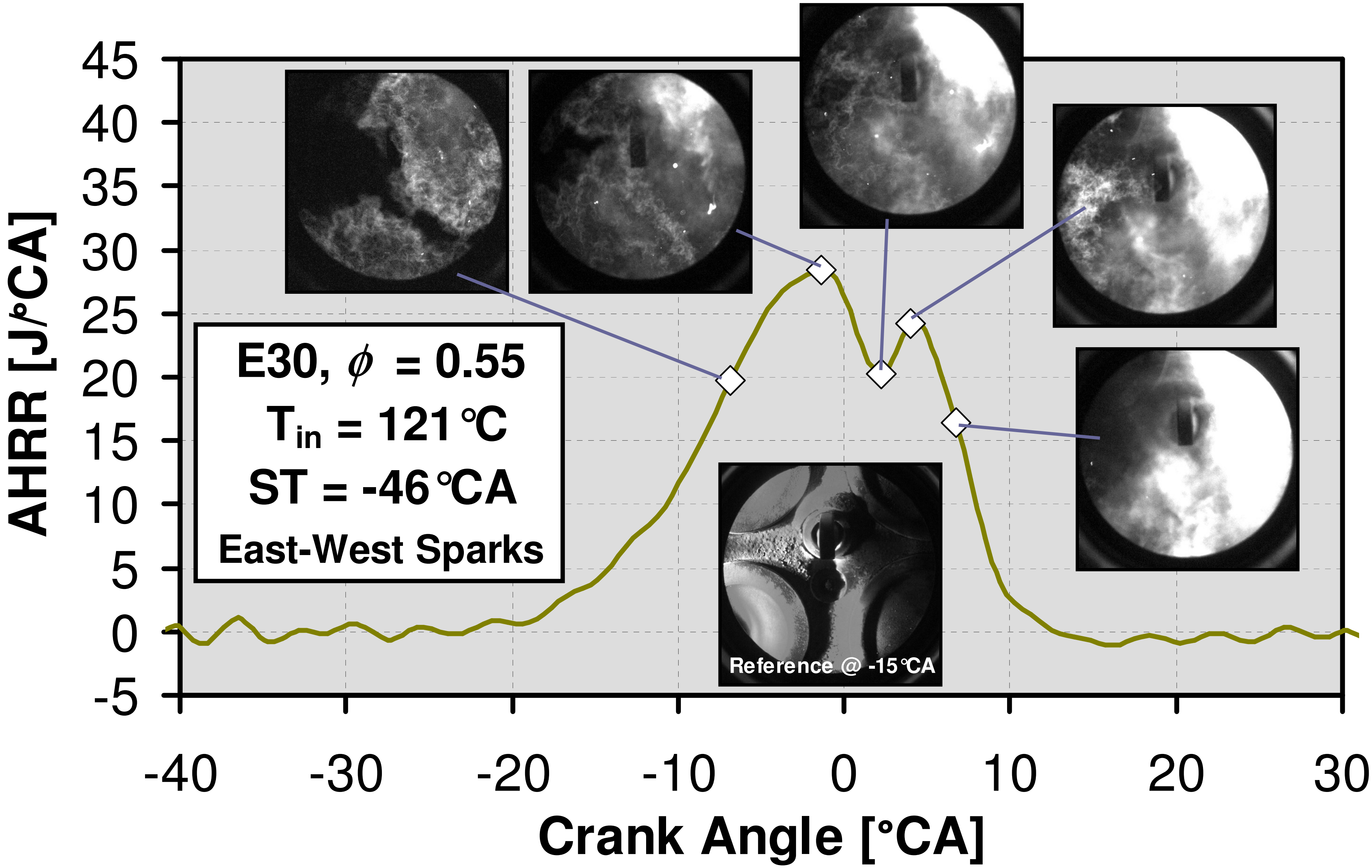




- Performed imaging of:
- ϕ = 0.55, T_{in} = 121℃, no swirl.
- Here, only examine East-West.
  - Multiple cycles with mixed-mode combustion.
- Presented movie is for "blue" cycle.



Imaging of End-gas Autoignition

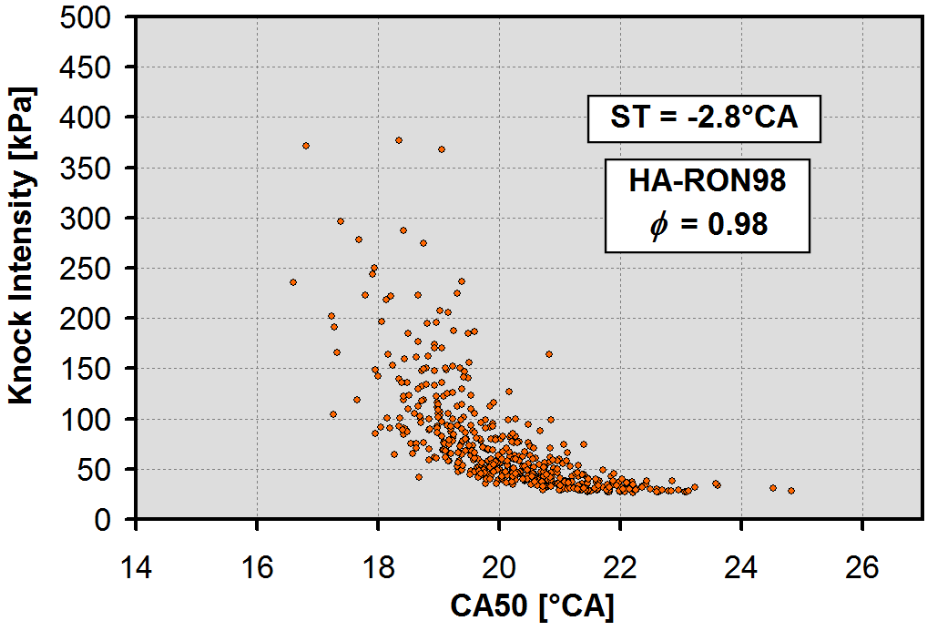


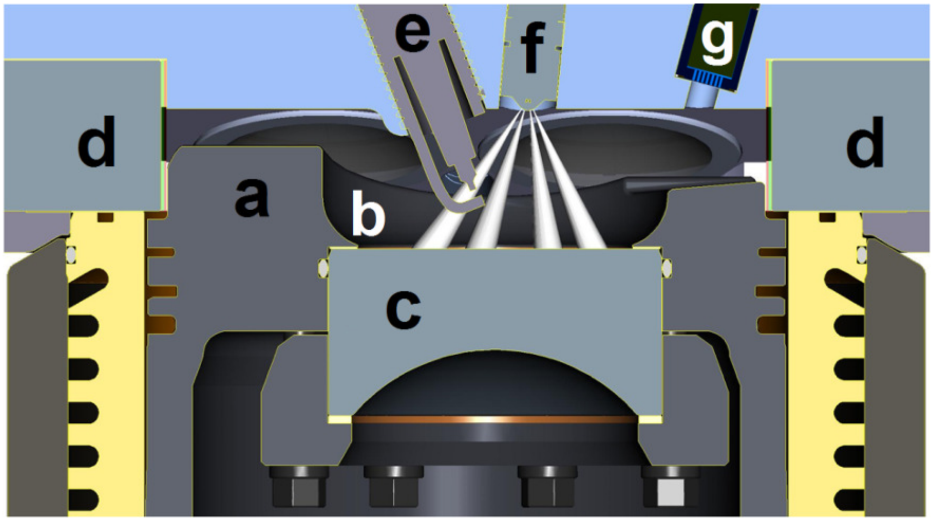
Common Autoignition Metric

- One of current Co-Optima tasks in Sandia Alternative Fuels DISI lab: Assess applicability of octane-index framework for ultra-lean mixed-mode combustion.
- Stoichiometric operation: Knock should be avoided.
- Ultra-lean operation: End-gas autoignition is required for complete combustion.
- $\Rightarrow$ Common metric: Conditions (CA50) for trace autoignition.

Acoustic Knock Intensity vs. CA50

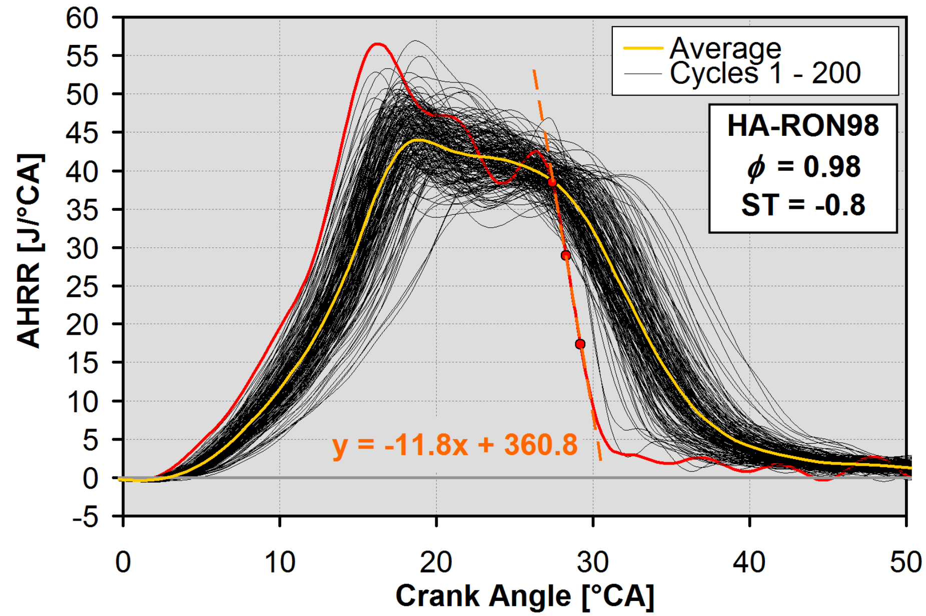
- Impossible to tell when autoignition occurs from KI alone.
- Large vertical spread for a given CA50.
- Need another metric.
- Acoustic knock is essentially a point measurement.

