

A Computational Study of the Combined Effects of EGR and Boost Pressure on HCCI Autoignition

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ABSTRACT

This study computationally investigates the combined effects of EGR and boost pressure on HCCI autoignition using iso-octane, PRF50 and n-heptane. The computations were conducted using the single-zone model of CHEMKIN included in CHEMKIN-PRO with detailed chemical-kinetics mechanisms for iso-octane, PRF and n-heptane from Lawrence Livermore National Laboratory (LLNL). To better reproduce the state of EGR addition in real engine, the EGR composition is determined after several combustion cycles under the constant amount of fuel. All data points were acquired with a CA50 of 5°CA aTDC by adjusting initial temperature to remove the effect of combustion phasing, which can influence on HCCI autoignition from any effect of the EGR and boost pressure themselves.

The results show that EGR increases the burn duration and reduces the maximum pressure-rise rate with lower peak of maximum heat-release rates for all fuels even for a boost pressure, which accelerates a HCCI autoignition propensity. However, above a certain EGR ratio with no boost pressure, the LTHR of two-stage ignition fuel PRF50 disappears, and its autoignition process is changed to that of single-stage ignition fuel, which exhibits a high maximum pressure-rise rate and lower IMEP. Boost pressure increases the autoignition reactivity, and especially pronounced on LTHR of two-stage ignition fuels n-heptane and PRF50. PRF50 turns into two-stage ignition fuel again by boost pressure even at high EGR ratio, and the autoignition process of PRF50 becomes similar to that of n-heptane. Moreover, boost pressure could also eliminate the need to increase the initial temperature for a fixed CA50 when applying EGR, which provides potential to allow higher power output due to the increased charge mass inducted. Finally, the combined effects of EGR and boost pressure provide substantial advantages for controlling low-temperature heat-release and reducing peak of heat-release rate. These advantageous effects allow higher IMEP with lower maximum pressure-rise rate across a wide EGR ratio range, especially on the two-stage ignition fuel.

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INTRODUCTION

The homogeneous charge compression ignition (HCCI) combustion is the process in which a homogeneous mixture is auto-ignited through compression, providing both high efficiencies and very low nitrogen-oxide (NO_x) and particulate matter (PM) [1]. Although HCCI combustion is beneficial to fuel economy and emissions compared to spark-ignited (SI) gasoline combustion and compression ignition (CI) diesel combustion, it is very challenging to control autoignition processes while maintaining acceptable heat-release rate (HRR) due to no direct control mechanism such as spark discharge or fuel injection. Among the methods for controlling HCCI autoignition, exhaust gas recirculation (EGR) can be an effective means over a wide range of engine operating conditions. Hot EGR (internal EGR), usually in the

form of retained residuals, is often used to achieve HCCI autoignition of single-stage ignition fuels in engines with the relatively low compression ratios [2]. The presence of hot EGR heats the incoming charge, and causes advanced the autoignition timing, rapid HRR and moderate reduction of combustion duration [3]. Alternatively, cooled EGR (external EGR) is added to intake charges for controlling amount of heat release across a wide engine-speed range [4]. EGR addition increases the mole-specific heat capacity (C_v) of intake charges mainly by means of CO₂ and H₂O, and it leads to a significant reduction of the compressed-gas temperature, and finally limits HCCI autoignition. The use of EGR also reduces intake O₂ concentration by the displacement of air, and this extends the combustion duration and slows down the HRR. Consequently, a combination of increase of C_v and

