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# Uncertainty Assessment of Octane Index Framework for Stoichiometric Knock Limits of Co-Optima Gasoline Fuel Blends

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# Acknowledgements

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Co-Optimization of
Fuels & Engines

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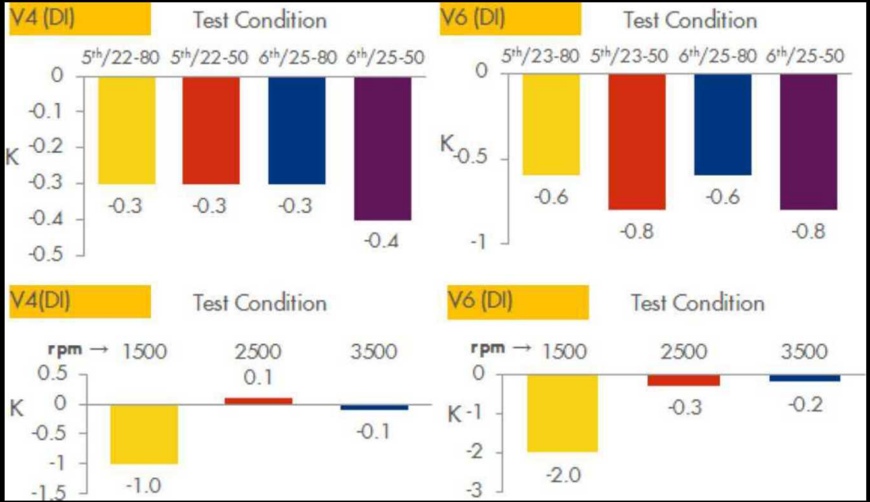
# Introduction

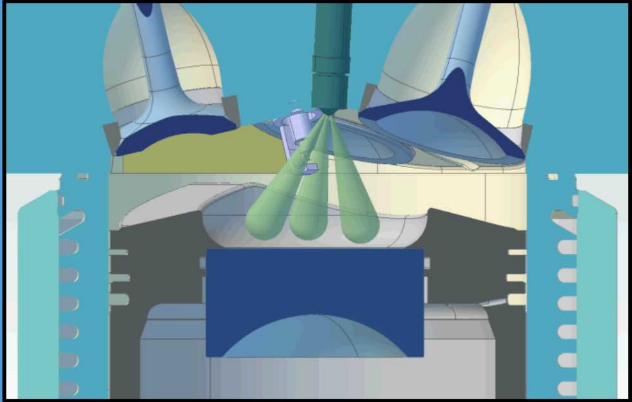
- Need to quantify fuel knock-resistance for Spark Ignition Engines
- Octane Index generally works well for this purpose, but does it hold up at extreme conditions and with uncommon fuel formulations?

Octane Index = RON – K • S




**Prakash *et al.*, SAE 2016-01-0834**

# Research Engine Characteristics



Directly Injected Spark Ignition (DISI)

CR = 12:1

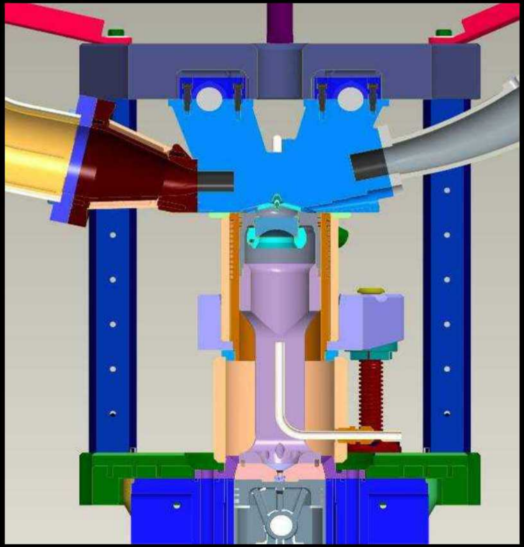
0.55 L displacement

High-swirl operation

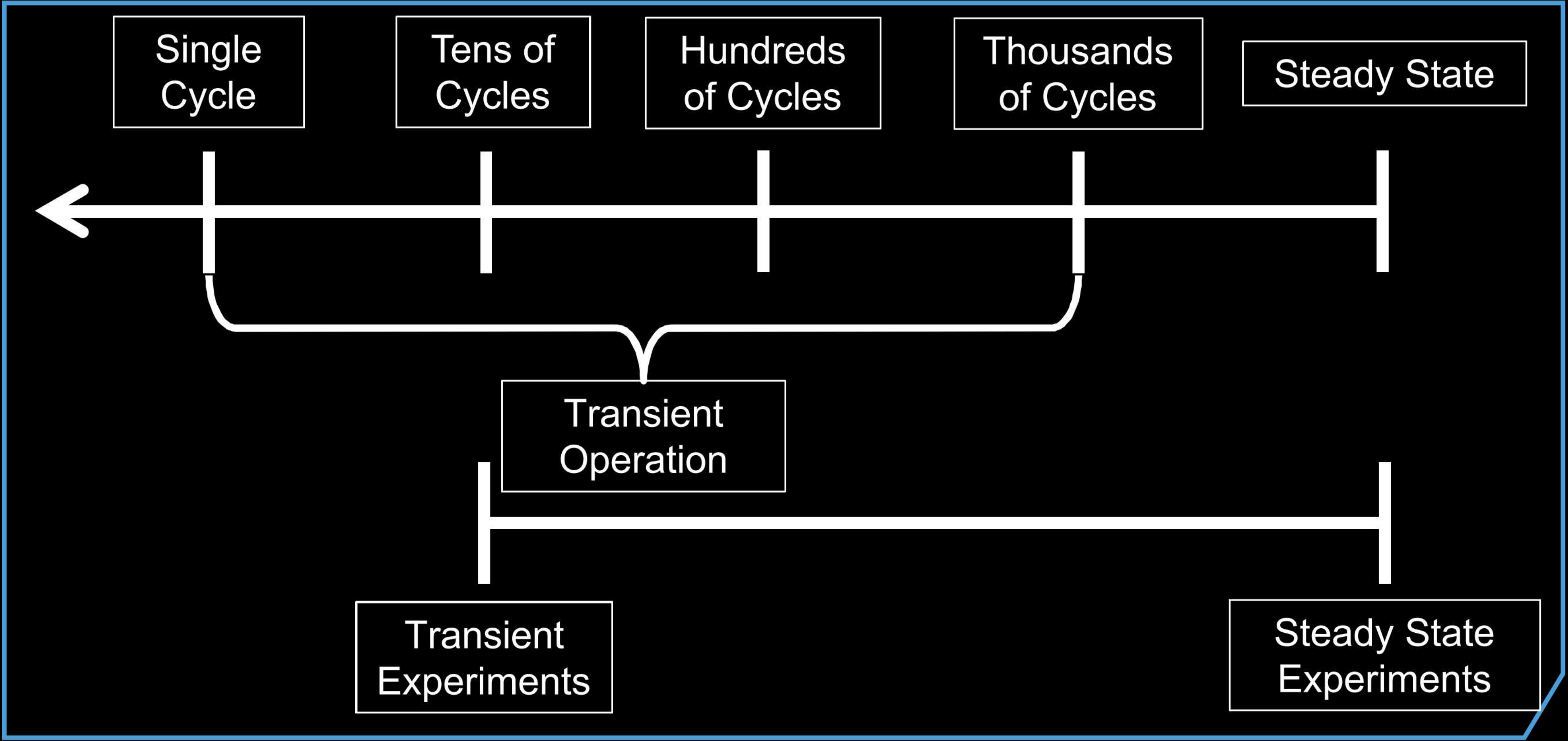
Low residuals - No valve overlap

KL-CA50 measured at 1400 RPM

Well-mixed charge operation for low PM emissions.



