

The Effects of Charge Preparation, Fuel Stratification, and Premixed Fuel Chemistry on Reactivity Controlled Compression Ignition (RCCI) Combustion

Dan DelVescovo
 Oakland University

Sage Kokjohn and Rolf Reitz
 University of Wisconsin

ABSTRACT

Engine experiments were conducted on a heavy-duty single-cylinder engine to explore the effects of charge preparation, fuel stratification, and premixed fuel chemistry on the performance and emissions of Reactivity Controlled Compression Ignition (RCCI) combustion. The experiments were conducted at a fixed total fuel energy and engine speed, and charge preparation was varied by adjusting the global equivalence ratio between 0.28 and 0.35 at intake temperatures of 40°C and 60°C. With a premixed injection of isooctane (PRF100), and a single direct-injection of n-heptane (PRF0), fuel stratification was varied with start of injection (SOI) timing. Combustion phasing advanced as SOI was retarded between -140° and -35°, then retarded as injection timing was further retarded, indicating a potential shift in combustion regime. Peak gross efficiency was achieved between -60° and -45° SOI, and NO_x emissions increased as SOI was retarded beyond -40°, peaking around -25° SOI. Optimal cases in terms of both gross efficiency and peak pressure rise rate (PPRR) were in the mid-range SOI timings centered about -50° SOI, while late SOI resulted in decreased gross efficiency, decreased combustion efficiency, and high NO_x.

To assess the effect of the premixed fuel chemistry on RCCI combustion, a representative reformed fuel referred to as syngas (50% H₂, 50% CO by volume), and methane were substituted for PRF100. A reference baseline PRF condition with an SOI timing of -50° at T_{in} = 40°C and $\phi = 0.30$ was used for comparison purposes. Matching combustion phasing to the baseline case by adjusting the premixed percent or SOI timing resulted in reduced gross efficiency (η_g) and increased NO_x emissions for both the syngas and methane cases. Matching the bulk heat release rate (HRR) characteristics by fixing the DI SOI quantity and duration and adding a premixed injection of n-heptane was able to regain most of the lost efficiency while decreasing NO_x emissions close to the baseline level.

CITATION: DelVescovo, D., Kokjohn, S., and Reitz, R., "The Effects of Charge Preparation, Fuel Stratification, and Premixed Fuel Chemistry on Reactivity Controlled Compression Ignition (RCCI) Combustion," *SAE Int. J. Engines* 10(4):2017, doi:10.4271/2017-01-0773.

INTRODUCTION

In an effort to avoid the pollutant emissions associated with conventional diesel and spark ignited (SI) engines [1], researchers have turned towards low temperature combustion (LTC) strategies, such as homogenous charge compression ignition (HCCI) [2, 3, 4], and reactivity controlled compression ignition (RCCI) [5, 6, 7]. These strategies reduce peak cylinder temperatures and operate locally lean to avoid forming oxides of nitrogen (NO_x) and particulate matter (PM), respectively.

Low temperature combustion strategies have demonstrated high thermal efficiency [8] with low NO_x and PM emissions [5,9]. The RCCI strategy, which involves the port injection of a low reactivity fuel such as gasoline, ethanol, or natural gas, and a direct injection of a high reactivity fuel, such as diesel, has demonstrated excellent control over the heat release event due to the introduction of in-cylinder stratification of equivalence ratio and reactivity. This stratification provides excellent control of the combustion phasing

(defined by CA50), and combustion duration (defined by CA10-90), but care must be taken to avoid overly stratified mixtures [10], which are prone to excessive NO_x and PM emissions [11]. In order to better understand the role of this stratification on the RCCI heat release, and the effects of intake conditions such as temperature and equivalence ratio, the following experimental study initially seeks to assess the role of injection timing on the performance and emissions of a representative low-load RCCI condition with primary reference fuels (PRF) isooctane (PRF100) and n-heptane (PRF0).

