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# Using Chemical Kinetics to Understand Effects of Fuel Type and Compression Ratio on Knock-Mitigation Effectiveness of Various EGR Constituents

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# Introduction

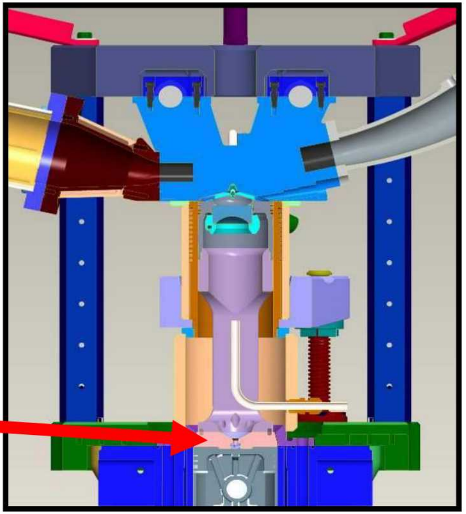
- **Knocking is caused by the strong autoignition of the fuel-oxidizer charge "end-gas" resulting in pressure oscillations.**
- **Autoignition processes are influenced by temperature, pressure, fuel concentration, oxygen concentration, and the temporal evolution of these parameters.**
- **Does EGR effect all fuels equally?**
- **A matrix of three fuels and nine diluent combinations used to investigate competing effects in the previous study. (SAE 2018-01-1677)**

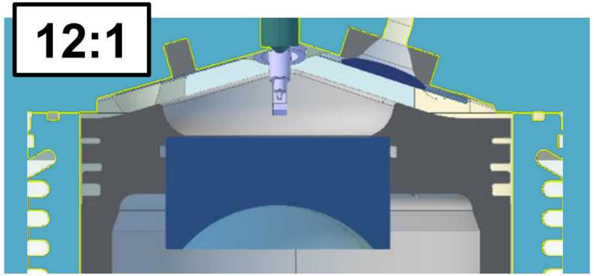
| | |
|---|---|
| **Engine Compression Ratios** | 12:1, 10:1 |
| **Fuels (RON ≈ 98)** | Alkylate, High Aromatic, E30 |
| **Diluents** | Air, $N_2$, $CO_2$, $H_2O$, Dry CSP, Wet CSP, Air + CSP, EGR, Air+EGR |
| **Dilution Levels** | $\phi_m = 0.92$, $\phi_m = 0.85$ |

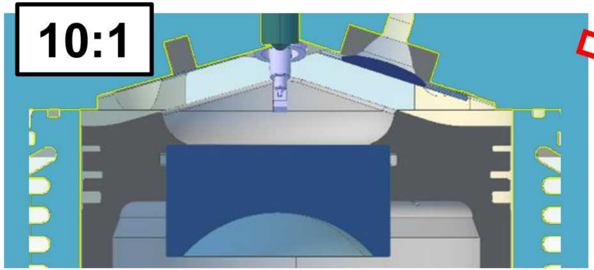
| | Alkylate | High Aromatic | E30 |
|---|---|---|---|
| S | 1 | 11 | 10 |
| RON | 98 | 98 | 98 |
| MON | 97 | 87 | 88 |
| Ethanol [vol.%] | 0 | 0 | 30 |
| Aromatics [vol.%] | 0 | 31 | 8 |
| T90 [°C] | 106 | 158 | 155 |

# Research Engine used for Experiments (Recap of Previous Study: SAE 2018-01-1677)

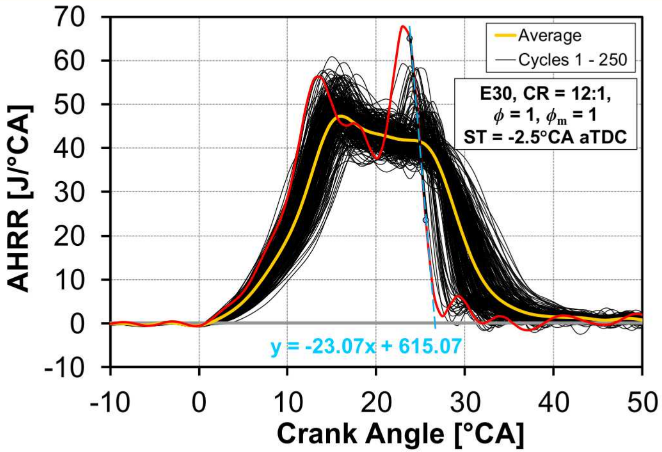
- **DISI, 0.55 L displacement.**
- **High-swirl operation.**
- **Low residuals.**
- **Conventional high-energy ignition system.**
- **Well-mixed charge operation.**
- **CR = 12:1 or 10:1.**
  - Use adaptor plates with various thicknesses.

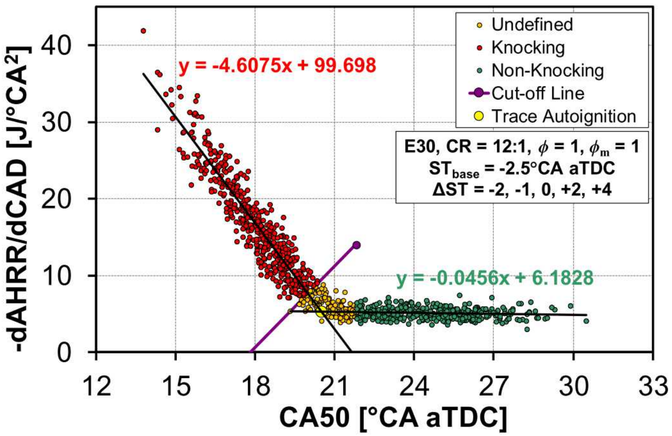





# Definition of Trace Autoignition (Recap of Previous Study: SAE 2018-01-1677)



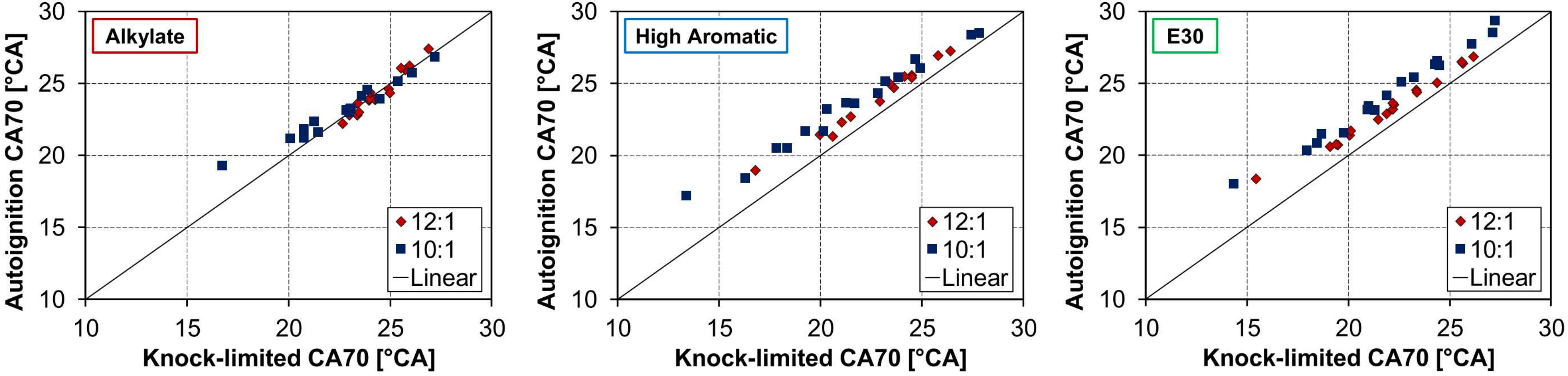




- **Knock vs. Autoignition: Knocking is the phenomena which is a problem for SI engines.**
- **However, the problem is rooted in the autoignition of the end-gas.**
- **To begin to decouple these two phenomena, the phasing required for end-gas autoignition is measured by observing the heat-release characteristics of the charge.**
  - Increased rate of decay of the heat release rate indicates light autoignition event.

❖ **Knock-limited CA50 is different from Trace Autoignition CA50.**
**(KL-CA50 is determined based on Knock Intensity.)**

# Knock-Limited CA70 vs Trace Autoignition CA70 (Recap of Previous Study: SAE 2018-01-1677)

**All °CA is referenced at aTDC.




- **E30 and High Aromatic Fuels were able to operate with phasing advanced from the autoignition limit.**
- **Indicates that these fuels can tolerate light autoignition without exceeding knock limit.**
- **Conversely, Alkylate cannot operate in advance of the autoignition limit without exceeding the knock limit under most conditions.**
  - Suggests that this fuel is less tolerant of end-gas autoignition. Why?