reduction of O_2 concentration associated with EGR addition results in suppression of autoignition and combustion-phasing retard, allowing high-load operation without knock. However, the underlying mechanisms of EGR responsible for the HCCI autoignition are different depending on the fuel-type, and it makes the analysis complicated to explain. A recent study by Magnus et al. [5] shows that the partial-burn products retained in residuals enhance the autoignition for iso-octane, but suppress autoignition for PRF80. They also found that the autoignition propensity of single-stage ignition fuels (e.g. iso-octane and gasoline) are more sensitive to compressed-gas temperature, while the two-stage ignition fuels (e.g. PRF80 and PRF60) stand out with significantly higher sensitivity to the reduction of O_2 concentration [6]. In addition, the species presented in the EGR respond differently to fuel-type during autoignition reactions. Dimethylether (DME) exhibits two-stage ignition, but shows much lower sensitivity to the reduction of O_2 concentration contrary to PRF80 and PRF60, which could be possibly explained by DME's very different molecular structure [7]. The question is: if an in-cylinder charge density becomes be doubled just by increasing initial pressure at twice under the EGR addition with a same mole fraction of in-cylinder charge, can all effects of EGR on HCCI autoignition be still valid? This question provides a motivation to investigate the underlying mechanisms of EGR addition on HCCI autoignition under boost pressure operation. Several studies have shown that intake pressure boost can increase the autoignition reactivity. The boost pressure is especially pronounced for fuels that transition from single- to two-stage ignition by enhancing low-temperature heat release (LTHR). In the open literature, this has been shown to happen for gasoline and methylcyclohexane [8], and for iso-octane [9]. More fundamental experiments have examined this for n-pentane [10]. This LTHR-boosting effect of pressure opens up the possibility of maintaining LTHR at higher EGR ratio. A combination of the different autoignition propensity of fuel on EGR and other operating parameters affected by EGR addition such as combustion phasing, which can influence the autoignition independently from any effect of the EGR, makes it more difficult to understand direct effects of EGR on HCCI autoignition themselves. To better understand the underlying mechanisms of EGR on HCCI autoignition, it needs to focus on chemical kinetics of the autoignition of each fuel after isolating EGR effects from other operating parameters due to the chemical kinetic nature of the HCCI autoignition processes.

The main objective of this study is to computationally investigate the combined effects of EGR and boost pressure on HCCI autoignition, and to clarify the underlying mechanisms for both single- and two-stage ignition fuels. The fuels considered are iso-octane, PRF50 and n-heptane. The "Contribution matrix to heat release" and "Absolute heat-release rate" [11, 12] for important elementary reactions were plotted for various cases of each fuel, which are: 1) Cases

between no EGR addition and EGR addition for both at naturally aspirated operation, and 2) Cases between EGR addition at naturally aspirated operation and EGR addition at boost pressure operation.

CHEMICAL-KINETICS MODELING SETUP

Single-zone Model

The computational investigations have been conducted using the single-zone model of CHEMKIN [13, 14] included in CHEMKIN-PRO [15]. The single-zone model treats the in-cylinder charge as a single lumped mass with uniform composition and thermodynamic properties [16, 17]. Heat-transfer and blow-by effects were not included. It is recognized that this is a considerable simplification of a real engine in which the charge will never be completely mixed and there will be residuals from the previous cycle. In addition, heat transfer during intake can affect the initial charge temperature, and heat transfer to the cylinder wall and in crevices will always produce some temperature inhomogeneities. Because these effects will alter the maximum pressure-rise rate (PRRmax), HRR, the peak pressure, peak temperature, and the amount of emissions, the single-zone model is not expected to accurately predict these values over the operating range [9, 18, 19, 20]. Nevertheless, the single-zone model is a useful tool for investigating certain fundamental aspects of HCCI combustion. It allows the bulk-gas chemical kinetics and thermodynamics to be isolated in order to understand how they alone influence the in-cylinder processes. Eliminating the complexities of walls, crevices, and mixture inhomogeneities simplifies the analysis and allows cause-and-effect relationships to be more easily identified. The single-zone model also takes relatively short computational time even with the detailed chemical-kinetic mechanisms, which readily allow numerous changes in operating conditions of interest. Typical computational times for the LLNL mechanisms on the 3.2 GHz processor are about 3 minutes for a single-zone calculation.

Compression / expansion was modeled according to the standard slider-crank relationship [21], using the geometry and specifications of the single-cylinder HCCI engine shown in Table 1. The calculation starts from the intake valve close (IVC) of -132°CA aTDC to the exhaust valve open (EVO) of 132°CA aTDC.

