PRESSURE-TEMPERATURE DOMAIN ANALYSIS TO PROVIDE INSIGHT INTO AUTOIGNITION PROCESSES IN SI ENGINES AT HIGH OPERATING LOAD

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Why Work on SI Combustion?

- Gasoline consumption in SI engines accounts for approximately 75% of on-highway petroleum consumption in the U.S.
- Moving forward with electrified architectures, OEMs are looking for cost-effective engine and aftertreatment systems
  - Stoichiometric SI engines offer lower cost than diesel or low temperature combustion (lower peak cylinder pressure, lower pressure fueling system, less complex controls)
  - Stoichiometric SI engines use 3-way catalyst to meet emissions standards, a mature technology
    - Lean equivalence ratio for low temperature combustion and diesel will require lean NOx emissions control
- Efficiency for SI engines has been rapidly closing the gap relative to diesel and low temperature combustion
  - Toyota has 2 engines in production achieving 40% brake thermal efficiency
  - Emerging stoichiometric SI approaches exceed 40% brake thermal efficiency
    - Southwest D-EGR strategy has reported 42% brake thermal efficiency
    - Honda projecting 45% brake thermal efficiency for their long-stroke engine

Purpose of Anti-Knock Indices is to Rank Fuel Quality. Ranking Changes Based on Operating Condition.

- Research octane number (RON) and motor octane number (MON) differ in intake temperature and engine operating speed
- Octane Index (OI), pioneered by Kalghatgi, uses a variable K to account for changing operating conditions
  - OI = RON – K*(RON – MON)
  - Superior correlation to knock in modern engines, negative K

Notional Set of Fuels

	RON	MON
Fuel 1	98	98
Fuel 2	95	85
Fuel 3	93	87
Fuel 4	97	91
Fuel 5	92	82

Which Fuel is Best? It Depends.

Fuel Ranking	RON Conditions	MON Conditions	AKI	K = -0.5	K = -1	K = -2
Best	Fuel 1	Fuel 1	Fuel 1	Fuel 2	Fuel 2	Fuel 2
	Fuel 4	Fuel 4	Fuel 4	Fuel 4	Fuel 4	Fuel 5
	Fuel 2	Fuel 3	Fuel 2	Fuel 1	Fuel 5	Fuel 4
	Fuel 3	Fuel 2	Fuel 3	Fuel 5	Fuel 3	Fuel 3
Worst	Fuel 5	Fuel 5	Fuel 5	Fuel 3	Fuel 1	Fuel 1

Fuel Sales Based on RON in EU

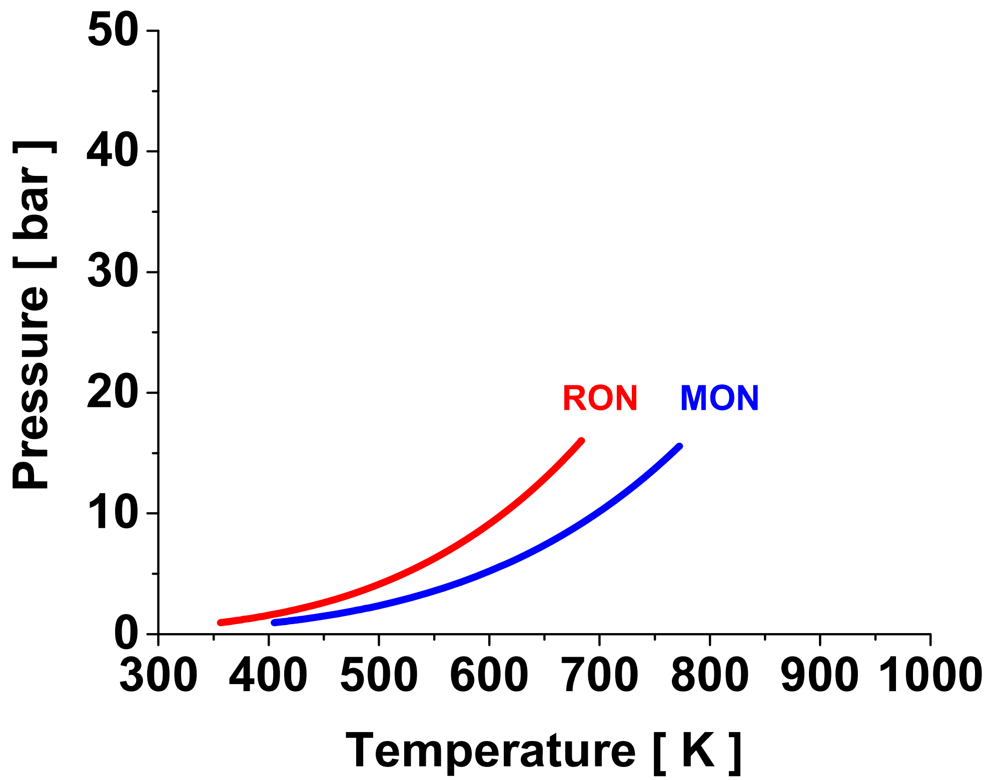
Fuel Sales Based on AKI in US

Negative K for Boosted SI Engine

Changing Reactivity Ranking can be Better Understood by Analysis in the Pressure-Temperature Domain, Coupling to Kinetics

- Engines are thermodynamic devices where pressure and temperature are linked
- Intake valve closing (IVC) conditions sets up the pressure-temperature trajectory of the unburned air and fuel mixture
- IVC conditions are dependent on engine speed and load as well as operating strategy
  - Engine compression ratio determines the end point on the trajectory
  - Relevant kinetic timescale determined by engine speed and engine geometry (stroke-to-bore ratio)

Initial In-Cylinder Conditions Determine Pressure-Temperature Trajectory; Autoignition Chemistry is Dependent on Trajectory



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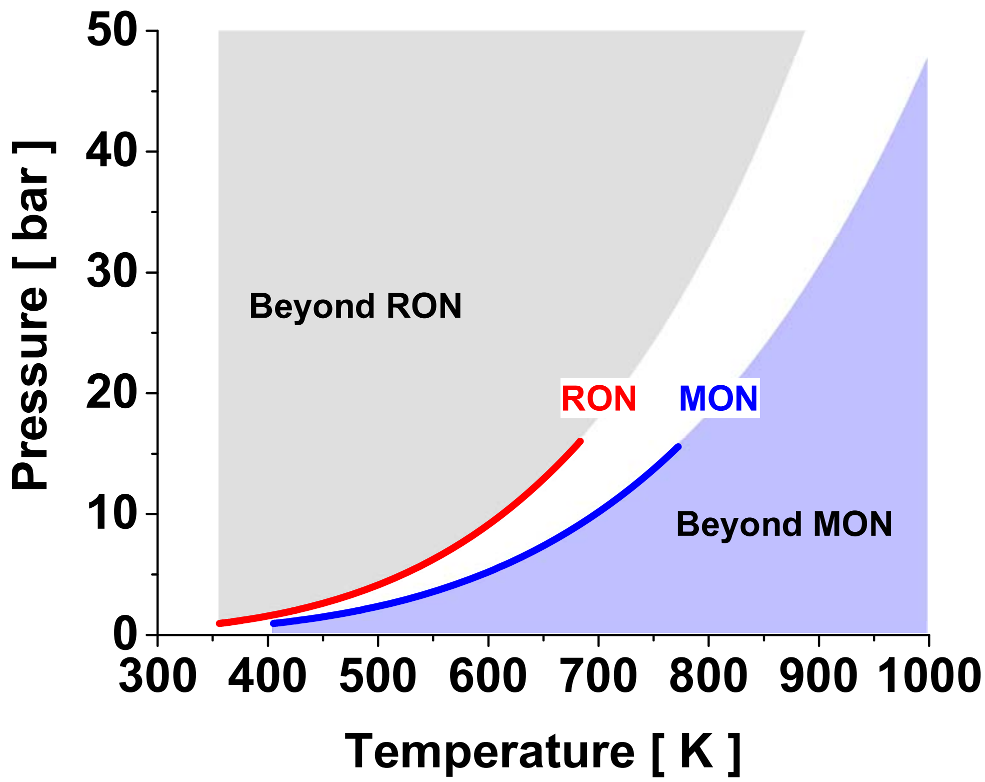

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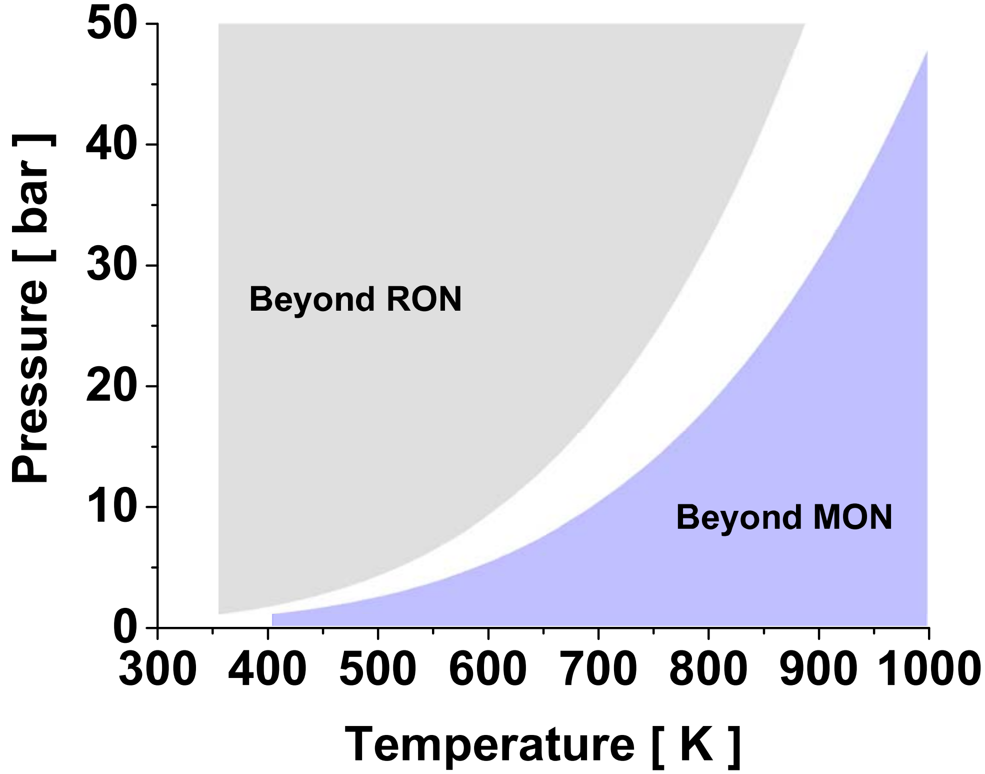

