

**Title:** Single-fuel reactivity controlled compression ignition through catalytic partial oxidation reformation of diesel fuel

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## **Abstract**

A single-fuel RCCI concept has been proposed to avoid the need for a secondary fuel system required for conventional RCCI by generating the secondary fuel from the primary fuel through catalytic partial oxidation (CPOX) reformation. In conventional RCCI, gasoline or natural gas can be used as the low-reactivity fuel, and diesel can be used as the high-reactivity fuel. In this study, two reformat mixture generated by reforming diesel fuel at different operating conditions were used as the low-reactivity fuel, with the parent diesel as the high reactivity fuel. The combustion characteristics of reformat-diesel RCCI were compared with gasoline-diesel RCCI and natural gas-diesel RCCI. A CFD model was also developed and validated against the experimental results. The model was then used to validate a necessary approximation of the reformat mixture's species concentrations.

Compared to conventional RCCI fuel pairs, reformat-diesel RCCI shows marginally better thermal efficiency, approximately 10% better THC emissions, approximately 50% lower NO<sub>x</sub> emissions, and good controllability. Because the reformat mixture has a high concentration of diluents (higher than 80% by mole), it displaces a large fraction of intake air and acts similarly to EGR. Therefore, the intake pressure needed to be boosted to 1.4 bar to resolve the oxygen deficiency. The combustion behavior of reformat-diesel RCCI is in between that of gasoline-diesel and natural gas-diesel conventional RCCI since the reactivity of the reformat mixture is in between that of gasoline and natural gas. From the results, it can be concluded that reformat-diesel RCCI is not overly sensitive to the reformation process itself and the exact species concentrations in the reformat mixture. A small change in the start of injection of diesel, blend ratio, and EGR fraction can be used to compensate for reformat mixture concentration differences.

## **Introduction**

Compression Ignition (CI) engines have higher thermal efficiency due to their ability to operate at leaner air-fuel ratios and higher compression ratios compared to Spark Ignition (SI) – the other conventional combustion mode. However, due to the stratified mixtures and high combustion temperatures, conventional CI combustion results in high particulate matter emissions and NO<sub>x</sub> emissions, respectively. Thus, Low Temperature Combustion (LTC) strategies such as Homogeneous Charge Compression Ignition (HCCI) have been introduced. In HCCI, a homogeneous, lean air-fuel mixture is autoignited at mid-range compression ratios. Therefore, HCCI has ultra-low NO<sub>x</sub> and particulate matter emissions paired with high thermal efficiencies. Despite these benefits, HCCI lacks a direct control mechanism over combustion since the combustion process is controlled by chemical kinetics and thermal stratification. This results in an inability to operate at high loads due to the engine limitations of pressure rise rates and heat release rates. To address the drawback of HCCI and introduce a direct control mechanism over the

combustion process, researchers have proposed using a secondary, high reactivity fuel that is direct injected into the cylinder at a specific time during the engine cycle, while the primary fuel with lower reactivity is premixed with air to create a homogeneous air-fuel mixture. This combustion mode is known as Reactivity-Controlled Compression Ignition (RCCI) [1 – 3]. Gasoline and diesel are the two most commonly used low and high reactivity fuels, respectively, as their reactivity separation is large enough to provide good control over the combustion process [4 – 7].

In RCCI, by altering the ratios of the two fuels and/or adjusting the start of injection (SOI) timing of the high reactivity fuel, the combustion process can be controlled [8 – 10]. Due to this enhanced control over combustion, the operating range in RCCI is wider and shifted to higher loads compared with HCCI. In addition to the conventional fuels, researchers have studied RCCI with various alternative fuels, since the main requirement of RCCI is that there is sufficient reactivity separation between the two fuels. Along with the conventional fuels (i.e., gasoline and diesel), a wide range of alternative fuels such as polyoxymethylene dimethyl ethers (PODE) [53], natural gas [54, 55], and primary reference fuels (PRF) [56] were also studied in RCCI combustion. Although RCCI has these advantages, there is the specific shortcoming of the requirement of two separate fuel systems. Thus, an adaptation of this technology - "Single-Fuel RCCI" - has been introduced and is being investigated to enable RCCI combustion from a single parent fuel, thereby resolving the main drawback of conventional dual-fuel RCCI.

"Single-Fuel RCCI" was initially proposed with the addition of a cetane improver such as di-tert-butyl-peroxide (DTBP) [11 – 13] to gasoline. The gasoline + DTBP was used as the high reactivity fuel, while the unaltered gasoline was used as the low reactivity fuel. With 2% DTBP by volume added to the parent gasoline, the fuel's reactivity was found to be sufficient to enable RCCI combustion with the parent gasoline as the low reactivity fuel [13]. Although this concept was successful at enabling effective RCCI combustion in the cylinder, the goal was for the additive consumption to be such that the tank could be refilled at oil-change intervals, and with DTBP, the consumption was too high to achieve this goal. Therefore, researchers attempted using a stronger cetane improver: 2-Ethyl-Hexyl Nitrate (EHN) [14 – 16].

Although 2-EHN is a stronger cetane improver than DTBP, 2-EHN has its own specific shortcomings. For example,  $\text{NO}_x$  formed during combustion is generally called "thermal  $\text{NO}_x$ " because it is produced from the dissociation of  $\text{O}_2$  and  $\text{N}_2$ . However, the consumption of 2-EHN linearly increases the  $\text{NO}_x$  emissions due to the fuel-bound nitrate group [17, 18]. Kaddatz et al. [19] studied E10 gasoline with up to 3% of 2-EHN and found that when comparing gasoline-gasoline+2-EHN RCCI to conventional gasoline-diesel RCCI at a similar SOI timing, the gasoline-gasoline+2-EHN RCCI had significantly higher  $\text{NO}_x$  emissions. In order to reduce the  $\text{NO}_x$  emissions to match the near-zero levels of conventional RCCI, the SOI timing had to be advanced significantly to retard combustion phasing. As the SOI timing advanced and the start of combustion retarded, the peak temperatures decreased, which was able to reduce the  $\text{NO}_x$  emissions [19]. However, retarding the combustion phasing had adverse effects on the efficiency and some other emissions. In addition to the elevated  $\text{NO}_x$  emissions, 2-EHN is thermally unstable above 140 °C [20], which poses practical challenges related to storage in a vehicle application.

