

# Engine Operating Conditions and Fuel Properties on Pre-Spark Heat Release and SPI Promotion in SI Engines

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## ABSTRACT

This work explores the dependence of fuel ignition delay on stochastic pre-ignition (SPI). Findings are based on bulk gas thermodynamic state, where the effects of kinetically controlled bulk gas pre-spark heat release (PSHR) are correlated to SPI tendency and magnitude. Specifically, residual gas and low temperature PSHR chemistry effects and observations are explored, which are found to be indicative of bulk gas conditions required for strong SPI events. Analyzed events range from non-knocking SPI to knocking SPI and even detonation SPI events in excess of 325 bar peak cylinder pressure. The work illustrates that singular SPI event count and magnitude are found to be proportional to PSHR of the bulk gas mixture and residual gas fraction. Cycle-to-cycle variability in trapped residual mass and temperature are found to impose variability in singular SPI event count and magnitude. However, clusters and short lived bursts of multiple SPI events are found to better correlate with fuel-wall interaction. The results highlight the interplay of bulk gas thermodynamics and SPI ignition source, on SPI event magnitude and cluster tendency. Moreover, the results highlight fundamental fuel reactivity and associated hypersensitivity to operating conditions at SPI prone operating conditions.

**CITATION:** Splitter, D., Kaul, B., Szybist, J., and Jatana, G., "Engine Operating Conditions and Fuel Properties on Pre-Spark Heat Release and SPI Promotion in SI Engines," *SAE Int. J. Engines* 10(3):2017, doi:10.4271/2017-01-0688.

## INTRODUCTION

In recent years, use of downsized, turbocharged engines has increased significantly as a means for industry to meet corporate average fuel economy (CAFE) standards and reduce CO<sub>2</sub> emissions [1,2]. This approach has been effective, enabling significant improvements in vehicle fuel economy. However, the high specific loads encountered with this approach have made pre-ignition phenomena, which had not generally been observed since the reduced compression ratios of the unleaded gas era, relevant again [3]. In these engines, this is exhibited as combustion abnormalities typically termed low-speed pre-ignition (LSPI), or stochastic pre-ignition (SPI), which are often accompanied by very strong knock events that can cause significant damage to engine hardware, including catastrophic engine failure.

SPI is characterized by the initiation of a flame front before the spark is fired, and typically occurs at engine speeds of 2000 r/min and below, under very high load conditions. This flame front often initially propagates normally, but with significantly advanced combustion phasing due to the earlier ignition. In many cases, the pressure rise due to combustion will lead to violent end-gas autoignition, causing rapid pressure rise and severe pressure oscillations commonly termed "super-knock" [4]. While the pre-ignition event and the resulting super-knock event are related, they

are distinct phenomena, and not all SPI cycles exhibit knock [5]. The initial SPI cycle is apparently stochastic and typically occurs on the order of once per 10,000 cycles at operating conditions conducive to it. However, the initial SPI cycle is often followed by a cluster of several more SPI events in the subsequent cycles. This usually occurs in an alternating pattern, i.e. an SPI cycle followed by a normal cycle, followed by an SPI cycle, etc., but consecutive SPI cycles have rarely been observed as well [6].

A number of studies have been performed to examine the relevant factors contributing to SPI frequency. Zahdeh, et al. [6] evaluated an engine's SPI frequency over extensive operating condition sweeps and varying hardware configurations (e.g. injector targeting, piston top/ring geometry, etc.). The results of these experiments illustrated the sensitivities of SPI to different operating conditions and even provided some strategies to greatly reduce the frequency of pre-ignitions. These strategies include the use of a high volatility fuel, targeting the piston top rather than the cylinder liner with the fuel injection spray, and using multiple fuel injections.