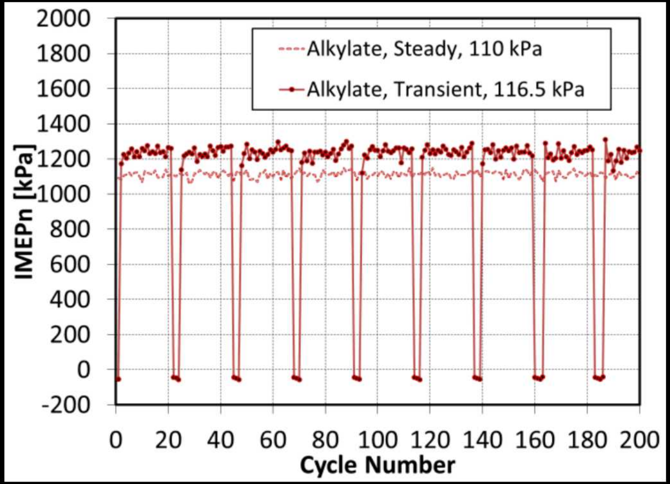
# Test Regimes: Steady State & Transient

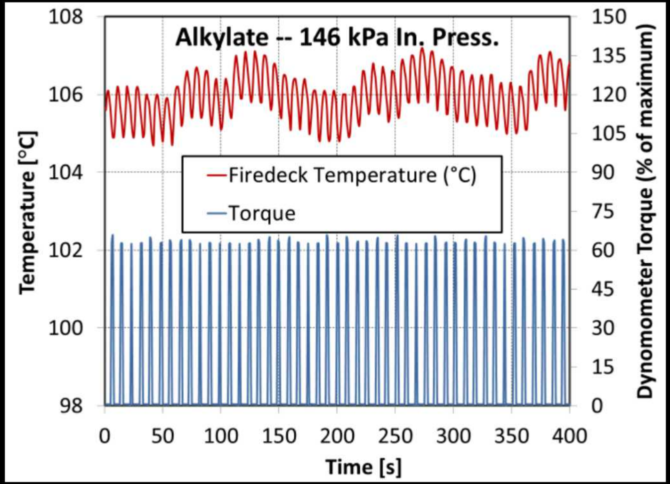


# Test Regimes: Steady State & Transient

**IMEP fluctuations of transient operation are on same order as steady-state, when first 3 cycles are omitted (CoV IMEP < 2%)**

**Firedeck temperatures of transient operation are significantly lower than steady state operation (~105 °C vs 130 °C)**

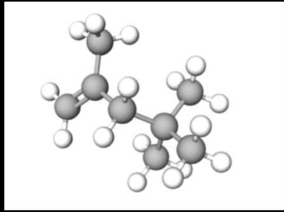


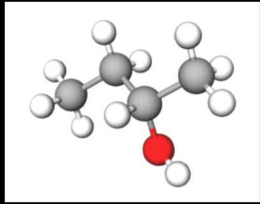
# Fuels Matrix

| | *Isobutanol Blend* | *2-Butanol Blend* | *Diisobutylene Blend* | *High Olefins* | *High Cycloalkanes* | *Alkylate* | *E30* | *High Aromatic* | *RD5-87 E10* |
|---|---|---|---|---|---|---|---|---|---|
| **#** | **1** | **2** | **3** | **4** | **5** | **6** | **7** | **8** | **9** |
| **RON** | 98.1 | 98.2 | 98.3 | 98.3 | 97.8 | 98.0 | 97.9 | 98.1 | 92.1 |
| **MON** | 88.0 | 89.1 | 88.5 | 87.9 | 86.9 | 96.7 | 87.1 | 87.6 | 84.8 |
| **Octane Sensitivity** | 10.1 | 9.1 | 9.8 | 10.4 | 11.0 | 1.3 | 10.8 | 10.5 | 7.3 |
| **AKI** | 93.1 | 93.7 | 93.4 | 93.1 | 92.3 | 97.3 | 92.5 | 92.8 | 88.5 |
| **Oxygenates [vol.%]** | 24.1 | 28.4 | 0.0 | 0.0 | 0.0 | 0.0 | 30.4 | 0.0 | 10.6 |
| **Aromatics [vol.%]** | 19.0 | 17.9 | 20.1 | 13.4 | 33.2 | 0.7 | 13.8 | 39.8 | 20.9 |
| **Alkanes [vol.%]** | 53.1 | 50.1 | 56.3 | 56.4 | 40.6 | 98.8 | 40.5 | 46.2 | 49.4 |
| **Cycloalkanes [vol.%]** | 0.0 | 0.0 | 0.0 | 2.9 | 24.2 | 0.0 | 7.0 | 8.0 | 11.3 |
| **Olefins [vol.%]** | 3.8 | 3.6 | 23.6 | 26.5 | 1.6 | 0.1 | 5.6 | 4.5 | 4.9 |
| **T10 [°C]** | - | - | - | 77 | 56 | 93 | 61 | 59 | 57 |
| **T50 [°C]** | - | - | - | 104 | 87 | 100 | 74 | 108 | 98 |
| **T90 [°C]** | - | - | - | 136 | 143 | 106 | 155 | 158 | 156 |
| **TF [°C]** | - | - | - | 198 | 204 | 161 | 204 | 204 | 203 |
| **Net Heat of Combustion [MJ/kg]** | 40.6 | 40.1 | 43.2 | 44.1 | 43.2 | 44.5 | 38.2 | 43.0 | 41.9 |
| **Heat of Vaporization [kJ/kg]** | 412 | 415 | 337 | 333 | 373 | 308 | 532 | 361 | - |
| **Stochiometric Air/Fuel Ratio** | 13.8 | 13.6 | 14.7 | 14.8 | 14.5 | 15.1 | 12.9 | 14.5 | 14.1 |
| **Heat of Vaporization [kJ/kg stoichiometric charge]** | 27.9 | 28.5 | 21.5 | 21.1 | 24.0 | 19.1 | 38.4 | 23.3 | - |
| **Particulate Matter Index** | 0.40 | 0.37 | 0.47 | 1.00 | 1.54 | 0.22 | 1.28 | 1.80 | - |
| **Average Molecular Formula** | C: 6.299<br>H: 12.744<br>O: 0.326 | C: 6.122<br>H: 12.532<br>O: 0.378 | C: 7.519<br>H: 14.420 | C: 7.130<br>H: 14.23 | C: 6.460<br>H: 11.71 | C: 7.76<br>H: 17.45 | C: 4.49<br>H: 9.87<br>O: 0.5 | C: 6.92<br>H: 12.41 | C: 6.01<br>H: 11.84<br>O: 0.2 |