While researchers have shown that high octane fuels such as ethanol, and methane are capable of extending the high load limit of RCCI [7, 12, 13, 14, 15, 16], DelVescovo et al. [11] showed that at mid load in RCCI combustion, without adjusting the direct injection strategy for the specific fuel combination, matching combustion phasing resulted in decreased efficiency and increased emissions for high octane fuels (in this case isobutanol). The authors suggest that the direct injection strategy should be tailored for the specific fuel

combination to maximize performance and minimize emissions [11]. Simulations showed that the high DI fueling requirements of the less reactive premixed fuel (isobutanol compared to gasoline) resulted in locally rich regions in the cylinder, thereby causing high local temperatures near the piston, increased heat transfer, and high NO_x emissions [11]. This previous work served as the motivation for the experimental work discussed in the final two sections in which premixed isooctane was replaced with premixed syngas and methane respectively. This work seeks to determine an appropriate method by which to compare fuels with vastly different physical and chemical properties at a given operating condition.

EXPERIMENTAL SETUP

The engine experiments presented in the following sections utilized a heavy-duty 2.44L displacement Caterpillar 3401 Single Cylinder Oil Test Engine (SCOTE). The engine is a single-cylinder variant of the commercially produced Caterpillar 3406E six-cylinder diesel engine, rated at 62kW (83hp) at 1800rev/min. The specific engine geometry can be seen in Table 1. A representation of the piston bowl geometry at top dead center (TDC) used in the experimental work presented here is shown in Figure 1.

Table 1. Stock 3401E SCOTE engine geometry

Displacement	2.44L
Bore x Stroke	13.72 x 16.51cm
Connecting Rod Length	21.16cm
Swirl Ratio	0.7
Number of Valves	4
Intake Valve Opening (IVO)	335°CA ATDC Firing
Intake Valve Closing (IVC)	-143°CA ATDC Firing
Exhaust Valve Opening (EVO)	130°CA ATDC Firing
Exhaust Valve Closing (EVC)	-355°CA ATDC Firing
Compression Ratio (-)	16.1:1
Piston Bowl Type	Stock

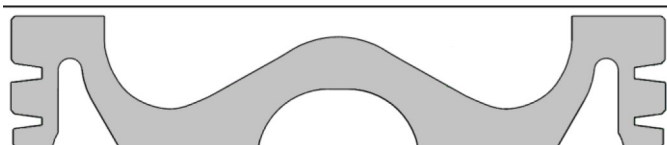


Figure 1. Stock SCOTE 3401E piston profile ($r_c=16.1:1$). Horizontal black line indicates location of fire deck at TDC

Laboratory Setup and Hardware

Compressed building air was introduced into a choked flow orifice rack, which allowed for the metering of the air mass flowrate by controlling the upstream pressure. The air was then heated to the desired temperature using two 4.5kW immersion style air heaters and introduced into the intake surge tank. Intake and exhaust surge tanks were used to provide stable steady-state measurement points for temperature, pressure, and emissions, and the relationship between the exhaust and intake pressure was used to simulate a turbocharger using the relationship for turbocharger efficiency outlined in Wissink et al. [18]. More details regarding the engine geometry and laboratory setup can be found in [5,9].