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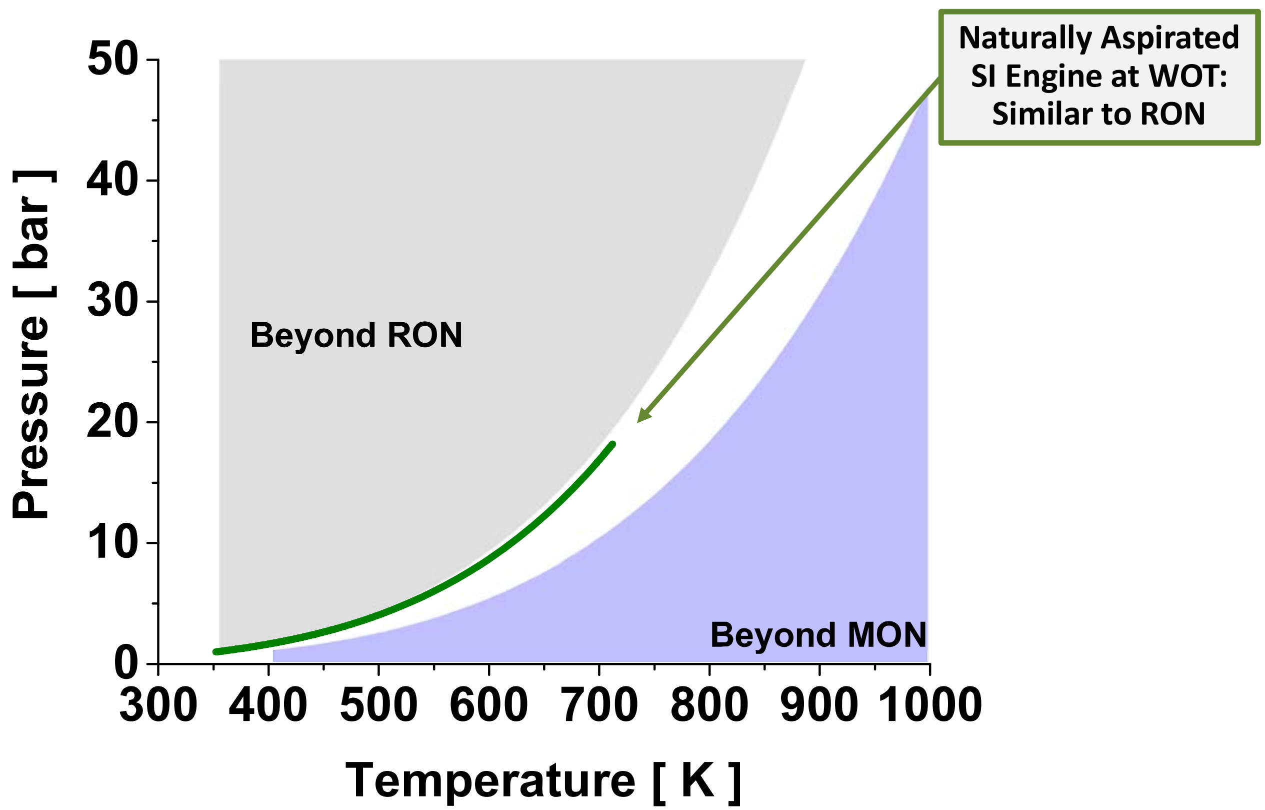

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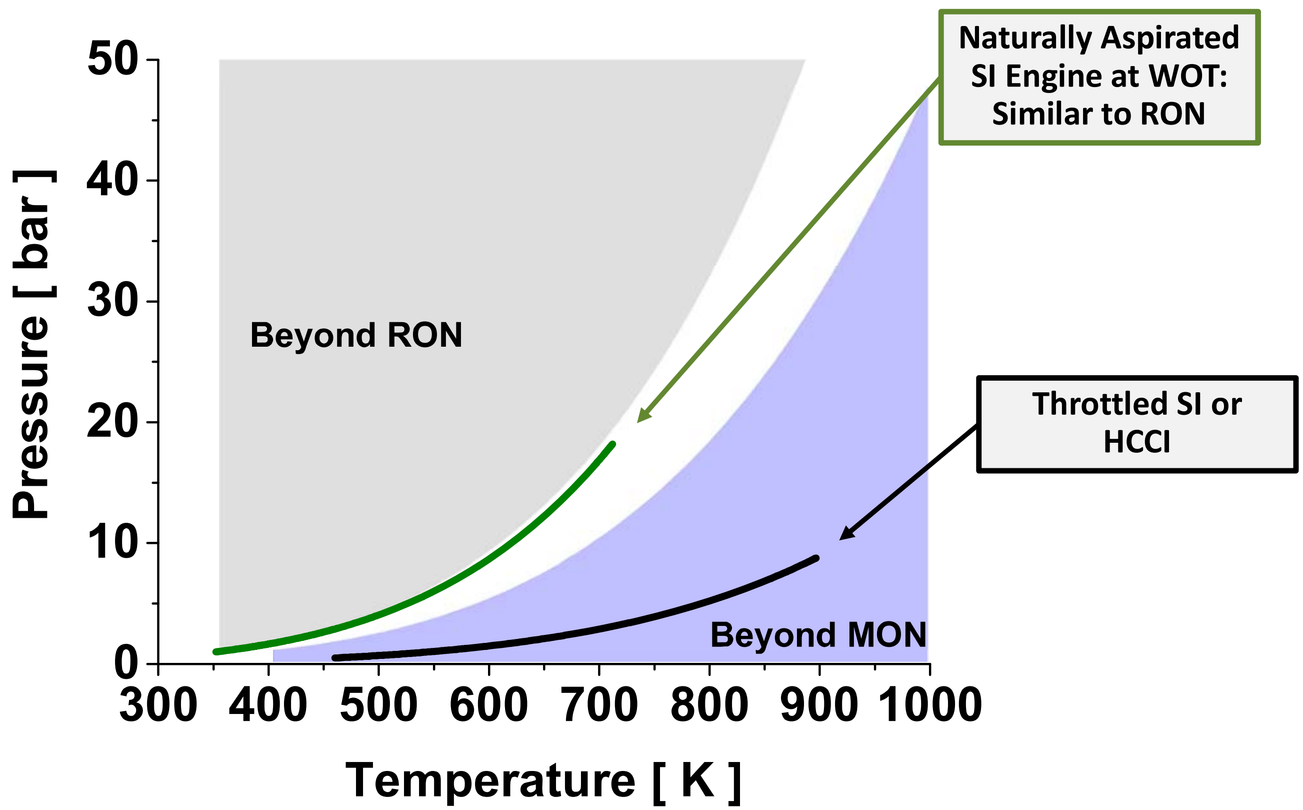

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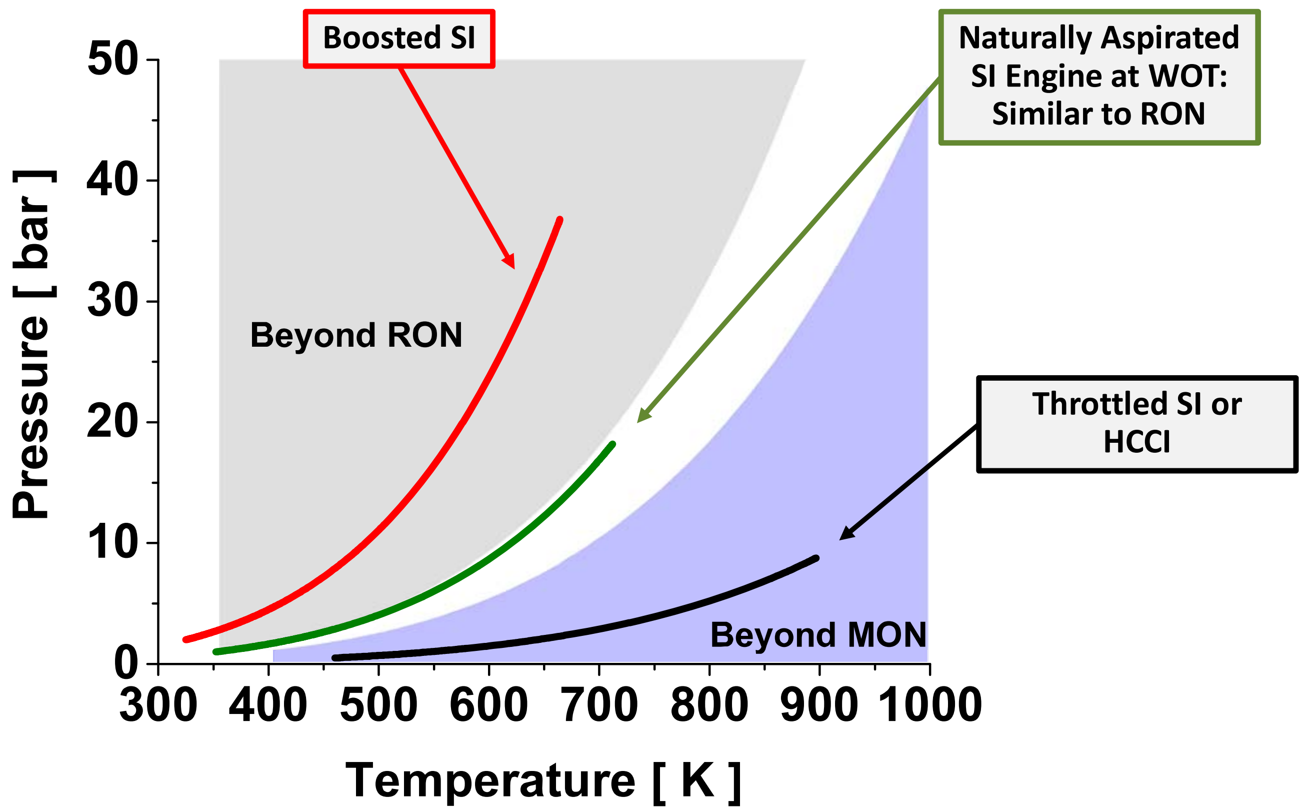