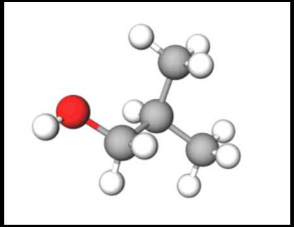
2,4,4-trimethyl-1-pentene



2-butanol



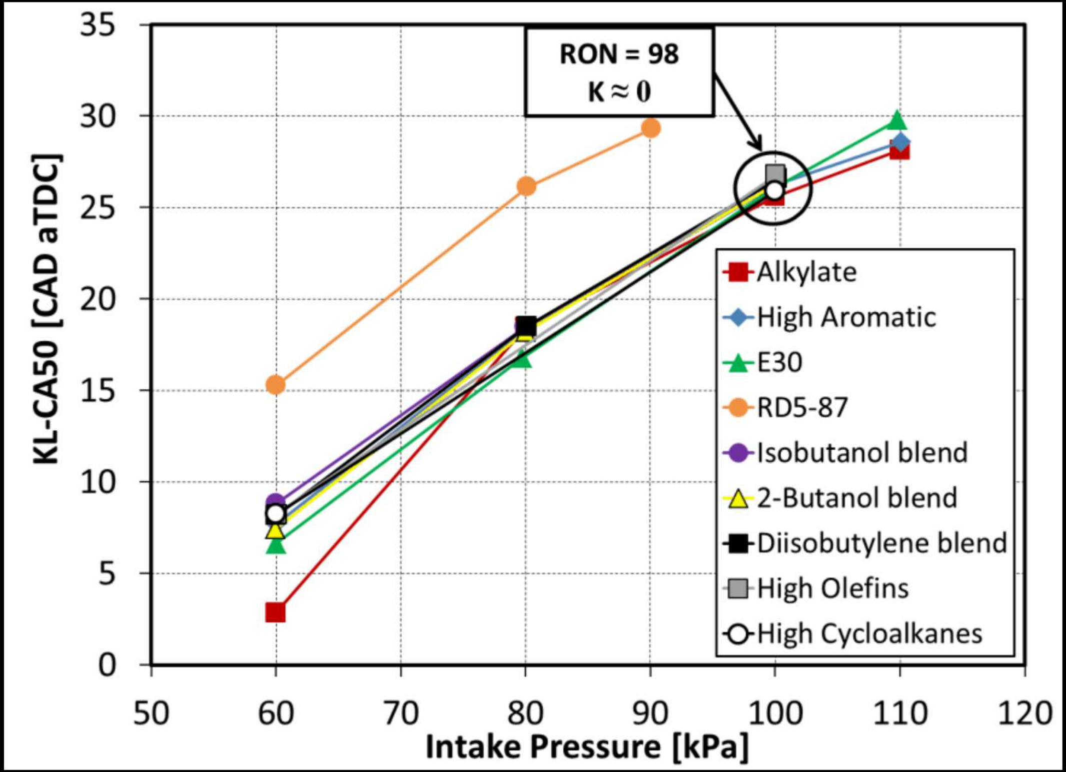
iso-butanol



# Knock Limits: Steady-State 30 °C

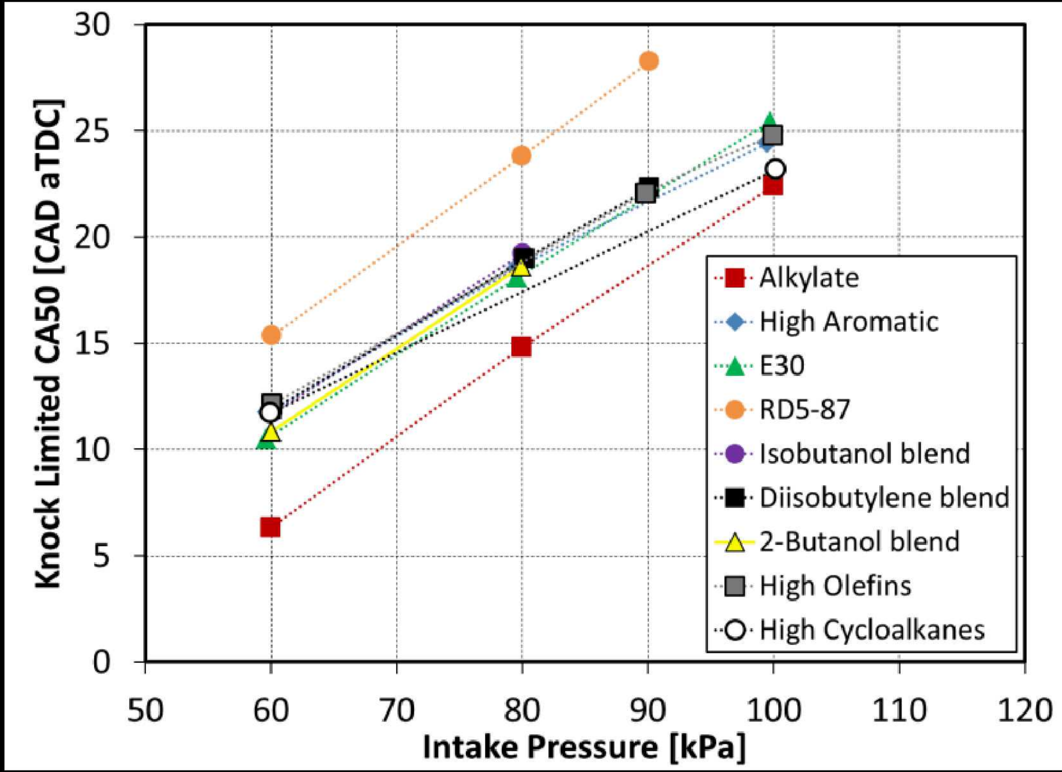
**Under steady-state naturally aspirated conditions, all RON = 98 fuels behave similarly**

**Indicates K ≈ 0**



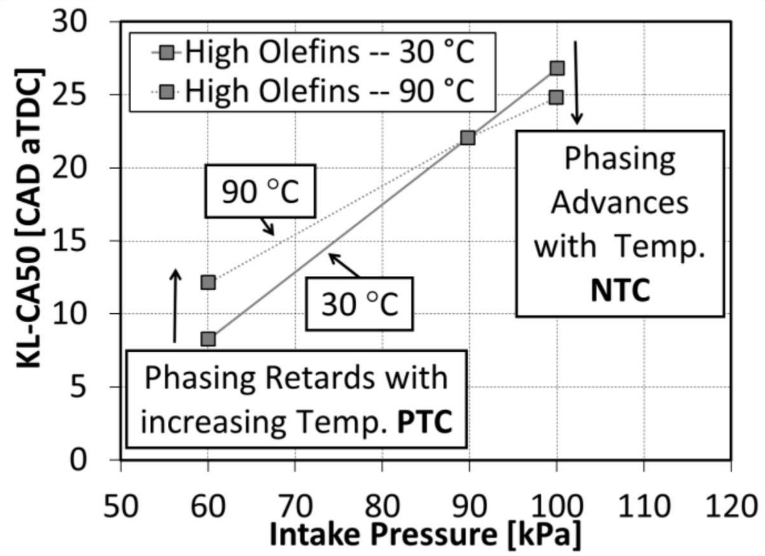
# Knock Limits: Steady-State 90 °C

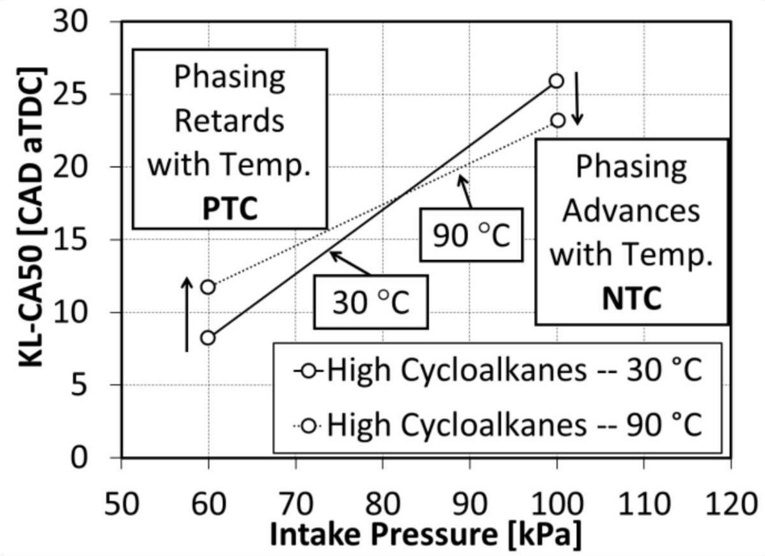
**Under heated steady-state naturally aspirated conditions, differences emerge among RON = 98 fuels**