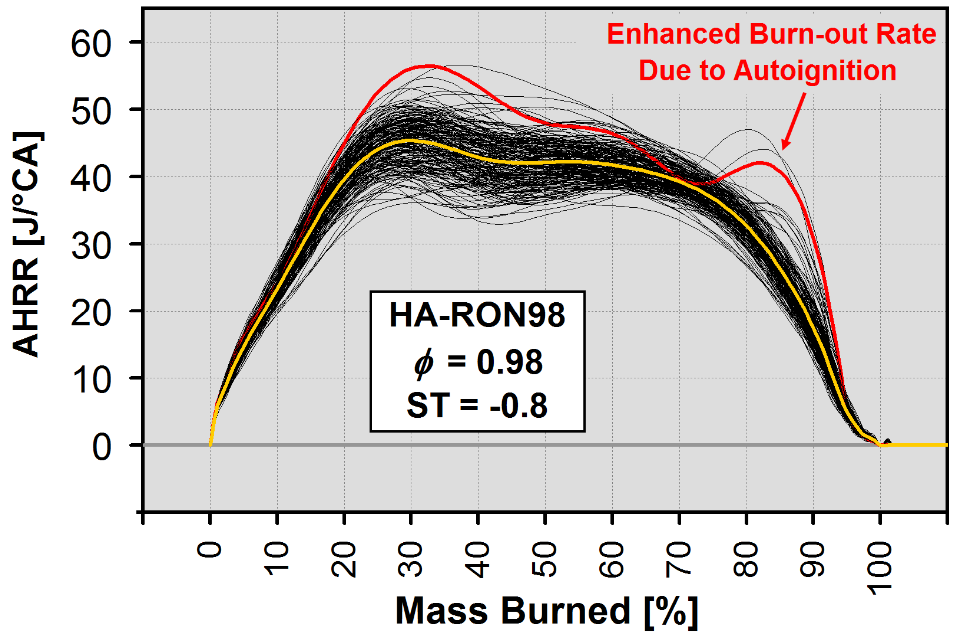




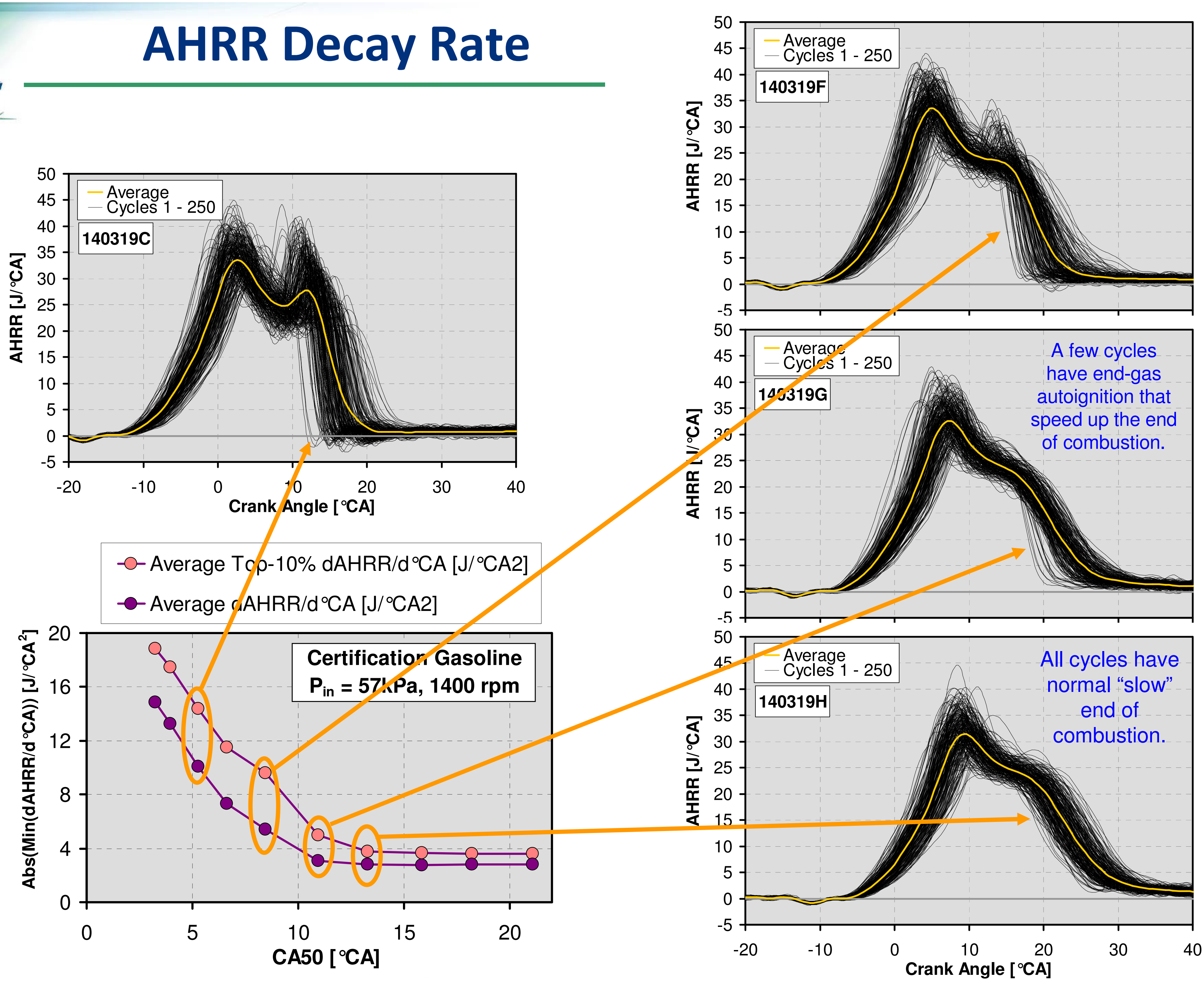
AHRR Decay Rate

- Examination of the AHRR decay rate allows detection of end-gas autoignition.
- Computed from low-pass filtered pressure.
  - Insensitive to orientation of acoustic wave associated with knock.
- The use of AHRR decay rate for knock research was discussed by Borg & Alkidas in SAE 2006-01-3341