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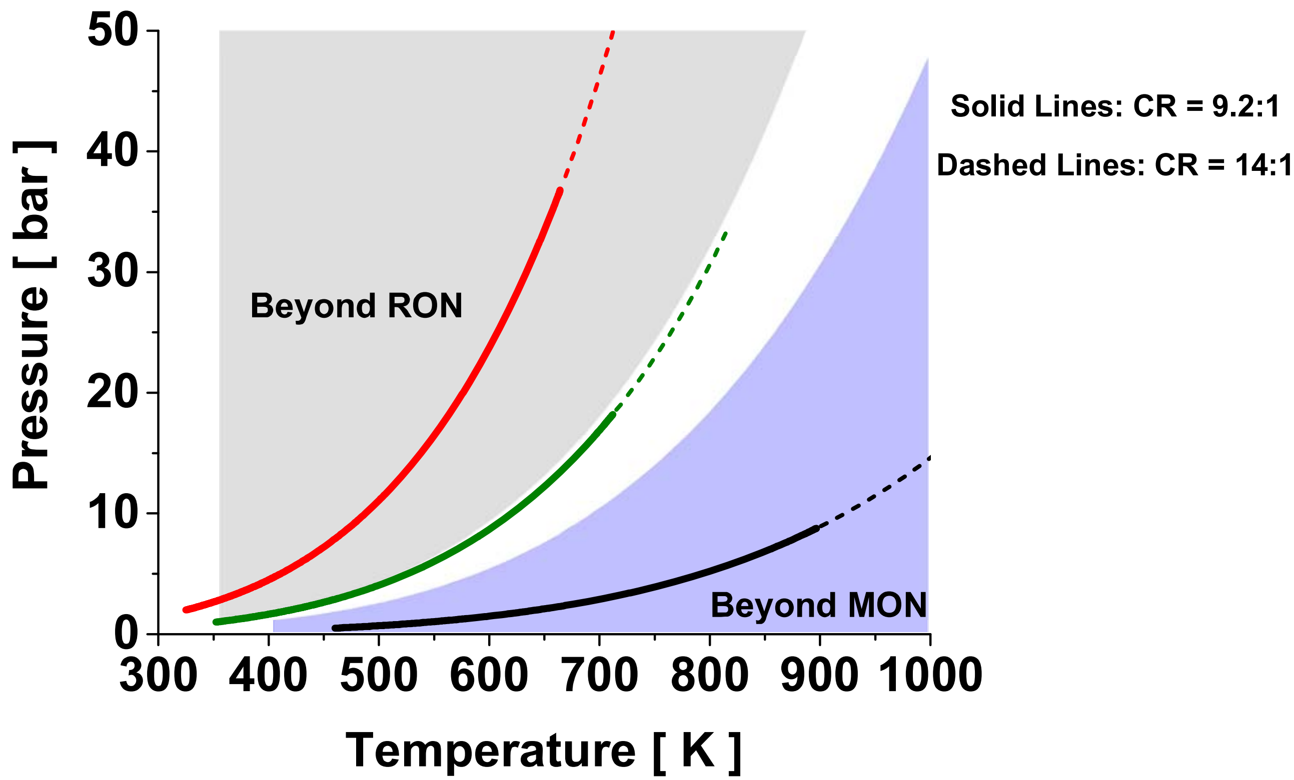

Higher Compression Ratio Maintains Trajectory, Changes Endpoint

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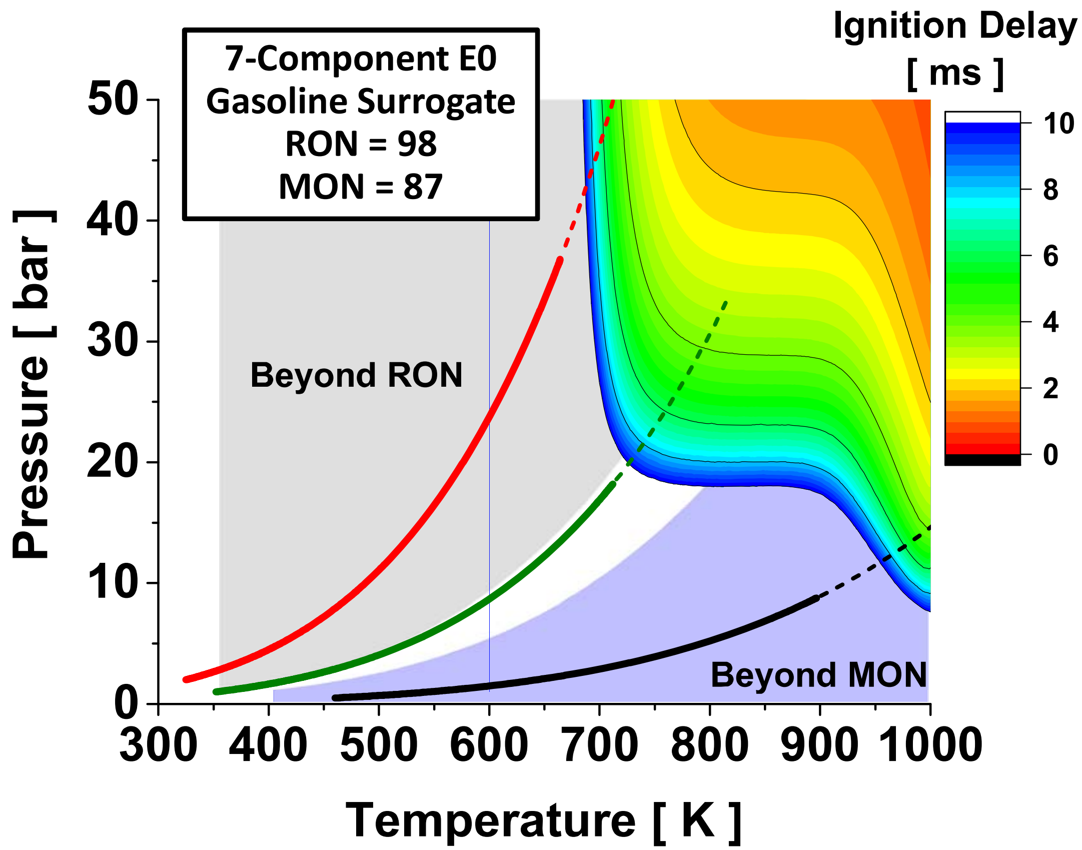