# Knock Limits: Intake Temperature Response

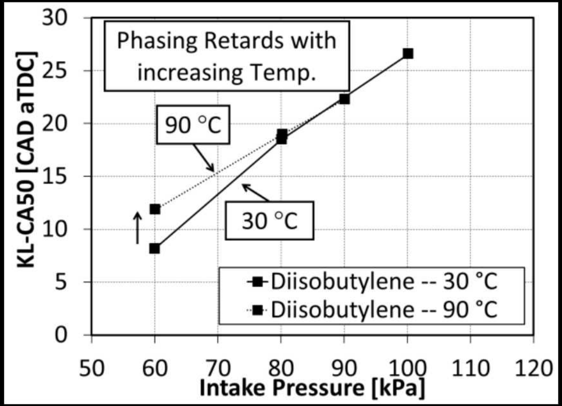
**NTC behavior observable in High Olefins and High Cycloalkanes fuels**
**Similar to behavior observed with other RON = 98, S ≈ 10 core fuels**

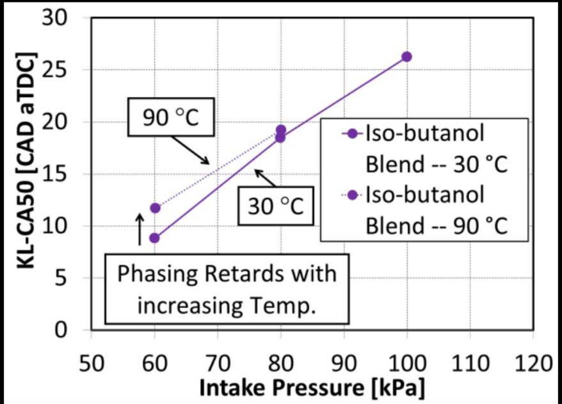


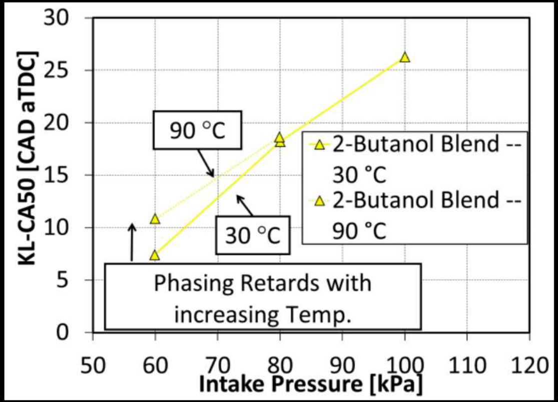



# Knock Limits: Intake Temperature Response

**NTC behavior not observable in TIER III blends, however, likely would be observable if operating range were not limited by pre-ignition**

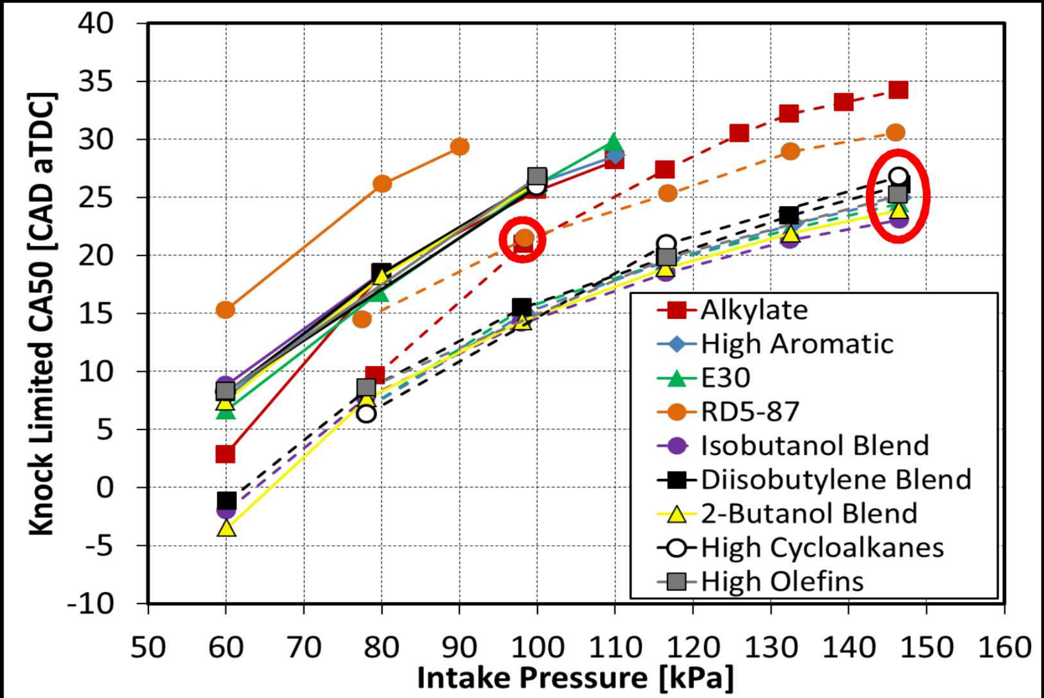


# Knock Limits: Transient Response

- 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

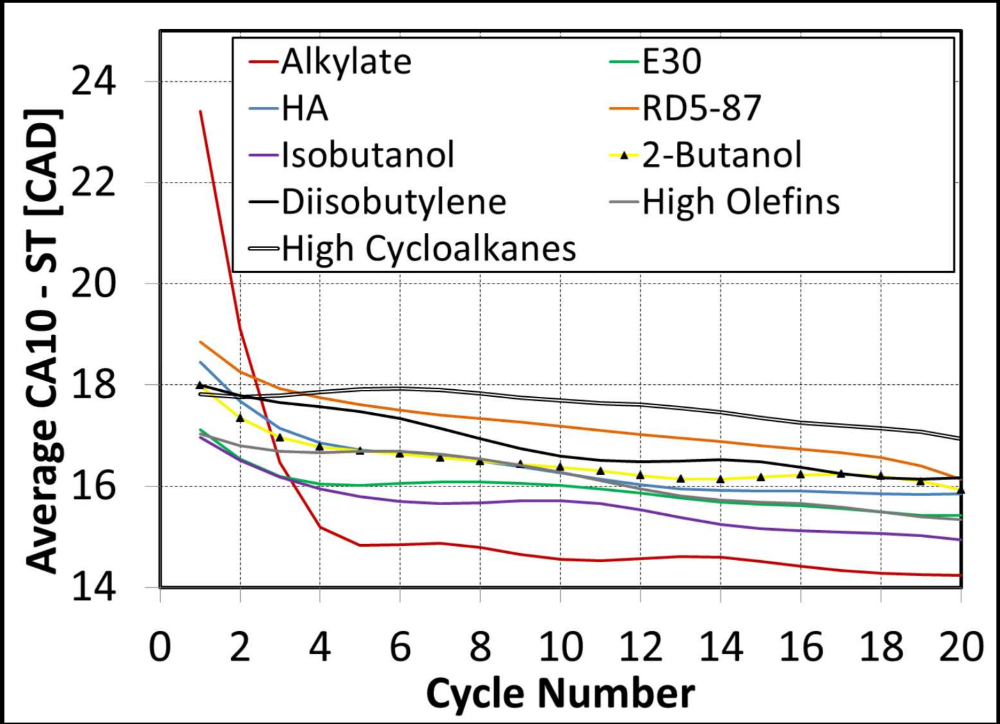


# Response to Transient Operation

Fuels exhibit varying sensitivities to the first fired cycle

First fired cycles has cold residuals composed of air rather than combustion products

