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Comparing Late-cycle Autoignition Stability for Single- and Two-Stage Ignition Fuels in HCCI Engines

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Abstract

The characteristics of autoignition after top-dead-center (TDC) for both single- and two-stage ignition fuels have been investigated in a homogeneous charge compression ignition (HCCI) engine. The single-stage ignition fuel was iso-octane and the two-stage ignition fuel was PRF80 (80% iso-octane & 20% n-heptane). The results show that the heat-release rate and pressure-rise rate both decrease as the combustion is retarded later into the early expansion stroke. This is an advantage for high-load HCCI operation. However, for both fuel-types, cycle-to-cycle variations of the ignition and combustion phasing increase with combustion-phasing retard. Also, the cycle-to-cycle variations are higher for iso-octane compared to PRF80. These observations can be explained by considering the magnitude of random temperature fluctuation and the temperature-rise rate just prior to thermal run-away. Furthermore, too much combustion-phasing retard leads to the appearance of partial-burn or misfire cycles, but the response of the two fuels is quite different. The different behaviors can be explained by considering the thermal and chemical state of the residual exhaust gases that are recycled from one cycle to the next. The data indicate that a partial-burn cycle with iso-octane produces residuals that increase the reactivity of the following cycle. However, for the already more reactive PRF80 fuel, the partial-burn products present in the residuals do not increase the reactivity enough to overcome the retarding effect of cool residual gases.

Keywords: HCCI; autoignition; variations; residuals; single-stage; two-stage

1. Introduction

The homogeneous charge compression ignition (HCCI) combustion process holds the promise of both good fuel economy and very low emissions of nitrogen oxides (NO_x) and soot. Therefore, HCCI is considered as a high-efficiency alternative to spark-ignited (SI) gasoline operation [1] and as a low-emissions alternative to traditional diesel compression ignition (CI) combustion [2]. However, several technical hurdles need to be overcome before HCCI can be widely implemented in production engines. Among these, controlling the rate of energy release and pressure-rise rate at high loads continues to be a major issue. Too high pressure-rise rates lead to strong acoustic oscillations in the combustion chamber, which can result in unacceptable noise and possibly engine damage. To reduce the combustion rate and pressure-rise rate at high loads, a recent study by the authors demonstrated the strong potential of combustion-phasing retard [3]. The benefits of combustion-phasing retard are realized because the effects of the naturally-occurring thermal stratification produced by heat transfer are amplified when autoignition occurs during the expansion stroke [4,5]. This extends the duration of the staged autoignition event, thus lowering the peak heat-release rate. Changes to the chemical-kinetic rates due to slightly lower combustion temperatures only play a minor role for equivalence ratios (ϕ) of 0.38 and higher [6].

However, there are limits to how far combustion-phasing retard can be exploited to reduce the pressure-rise rates. If the combustion is retarded enough, ultimately the combustion becomes very erratic with misfire or partial-burn cycles. Principally, this happens because the charge cooling due to piston expansion is too strong compared to the exothermic reactions of the autoignition event, thus preventing the charge from undergoing "hot" ignition. However, the exact combustion-retard limits and the behavior of the combustion for these conditions are not well known. In addition, the performance of retarded operation is dependent on the fuel-type, as identified in a concurrent study by the authors [7]. In that study, the engine was operated with both pure iso-octane (2,2,4-trimethylpentane), which exhibits single-stage autoignition, and PRF80 (primary reference fuel with 80% iso-octane and 20% n-heptane) which exhibits two-stage ignition with low-temperature heat release (LTHR) for these operating conditions. (Note that gasoline is expected to perform closely to iso-octane for the non-boosted conditions studied here [8].) The similarities and differences between these two fuel-types will be further investigated in the current paper.

2. Objectives and methods

2.1 Objectives and approach

The purpose of the current study is to investigate the combustion behavior of both single- and two-stage-ignition fuels for operation with combustion retarded to occur during the first part of the expansion stroke. This is accomplished with a combination of experiments and chemical-kinetics modeling.