Chemical-kinetic Mechanism

This study has used the most current detailed chemical-kinetic mechanisms and thermodynamic parameters for iso-octane [22, 23], primary reference fuel (PRF) [24] and n-heptane [25, 26] from Lawrence Livermore National Laboratory (LLNL). The LLNL mechanism consisted of 874 species and 3796 reactions for iso-octane, 1034 species and 4236 reactions for PRF, and 654 species and 2827 reactions for n-heptane. The chemical-kinetic mechanism for PRF is

Table 1. Engine Specification

Displacement (single-cylinder)	1322 cc
Stroke	115 mm
Bore	112 mm
Connecting Rod	255 mm
Compression Ratio	16:1
IVC	-132 aTDC
EVO	132 aTDC

Table 2. Fuel Properties

Fuel	Iso-Octane	PRF50	n-Heptane
Iso-Octane % vol.	100	50	0
n-heptane % vol.	0	50	100
RON	100	50	0
C-atoms	8	7.47	6
H-atoms	18	16.94	16
Molecular weight	114.23	106.797	100.205

developed by combining the same LLNL mechanisms of iso-octane and n-heptane [27]. The fuels considered in this study are iso-octane, PRF50 and n-heptane, and Table 3 shows the properties of these fuels. The air was modeled using N₂, O₂ and argon (Ar) with a molecular ratio of 78/21:1:1/21, where atmospheric CO₂ has been lumped as atmospheric N₂.

Contribution Matrix to Heat Release

This study employs the “Contribution matrix to heat release” to explain the underlying mechanisms of EGR addition on HCCI autoignition by identifying and quantifying chemical kinetics in the autoignition processes. The “Contribution matrix to heat release” extracts important elementary reactions by reducing detailed chemical-kinetics mechanisms. CHEMKIN included in CHEMKIN-PRO provides results of HRR of all reactions at transient temperatures (T_t) during reaction processes [11, 12]. Using the results of HRR of all reactions at T_t , this study derived the contribution ratio of the j^{th} elementary reaction to heat release at T_t (CHR_{j,T_t}) from dividing the HRR of a j^{th} elementary reaction at T_t (HR_{j,T_t}) by the sum of absolute HRR from j to N elementary reactions at T_t , as shown in Eq. (1). The CHR_{j,T_t} indicates a significance of j^{th} elementary reaction at T_t , thus important elementary reactions at T_t can be determined by the value of CHR . This study considers reactions as important elementary reactions when the CHR_{j,T_t} is beyond 5.0% at T_t .

$$CHR_{j,T_t} = \frac{HR_{j,T_t}}{\sum_{j=1}^N abs(HR_{j,T_t})} \times 100 [\%] \quad (1)$$

CHR_{j,T_t} : Contribution ratio of the j^{th} elementary reaction to heat release at a transient temperature T_t . HR_{j,T_t} : Heat-release rate of the j^{th} elementary reaction at T_t .

BASIC EGR CONSIDERATION

After a complete combustion of fuel with sufficient air, complete stoichiometric products (CSP), namely CO₂, H₂O and N₂, are generated with unused air. A mixture of CSP and unused air generated from previous cycles can be called an exhaust gas recirculation (EGR) when adding it to inducted air of next cycle. The use of EGR significantly alters the charge mixture composition and thermodynamic properties so that it directly influences HCCI autoignition reactions. Typically there are combustion inefficiencies, and this generates traces species like carbon monoxide (CO), hydrocarbons (HC) and partially oxidized hydrocarbons that can also influence the autoignition. However, it is difficult to clearly identify the amount of these species in recirculated gases since its amount is dependent on the specific fuel type and the engine operating conditions. For this modeling work, no attempt is made to capture the effect of trace hydrocarbon species such as CO, HC and partially-oxidized hydrocarbons encountered experimentally in real EGR. Here EGR ratio (γ) is defined as the ratio of the mole fraction of EGR (n_{EGR}) of in-cylinder charge to the mole fraction of sum of EGR and air ($n_{EGR} + n_{air}$) of in-cylinder charge, as shown in Eq. (2). Fuel is an important constituent of the intake charge, and especially the amount of fuel significantly influences on a power and/or efficiency of engines. In practical engine operations, the amount of supplied fuel should be constant to maintain the power even in an increase of EGR. For the reason, it is assumed that the amount of fuel is not varied by changes in γ after initial equivalence ratio (ϕ_0) is determined