# Numerical Study: Conditions of Interest & Methodology

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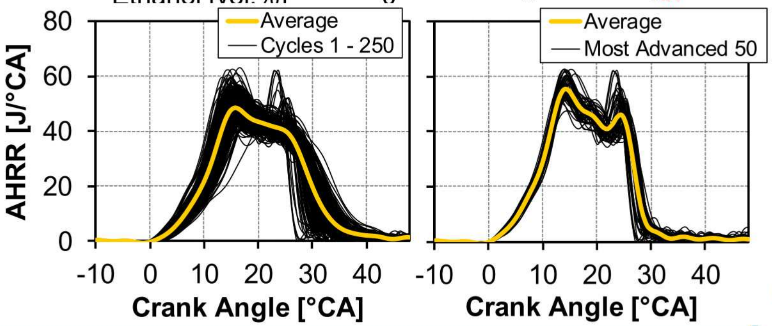
- **Numerical study was conducted for the combinations of CR, diluents, and three fuels listed in the table.**
- **Closed, homogeneous, adiabatic reactor models used to model end-gas.**
- **Experimental pressure trace imposed to mimic compression (due to piston and flame induced)**
  - Experimental pressure trace was downsampled to 10% most advanced cycles.
  - Resulting heat release cases with observable autoignition shown in figure.
- **Included trace species in residual gas such as NO which plays significant role in autoignition chemistry.**

| | |
|---|---|
| CR | 10:1, 12:1 |
| Diluent | None, Air, CO2, N2 |
| Dilution level | $\phi_m$ = 0.85 |
| Fuels | Alkylate, High Aromatics, E30 |

| | Alkylate | High Aromatic | E30 |
|---|---|---|---|
| S | 1 | 11 | 10 |
| RON | 98 | 98 | 98 |
| MON | 97 | 87 | 88 |
| Ethanol [vol.%] | 0 | 0 | 30 |



# Definitions on Mass-Based Equivalence Ratio, Autoignition Timing, and Burned Mass-Fraction (MFB) at Autoignition Timing

**Conventional $\phi$**

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

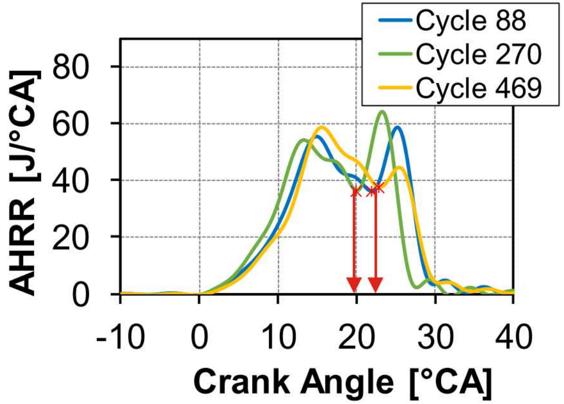
**Mass-based $\phi$**

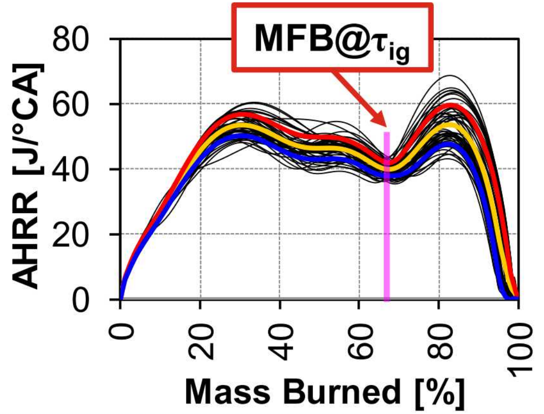
$$\phi_{\mathrm{m}} \equiv \frac{\left(F/C\right)_{Actual}}{\left(F/A\right)_{Stoichiometric}}$$

F = **F**uel mass.
A = **A**ir mass.
C = Gas **C**harge Mass (Example: Air + $N_2$).

| Diluent | $\phi$ | $\phi_m$ |
|---|---|---|
| None (baseline) | 1 | 1 |
| Air | 0.85 | 0.85 |
| $N_2$, $CO_2$ | 1 | 0.85 |

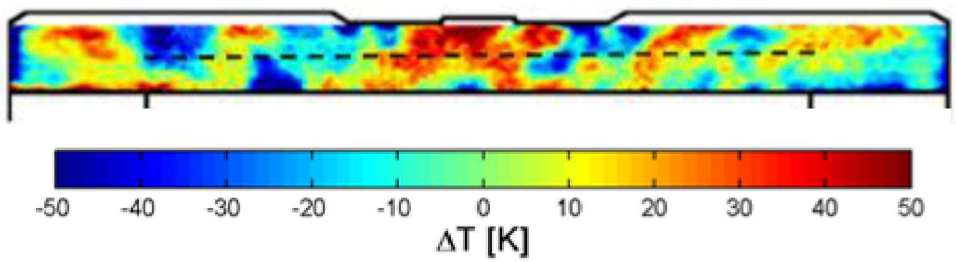
- **$\phi_m$ is a measure of chemical energy per reactant mass, regardless of type of diluent.**
- **Allows plotting data for operation lean and with EGR on the same scale.**



# Study Effects of Thermal Stratification in the End Gas: Previous HCCI Work

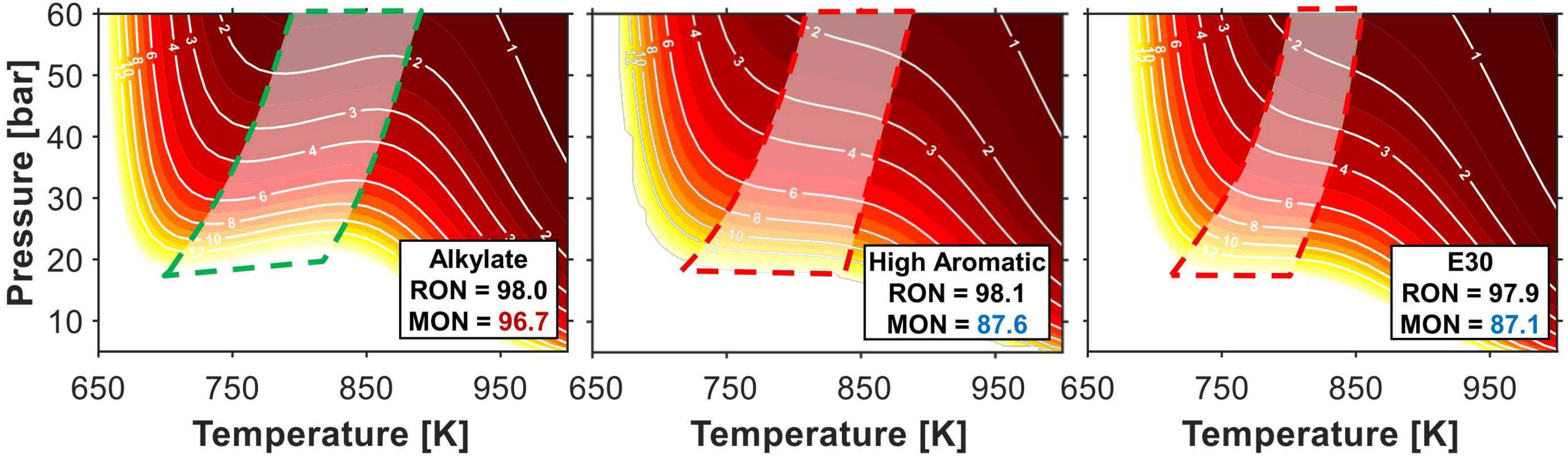
- **Natural thermal stratification is created by heat-transfer from the compressed and heated gas to the surrounding combustion chamber walls.**
  - Planar thermal imaging SAE 2012-01-1111.
  - Cold pockets entrain from walls.




