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COMBUSTION RESEARCH FACILITY

Applicability of the Octane-Index Framework for Stoichiometric and Lean End-gas Autoignition in a DISI Engine

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AEC Meeting

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Abstract:

Nine gasoline fuels have been tested under a wide range of stoichiometric, knock-limited Spark Ignition (SI) combustion conditions. Testing revealed that fuels with matched Research and Motor Octane Number (RON & MON) ratings exhibited similar resistance to autoignition at all conditions, and only showed measurable differences at well "beyond-RON" conditions. An uncertainty analysis of the Octane Index approach to ranking fuels was completed, and under the farthest from RON condition tested, the Octane Index described approximately 85% of the observed variation between the fuels. The focus of the project is now shifting to understanding fuel autoignition behavior under lean and dilute conditions, using the same palate of fuels.

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Mike Weismiller, Alicia Lindauer

U.S. DEPARTMENT OF ENERGY

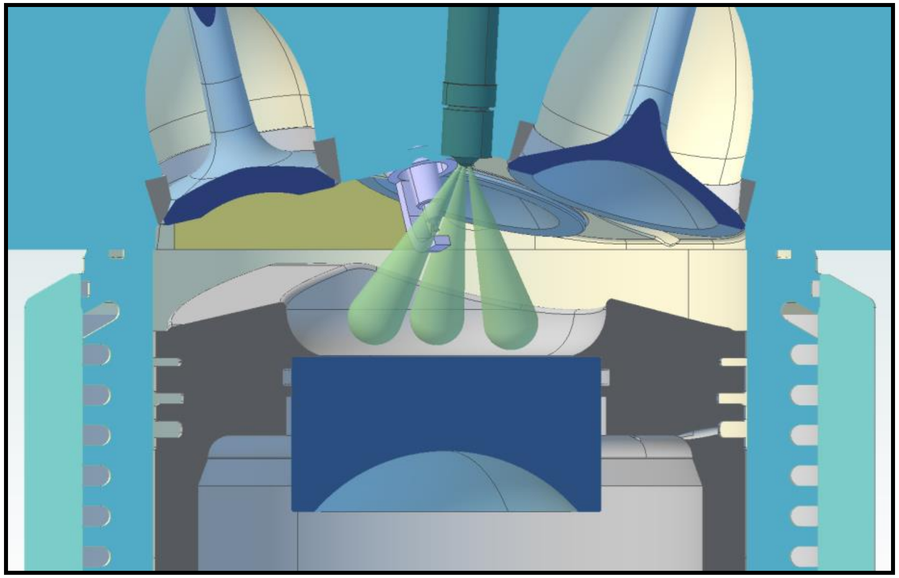
Co-Optimization of Fuels & Engines

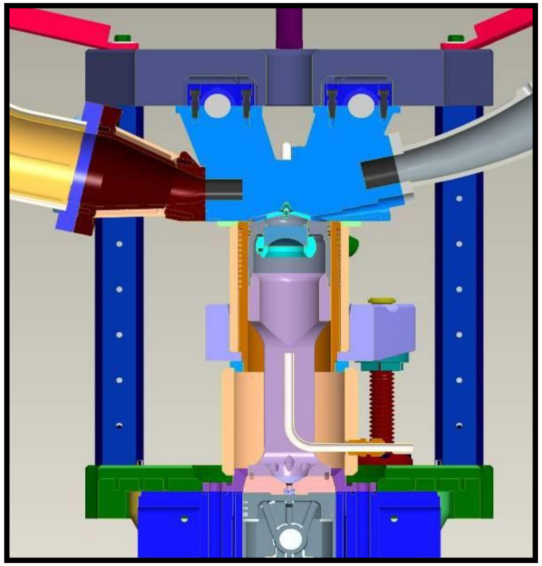
Outline

1. Stoichiometric Knock Limits Wrap-Up
2. Octane Index Uncertainty at Stoichiometric Conditions Wrap-Up
3. Mixed-Mode Combustion for High Efficiency and Low Emissions
4. Future Directions

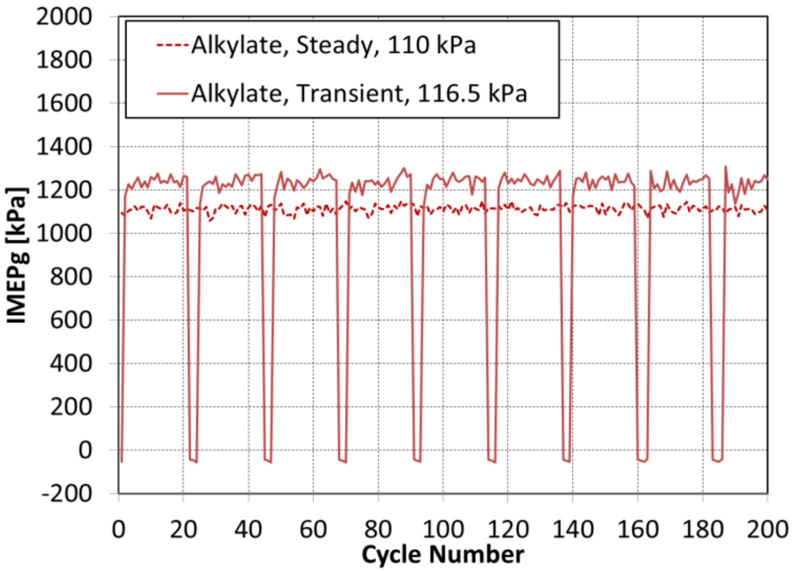
Research Engine Characteristics

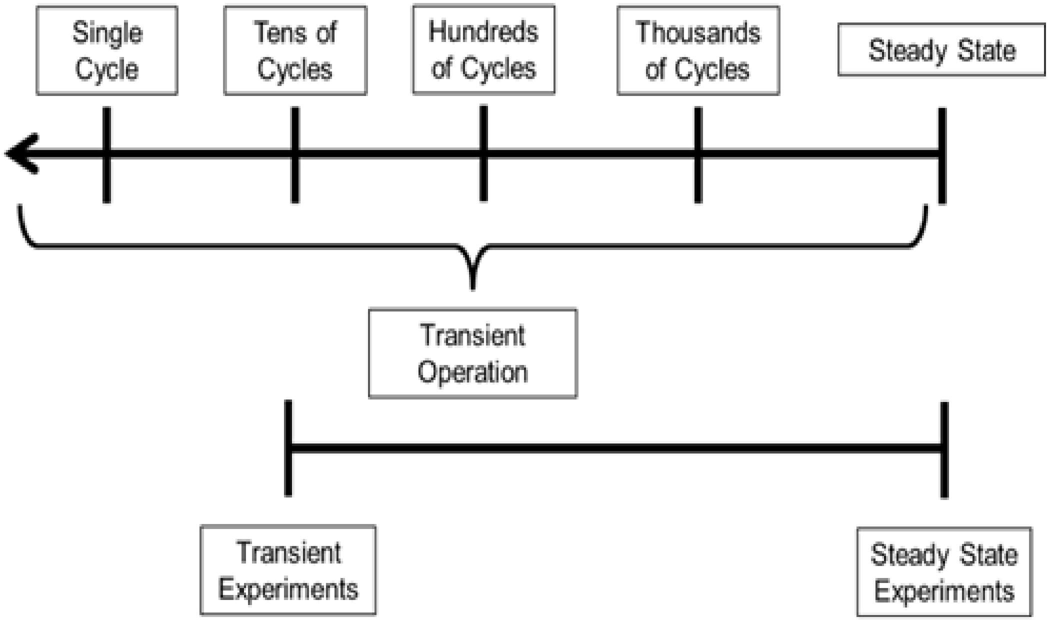
- DISI
- CR = 12:1
- 0.55 L displacement
- High-swirl operation
  - Single intake valve
- Low residuals
  - No valve overlap
- KL-CA50 measured at 1400 RPM
- Conventional High-Energy Ignition System used
- Well-mixed charge operation
  - 3- or 4- injection strategy for low PM emissions.





Test Regimes: Steady State and Transient





Single Cycle

Tens of Cycles

Hundreds of Cycles

Thousands of Cycles

Steady State

Transient Operation

Transient Experiments

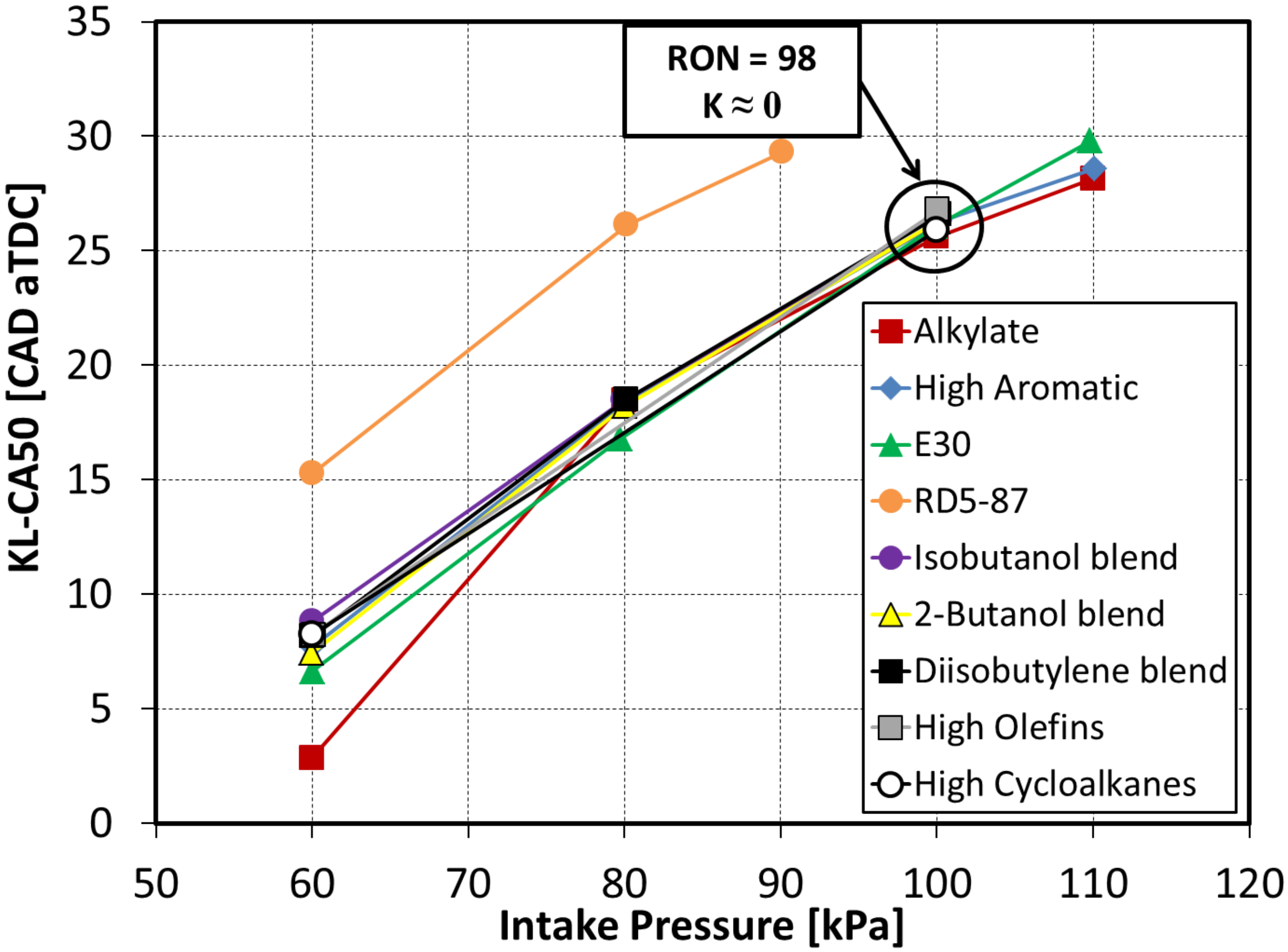
Steady State Experiments

- Steady-state operation reflects knock-limited operation at throttled and naturally aspirated conditions
- 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

