

Title: Exploring the effects of piston bowl geometry and injector included angle on dual-fuel and single-fuel RCCI

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Abstract

Reactivity Control Compression Ignition (RCCI) is a Low-Temperature Combustion (LTC) technique that have been proposed to meet the current demand for high thermal efficiency and low engine-out emissions. However, its requirement of two separate fuel systems (i.e., a low-reactivity fuel system and a high-reactivity fuel system) has been one of its major challenges in the last decade. This leads to the single-fuel RCCI concept, where the secondary fuel is generated from the primary fuel through CPOX reformation. After studying three different fuels, diesel was found to be the best candidate for the reformation process, where the reformed gaseous fuel (with lower reactivity) was used as the secondary fuel and the parent diesel fuel (with higher reactivity) was used as the primary fuel. In-depth analysis of the reformat fuel and its benefits as the low-reactivity fuel with diesel were studied previously by the authors. Additionally, the effects of the start of injection (SOI) timing of diesel and the energy-based blend ratio were also studied in detail. In this study, the effect of piston profile and the injector included angles were experimentally studied using both conventional fuel pairs (gasoline – diesel and natural gas – diesel) and reformat RCCI.

A validated CFD model was also used for a better understanding of the experimental trends. Comparing a re-entrant bowl piston with a shallow bowl piston at a constant compression ratio and SOI, the latter showed better thermal efficiency, regardless of the fuel combination, due to its 10% lower surface area for the heat transfer. Comparing the 150-degree included angle and 60-degree included angle on the shallow bowl piston, the latter showed better combustion efficiency, regardless of the fuel combination, due to its earlier combustion phasing (at constant SOI timing). The effect was particularly prominent on reformat RCCI because of its incredibly high diluent concentration, which retards the combustion further for the 150-degree injector. Later, using CONVERGE CFD, seven different injector included angles were studied at a constant SOI. With the change in injector included angle, the region of the cylinder targeted

by the fuel spray varies significantly, and it was found to have a significant impact on the combustion efficiency and the engine-out emissions.

Introduction

Low-temperature combustion, or advanced compression ignition combustion, shows promising results in achieving high thermal efficiencies with ultra-low emissions. Homogeneous charge compression ignition (HCCI) is one of the first LTC modes, where a lean mixture of fuel and air is premixed and inducted into the combustion chamber and combustion is achieved via autoignition [1 – 4]. HCCI exhibits the above-mentioned benefits; however, there are associated tradeoffs, such as low combustion controllability and restricted operable load range.

To overcome these shortcomings, researchers have created second generation LTC strategies such as premixed charge compression ignition (PCCI), gasoline compression ignition (GCI), partial fuel stratification (PFS), and thermally stratified compression ignition (TSCI). In TSCI, the latent heat of vaporization of a liquid that is direct-injected during the compression stroke is used to amplify the level of thermal stratification in the combustion chamber. TSCI can be enabled by using either a non-combustible liquid, such as water [5, 6], or a fuel with a high latent heat of vaporization and low ϕ -sensitivity, such as ethanol [7 – 9]. The enhanced thermal stratification elongates the combustion process, providing control over the heat release process to increase the operable load range. In other combustion modes, equivalence ratio stratification is induced either by adjusting the injection timing of the fuel (e.g., in PCCI [10, 11] or GCI [12, 13]) or by using multiple injections of fuel in a split injection strategy (PFS) [14, 15]. Using ϕ -sensitive fuels, the heat release process can be elongated by the equivalence ratio stratification, providing controllability over combustion. All of these combustion processes use a single fuel. To provide better controllability, researchers also proposed the use of two different fuel with a reactivity separation between them, called reactivity-controlled compression ignition (RCCI) [16 – 18].

In RCCI, a low-reactivity fuel, such as gasoline, natural gas, ethanol, or others, is premixed with air while a high reactivity fuel, such as diesel, dimethyl ether (DME), or others, is direct-injected into the cylinder during the compression stroke. The injection timing of the high reactivity fuel is early enough to avoid mixing-controlled combustion. By adjusting the blend ratio (i.e., the ratio of the low-reactivity fuel to the total fuel in the cylinder) and the start of injection timing of the high reactivity fuel, the combustion process can be controlled effectively [19, 20]. Since it is the reactivity gradient in the cylinder that drives

the combustion process, researchers have studied various alternative fuels, such as ethanol, DME, etc. [21 – 24] to determine whether these alternative fuels could provide benefits over conventional fuels (i.e., gasoline and diesel). The main shortcoming of RCCI is the requirement of the secondary fuel and injection system. To overcome this, *single-fuel RCCI* has been proposed and studied by various researchers, as discussed below.

Single-fuel RCCI was first approached by using a cetane improver to modify the reactivity of the low-reactivity fuel to produce the high-reactivity fuel. Gasoline was doped with either di-tert butyl peroxide (DTBP) [25, 26] or 2-ethylhexyl nitrate (2-EHN) [27 – 29] (two commonly used cetane improvers) to increase its reactivity. The doped gasoline served as the direct-injected high-reactivity fuel while the undoped gasoline remained as the premixed, low-reactivity fuel. Although this approach was promising, the consumption of DTBP was found to be too high, i.e., a DTBP tank would need to be refilled more frequently than the oil change intervals. This left 2-EHN, a more effective cetane improver, as the primary candidate to enable single-fuel RCCI with cetane improvers. Although it provided acceptable cetane improver consumption rates, the higher decomposition tendency of 2-EHN at higher temperatures and the increase in NO_x emissions from the fuel-bound nitrogen group of 2-EHN were drawbacks. Additionally, this approach still uses two fluids that require refilling, rather than a single fuel. A new, truly single-fuel approach was proposed to address these drawbacks where a fraction of fuel is reformed through an onboard fuel reformer to produce a second fuel whose reactivity is distinct from the parent fuel such that RCCI combustion can be enabled from a single parent fuel [30].

The reformat fuel mixture produced by the onboard fuel reformer is a mixture of completely oxidized products, unreacted fuel, and partially oxidized products, mainly consisting of a mixture of diatomic hydrogen (H₂) and carbon monoxide (CO), sometimes called syngas. The fuel being reformed is referred to as the *parent fuel*, while the fuel resulting from the reformation process is typically referred to as *reformat*. The external reforming process is primarily categorized into three types: steam reforming or steam methane reforming (SMR), catalytic partial oxidation (CPOX), and Autothermal reforming (ATR). In a previous study, gasoline, diesel, and natural gas were externally reformed through a CPOX reformation process at various equivalence ratios and pressures. The autoignition characteristics of the reformat mixtures were studied in HCCI combustion, with their effective octane ratings determined with the help of a primary reference fuel (PRF) mapping at similar operating conditions. From this study, it

was found that the diesel reformates were the best candidate to enable single-fuel RCCI, because of the significant reactivity separation between the reformat fuel and the parent fuel [31].

Single-fuel RCCI, enabled by employing CPOX reformation with diesel as the parent fuel, was demonstrated in previous studies by the authors [32, 33]. In these previous studies, the combustion characteristics of reformat-diesel RCCI were studied and compared with that of conventional dual-fuel RCCI (gasoline-diesel RCCI and natural gas-diesel RCCI). Following that, the effects of the start of injection timing of the diesel fuel and the effects of blend ratio on the combustion and emissions characteristics of reformat-diesel RCCI were studied. Both of these studies were conducted with a diesel-style re-entrant bowl piston and with an injector whose included angle is 150° .

In the past, researchers have studied the influence of piston bowl profile on various combustion modes. In the conventional combustion modes, the influence of the piston bowl geometry on the emissions and heat transfer losses have been studied extensively [34 – 38]. Additionally, similar studies were conducted in advanced low-temperature combustion modes such as PPC [39] and RCCI [40 – 42]. Splitter et al. experimentally studied the effects of the nominal depth of the piston bowl on thermal efficiency to minimize heat transfer losses and THC emissions by reducing the squish volume [43]. Dempsey et al. showed that at low loads, due to reduced heat transfer losses and better combustion efficiency, the shallow bowl piston shows significantly better combustion efficiency over a re-entrant bowl piston [44]. These studies inspired the authors to explore the advantages that could be realized by using a wide, shallow bowl piston when employing single-fuel reformat-diesel RCCI. In addition to the piston profile, the effect of injector included angle has also been extensively researched in various combustion modes and engine architectures, such as SIDI [45 – 47], two-stroke direct injection [48], conventional diesel engines [49, 50], and PFS [51]. In this study, both single-fuel reformat RCCI and the conventional dual-fuel RCCI were studied on a light-duty engine with two different piston bowl profiles, a) re-entrant bowl and b) shallow bowl and with two different injector included angles, a) 150° and b) 60° .