- **Thermal broadening provides an opportunity for sequential autoignition.**
- **Shown to reduce HRR in HCCI engines.**
- **Could reduce knock intensity in SI engines?**

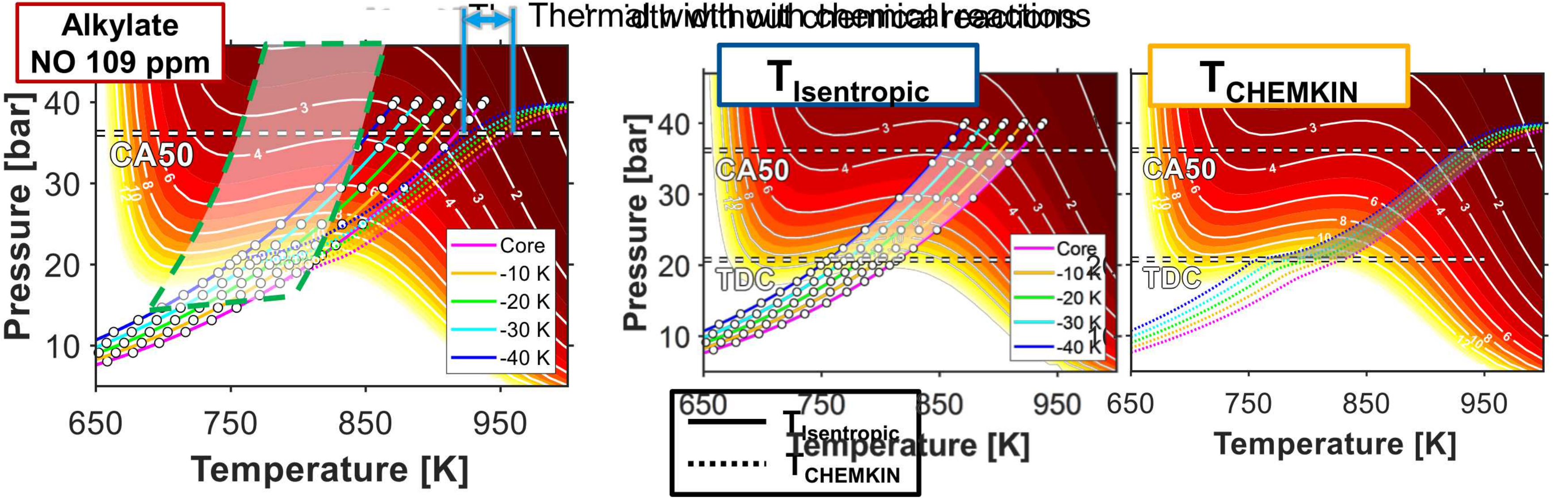
➢ Heat transfer and boundary layer effects mimicked by initializing six reactor models with 10K variations in initial temperature (for a 50K span).

# Comparison of Constant Volume Ignition-Delay Maps for Three RON ≈ 98 Fuels




- **The Alkylate fuel is the only fuel that exhibits strong NTC behavior.**
- **Region of reduced temperature sensitivity is wider for the High Aromatic fuel compared to the E30 fuel.**
  - Suggests differences in autoignition chemistry despite having nearly identical RON and MON.

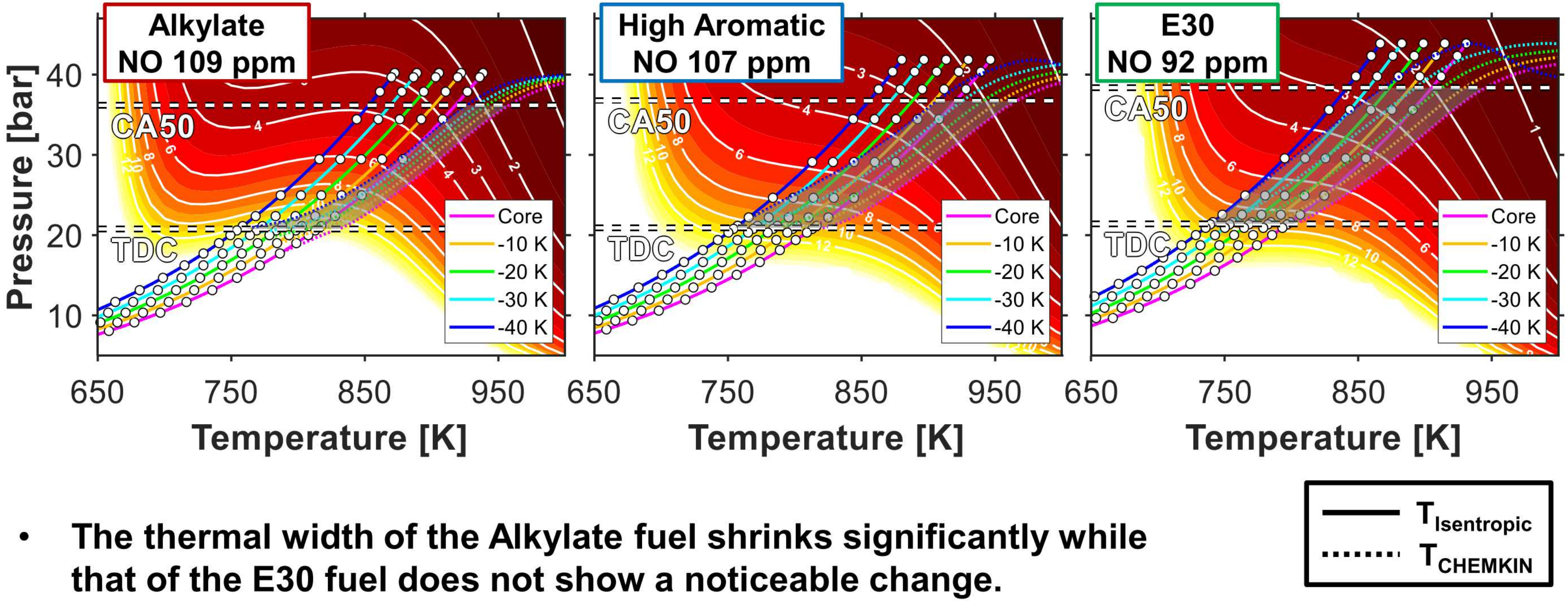
# Temporal Evolution of Thermal Stratification for Three RON ≈ 98 Fuels (Non-diluted, CR 10:1)




- **Temperature-pressure (TP) trajectories of lower temperature zones traverses through and spend significant amount of time in NTC regime.**
- **Chemical reactions play important role in altering thermal width.**

$T_{Isentropic}$
$T_{CHEMKIN}$

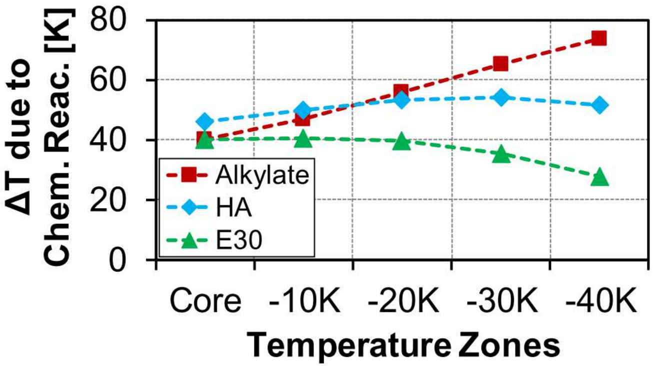
# Temporal Evolution of Thermal Stratification for Three RON ≈ 98 Fuels (Non-diluted, CR 10:1)

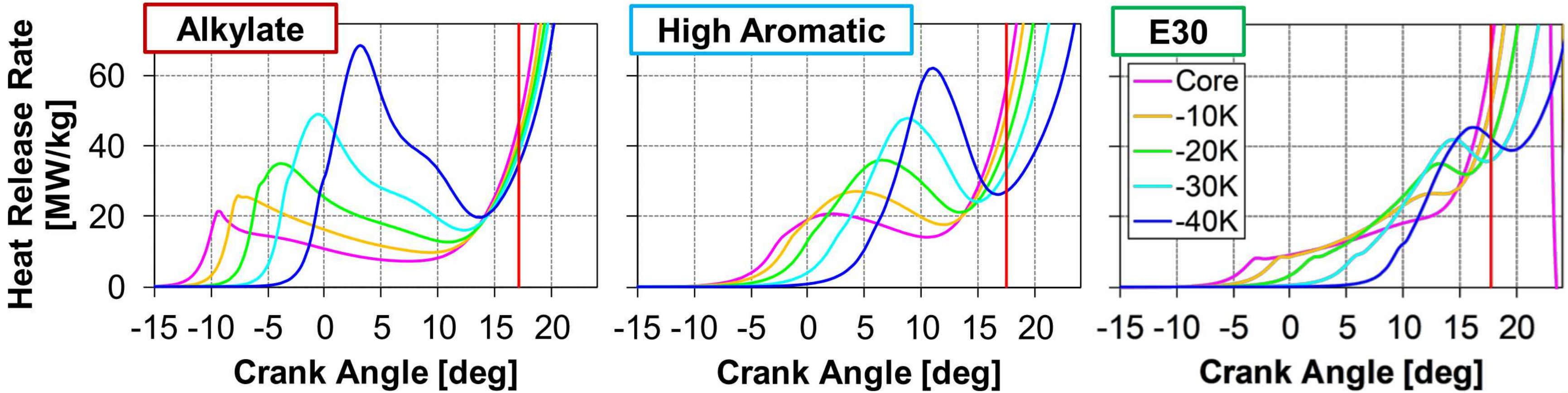



- **The thermal width of the Alkylate fuel shrinks significantly while that of the E30 fuel does not show a noticeable change.**
  - This is a consequence of a greater temperature rise in the coldest zone of the Alkylate fuel compared to the other zones.