The fundamental causes of SPI, however, remain poorly understood, and there is not a firm consensus on the underlying mechanism. Zaccardi [7] describes several possible mechanisms, including autoignition in the gaseous phase as well as autoignition due to

interactions between the gaseous mixture and either liquid droplets or solid particles. In all cases, favorable thermodynamic conditions are required. Some authors have shown that solid particulates of sufficient size, e.g. flaking deposits or large soot particles, can initiate pre-ignition events [8,9,10]. Other research has shown a much stronger probability of fuel/lubricant droplets serving as the primary ignition source [6,11], and a great deal of recent work has focused on understanding the effects of fuel [12,13,14,15] and lubricant [16,17,18,19,20,21,22,23] properties, and the interaction of fuel sprays and lubricating oil in the top crevice region [6,24,25].

Variations in piston ring motion [6] and turbulence [26] have also been proposed as possible transport-related causes of the apparently stochastic nature of SPI.

Some efforts have been made to consider the pre-ignition and end-gas autoignition phenomena from a chemical kinetics perspective, and to distinguish between deflagration and detonation in super-knock events [4]. Kalghatgi, et al. [27,28] evaluated the formation of propagating flames from pre-ignition hotspots (which could be particles, fuel/oil droplets, etc.) and the severity of any resulting super-knock events based on analysis of ignition delays of surrogate fuels. Rudloff, et al. [29] expanded upon this work to develop an analysis method for characterizing the deflagration-detonation transition in super-knock events with more detailed fuel chemistry rather than simple surrogates. Lecoq, et al. [30] have developed an LES model with an integrated chemical-kinetics-based autoignition model to simulate the formation of a flame front from a hotspot. These approaches focus on the kinetics of the fuel/air mixture rather than the ignition source itself.

Recently, Szybist and Splitter [31] observed kinetically controlled bulk gas pre-spark heat release (PSHR) of gasoline and gasoline-like fuels as a function of operating conditions. It is imperative to note that [31] demonstrated that PSHR is a bulk gas kinetically controlled heat release and not a deflagration. Moreover, [31] highlighted that fuels with reduced sensitivity (i.e., research octane number (RON)-motor octane number (MON)) at elevated temperature and boosted conditions exhibited PSHR. That work explained the PSHR effect in terms of the bulk gas ignition delay and the associated in-cylinder pressure-temperature trajectories. A major finding of that work was that an island of low-temperature heat release exists where PSHR is enhanced but the transition time from low-temperature reactions to main ignition is extended. The present work builds upon that analysis and explores conditions at more elevated boost pressures and compression ratio, resulting in pressure-temperature trajectories that are beyond those explored in Szybist and Splitter [31]. The conditions in the present work are representative of those at very highly boosted SPI-prone operating conditions. Analysis of the relationship between bulk-gas kinetic state and PSHR within the context of SPI frequency and magnitude of associated super-knock events is conducted. The intermittency of SPI events is evaluated from the perspective of cycle-to-cycle variations in the trapped mass and thermodynamic

properties of the mixture, rather than the properties or transport of the ignition source. Additionally, comparison of operation with different lubricants is performed to elucidate the impact of fuel-wall interaction, where all presented analysis is performed with a certification gasoline and a market lubricant.

## METHODOLOGY

### Experimental Facility

The engine used in this study is based on a 1.6 L Ford Ecoboost engine equipped with the production center-mounted direct injection fueling system. Engine geometry details are presented in Table 1. The engine was converted to a single-cylinder engine by disabling cylinders 2, 3 and 4. The combustion chamber geometry and camshaft profiles were unchanged from the stock configuration. The engine specifics are highlighted in Table 1.

The engine was operated using laboratory fueling and air handling systems. The fueling system used a pneumatically-actuated positive displacement pump in conjunction with an electronic pressure regulator to provide fuel rail pressure. A constant fuel rail pressure of 150 bar was used throughout this study. Pressurized and dried facility air having less than 5% relative humidity was metered to the engine using a mass air flow controller, and no external EGR was used. Intake manifold temperature was a variable in this study and was controlled using an electrical heater upstream of the intake surge tank. The laboratory configuration has the ability to simulate turbocharger conditions by applying backpressure to the exhaust system, which was also a variable in the study.