Experimental Setup

A production light-duty 1.7L four-cylinder GM engine head on a single-cylinder Ricardo Hydra research engine block was used for this study. Three of the production cylinders were deactivated. All other subsystems of the engine, including the intake and exhaust system, were custom-built by the authors'

research group. The schematic of the test cell is shown in Figure 1 and the engine parameters, including geometry specifications and valve timings, are shown in Table 1.

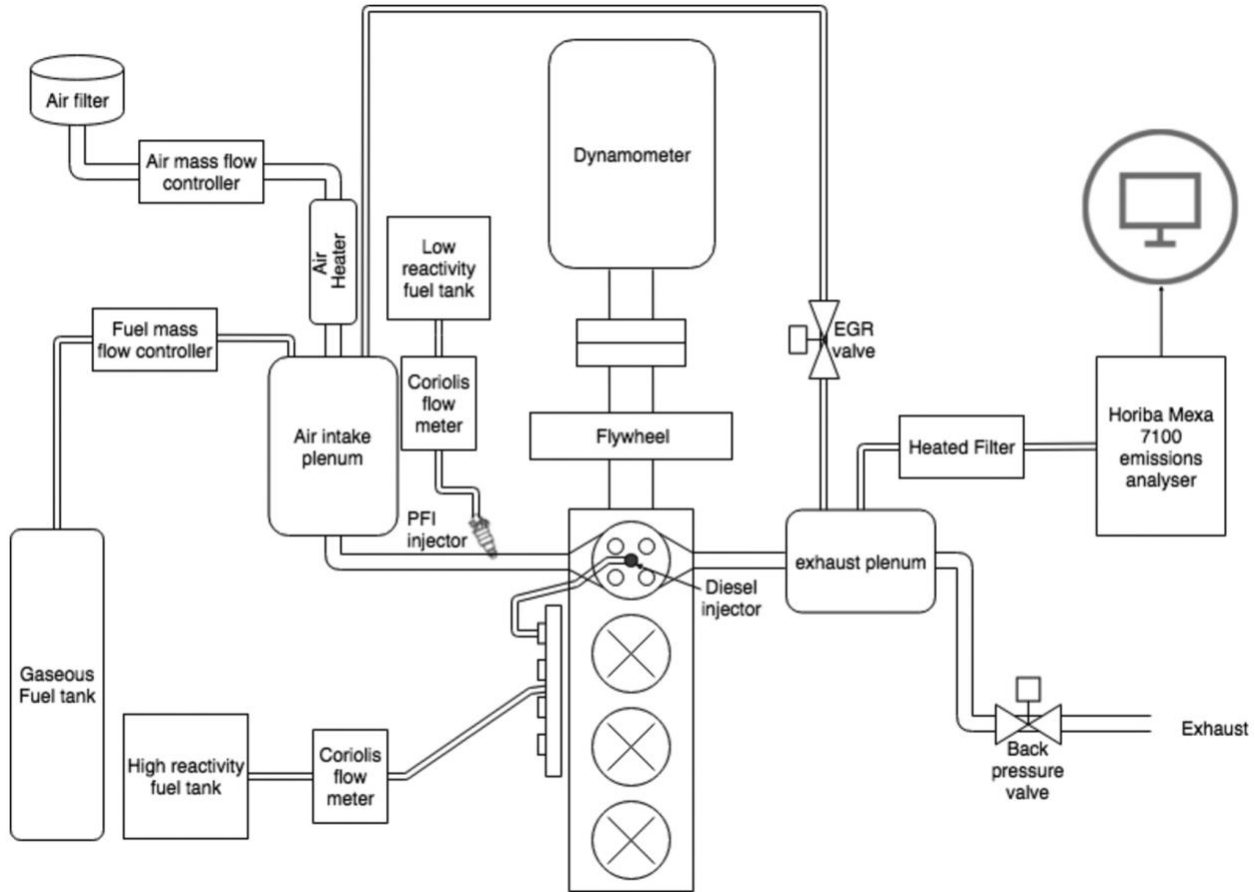


Figure 1: Test cell schematic

The engine intake system consists of a 5kW inline air heater used to maintain the intake air temperature constant, a large intake plenum to dampen the flow fluctuations caused by the gas exchange process, an Alicat intake air mass flow controller upstream of the intake heater and used to control and measure the airflow, a port fuel injector outfitted to the custom-built intake manifold, and a thermocouple and a high-speed piezoresistive pressure transducer to measure intake temperature and pressure, respectively. The exhaust system consists of an ECM LambdaCANp oxygen sensor in the exhaust manifold used to measure the oxygen fraction in the exhaust on a wet basis, an exhaust plenum, which mixes the exhaust gases prior to being sampled by a Horiba MEXA 7100 D-EGR, a gate valve downstream of the plenum to adjust and maintain constant exhaust backpressure, and a heated metal pipe with an electronically controlled valve that connects downstream of the exhaust plenum to the intake plenum to

enable exhaust gas recirculation (EGR). The Horiba MEXA 7100 D-EGR emissions bench passes exhaust gas through a heated filter and then measures O₂, CO₂, CO, THC, and NO_x emissions. A sample of gas from the intake plenum is also taken to calculate external EGR fraction by comparing the measured CO₂ concentration in the intake and exhaust.

Table 1: Engine specifications

Bore	79 mm
Stroke	86 mm
Connecting Rod Length	160 mm
Piston pin offset	0.6 mm
Compression ratio	15.5
Optical Shaft Encoder's Resolutions	0.1 Crank Angle Degrees (CAD)
Intake Valve Opening (IVO)	-366° deg aTDC
Intake Valve Closing (IVC)	-146° deg aTDC
Exhaust Valve Opening (EVO)	122° deg aTDC
Exhaust Valve Closing (EVC)	366° deg aTDC

The coolant and oil systems are maintained at a constant temperature of 353 K and 343 K, respectively. Both systems consist of an electric heater and a radiator which are controlled electronically by a PID controller to maintain a constant temperature. Similarly, the temperature of the intake air and external EGR are also controlled by a PID controller. The fuel system of this test cell is a custom-built fuel cart, which can supply two liquid fuels simultaneously, one for the PFI system and the other for the direct injection system. The fuel cart consists of two fuel tanks, low-pressure pumps, cooling fans, and MicroMotion Coriolis mass flow meters for both fuel systems. Gasoline and diesel were the two liquid fuels that were used in this study. The PFI system is pressurized and regulated to 35 psi using an axial pump and a pressure regulator. The DI system's low-pressure pump is used as a lift pump to supply a high-pressure Bosch CP3 pump. The high-pressure pump is used to supply diesel fuel at a constant fuel pressure of 700 bar to the production common rail. In addition to the two liquid fuels, the test cell is also

capable of testing gaseous fuels. Gaseous fuels are regulated using a gas regulator from the gas bottle and directed into the intake plenum through an electronically controlled Alicat mass flow controller. Natural gas and reformat fuels are the gaseous fuels that were tested during this study.

The two reformat fuels used in this study are diesel reformat-1 (DR1) and diesel reformat-2 (DR2). They were produced by a CPOX process of diesel fuel. Detailed information on how these reformat fuels were produced and why diesel was chosen over other conventional fuels is discussed in an earlier study [31]. The fuel properties of all the three gaseous fuels are tabulated in Table 2.

Table 2: Fuel properties

		DIESEL REFORMAT 1 (DR1)	DIESEL REFORMAT 2 (DR2)	NATURAL GAS (CNG)
MOLAR CONCENTRATION	Acetylene	0.048%	0.195%	-
	Carbon dioxide	11.090%	8.492%	0.706%
	Carbon monoxide	3.400%	8.251%	-
	Ethane	-	-	2.496%
	Ethylene	2.903%	3.445%	-
	Hydrogen	3.065%	5.605%	-
	Methane	1.346%	2.384%	94.986%
	Nitrogen	78.148%	71.628%	1.612%
	Propane	-	-	0.200%
H/C RATIO		1.1	1.3	3.9
LHV (MJ/KG)		2.3	3.8	47.6
EFFECTIVE OCTANE RATING (APPROX.)		105 [31]	102 [31]	140

A 30 hp DC active dynamometer is coupled to the engine and is controlled to maintain a constant engine speed of 1200 rpm. A Kistler encoder is coupled to the engine’s crankshaft, which measures the crank angle in increments of 0.1 crank angle degrees using a pulse multiplier. At each crank angle increment, the encoder triggers the high-speed pressure measurements in the engine subsystems: the cylinder pressure, common rail pressure, intake pressure, and exhaust pressure. All of the low-speed measurements, such as coolant pressure, oil pressure, fuel flow rate, airflow rate, and thermocouple

readings were measured at a frequency of 0.5 Hz. A custom-designed LabVIEW code is used to measure both the high-speed and low-speed data, as well as to control the temperatures of coolant, oil, intake charge, external EGR, mass flow, and the two fuel injection systems.