Second cycle has hotter residuals, but stoichiometry varies from unity



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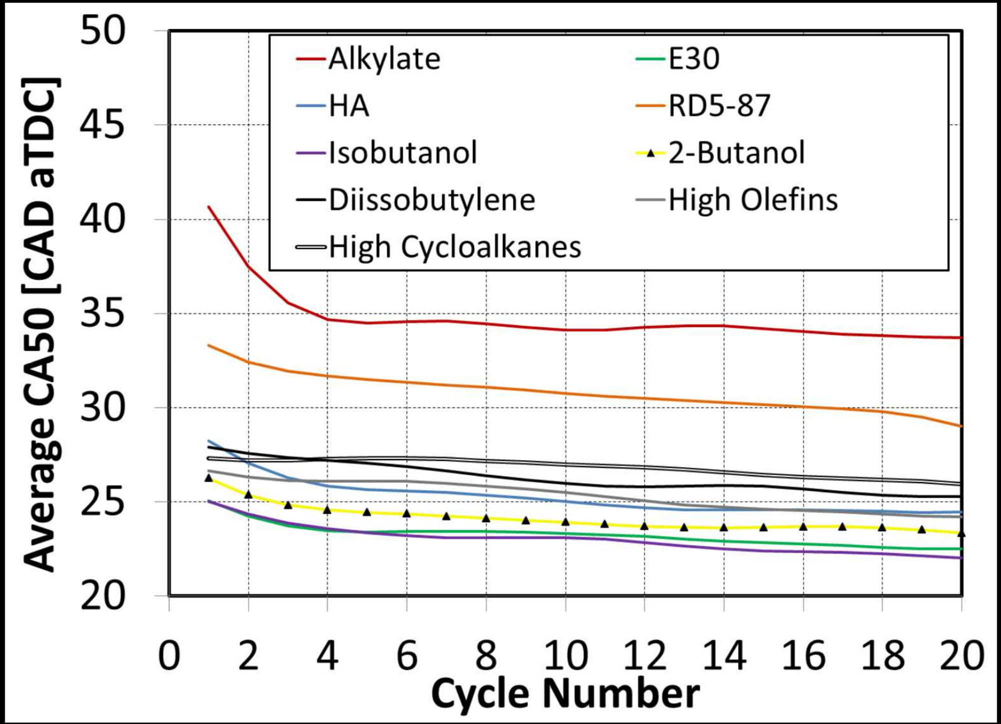

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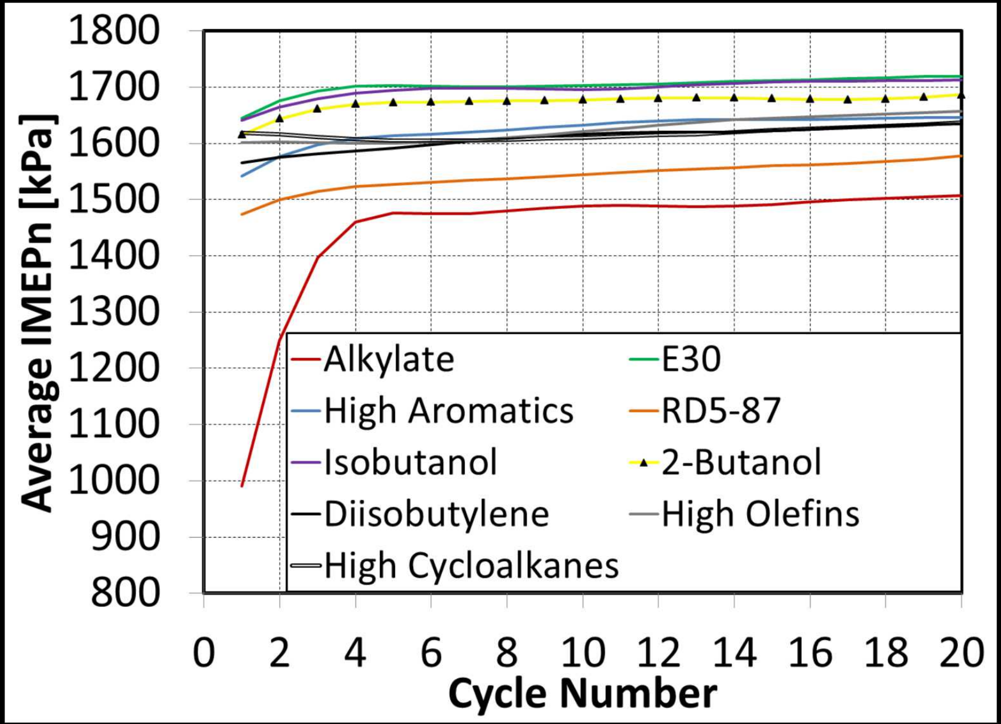

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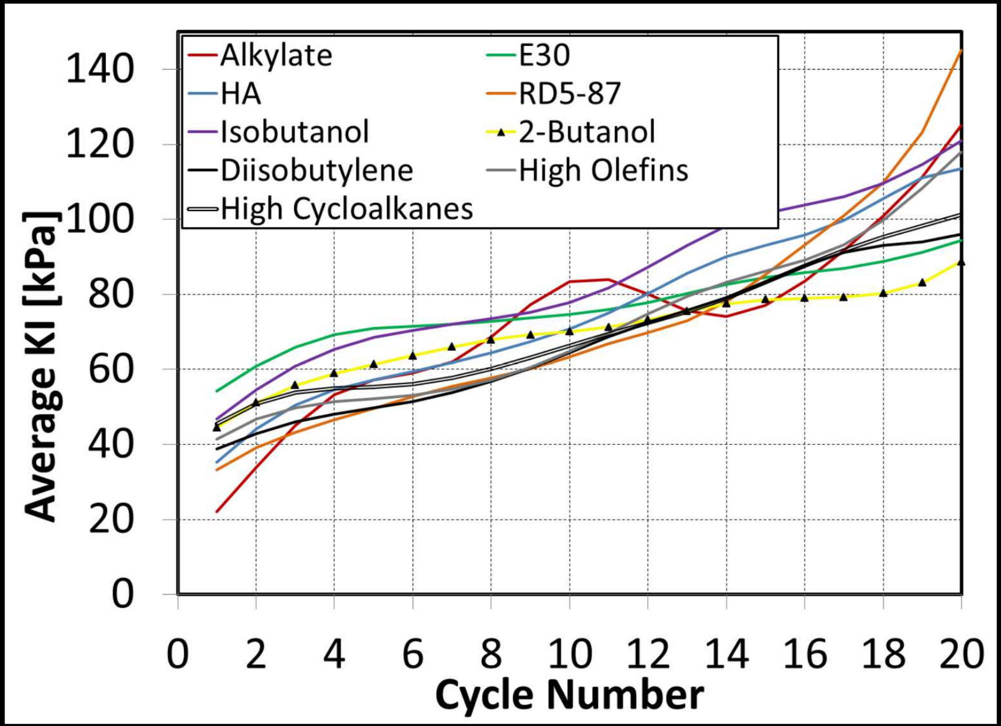
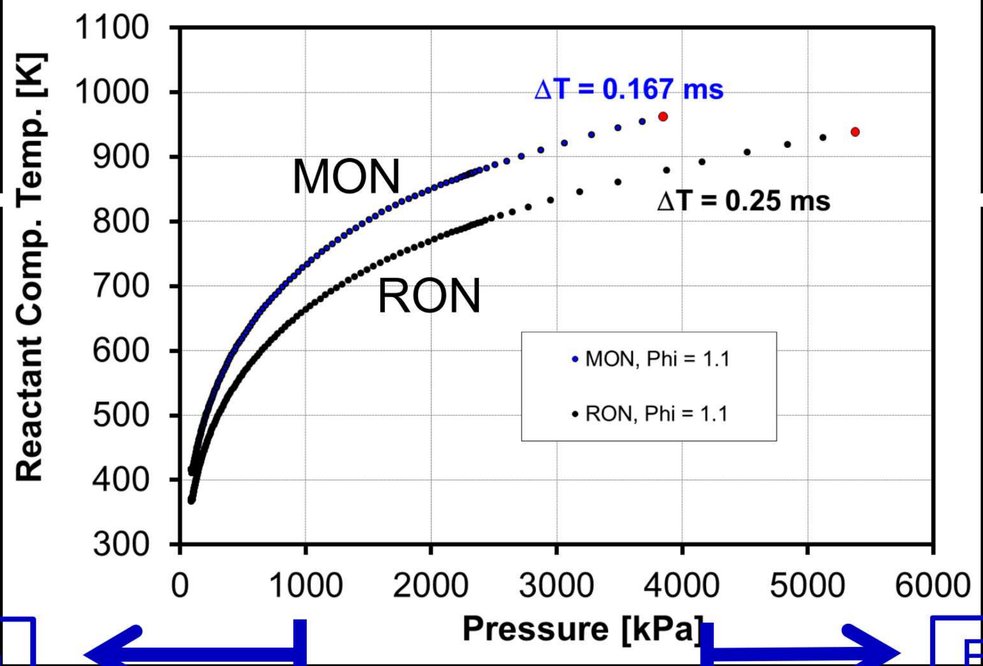