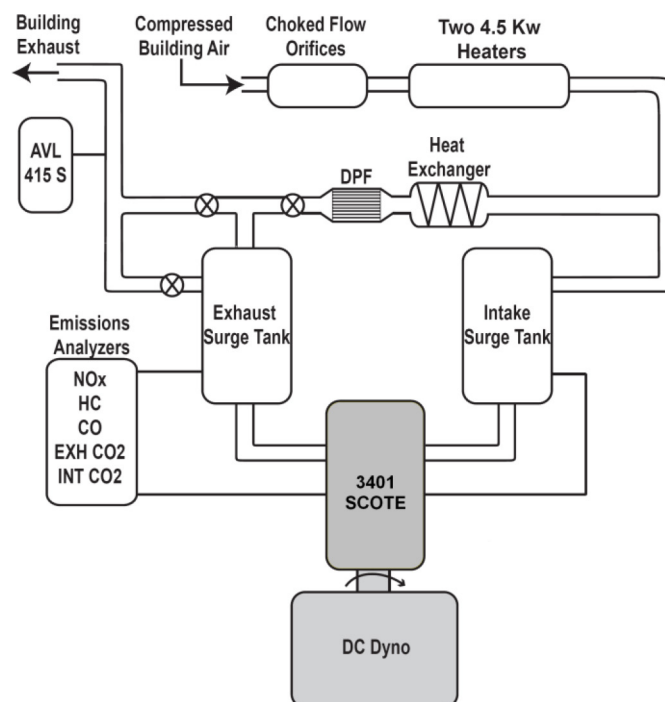


Figure 2. Caterpillar 3401 SCOTE Laboratory Setup

Fuels and Fuel Delivery

The laboratory is equipped with two independent liquid fuel systems each capable of supplying low pressure fuel to a port fuel injector (PFI) or high pressure fuel to a direct injector (DI), and a single gaseous fuel system capable of supplying low to intermediate pressures to a set of two gaseous port fuel injectors. The experiments conducted in this work utilized a stock 3401E SCOTE cylinder head that was modified to accept a Bosch CRI2 common rail injector with a 7 hole, 141 μm injector tip attached in place of the 315B HEUI injector. A detailed discussion of the design of the insert can be found in Splitter [19].

Important chemical and physical properties of the fuels tested in this work can be seen in Table 2. The experiments shown in the following sections included the addition of a lubricity improver (Infineum R655) to the direct injected n-heptane due to the fuel's low lubricity relative to the diesel fuel that the high pressure common rail injection system was designed for. The additive was splash blended to 100 ppm by volume in the fuel tank.

Table 2. Relevant Fuel Physical and Chemical Properties

Fuel	iso-Octane	n-Heptane	Methane	Syngas
Formula	C_8H_{18}	C_7H_{16}	CH_4	$0.5\text{H}_2 + 0.5\text{CO}$
MW [g/mol]	114.23	100.21	16.04	15.013
H/C Ratio	2.25	2.286	4	2
O/C Ratio	0	0	0	0.5
ρ [kg/m ³]	692	684	~0.7	~1.0
RON [-]	100	0	~120	N/A
MON [-]	100	0	~120	N/A
LHV [MJ/kg]	44.33	44.66	50.009	17.48

Data Analysis

Data analysis, post-processing of experimental data, and data visualization were all performed using custom MATLAB scripts. Low-speed instrument (e.g. fuel mass flowmeters and emission analyzers) voltages were saved at a frequency of 2Hz over a 1 minute sample period, and then converted into measured values through calibration curves for each instrument. The low-speed data arrays were then fit to a normal distribution to determine statistical quantities such as the mean, standard deviation, and the “precision” 95% confidence interval. The mean value was then fed back to the calibration curve to determine the “accuracy” 95% confidence interval of the measurement. The “precision” and “accuracy” error measures were then used to determine the total uncertainty of the measurement by summing the two quantities in quadrature.

High speed data measurements such as in-cylinder pressure, and heat release rate calculations (which were performed using the correlation for the ratio of specific heats of the fuel-air mixture, γ presented in DeVescovo et al. [20]), which are functions of crank angle, were collected over 250 cycles and fit to normal distributions at each crank angle index from the crankshaft encoder, thus resulting in the calculation of an ensembled mean, standard deviation, and 95% confidence interval as a function of crank angle.

Uncertainties were propagated through calculated quantities involving multiple measured values such as combustion efficiency, emissions indices, or trapped mass of the functional form $f = f(x,y,z,\dots)$ according to Equation (1).

Partial derivatives were calculated with MATLAB's Symbolic Math Toolbox™. This was accomplished by first representing each equation symbolically, then calculating the necessary partial derivatives for each independent variable at the specific mean value, next evaluating the symbolic expressions, and finally carrying out the uncertainty propagation as expressed in Equation (1). Thus, each calculated quantity has an associated uncertainty value which is defined as the 95% confidence interval through this work, unless otherwise indicated. This calculated confidence interval is represented on relevant plots by error bars above and below the mean value of the calculated or measured quantity. More details regarding the uncertainty propagation methodology can be found in DeVescovo [21].

$$\epsilon_f = \sqrt{\left(\frac{\partial f}{\partial x}\right)^2 \epsilon_x^2 + \left(\frac{\partial f}{\partial y}\right)^2 \epsilon_y^2 + \left(\frac{\partial f}{\partial z}\right)^2 \epsilon_z^2 + \dots} \quad (1)$$

RESULTS

RCCI Experiments with iso-Octane/n-Heptane (ϕ Study)

In order to assess the performance and emissions of RCCI combustion with primary reference fuels, which are commonly used chemical surrogates for gasoline and diesel [5,22], the first set

of experiments presented here examined the effect of start of injection (SOI) timing and global equivalence ratio (ϕ) for a fixed premixed mass fraction (PRE%) of isooctane ($\approx$ PRF). The relevant operating conditions of the first set of experiments are summarized in Table 3. Despite recent RCCI work, including [5,19], which demonstrated improved efficiency and emissions from a double direct-injection strategy, a single injection strategy was utilized in this work in order to limit the number of variables in the experimental operating space.