Kinetic Ignition Delay Calculations Illustrate Changing Autoignition Chemistry

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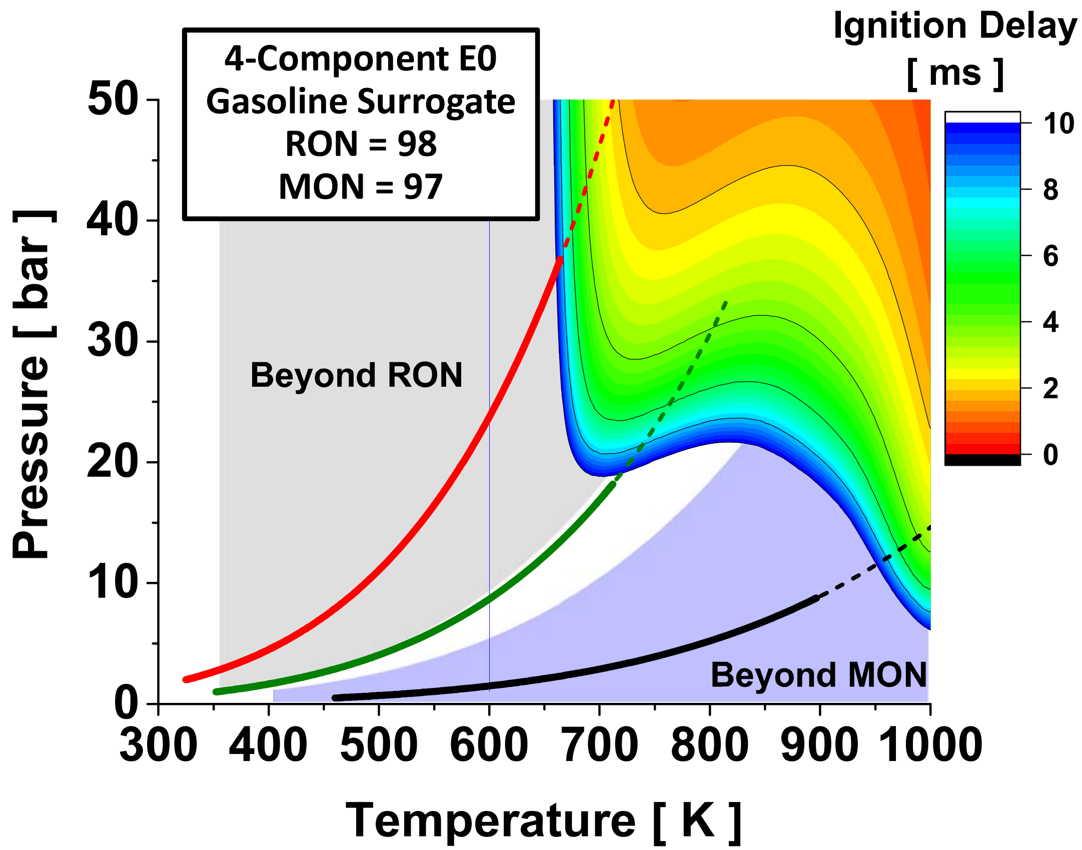
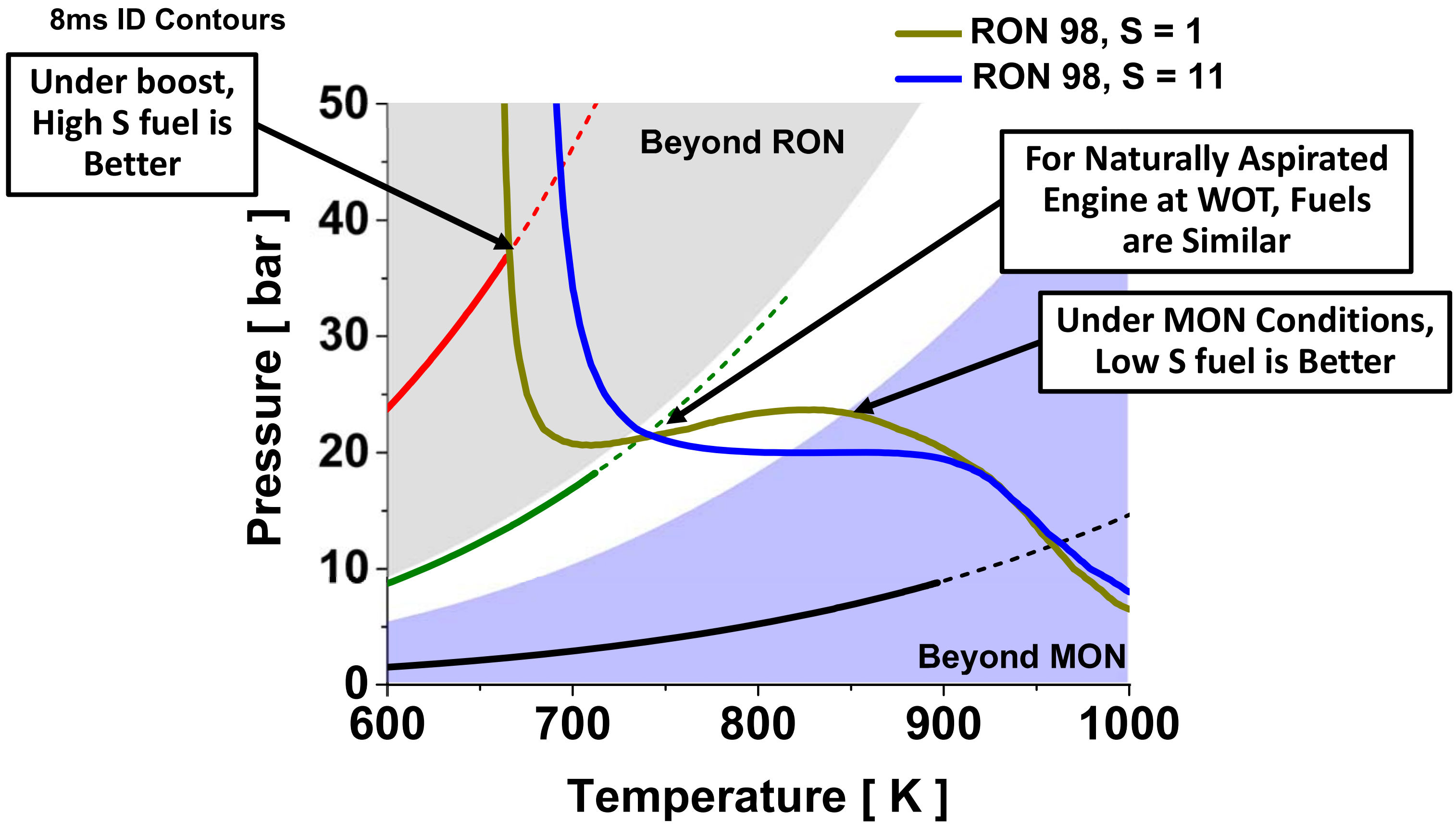


Kinetic Ignition Delay Calculations Illustrate Changing Autoignition Chemistry

Comparing Constant Ignition Delay for Different Fuels Enable a Better Understanding of RON, MON, and OI



Application of Pressure-Temperature Framework

1. Presence of pre-spark heat release under boosted SI conditions

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3. Importance of the thermodynamic state on low speed preignition

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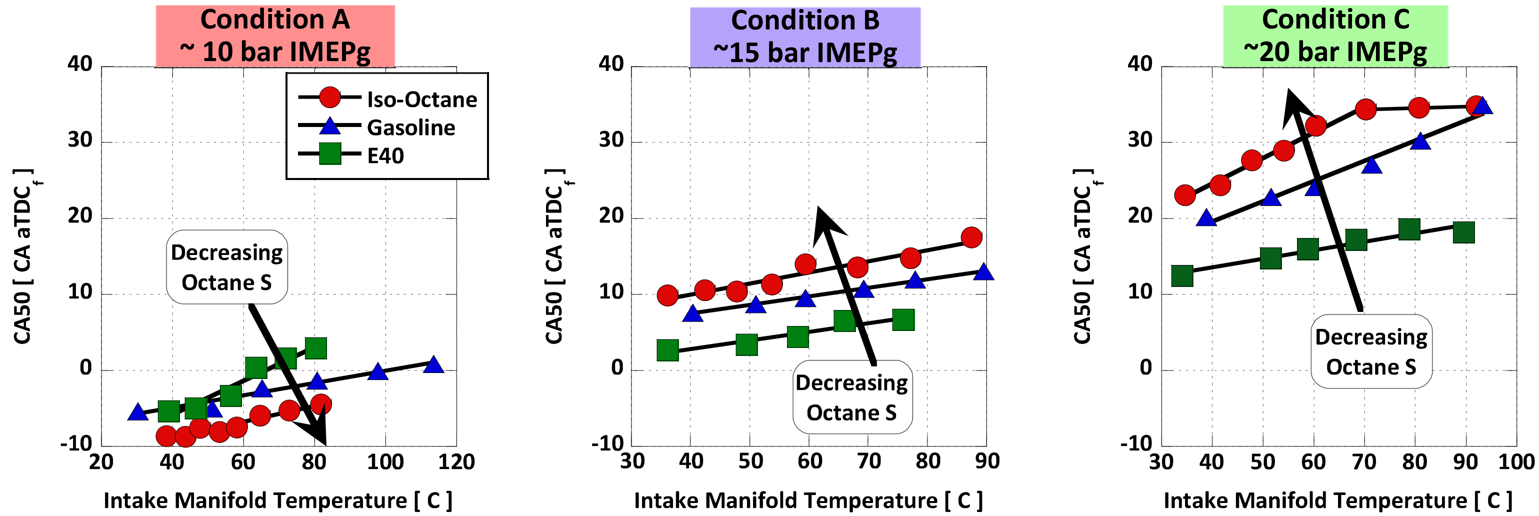
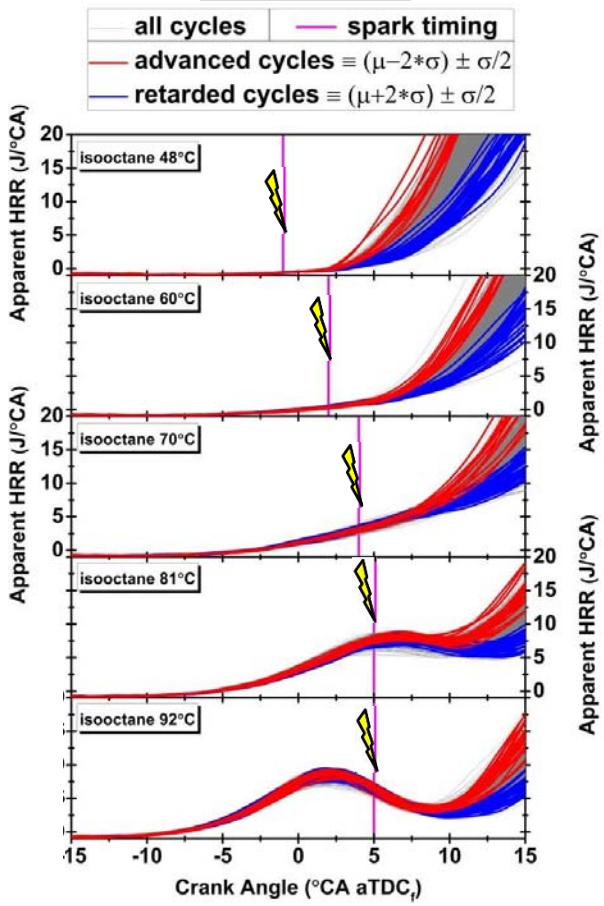
Fuels with Constant RON (RON = 100) Exhibit Fuel-Specific Differences in Knock Limited Phasing at Different Engine Conditions



- Condition A knock resistance: Iso-octane > Gasoline > E40 — **Low S is Good**
- Condition B knock resistance: E40 > Gasoline > Iso-octane — **High S is Good**
- Condition C knock resistance: E40 >> Gasoline >> Iso-octane — **High S is Really Good**
- In moving from Condition A to Condition C, the combustion phasing change for E40 is approximately half that of iso-octane

Pre-Spark Heat Release (PSHR) is Present for Iso-octane and Gasoline. Phenomenon is Extremely Repeatable, Increases with Intake T