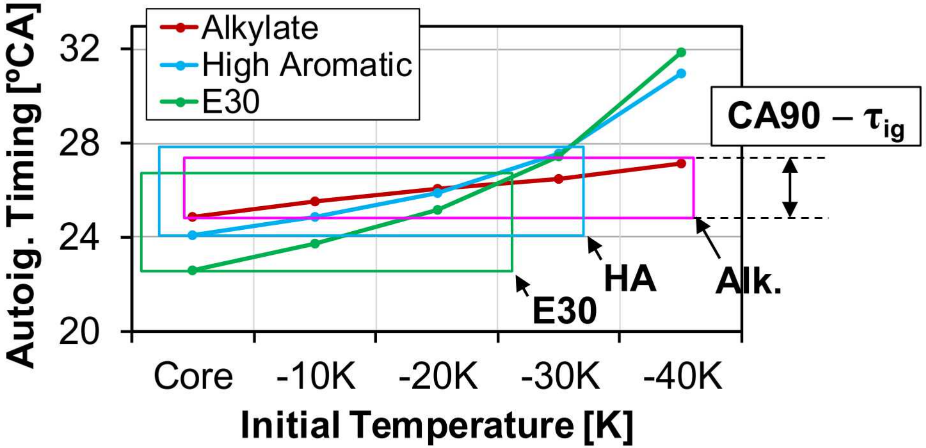
# Effect of Fuel Type on Thermal Stratification (Non-diluted, CR 10:1)

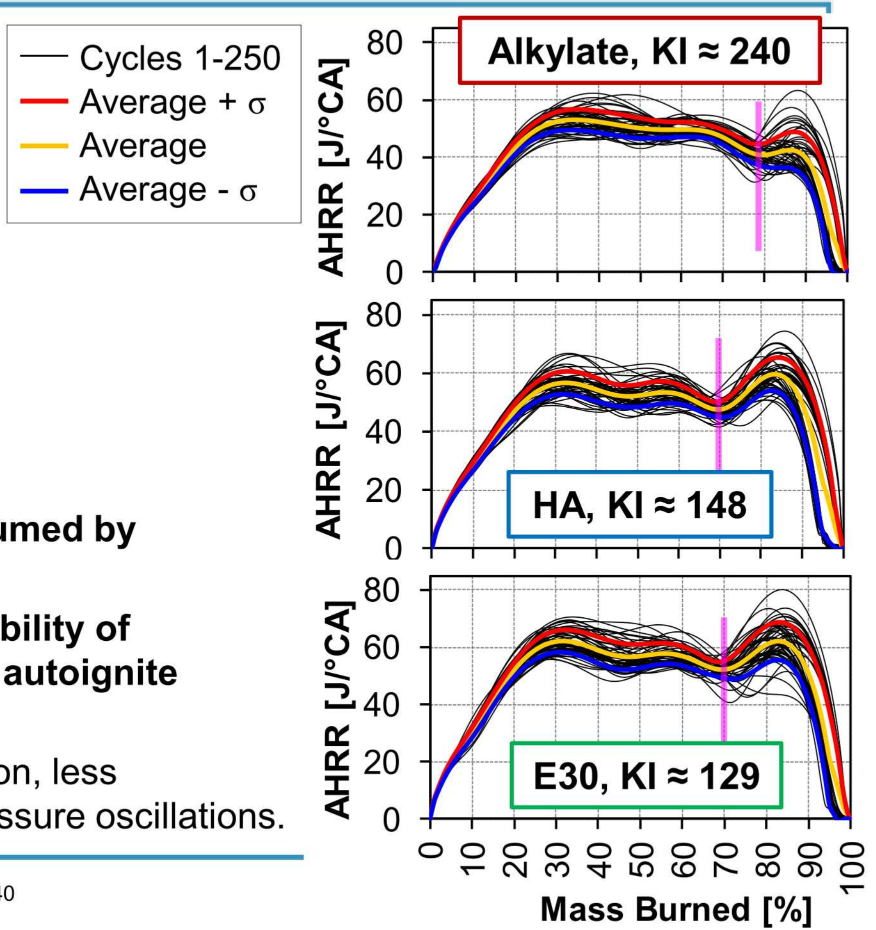
- **The coldest zone of Alkylate exhibits much stronger LTHR than the other fuels.**
  - Explains the greater temperature rise in the coldest zone of the Alkylate fuel.
- **The peak magnitude of LTHR of E30 increases moderately with a reduction of the initial temperature.**



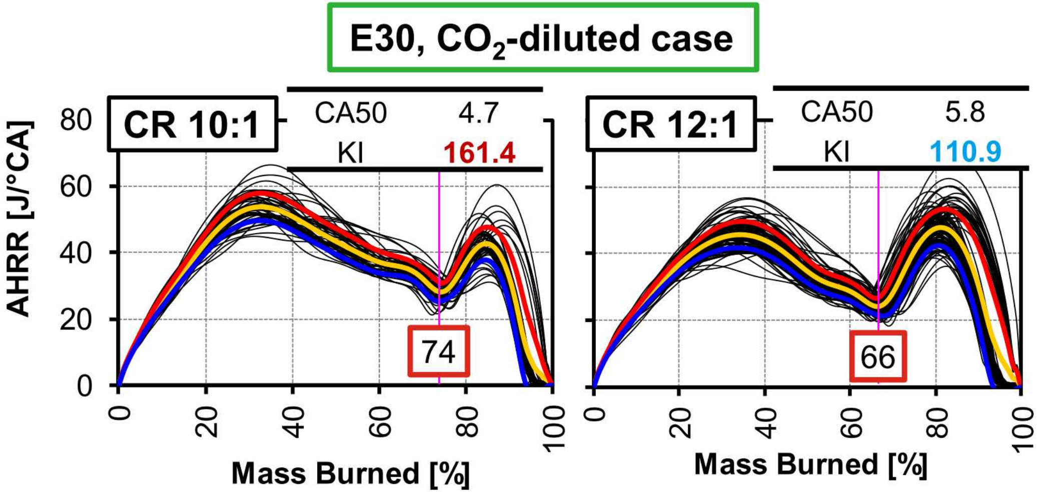
# Comparison of Sequential Autoignition and Its Relevance to Experimental Results (Non-diluted, CR 10:1)

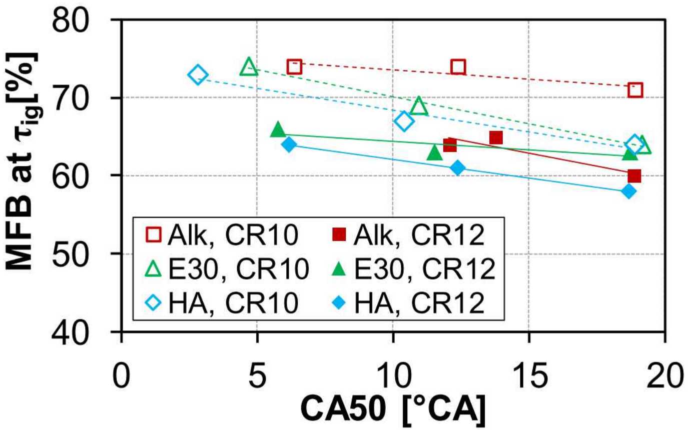


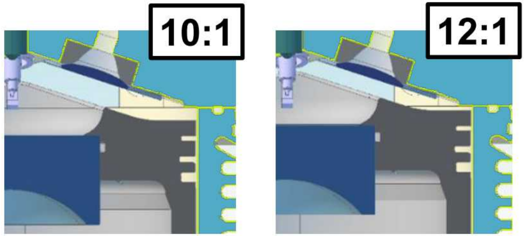




- **(CA90 - $\tau_{ig}$) → Time allowed for end-gas to be consumed by deflagration after adiabatic core autoignites.**
- **Comparison with the (CA90 - $\tau_{ig}$) indicate a ↑ probability of Alkylate's reactants in colder temperature zones to autoignite before deflagration reaches these cooler areas.**
  - Hypothesized that with a faster sequential autoignition, less autoigniting end-gas mass is sufficient to induce pressure oscillations.