Table 3. Nominal Operating Conditions for constant PRF SOI sweeps

Engine speed [rev/min]	1300
Fuel Energy, (Q_{fuel}) [J/cyc]	2590 (± 20)
Nominal Load (IMEP _n) [bar]	4.5-4.75
EGR [%]	0
Intake Temperature [°C]	40 (± 2.2)
PFI Fuel	iso-octane (PRF100)
PFI Timing [°CA ATDC]	-320
PFI Pressure [bar]	2.5
DI Fuel	n-heptane (PRF0)
DI Timing, (SOI) [°CA ATDC]	Swept
Rail Pressure [bar]	500
Global PRF [-]	88.1 (± 0.2)

The three intake conditions tested in the first set of RCCI experiments are summarized in Table 4. The fixed fuel energy condition required the adjustment of intake pressure to adjust the global equivalence ratio, (i.e., higher intake pressures were required to achieve leaner global equivalence ratios), which has implications in terms of interpreting the trends of the data since pressure and equivalence ratio are coupled.

Table 4. Intake conditions for constant PRF SOI sweeps

Intake Condition	1	2	3
Intake Pressure [kPa]	100.0 (± 0.7)	114.5 (± 0.7)	122.0 (± 0.7)
Exhaust Pressure [kPa]	118.6 (± 2.8)	135.8 (± 2.8)	144.8 (± 2.8)
Equivalence Ratio, ϕ [-]	0.35 (± 0.01)	0.30 (± 0.01)	0.28 (± 0.01)

Selected performance metrics including CA50, gross efficiency, and NO_x emissions as a function of SOI timing for the three global equivalence ratios can be seen in Figure 3. Combustion phasing advanced as SOI was retarded between about -140° and -35° SOI; however as SOI timing was further retarded, combustion phasing also retarded, potentially indicating the transition from a kinetically controlled regime to a mixing controlled combustion regime. Another possible explanation is that as equivalence ratio is increased, the relative sensitivity of ignition delay to equivalence ratio is decreased, as discussed by Kokjohn et al. [10]. This decrease in ignition delay sensitivity implies that despite more fuel existing in locally very rich regions as the SOI is retarded as a result of decreased mixing time, the time between the injection and ignition events does not decrease significantly due to the relatively unchanged ignition delay. In effect, the time between injection and ignition is then fixed, thus implying retarding injection will retard combustion phasing. Similar trends in combustion phasing as a function of injection timing have been observed in previous studies with premixed gasoline, ethanol, and hydrogen [23,24], and methane [25].