Irrespective of the cetane improver used, the additive itself is a secondary fuel and needs to be periodically refilled. Thus, researchers have recently proposed a different technique to enable RCCI combustion from a single parent fuel through onboard fuel reformation [21]. In this concept, a fraction of the primary fuel is directed into an onboard fuel reformer to produce *reformate*: a gaseous mixture of hydrogen ( $\text{H}_2$ ), carbon monoxide (CO), and other partially reacted hydrocarbon

species. Since the reactivity of the reformat is different from the parent fuel, the reformat can be used as a secondary fuel along with the parent fuel to enable RCCI combustion from a single fuel tank. The current study was conducted to experimentally investigate this concept of "single-fuel" RCCI with onboard fuel reformation.

There are different types of reformation processes including catalytic partial oxidation (CPOX or POX), steam methane reforming (SMR or SR for steam reforming), and autothermal reforming (ATR) [22]. In CPOX reforming, a very rich mixture of fuel and air is reacted over a catalyst, which produces CO and H<sub>2</sub> (i.e., products of rich combustion due to the oxygen deficiency), and other partially reacted hydrocarbon species [23 – 25]. CPOX is an exothermic process. SMR reacts steam and methane over a catalyst to produce CO and H<sub>2</sub> [23, 26]. SMR is endothermic and requires high temperatures and a high-temperature heat source. ATR is a combination of both SMR and CPOX and therefore can be endothermic, exothermic, or net neutral [27 - 30]. The details of these reforming processes have been, and will continue to be, the focus of much research; however, the goal of this paper is to evaluate RCCI combustion with a parent fuel and its reformat in the cylinder. Therefore, CPOX is chosen as the specific reformation process because it is the simplest to implement and easiest to control. Due to the requirements of high temperatures and a high-temperature heat source, SMR would be challenging to implement in a vehicle application.

In order to determine which parent fuel is most conducive to the concept of single-fuel RCCI with onboard fuel reformation, the gaseous fuel mixture that results from a CPOX reaction of various transportation-relevant fuels needed to be studied. Thus, three parent fuels, gasoline, diesel, and natural gas, were partially oxidized by a CPOX reformation method at various equivalence ratios and pressures in a previous study [31]. The reformat mixtures that were produced had different concentrations of CO and H<sub>2</sub>, along with inert species such as H<sub>2</sub>O, CO<sub>2</sub>, and N<sub>2</sub> (since air was used as the oxidizer). Selected mixtures from each parent fuel were studied in HCCI at a constant compression ratio of 16 and equivalence ratio of 0.3 to determine the reformates' reactivities in comparison to their respective parent fuels [31]. With the help of a PRF mapping that was generated on the same engine and operating conditions [32], an effective PRF number, or effective octane rating, for each of the selected reformat fuel mixtures was determined. Based on the comparisons between the octane rating of the reformat fuel mixtures and their parent fuels, diesel and diesel's reformat were chosen for further study of single fuel RCCI because diesel and its reformat fuel mixtures exhibited the largest reactivity separation, which is necessary for RCCI. The compositions of the reformat fuel mixtures are somewhat similar to *syngas*, which is a combination of H<sub>2</sub> and CO; however, the reformat fuel mixtures also have other partially oxidized hydrocarbons and inert gases, such as N<sub>2</sub>, H<sub>2</sub>O, and CO<sub>2</sub>. For more information on the reformat speciation, please refer to [31].

Various researchers have studied *syngas* in both conventional and low temperature combustion modes. Since hydrogen is one of the main components in *syngas*, *syngas* has been heavily researched in spark-ignited (SI) combustion to extend the lean limit due to hydrogen's high flame speed and low lean flammability limit [33, 34]. In dual-fuel combustion with diesel as the secondary fuel, researchers noted that by replacing a fraction of the diesel fuel with *syngas*, the NO<sub>x</sub> and CO<sub>2</sub> emissions decreased [35]. The fraction of H<sub>2</sub> in the *syngas* was found to have a significant effect on NO<sub>x</sub> emissions and the maximum possible replacement of diesel fuel with *syngas* [36]. Following this, Chuahy et al. [34] tested *syngas* with diesel in reactivity-controlled compression ignition and studied the effects of the concentrations of H<sub>2</sub> and CO in *syngas* on RCCI

combustion. There was no significant effect of H<sub>2</sub> concentration (between 20% and 60%) on the thermal efficiency at constant combustion phasing even though the burn duration shortened. For H<sub>2</sub> concentrations higher than 60%, the thermal efficiency decreases due to higher heat transfer losses [34]. Although the effects of various concentration of syngas have been tested extensively on various combustion modes, including RCCI, the concentration and reactivity of actual reformat mixture compositions that result from CPOX reformation of diesel fuel has not been studied in the literature. Therefore, this paper presents the first results of single-fuel RCCI with diesel and its realistic reformat mixture composition from CPOX reformation.

In this study, in addition to the effects of H<sub>2</sub> and CO, the effects of the other minor hydrocarbon species and the inert species (N<sub>2</sub> and CO<sub>2</sub>) were studied. The reformat of diesel was used as the low reactivity fuel and the parent diesel fuel was used as the high reactivity fuel to conduct experiments on RCCI combustion. Following that, a Computational Fluid Dynamics (CFD) model, including combustion and spray submodels, was performed using CONVERGE 3-D CFD software. The CFD model was validated against experimental results. The model was then used to validate the approximation of the molar concentration of the reformat fuel mixtures for experimental testing. Finally, the combustion characteristics of reformat-diesel RCCI were compared with conventional gasoline-diesel RCCI and natural gas-diesel RCCI.

## Experimental Set up

In a previous study [31], gasoline, diesel, and natural gas were reformed in a CPOX process and the mixture compositions were determined with gas chromatography-mass spectrometry (GCMS). From these experimentally determined reformat mixture compositions, two reformates mixtures were selected as representative compositions for each parent fuel. These representative mixtures were tested to experimentally determine their autoignition tendency in comparison to their parent fuel. This previous study found that diesel and its reformat mixture exhibit the largest reactivity separation between a given parent fuel and its reformat. Therefore, these two specific reformat compositions (created from a CPOX reaction of diesel fuel) were chosen for further analysis in RCCI using the reformat mixture as the premixed, low reactivity fuel, and the parent diesel as the high reactivity fuel. In order to experimentally test the reformat composition in RCCI combustion on a research engine, gas bottles were procured to mimic the reformat composition. However, due to practical constraints, the compositions of the reformat fuel that were procured in gas bottles and used for experimental testing were slightly different from the mixture compositions determined from the GCMS measurements. Therefore, this approximation of the reformat composition will be validated with the help of a CFD model in a subsequent section of the paper below.

The experimental setup for this study consists of a production light-duty 1.7L GM engine head mounted to a single cylinder Ricardo Hydra research engine block. The remaining three cylinders are deactivated. The Ricardo Hydra engine specifications are presented in Table 1 and a schematic of the engine is displayed in Figure 1.