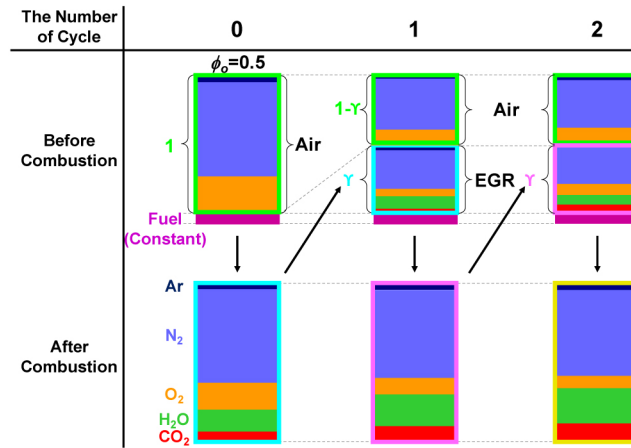


Figure 1. Illustration of an EGR addition during the cycle mode under constant amount of fuel.

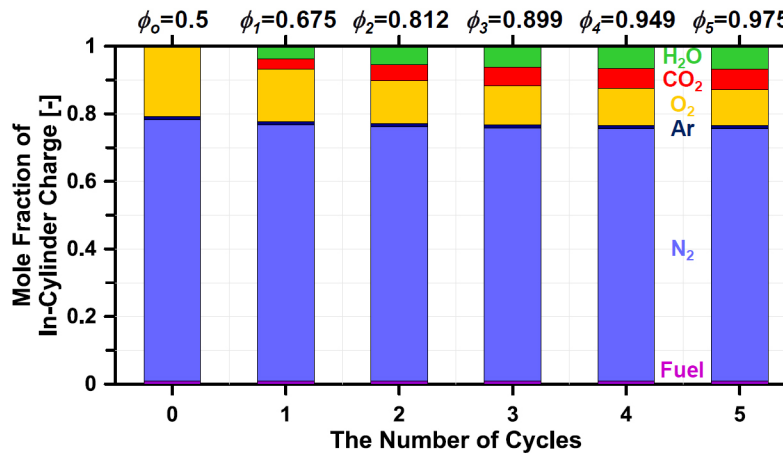


Figure 2. Changes of mole fraction of in-cylinder charge with cycles. $\phi_0=0.5$. $\gamma=0.5$. N-heptane.

at baseline point. The basic EGR consideration is illustrated in Fig. 1, which shows that the EGR is added to air after combustion by cycles under the constant amount of fuel. Figure 2 demonstrates how a mole fraction of in-cylinder charge changes with the cycles under basic EGR consideration. As expected, the equivalence ratio (ϕ) increases gradually with the number of cycles regardless of EGR addition due to the constant amount of fuel of in-cylinder charge. However, the increase of ϕ with the cycles gets smaller since the amount of oxygen of in-cylinder charge decreases, and in the end becomes constant with the number of cycles. Finally, the certain value of ϕ is determined after numerous cycles in having a trend that the higher γ , the higher ϕ . Figure 3 clearly represents the trend between γ and ϕ shown in n-heptane of $\phi_0=0.5$, and exhibits the sensitivity of ϕ to the number of cycles especially higher γ . It should be noted that the trend and the sensitivity stated with n-heptane of $\phi_0=0.5$ will vary naturally with fuel properties and/or ϕ_0 . Although the different fuel properties as shown in Table 3 leads to a different trend between γ and ϕ and the sensitivity of ϕ to the number of cycles, there are no distinct differences

between fuels used for this study. Figure 4 shows the mole fraction of in-cylinder charge and ϕ corresponding to 30th cycle in Fig. 3 for all γ . The highest γ of 0.5 considered in this study shows $\phi = 1$ at 30th cycle, and this is a double for ϕ_0 . Based on the results shown in Fig. 3 and 4, $\phi_0=0.5$ is chosen for iso-octane, PRF50 and n-heptane since it was observed that higher equivalence ratio is required to achieve combustion under high γ . To simulate various amounts of EGR, the γ has considered on the order of 0, 0.1, 0.125, 0.25, 0.315, 0.4, and 0.5.