The two piston profiles that were studied are shown in Figure 2. Figure 2a shows the production GM piston with the re-entrant diesel bowl geometry, whereas Figure 2b shows the custom shallow bowl piston geometry that was designed based on the literature [43, 44] to reduce heat transfer losses through a more favorable surface-area-to-volume ratio and avoid having a large squish region. The dimensions of the shallow bowl were designed to have the same compression ratio as the re-entrant diesel bowl. Figure 3 shows the two different injector included angles, a) 150 degrees and b) 60 degrees, which were studied in the shallow bowl piston.

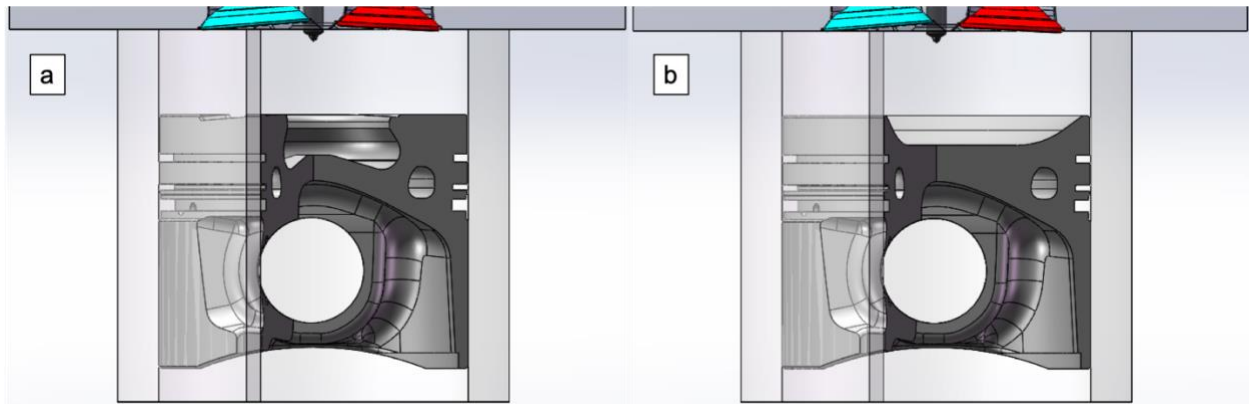


Figure 2: CAD models of the two different piston bowl profiles that were used in this study: a) re-entrant diesel bowl, and b) shallow bowl

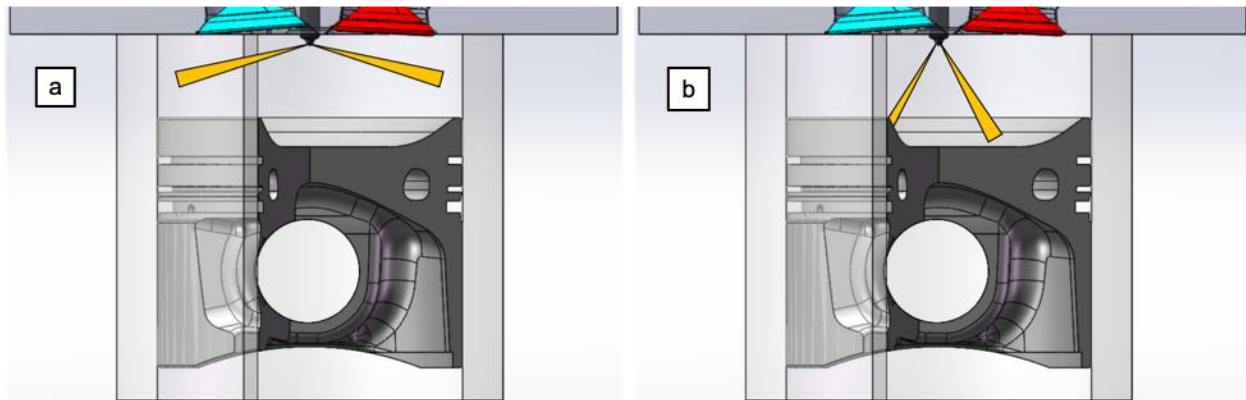


Figure 3: CAD models of the two injector included angles that were used in this study: a) 150 degrees, and b) 60 degrees

Results and Discussion

Before studying the effects of various piston geometries on reformat RCCI combustion, the engine was motored to ensure the cylinder pressure matches for both pistons. This comparison is necessary to exclude the influence of the compression ratio on the combustion characteristics. The cylinder pressure trace in Figure 4 shows that the compression ratio of both pistons was the same. Using these two pistons, three different low reactivity fuels were studied. Due to the vast reactivity differences between the fuels, the conditions required to enable healthy and stable combustion are different for each fuel. Therefore, comparisons across fuels will be difficult. However, the operating conditions for the same fuel across the different piston geometries were kept constant.

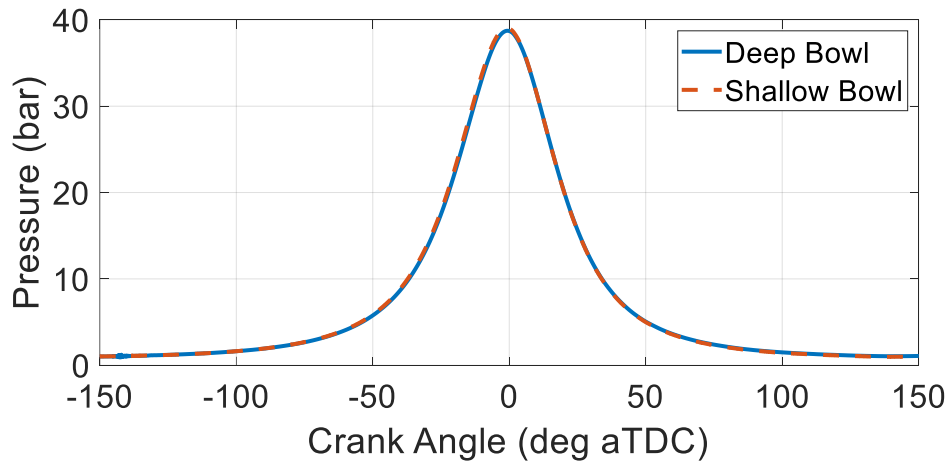


Figure 4: Comparison of the motoring cylinder pressure for the two different piston bowl profiles

1.1. Effect of piston bowl profile with the 150-degree injector

In RCCI combustion, the start of injection (SOI) timing of the high reactivity fuel has a significant effect on the combustion process, which has been studied in detail by various researchers in the past including the authors, who studied the effect of SOI timing on reformat-diesel RCCI [33]. By keeping the SOI constant, the amount of time for mixing of the high reactivity diesel fuel with the premixed low reactivity fuel and air before combustion was maintained constant. Therefore, comparing the combustion characteristics across both piston geometries can help illuminate the differences in the mixing processes of the pistons. Figure 5 shows the effect of two different piston bowl profiles on the cylinder pressure and gross heat release rate (GHRR) at constant SOI. The gross heat release rate is the sum of the net heat release rate (calculated from the measured cylinder pressure) and the heat transfer rate (calculated using the Chang heat transfer correlation [52]). The high reactivity fuel in all three cases is diesel and the low

reactivity fuels are a) gasoline, b) diesel reformat 1 (DR1), and c) diesel reformat 2 (DR2). Other combustion parameters including the input parameters for the experiments are presented in Table 3.

Input parameters in each data set with the same low reactivity fuel, such as blend ratio, intake temperature, intake pressure, and the start of injection of diesel, were kept constant for the two piston geometries. These parameters needed to change across the low-reactivity fuels since each fuel has drastically different autoignition tendencies. The blend ratio reported throughout the study is on an energy basis, which is the ratio of fuel energy input from the low-reactivity fuel to the overall fuel energy in the cylinder. The energy-based blend ratio is chosen due to the significant differences in the energy densities of the low-reactivity fuels used in this study. The mass of fuel for each data set with the same low reactivity fuel is adjusted to obtain a constant load. The load is defined as the gross indicated mean effective pressure (IMEPg). IMEPg is the ratio of gross work output to the displaced volume. From Figure 5, it can be seen that the effect of piston profile on the cylinder pressure and heat release rate is insignificant. This shows that the combustion phasing was not significantly affected by the piston bowl profile since the compression ratio was kept constant. The CA50 values in Table 3 confirm this observation. The main differences can be seen in Figure 6, where the effects of two different piston bowl profiles on the thermal efficiency and combustion efficiency are shown.