Fuel Properties

	Iso-butanol blend	*2-butanol blend*	*Diisobutylene blend*	*High Olefins*	*High Cyclo-alkanes*	*Alkylate*	*E30*	*High Aromatic*	*RD5-87*
#	1	2	3	4	5	6	7	8	9
RON	98.1	98.2	98.3	98.2	97.8	98.0	97.9	98.1	92.1
MON	88.0	89.1	88.5	88.0	86.9	96.7	87.1	87.6	84.8
AKI (R+M)/2	93.1	93.7	93.4	93.1	92.3	97.3	92.5	92.8	88.5
Octane Sensitivity (RON - MON)	10.1	9.1	9.8	10.2	11.0	1.3	10.8	10.5	7.3
T10 (°C)	-	-	-	77	56	93	61	59	-
T50 (°C)	-	-	-	104	87	100	74	108	-
T90 (°C)	-	-	-	136	143	106	155	158	-
TF (°C)	-	-	-	198	204	161	204	204	-
Aromatics (Vol. %)	19.0	17.9	20.1	13.4	33.2	0.0	8.1	30.8	20.9
Olefins (Vol. %)	3.8	3.6	4.0	26.5	1.6	0.0	5.0	4.2	4.9
Paraffins (Vol. %)	53.1	50.1	56.3	56.4	40.6	100.0	57.1	65.0	60.0
Cycloalkanes (Vol. %)	0.0	0.0	0.0	2.9	24.2	0.0	7.0	8.0	11.3
Ethanol (Vol. %)	0.0	0.0	0.0	0.0	0.0	0.0	30.0	0.0	10.6
Net Heat of Combustion (MJ/kg)	40.6	40.1	43.5	44.1	43.2	44.5	38.2	43.0	41.9
Stoichiometric Air to Fuel Ratio (-)	13.8	13.6	14.7	14.8	14.5	15.1	12.8	14.5	14.1
Heat of Vaporization (kJ/kg)	416	422	330	-	-	309	536	363	-
Heat of Vaporization Per Mass of Stoichiometric Charge (kJ/kg)	28.2	28.9	21.1	-	-	19.1	38.8	23.4	-
Average Molecular Formula	C: 6.299 H: 12.744 O: 0.326	C: 6.122 H: 12.532 O: 0.378	C: 7.519 H: 14.420	C: 7.125 H: 14.23	C: 6.46 H: 11.71	C: 7.76 H: 17.45	C: 4.49 H: 9.87 O: 0.5	C: 6.92 H: 12.41	C: 6.01 H: 11.84 O: 0.2

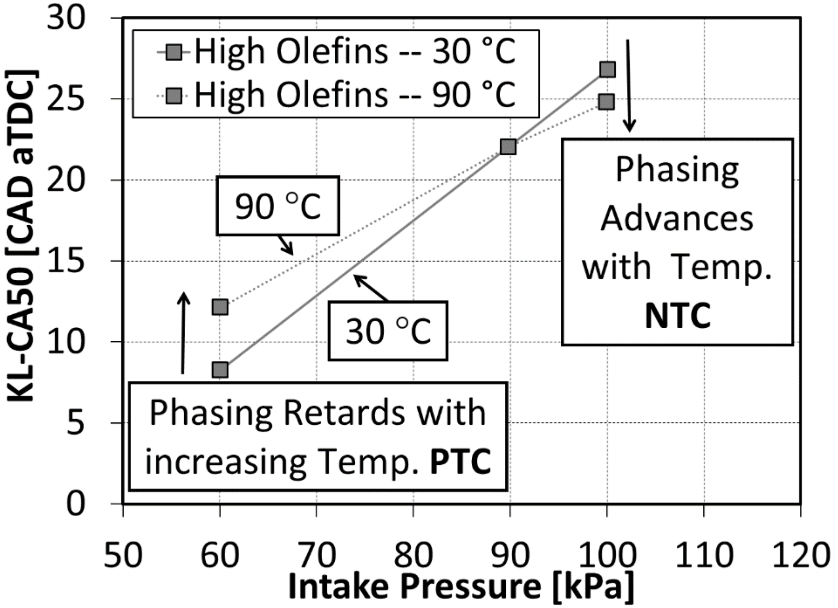
Knock Limits: Steady-State 30 °C

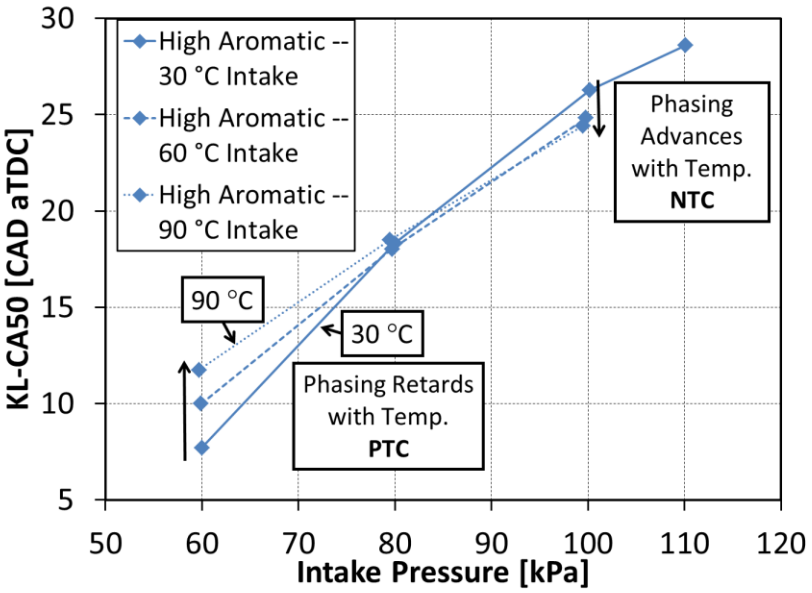


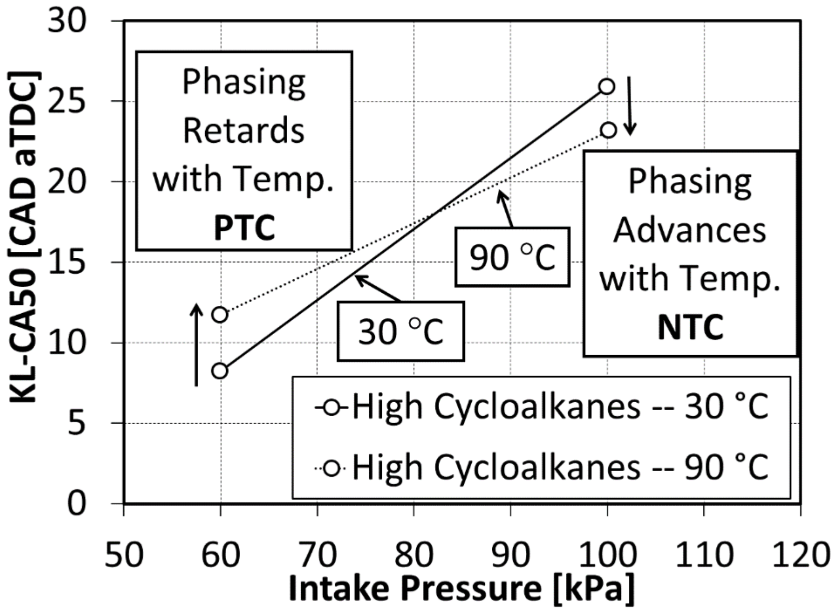
- Under steady-state naturally aspirated conditions, all RON = 98 fuels behave similarly
  - Indicates K ≈ 0

Knock Limits: Intake Temperature Response

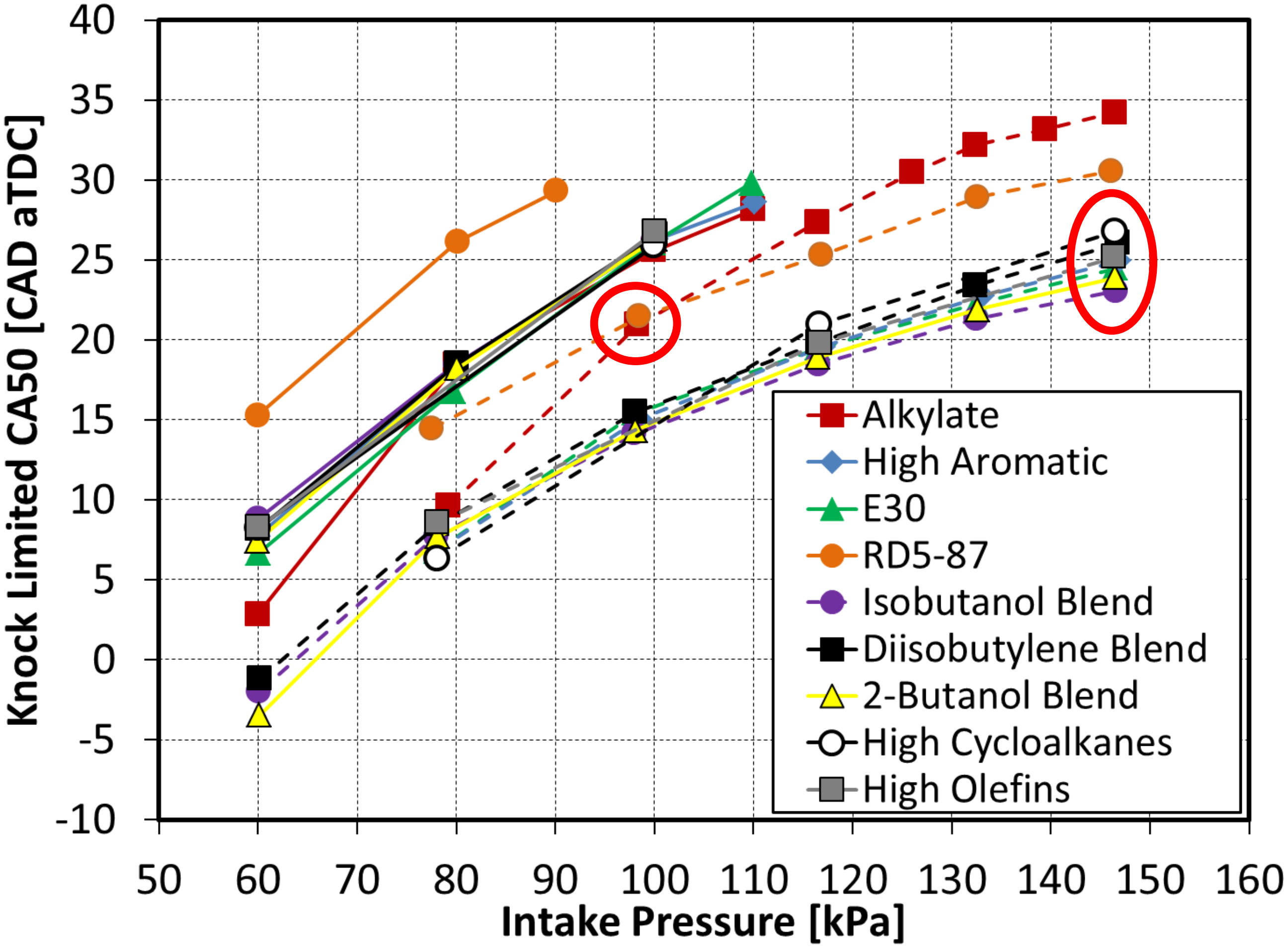
- NTC behavior observable in High Olefins and High Cycloalkanes fuels
  - Similar to behavior observed with other RON = 98, S ≈ 10 core fuels