$$\gamma = \frac{n_{EGR}}{n_{EGR} + n_{air}} \quad (2)$$

n_{EGR} : Mole fraction of EGR of in-cylinder charge
 $n_{EGR} + n_{air}$: Mole fraction of sum of EGR and air

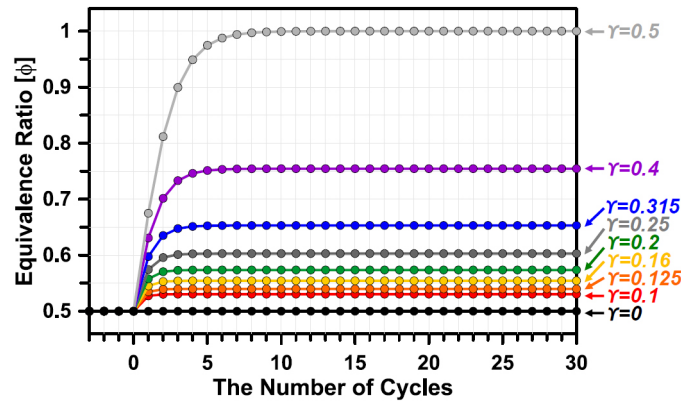


Figure 3. Equivalence ratio as a function of the number of cycles corresponding to EGR ratio from $\gamma=0$ to $\gamma=0.5$. N-heptane.

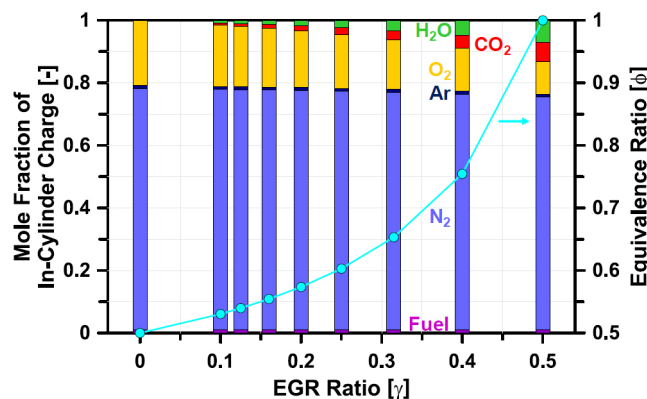


Figure 4. Mole fraction of in-cylinder charge and equivalence ratio as a function of EGR ratio after 30 cycles under constant amount of fuel. N-heptane.

BASELINE POINT CONSIDERATIONS

Control of an Initial Temperature for a Fixed CA50

EGR has a strong effect on autoignition retard under the condition of constant initial temperature (T_0) and naturally aspirated operation, as shown in Fig. 5a. The 50% burn point (CA50) becomes more retarded with an increase of γ , finally a misfire happens at $\gamma=0.5$. The retarding effect of EGR occurs mainly by means of a higher C_v of CO_2 and H_2O in EGR. CO_2 and H_2O stand out with C_v that are roughly 80% and 50% higher than that of air. For a higher C_v , more compression work is required to raise the charge temperature a certain amount. In addition, because of lower compression pressures caused by lower gas temperatures, the total piston-compression work tends to decrease slightly when C_v increases. The net result of the higher C_v and the slightly lower compression work is a significant reduction of the compressed-gas temperature, and retard the autoignition. Besides the effect of higher C_v , EGR reduces the oxygen