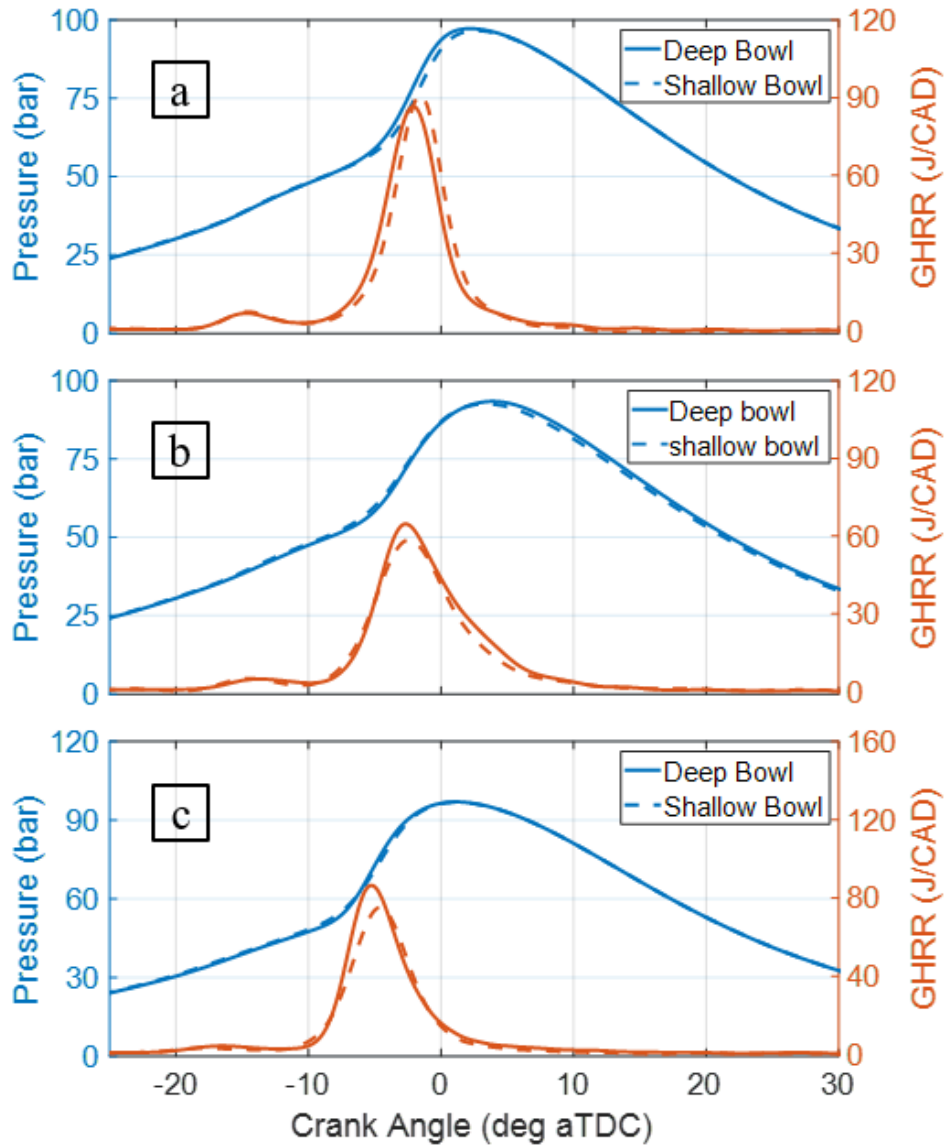


Figure 5: Effect of the two different piston profiles on the cylinder pressures and gross heat release rates (GHRR) at a constant SOI timing for the following three low reactivity fuels: a) gasoline, b) diesel reformate-1, and c) diesel reformate-2

In Figure 6a, it is seen that the shallow bowl piston geometry has a higher thermal efficiency than the re-entrant bowl piston geometry. For DR1-diesel and gasoline-diesel, the difference in efficiency is less than the efficiency difference of DR2-diesel, due to the difference in the peak heat release rate. Since the compression ratio and IMEP_g were kept constant, the effect of heat transfer losses remains the only major factor influencing thermal efficiency. The factors that affect the heat transfer losses are convective heat transfer coefficient, bulk temperature, and the surface area. By comparing the two piston bowl profiles, the re-entrant bowl has approximately 10% more surface area at TDC than the shallow bowl piston. Figure 6b shows that the combustion efficiency was marginally higher for the re-entrant bowl

piston than the shallow bowl piston. However, the difference in combustion efficiency is very small and falls within the uncertainty of the emissions measurements.

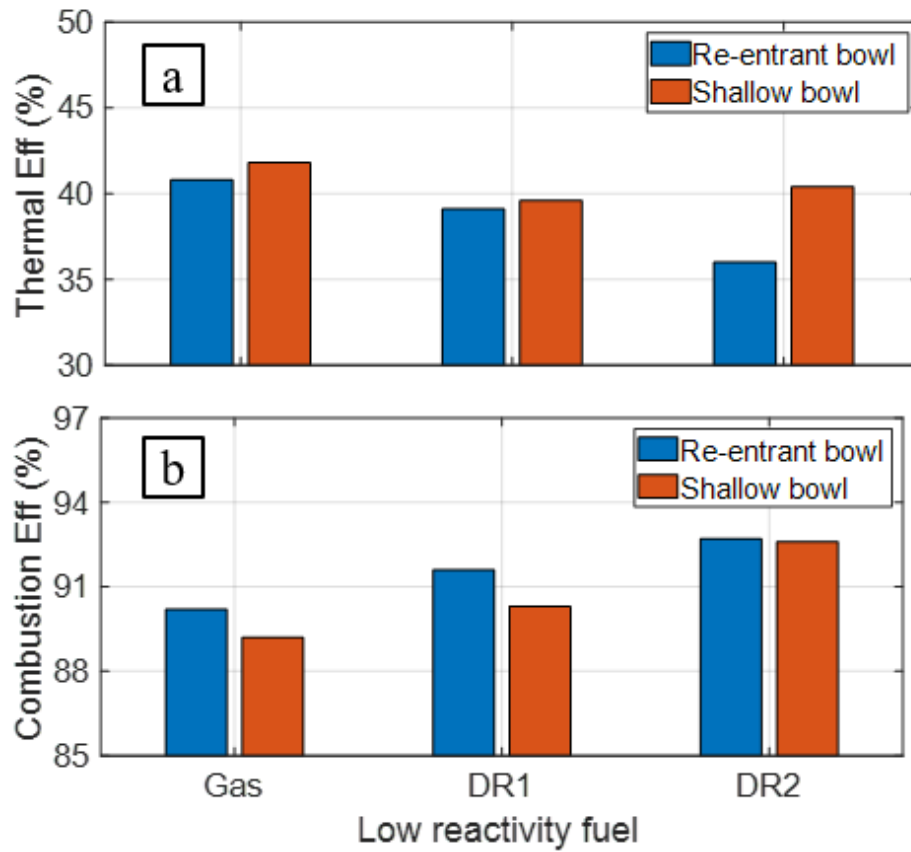


Figure 6: Effect of piston bowl geometry for the three different low reactivity fuels with diesel as the high reactivity fuel in RCCI at a constant SOI timing on a) the gross thermal efficiency and b) the combustion efficiency

The emissions values from the piston bowl comparison were also studied and they are presented in Table 3. Similar to the combustion phasing, the piston profile's effects on emissions were minimal. More importantly, the emissions values from both conventional RCCI and reformat RCCI are comparable. These results provide evidence that there is no major effect of reformat RCCI on the emissions, unlike the negative effect that cetane improvers can have on the NO_x emissions.