Table 1. Engine geometry.

|                                                       |                                                              |
|-------------------------------------------------------|--------------------------------------------------------------|
| <b>Bore x Stroke (mm)</b>                             | <b>79.0 x 81.3</b>                                           |
| <b>Connecting rod length (mm)</b>                     | <b>133</b>                                                   |
| <b>Wrist pin offset towards expansion stroke (mm)</b> | <b>0.8</b>                                                   |
| <b>Compression ratio (-)</b>                          | <b>10.1:1</b>                                                |
| <b>Fuel injection system</b>                          | <b>Direct injection, center-mounted, production injector</b> |

The engine was controlled through a custom DRIVEN-based engine controller, with automatic engine controls developed at ORNL with calibration based on manual engine mapping. The controller used a mass airflow based, PID-enabled tabular engine map for fully automatic control of fuel, air, spark timing, and camshaft phasing. The present measurements were acquired in automated operation using a time varying load square-wave at 2000 r/min. The specifics of the test cycle are illustrated in Figure 1. The exploratory analysis presented in this study is based on two consecutive 20-minute duration high load segments. Although the combustion phasing of the high load operating condition is very late, CA50 of 38°CA aTDC<sub>p</sub>, the CoV of IMEP was 3 at the baseline condition.

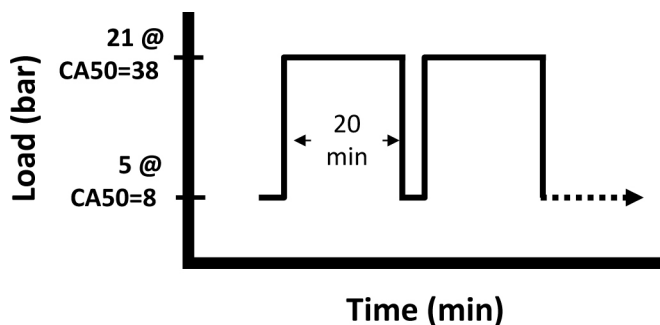


Figure 1. Automatized engine operating cycle.

For each tested fuel-condition, fuel injection timing, spark discharge, and cylinder pressure were recorded at either 0.2°CA (backpressure sweep) or 0.5°CA (all other reported conditions) resolution. Cylinder pressure was measured using a reinforced-diaphragm flush-mounted piezoelectric pressure transducer from Kistler (6052), which also had a flame arrestor installed. Start of fuel injection timing was commanded during the intake stroke and held constant at 250°CA bTDC<sub>r</sub>. Spark timing was adjusted as-needed to achieve the desired crank angle of 50 percent mass fraction burned (CA50) combustion phasing, and spark dwell was held constant at 1.8ms with the stock 4-wire ignition coil from a GM LNF engine. Engine fuel flow was measured with a coriolis-based fuel flow meter. To exacerbate SPI, the engine coolant temperature was maintained at 68°C.

To prevent hot-spot run-away at high-load, a spark plug with 2 heat ranges colder than the production engine's plug was used. The corresponding colder spark plug was identified through cross-referencing current production spark plugs with the same thread and reach as the OEM spark plug, and a Denso Iridium HP ITV24 spark plug was identified as being compatible. Note the Denso spark plug is a 25 mm reach where the production spark plug is a 26.5 mm reach, however the 1.5 mm shorter reach Denso spark plug resulted in flush mounting of the spark plug to the combustion chamber while the stock 26.5 mm reach protruded into the combustion chamber approximately 1.5 mm.