*Table 1: Ricardo Hydra 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)	-354° deg aTDC
Intake Valve Closing (IVC)	-146° deg aTDC
Exhaust Valve Opening (EVO)	122° deg aTDC
Exhaust Valve Closing (EVC)	366° deg aTDC

Even though the engine setup has the production diesel engine head, the intake, exhaust, fuel, coolant, and oil subsystems are all custom built to meet research needs. A 30 hp DC active dynamometer is used in this engine setup. A Kistler encoder with a resolution of 0.1 degrees is coupled to the crankshaft and triggers the high-speed cylinder pressure measurements. Meanwhile, most of the low-speed measurements are measured at 2-second resolution. A custom LabVIEW code is used for both low- and high-speed data acquisition and for engine controls of temperatures, pressures, and injection characteristics.

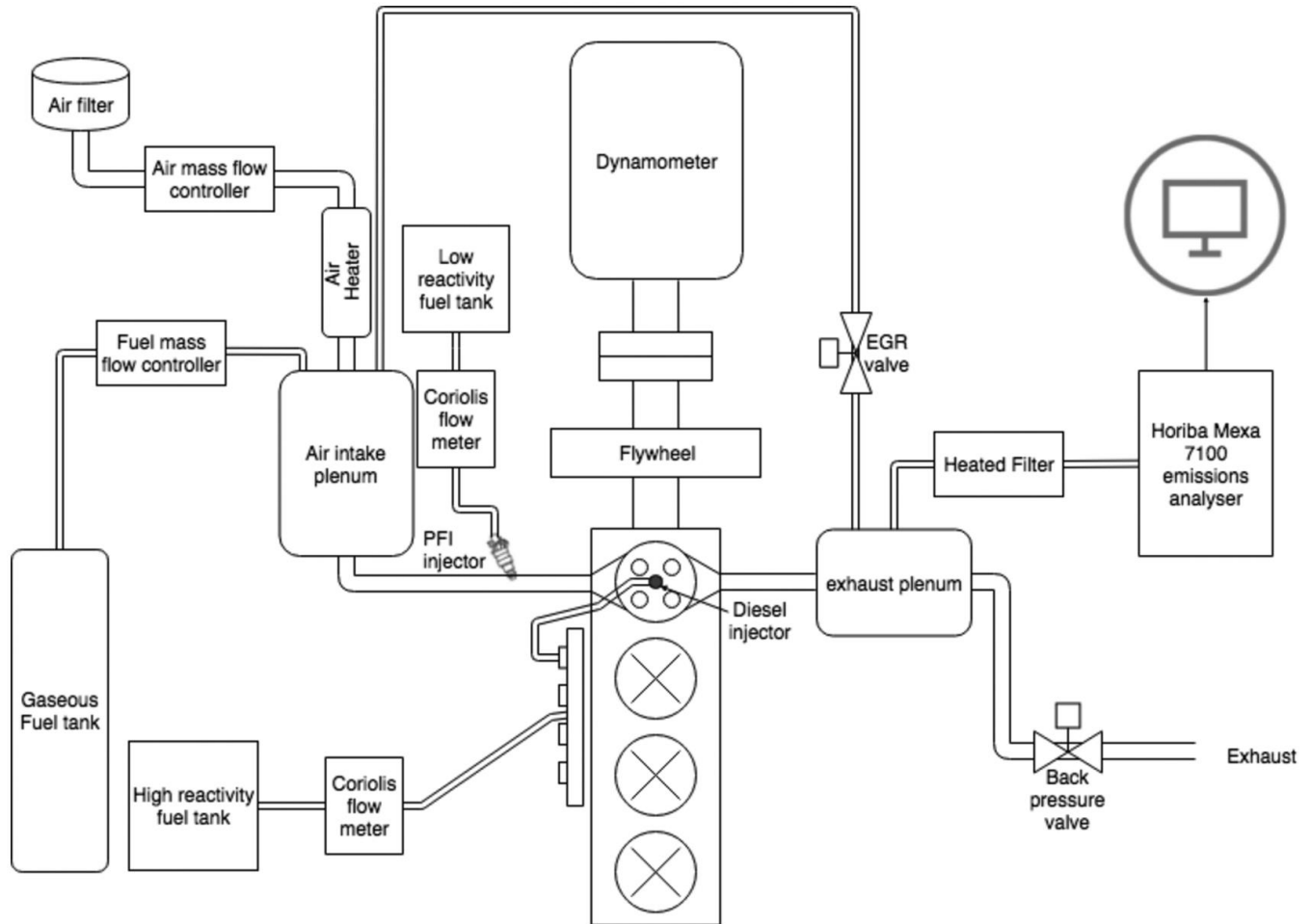


Figure 1: Schematic of the Ricardo Hydra engine

The intake system starts at an air filter, followed by an MCR Alicat mass flow meter/controller to measure and control the intake air mass flow rate. Downstream of the flow meter is a 5kW intake heater to heat the intake air and an intake plenum to prevent the gas exchange process from causing fluctuations in the air flow upstream in the air flow meter. The intake system has two pressure transducers, a Kistler high-speed piezoresistive pressure transducer located in the intake manifold to measure and record the intake pressure on a high-speed basis and a low-speed, high-accuracy barometer in the intake plenum used for daily calibration of the high-speed transducer. The exhaust system has a plenum, similar to the intake system, and a throttle valve to control the exhaust pressure. A high-speed, water-cooled pressure transducer has been located in the exhaust manifold to read the exhaust pressure on a high-speed basis. An ECM Lambda CAN oxygen sensor is located upstream of the exhaust plenum to measure the oxygen fraction in the exhaust and calculate the air-fuel ratio. A sample of exhaust gas from the exhaust plenum is directed to a Horiba MEXA 7100 D-EGR emissions bench. Additionally, this engine setup is capable of running external exhaust gas recirculation (EGR). The EGR line runs from the exhaust plenum to the intake plenum and is controlled by an electronically controlled valve.

The engine has a custom-built fuel cart which can supply two liquid fuels simultaneously; one for direct injection and the other for port fuel injection. The engine uses a production Bosch, solenoid-style diesel direct injector and a port fuel injector, both controlled by the custom

LabVIEW code. Both of the fuel systems have their respective fuel tanks and Micro Motion Coriolis mass flow meters. In the port fuel injection system, the pump pressurizes the fuel to 35 psi and the fuel is routed through the flow meter to the injector. In the direct injection system, a low-pressure pump pressurizes the fuel to 7 psi to feed a Bosch CP3 pump. The CP3 pump can pressurize the fuel up to 2000 bar, but in the current study, the injection pressure was maintained at 700 bar. The pressurized fuel is directed to the production direct injector through a common rail where the three unused outlets are capped. A high-speed pressure transducer is located in the high-pressure line as close to the injector as possible to measure the fuel injection pressure. Table 3 lists more information regarding the injector.