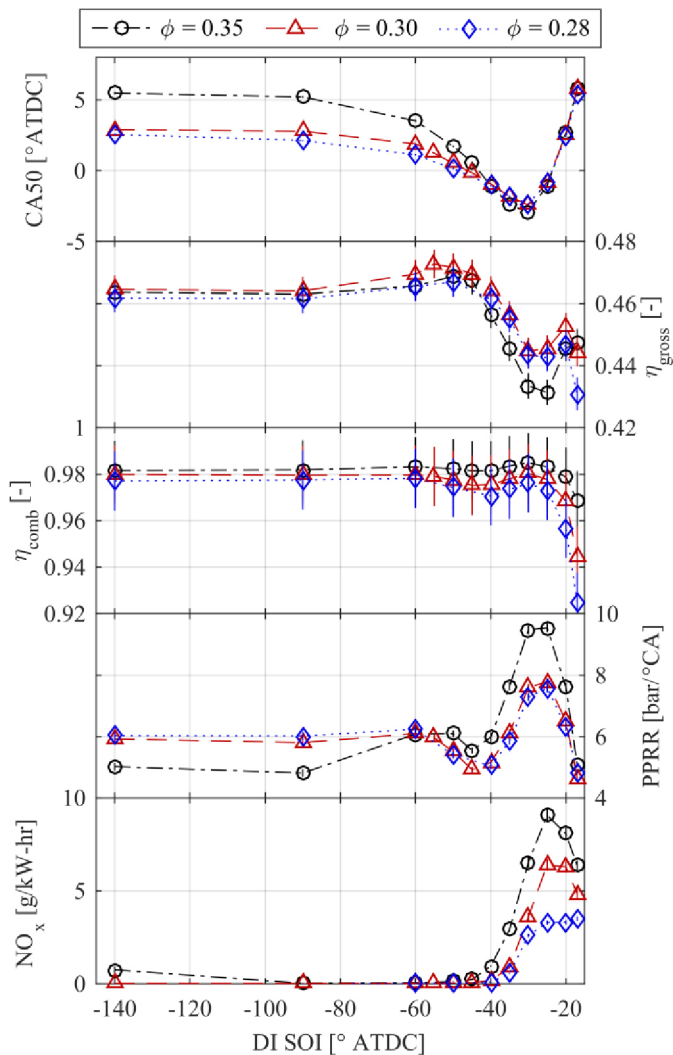


Figure 3. Selected performance and emissions metrics for PRF RCCI combustion as a function of SOI for three global equivalence ratios at $T_{in} = 40^\circ\text{C}$, and PRF88 including CA50 (top), gross efficiency (second), combustion efficiency (third), PPRR (forth), and NO_x emissions (bottom)

The combustion phasing advancement seen for decreased equivalence ratio was a function of the increased cylinder pressure required to increase air flowrate and decrease ϕ , as for a fixed inlet pressure condition, decreasing equivalence ratio would be expected to retard combustion phasing. The combustion phasing of the three global ϕ lines converged around an SOI of about -30° and follow the same path, indicating a decrease in the sensitivity of combustion phasing to the intake pressure (and ϕ), supporting the idea of a change in combustion regime. This decrease in combustion phasing sensitivity can be seen in the pressure and HRR traces shown in Figure 4 for an early SOI timing (-140°), which is sensitive to the intake pressure and ϕ , and a late SOI timing (-20°), which showed only minor sensitivity in the start of combustion to the intake pressure and ϕ .

Peak gross efficiency was achieved in the range of -60° and -45° SOI for all three global equivalence ratios; however, it is difficult to decouple the link between combustion phasing and gross efficiency from this test. The combustion efficiency was relatively constant around $\sim 98\%$ until combustion phasing retarded at late SOI timings, decreasing sharply, particularly for the leanest global case, $\phi = 0.28$.