### Combustion Analysis Approach

Combustion analysis was performed using a MATLAB based routine, which was applied on a per-cycle basis. For each cycle, trapped mass was calculated using the cam position with measured in-cylinder pressure and applying the methodology described by Fox et al., [32] with the measured cycle-by-cycle based polytropic compression and expansion coefficients. Apparent heat release was then solved from zero-phase filtered in-cylinder pressure cycle-by-cycle trapped mass. For all cycles, a check for PSHR was conducted and PSHR was identified if at least 0.1% cumulative heat release occurred before the spark discharge. Note that because apparent heat release rate (AHRR) was used in the analysis, there is a small negative heat release near TDC inherent in the calculations due to neglecting heat transfer, which results in negative values of PSHR for cycles that do not

exhibit PSHR. Thus the 0.1% cumulative threshold at spark discharge is inherently incorporating and integrating the negative AHRR near TDC, resulting in the 0.1% positive PSHR threshold requiring non-trivial actual PSHR.

If PSHR was identified, the heat release analysis was separated into the deflagration and kinetic bulk gas reaction portions with independent analysis of each process. Depending on the PSHR behavior, the transition point from PSHR to deflagration differed. For PSHR with negative temperature coefficient (NTC) behavior (i.e., a rise and fall in the AHRR prior to the main combustion event, see red 80°C data in Figure 4), the deflagration portion was identified by the minimum AHRR of the NTC. Conversely, for PSHR without any NTC, the transition to deflagration was empirically determined by windowing the heat release between the crank angle at spark discharge and the crank angle at 5 percent of the cumulative heat release (CA05), and identifying the location of maximum heat release rate acceleration within the window.

Regardless of PSHR presence, the presence of SPI was identified on a cycle-by-cycle basis using an approach similar to that described by Mansfield et al. [14]. The present approach identified SPI cycles that exhibited both statistically significant early combustion and maximum cylinder pressure, thus focusing on cycles that exhibited early heavy knock and super-knock rather than all pre-igniting cycles. The threshold used to identify statistical significance was defined as at least 3.85 standard deviations from the mean in both the crank angle of CA05 and peak cylinder pressure ( $P_{max}$ ). The results of this approach clearly identified significant pressure and early heat release events, where a typical SPI would have a peak pressure of 100 bar greater than the ensemble average peak pressure.

For all cycles the bulk gas temperature was solved for using ideal gas relations. For each cycle the trapped mass was converted to moles by accounting for trapped residual and fresh air-fuel charge. Since mass is conserved but moles are not, the number of moles were calculated for each crank angle as a function of the normalized heat release, where no dissociation or chemical equilibrium effects were assumed. The number of moles before heat release was assumed to be equal to the trapped moles, the number of moles at the end of heat release was assumed to be the moles of exhaust gas based on the ensemble measured exhaust species, and the number of moles during heat release was estimated by being directly proportional to the normalized heat release times the difference between the initial and final number of moles. The trapped moles were determined through the assumption of residual gas having the molecular weight of the ensemble average of wet measured exhaust gas species, the fresh intake air having the molecular weight of dry air, and the fuel having the molecular weight of isooctane. Thus this approach results in calculating the number of moles at crank angle in a zero-dimensional approach for bulk gas temperature with shifting number moles based on proportional equilibrium.

### Experimental Steady State Operating Conditions

All data presented in the analysis were acquired under steady-state conditions during an automated square-wave load schedule (Figure 1). In the analysis, the transient portions of the acquired data were ignored. Steady state operation was found to occur approximately 450 seconds into the low-to-high load transition (~7000 cycles at 2000 r/min). The transient response of one such low-to-high load transition is plotted in Figure 2, where the time to steady state operation is indicated. Note the bottom plot in Figure 2,  $\Delta P_{\text{engine}}$ , is defined according to Equation 1.

$$\Delta P_{\text{engine}} = P_{\text{intake}} - P_{\text{exhaust}} \quad (1)$$

Thus, a positive value of  $\Delta P_{\text{engine}}$  indicates a flipped pumping loop which was present for all high-load cases in the present study.