Knock Limits: Transient Response



- Transient high-load testing shows clear crossover in performance of high- and low-octane sensitivity fuels
  - Indicates need for Octane Index (OI) approach in assessing fuel knock limits
- Observable differences in performance for 7 RON = 98, S ≈ 10 gasolines

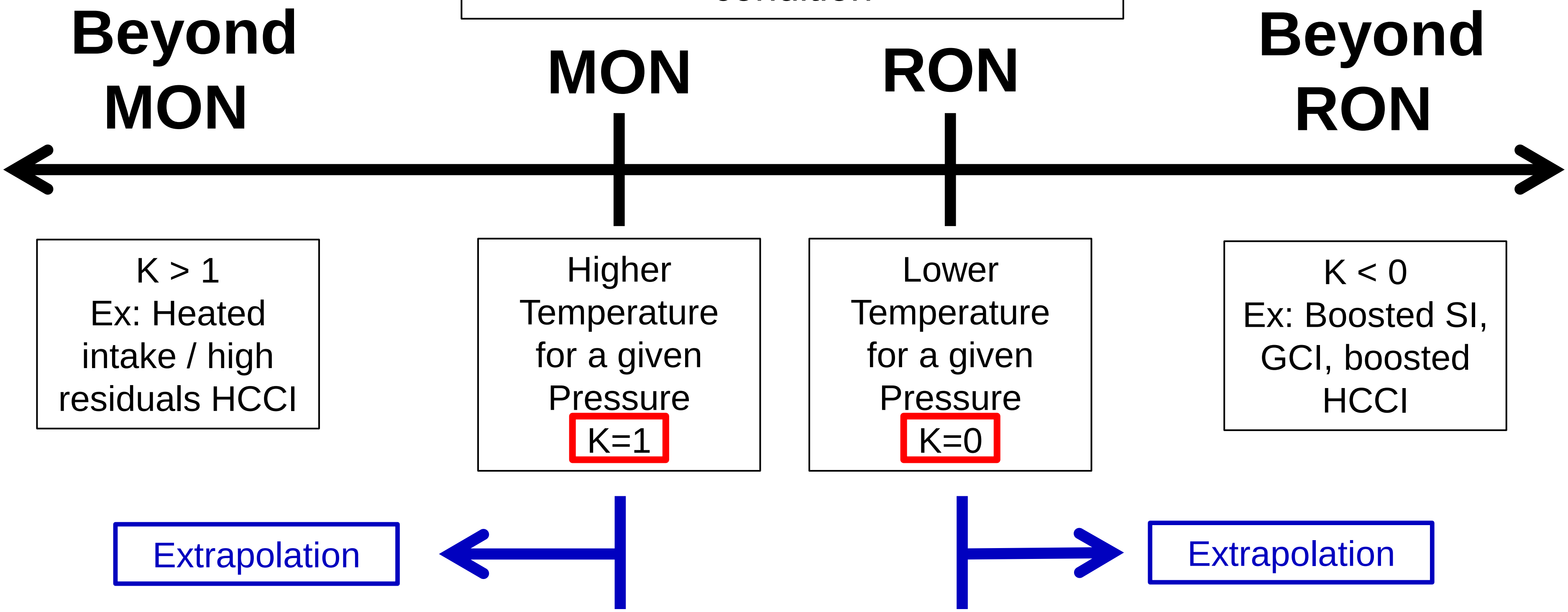
SHIFTING GEARS: OCTANE INDEX CALCULATION AND UNCERTAINTY

Octane Index Framework

Octane Index = RON – K • S

S = RON - MON

K = Dependent on operating condition



Beyond MON

MON

RON

Beyond RON

K > 1
Ex: Heated intake / high residuals HCCI

Higher Temperature for a given Pressure
K=1

Lower Temperature for a given Pressure
K=0

K < 0
Ex: Boosted SI, GCI, boosted HCCI

Extrapolation

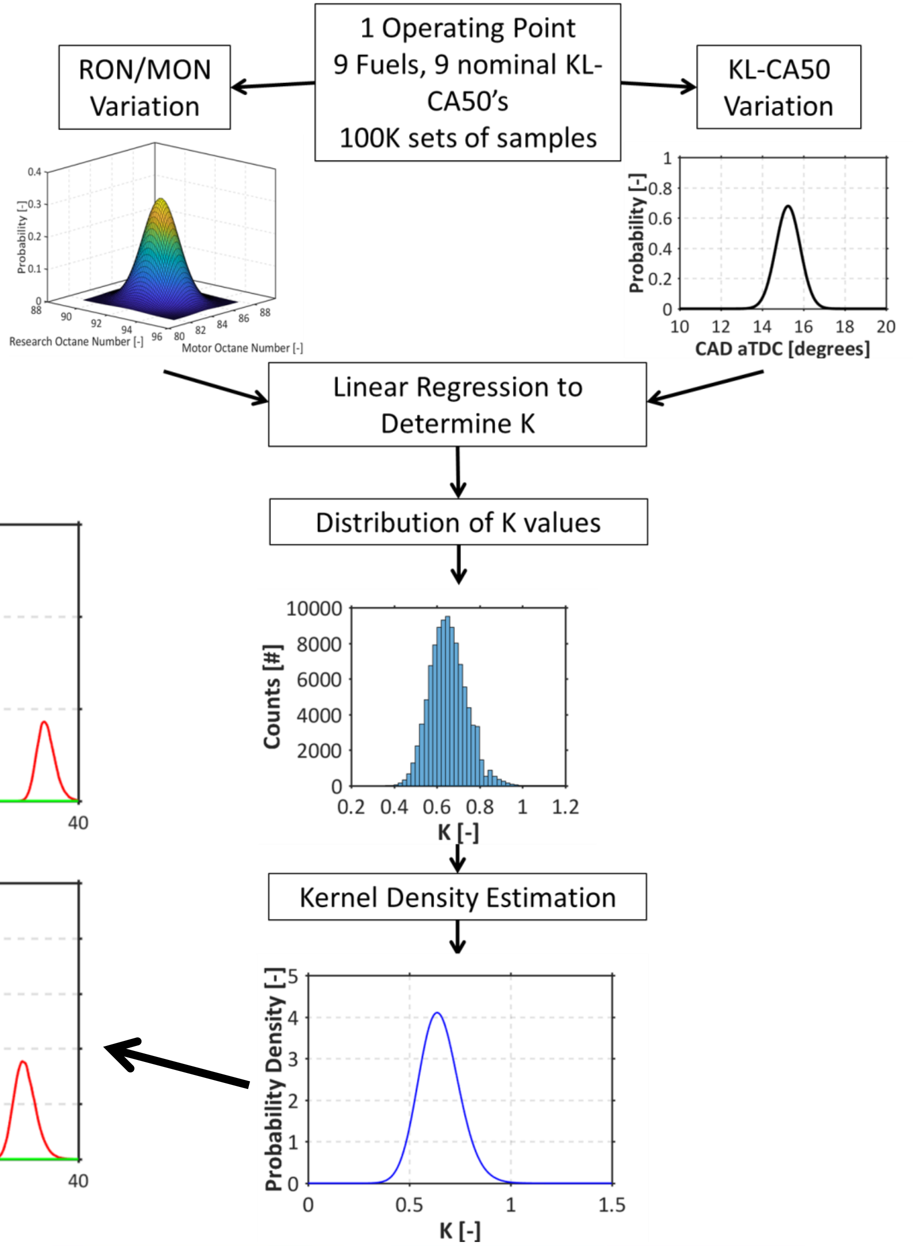
Extrapolation

OI Reference: SAE #2001-01-3584

Modern SI Engines

Monte Carlo Sampling Procedure

- Goal: Determine effects of RON/MON/KL-CA50 uncertainty on K calculations
- Use Monte Carlo sampling scheme to assess distribution of possible K values at each operating point