Table 3: Effect of two different piston bowl geometries on the combustion characteristics including emissions at a constant SOI timing for the three fuel combinations

Piston Profile	Low-reactivity fuel	EGR	IMEP_g	BRe	T_{int}	SOI	CA50	IS CO	IS CO₂	IS NO_x	IS THC
-	-	%	bar	%	K	deg aTDC	deg aTDC	g/kWh	kg/kWh	g/kWh	g/kWh
'Deep bowl'	'Gas'	33	5.2	44	320	-60	-2.2	18.6	1.1	0.10	19.3
'shallow bowl'	'Gas'	32	5.3	45	321	-60	-1.9	20.4	1.1	0.34	20.2
'Deep bowl'	'DR1'	0	5.2	30	320	-50	-1.6	31.1	1.0	0.48	13.4
'shallow bowl'	'DR1'	0	4.9	30	320	-50	-1.8	40	0.9	0.30	13.7
'Deep bowl'	'DR2'	0	4.9	30	340	-56	-4.5	20.3	0.9	0.50	12.9
'shallow bowl'	'DR2'	0	4.9	32	340	-56	-4.4	20.3	0.9	0.38	12.9

1.2. Effect of two different injector included angles

The injector included angle is the angle between the fuel jets spraying out of the injector's nozzles (as shown in Figure 3). Similar to SOI timing, the injector included angle also has a large influence on the mixing of the high reactivity fuel with the background mixture, since the angle determines whether the fuel spray is directed toward the piston or the cylinder liner. In this study, injector included angles of 150 degrees and 60 degrees were experimentally studied at similar operating conditions across the three different low reactivity fuels: diesel reformat-1 (DR1), gasoline, and natural gas (CNG). Diesel was used as the high reactivity fuel. DR1 was used for brevity as an example of single-fuel reformat RCCI. Figure 7 shows the effect of two different injector included angles on the cylinder pressure and gross heat release rate (GHRR) at a constant SOI timing. Unlike the piston profile comparison, the injector included angle has a significant influence on the combustion phasing. The exact cause of the earlier combustion phasing with the narrower injector angle will be explored in more detail in the last part of this manuscript which uses CFD simulations in CONVERGE CFD.

Even though the start of injection was kept constant, the start of combustion, combustion duration, and CA50 changed noticeably. Regardless of the low reactivity fuel, blend ratio, or start of injection timing, the combustion phasing using the 60-degree included angle is always earlier than the 150-degree included angle. Considering gasoline-diesel RCCI in Figure 7.a, even though the start of injection is kept constant at -75 deg aTDC, the start of combustion for the 60-degree injector is 9 degrees earlier than the 150-degree injector. Similarly, for the natural gas-diesel RCCI and DR1-diesel RCCI, the start of combustion advanced by 2 degrees and 11 degrees, respectively. Additionally, the combustion duration is also invariantly longer for the 150-degree injector for all fuel combinations because of the retarded combustion phasing. These trends can be seen in Table 4, where all the combustion characteristics, including the emissions, are tabulated.

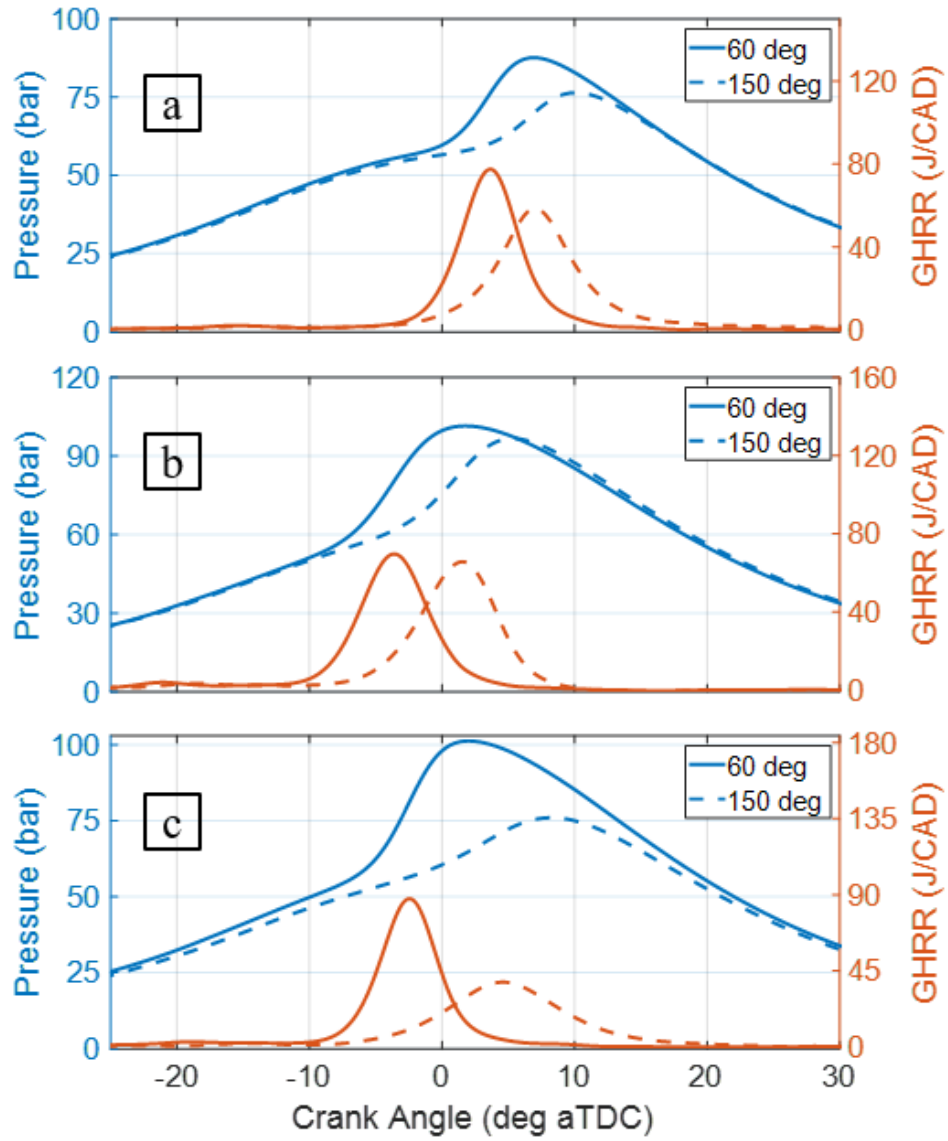


Figure 7: Effect of the two different injector included angles on the cylinder pressures and gross heat release rates (GHRR) at a constant SOI timing for the following three low reactivity fuels: a) gasoline, b) natural gas, and c) diesel reformate-1

Table 4: Effect of two different injector included angles on the combustion characteristics including emissions at constant SOI timing for the three low-reactivity fuels

Injector included angle	Low reactivity fuel	EGR	IMEP_g	BRe	T_{int}	SOI	CA50	IS CO	IS CO₂	IS NO_x	IS THC
-	-	%	bar	%	K	deg aTDC	deg aTDC	g/kWh	kg/kWh	g/kWh	g/kWh
'60 deg'	'Gas'	46	5.1	75	340	-75	3.5	30.3	1.9	0.03	23.5
'150 deg'	'Gas'	40	5.1	77	340	-75	7.3	33.4	1.4	0.02	25.1
'60 deg'	'CNG'	25	5.0	60	340	-85	-3.9	16.8	1.0	0.20	21.6
'150 deg'	'CNG'	31	5.2	58	341	-85	0.7	16.8	1.0	0.05	20.4
'60 deg'	'DR1'	0	5.0	43	340	-58	-2.9	19.7	1.1	0.28	14.6
'150 deg'	'DR1'	0	4.8	40	340	-57	4.7	43.5	0.9	0.05	14.9

The longer combustion duration of the 150-degree injector is due to the later start of combustion. From both the start of combustion and the combustion duration values, the effect of the injector angle seems to be lower on natural gas-diesel RCCI compared to the other two fuel combinations. The lower effectiveness is due to the high-octane rating of the natural gas and the earliest SOI timing between the fuel combinations of -85 deg aTDC.

The effects of the injector included angle on the combustion efficiency and the thermal efficiency are shown in Figure 8. In Figure 8.a, the change in thermal efficiency has been compared for the three different low reactivity fuels. In general, thermal efficiency is mainly influenced by the combustion phasing and the combustion duration, where shorter durations result in higher efficiencies and combustion phasing in the optimal window of about 5-8 degrees aTDC results in the highest efficiency.

In Figure 8.b, the change in combustion efficiency also follows the changes in combustion phasing, where later combustion phasing resulted in somewhat lower combustion efficiency. In addition, the 150-degree injector most likely results in the fuel impingement and “wall wetting” of the cylinder liner, and unburned fuel closed to the walls being trapped in the crevices. All of these effects are minimized by using a 60-degree injector, where the fuel is directed toward the piston rather than cylinder liner.