concentration $[\text{O}_2]$ of air, thus also retarding the autoignition. Moreover, a combination of higher C_v and $[\text{O}_2]$ reduction effects of EGR affects other operating parameters such as combustion phasing, which can in turn influence the autoignition independently from any effect of the EGR gases themselves. For the sake of keeping as many operating parameters as possible constant, this study decides to maintain the CA50 at 5°CA aTDC for all data sets by controlling T_0 . Figure 5b presents an example of cylinder pressure traces held at CA50=5°CA aTDC by increasing T_0 for all γ of Fig. 5a, and significant combustion-phasing retard effects on the cylinder pressure could be observed. Boost pressure operation with lower γ can lead to overly advanced combustion phasing, thus reducing the T_0 for CA50 at 5°CA aTDC.

Autoignition Characteristics of Test Fuels

As outlined above, this study computationally investigates the combined effects of EGR and boost pressure on HCCI autoignition for iso-octane, PRF50 and n-heptane using the single-zone model of CHEMKIN. For each fuel, it is important to understand the differences of autoignition

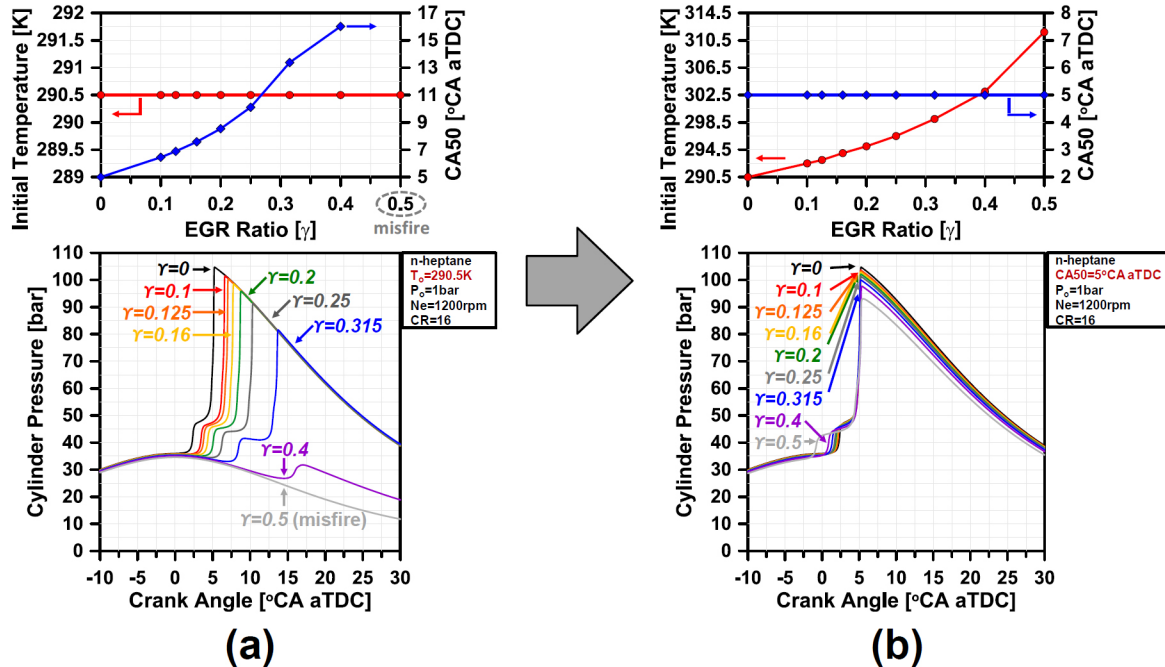


Figure 5. Intake temperature, T_0 and CA50 as a function of EGR ratio with cylinder pressure corresponding to each EGR ratio. N-heptane. (a) EGR addition without T_0 control. (b) EGR addition with T_0 control for $CA50=5°CA aTDC$.