# Effect of Compression Ratio on Thermal Stratification (Physical effect)



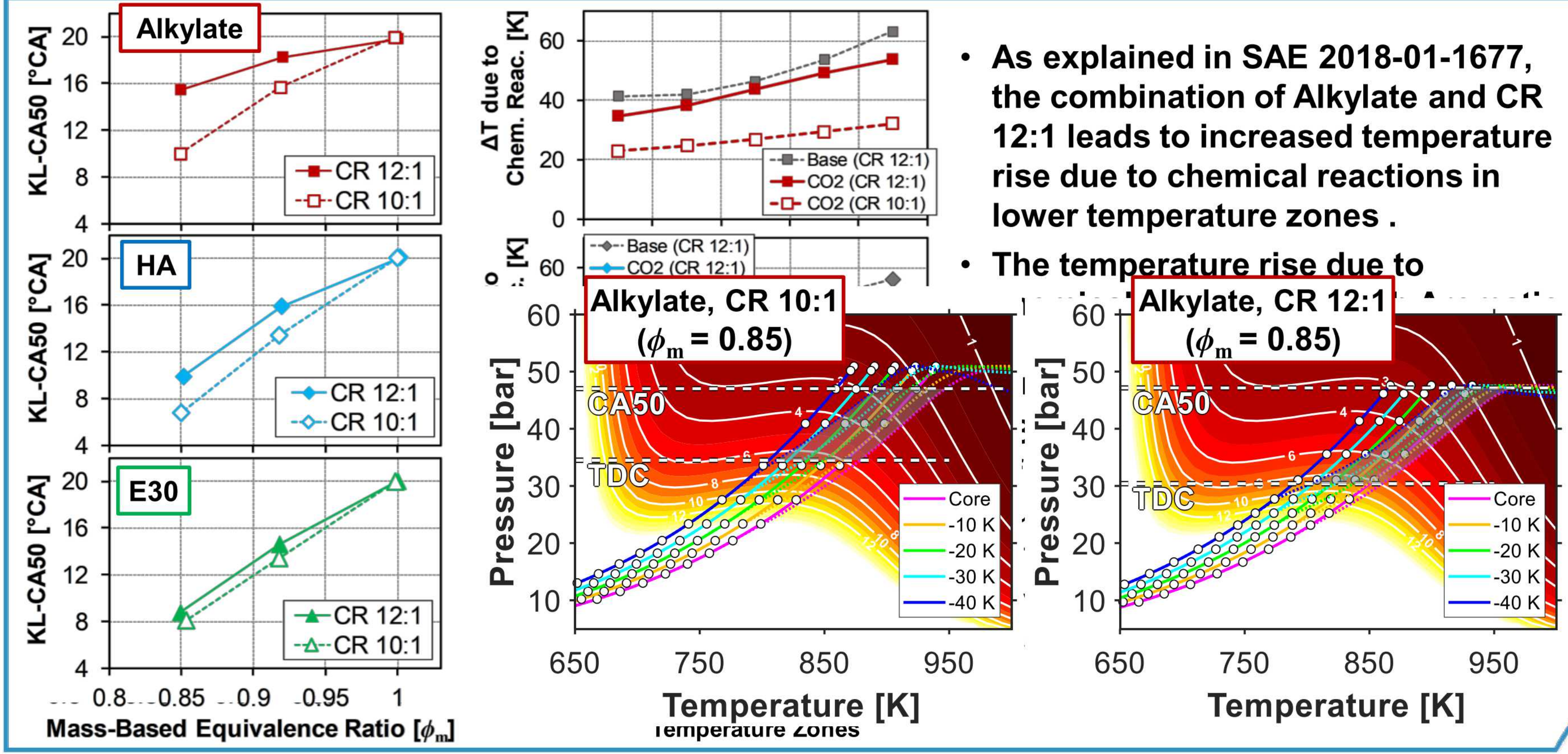



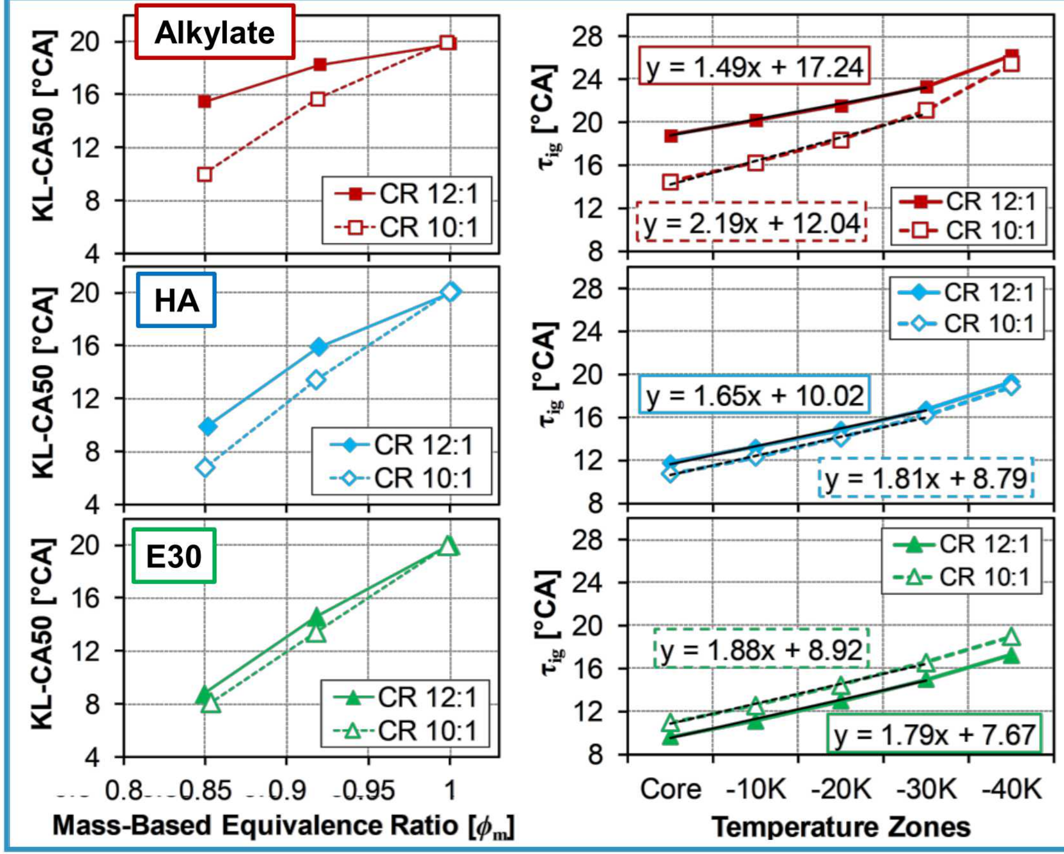

- **At any given combination of fuel and CA50, CR 12:1 case tolerated a larger autoigniting end-gas mass.**
  - Hypothesized that for the higher CR, heat transfer in the end-gas region is stronger and enhances the thermal stratification.
  - $IMEP_g$ at CR = 10:1 and 12:1 were -37.9 kPa and -51.0 kPa.

# Effect of Compression Ratio on Thermal Stratification (Chemical effect; $CO_2$-diluted condition)

- As explained in SAE 2018-01-1677, the combination of Alkylate and CR 12:1 leads to increased temperature rise due to chemical reactions in lower temperature zones .
- The temperature rise due to