First, the benefits of combustion-phasing retard are demonstrated. Second, the limits of combustion-phasing retard and the trends of increasing cycle-to-cycle variations are identified. Third, the source of these variations is explained, and the reasons for the different trends between fuels is clarified. Last, the reasons behind the differences in behavior between the fuel types for very retarded operation with partial-burn and misfire cycles are investigated by considering the thermal and chemical state of the residual gases retained from the preceding cycle.

For the current study, the combustion phasing (averaged over many cycles) was controlled by adjusting the temperature of the supplied fresh charge. For all conditions reported here, the engine speed was 1200 rpm. The intake pressure was maintained at 100 kPa, simulating naturally-aspirated operation.

2.2 Experimental setup

The engine used for the experiments is derived from a Cummins B-series diesel engine that has been converted for single-cylinder HCCI operation. The displacement is 0.98 liters/cylinder. The engine is equipped with a custom piston that provides an open combustion chamber with small top ring-land crevice. The piston dimensions produce a nominal compression ratio (CR) of 14:1. The valve timings are such that residual levels are low (≈4-5% by mass) for the conditions investigated.

For all engine operation, fuel and fresh air were well mixed in the intake system before being inducted. The supplied fuel-air equivalence ratio (ϕ) was kept at 0.40 throughout the study (air/fuel mass ratio = 37.8). Accounting for the additional dilution due to residual exhaust gases retained from the preceding cycle, the in-cylinder gas/fuel mass ratio is ≈39.8.

For each operating point, pressure traces were acquired for at least 200 cycles. The heat-release rate (HRR) and maximum pressure-rise rate (PRR_{max}) were computed for each individual cycle, and then averaged. However, the plotted temperature and heat-release traces were computed from the ensemble-averaged pressure trace. It should be noted that 0°CA (crank angle) is taken to be TDC (top dead center) intake, so TDC combustion is 360°CA. For more details on the engine, the fueling system, the combustion chamber geometry, and the experimental setup the reader is recommended Refs. [7,9].

2.3 Chemical kinetics modeling

The modeling part of this investigation used the Senkin application of the CHEMKIN-III kinetics rate code [10]. This adiabatic single-zone model was setup analogous to that of Refs. [8,9], except that CR = 12.4 was used to match the compression pressure of the current CR = 14 engine. The most current detailed reaction mechanisms for iso-octane and PRF from Lawrence Livermore National Laboratory [11,12] were used. To achieve the same amount of LTHR as found experimentally for PRF80 fuel, PRF30 was used computationally. This discrepancy between the experiment and the PRF mechanism is described in Ref. [13]. To match the dilution level of the experiment, the computations were performed with an air/fuel mass ratio of 39.8.

3. Results and Discussion

3.1 Benefits of combustion-phasing retard.

Figure 1 shows the average PRR_{max} as a function of 50% burn point (CA50) for the two fuels: iso-octane and PRF80. PRR_{max} decreases rapidly with combustion-phasing retard, and this is a benefit for high-load operation. As described in Ref. [4], this happens because the compressed charge has a temperature distribution. For a given combustion phasing, the pressure rise associated with the combustion of the hottest zone drives the next colder zone into autoignition and a chain event of autoignition occurs until all the in-cylinder charge has reacted, except for small amounts in boundary layers and crevices. When the combustion phasing is retarded by reducing the intake temperature, the autoignition of the hottest zone is delayed. The faster piston expansion at these later crank angles now more strongly counteracts the pressure rise associated with combustion, causing the autoignition of subsequently colder zones to be even more delayed than the hottest zone. This leads to a longer combustion event, as shown in the top portion of Fig. 1. The combination of lower peak heat-release rate and higher piston-expansion rate leads to the benefit of lower PRR_{max}. For reference, the acceptable limit is ≈8 bar/°CA for this combination of engine speed, CR, and intake pressure. Above this level the engine operation becomes too noisy [3,6].