The properties of the reformat fuel mixtures, i.e., diesel reformat 1 (DR1) and diesel reformat 2 (DR2), and the composition of the natural gas (CNG) used in this study are tabulated in Table 2. DR1 and DR2 were formed through a catalytic partial oxidation reformation process of diesel fuel at different equivalence ratios and pressures. For more information on the reformation of diesel to form DR1 and DR2, please refer to [31]. **These three gaseous fuels, along with the fourth premixed fuel of gasoline, were the four low reactivity fuels that were studied in RCCI combustion using diesel as the high reactivity fuel.** The combustion characteristics, efficiencies, and indicated specific emissions of single-fuel RCCI (reformat-diesel RCCI) are compared against conventional gasoline-diesel RCCI and natural gas-diesel RCCI below. The comparison was made at a constant gross indicated mean effective pressure (IMEPg) and combustion phasing to study the similarities and differences between reformat RCCI and RCCI with conventional fuel pairs.

Table 2 : Properties of the gaseous low reactivity fuels

	Diesel Reformat 1 (DR1)	Diesel Reformat 2 (DR2)	Natural Gas (CNG)	
<b>Molar Concentration</b>	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%
<b>H/C ratio</b>	1.1	1.3	3.9	
<b>LHV (MJ/kg)</b>	2.3	3.8	47.6	

Table 3. Injector specifications

Number of nozzle holes	6
Injection spray type	Solid cone spray
Nozzle diameter	0.13 mm
Spray included angle	150°
SOI	-49° to -59° aTDC
Injection pressure	700 bar
Injection temperature	330 K
Injector mounting type	Centrally-mounted

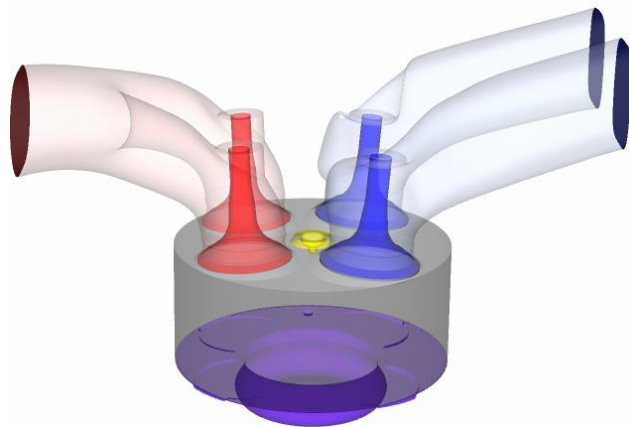
### Computational Setup

In addition to the experimental test results that will be described below, a Computational Fluid Dynamics (CFD) model is used in this study to validate the approximation of the experimentally tested reformat composition (described in more detail below). The CFD modeling, including combustion and spray submodels, was performed using CONVERGE 3-D CFD software. CONVERGE uses the Lagrangian-parcel Eulerian-fluid approach to convert the injected liquid parcels to Lagrangian parcels and discretize the gaseous fluid to Eulerian cells [37]. The modeled geometry was based on the experimental setup described above (a 4-cylinder production, diesel 1.7 General Motors/Isuzu engine with a re-entrant bowl piston). Only the cylinder that was mounted to the Ricardo Hydra engine block was modeled in the simulations. A schematic of the engine in CONVERGE CFD is shown in Figure 2. The engine operated at 1200 rpm at a load of 5.2 – 5.4 bar IMEPg for all of the simulated cases. The engine was fueled using the low reactivity gaseous reformat fuel and parent diesel fuel which contained 46% and 54% of the total energy of the system, respectively. The ratio of the premixed fuel’s energy content in the cylinder to the total fuel energy in the cylinder will be called the *blend ratio (BRe)*. A homogenous mixture of gaseous reformat and air was inducted into the combustion chamber through the intake manifold while the diesel fuel was injected directly into the cylinder at 700 bar using a production, Bosch, solenoid-style, centrally mounted diesel injector.

The spray is modeled using the hybrid KH-RT model for atomization and breakup of the droplets [38 – 40], the dynamic drop drag model for modeling the drag of the spray droplets [41], the No Time Counter (NTC) method for drop collision [42], the Chiang correlation for spray evaporation [43], and the built-in wall film model for spray-wall interactions [37]. In the simulation, the physical properties of the injected liquid droplets are represented using that of tetradecane and the injected liquid is modeled as n-heptane once each droplet evaporates. This is common practice in CFD modeling to represent the liquid properties of diesel by tetradecane and its chemical kinetics pathways as n-heptane. The n-heptane chemical kinetics pathway is represented using a PRF mechanism presented by Liu et al. [44] which consists of 41 species and

124 reactions. This mechanism was validated previously using experimental data from shock tubes, jet-stirred reactors, and flow reactors, and the ignition delay and the species evolution of this mechanism showed good agreement with various experimental advanced combustion data sets [44]. This mechanism was also validated in an HCCI engine using a 3D CFD model developed in KIVA-3V [47] for PRF73 and PRF70 and showed the ability to predict HCCI combustion. Also, since all of the reformat fuel species were partially oxidized species from the parent diesel fuel, they were present in this mechanism already and therefore the mechanism can also represent the reformat fuel.

Turbulence is modeled via a Reynolds-Averaged Navier-Stokes (RANS) method and the Reynolds stress term in the Navier-Stokes equations is modeled using the renormalization group (RNG)  $k-\epsilon$  model [45, 46]. The flow near the wall is treated with the law of the wall model and the heat transfer is modeled using the O'Rourke and Amsden [47, 48] heat transfer model. Additionally, combustion is modeled using the SAGE chemistry solver [49] coupled with the multi-zone model of Babajimopoulos et al. [50] to accelerate the simulations while maintaining the accuracy of the results [51].



*Figure 2. CFD model of the Ricardo Hydra engine*

Full simulations of the 360° engine geometry were performed (as opposed to a sector mesh) starting from the Exhaust Valve Opening (EVO). This allows for a more accurate prediction of the internal residual fraction and the temperature before Intake Valve Opening (IVO). Additionally, multiple cycle simulations were performed to find the number of cycles that are required to have an accurate simulation result for this engine and operating condition. Comparing the results of first and second cycle, shown in Figure 3, the difference between these two cycles is negligible indicating that the simulation of only one cycle is sufficient for accurate results. This can be expected due to the low internal residual gas fraction (RGF) of this Ricardo Hydra engine and conventional valve strategy (about 3-6% internal residuals), which results in a low dependence of the current cycle's combustion process on the previous cycle.