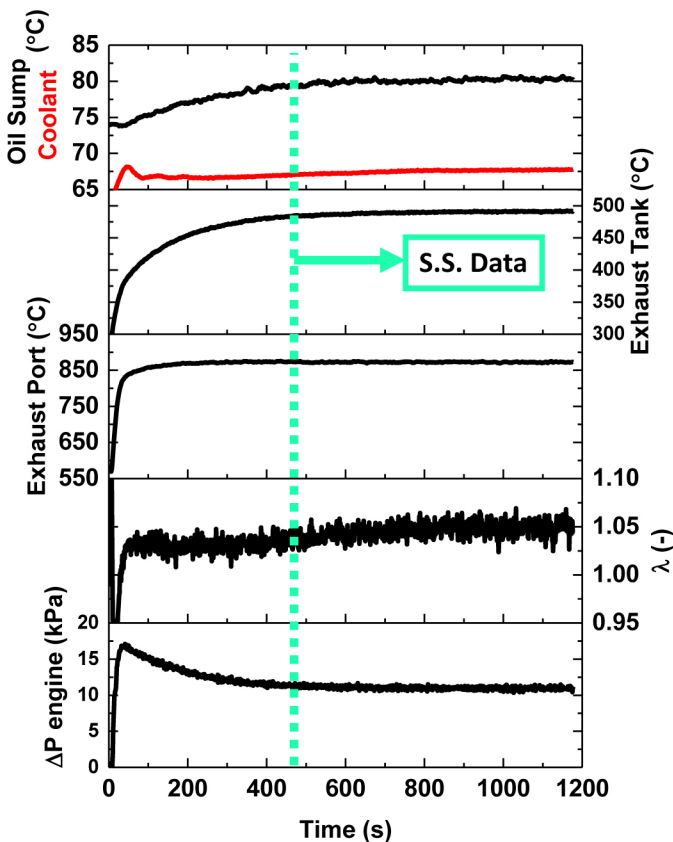


Figure 2. Transient response of engine thermodynamic state through one upload segment.

### Fuel

Premium grade Tier II certification fuel, acquired from Haltermann products, product code HFO437 was used for this study. The specific properties from the certificate of analysis of the fuel used are in Table 2.

Table 2. Fuel properties of Haltermann EEE premium grade fuel

|                                 |       |
|---------------------------------|-------|
| RON (ASTM D2699)                | 96.3  |
| MON (ASTM D2700)                | 88.8  |
| S (RON – MON)                   | 7.5   |
| IBP (°F) (ASTM D86)             | 87    |
| T5 (°F) (ASTM D86)              | 114   |
| T10 (°F) (ASTM D86)             | 127   |
| T20 (°F) (ASTM D86)             | 148   |
| T30 (°F) (ASTM D86)             | 171   |
| T40 (°F) (ASTM D86)             | 200   |
| T50 (°F) (ASTM D86)             | 220   |
| T60 (°F) (ASTM D86)             | 231   |
| T70 (°F) (ASTM D86)             | 241   |
| T80 (°F) (ASTM D86)             | 257   |
| T90 (°F) (ASTM D86)             | 315   |
| T95 (°F) (ASTM D86)             | 340   |
| FBP (°F) (ASTM D86)             | 411   |
| C (wt. %) (ASTM D5291)          | 86.58 |
| H (wt. %) (ASTM D5291)          | 13.42 |
| O (wt. %) (ASTM D4815)          | 0     |
| LHV (kJ/kg) (ASTM D3338)        | 42984 |
| Aromatics (vol. %) (ASTM D1319) | 28    |
| Saturates (vol. %) (ASTM D1319) | 71    |
| Olefins (vol. %) (ASTM D1319)   | 1     |

### Lubricant

All experiments were performed with commercially obtained Mobil 1 5W-20 lubricant. Independent lubricant analyses of this API service SN lubricant are listed in Table 3.