Furthermore, it can be observed that for a given CA50, PRF80 has shorter burn duration and higher PRR_{max} than iso-octane. This is caused by a higher charge density for the PRF80 case, leading to a larger fuel mass being inducted per cycle. The density is higher because it is necessary to reduce the intake temperature to obtain the same combustion phasing. This is explained using Figs. 2 and 3.

Figure 2 shows that PRF80 has a two-stage autoignition process, with the LTHR centered around 344°CA. This accelerates the temperature rise during the late compression stroke, as shown in Fig. 3. Therefore, the temperature at the beginning of the compression stroke (T_{bdc}) has to be lowered to achieve the same combustion phasing of the main heat release. This increases the density of the inducted charge resulting in a 36% increase in the power output (as measured by the indicated mean effective pressure - $IMEP_g$) for PRF80 compared to iso-octane, as indicated in the legend of Fig. 3.

3.2 Increase of cycle-to-cycle variations with combustion-phasing retard

From Fig. 1, it appears that extensive combustion-phasing retard is desirable to obtain quiet engine operation and to allow higher fueling rates. However, combustion-phasing retard has to be exercised with caution, or erratic engine combustion results. This is illustrated in Fig. 4 which shows the standard deviation of $IMEP_g$ as a function of CA50.

Both iso-octane and PRF80 experience increasing cycle-to-cycle variations as CA50 is retarded. However, the increase is small for PRF80 and much greater for iso-octane. For this study, $\mathrm{IMEP_g}$ variations above 2% are deemed unacceptable for both fuels as this corresponds to the appearance of (>1% occurrence) partial-burn cycles. A cycle is considered a partial-burn cycle if its total heat release is reduced 10% or more, compared to a well-burning cycle. This means that the latest acceptable CA50 is 373°CA for iso-octane. For CA50 beyond 373°CA, a high frequency of partial-burn cycles occurs. In contrast, Fig. 4 shows that PRF80 can tolerate more combustion-phasing retard while maintaining stable combustion. This provides an advantage for PRF80. In fact, PRF80 never exhibits a significant occurrence of partial-burn cycles for steady-state operation. However, if CA50 is retarded beyond 376°CA, very soon all cycles start to misfire. This abrupt and total loss of combustion for PRF80 will be further discussed in section 3.3.

To understand why PRF80 exhibits lower cycle-to-cycle variations of $\mathrm{IMEP_g}$ for CA50 in the 370 – 376°CA range, and to explain why the variations increase with combustion-phasing retard for both fuels, it is beneficial to study and compare the autoignition processes. Figure 5 shows the standard deviation of CA10 plotted as a function of its average value. CA10 is the 10% burn point of the main combustion event. For PRF80, the LTHR was excluded from the computation of CA10 (and CA50) by initializing the integration of the heat release at the crank angle of minimum HRR between the low- and high-temperature combustion phases. As such, CA10 is here used as a measure of the crank-angle phasing of "hot" ignition, as was done in Ref. [13]. Both fuels exhibit increasing variations with combustion-phasing retard. Furthermore, iso-octane has substantially larger variations for a given CA10 timing. These two observations can both be explained by considering the charge-temperature history. Both explanations rely on the concept of a critical temperature for which thermal run-away occurs.

First however, analysis of motored (non-fired) operation is discussed to provide insight into how the magnitude of the random temperature variations changes with operating conditions. This analysis shows that the mass-averaged temperature at TDC (derived from the pressure trace) has a standard deviation of 1.1 K for PRF80 and 1.8 K for iso-octane. This difference occurs because the magnitude of the variations depends on the intake temperature, with higher intake temperatures showing larger variations. These variations of the compressed gas temperature are primarily caused by random variations of the turbulent heat-transfer processes during the compression stroke [5]. (It should be noted that a portion, estimated to ≈20%, of the apparent cycle-to-cycle variations stated above stem from pressure-measurement errors and small variations of the trapped mass from cycle to cycle.) For fired operation, variations of the residual temperature from the preceding cycle add to the total variations. These small, but inevitable, variations influence the crank-angle phasing when the charge reaches the critical temperature for thermal run-away (hot ignition). Depending on the temperature-rise rate just prior to hot ignition, a certain degree of cycle-to-cycle temperature variation will have a different impact on the timing of hot ignition. To illustrate this point, Fig. 6 shows model results for iso-octane.