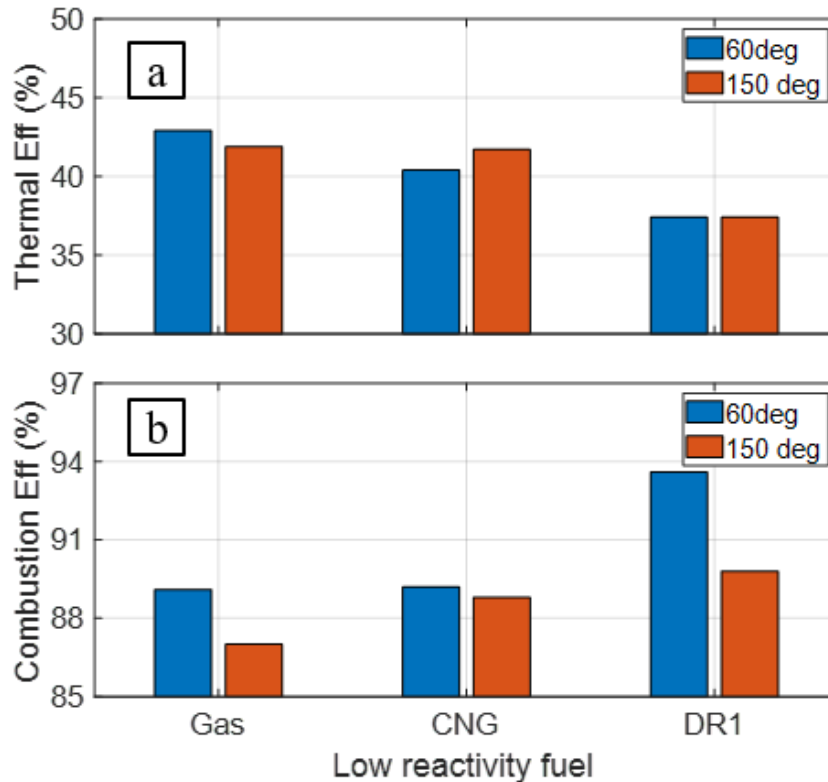


Figure 8: Effect of injector included angle for the three different low reactivity fuels with diesel as the high reactivity fuel in RCCI combustion at constant SOI timing on a) gross thermal efficiency and b) combustion efficiency

To better understand the effects of the injector include angle on single-fuel reformatе RCCI combustion, a CFD model was constructed and used to explain the trends in the experimental results. The CFD model and results are described below.

1.3. CFD Simulations to understand the effects of injector included angle

In the authors' previous paper, a CONVERGE CFD model was constructed for the engine described above and validated against experimental data [32]. In the interest of brevity, a brief description of the model will be included here; however, for the validation of the CFD model and the detailed explanation of sub-models used for capturing physical phenomena, please refer to [32]. The Reynolds-Averaged Navier-Stokes (RANS) CONVERGE CFD 3D model with detailed chemical kinetics uses the mechanism by Liu et al. [53] for Primary Reference Fuels (PRFs). The diesel fuel was modeled as tetradecane for the injection process and as n-heptane for the chemical kinetics. All the reformatе species were available in the mechanism as they are the partially oxidized species from the parent diesel fuel. An orthogonal cut-cell grid of 4 mm is used in the intake and exhaust ports while the mesh size is reduced around the intake and exhaust valves to 0.5 mm, in the entire combustion chamber to 1 mm, and around

the injector to 0.25 mm. Adaptive mesh refinement (AMR) refines the mesh in regions with high gradients of temperature, velocity, and HO_2 , OH , CO , and O_2 species mass fraction. Lastly, the full engine cycle simulation was performed from EVO to improve the accuracy of predicted residual gas fraction and temperature as well as intake and exhaust flow. Figure 9 shows the CONVERGE CFD model of the Ricardo Hydra engine.

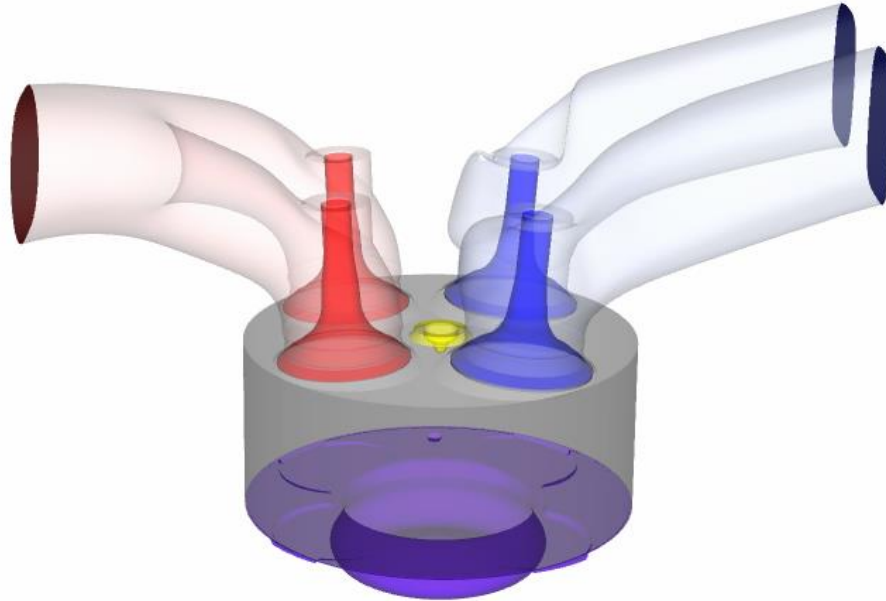


Figure 9. CONVERGE CFD engine model of the Ricardo Hydra engine

The CFD engine model was validated against experimental data collected on the Ricardo Hydra engine operating in RCCI with diesel as the parent fuel and diesel's gaseous reformat fuel mixture as the low-reactivity fuel in the previous paper [32]. In the experiment, it is relatively difficult to change the injector's included angle because different custom injector tips would need to be made for each included angle. Experimentally, two injector tips were available to test reformat RCCI and generate the results presented above. However, the CFD model is incredibly well-suited to conduct a more thorough screening of the effect of the injector spray angle on the behavior of RCCI combustion. CFD simulation results are shown in Figure 10 and Table 5 below to determine the effect of injector included angle on the characteristics of reformat RCCI combustion.

From Figure 10, it can be seen that combustion is relatively retarded and elongated for included angles of 150° , 135° , 120° , and 105° . At an included angle of 90° and 75° , the combustion phasing advances considerably, and the burn duration is reduced. At an included angle of 60° , the combustion is

slightly retarded compared to 75° and 90° but has a lower peak heat release rate and a slightly broader heat release process. This trend in combustion phasing with included angle will be expanded upon below. The 60° included angle injector exhibits earlier combustion phasing than the 150° included angle injector which agrees well with the trend observed in the experiment. Table 5 shows that the NO_x emissions were highest for the cases with the earliest combustion phasing and shortest burn duration (75° and 90°), which is to be expected. However, combustion efficiency, CO emissions, and UHC emissions do not necessarily follow an intuitive trend, which will be explained in more detail below.

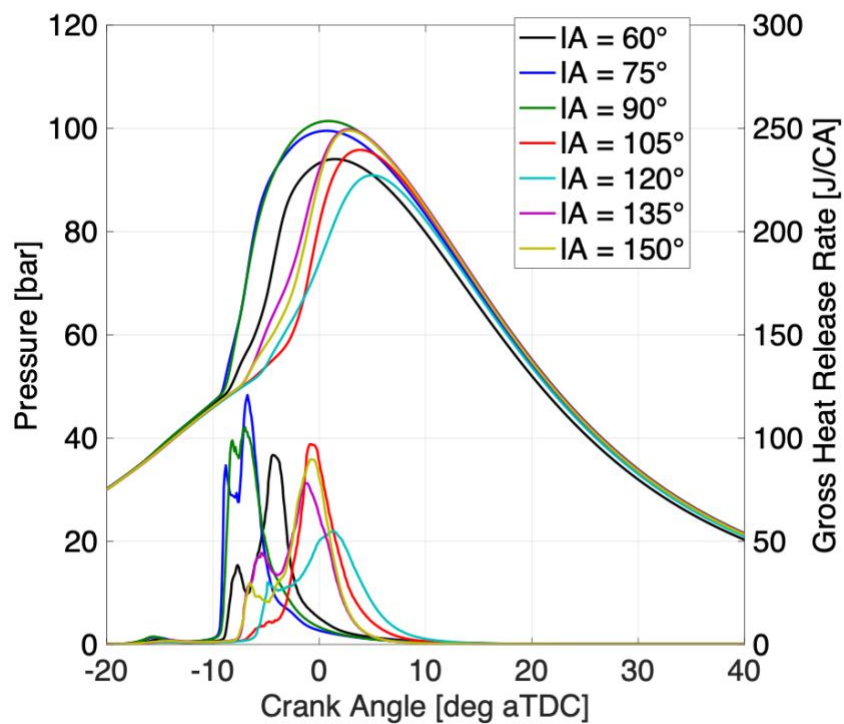


Figure 10. Pressure and heat release rate results from the computational fluid dynamics model that show the effect of varying the included angle of the injector. IA stands for Included Angle.