1 Operating Point
9 Fuels, 9 nominal KL-CA50's
100K sets of samples

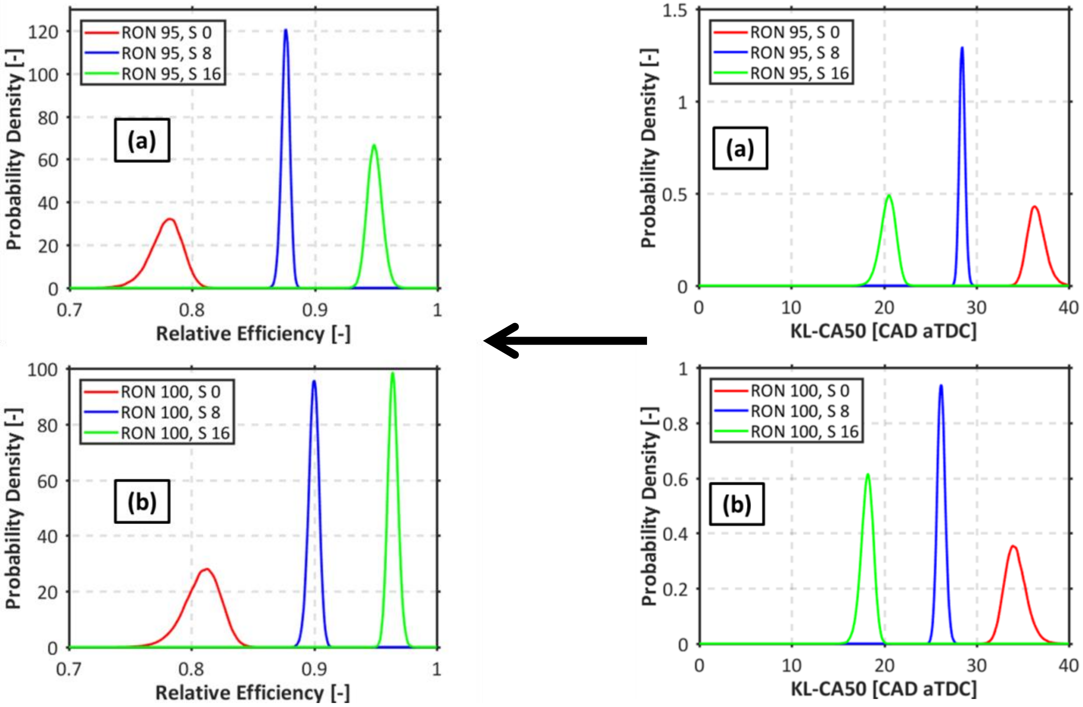
RON/MON Variation

KL-CA50 Variation

Linear Regression to Determine K

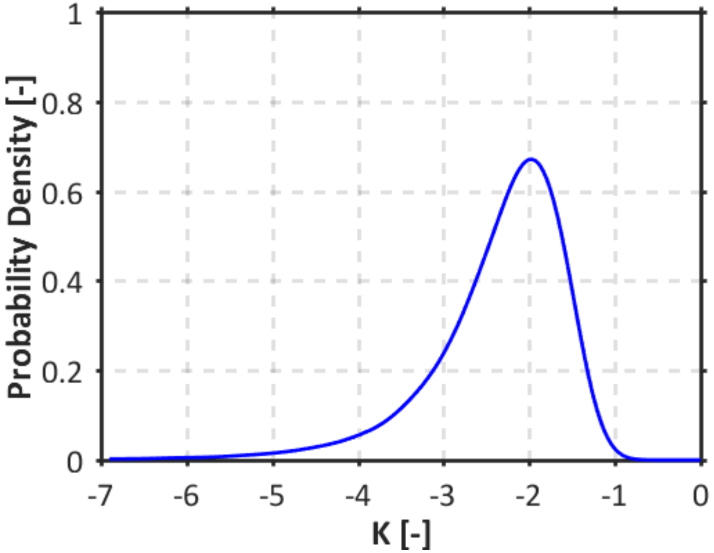
Distribution of K values

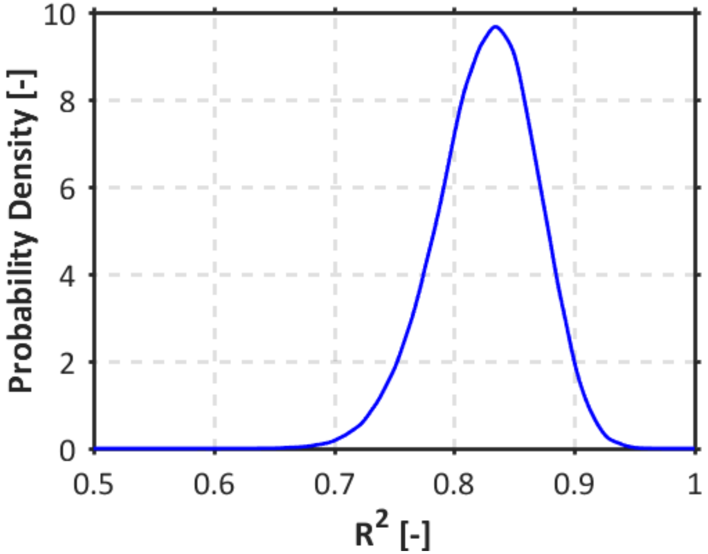
Kernel Density Estimation

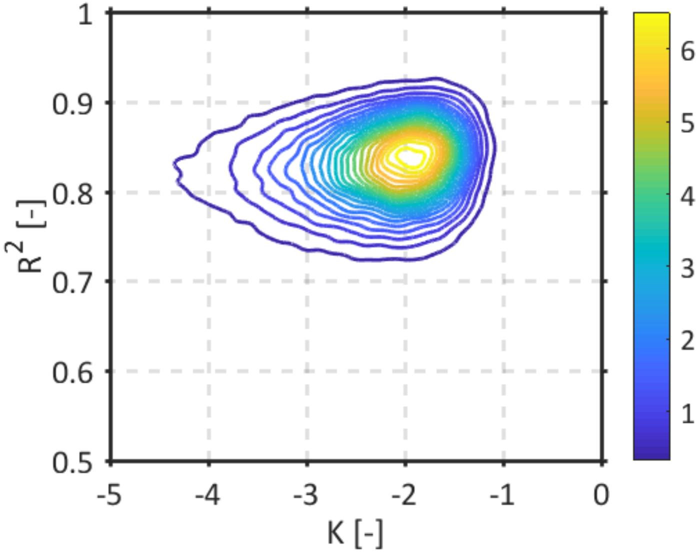


K Uncertainty Results: 146 kPa Intake, Transient

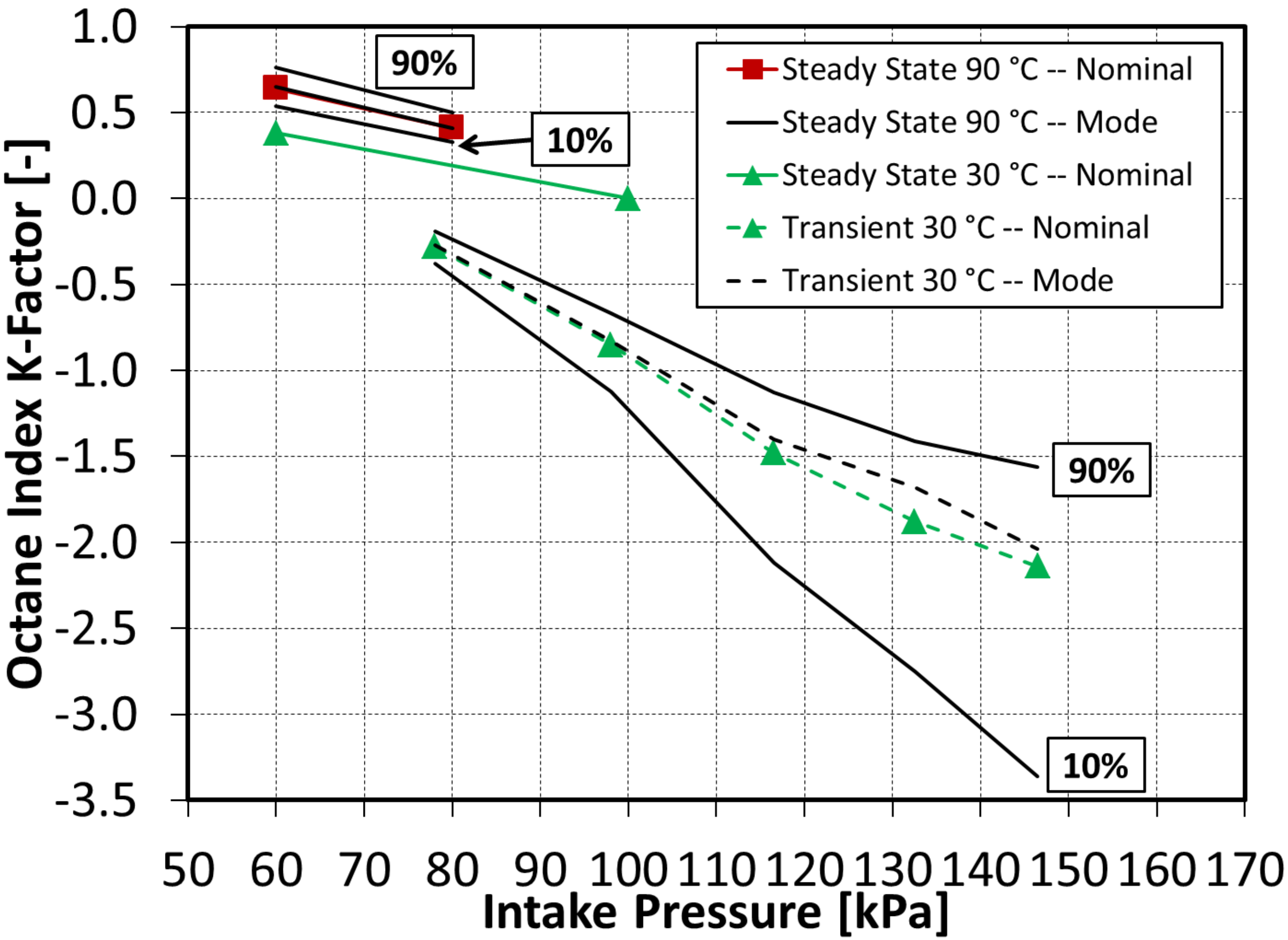
- "Beyond RON" condition exhibits large K value distribution
  - Distribution skewed
- R^2 distribution closer to 1 than for other example, despite wide K distribution





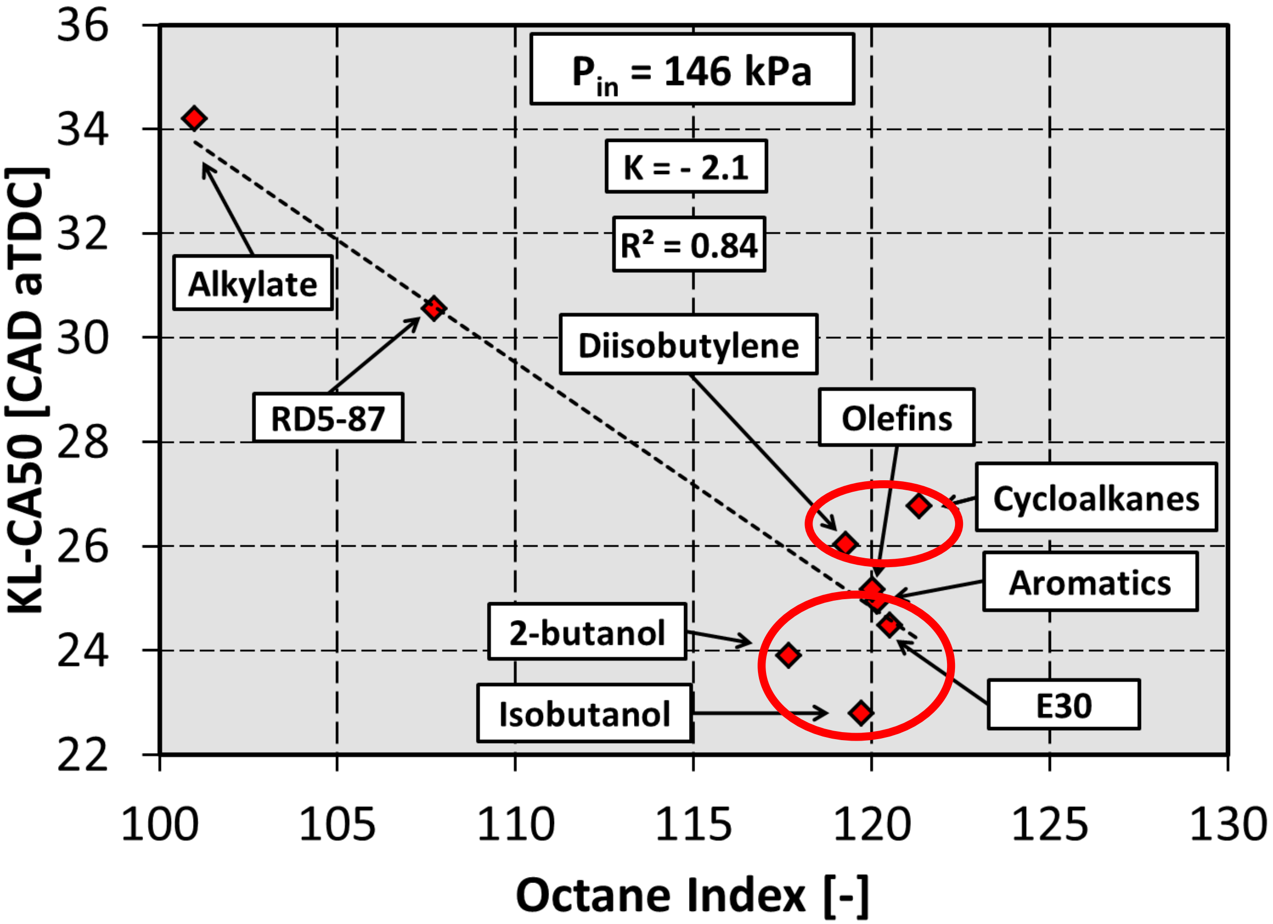


K Uncertainty Results



- 80% probability range grows as K becomes more negative
- Results less dramatic and more symmetric in interpolation region
- Large uncertainty in K, but does it matter?