# Octane Index Calculation & Uncertainty Analysis

## Beyond MON

K > 1
Ex: Heated intake / high residuals
HCCI




## Beyond RON

K < 0
Ex: Boosted SI,
GCI

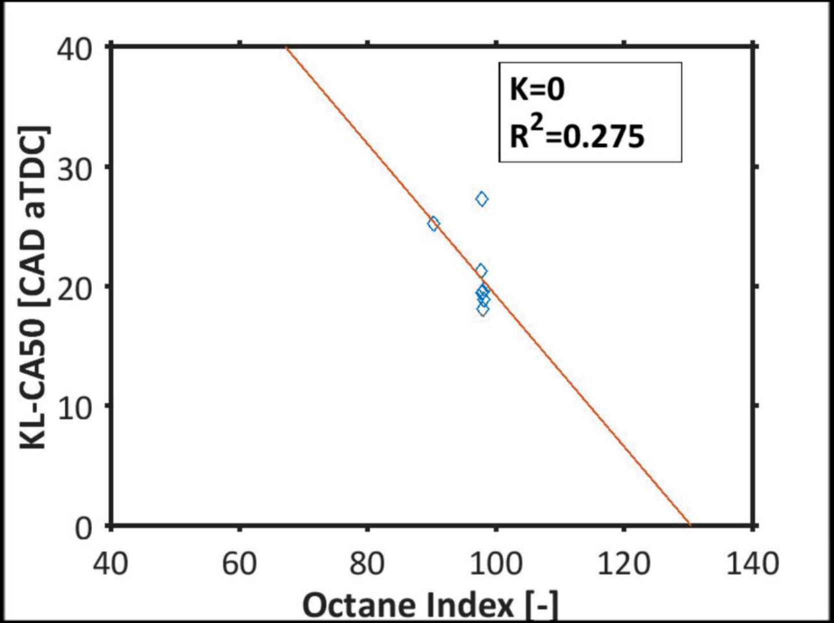
Extrapolation

Extrapolation

Modern SI Engines

OI Reference: SAE #2001-01-3584

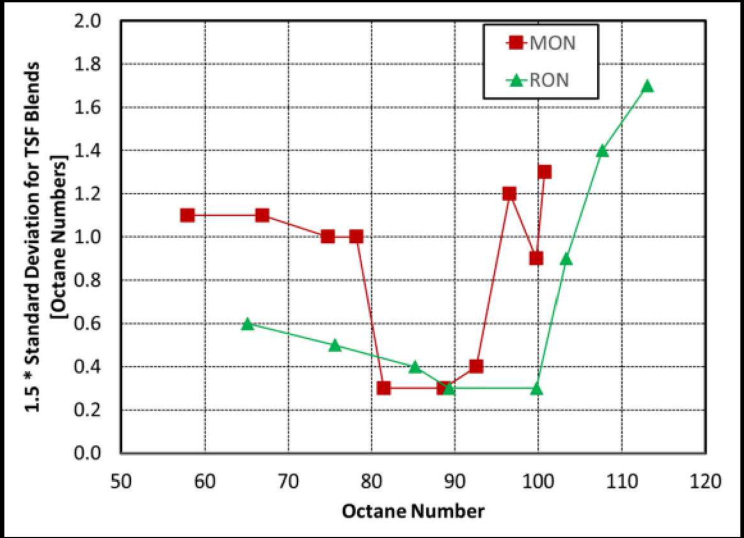
# Calculation of K



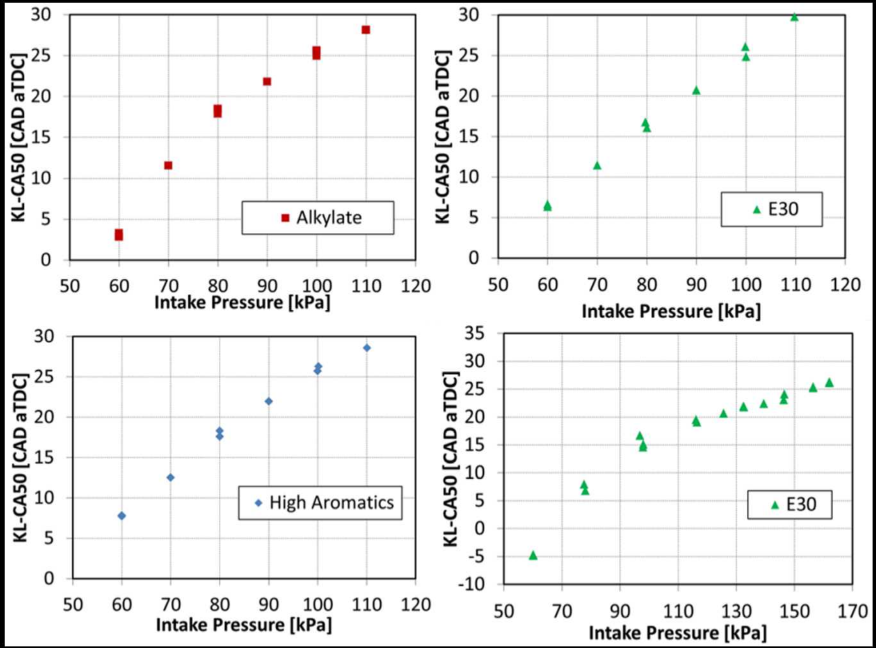

Linear regression between KL-CA50 and Octane Index is performed over a wide range of K values

K value yielding highest coefficient of determination is taken as “best fit” K value