Table 3. Lubricant properties

|                    |      |
|--------------------|------|
| Silicon (ppm)      | 3    |
| Boron (ppm)        | 93   |
| Molybdenum (ppm)   | 76   |
| Phosphorus (ppm)   | 703  |
| Zinc (ppm)         | 803  |
| Sodium (ppm)       | 0    |
| Calcium (ppm)      | 1157 |
| Magnesium (ppm)    | 411  |
| Tungsten (ppm)     | 0    |
| Viscosity at 100°C | 8.9  |
| Viscosity at 40°C  | 47.6 |
| Viscosity Index    | 171  |
| Total Base Number  | 7.01 |

### Kinetic Modeling

Kinetic simulations of ignition delay were performed using ANSYS Chemkin release 15151. All ignition delay simulations were performed under adiabatic conditions using the closed homogeneous reactor simulation with a constant volume. Ignition delay calculations were performed for 20 ms, equivalent to 240°CA at 2000 r/min. All ignition delay calculations are performed for engine conditions with air ranging from 0.75-1.25  $\lambda$ .

The detailed gasoline surrogate mechanism from LLNL containing 1389 species and 5935 reactions [33] was used in the kinetic simulation. Gasoline was represented using a surrogate composition shown in Table 4, a formulation that was calculated using the

methodology presented by Morgan et al. [34]. Using this ternary mixture, however, it is not possible to simultaneously match the RON, MON, and aromatic content of the experimental gasoline. As a result, the fuel has matched RON and MON, but the aromatic content is higher than the experimental fuel (30 vs. 28 vol. %).

Table 4. Surrogate formulations for the chemical kinetic mechanisms.

|                     |       |
|---------------------|-------|
| iso-octane (vol. %) | 56.23 |
| n-heptane (vol. %)  | 13.77 |
| toluene (vol. %)    | 30.00 |

Additional deviation in the simulations relative to the experiments existed in the exhaust residual composition. In all simulations the exhaust residual composition was fixed at the concentrations in Table 5, which represent the nominal composition of a representative measured case. Note that HC are not included as the experiments measured only ~130 ppm of HC at the high load test condition. Using the fuel and residual composition in Table 4 and Table 5,  $\lambda=1.048$  charge condition was assumed for all cases in the simulations.

Table 5. Simulated residual composition

|                           |         |
|---------------------------|---------|
| CO <sub>2</sub> (mol. %)  | 9.81    |
| O <sub>2</sub> (mol. %)   | 0.81    |
| CO (mol. %)               | 0.00053 |
| H <sub>2</sub> O (mol. %) | 11.17   |
| N <sub>2</sub> (mol. %)   | 78.21   |

## RESULTS AND ANALYSIS

### Intake Temperature Effects

Previous findings by Szybist and Splitter [31], illustrated that at "beyond RON" conditions PSHR was observed with gasoline. The present work also explores intake temperature effects, but at conditions even further "beyond-RON," where engine operation with constant CA50 phasing of 38°CA aTDC<sub>f</sub> at 21 bar IMEP<sub>g</sub> was maintained through adjusting spark timing as needed. Although this is a very late CA50, the measured CoV of IMEP 3 at the baseline condition. Intake temperature was swept from 35°C to 80°C in 15°C increments, where Table 6 highlights the operating conditions of the sweep. Note that since the laboratory used a mass flow rate controller for intake airflow, the mass of air and AFR are constant for all tests and intake density (i.e., not intake pressure) was constant with intake temperature. Additionally, the trapped residual fraction was effectively kept constant for this sweep by maintaining very similar pressure differential across the engine at all intake temperatures.