Deviations from OI-based Ranking

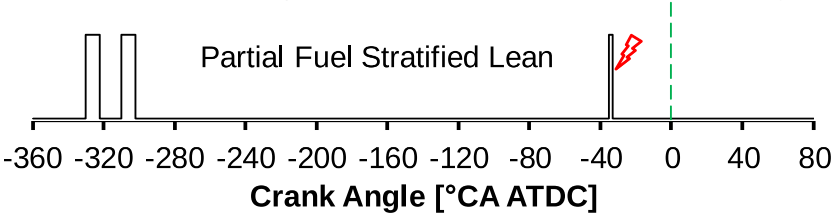


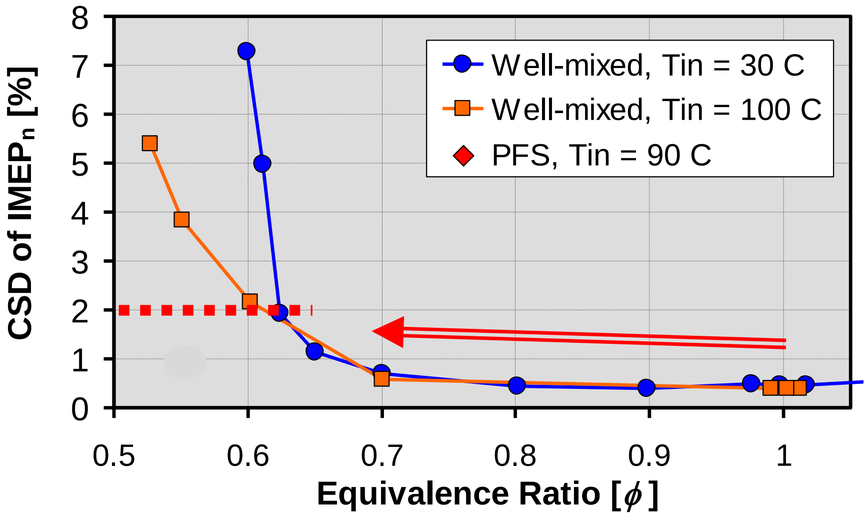
- Alcohol blends outperform OI predictions.
- Diisobutylene (iso-octene) and High-Cycloalkanes underperform.

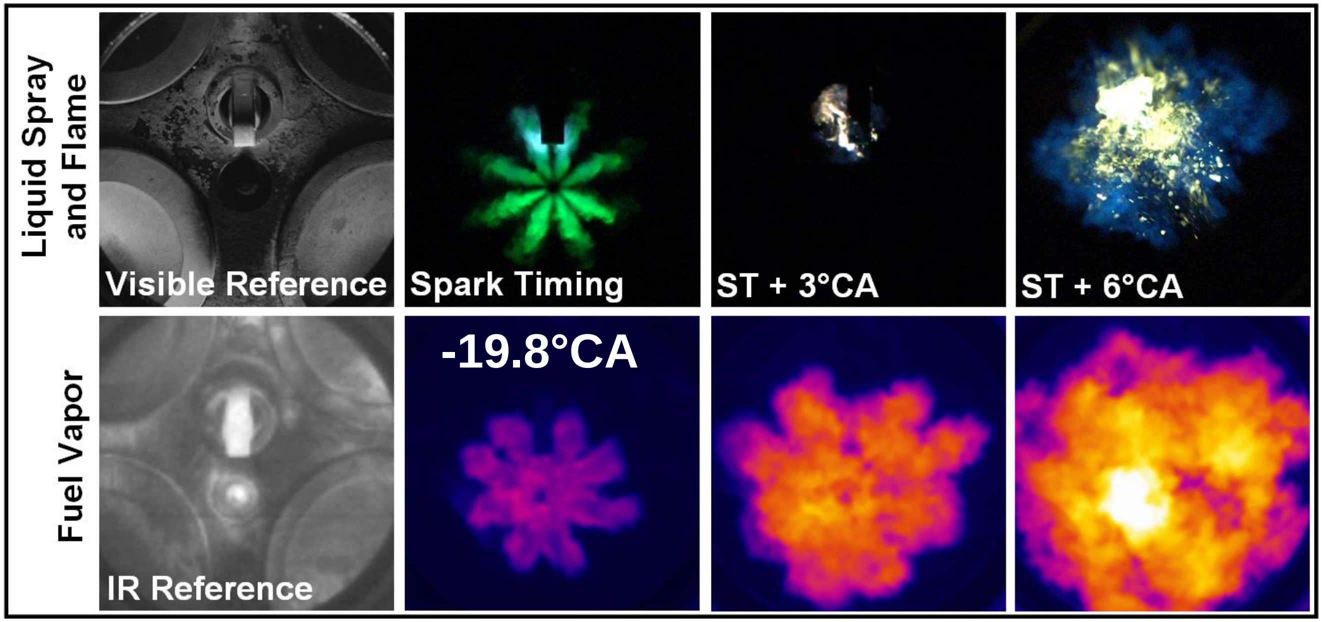
SHIFTING GEARS: MIXED-MODE COMBUSTION

Partial Fuel Stratification for Stable Ultra-lean Operation

- Need to stabilize deflagration to facilitate mixed-mode combustion studies.
- Use small injection at the time of spark.

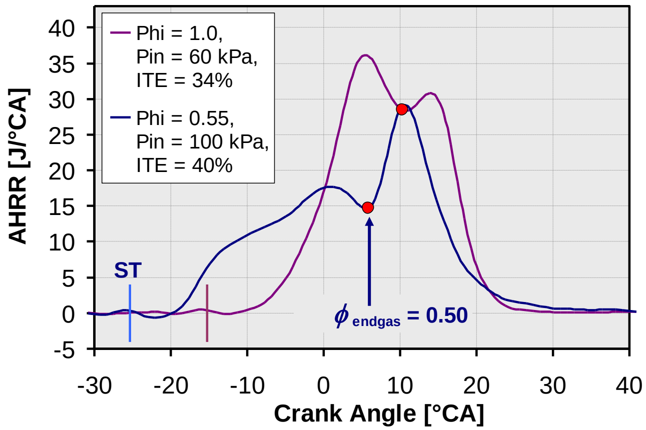


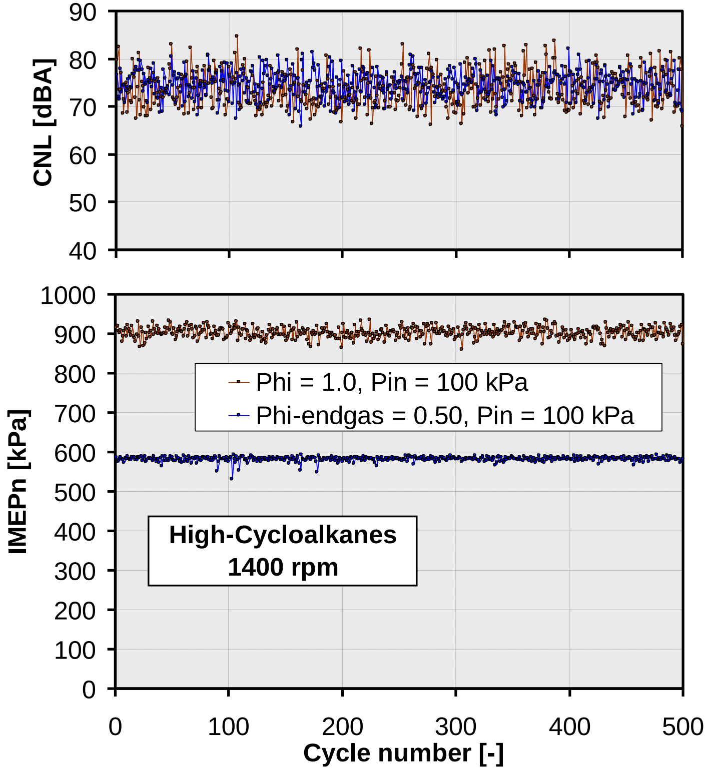


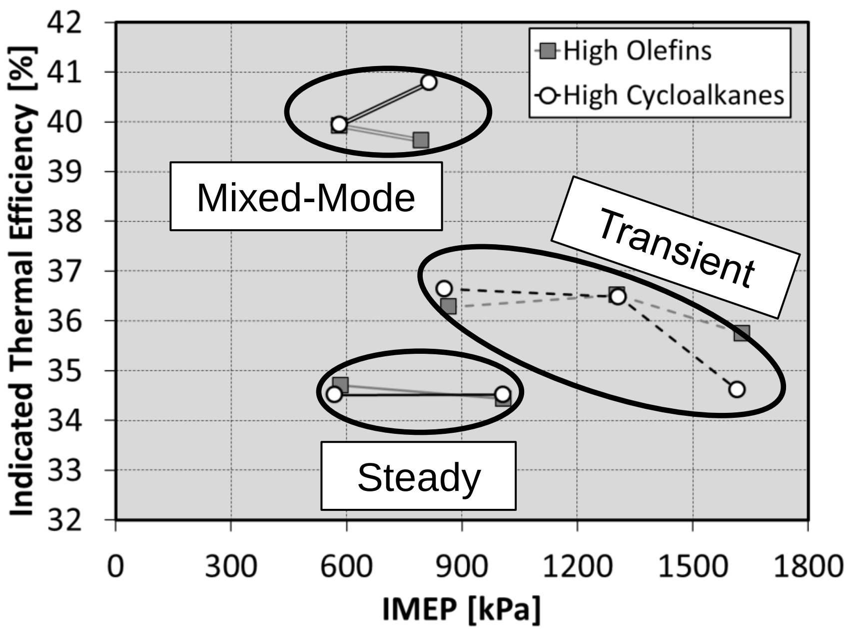


Efficiency Benefit of Lean Operation

- Lean operation provides substantial efficiency benefits, $34 \Rightarrow 40\%$.
- Naturally-aspirated 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: $\phi_{global} = 0.55$