Iso-Octane



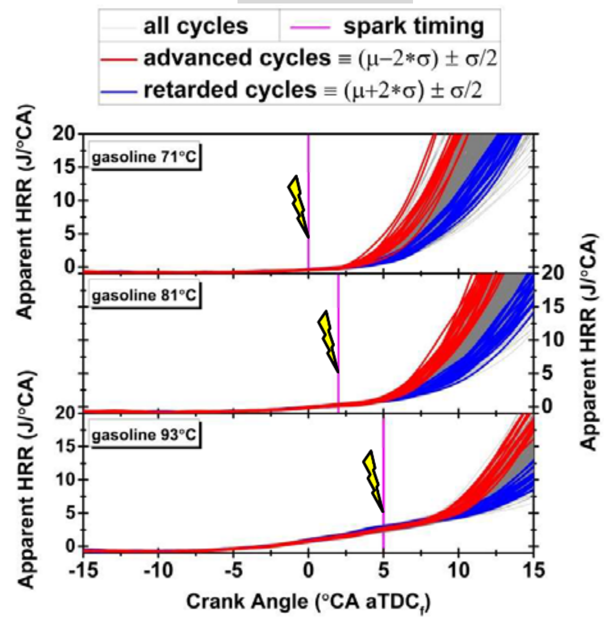
Beginning Stages of PSHR

Stronger PSHR

PSHR with NTC

Stronger PSHR with NTC

Gasoline



Gasoline requires higher intake temperature for similar behavior (20-25 deg C)

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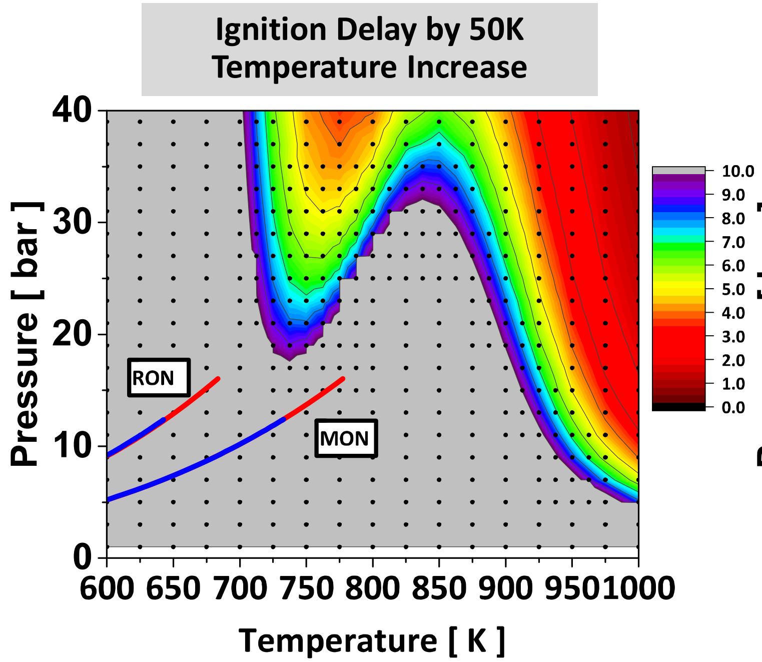
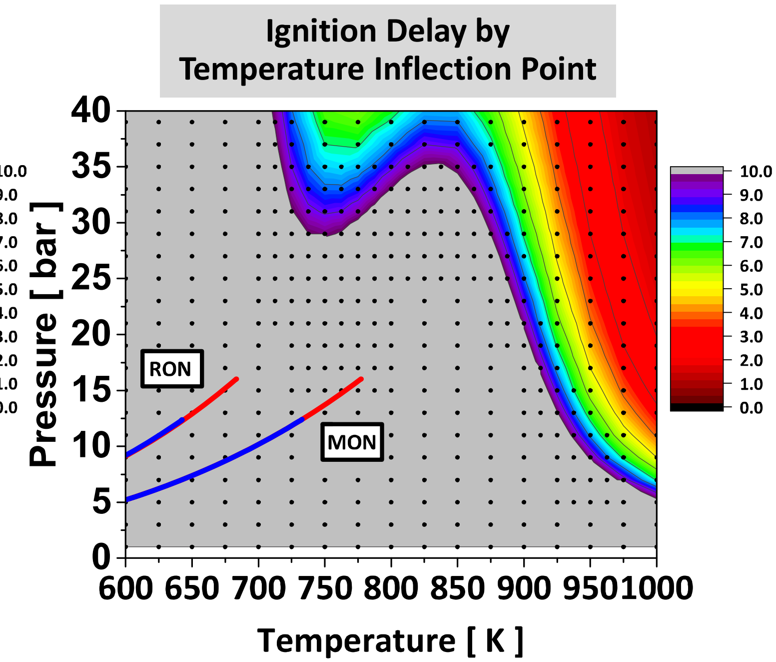
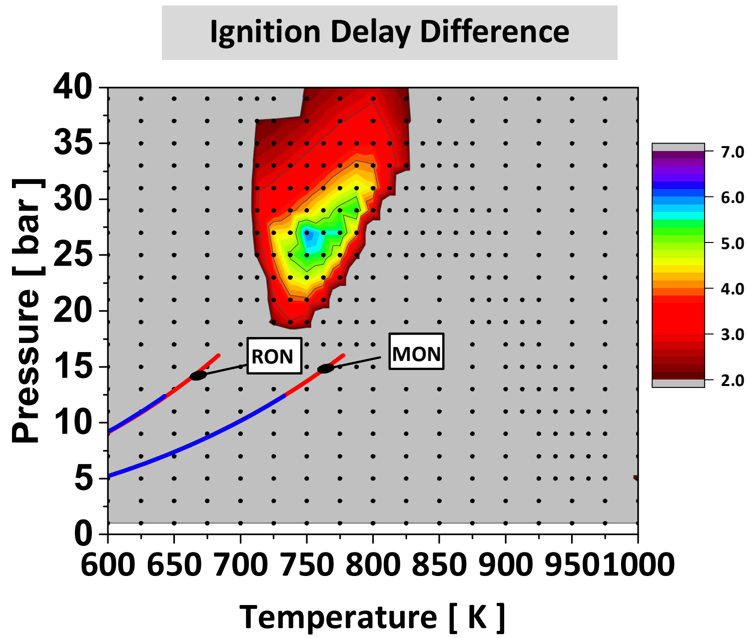
Comparison of the Ignition Delay Definitions for Iso-Octane. Substantial Differences for T < 850K.





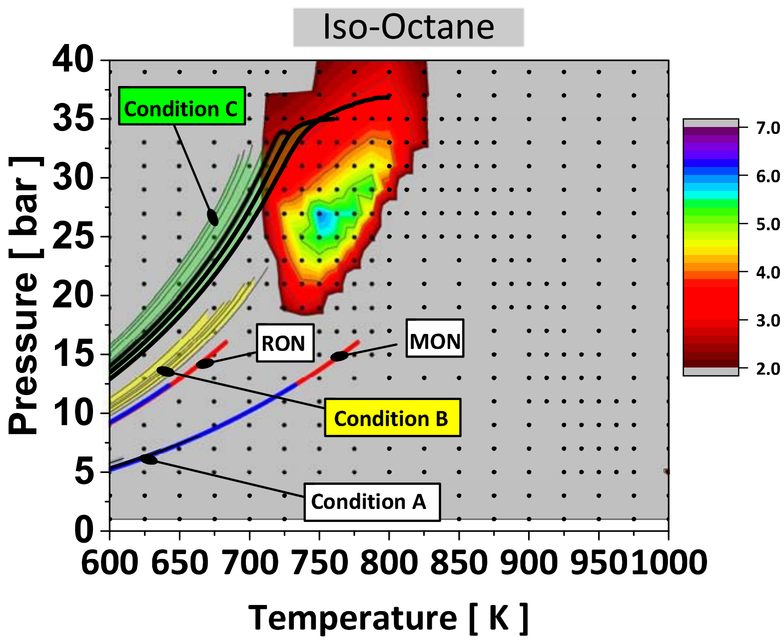
- Above 850K, the two methods show very little difference
- Below 850K, ignition delays are much shorter for the 50K temperature increase methodology
- This region of activity is indicative of low temperature heat release!

Ignition Delays from the Two Definitions Can Be Subtracted to Identify Islands of Low Temperature Chemistry



- **Island of low temperature chemistry can be thought of as being similar to the islands of NOx and soot formation in the phi/T domain**
- Note: Ignition delay threshold of > 2ms applied

Experimental Temperature/Pressure Trajectories Show Interaction with the Low Temperature Chemistry Island for Different Fuels



- Iso-octane has the largest low temperature chemistry island
  - Condition C transitions into the low temperature chemistry island prior to ignition at high intake manifold temperatures
  - Fully consistent with the PSHR observed in the experimental data
  - Conditions A & B, as well as RON and MON, do not enter low temperature chemistry island prior to ignition