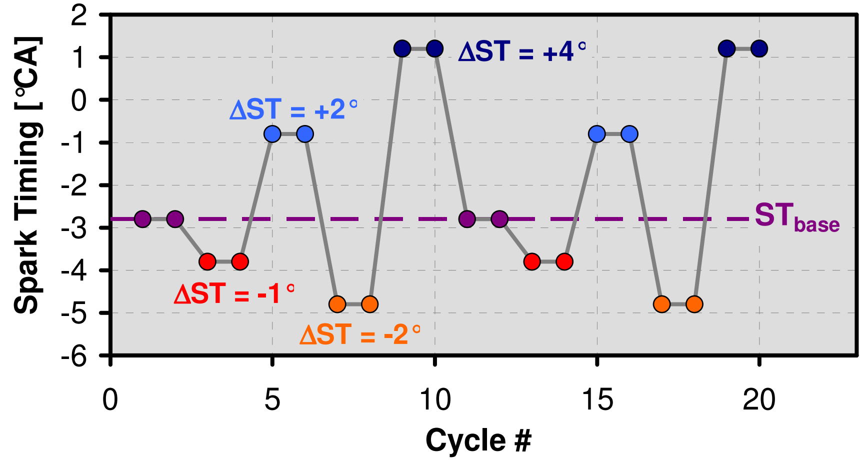


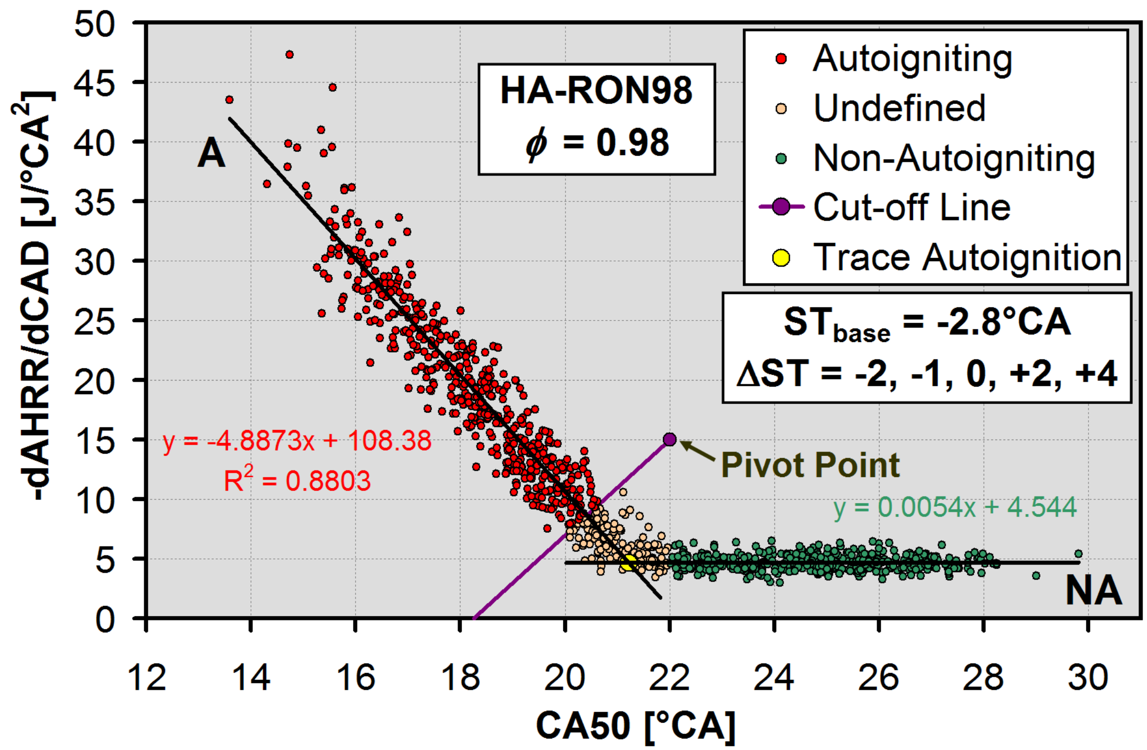
AHRR Decay Rate



Detecting Onset of Autoignition

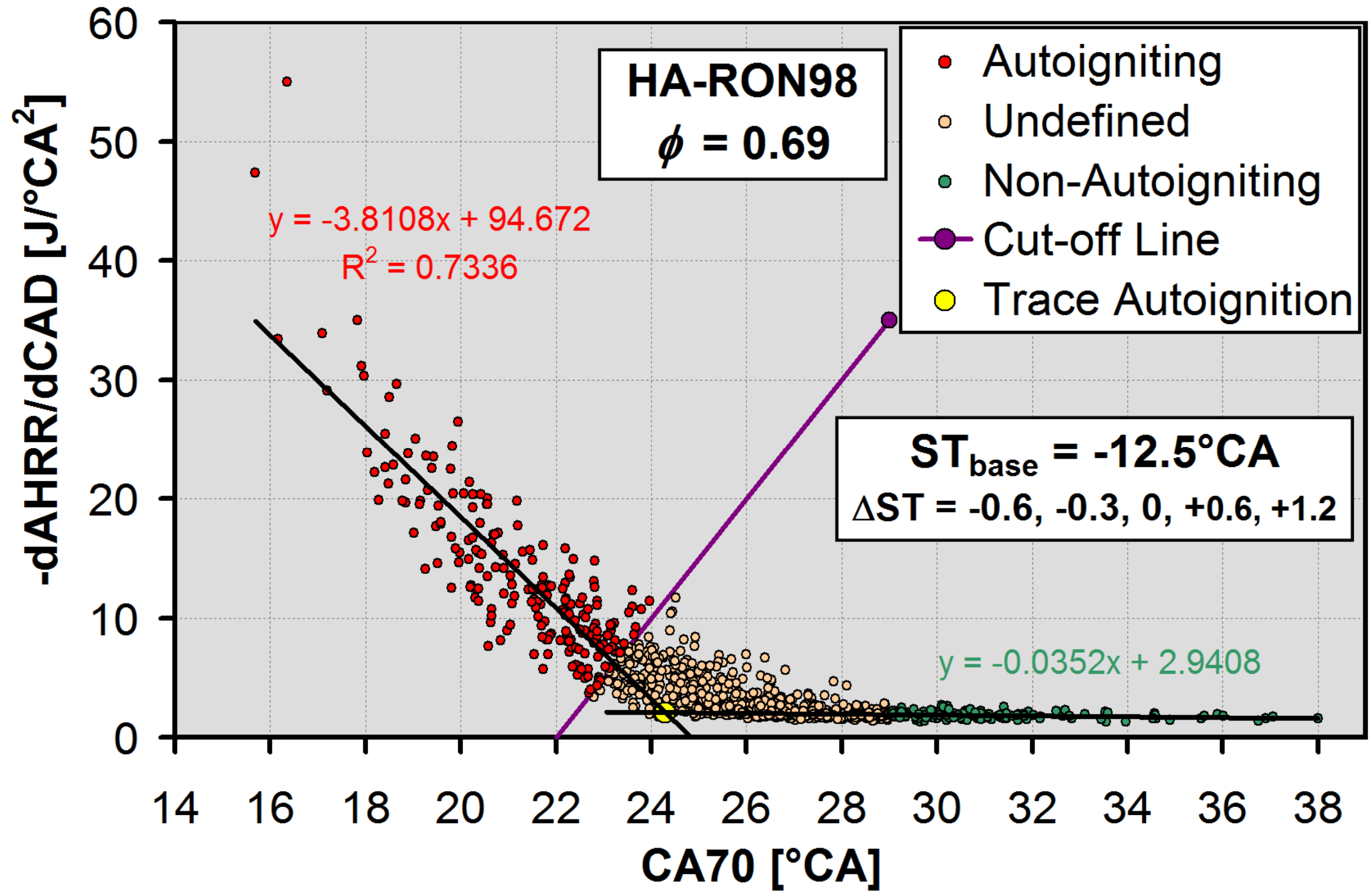
- For each operating point, 1000 extra cycles with alternating ST were acquired.
- dAHRR/d°CA plotted against CA50 creates a very well behaved correlation.
- Use intersection of two linear fits to determine CA50 for trace autoignition.





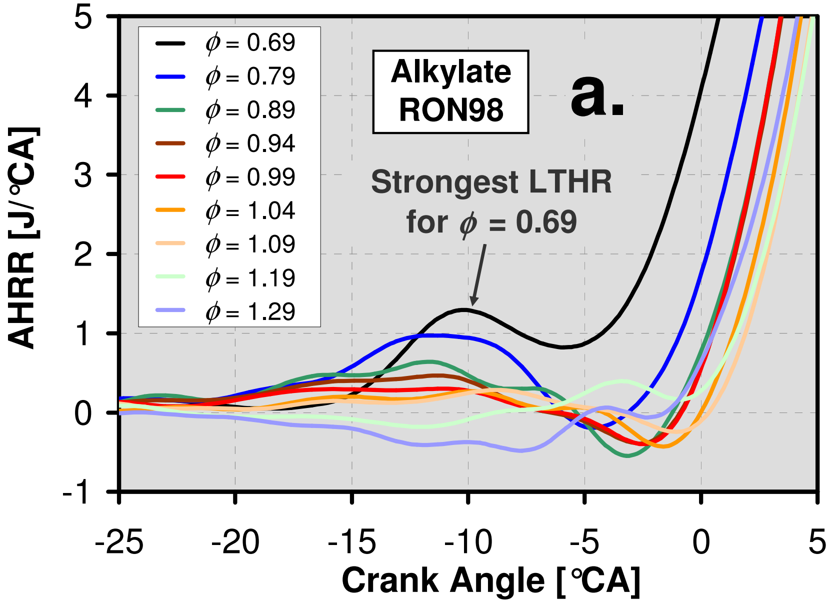
dAHRR/d°CA vs. CA70

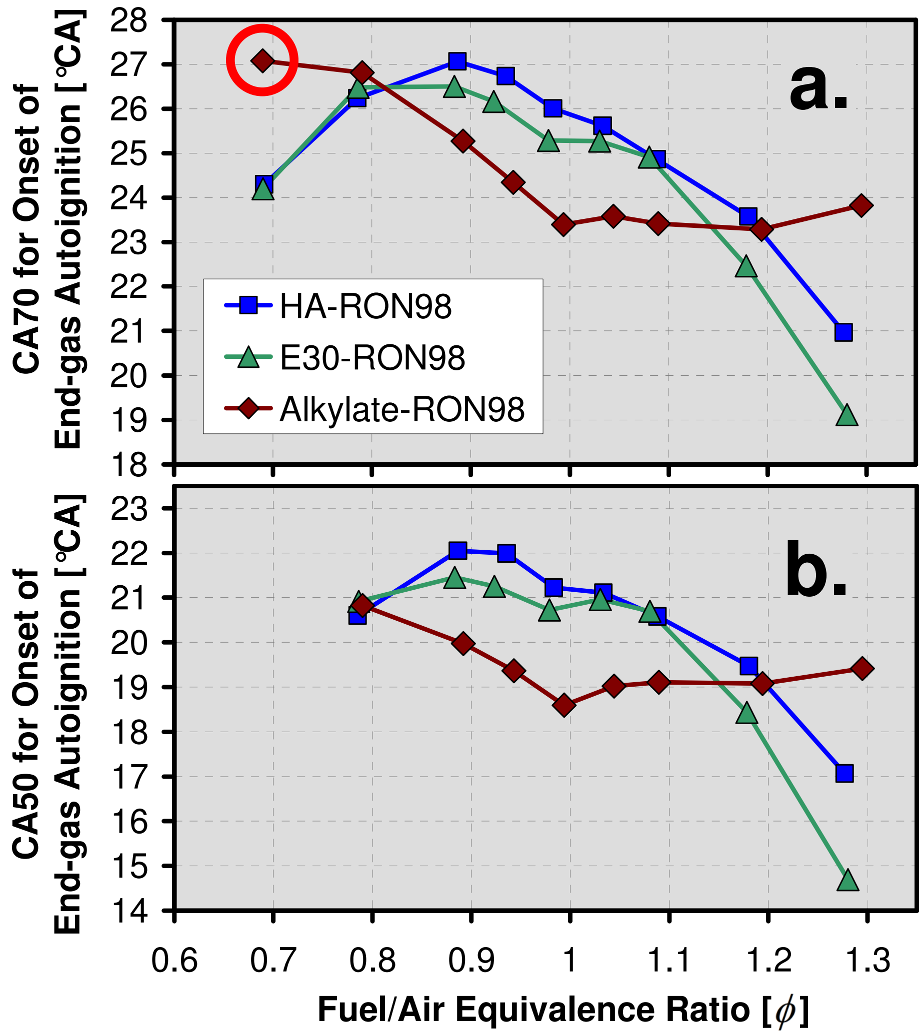
- For ϕ = 0.69, correlating dAHRR/d°CA with CA70 works better.
- CA70 is near the time of end-gas autoignition, so it is a more robust indicator of end-gas compression heating.