characteristics between fuels at each baseline point ($CA50=5°CA aTDC$, $P_0=1bar$, $\gamma=0$). Figure 6 shows the cylinder temperature (Top), HRR (Middle) and an expanded scale of HRR (Bottom) for iso-octane, PRF50 and n-heptane when CA50 is set at $5°CA aTDC$. As can be seen, iso-octane exhibits single-stage ignition at this operating condition. This requires high T_0 of 418.8K to position CA50 at $5°CA aTDC$, and results in the highest peak temperature and HRR. On the other hand, PRF50 and n-heptane exhibit two-stage ignition with low temperature heat release (LTHR) for this operating condition, as shown in expanded scale of HRR. The presence of strong LTHR accelerates the temperature rise and makes n-heptane undergo high-temperature heat release (HTHR) at about the same crank angle as iso-octane, despite a much lower T_0 of 290.5K. The n-heptane exhibits more, but retarded LTHR than that of PRF50. It may seem that substantial amount of LTHR of n-heptane requires low T_0 for CA50, and the reduced T_0 leads to retarded LTHR timing and short burn duration, as shown in Fig. 7. Furthermore, Fig. 7 shows that n-heptane exhibits the highest IMEP and iso-octane the lowest. This happens because the LTHR significantly reduces the required T_0 for CA50, which inducts more air and fuel for an given P_0 , and finally this helps to increase the IMEP under constraints of low pressure-rise rate (PRR).

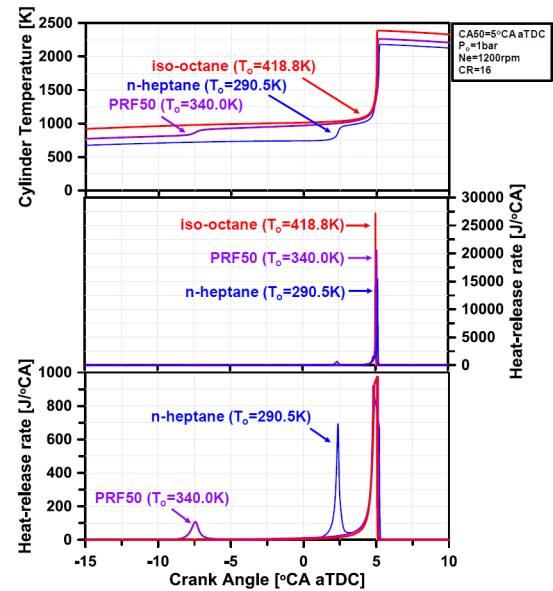


Figure 6. Comparison of the cylinder temperature and HRR for iso-octane, PRF50, and n-heptane. $CA50=5°CA aTDC$. $\phi_0=0.5$. $\gamma=0$.

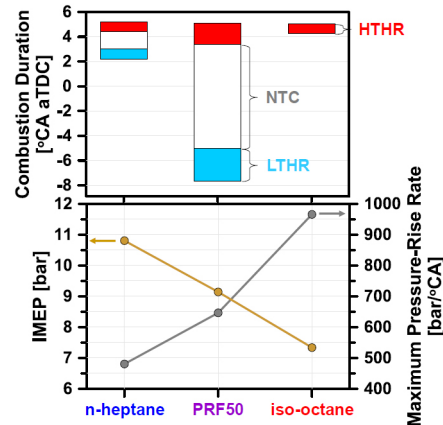


Figure 7. Comparison of the combustion duration, IMEP and maximum pressure-rise rate. $\phi_o=0.5$. $\gamma=0$. $CA_{50}=5^\circ CA$ aTDC.