Table 6. Intake temperature sweep operating conditions

|                                       |     |     |     |     |
|---------------------------------------|-----|-----|-----|-----|
| $\Delta P_{\text{engine}}$ (kPa)      | 24  | 24  | 25  | 25  |
| $P_{\text{intake}}$ (kPa)             | 209 | 211 | 214 | 217 |
| $P_{\text{exhaust}}$ (kPa)            | 184 | 187 | 189 | 192 |
| $T_{\text{intake}}$ (°C)              | 35  | 50  | 65  | 80  |
| Spark Timing (°CA aTDC <sub>f</sub> ) | 6.5 | 7.5 | 9   | 10  |
| PSHR (% of total HR)                  | 0.0 | 0.0 | 0.4 | 1.8 |

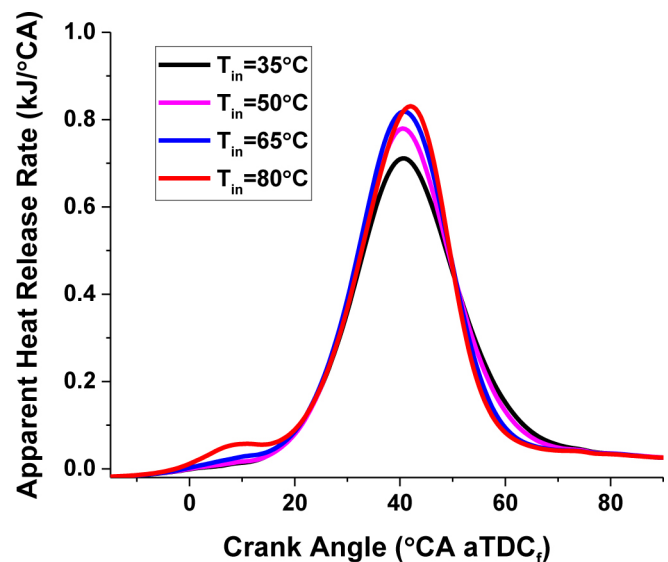


Figure 3. Ensemble average of apparent heat release as a function of intake temperature at constant CA50 phasing.

As intake temperature increased, PSHR behavior emerged and increased. The specifics of the PSHR as a function of intake temperature are magnified in Figure 4, where spark timing is also depicted by colored lightning bolts for the respective intake temperatures.

The trends of Figures 3 and 4 clearly show that PSHR increases proportional to intake temperature, with developed NTC PSHR occurring at the 80°C condition. Note that for all intake temperatures AHRR is slightly negative prior to TDC, an artifact of in-cylinder heat transfer. To avoid artifact bias of the cumulative heat release, AHRR integration only considered positive value of AHRR near TDC. The justification and results of the heat release integration and calculation is supported by the trends in Figure 5, which displays cylinder pressure as a function of in-cylinder bulk gas temperature for the four intake temperatures. Also plotted in Figure 5 are contour lines of simulated ignition delay of the surrogate fuel in constant volume reactor simulations at  $\Phi=0.95$ , the corresponding experimental air fuel condition. Note that the trends in Figure 5 are plotted up to the respective spark timing of the four intake temperatures.

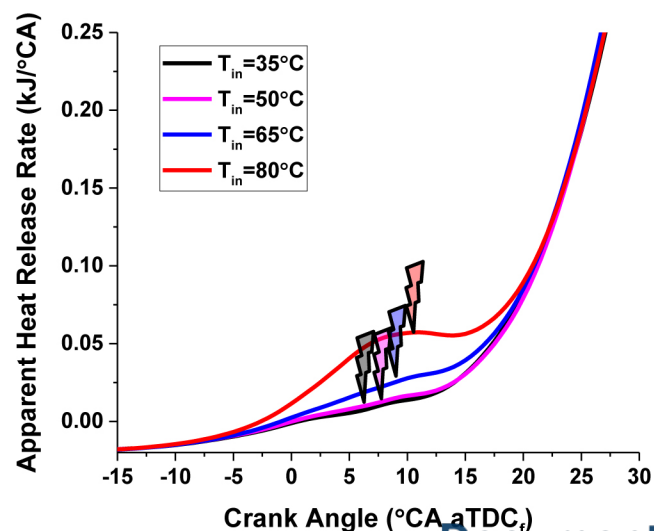


Figure 4. Detailed view of apparent heat release and spark timing as a function of intake temperature.