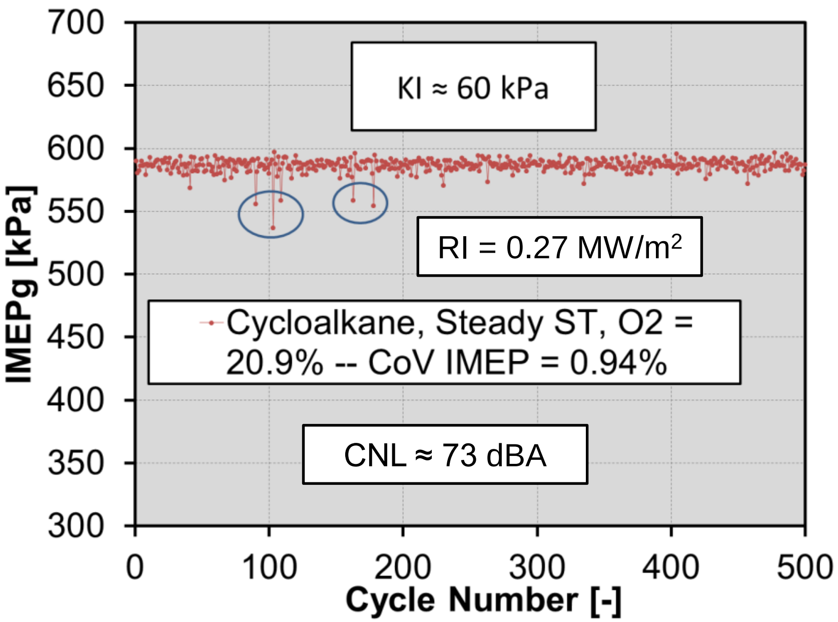


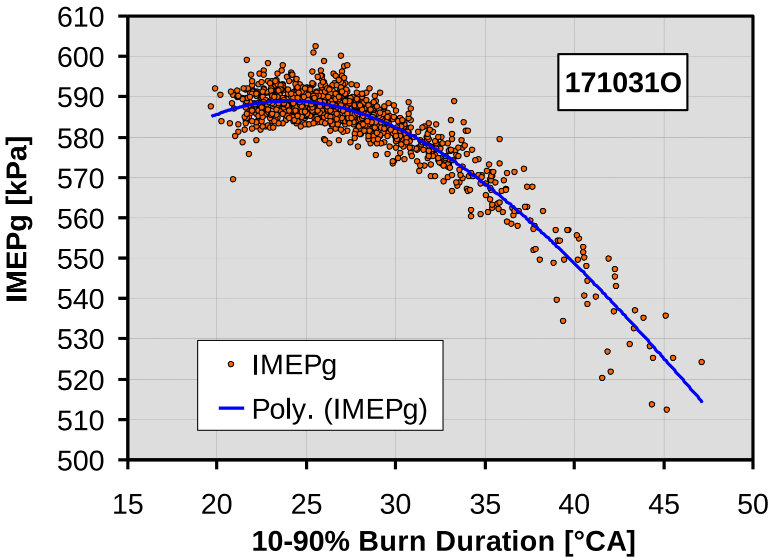


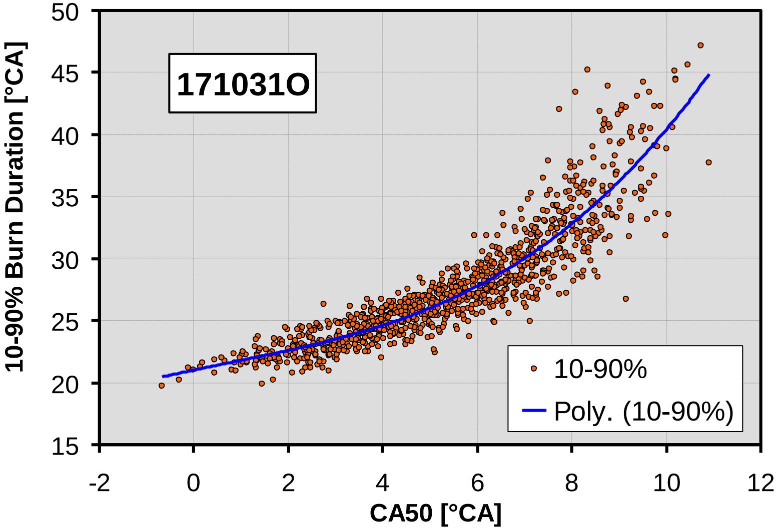


IMEP Variability and CA50 Requirement

- CoV of IMEP = 0.94% (lower than 1.4% of ϕ = 1.0.)
- Combustion Noise Level is comparable to ϕ = 1.0 operation
- Near-TDC combustion phasing required for end-gas autoignition
  - End-gas autoignition required for efficient operation

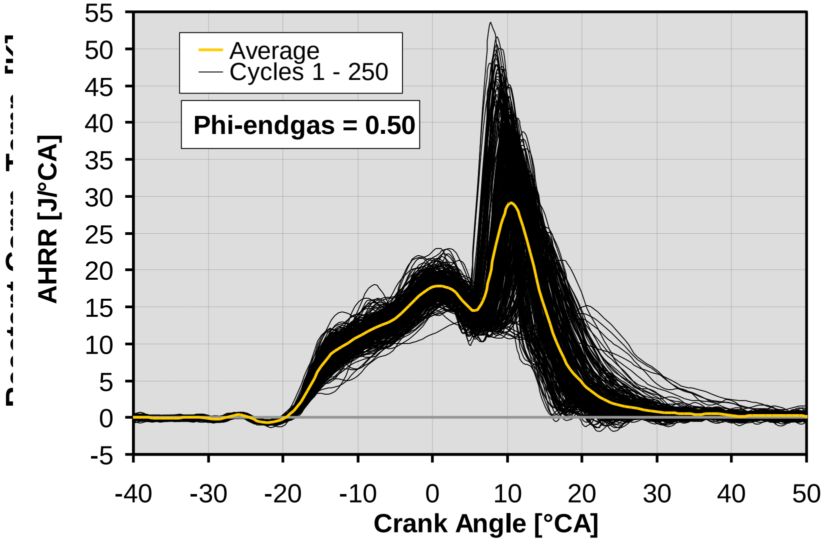


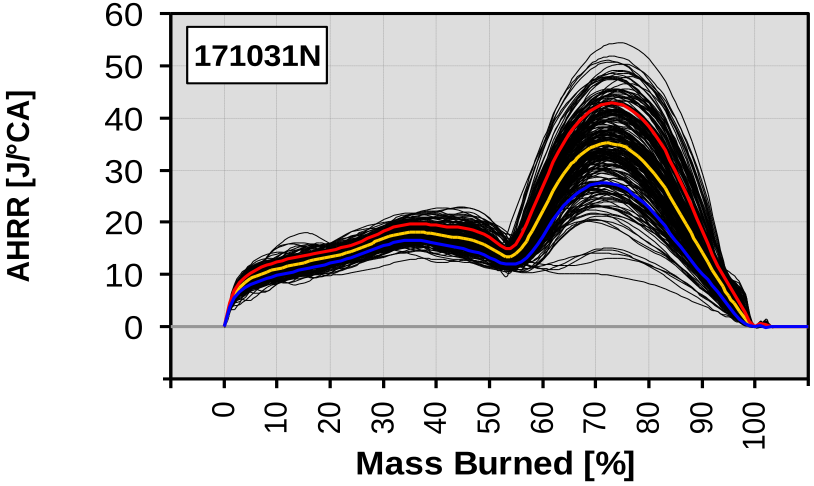




Autoignition for High-Cycloalkane

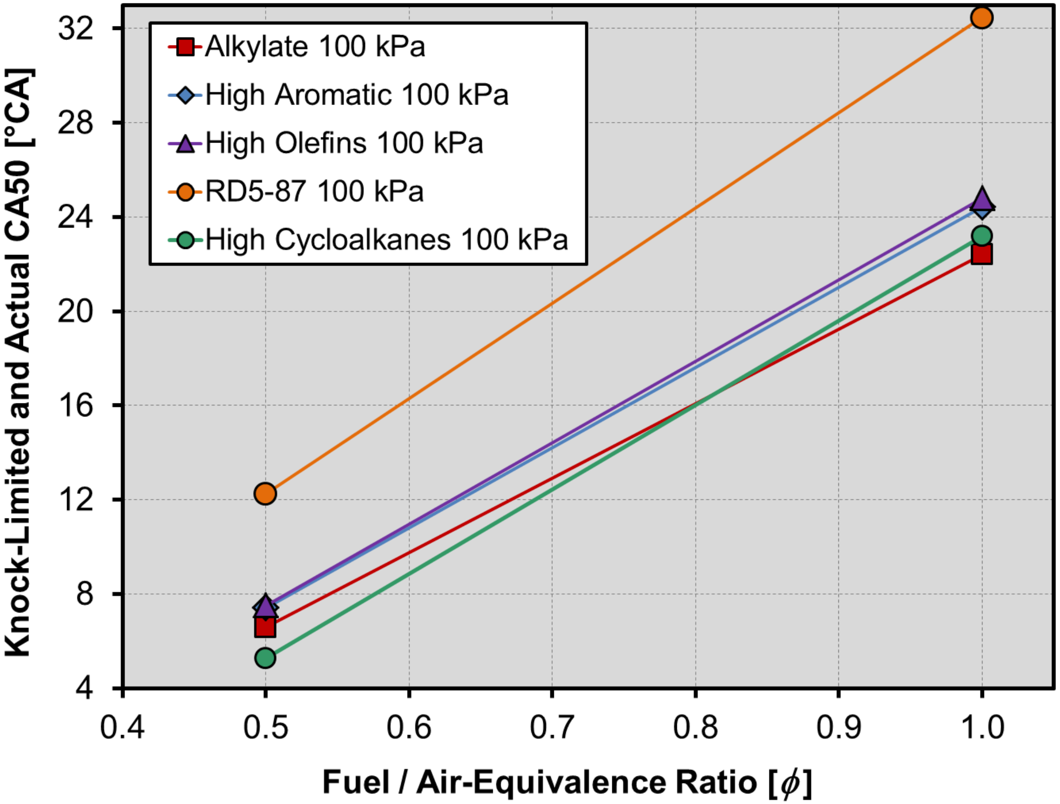
- $[O_2]$ = 20.9%, 100 kPa intake pressure
- Steady ST = -25.3°CA.
- Average CA50 = 5.3°CA.
- Significantly higher temperature and pressure required to achieve autoignition compared to stoichiometric conditions
- End-gas autoignition dominates last 47% burned.
  - At constant KI level, autoignition percentage varies by fuel
- Despite significant autoignition event, CNL / KI / RI





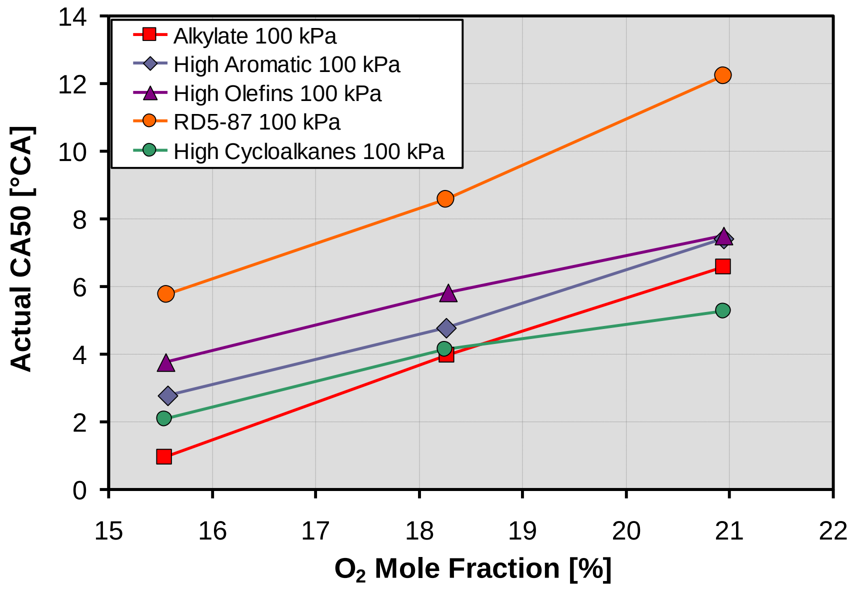
Effect of Equivalence Ratio for P_{in} = 100 kPa

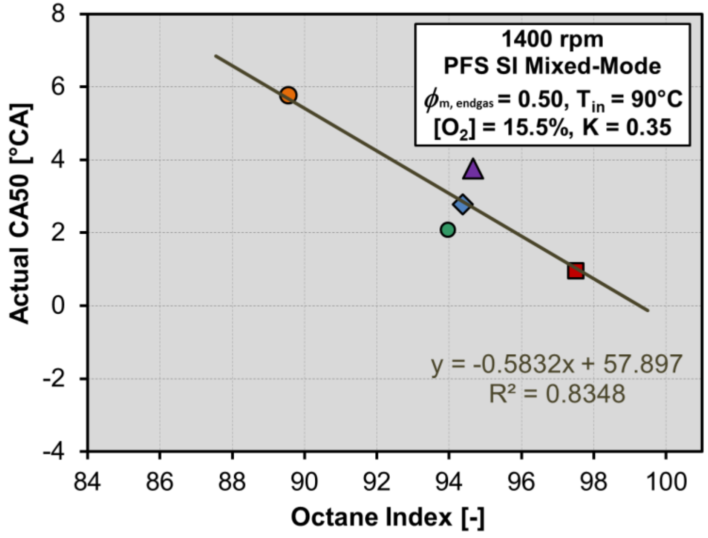
- 1400 rpm, P_{in} = 100 kPa, T_{in} = 90°C. Same intake conditions for stoichiometric and lean operation.
- Use actual CA50 as reactivity metric for all lean operation.
- For a fixed P_{in} = 100 kPa, ultra-lean operation requires strong advancement of CA50 to ensure end-gas autoignition.
- Small differences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

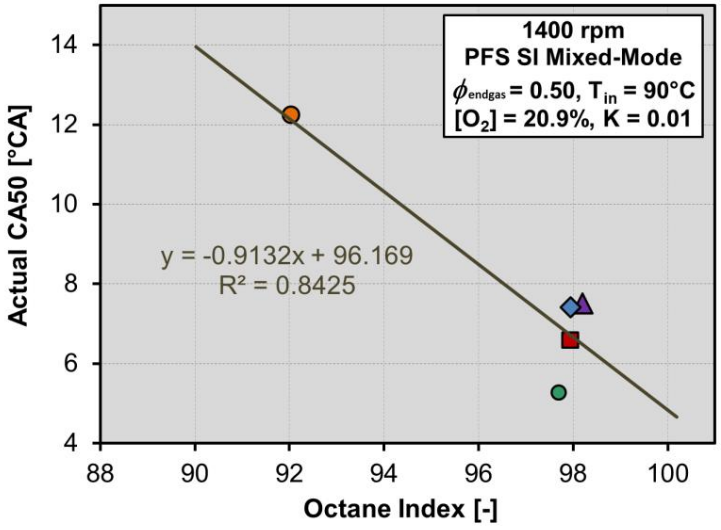


Effect of Intake [O_2] for Mixed-Mode Comb.