# Consideration of Experimental Uncertainty

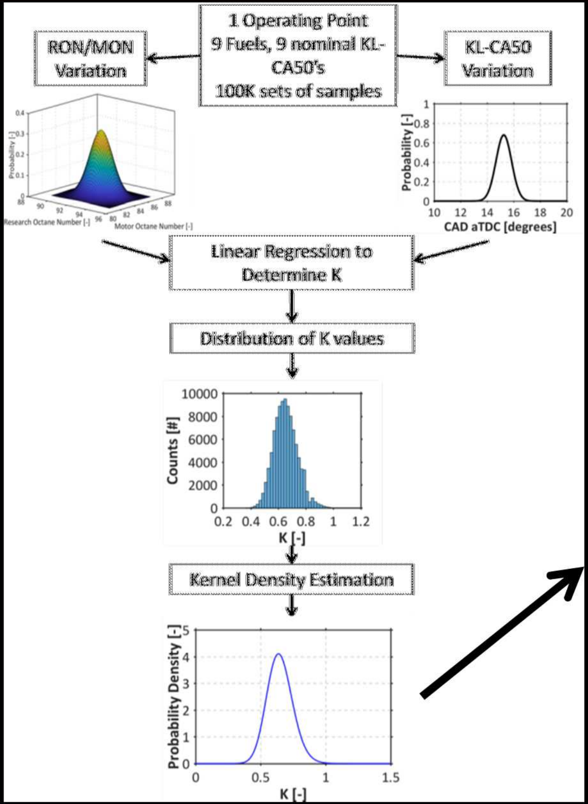



**RON and MON uncertainty depends on Octane Number**

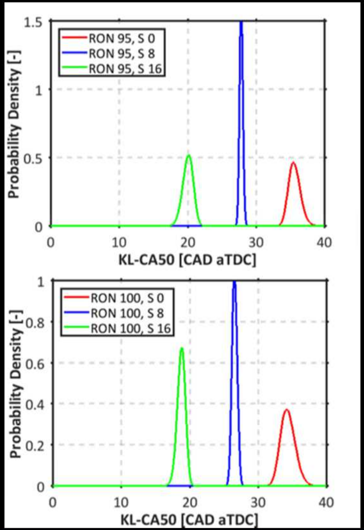


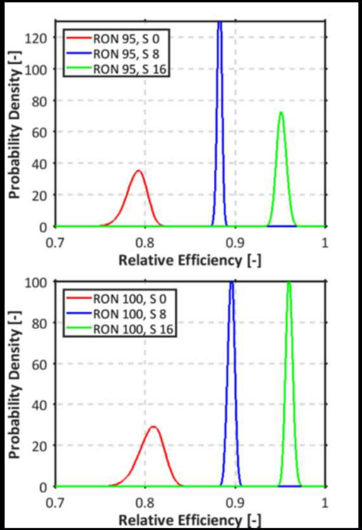

**Standard Deviation of KL-CA50 ≈ 0.41 CAD**

# Consideration of Experimental Uncertainty

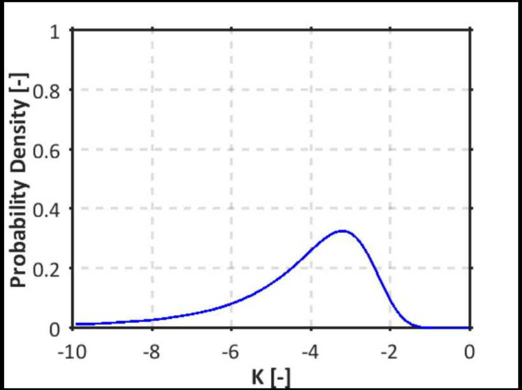


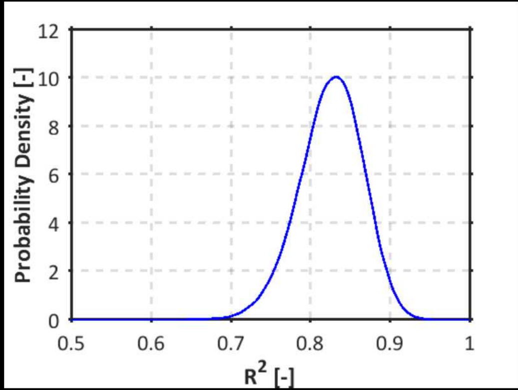

**Monte Carlo sampling procedure used to consider joint RON/MON & KL-CA50 uncertainty on determination of K values and assessment of hypothetical fuels**



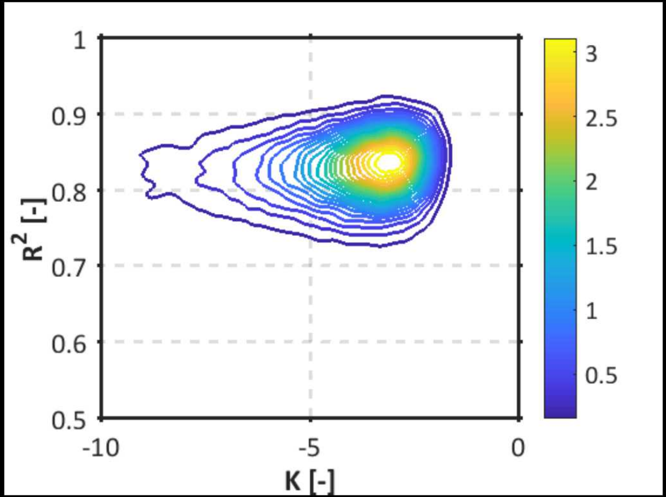



# K Uncertainty: 146 kPa Intake, Transient




- **"Beyond RON" condition exhibits large K value distribution**
  - Distribution skewed
- **Highly unlikely that a perfect fit could be obtained**