Table 5: Efficiencies, emissions, and CA50s for the different simulated injector included angle

BR	Tint [K]	Spray angle	SOI [CAD]	η_{th} [%]	η_c [%]	CA50	CO [g/kwh]	CO2 [g/kwh]	NOx [g/kwh]	UHC [g/kwh]
45	380°	150°	-55°	48	90.7	-1.2	1.48	704	1.3	0.564
		135°		48.6	90.8	-1.6	1.54	696	2.43	0.78
		120°		50.2	83.2	0.8	8.68	684	0.58	1.84
		105°		49.8	87.6	-0.2	6.36	681	0.44	2.2
		90°		47.9	90.8	-6.4	15.3	695	9.06	1.57
		75°		47.4	88	-6.5	29.15	697	8.18	2.1
		60°		49.2	78.6	-4	40.25	685	4.32	4.11

Figure 11 shows cut planes of the equivalence ratio distribution for four of the simulated injector include angles. The cut-planes show that the fuel is distributed primarily in the squish region for an included angle of 150°. At 120°, the majority of the diesel fuel is still deposited into the squish region, although it is also possible to see that some of the direct-injected diesel fuel is present in the bowl. At 90° and 60°, the majority of the direct-injected diesel fuel is in the piston bowl. Considering that the bowl region also has the hottest temperatures, this explains why the combustion phasings of the 60°, 75°, and 90° cases were significantly advanced compared to the remaining cases. However, the cut-planes alone are not sufficient to explain all of the trends in Figure 10 and Table 5.

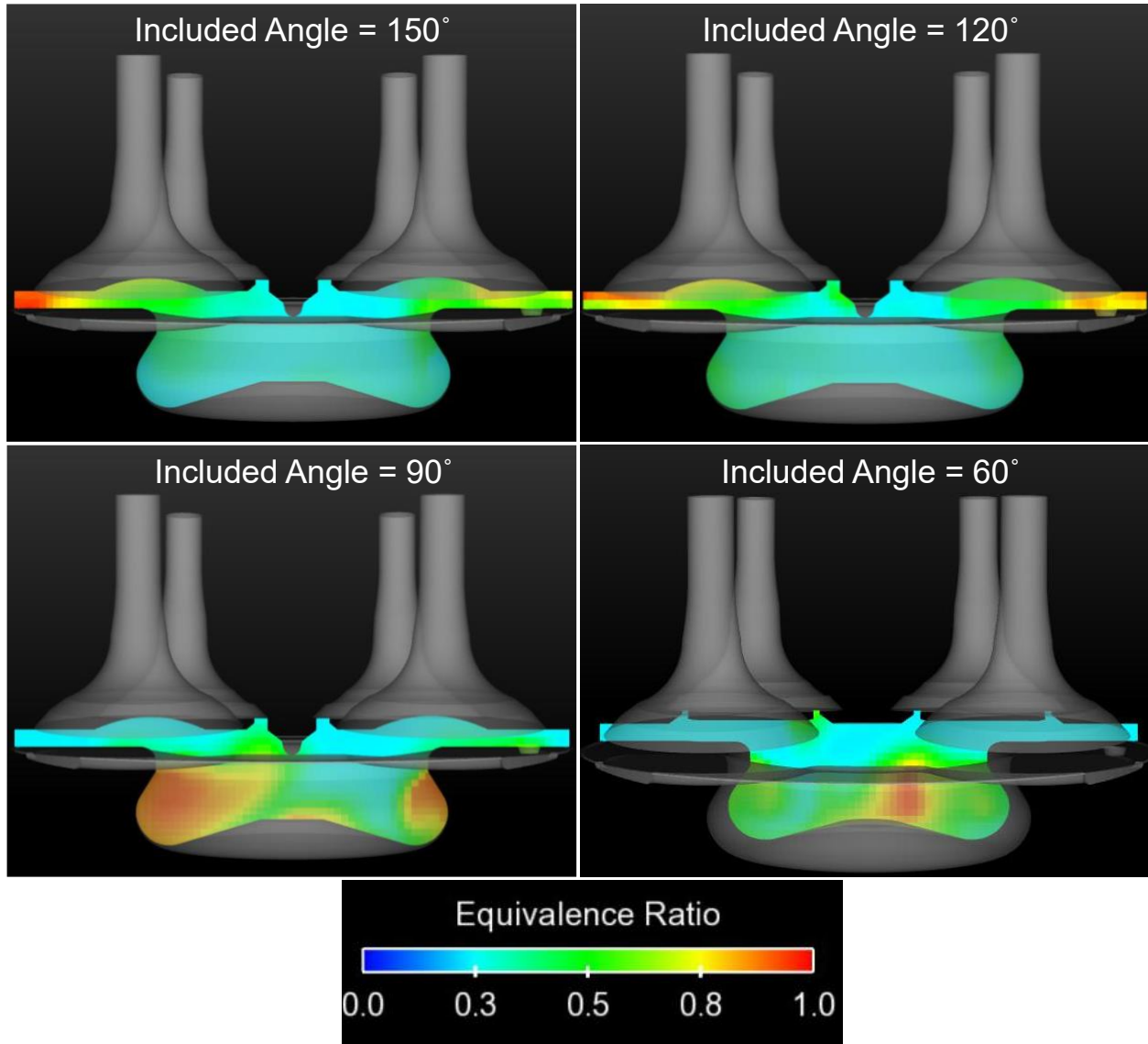


Figure 11. Cut-planes of equivalence ratio for different included angles at -10° CAD showing that the diesel is deposited primarily in the squish region for included angles of 120 degrees and 150 degrees, whereas the diesel fuel is deposited primarily in the production diesel, re-entrant bowl for included angles of 90 degrees and 60 degrees

Figure 12 shows the film mass for each of the included angle simulations. An included angle of 150° and 135° results in a moderate amount of fuel being deposited into the wall film due to spray-wall impingement. At 120° , the amount of fuel that is deposited into the wall film is very large, which helps to explain why the combustion efficiency and peak heat release rate for the 120° case are much lower than some of the other cases. An included angle of 90° and 75° both exhibited the lowest fuel film mass, which, in combination with the fact that the higher reactivity fuel is targeted at the bowl region that is generally higher temperature, is why their peak pressures, heat release rates, and combustion efficiencies were the highest. An included angle of 60° shows the largest amount of fuel mass in the film which must be due to

the small included angle causing plume-plume interactions and causing the spray plumes to collapse on each other, which negatively impacts their break-up and evaporation. This explains why the 60° had the lowest combustion efficiency and lower peak heat release rate, even though the majority of the high reactivity fuel was deposited into the bowl. To further help visualize the wall film mass for the different injector included angles, Figure 13 shows the film mass color-coded by its thickness. These results show that the combustion process is very sensitive to the injector included angle for at least two reasons. First, the high-reactivity fuel can either be deposited in the bowl where the temperatures are generally higher, or in the squish region where the temperatures are generally lower, or some combination of the bowl and squish regions. Second, the injector included angle has a large impact on the fuel film deposition, and since diesel fuel is not very volatile, when the diesel fuel is deposited in the fuel film, it struggles to evaporate off of the film. In conventional diesel combustion, the diesel fuel mixes with the air and combusts before a significant fraction can be deposited into the wall-film. Therefore, advanced combustion strategies like RCCI and PCCI, although better for particulate mass emissions, their early injection timings of a low volatility fuel like diesel can result in a large fraction of the fuel mass being deposited in the wall film, therefore resulting in a lower combustion efficiency. Since single-fuel RCCI with onboard fuel reformation is between conventional RCCI and PCCI in terms of its diesel fuel mass and the injection timings, this is a larger consideration for single-fuel RCCI than for conventional diesel-gasoline RCCI where the energy blend ratios would result in a lower amount of diesel being direct-injected.