Figure 6 shows that thermal run-away occurs at ≈1050 K, regardless of combustion phasing. It is clear that the temperature-rise rate prior to thermal run-away is less for more retarded combustion phasing. This happens because the piston expansion rate is greater with combustion-phasing retard, which produces more charge cooling. This counteracts the temperature rise associated with early exothermic reactions, reducing the temperature-rise rate. Consequently, a certain perturbation of the charge temperature has a larger effect on the crank-angle timing for thermal run-away, as illustrated in Fig. 6. This observation explains the trend of increasing cycle-to-cycle variations with combustion-phasing retard for both fuels, as shown in Fig. 5.

Furthermore, for a given CA10, Fig. 5 shows that PRF80 has smaller variations of CA10 than iso-octane. There are three reasons for this. First, the gas temperature is lower during the compression stroke. Because of this, random variations of the heat transfer are somewhat smaller, as discussed above. The second, and more important reason, is the presence of LTHR for PRF80. Looking back at Fig. 2 shows that iso-octane has very little heat-release prior to hot ignition at 366°CA. In contrast, PRF80 shows a distinct bump centered around 344°CA, but also elevated HRR after “the LTHR bump”. This makes the temperature-rise rate higher prior to hot ignition, compared to that of iso-octane. Indeed, careful examination of Fig. 3 shows that this is the case. For clarity, Fig 7 shows a magnified view of the temperature histories for the two fuels. It shows that the temperature-rise rates are comparable before the onset of PRF80’s LTHR. The LTHR then strongly accelerates the temperature rise between 340 and 349°CA. More importantly, PRF80 maintains higher temperature-rise rate near TDC. Analogous to the discussion in conjunction with Fig. 6, a higher temperature-rise rate should make the transition into hot ignition less sensitive to cycle-to-cycle variations of the compressed gas temperature.

Third, there is an additional factor related to the presence of LTHR for PRF80 that helps to explain why PRF80 has lower CA10 variations compared to iso-octane (Fig. 5). For alkane fuels, the low-temperature reactivity has been shown to increase with pressure (*e.g.* Ref. [14]). Therefore, if the charge is initialized with a lower temperature at BDC it will pass through the 760 – 880 K window (where LTHR is most active) at a later crank angle. Since the pressure now is higher, the amount of LTHR increases. The effect of this on the charge temperature is demonstrated in Fig. 8. Figure 8a shows that the onset of LTHR is delayed when the charge temperature is reduced. However, since the pressure is higher once the LTHR commences, more heat is released during this stage. Consequently, Fig. 8b shows that the temperature difference between the two cases is reduced from 21 K before the LTHR to 13 K after, at a crank angle of 353°CA. Effectively, the characteristics of LTHR tend to compensate for cycle-to-cycle variations of the charge temperature that occur prior to the onset of LTHR at 339°CA. This acts to dampen variations of the charge temperature before TDC, and this is the third reason why PRF80 exhibit less variations of CA10 compared to iso-octane.

3.3 Behavior under excessive combustion-phasing retard

As pointed out in conjunction with Fig. 4, another difference between these fuels is that PRF80 cannot be operated steady-state with high IMEP_g variations. Since misfire and very erratic combustion are not acceptable, it is important to understand the limits of combustion-phasing retard, how the combustion fails beyond this limit, and how easily stable combustion can be restored. Therefore, this section is dedicated to characterizing and explaining the failure modes for both fuels.