Effect of ϕ Around Stoichiometry

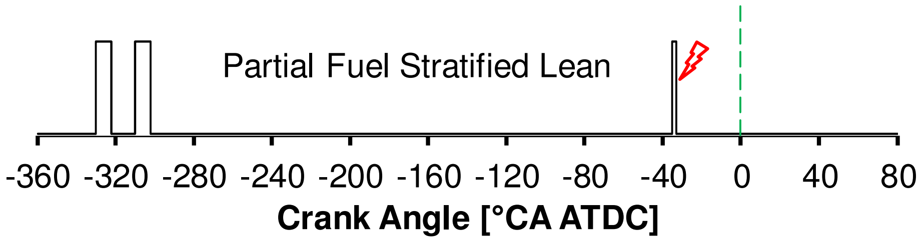
- Fuels show differences in response to changes of ϕ.
- Alkylate shows no benefit of enrichment.
- Lean operation is only detrimental for Alkylate. Increases LTHR.

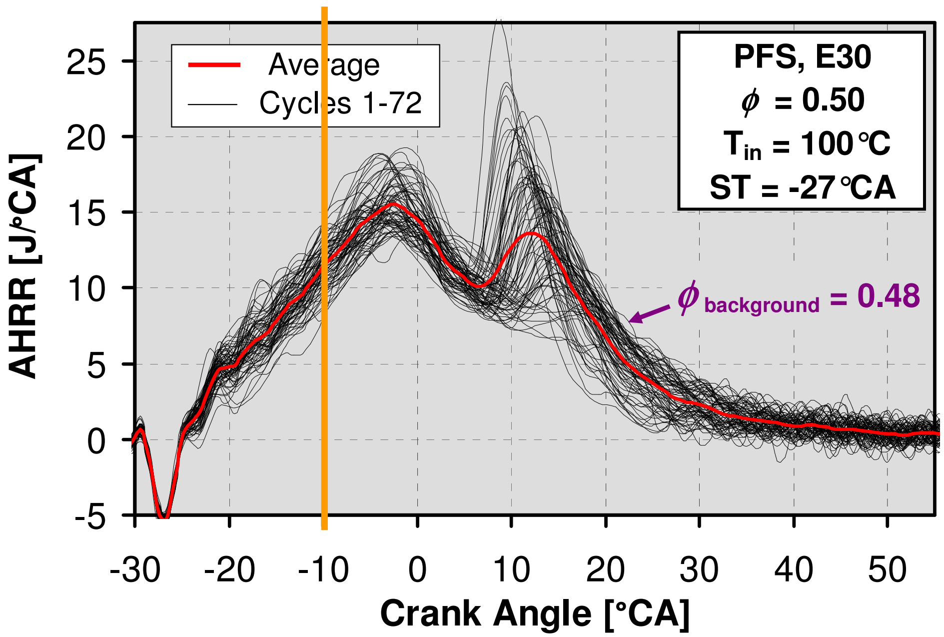


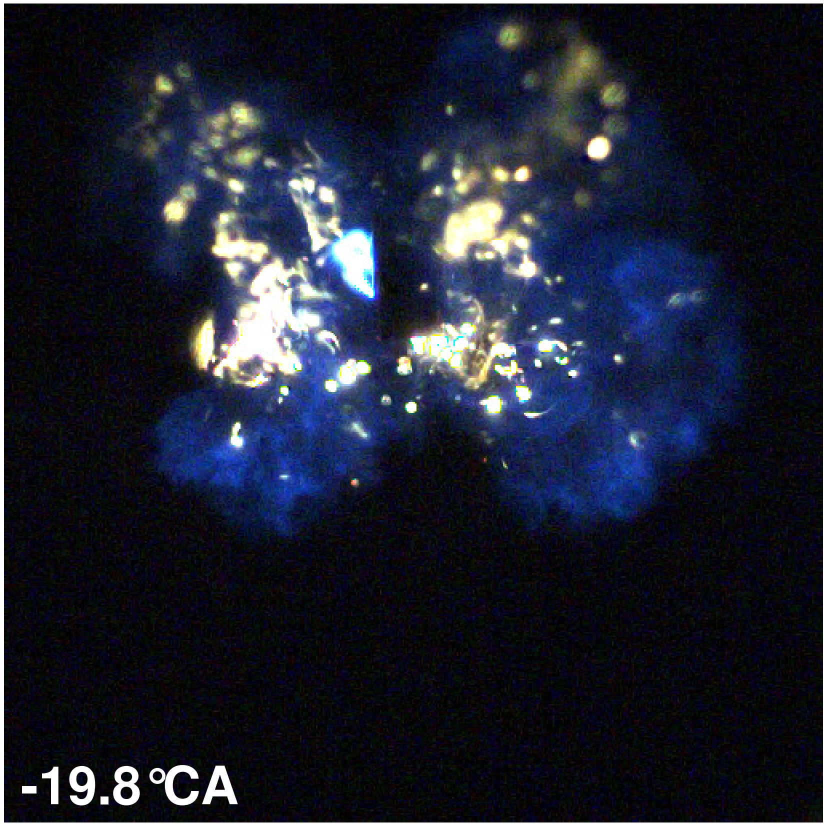


Partial Fuel Stratification for Stable Ultra-lean Operation

- Need to stabilize deflagration to facilitate mixed-mode studies.
- Use small injection at the time of spark.
- Liquid fuel vaporizes quickly.
- Flame spread is relatively slow in the outer parts of the piston-bowl area.
- Flames fronts propagate outside field of view by -10°CA.