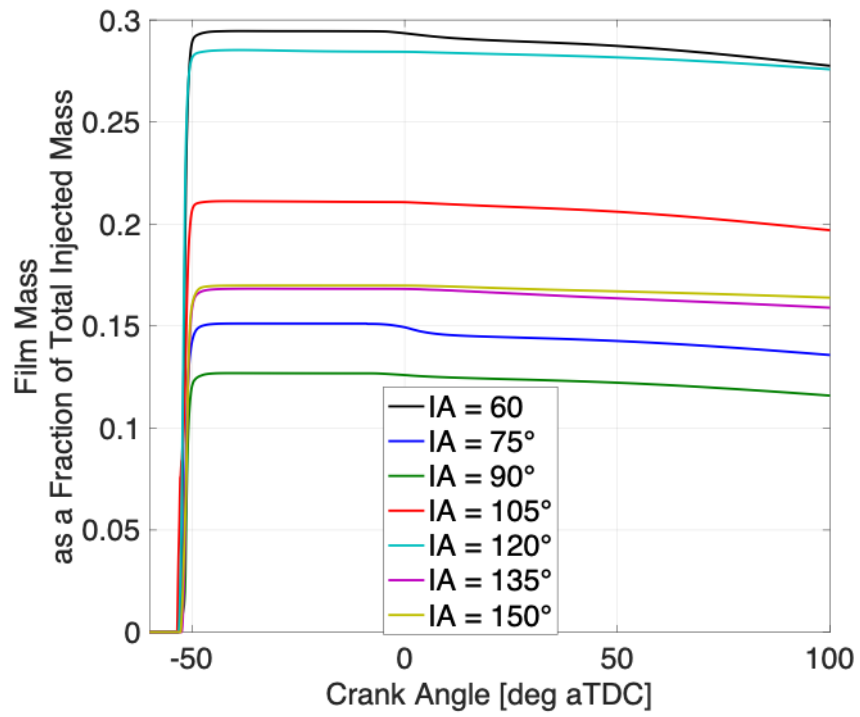


Figure 12. Film mass as a function of crank angle for each of the simulated included angle

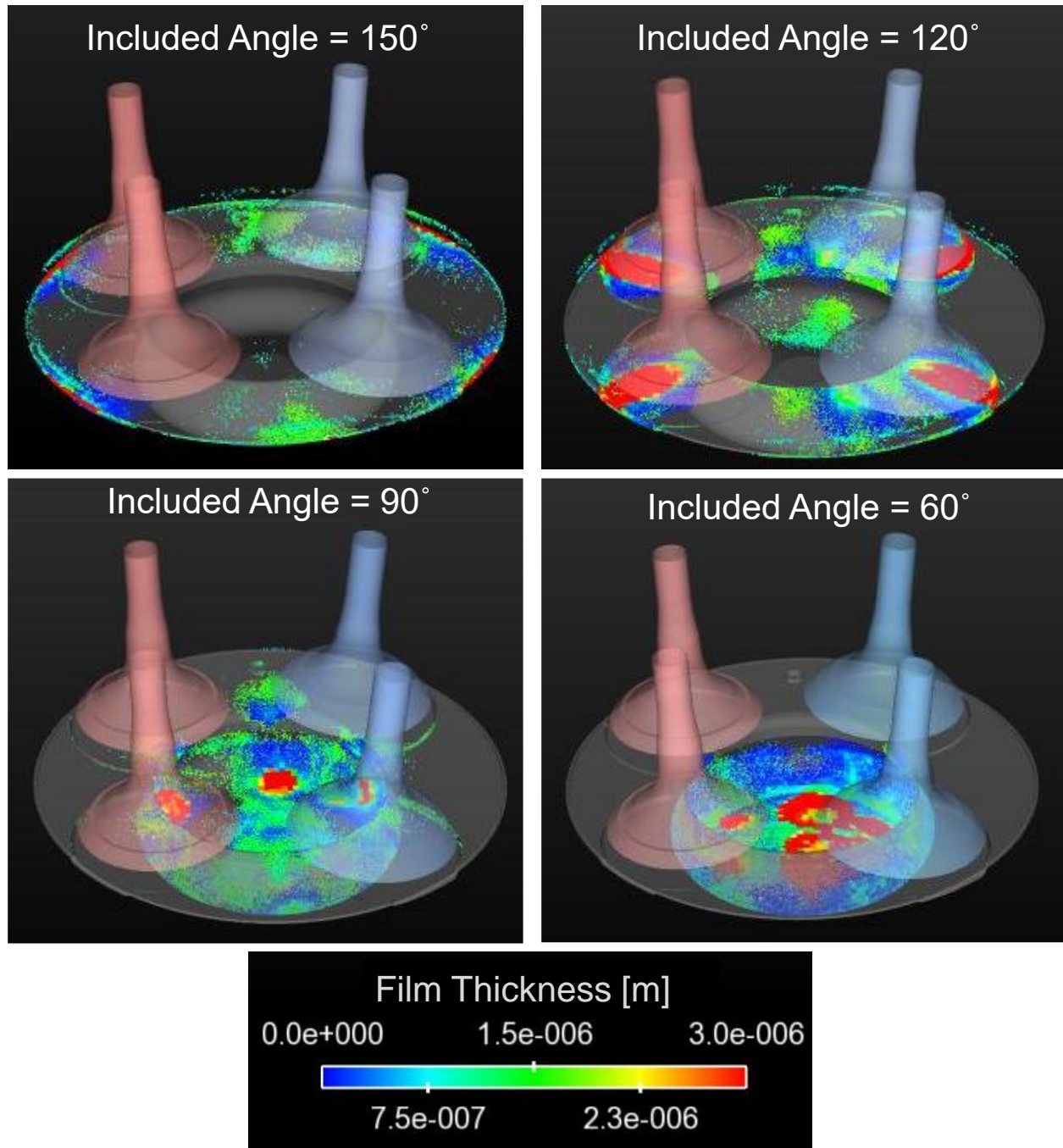


Figure 13. Surface visualization of the film thickness for the different included angle simulations at -10 CAD

In summary, the CFD simulations were able to illuminate the reason for the combustion phasing trend with injector included angle that was observed in the experiment. The reason for the advanced combustion phasing associated with the narrower included angle is explained when considering the regions in the combustion chamber targeted by the spray. In RCCI combustion, the high-reactivity fuel (i.e., diesel fuel) initiates the progression of autoignition. The basic concept is that the richer regions, with

more diesel fuel, ignite first and the increase in pressure and temperature from this combustion further compresses the leaner regions, containing primarily low-reactivity fuel until eventually, the low reactivity fuel ignites. Therefore, when the fuel is injected using the 60° injector, the fuel is directed toward the hot center of the combustion chamber compared to the 150° injector where the fuel is directed into the cooler region (i.e., near the cylinder liner). This difference advances the start of combustion for the 60° injector case compared to the 150° injector case since the richer regions are collocated with the generally hotter regions.

Conclusions

The effects of two different piston bowl profiles (i.e., a re-entrant bowl and a shallow bowl) and two different injector included angles (60 degrees and 150 degrees) were experimentally studied on conventional RCCI (i.e., gasoline-diesel and natural gas-diesel) and reformat RCCI. A validated CFD model was also used to study seven different injector included angles (from 60 degrees to 150 degrees), for a better understanding of the injector included angle effect on the combustion characteristics. From the detailed analysis, the following conclusions can be drawn:

1. At a constant compression ratio and SOI timing of diesel, the two different piston profiles were compared.
 - a. There was no significant effect on the combustion phasing or combustion duration, regardless of the fuel pair.
 - b. However, the shallow bowl piston showed slightly better thermal efficiency, due to its 10% less surface area availability for heat transfer. The improvement in thermal efficiency was minimal for the conventional fuel, but it was significantly better (~13% higher than re-entrant bowl) on the reformat fuel.
2. At a constant compression ratio and SOI timing of diesel, the two different injector included angles were compared.
 - a. Unlike the piston bowl profiles, changing the injector included angle from 150 degrees to 60 degrees had a significant impact on the combustion phasing and combustion duration for all the fuel combinations (gasoline-diesel – 3.8 degrees, natural gas-diesel – 4.6 degrees, and reformat RCCI – 7.6 degrees).
 - b. Although the differences in the thermal efficiencies were minimal across all the fuel combinations, the combustion efficiency of 60-degree injector was noticeably better (3% for gasoline-diesel, 1% for natural gas-diesel, and 5% for reformat RCCI), due to their earlier combustion phasing and probable wall wetting with the 150-degree injector.
3. To further analyze the injector included angle, CFD simulations were conducted for seven different injector included angles which determined the two important parameters that affect the combustion process:

- a. The regions of the cylinder that are targeted by the injected fuel. For the injector included angles of 75 degrees and 90 degrees, the majority of the fuel was targeted into hot center of the combustion chamber (i.e., the piston bowl), which results in earlier combustion phasing. Alternatively, for wider injector included angles (greater than 100 degrees), the majority of the fuel is targeted toward the colder region of the combustion chamber, which retards combustion phasing.
- b. Fuel film deposition: Especially with the significantly lower BRe required by reformat RCCI (more energy input through the direct-injected diesel fuel), the fuel film deposition has a significant effect as it was found that a significant fraction of the injected fuel can be deposited into the wall film.

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