Figure 9 shows what happens when CA50 is retarded beyond 376°CA for PRF80. This transient was accomplished by reducing ϕ from 0.408 to 0.404 at cycle 50. For clarity, only 101 cycles out of the 500-cycle sample are shown. Fig. 9a shows that the average CA50 is being retarded past 377°CA in this cycle window. This retarding trend is a slow thermal effect caused by the slight cooling of the in-cylinder surfaces as a result of the slight reduction of the supplied ϕ. At this CA50 of 377°CA, PRF80 starts exhibiting occasional partial-burn cycles with incomplete combustion and reduced IMEP_g. Cycles 379 - 380, and 390 – 392 are examples of this. As Fig. 8b shows, a partial-burn cycle is often followed by another partial-burn cycle. This happens because a partial-burn cycle tends to have lower exhaust-residual temperature. (The plotted residual temperature is computed from the cylinder pressure prior to exhaust valve opening, accounting for cooling during blow-down using Eq. 9 in Ref. [15].) As the cooler exhaust residuals mix with the fresh charge of the following cycle, a lower-than-average charge temperature results. Thus, the cycle following a partial-burn cycle has a higher probability for very late hot ignition, likely resulting in a second partial-burn cycle.

This is a precarious combustion mode which eventually leads to a total loss of the main combustion event. For this particular case, this happens around cycle 426. Cycle 425 burns well with an IMEP_g of 545 kPa and high residual temperature. However, due to random variations of heat transfer, cycle 426 becomes a late-burning partial-burn cycle with an IMEP_g of 392 kPa and an estimated residual temperature of 603 K. Unlike for the earlier partial-burn cycles, the combustion does not recover from this, and the combustion for cycle 427 is very late and incomplete, rendering a very low residual temperature of 456 K. At this point onward, the cold residuals, which are recycled from one cycle to the next, prevent hot ignition for any subsequent cycle and only the LTHR takes place, producing low IMEP_g (≈35 kPa). In fact, the intake temperature has to be raised considerably to resume hot ignition and full power output.

In stark contrast, iso-octane can be operated with partial-burn cycles on a continuous basis, as illustrated in Fig. 10. The standard deviation of $IMEP_g$ is 10.1% for this operating point, which corresponds to the CA50 = 376.1°CA data point in Fig. 4. Careful examination of the data shows that a partial-burn cycle is always followed by well-burning cycle with high $IMEP_g$ and a more advanced combustion phasing than the average cycle. This is the opposite behavior of PRF80. Careful examination of Fig. 10 shows that for iso-octane a low $IMEP_g$ cycle universally results in low residual temperature, just like for PRF80. Therefore, the variations of residual temperature cannot explain why iso-octane recovers so well after each partial-burn cycle.

Further insight is gained by plotting the influence of residual temperature on the $IMEP_g$ of the cycle that follows, as shown in Fig. 11. Two observations can be made. First, well-burning cycles that produce residual temperatures around 720 K can be followed by a cycle with any level of $IMEP_g$. In other words, having a well-burning cycle that produces high residual temperature does not guarantee that a well-burning cycle will follow. This implies that a late partial-burn cycle is randomly produced by random fluctuations of the heat-transfer processes during the compression stroke, not cool residuals. Second, and more importantly, Fig. 11 shows that all cycles that burn poorly and produce low residual temperatures (< 700 K) are followed by a well-burning cycle with high $IMEP_g$. This strongly suggests that the residuals from a poorly burning cycle contain species that enhance the ignition of the following cycle. The effect is so strong that it overcomes the cooling effect of the lower residual temperature. This is an important finding with practical implications since this chemical effect prevents total loss of combustion and makes a recovery of stable combustion significantly easier than for PRF80. It should be noted that the residual level is low for this engine. For a high-residual engine this chemical effect would likely be even more prominent.

While the available data strongly suggests that the residuals from a partial-burn cycle with iso-octane contain species that enhance the ignition, it is unclear why the same chemical effect is not present for PRF80 operation, and that total loss of hot ignition happens when the residuals become sufficiently cool. Full treatment of this is beyond the scope of this paper. Nonetheless, it was decided to perform a limited study using CHEMKIN to examine the effects of selected species on the ignition processes for both iso-octane and PRF80. A recent HCCI exhaust speciation study by Kaiser *et al.* [16] was used to guide the selection of species worth examining. For HCCI combustion with low combustion efficiency, they reported ethene, propene, iso-butene, and formaldehyde to be the most prevalent exhaust hydrocarbon species, excluding fuel constituents.