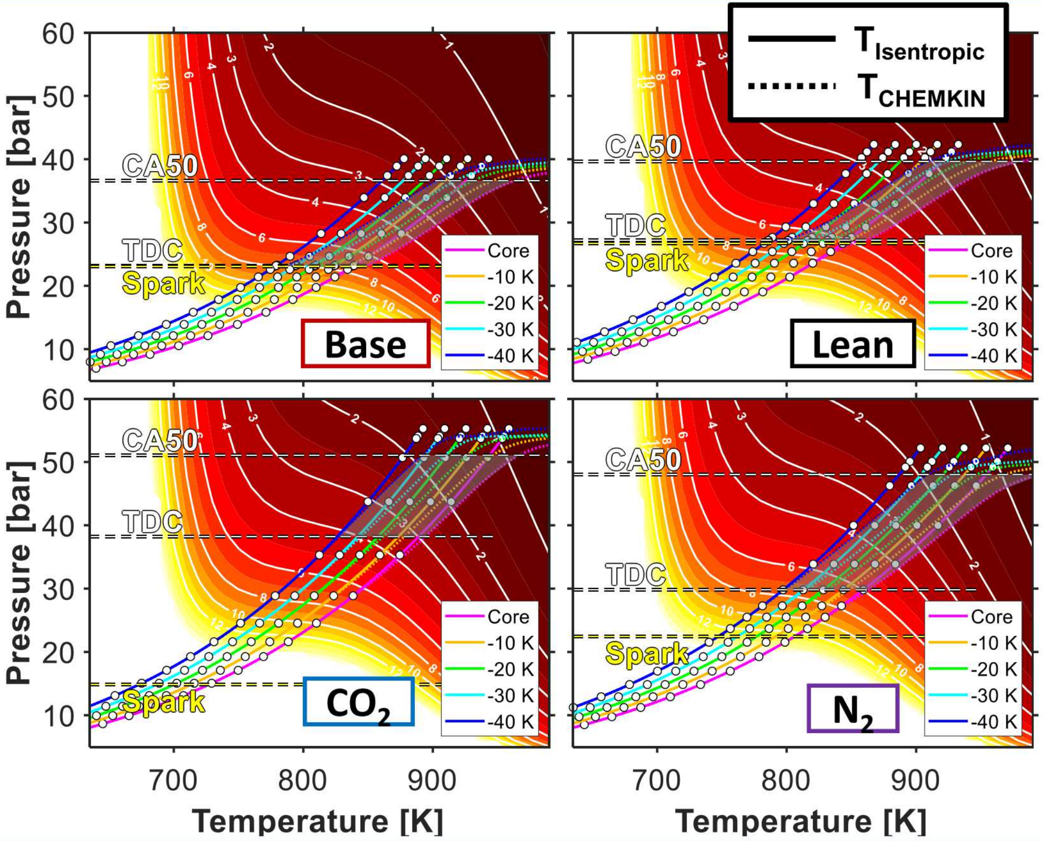


# Effect of Compression Ratio on Thermal Stratification (Chemical effect; $CO_2$-diluted condition)



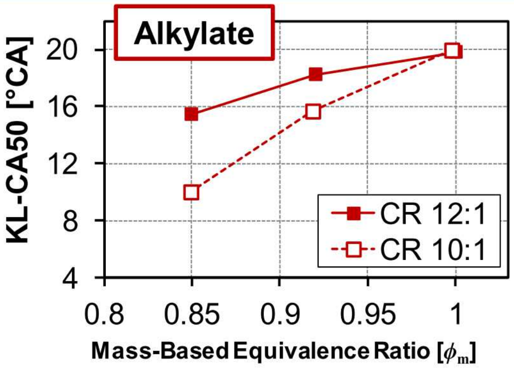

- **The slope of the linear fit and differences in the slopes of two CRs agree well with the characteristics of temperature rise due to chemical reactions.**
  - Maintaining thermal stratification despite ongoing early autoignition reactions is important for achieving sequential autoignition.
- **However, the sequential autoignition itself is not sufficient to explain some of the differences in KL-CA50 of different fuels.**
  - Suggests that both the sequential autoignition and a reduction in the overall temperature rise due to chemical reactions are important.

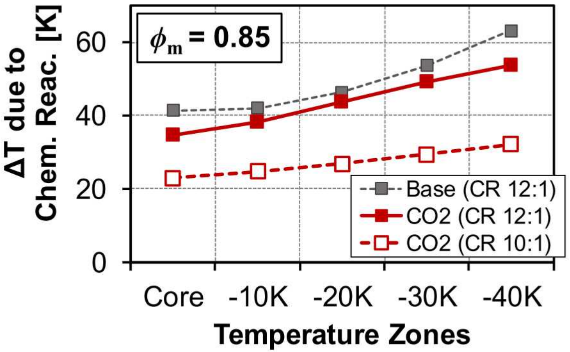
# Effect of Diluent Types on Thermal Stratification (E30, CR = 12:1)

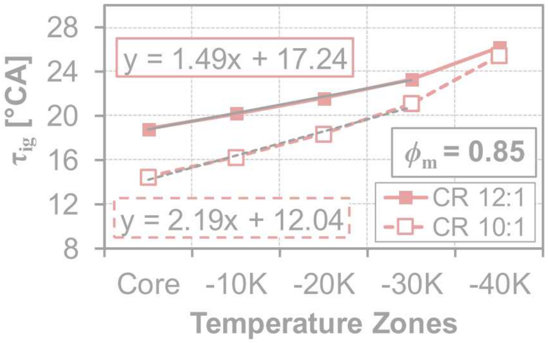



- **When $N_2$ or $CO_2$ is added, the contours of the constant-volume ignition delay are shifted, indicating that the reactants become less reactive for a given initial T and P.**
- **The thermal width of the $CO_2$-diluted case exhibits the smallest change when phasing spans from TDC to CA50.**
  - Reduced reactivity due to ↓ $T_{comp}$, ↓ $\gamma$, and ↓ $O_2$ mole fraction.
  - Reduced residence time due to advanced CA50.
  - Combined effects of a lower reactivity and faster traverse through TP space compound to allow a strong advancements of CA50.

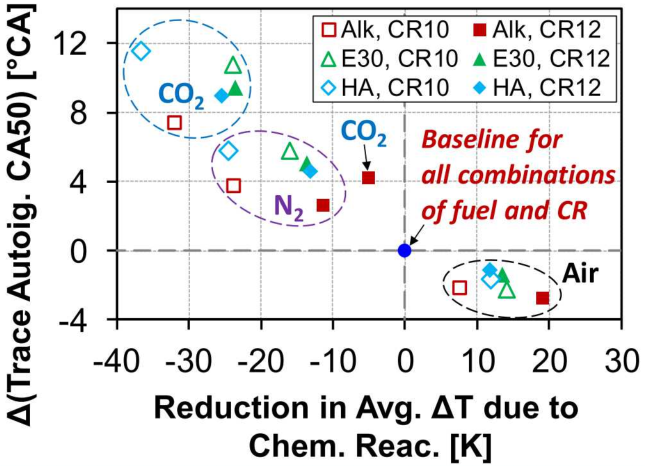
# Summary of Simulation Results



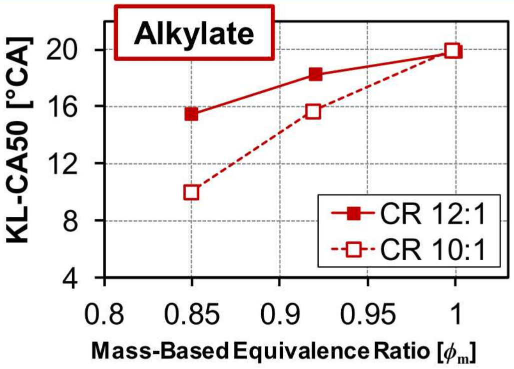



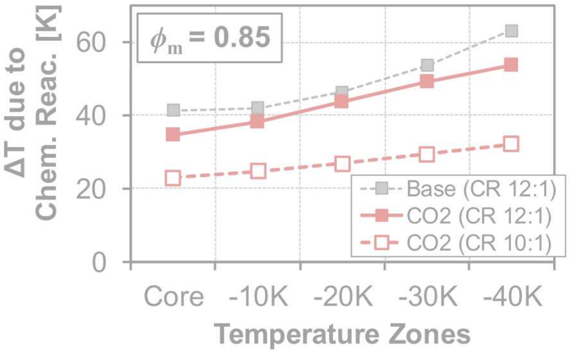



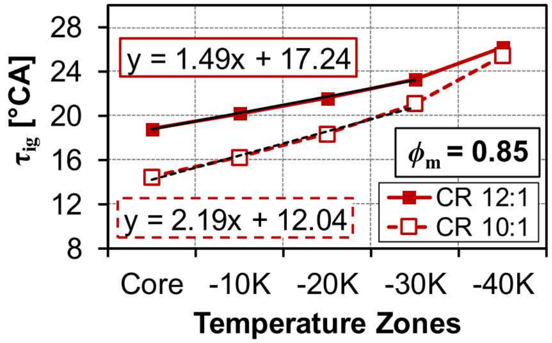

- **Compare diluted cases to their baseline conditions, and how this corresponds to the change in Trace Autoignition CA50.**
- **Dilution with air results in a greater temperature increase in the end-gas compared to the baseline condition, whereas dilution with $CO_2$ significantly reduces the temperature rise in the end-gas.**
- **Strong correlation confirms that the temperature is the key parameter that triggers autoignition.**