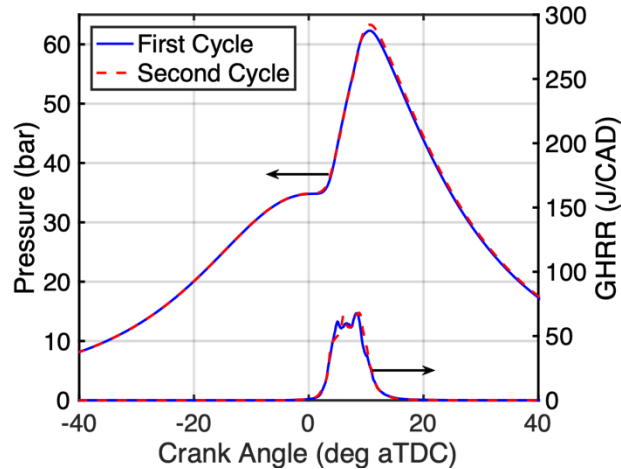


Figure 3. Comparison of first and second cycle simulations of the Ricardo Hydra model to demonstrate that under the current conditions and operating strategy, only one cycle is sufficient to provide accurate results

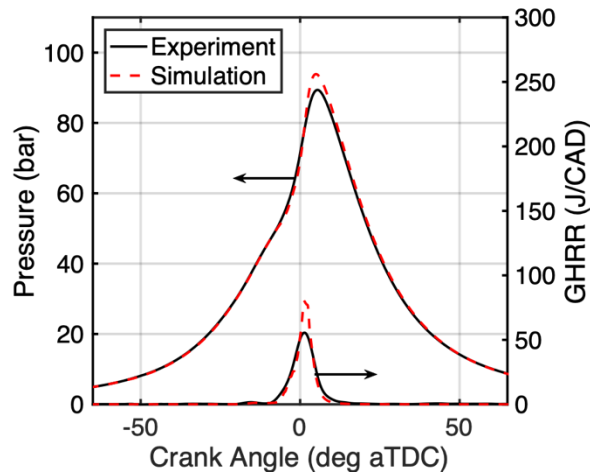
The computational domain was divided into three regions including the intake port, the exhaust port, and the combustion chamber. The combustion chamber is initialized using the experimental bulk temperature and in-cylinder pressure at the start of the simulation and the intake and exhaust regions are initialized using the experimental manifold pressures and temperatures. The boundary temperatures are estimated based on the experimental average boundary temperature and the location of each boundary in the model. The boundary temperatures were between 390 K and 550 K. For example, the cylinder liner's temperature was 390 K and the exhaust valve's temperature was 550 K. The CFD code uses a modified cut-cell cartesian method to generate the mesh automatically [37]. The base grid sizes of 1 mm inside the combustion chamber and 4 mm in the intake and exhaust port were used and then refined to 0.5 mm when the valves were open in the areas where the incoming or outgoing flows were present. Additionally, to resolve the flow near the injector, the grid near the injector was refined to 0.25 mm around the injection timing. Lastly, Adaptive Mesh Refinement (AMR) was incorporated into the model to refine the grid when the gradient of temperature, velocity, or CO, OH, HO<sub>2</sub> mass fraction exceeded specified criteria. **Each full-cycle simulation lasted for 30 hours on total of 112 processors.**

## Validation

### Validation of CFD model against experimental results

The CFD model was validated against experimental data collected on the Ricardo Hydra engine operating in RCCI with diesel as the direct injected parent fuel and diesel's gaseous reformat mixture as the low reactivity premixed fuel. The compression ratio in the CFD model was slightly different from the estimated experimental value (16.1 versus 15.5 for the experiment). The intake temperature was adjusted from the experimental value to account for slight differences between the chemical kinetics mechanism and the actual kinetics in the experiments. Additionally, the mass of fuel was adjusted in the CFD simulations to account for the following considerations: 1) the lack of blow-by or crevice model in the CFD model, 2) losses in the fuel mass due to the fuel wall-film wetting (CFD predicted the wall film from the simulation of only one cycle whereas in the experiment, the wall-film mass will reach a steady-state thickness and not constitute a loss),

and 3) the over-estimated combustion efficiency in the CFD simulations. The rest of the parameters, including the intake pressure and valve timings, were taken from the experimental cases. Figure 4 compares the simulation and experimental results of single-fuel RCCI combustion with diesel as the parent fuel. While there are slight differences between the experimental and simulation results, there is generally good agreement for the cylinder pressure and heat release rate between the experimental and simulation results. The simulation shows a higher peak heat release rate than the experiment, which is very common in engine CFD simulations. This could be due to slight differences between the actual thermal and/or equivalence ratio stratification and the thermal and equivalence ratio distribution predicted by the CFD. However, the agreement shown in Figure 4 is generally acceptable.

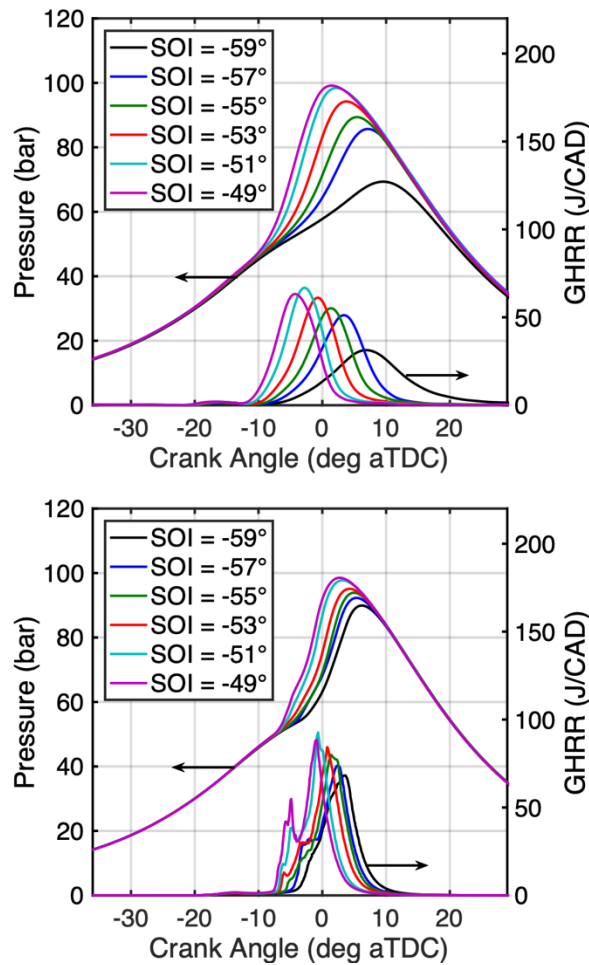


*Figure 4. Validation of the CFD model of the Ricardo Hydra engine against experimental data of single-fuel RCCI with diesel as the parent fuel*