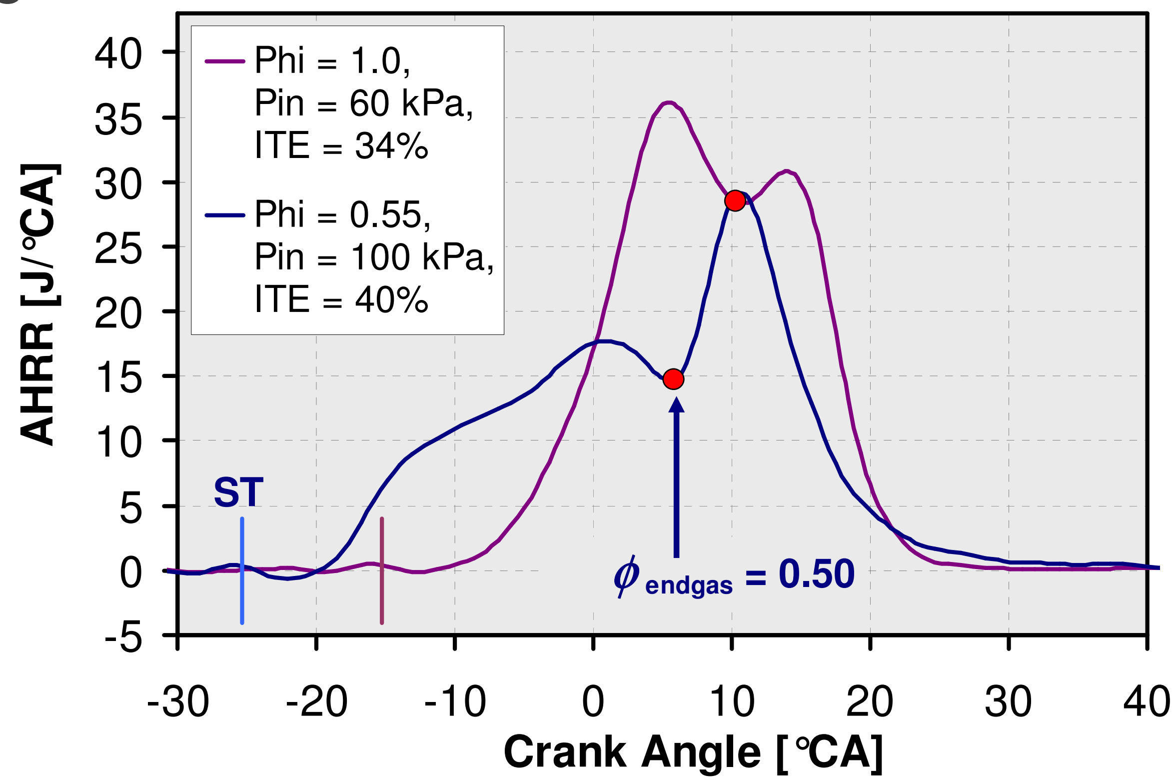


E30 fuel with RON = 105

17.9 + 1.1 = 19.0 mg

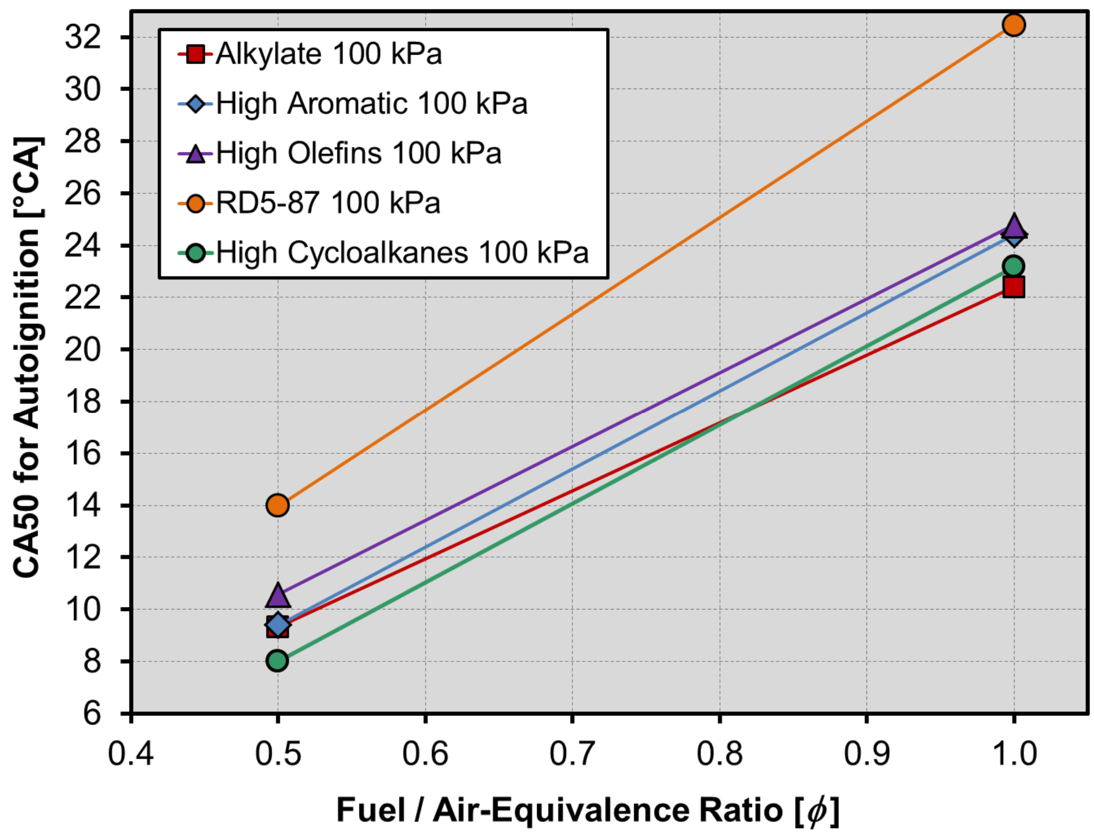
Efficiency Benefit of Lean Operation

- Lean operation provides substantial efficiency benefits, 34 ⇒ 40%.
- $IMEP_n \approx 580$ kPa, 1400 rpm.
- Here, partial fuel stratification uses 1.6mg.
- Early injections provide 17.0 mg, for $\phi_{endgas} = 0.50$
  (Metric used for further slides.)
- 18.6 mg total: $\phi_{global} = 0.55$



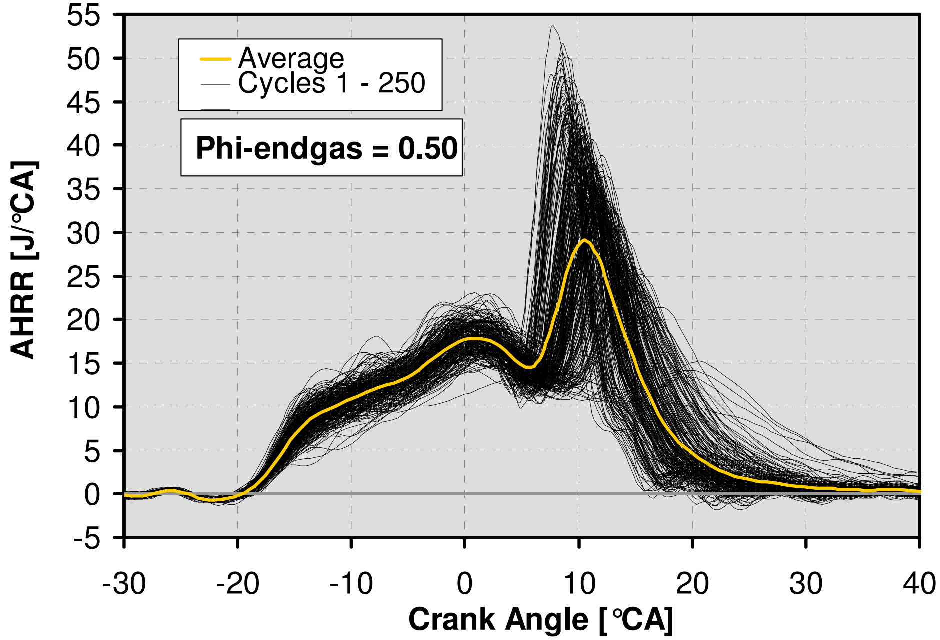
Effect of Equivalence Ratio for P_{in} = 100 kPa

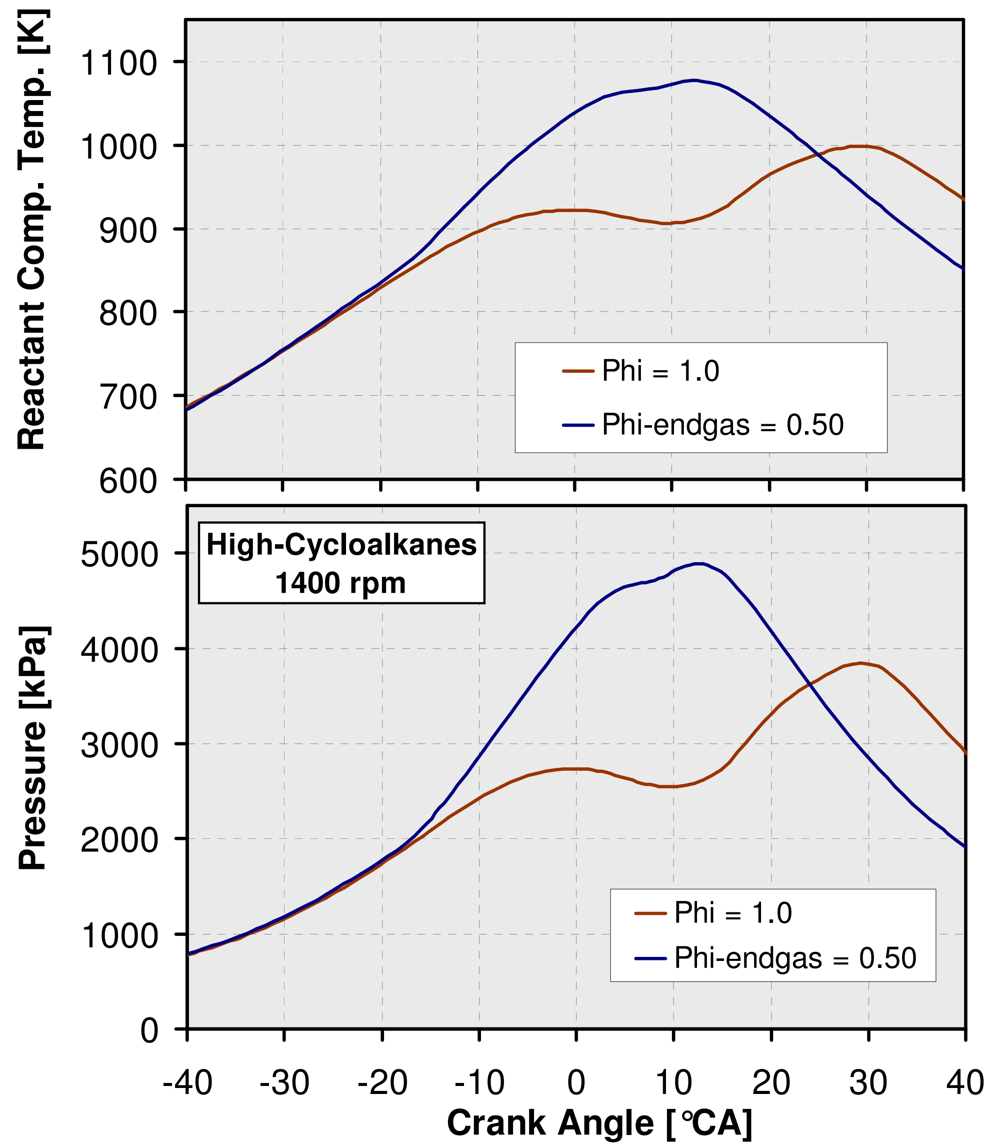
- 1400 rpm, P_{in} = 100 kPa, T_{in} = 90℃. Same for stoichiometric and lean.
- Use CA50 for trace autoignition as reactivity metric for all lean operation.
- For a fixed P_{in} = 100 kPa, ultra-lean operation requires strong advancement of CA50 to ensure end-gas autoignition.
- Small differences in ϕ sensitivities (slopes).