The CHEMKIN results for these species show that ethene, propene and iso-butene all have fairly small effect on the ignition processes for both iso-octane and PRF80. On the other hand, formaldehyde stands out with a fairly strong effect on the ignition processes. Interestingly, mixed with fresh charge to a concentration of 250 ppm, it advances CA50 from 370.0°CA to 369.0°CA for iso-octane, but it retards CA50 from 370.0°CA to 371.8°CA for PRF80. This demonstrates that certain species can have an advancing effect for one fuel-type, but a retarding effect for another fuel-type. The retarding effect of formaldehyde for two-stage ignition fuels has been demonstrated experimentally by Yamaya *et al.* [17]. It is also worth noting that LTHR has been found to produce significant amounts of formaldehyde for PRF-fuels [18]. Therefore, elevated levels of formaldehyde in the residuals can be expected following a partial-burn cycle, and this could contribute to PRF80's inability to recover the main combustion event. However, more research is needed to fully clarify the chemical role of residuals on HCCI combustion.

4. Conclusions

Combustion-phasing retard reduces the peak heat-release rate, the maximum pressure-rise rate, and engine knock for both iso-octane and PRF80. However, combustion-phasing retard increases cycle-to-cycle variations of the combustion phasing and IMEP_g. This occurs for both the single-stage ignition (iso-octane) and two-stage ignition (PRF80) fuels, but for any given combustion phasing the variations are smaller for PRF80. The reason for the increased variations with timing retard, and the differences between the fuels can be explained by considering the temperature-rise rate just prior to thermal run-away (*i.e.*, "hot" ignition).

With higher temperature-rise rates, random fluctuation of the charge temperature have less influence on the hot ignition timing. Retarding the combustion phasing decreases the temperature-rise rate prior to hot ignition because the piston-expansion rate is greater at later crank angles. This increases the variations for both fuels. However, the temperature-rise rate is always higher for PRF80 due to its elevated reactivity prior to hot ignition. In addition, the magnitude of the random temperature fluctuations is less for PRF80 because the lower charge temperature leads to less heat transfer. Finally, the low-temperature heat release tends to dampen charge temperature fluctuations.

With too much combustion-phasing retard, partial-burn and/or misfire cycles start to appear. However, the two fuels behave very differently. For PRF80, the appearance of partial-burn cycles is typically followed by a complete loss of hot ignition for all following cycles. This is due to the recirculation of cooler residual gases following a partial-burn cycle. In contrast, for iso-octane a partial-burn cycle is always followed by a more advanced, well-burning cycle, despite the cooler residual gases. This happens because a partial-burn cycle with iso-octane produces species that enhance the autoignition of the following cycle.

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Fig 1. PRR_{max} and burn duration for iso-octane and PRF80. $\phi = 0.40$.

Fig 2. Heat-release traces for iso-octane and PRF80.

Fig 3. Temperature and pressure traces for iso-octane and PRF80.

Fig 4. Standard deviation of $IMEP_g$ divided by ($IMEP_g$-$IMEP_{g,motored}$) as a function of CA50.

Fig 5. Cycle-to-cycle variation of the phasing of hot ignition, here measured as CA10, as a function of average CA10.

Fig 6. CHEMKIN predictions of the influence of ±1.9K variations of compressed gas temperature at 350°CA (T_{350}) on the timing of hot ignition, for two different baseline combustion phasings. Iso-octane.

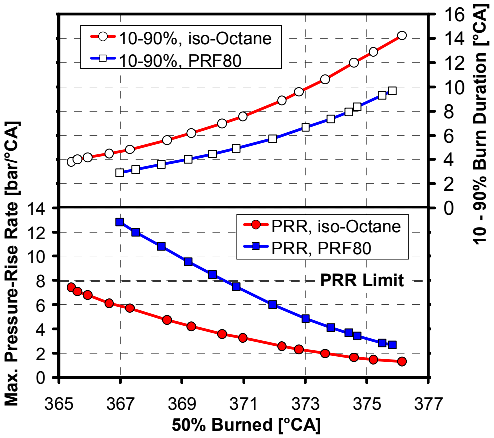
Fig 7. Temperature traces for iso-octane and PRF80. (Magnified view of Fig. 3.)