To further validate the CFD model and explore its ability to capture the physical trends, an injection timing sweep was compared between the experiment and the CFD simulation results in Figure 5. In both cases, all of the parameters were kept constant while the injection timing varied from  $-59^{\circ}$  CAD aTDC to  $-49^{\circ}$  CAD aTDC. In both the experiment and the CFD simulations, as the injection timing retarded, the combustion phasing advanced, which is an intrinsic feature of RCCI combustion due to the richer regions that exist around TDC when the injection timing is delayed. This result verifies that the experimental operating mode is RCCI combustion, and that the CFD model is able to capture the same trends as the experiment and capture the behavior of RCCI combustion. There is a very slight low-temperature heat release event in both the experiments and the simulation, which is smaller than typically seen with gasoline-diesel RCCI. The reason that the low-temperature heat release event for reformat-diesel RCCI is smaller than gasoline-diesel RCCI is that the premixed fuel (i.e., the reformat) does not exhibit any low-temperature heat release itself, as was previously determined [31], whereas gasoline would exhibit some low-temperature heat release at these conditions. This effect will be described again later in the paper when reformat-diesel RCCI is directly compared to gasoline-diesel RCCI. It is encouraging that the simulation results and experimental results generally agree about the amount of low- versus high-temperature heat release.

As can be seen in Figure 5, the trend of combustion phasing with injection timing is stronger in the experiment and the CFD simulations show a decreased sensitivity to injection timing compared to the experiment. Additionally, the simulation results for the latest injection timing cases portray two peaks in the high-temperature heat release process, whereas the experimental results do not exhibit this behavior. These discrepancies between the experimental and simulation results could be due to a

variety of reasons. For example, it could indicate that the spray break-up, evaporation, and turbulence models are not perfectly capturing the injection process and the resulting equivalence ratio distribution, meaning that the constants of these sub-models require some adjustment for this specific combustion mode. It could also be that the chemical kinetics mechanism does not perfectly capture the equivalence ratio sensitivity of the direct injection diesel and that results in a decreased sensitivity of combustion phasing to injection timing in RCCI. Despite the differences between the experimental and simulation results, it is encouraging that the simulation was able to capture the trend of RCCI combustion with injection timing, as well as the amount of low- versus high-temperature heat release. Additionally, Figure 4 shows generally good agreement between the pressure and heat release for the phasing matched case. Since the goal of this study is to evaluate the performance of single-fuel RCCI using experiments and CFD models and to capture the trends and the behavior of RCCI combustion, the level of agreement shown in Figure 4 and Figure 5 is sufficient to capture such trends.



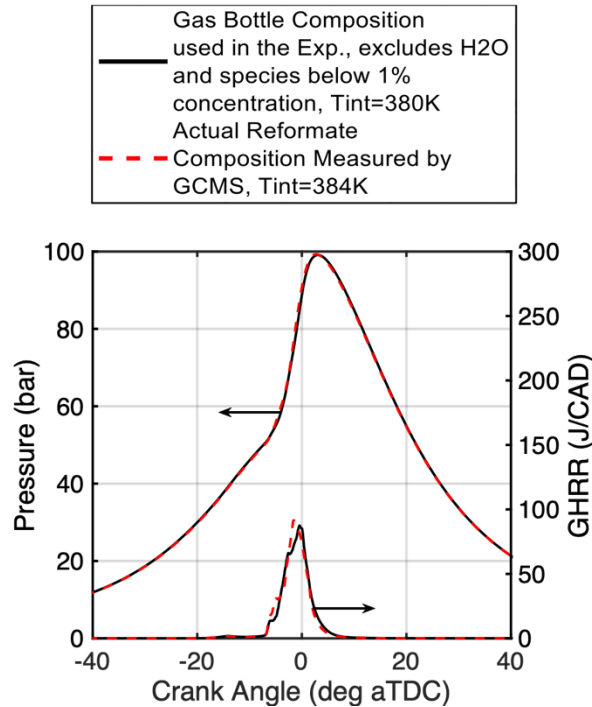
*Figure 5. Experimental (top) and simulation (bottom) pressure and heat release results for a start of injection (SOI) timing sweep. Gross load: 5.2-5.4 bar IMEPg. Intake pressure: 1.4 bar absolute.*

### **Validation of the approximation of reformate species for experimental testing**

In order to test the reformate fuel mixtures experimentally in the Ricardo Hydra engine, gas bottles were acquired with a composition of gas species that matched the composition of the reformate fuel mixtures measured by the GCMS as closely as possible. All of the engine testing used gas bottles

to approximate the reformat mixture. However, a practical consideration for experimental testing of diesel with its reformat fuel mixture is that the products of reformation contained a large number of different species with very low concentrations, especially when reforming diesel. Additionally, there is some water vapor in the reformat fuel mixture and some unreacted fuel that might condense on the walls as the reformat fuel mixture leaves the reformer and is directed to the engine in a practical application of the proposed concept. It is not possible for the gas bottle to contain water vapor or unreacted fuel, and it is impractical for the gas bottles to contain all of the species that resulted from the reformation of diesel. Therefore, the gas bottles only contained the species whose concentrations in the reformat mixture were larger than 1%, with three exceptions. First, any unreacted liquid parent fuel (i.e., diesel) cannot be present in the bottle and instead is assumed to be condensed and recirculated to the fuel tank in a vehicle embodiment of single-fuel RCCI with onboard fuel reformation. Second, since acetylene has been shown to play a significant role in the autoignition timing of reformed fuel mixtures [52], the exact concentration of acetylene in the reformat fuel mixture was used in the gas bottles regardless of its absolute concentration. Third, due to the practical difficulties of having gaseous H<sub>2</sub>O in gas bottles, the concentration of the components in the gas bottles were normalized without water. Due to these factors, the concentrations of species that were tested experimentally in the Ricardo Hydra engine do not perfectly match the concentrations that exited the fuel reformer, which creates some uncertainty that the combustion results will be representative of single-fuel RCCI with onboard reforming.