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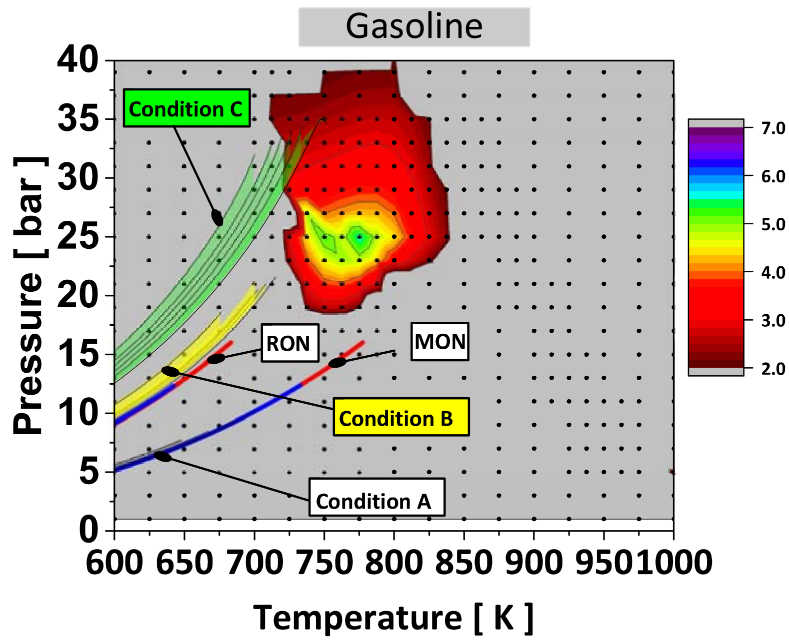
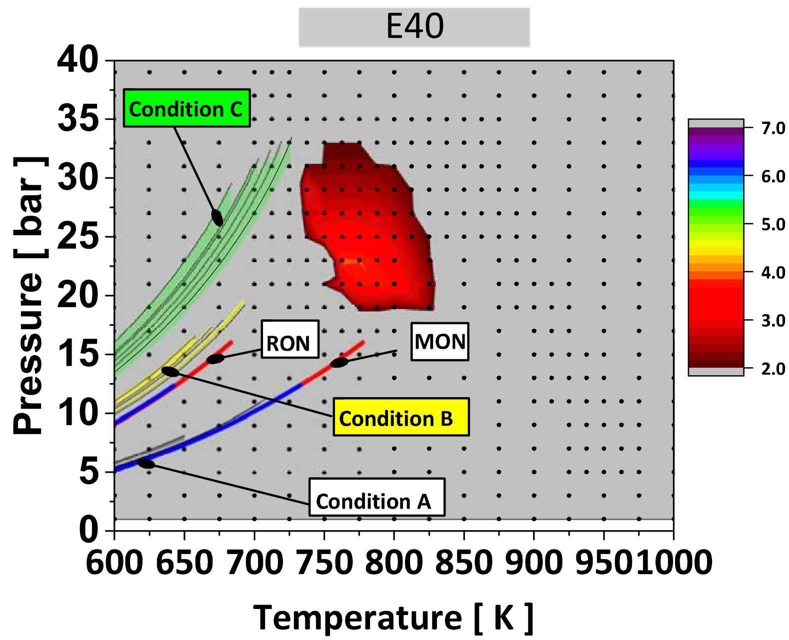


- Gasoline has a slightly smaller low temperature chemistry island, starts at higher T
  - Condition C for gasoline also enters the low temperature chemistry island prior to ignition
  - Fully consistent with the PSHR observed in the experimental data

Experimental Temperature/Pressure Trajectories Show Interaction with the Low Temperature Chemistry Island for Different Fuels



- E40 has a significantly smaller low temperature chemistry island
  - Island starts at ~735K for E40 vs. ~710 for iso-octane
  - Condition C for avoids the low temperature chemistry island for E40 prior to ignition
  - Consistent with the lack of ITHR and LTHR observed in the experimental data

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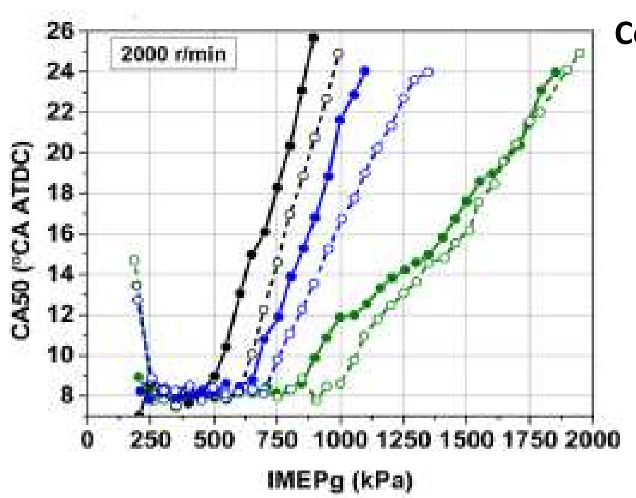
EGR is Capable of Mitigating Knock at High Loads, Right???

- Alger et al. (SAE 2011-01-1149) showed CA50 phasing advance of ~16 CAD due to knock mitigation with 20% EGR at 8 bar BMEP
  - Every % EGR is equivalent to 0.5 AKI increase
- Hoepke et al. (SAE 2012-01-0707) found that CA50 phasing advance of ~8 CAD due to knock mitigation at 14 bar BMEP
- Splitter and Szybist (Energy & Fuels, 2013) showed EGR loses effectiveness at mitigating knock at higher engine loads (15 bar IMEP and higher)



Colors represent different fuels

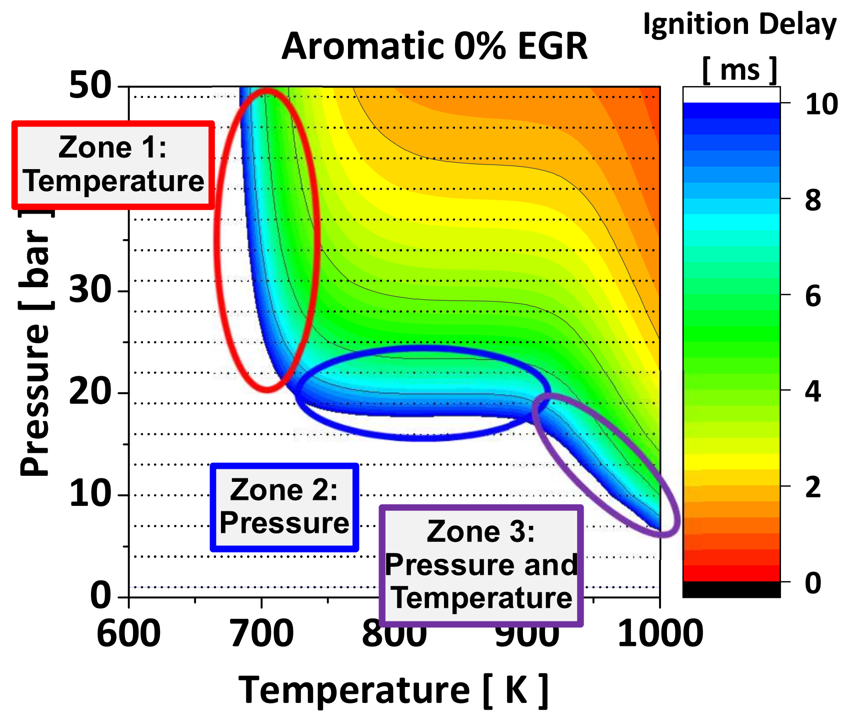
Closed Symbols: 0% EGR

Open Symbols: 15% EGR

Pressure-Temperature Analysis can be used to develop a better understanding of the ability of EGR to mitigate knock across the operating space.

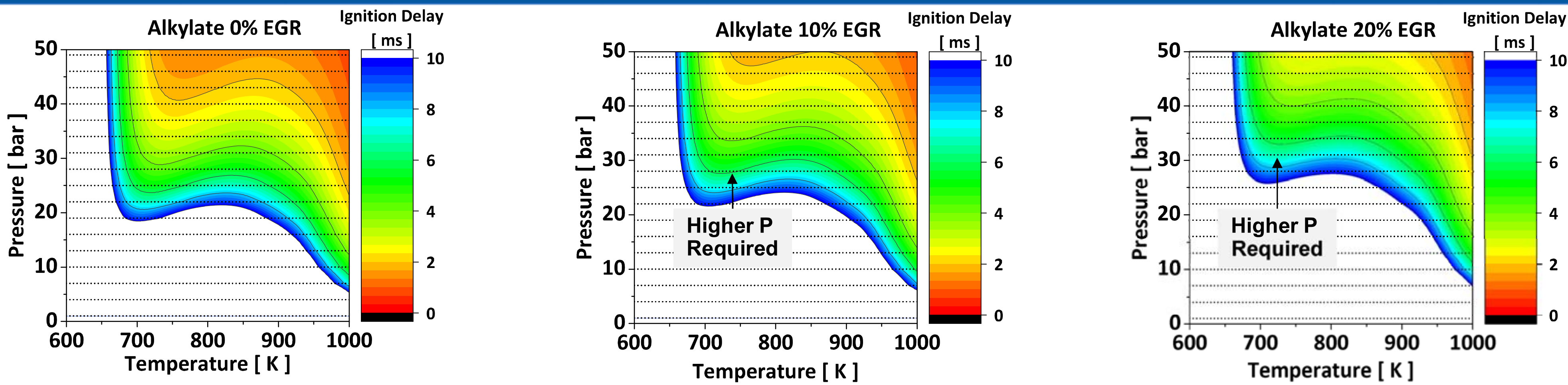
Analyzing Constant Volume Ignition Delay Contours Allows Us to Identify 3 Zones of Ignition Chemistry

- Ignition delay calculations performed by LLNL team (Scott Wagnon, Bill Pitz, Marco Mehl)
- Zone 1: Ignition delay contours are nearly vertical
  - Ignition delay is sensitive to temperature, less sensitive to pressure
  - In this region, LTHR is promoted because alkylperoxide and hydroperoxide radicals are relatively stable
- Zone 2: Ignition delay contours are nearly horizontal
  - Ignition delay is sensitive to pressure, less sensitive to temperature
  - In this region alkylperoxide and hydroperoxide radicals are thermally unstable, decreasing LTHR propensity

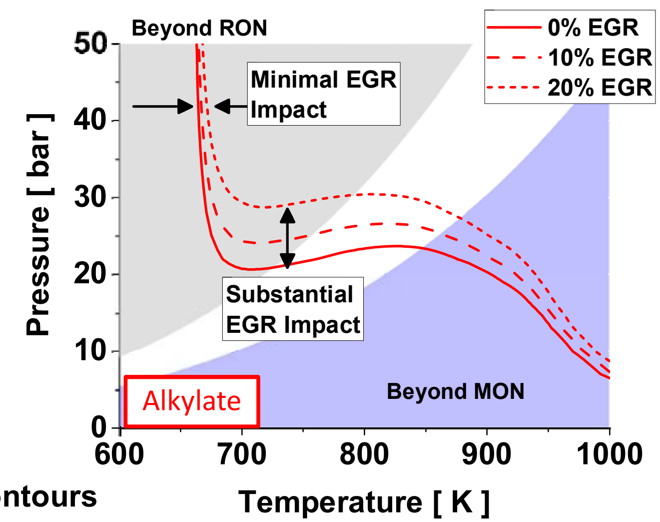


- Zone 3: Ignition delay is a strong function of both temperature and pressure
  - Exhibits third-body enhanced formation of hydroperoxyl radicals from O_2 and H radicals and the abstraction reactions HO_2 radicals on the fuel
  - Leads to the formation of hydrogen peroxide that subsequently decomposes to two reactive OH radicals