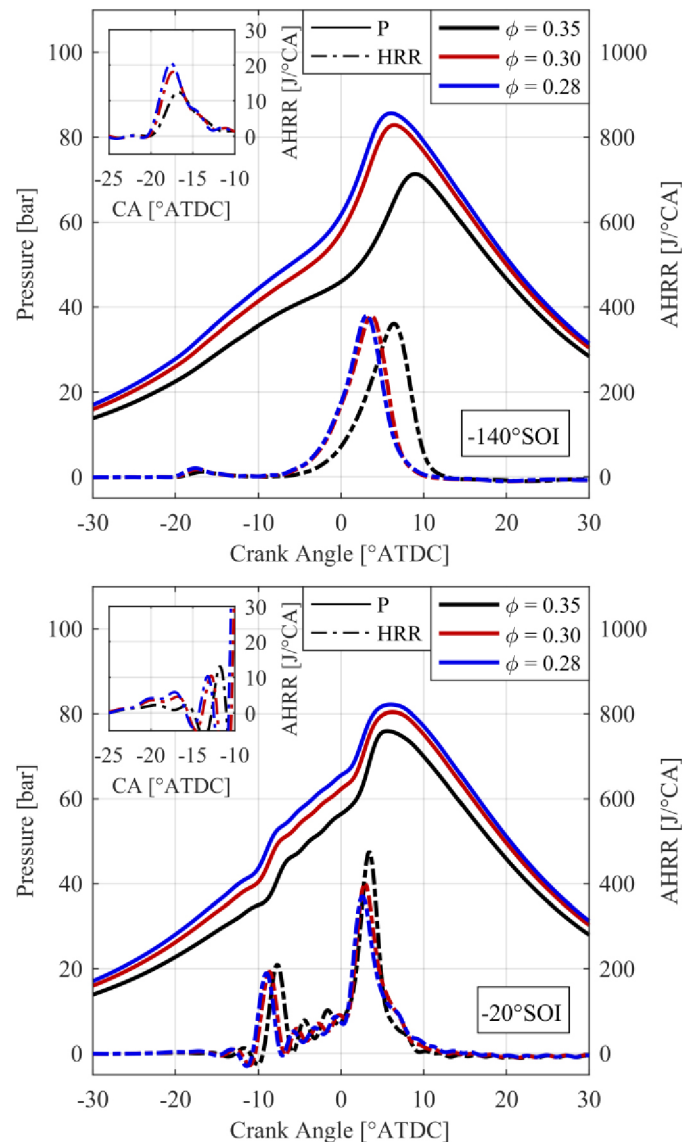


Figure 4. Pressure (solid) and AHRR (dash-dotted) for SOI of -140°ATDC (top) and -20°ATDC (bottom) for three global equivalence ratios at $T_{in} = 40^\circ\text{C}$, and PRF88.

At early SOI timings, peak pressure rise rate (PPRR) was highest for the leanest cases; however, this trend is reversed at late SOI timings. The early SOI timings exhibit higher PPRR for the lean cases due to the advanced combustion phasing caused by the increased pressure condition. At late SOI timings, when the combustion phasing does not depend on the equivalence ratio, the expected trend in PPRR (i.e., richer mixtures have higher PPRRs) is observed. NO_x emissions increased considerably as SOI was retarded beyond about -40° SOI likely due to regions of high local equivalence ratios resulting from decreased mixing time; and peaking around -25° SOI only to decrease again as combustion phasing retarded and peak cylinder temperatures decreased.

Figure 5 shows the pressure and heat release rate profiles for the early and late SOI cases. A fully premixed port injected HCCI case at the same intake conditions and PRF blend from DeVescovo et al. [20] is included for reference. For the early SOI timings, as the start of injection was retarded combustion phasing advanced and the duration of combustion increased. This is thought to be the result of increasing;

reactivity and equivalence ratio stratification in the cylinder. Due to the fixed fuel energy constraint, this increase in combustion duration also resulted in a decrease in the peak heat release rate as the area under the heat release rate corresponds to the total energy released, which is equal for all the cases assuming the same combustion efficiency [26,27]. For the late SOI timings, the opposite trend is seen in combustion phasing in relation to the injection timing, as retarding the injection timing retarded the combustion phasing. The combustion duration is largely unchanged by the injection timing for the late SOI timings, except in the case of the most retarded phasing, which is likely due to the expansion of the charge cause by the piston motion after TDC.