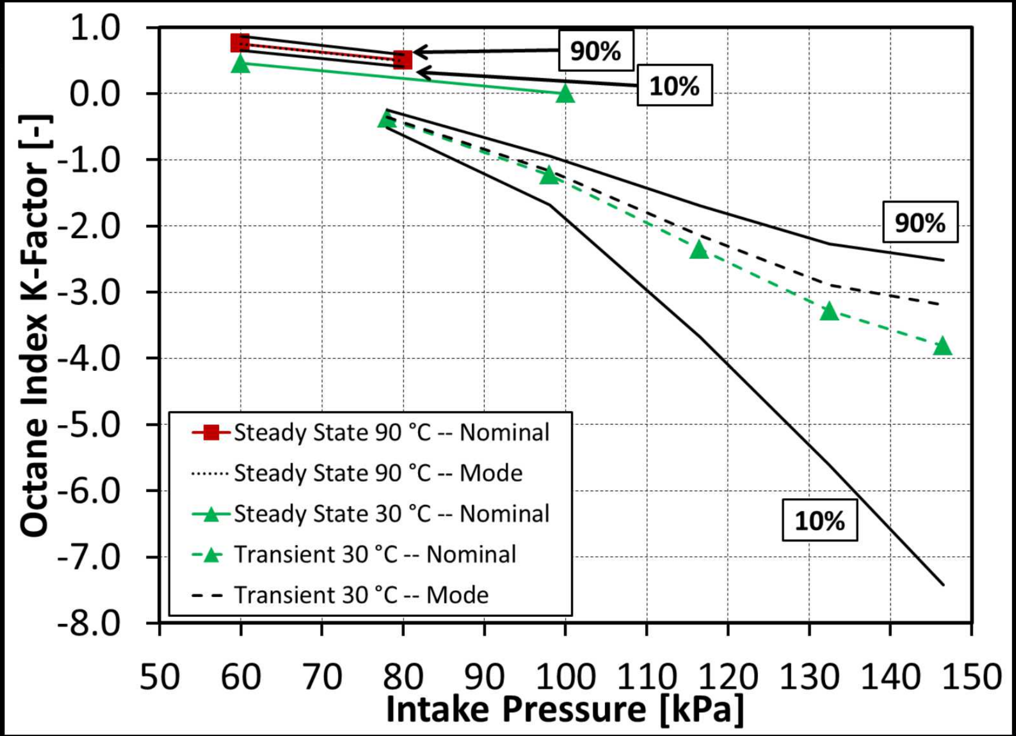


# Effect of Engine Operating Conditions on K

Heated intake temperature drives operation towards MON condition

Higher intake pressures drive operation towards RON condition

Transient operation, with lower thermal state, leads to "Beyond RON" conditions

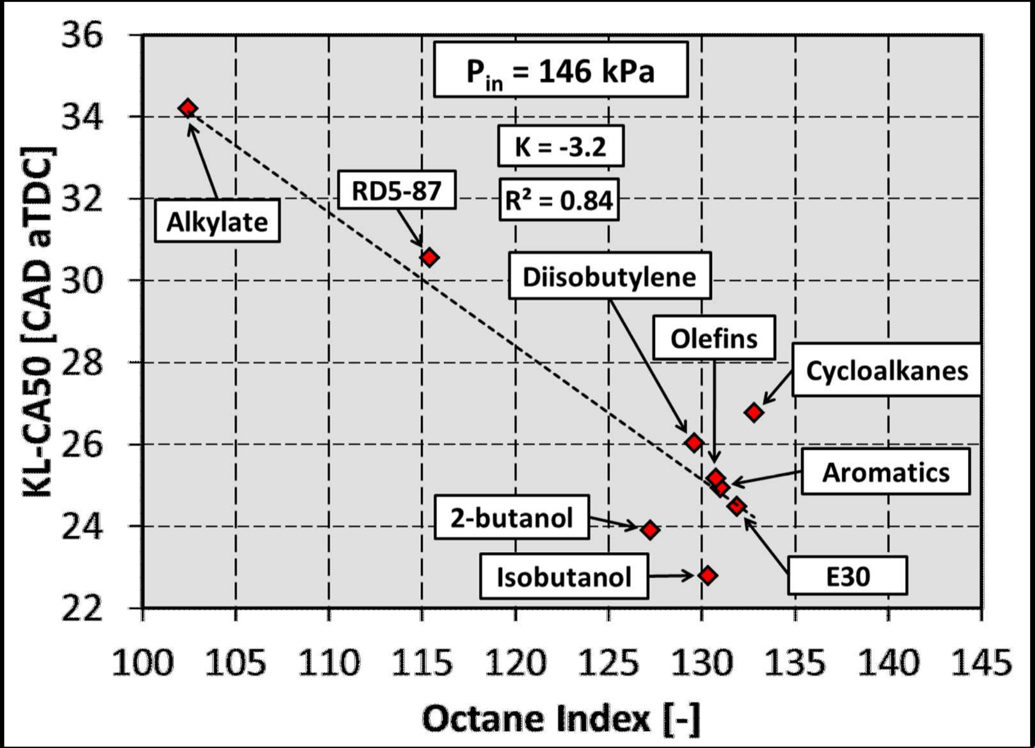


# Deviations from OI-based Ranking

Butanol blends outperform OI predictions.

Diisobutylene (iso-octene) and High-Cycloalkanes underperform.

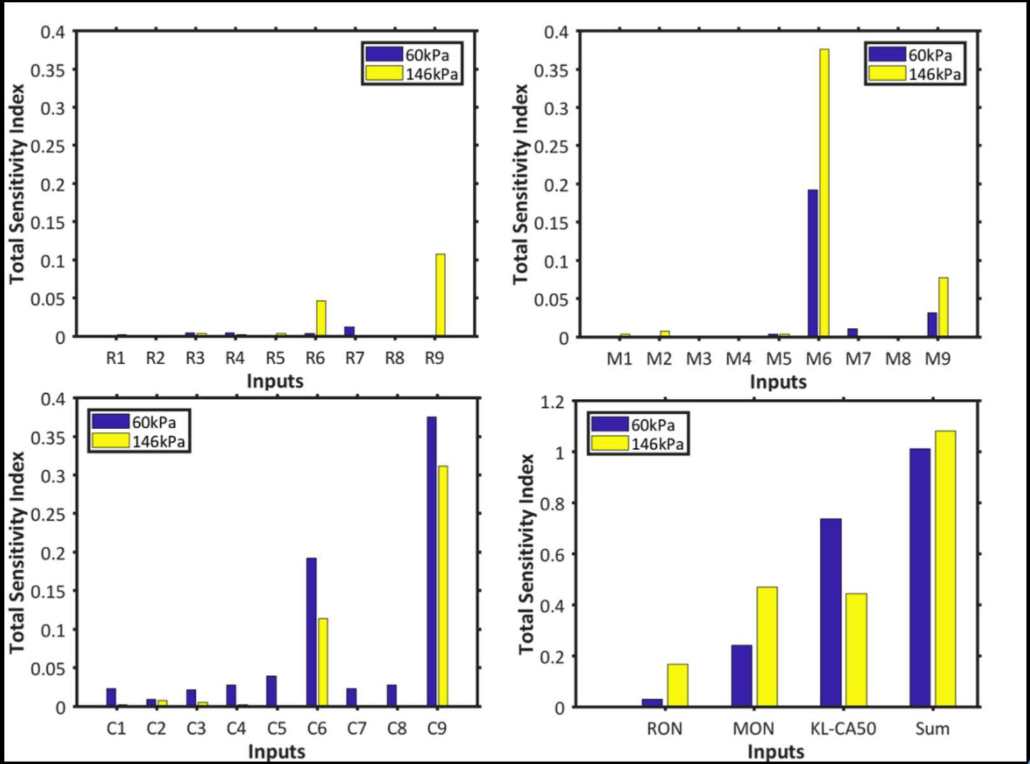
Olefins, Aromatics, and E30 core fuels behave according to OI predictions



# Global Sensitivity Analysis

60 kPa: With 0 < K < 1, KL-CA50 measurement uncertainty dominates the overall uncertainty

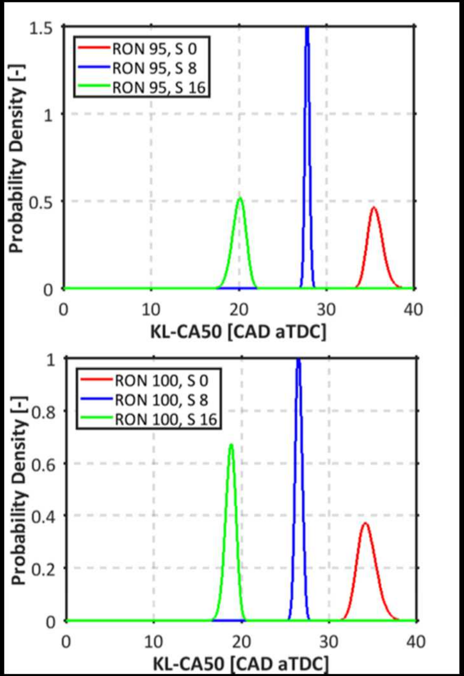
146 kPa: With K << 0, RON-MON uncertainty dominates the overall uncertainty

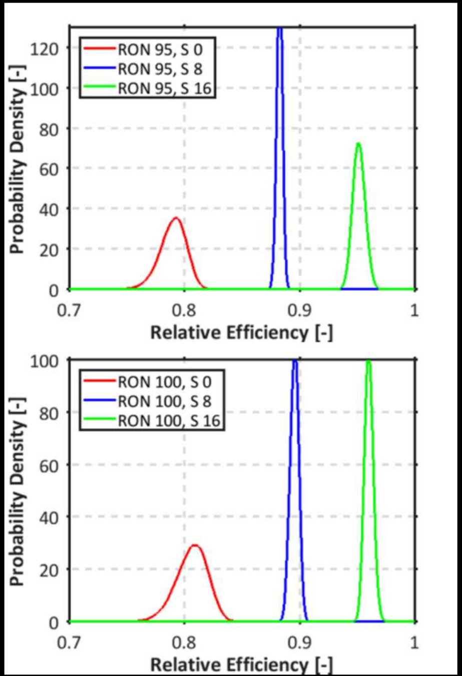


# Uncertainty Assessment of Hypothetical Fuels

Uncertainty of hypothetical fuels related to RON/MON of fuel compared to matrix of test fuels

Hypothetical fuels which fall between test fuels have greater certainty than those falling outside of tested fuels



# Conclusions

- “Beyond RON” conditions demonstrate improved knock-limited performance of tested Tier III blendstocks & high-S fuels over pump- and low-sensitivity gasolines
- 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

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# Thank you

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