- 1400 rpm, P_{in} = 100 kPa, T_{in} = 90°C, $\phi_{m,\ endgas}$ = 0.50.
- 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 to describe fuel behavior to first order at both conditions

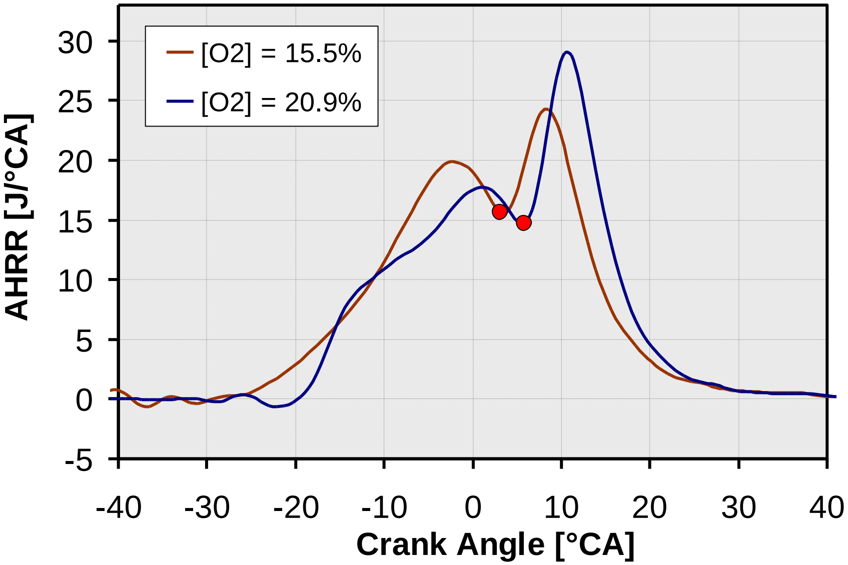


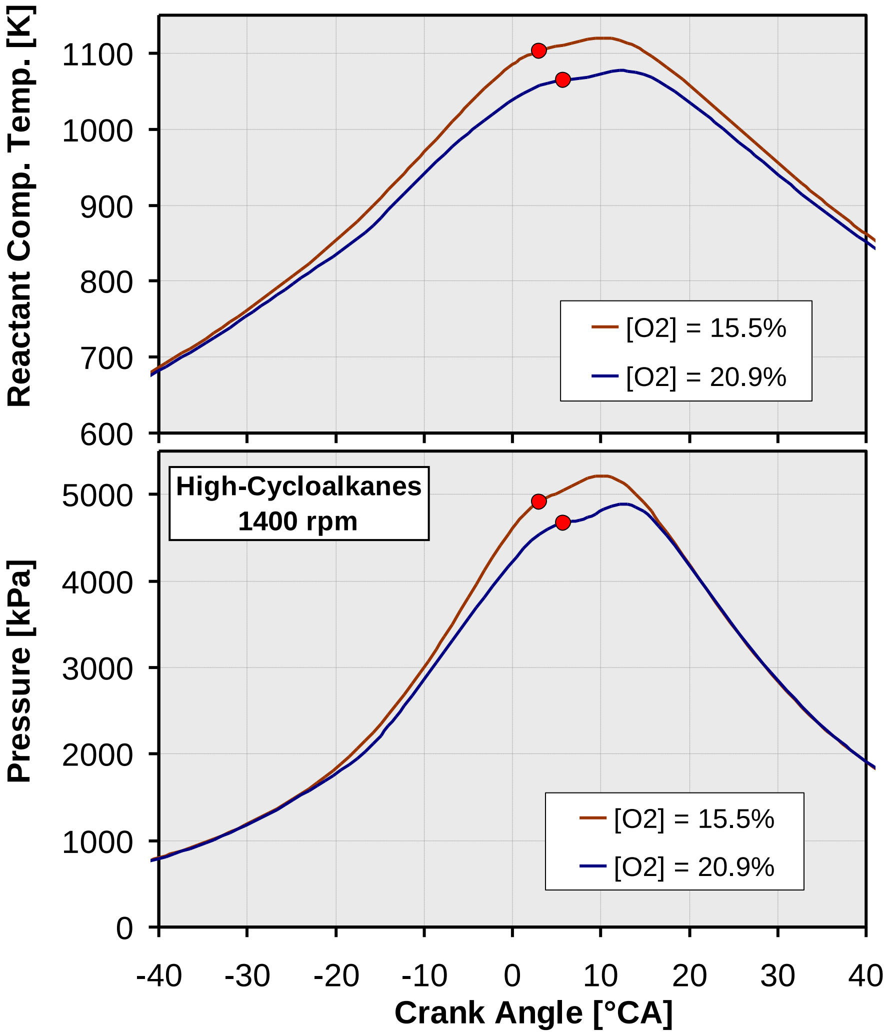




Effect of Intake [O_2] for High Cycloalkanes

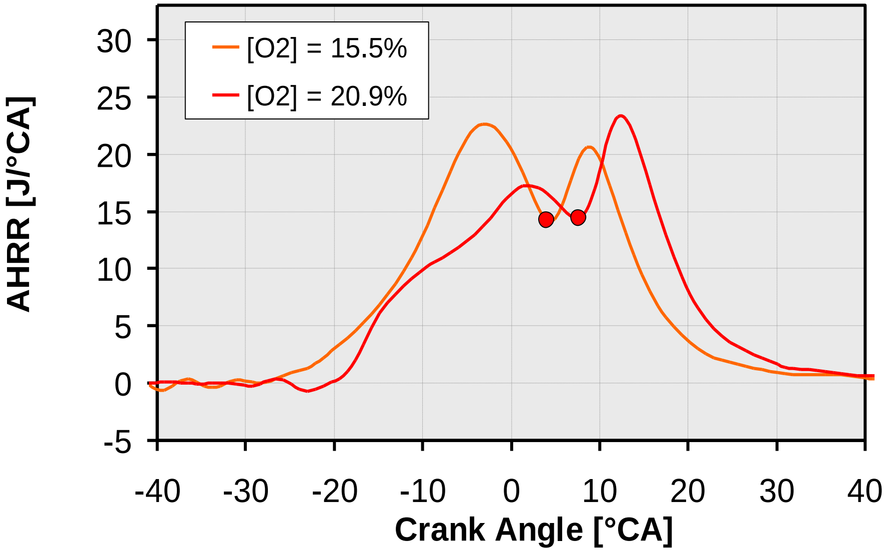
- 1400 rpm, P_{in} = 100 kPa, T_{in} = 90°C, $\phi_{m,\ endgas}$ = 0.50.
- High Cycloalkane has lowest sensitivity to [O_2].
- Relatively small increase of compressed-gas temperature is required to induce autoignition.

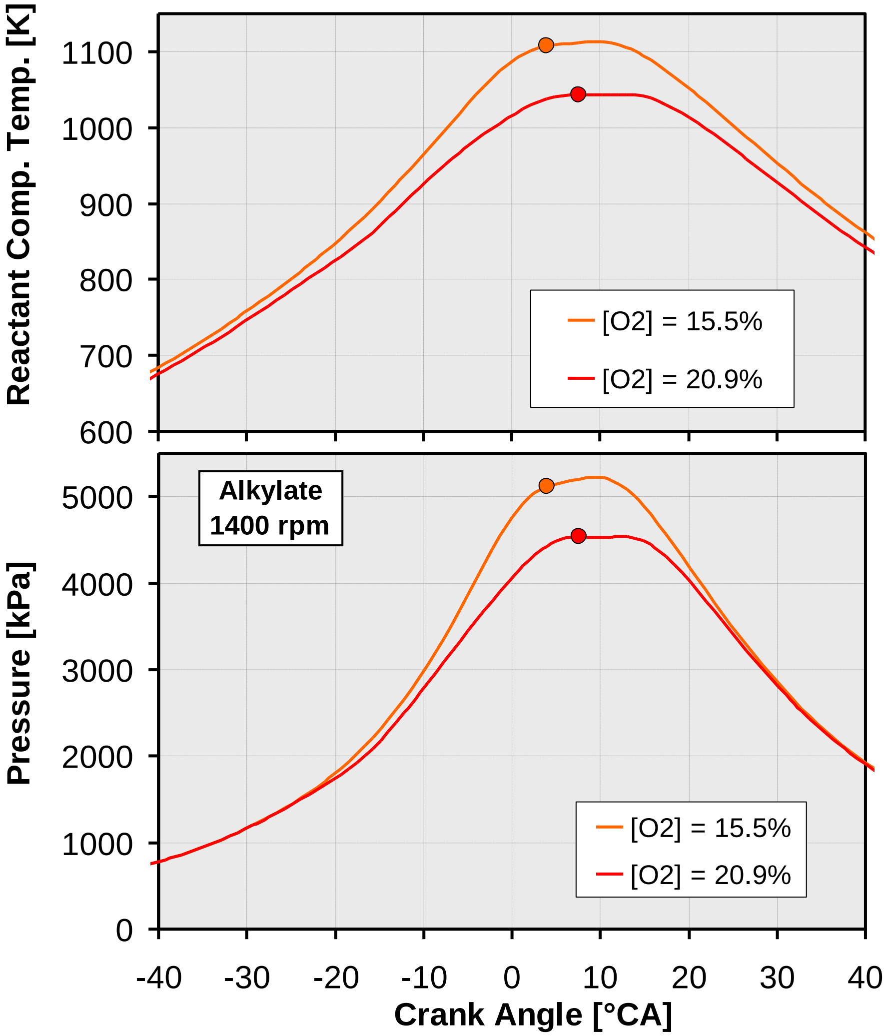




Effect of Intake [O_2] for Alkylate.