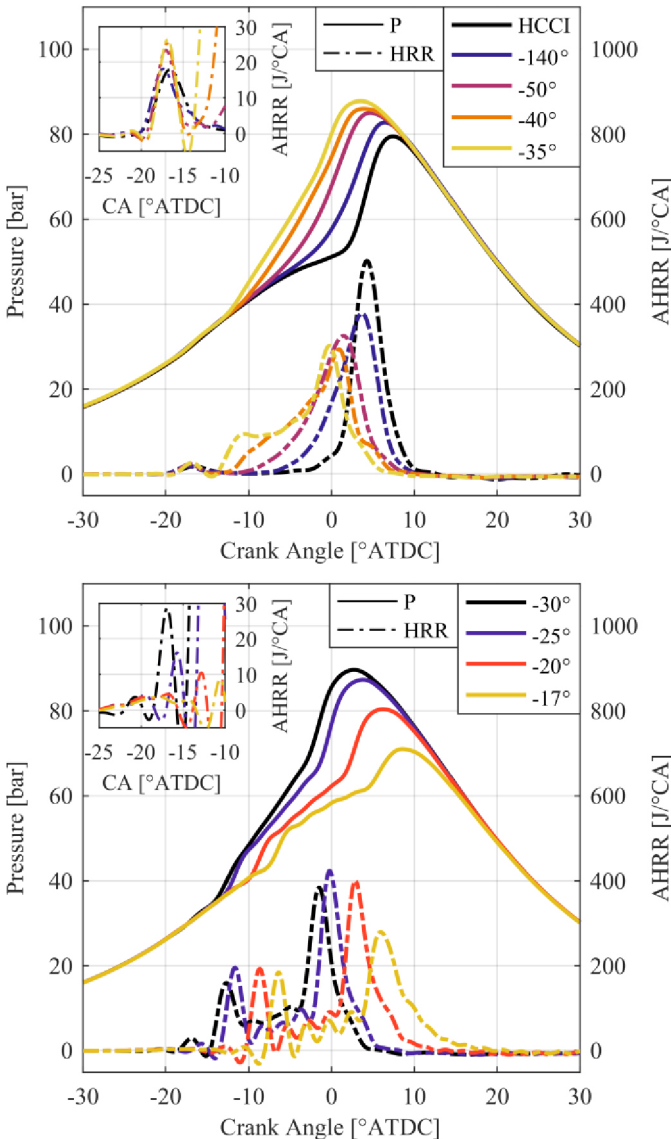


Figure 5. Pressure (solid) and AHRR (dash-dotted) for RCCI SOI sweep at $\phi = 0.30$, $T_m = 40^\circ\text{C}$ for a fixed global PRF of 88.1 ± 0.2 for early SOI timings including port fueled HCCI (top), and late SOI timings (bottom). Legend items denote SOI timing

In order to eliminate the influence of combustion phasing on the performance and emissions of the experimental results, a separate test was conducted where the combustion phasing was held constant at

the peak efficiency location from the previous data set ($\text{CA}_{50} \sim 0.75^\circ\text{CA}$) corresponding to the -50° SOI case. The injection timing was swept and the ratio of premixed to direct injected fuel (global PRF) was adjusted to match the combustion phasing. The operating conditions of this test are summarized in Table 5, and the intake conditions are listed in Table 6.

Figure 6 shows the performance and emissions metrics for the fixed CA_{50} sweeps as a function of SOI. Initially, as injection timing was retarded, the required PRF to achieve the desired combustion phasing was increased to counter the increased reactivity and equivalence ratio stratification. After -25° SOI, however, the required PRF decreased significantly as the combustion process became dominated by the vaporization and mixing processes. In order to match combustion phasing with a late injection, the reactivity of the global mixture had to increase significantly. The design of the experiment meant that this increase in reactivity could only be achieved by direct injecting more n-heptane, making the late phasing cases more reliant on the mixing process. Gross efficiency again peaked between -60° and -45° SOI, and the two equivalence ratios performed similarly across the entire SOI range for the metrics shown, though the differences in the intake conditions were minor. PPRR reached a minimum in the range of SOI timings where the highest gross efficiencies were observed (between -60° and -30°). The NO_x emissions increased as SOI was retarded beyond -35° due to high local ϕ 's.

Table 5. Nominal operating conditions for constant CA_{50} SOI sweeps

Engine speed [rev/min]	1300
Fuel Energy, (Q_{net}) [J/cyc]	2590 (± 20)
Nominal Load (IMEP _n) [bar]	4.3-4.75
EGR [%]	0
Intake Temperature [$^\circ\text{C}$]	40 (± 2.2)
PFI Fuel	iso-octane (PRF100)
PFI Timing [$^\circ\text{CA ATDC}$]	-320
PFI Pressure [bar]	2.5
DI Fuel	n-heptane (PRF0)
DI Timing, (SOI) [$^\circ\text{CA ATDC}$]	Swept
Rail Pressure [bar]	500
CA_{50} [$^\circ\text{CA ATDC}$]	0.75 (± 0.25)

Table 6. Intake conditions for constant CA_{50} SOI sweeps

Intake Condition	1	2
Intake Pressure [kPa]	114.5 (± 0.7)	122.0 (± 0.7)
Exhaust Pressure [kPa]	135.8 (± 2.8)	144.8 (± 2.8)
Equivalence Ratio, ϕ [-]	0.30 (± 0.01)	0.28 (± 0.01)

Figure 7 shows the early SOI and late SOI pressure and HRR profiles for the fixed CA_{50} cases. As SOI is retarded in the early injection timing cases, the PRF required to match combustion phasing increases, and the combustion duration increases due to the greater induced stratification. The peak heat release rate thereby decreases for the reasons discussed previously. For the late SOI cases with fixed CA_{50} , delaying the SOI beyond -25° delayed the onset of the first stage combustion, indicated by the first peak in HRR, by an approximately equal amount. The second stage combustion, indicated by the second large peak in HRR, occurred at nearly identical timing regardless of SOI. This differs from the