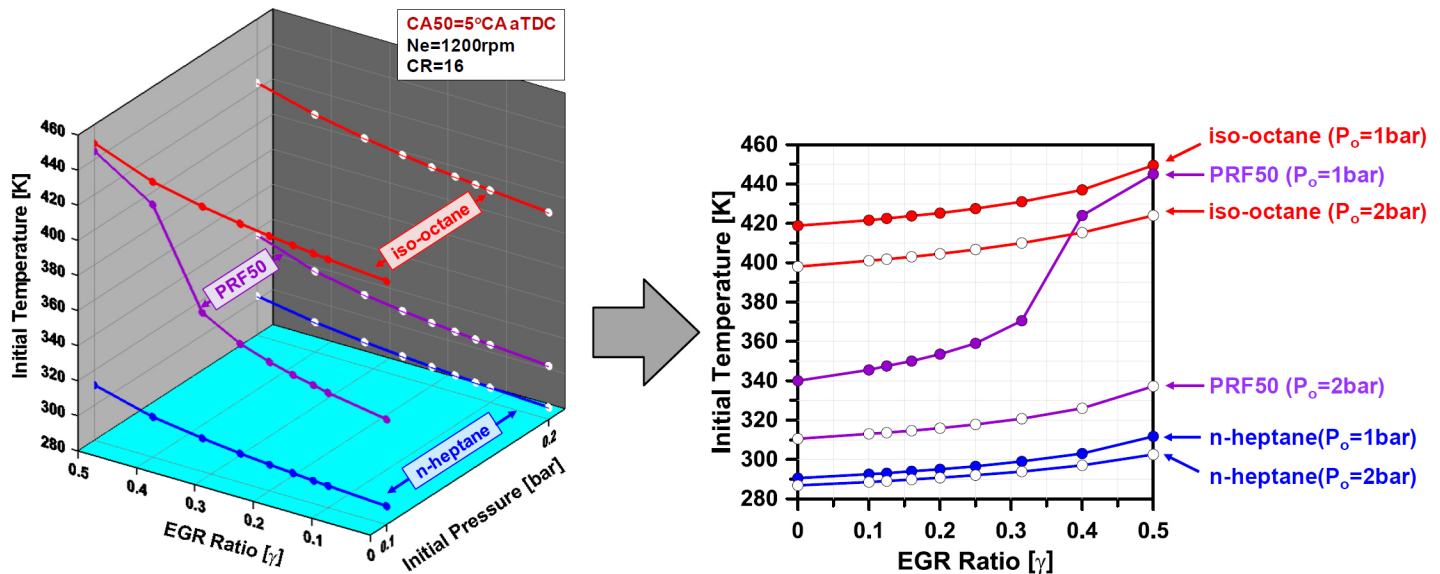


Figure 8. All data sets acquired at $CA_{50}=5^\circ CA$ aTDC for iso-octane, PRF50 and n-heptane.

RESULTS

Figure 8 shows all data sets acquired for iso-octane (red line), PRF50 (purple line) and n-heptane (blue line) at $CA_{50}=5^\circ CA$ aTDC. All data sets presented below were established by single-zone model calculations at 1200rpm. The initial equivalence ratio (ϕ_o) of all fuels is 0.5 for $\gamma=0$. (i.e. only air dilution). The initial pressure (P_o) was set to 1bar to simulate naturally aspirated operation, and 2bar for boost pressure operation. For all calculations, CA_{50} was maintained at $5^\circ CA$ aTDC by adjusting initial temperature (T_o) as EGR level and initial pressure were changed. As discussed above, controlling CA_{50} is important since excessive retarded CA_{50} by EGR addition can lead to misfire, and overly advanced CA_{50} by boost pressure increases PRR and knock. Maintaining a constant CA_{50} reduces the number of variables and allows cause-and-effect

relationships to be clearly identified. To facilitate comparison, the data sets in a 3-dimensional graph (left) are replotted on a 2-dimensional graph (right). As can be seen, iso-octane requires relatively high T_o for both conditions of $P_o=1$ bar and 2bar while boost pressure makes T_o drop on the order of 20K. It is noteworthy that the sensitivity of required T_o to EGR addition is similar to both conditions of $P_o=1$ bar and 2bar. On the other hand, n-heptane is so reactive enough to produce LTHR at the highest γ , and it can drop required T_o for CA_{50} well below ambient, which is clearly impractical. N-heptane also shows the similar sensitivity of required T_o to EGR addition for both conditions of $P_o=1$ bar and 2bar, but boost pressure effect is relatively weak on required T_o compared to iso-octane and PRF50. It should be noted that for operation with $P_o=1$ bar of PRF50, significantly larger changes of T_o is required to achieve a certain CA_{50} ,