Fig 8. Influence of a change of T_{bdc} from 349 to 362 K on LTHR and resulting temperature trace. PRF80.

Fig 9. CA50 trend, $IMEP_g$ and residual gas temperature as a function of consecutive cycle number for PRF80.

Fig 10. $IMEP_g$ as a function of consecutive cycle number for iso-octane. CA50 = 376.1°CA.

Fig 11. $IMEP_g$ of next cycle plotted against residual temperature for iso-octane. CA50 = 376.1°CA.



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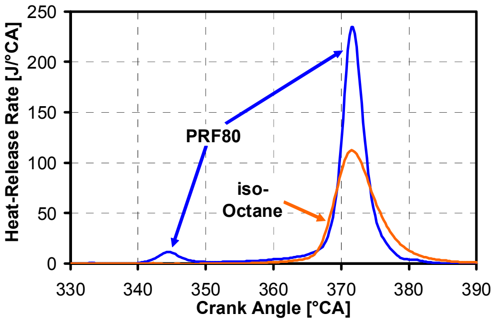
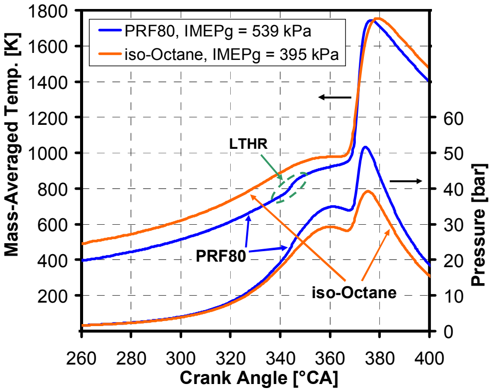


Fig 2. Heat-release traces for iso-octane and PRF80.



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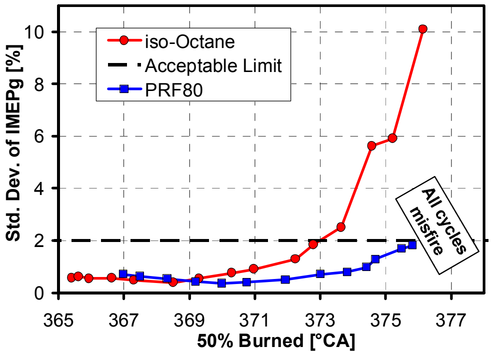
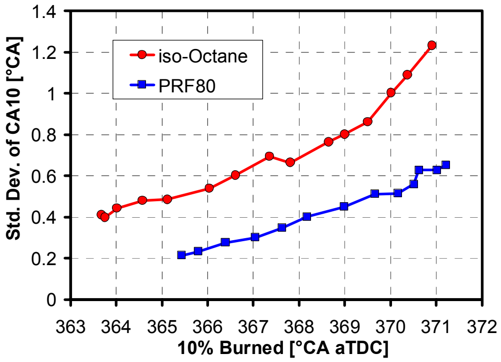


Fig 4. Standard deviation of $IMEP_g$ divided by ($IMEP_g$-$IMEP_{g,motored}$) as a function of CA50.



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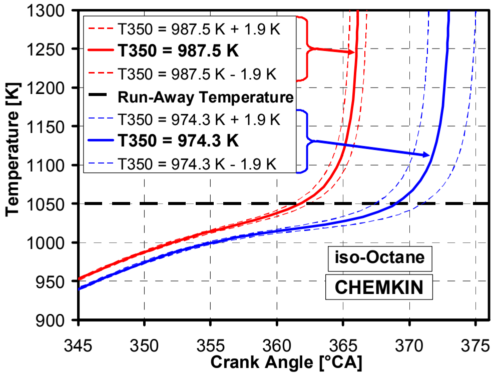