AHRR Variability of Mixed-mode Combustion

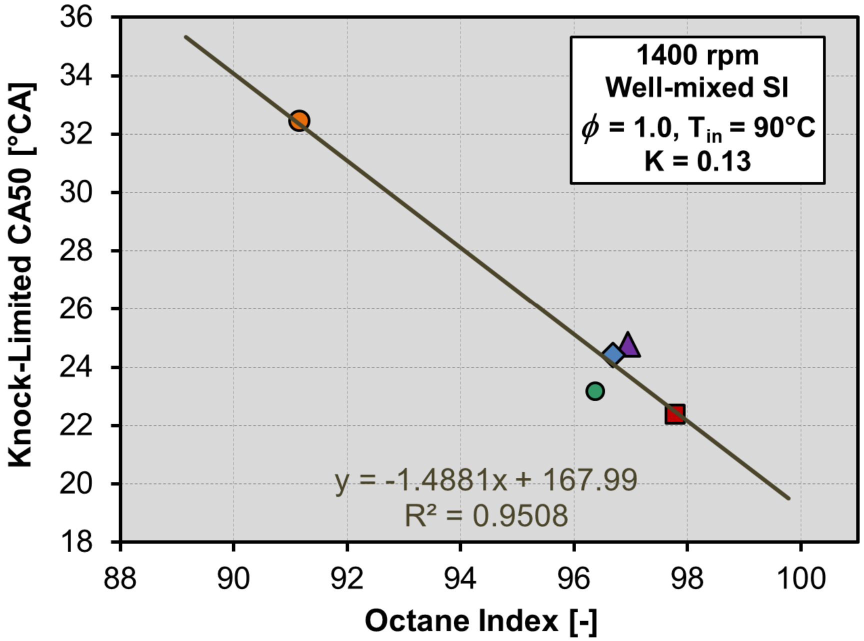
- Ultra-lean operation requires strong advancement of CA50 to ensure end-gas autoignition.
- High combustion pressure induces repeatable end-gas autoignition.
- CSD of IMEP = 0.9%
  (lower than 1.4% of $\phi = 1.0$.)

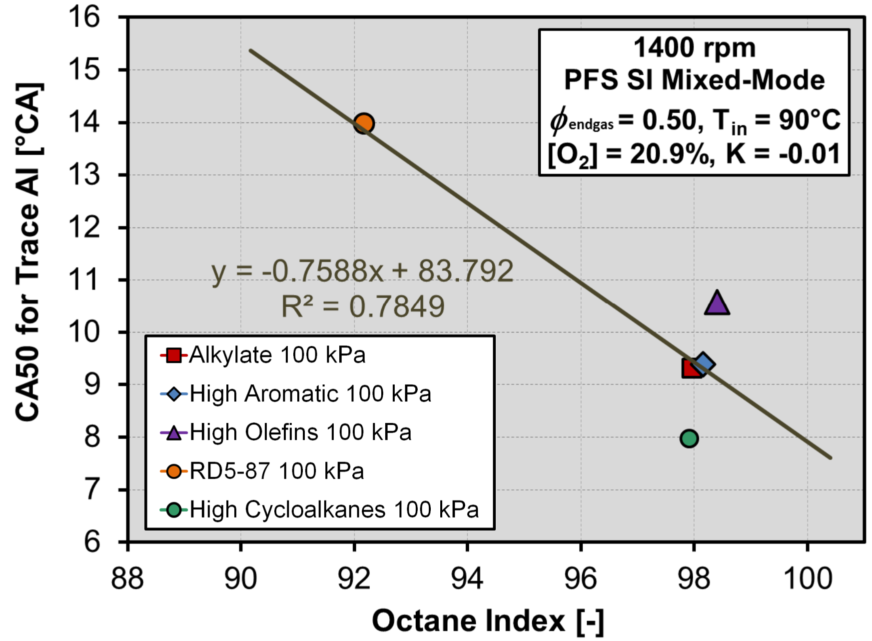




Effect of Equivalence Ratio on K-Factor

- 1400 rpm, P_{in} = 100 kPa, T_{in} = 90℃. Same for stoichiometric and lean.
- The reduction of ϕ from 1.0 to 0.50 decreases K slightly.
- Change of K may not be significant, given that linear fit deteriorates.

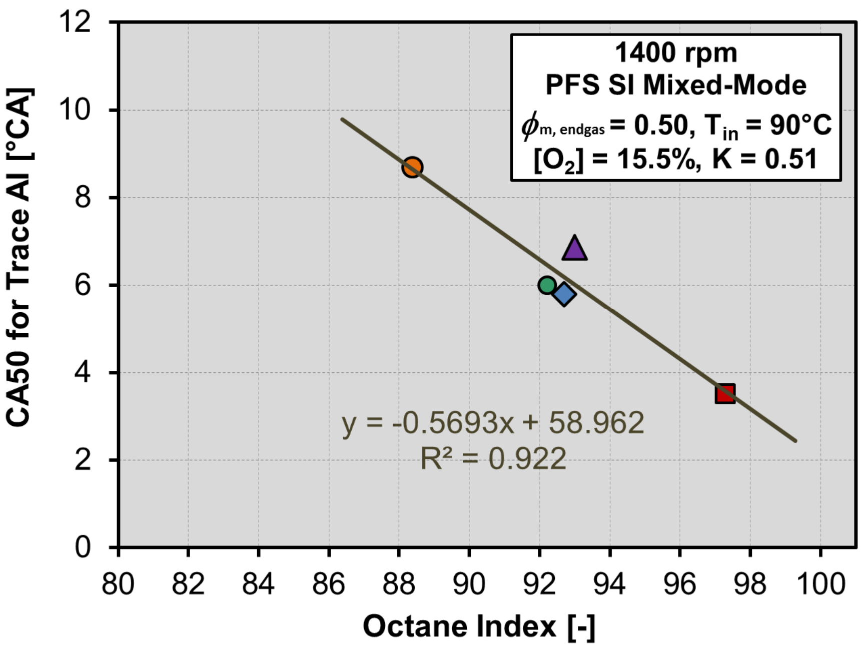


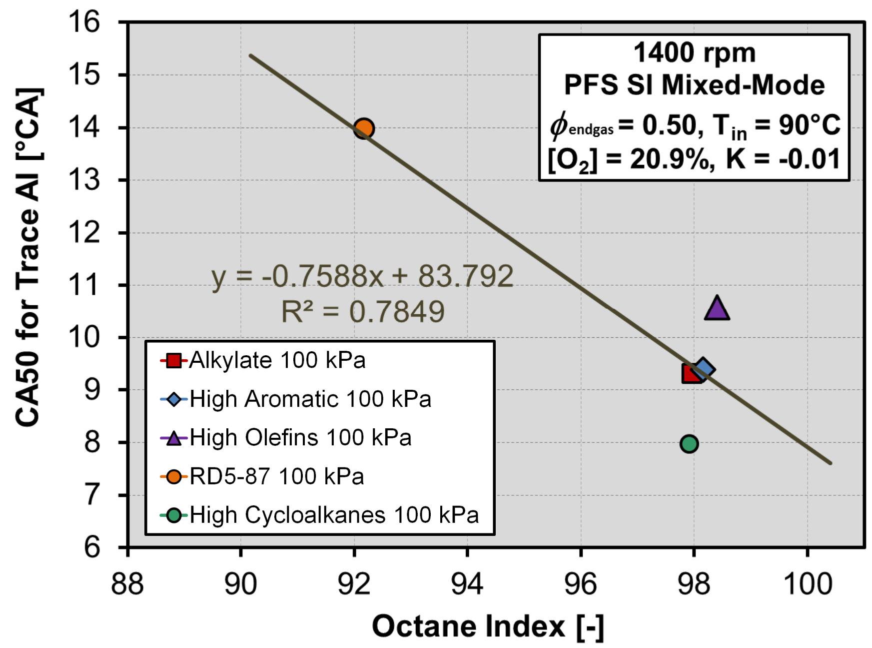


Effect of Intake $[O_2]$ for Mixed-Mode Comb.

- 1400 rpm, P_{in} = 100 kPa, T_{in} = 90℃.
- Use N_2 dilution to simulate $[O_2]$ – reducing effect of retained residuals or hot EGR.
- Fuel/Gas mass ratio maintained constant.

$$\phi_m \equiv \frac{\left(F/C\right)_{Actual}}{\left(F/A\right)_{Stoichiometric}}$$