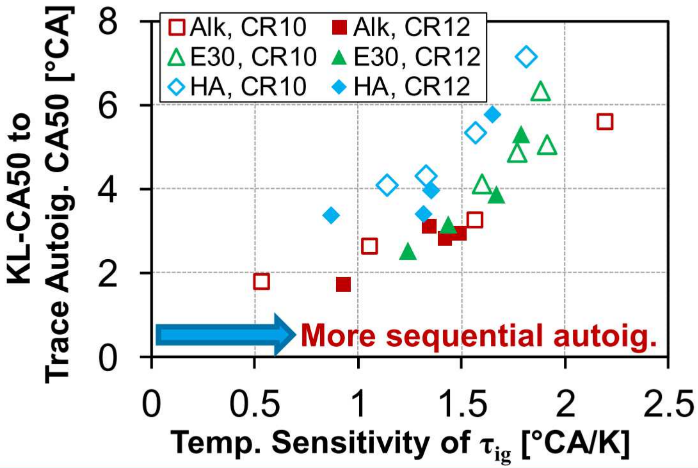


# Summary of Simulation Results




- **KL-CA50 – Trace Autoignition CA50**
  - Indicates how far CA50 can be advanced without incurring strong knock relative to CA50 at which end-gas autoignition starts to occur.
- **When the model indicates a more sequential autoignition for a given amount of thermal stratification, engine can be operated with a KL-CA50 that is further advanced beyond the Trace Autoignition CA50.**

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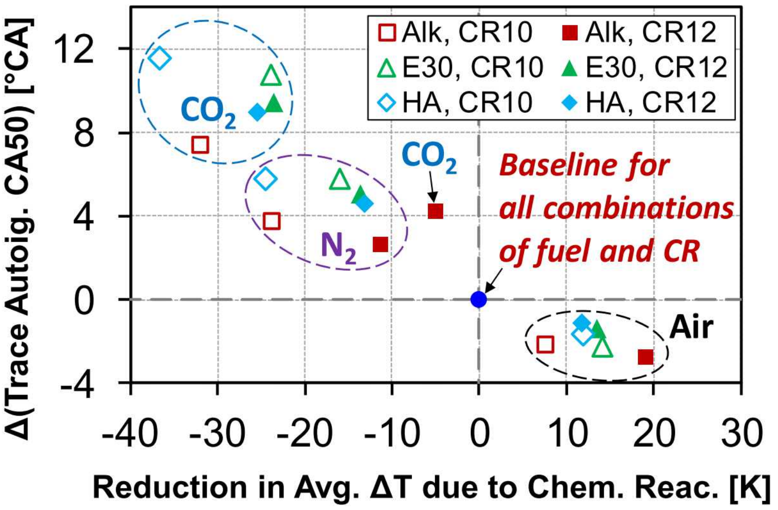
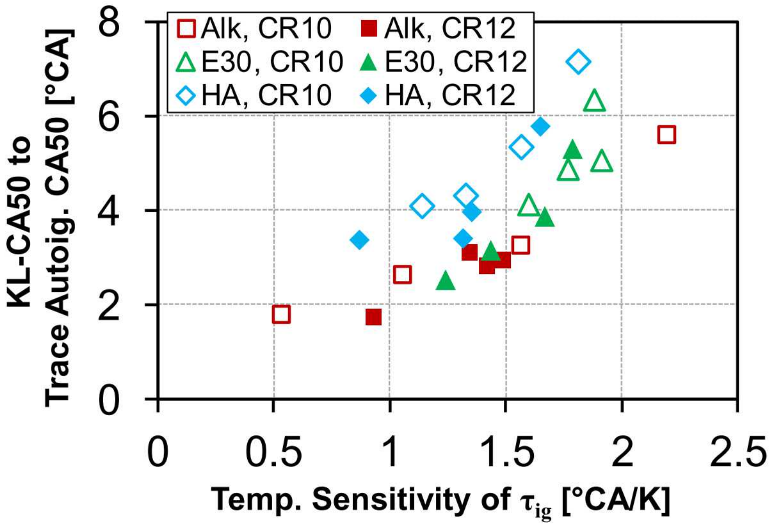
# Summary of Simulation Results




- **Thus, for a diluent to be effective in suppressing knock and enable more advanced KL-CA50,**
  - achieve a reduction in the end-gas temperature to achieve a more advanced Trace Autoignition CA50
  - induce a more sequential autoignition in the end-gas to enable the combustion phasing to be advanced relative to Trace Autoignition CA50 without incurring acoustic knock
- **Δ(KL-CA50) = Δ(Trace Autoignition CA50) + Δ(KL-CA50 − Trace Autoignition CA50)**

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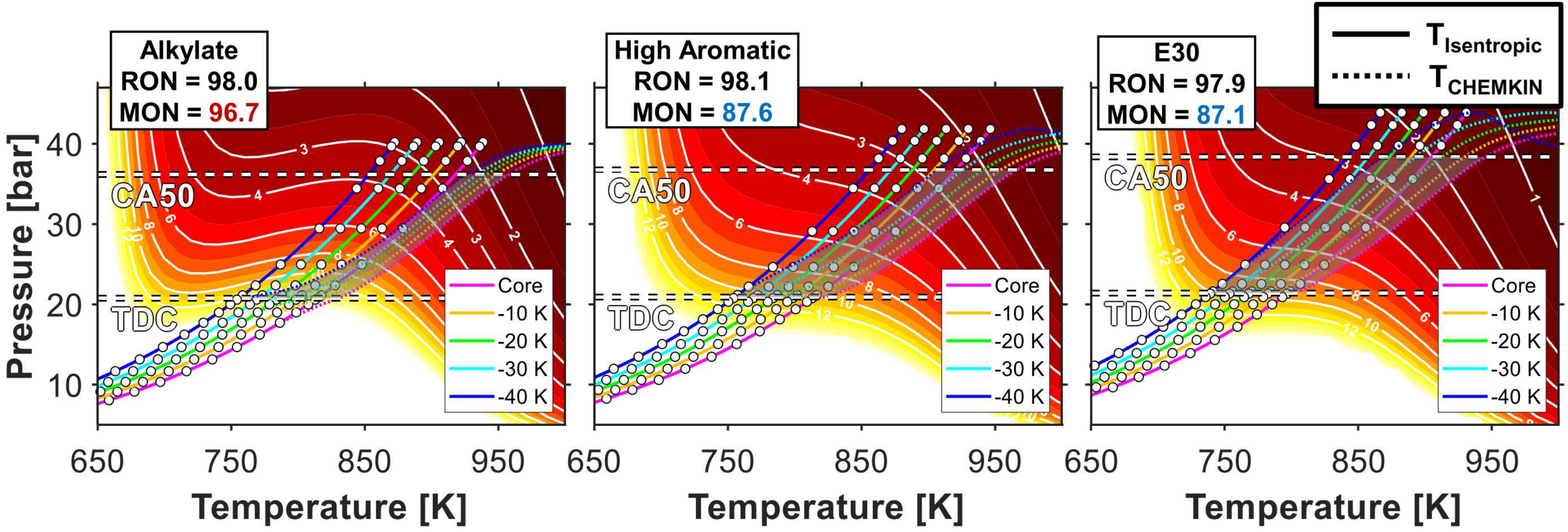
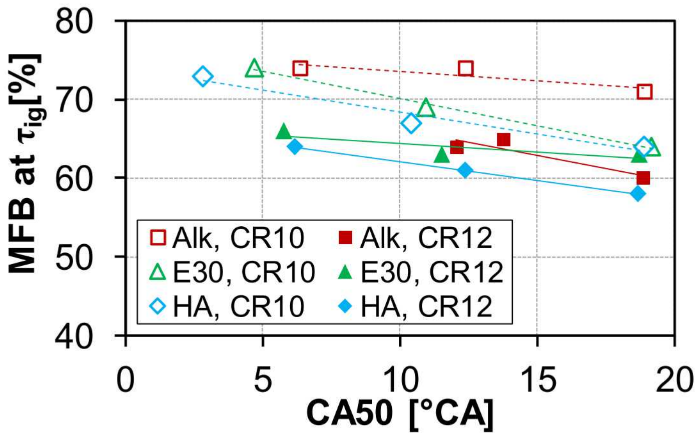
# Conclusions:
# (1) Effect of Fuel Type



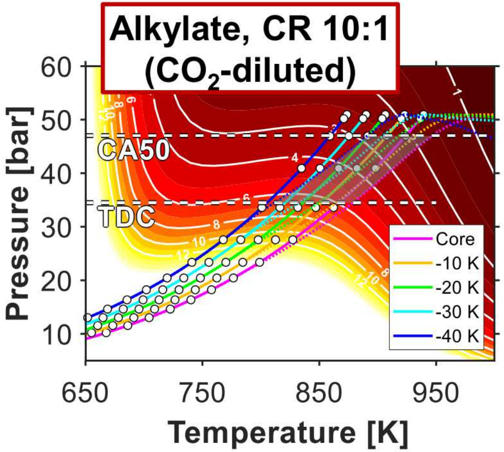

- **Due to the inherent NTC character of Alkylate's autoignition, its LTHR becomes stronger in regions that are cooler than the adiabatic core, and this counteracts a given thermal stratification, effectively making the end-gas more thermally uniform.**