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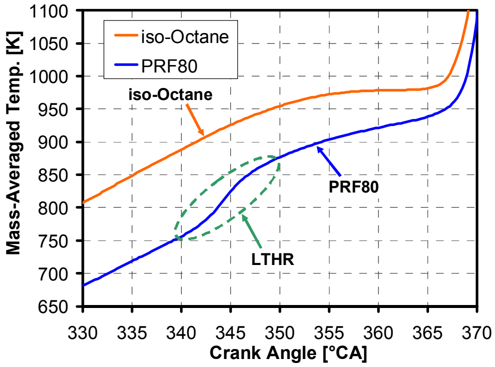

Fig 7. Temperature traces for iso-octane and PRF80. (Magnified view of Fig. 3.)

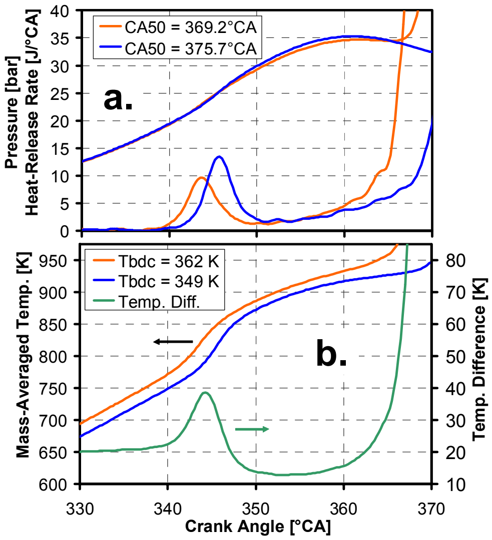

Fig 8. Influence of a change of T_{bdc} from 349 to 362 K on LTHR and resulting temperature trace. PRF80.

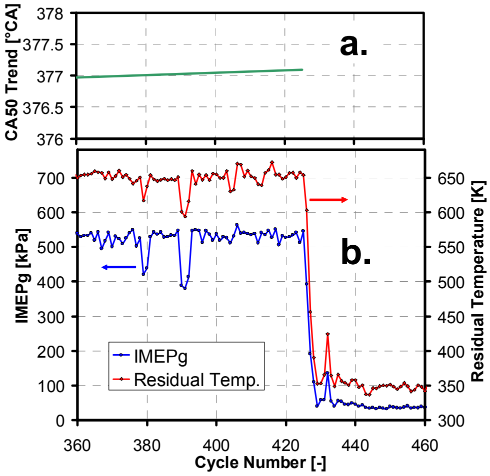

Fig 9. CA50 trend, $IMEP_g$ and residual gas temperature as a function of consecutive cycle number for PRF80.

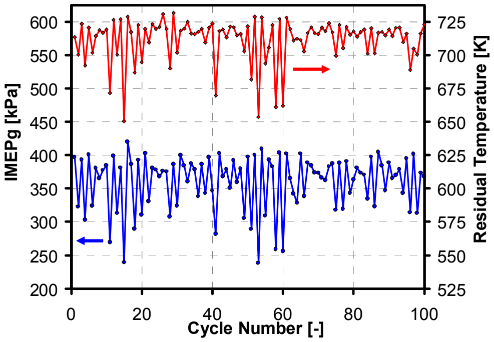

Fig 10. $IMEP_g$ as a function of consecutive cycle number for iso-octane. CA50 = 376.1°CA.

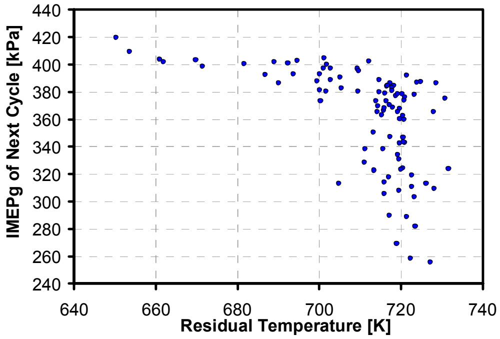

Fig 11. IMEP$_g$ of next cycle plotted against residual temperature for iso-octane. CA50 = 376.1°CA.