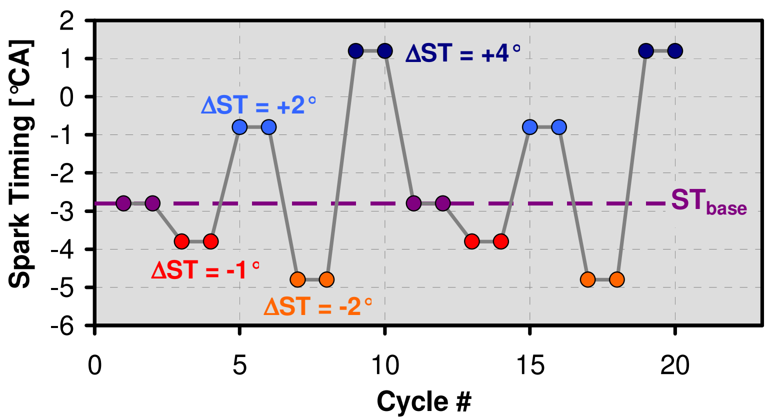


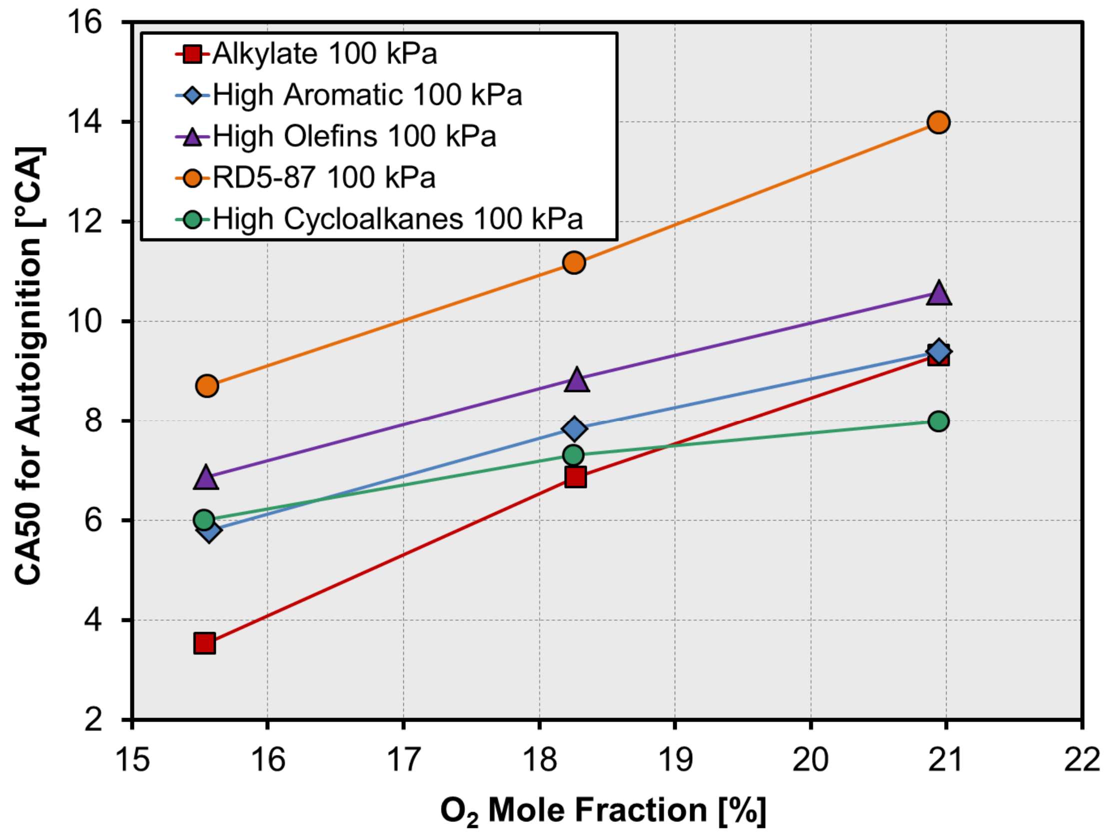


- The reduction of $[O_2]$ from 20.9 to 15.5% increased K slightly.
- Quality of linear fit improved.

Effect of Intake $[O_2]$ for Mixed-Mode Comb.

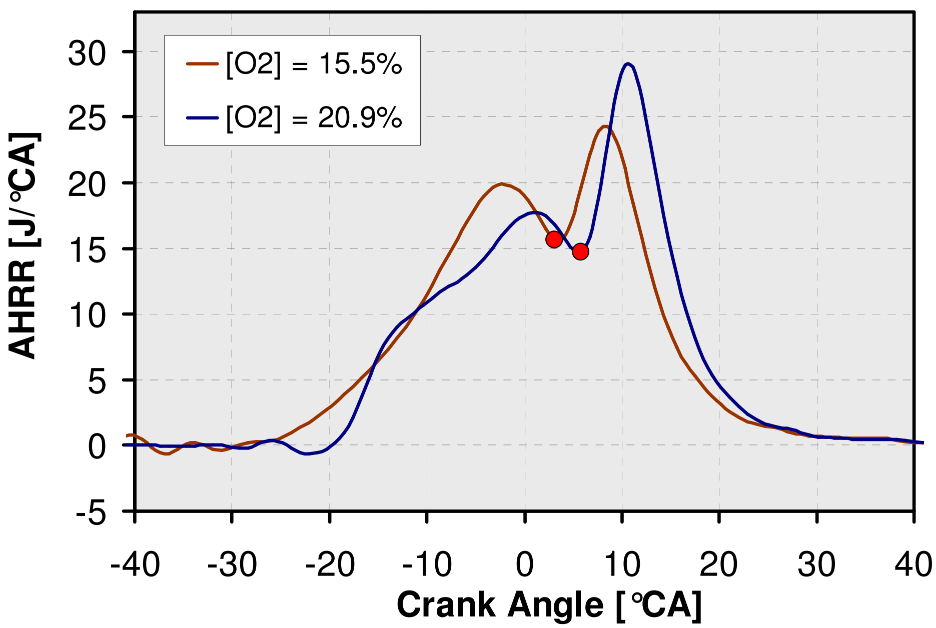
- 1400 rpm, P_{in} = 100 kPa, T_{in} = 90℃, $\phi_{m,\ endgas}$ = 0.50.
- The fuels show different sensitivities to $[O_2]$.
- High Cycloalkane has lowest sensitivity.
- Alkylate and RD5-87 have highest sensitivity.
- Alternate-ST used to induce sufficient variability to determine CA50 for trace autoignition.

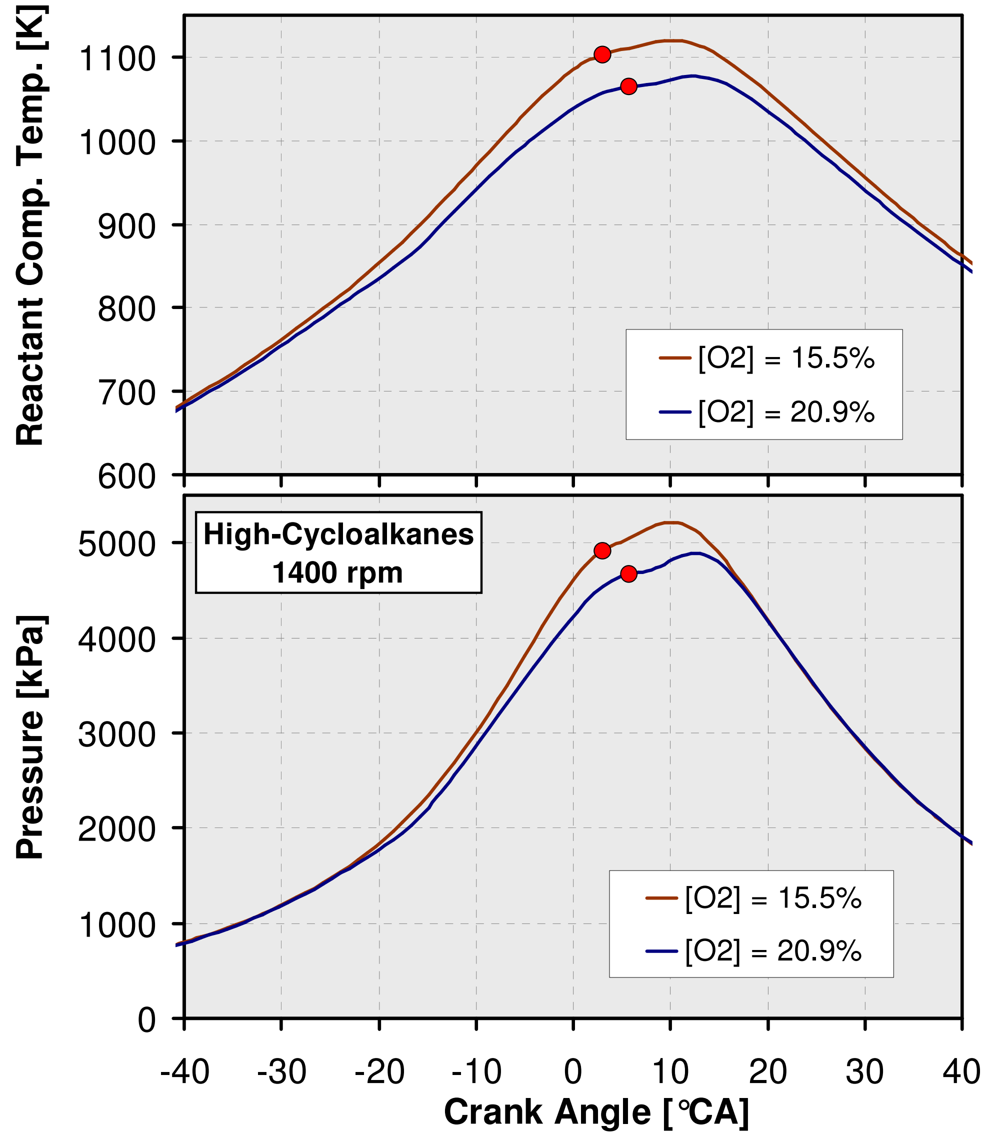




Effect of Intake [O_2] for High Cycloalkanes

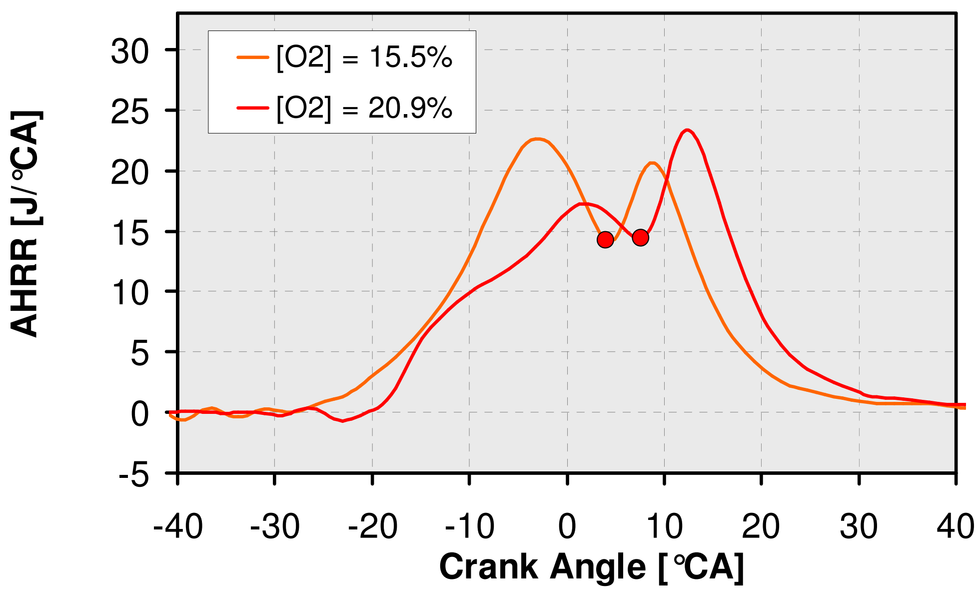
- 1400 rpm, P_{in} = 100 kPa, T_{in} = 90℃, $\phi_{m,\ endgas}$ = 0.50.
- High Cycloalkane has lowest sensitivity to [O_2].
- Relatively small increase of compressed-gas temperature is required to induce autoignition.