Kinetic Calculations show that EGR Attenuation of Ignition Delay is Uneven Across Pressure-Temperature Domain

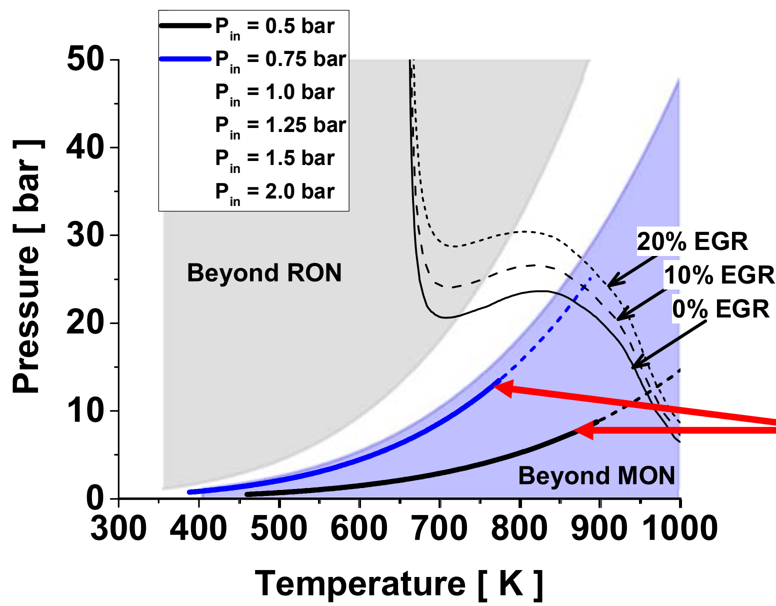


- Ignition delay contours maintain shape with EGR
  - Higher pressure for same ignition delay in Zone 2
- Direct comparison of constant ignition delay time for different EGR levels reveals more information
  1. Separation of ignition delay lines with different levels of EGR in Zone 2 → EGR Expected to have a substantial impact
  2. Ignition delay lines with different levels of EGR converge in Zone 1 → EGR Expected to have a minimal impact



8ms ID Contours

Boosted "Beyond RON" Conditions Interact with Ignition Zone 1, Minimal Impact on Knock



- Throttled operation interacts with ignition zone 3
- The operating conditions are typically far away from autoignition (i.e., not knock-limited)

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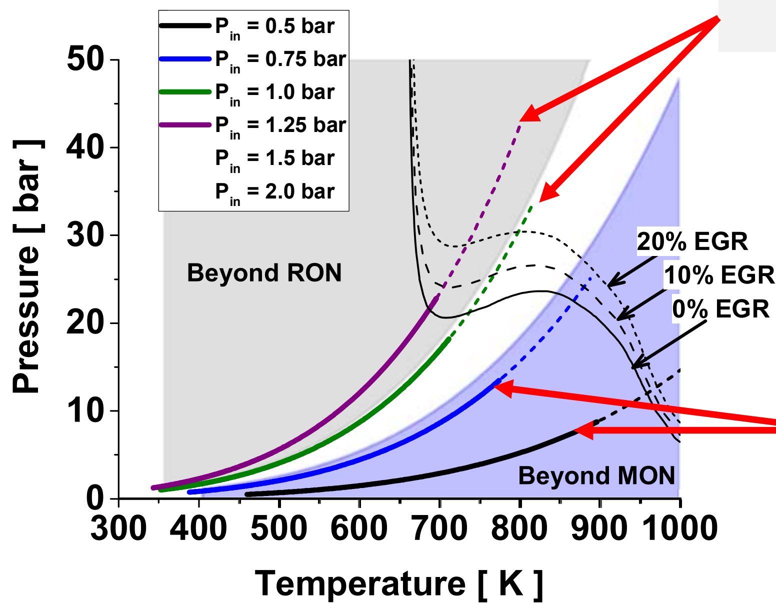


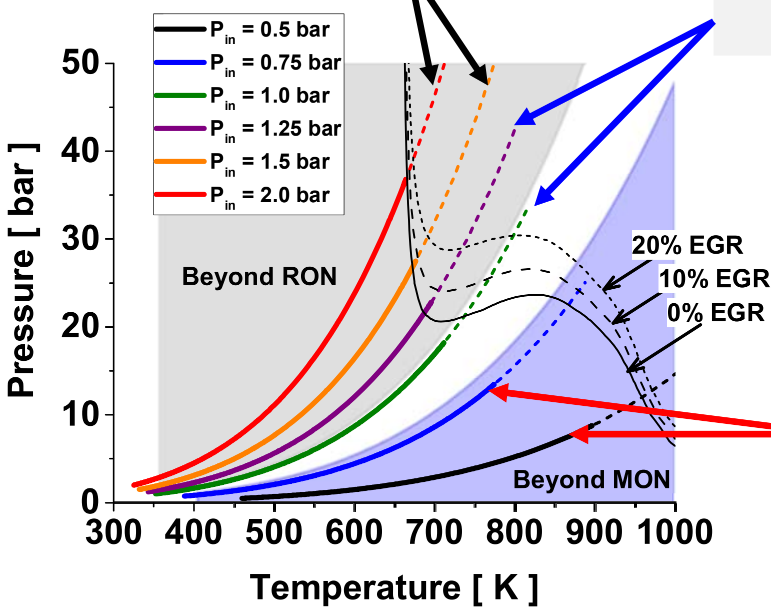
- WOT and modestly boosted operation interacts with Zone 2
- EGR is highly effective at knock-mitigation
- Conditions similar to where EGR is shown to be effective at mitigating knock

- Throttled operation interacts with ignition zone 3
- The operating conditions are typically far away from autoignition (i.e., not knock-limited)

Boosted "Beyond RON" Conditions Interact with Ignition Zone 1, Minimal Impact on Knock

- Higher levels of boost interact with ignition Zone 1
- At these conditions, EGR becomes increasingly ineffective at mitigating knock

- WOT and modestly boosted operation interacts with Zone 2
- EGR is highly effective at knock-mitigation
- Conditions similar to where EGR is shown to be effective at mitigating knock



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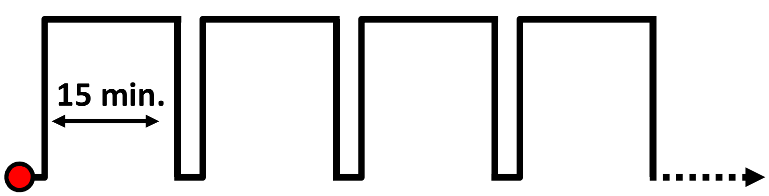
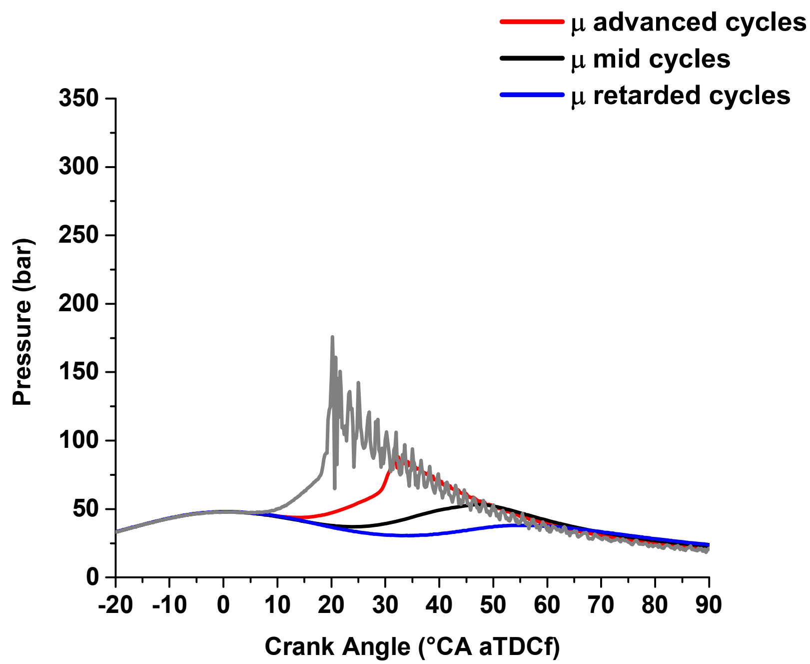
Stochastic Preignition is an Abnormal Combustion Event that Occurs at High Loads (boosted) and can Severely Damage Engines