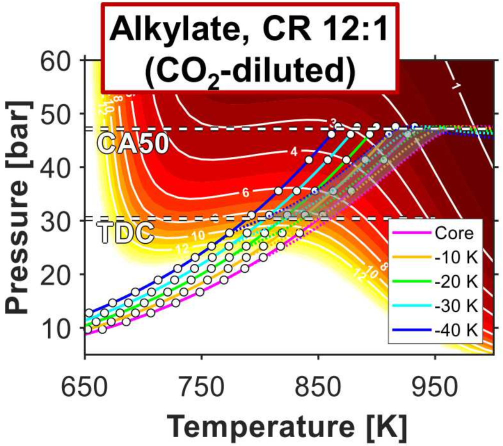
# Conclusions:
# (2) Effect of Compression Ratio

## Physical Effect



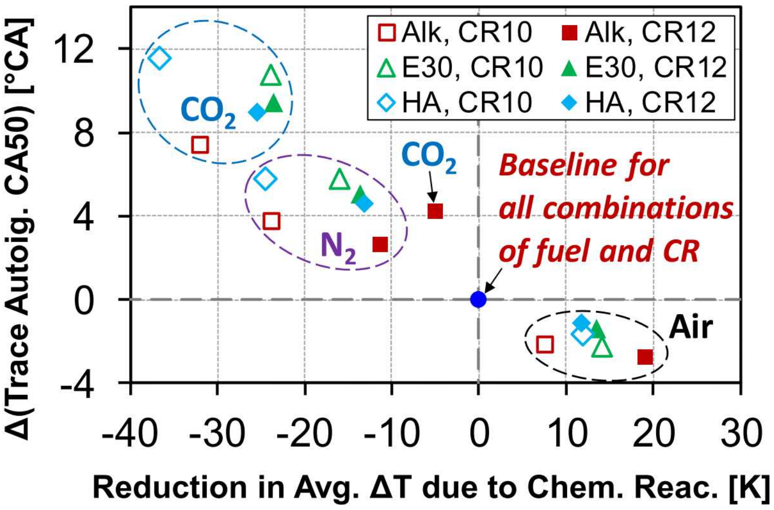

## Chemical Effect

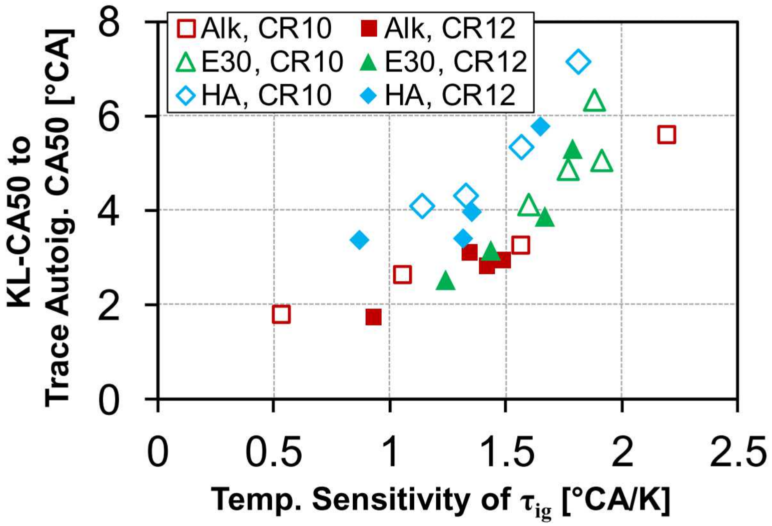



- **It is speculated that the smaller squish height at CR = 12:1 increases the heat transfer from the end-gas to the wall, which broadens the thermal width and promotes a sequential autoignition event with reduced peak HRR.**
- **Change in CR shifts TP trajectory and residence time spent in different regimes and hence alters initially-present thermal stratification.**

# Conclusions:
# (3) Effectiveness of Diluents on Knock Mitigation




- **To suppress knock with dilution, it is required to reduce temperature rise due to chemical reactions compared to the baseline condition without any dilution.**
- **Further advancement of KL-CA50 without incurring acoustic knock can be accomplished by inducing a more sequential autoignition in the end-gas.**
- **Δ(KL-CA50) = Δ(Trace Autoignition CA50) + Δ(KL-CA50 - Trace Autoignition CA50)**

**Thank you for your kind attention!**

# Acknowledgement

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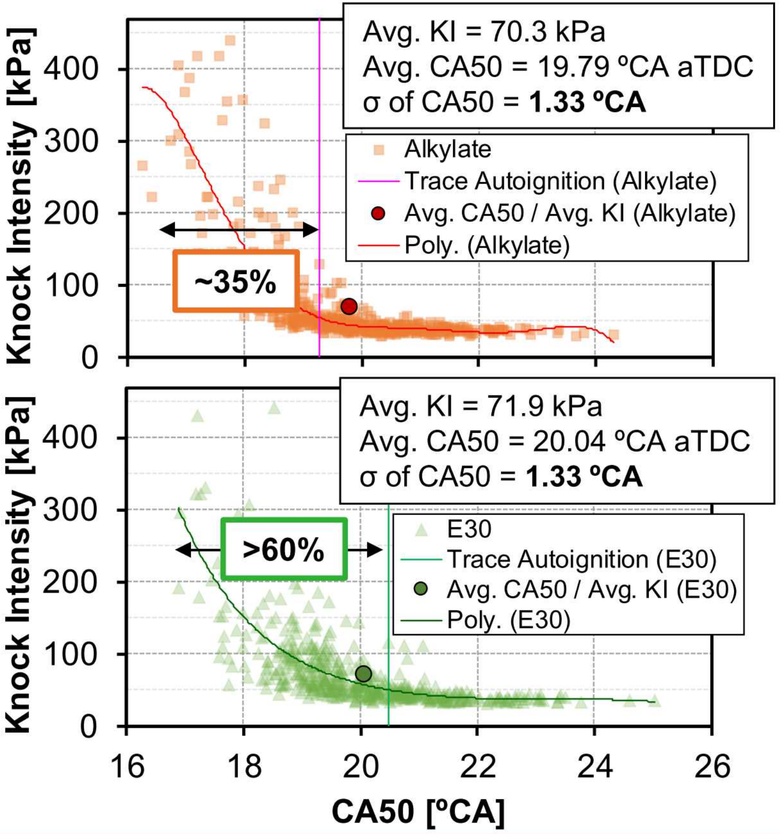
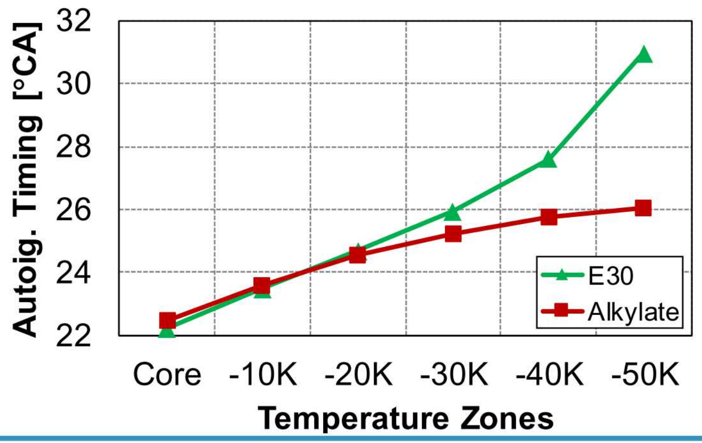
# Back-up Slides

# Implication of Sequential Autoignition on Knock Intensity Distribution (Non-diluted, CR 12:1)




- **Although the selected conditions have nearly identical average KI, CA50 and σ of CA50, KI vs CA50 presents very distinct KI distributions.**
- **Predicted autoignition in lower temperature zones occur more sequentially for E30.**
  - Supports hypothesis that sequential autoignition due to thermal stratification helps to mitigate acoustic knock of autoigniting cycles.



# Effect of phi-stratification (Non-diluted, CR 12:1)

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- To study effect of fuel stratification in mixture, it was necessary to quantify the effect of HoV and $\gamma$ on temperature.
- Utilized Chemkin to separate the contribution of HoV and $\gamma$ effects on changes in compressed gas temperature near °CA at which simulation is initiated.
- Variation of $\phi$ by ±0.2 resulted in less than 0.61°CA change in autoignition timing once the estimated temperature is compensated for effect of HoV and γ.