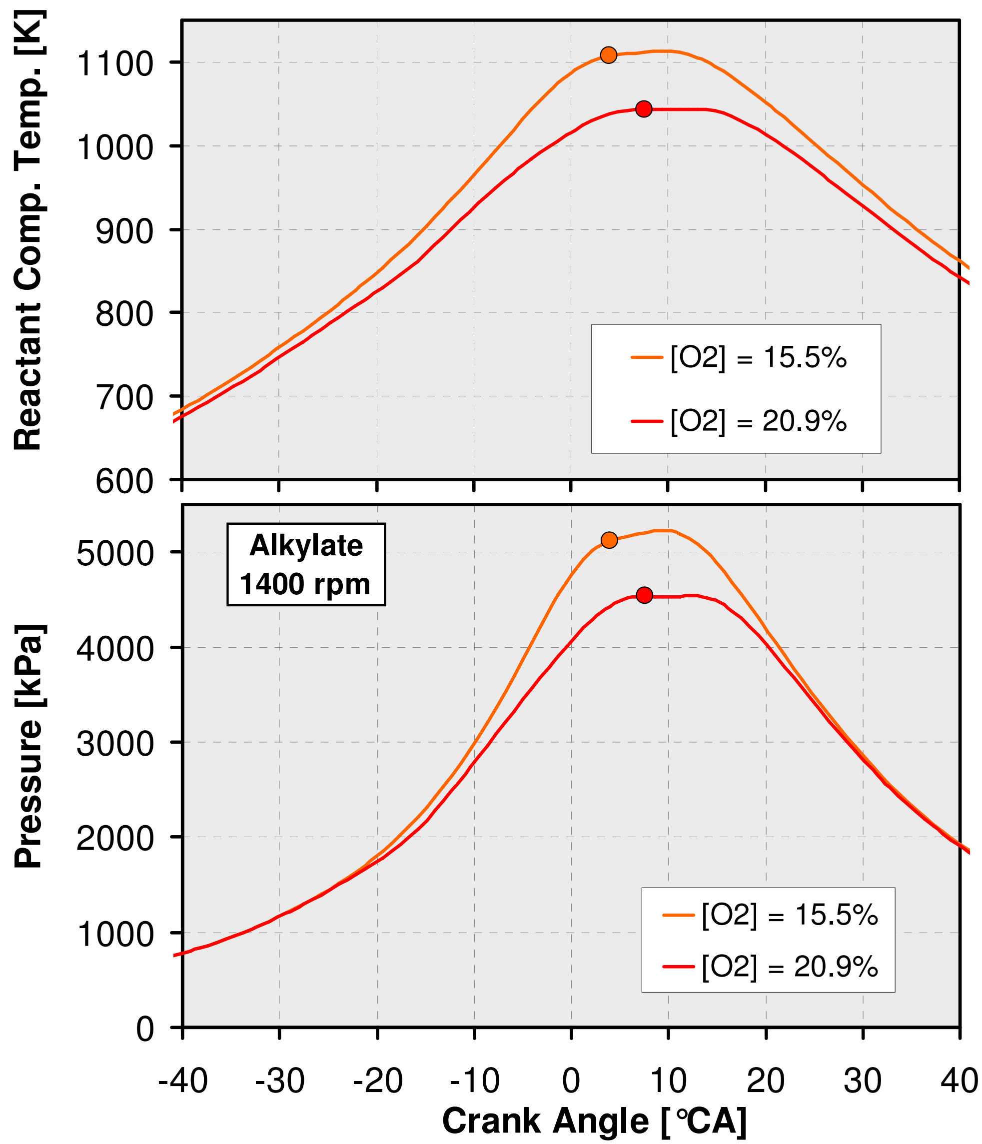




Effect of Intake $[O_2]$ for Alkylate.

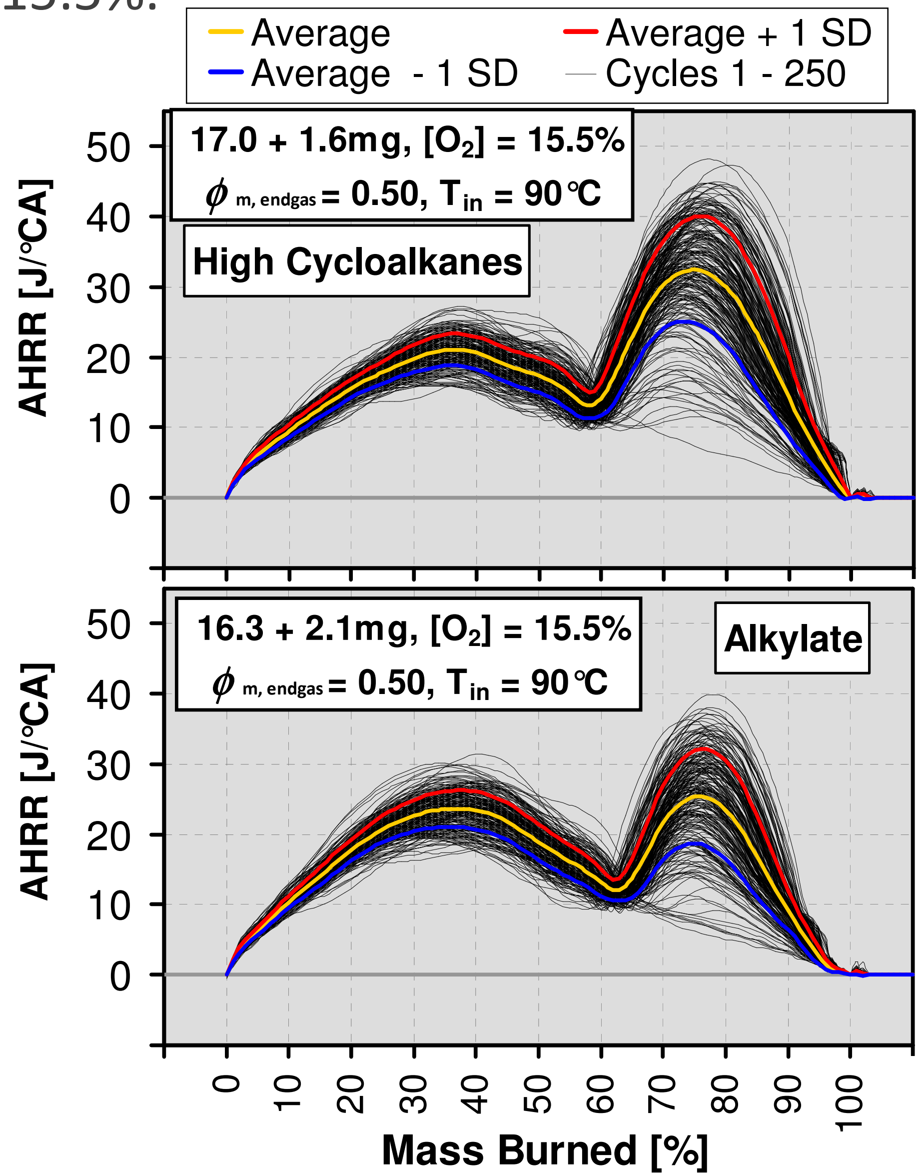
- 1400 rpm, P_{in} = 100 kPa, T_{in} = 90℃, $\phi_{m,\ endgas}$ = 0.50.
- Alkylate fuel has high sensitivity to $[O_2]$.
- Relatively large increase of compressed-gas temperature is required to induce autoignition.





Differences in Combustion Stability

- Compared to High Cycloalkanes, Alkylate fuel has tendency for higher cycle-to-cycle variability at $[O_2] = 15.5\%$.
- Due to lower inherent flame speed of Alkylate?
- Due to required earlier CA50?
- Or both?
- Here, compensate partly by increasing pilot from 1.6 to 2.1 mg.
- CSD of IMEP:
  - 1.8% for Alkylate.
  - 1.2% for High Cycloalkanes.
- Residual mass fraction ≈ 4%, but still important.
  - Especially for load-transient operation.
- Future work will shed more light on this.



Conclusions

- Load-transient operation results in significantly improved KL-CA50's relative to steady-state performance for all tested fuels.
- Boosted conditions lead to "beyond RON" conditions in which high-RON, high-S fuels exhibit improved performance over a high-RON, low-S fuel.
- The use of partial-fuel stratification is very effective in stabilizing ultra-lean SI operation.
  - Allows parametric fuels studies of lean autoignition.
- Differences are observed between fuels in sensitivity to equivalence ratio and intake [O_2].
- The octane-index is applicable to first order, even for ultra-lean mixed-mode combustion.
- Quality of linear regression varies with conditions.
- Future research will expand to slightly boosted operation, and address effect of residuals.

Acknowledgements

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