Due to the approximation of the reformat gas composition, verification is needed to ensure that the experimental testing of single-fuel RCCI with the approximated reformat gas composition can accurately capture the burn characteristics of single-fuel RCCI. Therefore, the CFD model that was previously validated against experimental data is now used to determine the differences in the combustion characteristics of the experimentally feasible reformat composition and the actual reformat composition as measured by the GCMS. Figure 6 shows simulation results of these two slightly different compositions. The solid black line corresponds to the approximated gas composition that was used in the experiments, while the dashed red line corresponds to the actual reformat composition as measured by the GCMS. For these cases, the intake temperature was adjusted to match the combustion phasing between the two cases. The difference in intake temperature was 4 K. The results show that there is a negligible difference in the heat release and pressure traces between the two composition once the combustion phasing is matched with the 4 K change in intake temperature. These results provide confidence that the approximated reformat composition is a good representation of the actual reformat composition that leaves the fuel reformer and that the practical limitations in gas bottle compositions will not affect the results or conclusions.



*Figure 6. Comparison between CFD results of the experimentally tested reformat composition that was capable of being ordered and stored in gas bottles and the actual reformat fuel mixture as measured by the GCMS showing that there is a negligible difference between the combustion characteristics of the two mixtures.*

## Experimental results

To experimentally study single-fuel RCCI, each of the diesel reformat mixtures were used as the low reactivity fuel and the parent diesel fuel was used as the high reactivity fuel. The combustion process was tested over a wide range of operating conditions, including two different piston profiles; a production diesel re-entrant bowl piston and a wide shallow bowl piston. For the experimental results in this paper, the shallow bowl piston is used. A future study will include a detailed comparison of the two different piston profiles and their influence on the combustion process. This paper focuses on the heat release, efficiency, and emissions characteristics of reformat-diesel RCCI compared to RCCI with conventional fuel pairs at a constant combustion phasing and IMEPg.

Cylinder pressure and heat release rates are shown in Figure 7. Figure 7 contains two conventional fuel pairs for RCCI combustion. One of the conventional fuel pairs in Figure 7 is diesel and gasoline, where diesel is the high reactivity fuel and gasoline is the low reactivity fuel. This case is referred to as “Gas - diesel” in the legend in Figure 7. The second conventional fuel pair is diesel as the high reactivity fuel and natural gas as the low reactivity fuel (labeled “CNG - diesel”). Figure 7 also shows the pressure and heat release rate for the two reformat-diesel RCCI cases (labeled “DR1 - diesel” and “DR2 - diesel”) such that single-fuel RCCI can be compared to the conventional fuel pairs. The peak of both the low- and high-temperature heat release of gasoline-diesel is much higher than the other three fuel pairs. The higher peak of the low-temperature heat release (LTHR) for gasoline-diesel is most likely caused by the addition of the LTHR from the direct injected diesel fuel and the LTHR from gasoline, which has been shown to exhibit LTHR at boosted and high compression ratio conditions. On the other hand, none of the

other three low reactivity fuels exhibit LTHR [31]. Therefore, all of the LTHR that can be observed from those fuel pairs is only contributed from the diesel fuel, which makes their LTHR peak significantly lower. Since gasoline has the lowest octane rating among the four low reactivity fuels, the reactivity separation between the direct injected diesel and the premixed fuel is lowest for the gasoline-diesel case. This lower reactivity separation results in the higher peak of the high-temperature heat release rate (HTHR) of gasoline-diesel RCCI that can be seen in Figure 7, due to the milder reactivity gradients that exist in the cylinder.

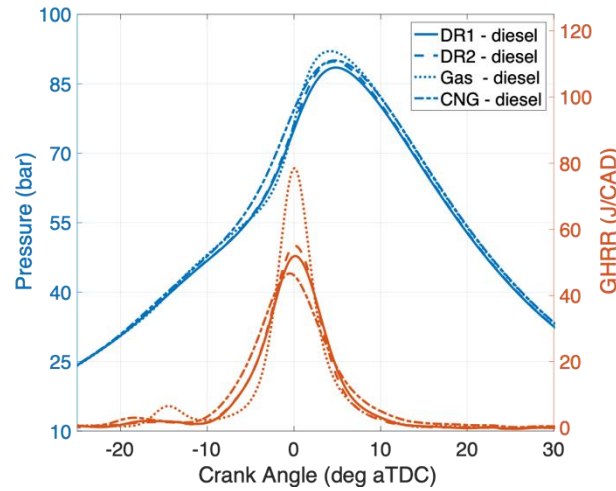


Figure 7: Cylinder pressure and gross heat release rate of RCCI combustion using both of the reformat fuel mixtures with diesel as the direct injected high reactivity fuel compared against the pressure and heat release rate of conventional RCCI fuel pairs (i.e., gasoline–diesel and natural gas–diesel) at 1200 rpm and a gross load of ~5.0 bar

In addition to the pressure and heat release results shown in Figure 7, other relevant operating conditions and combustion characteristics are compared in Table 4. To maintain combustion phasing and IMEP<sub>g</sub> constant while the fuel properties and reactivities changed significantly, a number of other operating conditions needed to change. Specifically, the large difference in the reactivity of the four premixed fuels (i.e., their octane ratings ranged from 87 to 130) requires changes to the control inputs of RCCI combustion. Intake temperature ( $T_{int}$ ), start of injection (SOI) timing of the diesel fuel, exhaust gas recirculation (EGR), and the energy-based blend ratio (BRe) are the most common input parameters to control the combustion phasing in RCCI and these four parameters were varied to attain a constant IMEP<sub>g</sub> and CA50. First, the two reformat mixtures are compared. Since air is used as the oxidizer during CPOX reformation, both the reformat fuels were highly diluted, mainly with nitrogen and the reformat mixtures have a similar octane rating [31]. This high concentration of diluents in the gaseous reformat mixture displaced intake air, which lowers the oxygen concentration in the cylinder and increases the equivalence ratio for a given load level. Therefore, the intake pressure needed to be elevated to 1.4 bar to counteract the oxygen deficiency. Additionally, the diluents in the reformat mixture act as a heat sink, in a similar way to EGR, which required the intake temperature to be raised to 340 K to achieve reasonable combustion phasing. The differences in the concentration of CO, CO<sub>2</sub>, and N<sub>2</sub> between the two reformat fuel mixtures (see Table 2) resulted in minor difference in their reactivity, which would have resulted in a slight change to the combustion phasing if all other parameters were held constant. Instead, this slight difference in reactivity was compensated for by

adjusting the SOI timing by 2 crank angle degrees (CAD) to match combustion phasing. This molar concentration difference in the two reformat mixtures is due to the variation in the operating condition of the reformation process. These results suggest that difference in the composition that results from the reformation process can be compensated for with slight changes to the blend ratio or injection timing. In other words, the combustion process of single-fuel RCCI with onboard fuel reformation is not overly sensitive to the exact reformat composition, which is beneficial for the potential commercial control strategy of reformat RCCI.

