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

Jim Szybist and Derek Splitter
Oak Ridge National Laboratory
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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

Which Fuel is Best? It Depends.

Notional Set of Fuels

<table>
<thead>
<tr>
<th>Fuel</th>
<th>RON</th>
<th>MON</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fuel 1</td>
<td>98</td>
<td>98</td>
</tr>
<tr>
<td>Fuel 2</td>
<td>95</td>
<td>85</td>
</tr>
<tr>
<td>Fuel 3</td>
<td>93</td>
<td>87</td>
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<tr>
<td>Fuel 4</td>
<td>97</td>
<td>91</td>
</tr>
<tr>
<td>Fuel 5</td>
<td>92</td>
<td>82</td>
</tr>
</tbody>
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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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- Naturally Aspirated SI Engine at WOT: Similar to RON
- Throttled SI or HCCI
Initial In-Cylinder Conditions Determine Pressure-Temperature Trajectory; Autoignition Chemistry is Dependent on Trajectory

Naturally Aspirated SI Engine at WOT: Similar to RON

Boosted SI

Beyond RON

Beyond MON

Throttled SI or HCCI
Initial In-Cylinder Conditions Determine Pressure-Temperature Trajectory; Autoignition Chemistry is Dependent on Trajectory.

Higher Compression Ratio Maintains Trajectory, Changes Endpoint.
Initial In-Cylinder Conditions Determine Pressure-Temperature Trajectory; Autoignition Chemistry is Dependent on Trajectory

7-Component E0 Gasoline Surrogate
RON = 98
MON = 87

Pressure [bar]
0 10 20 30 40 50

Temperature [K]
300 400 500 600 700 800 900 1000

Ignition Delay [ms]
0 2 4 6 8 10

Kinetic Ignition Delay Calculations Illustrate Changing Autoignition Chemistry
Initial In-Cylinder Conditions Determine Pressure-Temperature Trajectory; Autoignition Chemistry is Dependent on Trajectory

4-Component E0 Gasoline Surrogate
RON = 98
MON = 97

Kinetic Ignition Delay Calculations Illustrate Changing Autoignition Chemistry
Comparing Constant Ignition Delay for Different Fuels Enable a Better Understanding of RON, MON, and OI

For Naturally Aspirated Engine at WOT, Fuels are Similar

Under boost, High S fuel is Better

Under MON Conditions, Low S fuel is Better

8ms ID Contours

Pressure [bar]  
Beyond RON

Temperature [K]  
Beyond MON

RON 98, S = 1
RON 98, S = 11

For Naturally Aspirated Engine at WOT, Fuels are Similar

Under MON Conditions, Low S fuel is Better
Application of Pressure-Temperature Framework

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

2. Decreasing effectiveness of EGR to mitigate knock under boost

3. Importance of the thermodynamic state on low speed preignition
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
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
- Condition B knock resistance: E40 > Gasoline > Iso-octane
- Condition C knock resistance: E40 >> Gasoline >> Iso-octane
- In moving from Condition A to Condition C, the combustion phasing change for E40 is approximately half that of iso-octane

Low S is Good
High S is Good
High S is Really Good
Pre-Spark Heat Release (PSHR) is present for Iso-octane and Gasoline. Phenomenon is extremely repeatable, increases with intake temperature.

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

**Gasoline**
- Gasoline requires higher intake temperature for similar behavior (20-25 deg C)
Comparison of the Ignition Delay Definitions for Iso-Octane. Substantial Differences for $T < 850 \text{K}$.

- 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
• 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
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
Application of Pressure-Temperature Framework

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

2. Decreasing effectiveness of EGR to mitigate knock under boost

3. Importance of the thermodynamic state on low speed preignition
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)

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

Colors represent different fuels
Closed Symbols: 0% EGR
Open Symbols: 15% EGR
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 O₂ and H radicals and the abstraction reactions HO₂ 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
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)
Boosted “Beyond RON” Conditions Interact with Ignition Zone 1, Minimal Impact on 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

- 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
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Application of Pressure-Temperature Framework

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

2. **Decreasing effectiveness of EGR to mitigate knock under boost**

3. **Importance of the thermodynamic state on low speed preignition**
Stochastic Preignition is an Abnormal Combustion Event that Occurs at High Loads (boosted) and can Severely Damage Engines
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
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

![Graph showing constant volume ignition delay contours](image)

**Legend**
- \( \Phi = 0.95 \) calculated constant volume ignition delay time (ms)
- T\(_{\text{int.}}\) =35°C
- T\(_{\text{int.}}\) =50°C
- T\(_{\text{int.}}\) =65°C
- T\(_{\text{int.}}\) =80°C

**Marker**
- marker = 2°CA
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 autoignition propensity
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