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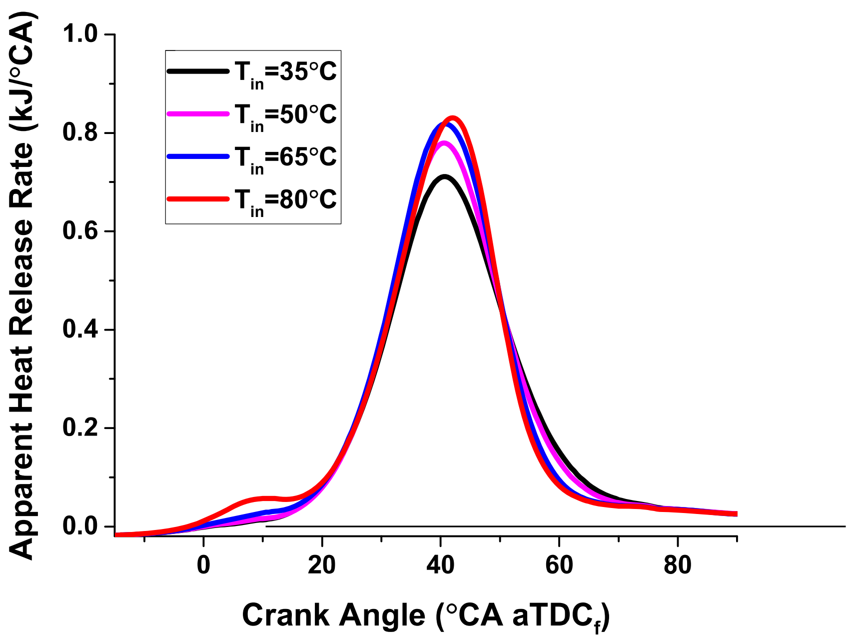
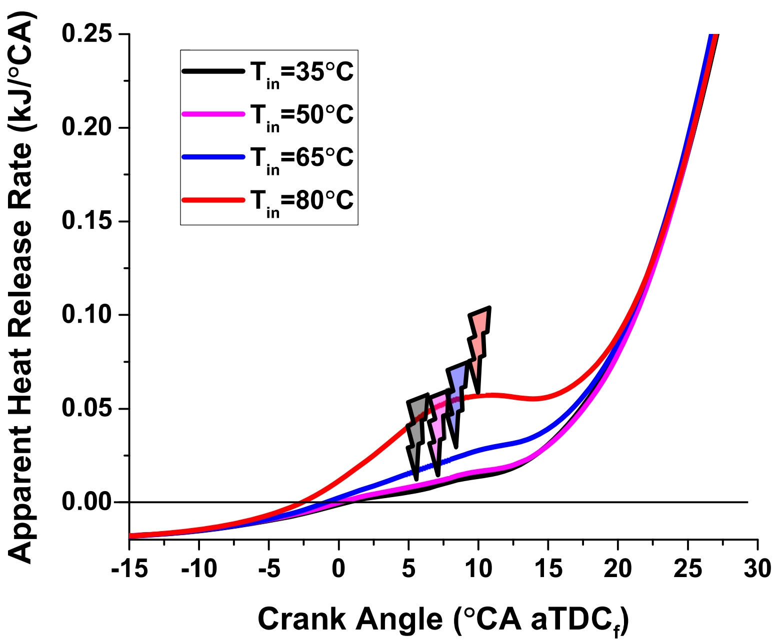
Similar to Prior Studies, Pre-Spark Heat Release Observed at Retarded Ignition Timing

- Pre-spark heat release increased with increasing intake temperature
- CA50 combustion phasing maintained with ignition timing





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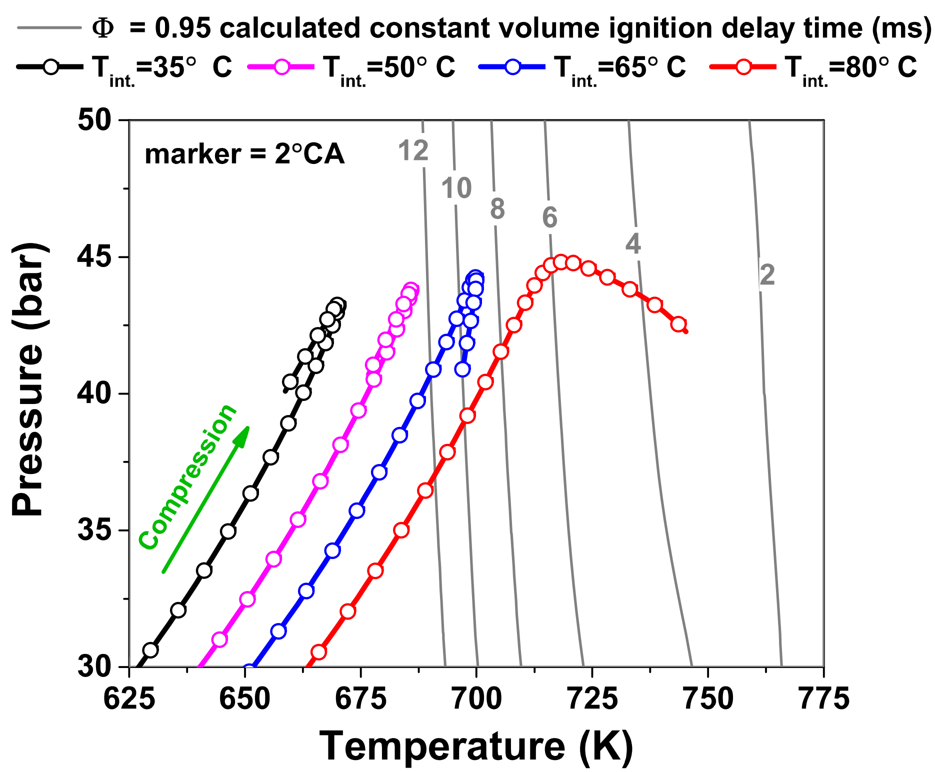
Constant Volume Ignition Delay Contours using 3-component Gasoline Allow Understanding of Data in Pressure-Temperature Domain

- Data plotted up to spark
- Reduced intake temp.
  - no PSHR and expansion temperature is reduced
- Increased intake temp.
  - PSHR developing and penetration into ignition delay contours
- Markers illustrate every 2 CA of time.
  - Slider crank mechanism increases TDC time
  - TDC ignition delay could be most dominant ignition delay state with very retarded CA50 phasing



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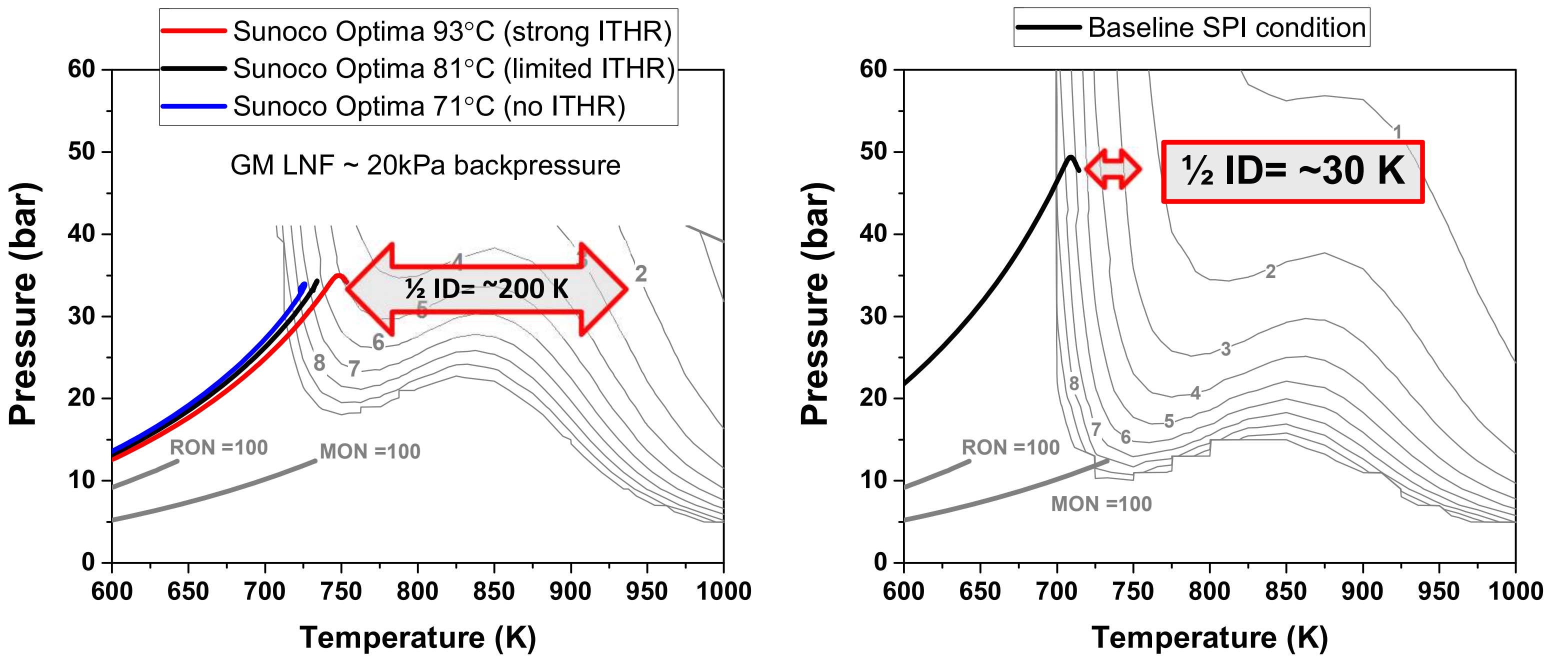
Analysis Reveals that for SPI Conditions, Interaction with a High-Gradient Portion of the Ignition Delay Contours



- At lower pressure condition, temperature increase to reduce ignition delay by 50% is 200K
  – Low temperature sensitivity because passing through negative temperature region
- At higher pressure SPI condition, ignition delay timescales are much shorter before negative temperature region, higher autoigition propensity

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Conclusion: Pressure-Temperature Framework is a Useful Way to Understand Kinetics and Experimental Data

- Fuel autoignition pathway and kinetics are determined by pressure-temperature trajectory
  - Different pressure-temperature trajectories interact with different rate-limiting steps in the autoignition chemistry
  - Initial conditions in engine setup pressure-temperature trajectory for unburned gas and determine the portion of the kinetic map that will be relevant
- Pressure-temperature analysis allow the relevant portion of the kinetic map to be understood
  - Revealed the role of PSHR for fuels of different octane sensitivity, and the role that plays on knock
  - Allowed an explanation of why effectiveness of EGR to mitigate knock is attenuated under boost
  - Provided insight into the thermodynamic conditions for stochastic preignition
- Technique allows for some level of error in kinetic ignition delay calculations
  - Dependent on trend-wise information from kinetic calculations to elucidate phenomenological differences
  - Avoids issue of small imperfections in kinetics at each timestep being integrated into a large error over the course of a full engine cycle