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





Chemkin Simulations of Mixed Mode Combustion

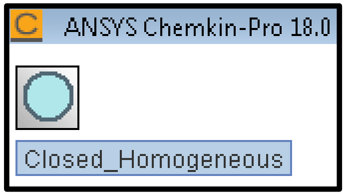
- Closed homogeneous reactor module with adiabatic assumption
- LLNL mechanism with 2,848 species and 12,201 reactions
- Variables : fuel type, intake O_2 mole fraction, initial temperature, NO mole fraction in residual gas, pressure traces (CA50)

❑ **Initial conditions**

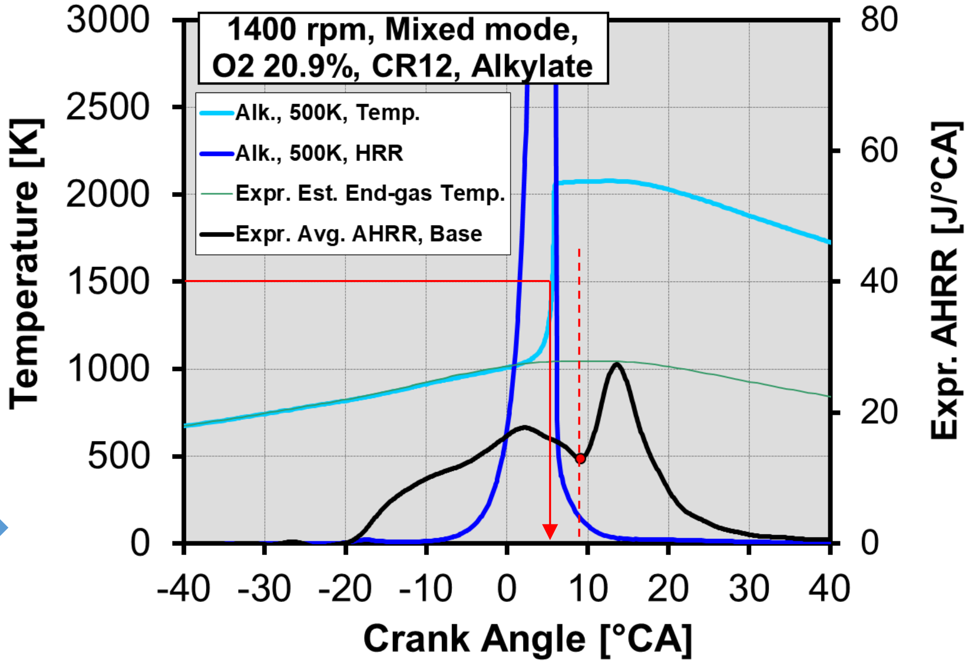
- Composition of oxidizer, residual
- Equivalence ratio
- Initial temperature

❑ **Boundary condition**

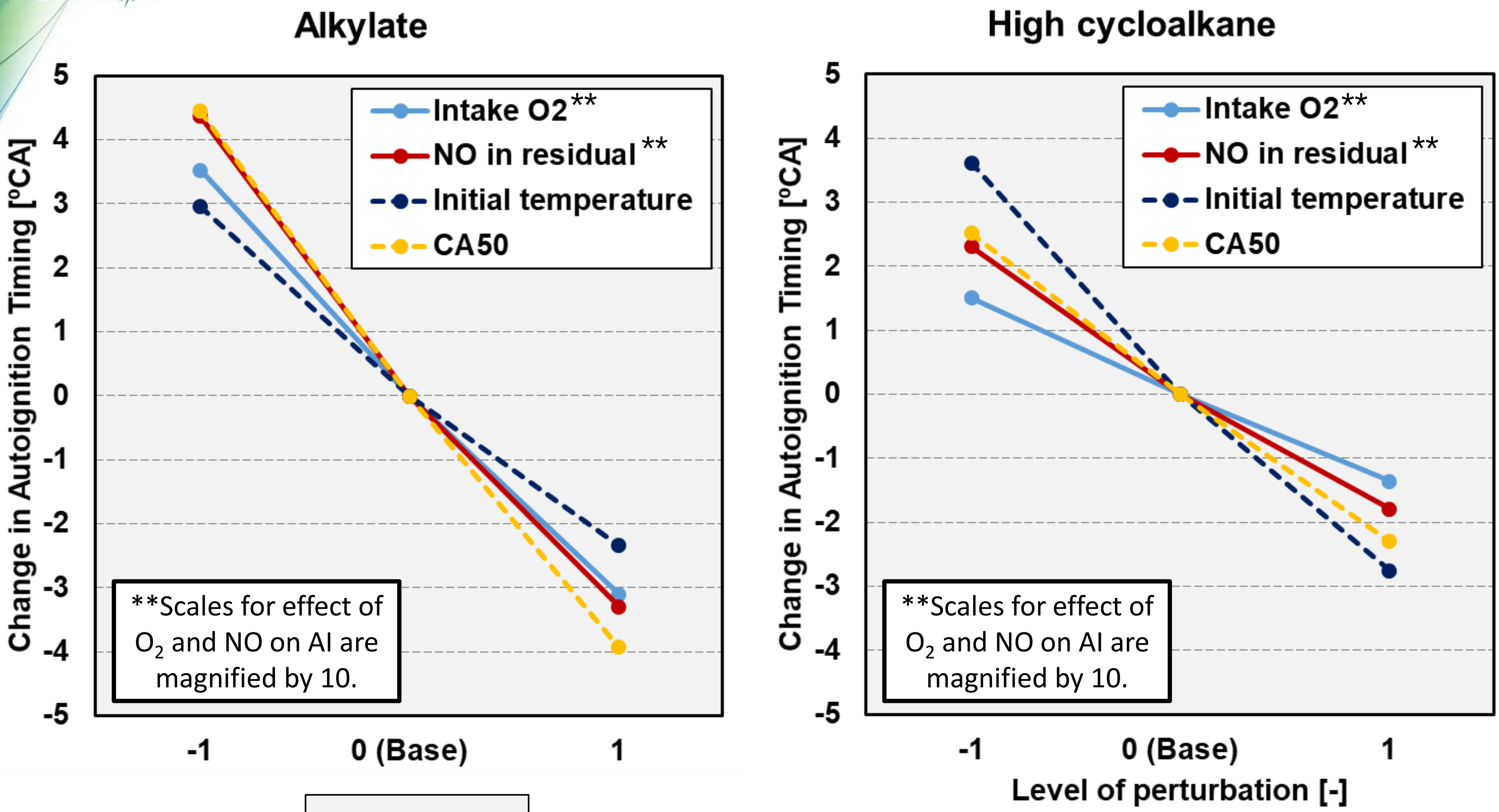
- Pressure from experimental data



Compare autoignition timing (t_{AI}).



Autoignition Phasing Sensitivity



**Scales for effect of O_2 and NO on AI are magnified by 10.

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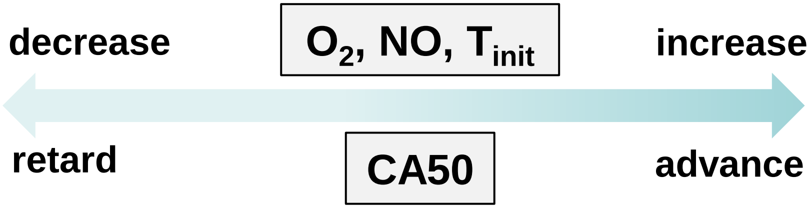


decrease

O_2, NO, T_{init}

increase

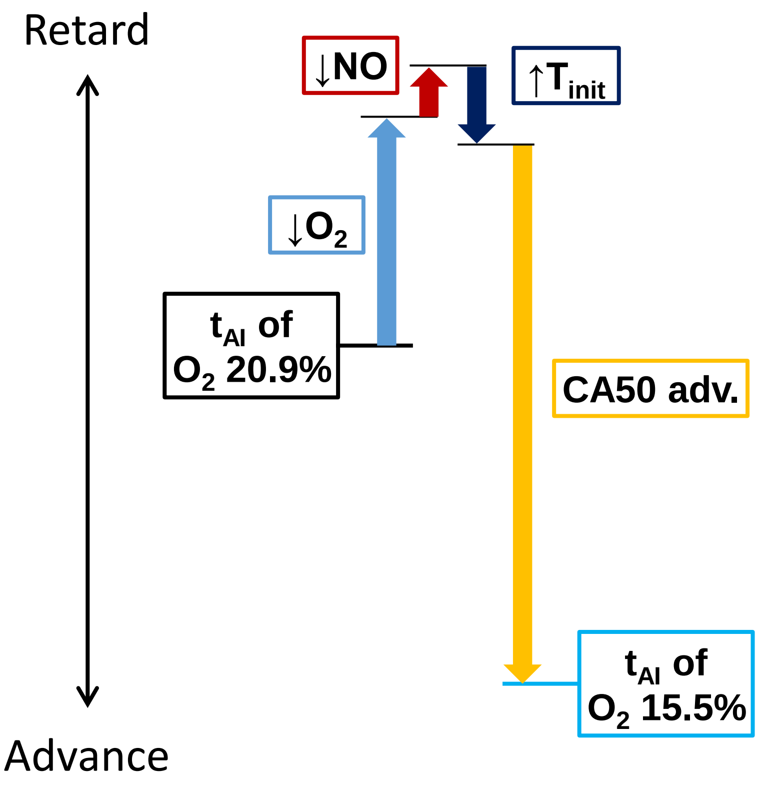
retard

CA50

advance

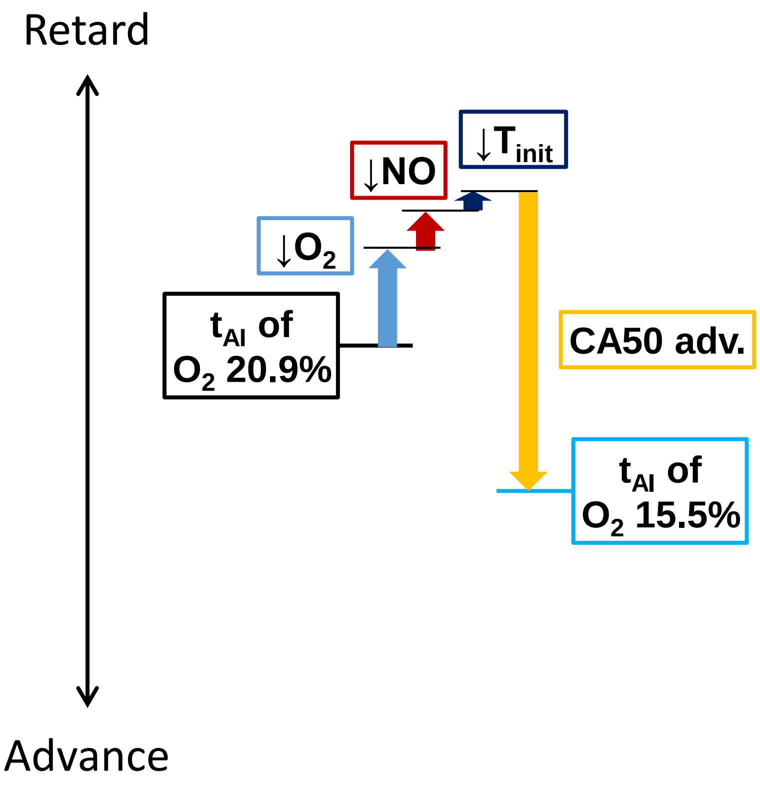
Linear Combination of Sensitivity Analysis

Alkylate



Experiment	Predicted	Error
3.41	2.64	-0.77

High cycloalkane



Experiment	Predicted	Error
1.24	1.25	0.01

Conclusions & Future Direction

- RON and MON provide at least 1st order description of fuel behavior under all stoichiometric, knock-limited conditions tested
- “Beyond RON” conditions result in a higher degree of uncertainty in Octane Index predictions, due to extrapolation of RON and MON results
- Mixed-mode combustion provides efficiency benefits expected by lean operation
- Octane Index framework appears to hold to first order at Mixed Mode conditions which have been tested so far

- Challenges remain:
  - Assuring stable flame development
  - Achieving a range of operation
  - Ensuring compatibility with a range of fuel compositions
- Many opportunities exist to improve Mixed Mode Combustion:
  - End-gas fuel stratification à la LTGC
  - Tailoring thermodynamic conditions at TDC
  - End-gas equivalence ratio

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