In addition to comparing the combustion characteristics of the two different reformat compositions with each other, reformat RCCI can also be compared with conventional RCCI with gasoline-diesel in Figure 7 and Table 4. Gasoline is much more reactive than either of the reformat fuels, as mentioned earlier, which required the input parameters to change to maintain IMEPg and CA50. It was not possible to achieve an IMEPg of 5 bar at the same blend ratio as the reformat RCCI cases, irrespective of the CA50 phasing, before being limited by the maximum pressure rise rate (MPRR). Therefore, the intake temperature was reduced by ~20 K and the injection timing was advanced by 15 degrees. With gasoline-diesel at these conditions, it was possible to achieve an IMEPg that was comparable to the reformat RCCI cases; however, the combustion phasing could not be delay enough to match the reformat RCCI cases. Therefore, 35% external EGR was applied to match the combustion phasing, at a slight penalty to combustion efficiency.

Finally, natural gas-diesel RCCI was compared with the reformat RCCI cases. Natural gas has the highest octane rating among the four low reactivity fuels that have been used (octane number ~ 130). Additionally, natural gas also has a significantly higher energy density than the reformat mixtures, due to the lack of diluents. Therefore, natural gas does not displace as much fresh intake air as the reformat mixtures, and at the same intake pressure, the equivalence ratio with natural gas was noticeably lower. This effect, along with the higher octane rating of natural gas, meant that some of the input parameters needed to be adjusted to match CA50 and load to the reformat RCCI cases, similarly to gasoline-diesel RCCI. It was not possible to achieve the same CA50 as the reformat RCCI cases with a BRe lower than approximately 49%. There were three ways to match the CA50 at the IMEPg of 5 bar: 1) increase the BRe, 2) add EGR and adjust the diesel SOI timing and fuel masses to maintain the BRe constant, or 3) increase the intake temperature and adjust the SOI timing. The first approach was used since it required fewer changes to the input parameter to match the combustion phasing and IMEPg. Therefore, the BRe was increased to 49% for the natural gas case.

The indicated thermal efficiency of the four cases are compared in Table 4. Since the IMEPg and combustion phasing were constant, the indicated thermal efficiencies are all fairly similar. The natural gas-diesel case has the lowest efficiency, possibly due to the long burn duration, although the burn duration for the reformat RCCI cases was also long without incurring an efficiency reduction. This could be due to a thermodynamic gamma benefit from the diluent species in the reformat mixtures but more analysis and case studies would be required to determine definitively. However, these results conclusively show that single-fuel RCCI with CPOX reformation is capable of achieving efficiencies that are at least equal to, if not greater than, conventional dual-fuel RCCI.

Table 4: Operating conditions and combustion characteristics of reformat–diesel RCCI compared to RCCI with conventional fuel pairs including gasoline–diesel and natural gas–diesel

Low reactivityfuel	EGR	IMEPg	BRe	T <sub>int</sub>	$\Phi$ (global)	SOI	Ind. Thermal Efficiency	Combustion Efficiency	CA50
-	%	bar	%	K	-	deg aTDC	%	%	deg aTDC
<b>DR1</b>	0	4.9	42	340	0.40	-53	43.5	92.5	0.1
<b>DR2</b>	0	4.9	42	340	0.36	-55	44	91.7	0
<b>Gasoline</b>	35	5.2	44	321	0.51	-70	42.3	92.4	0
<b>CNG</b>	0	5.1	49	340	0.35	-57	41.3	90.0	-0.2

The indicated specific emissions for the four cases are compared in Figure 8. Reformat RCCI has higher CO and CO<sub>2</sub> emissions compared with conventional RCCI when either gasoline or natural gas is used as the low reactivity fuel. This is due to the composition of the premixed fuels. In the case of the reformat fuels, both DR-1 and DR-2 have CO and CO<sub>2</sub> in the fuel itself, since they are products of CPOX reformation. Additionally, the H/C ratio contributes significantly to the CO and CO<sub>2</sub> emissions that are produced from combustion. From Table 2, it can be seen that natural gas has the most favorable H/C ratio among the four premixed fuels, which leads to the lowest CO and CO<sub>2</sub> emissions. Following natural gas, gasoline exhibits the second lowest IS-CO and IS-CO<sub>2</sub> and its H/C ratio is second highest. Finally, both of the reformat fuels have the least favorable H/C ratio since they are the partial oxidation products of the parent diesel fuel whose H/C ratio is the lowest (at approximately 1.77). Therefore, reformat RCCI has higher CO and CO<sub>2</sub> emissions than conventional dual-fuel RCCI.

However, unburned total hydrocarbons (THC) and NO<sub>x</sub> emissions display the opposite trend; reformat RCCI has lower emissions levels than conventional RCCI. The trend of THC is the opposite of the CO and CO<sub>2</sub> because, while the reformat fuels have CO and CO<sub>2</sub>, they do not have high levels of hydrocarbons. Therefore, any unburned premixed fuel in the crevices or colder/leaner regions of the cylinder will contribute to elevated CO emissions, but not THC emissions. Meanwhile, any unburned premixed regions in the gasoline or natural gas cases will not contribute to the CO emissions; however, they will directly contribute to the THC emissions. The NO<sub>x</sub> emissions are low for all the four cases due to the lean equivalence ratios and low peak combustion temperatures. It was therefore extremely difficult to determine a significant trend within the four different cases since their differences are within the limits of the accuracy of the NO<sub>x</sub> analyzer. However, it can be concluded that the NO<sub>x</sub> emissions of single-fuel RCCI with CPOX reformation are at least as low as conventional RCCI combustion.

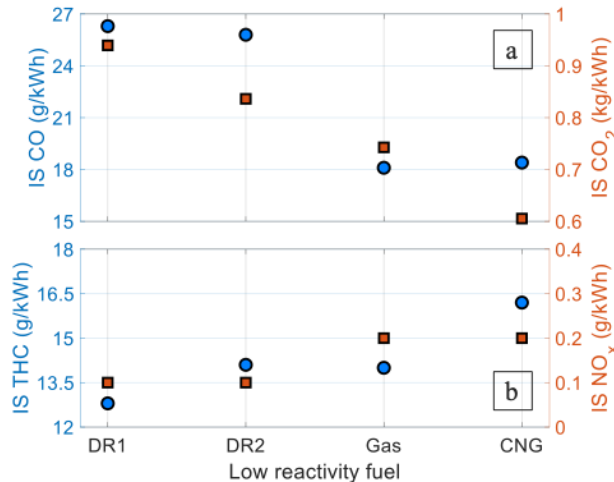


Figure 8: a) IS CO and IS CO<sub>2</sub> and b) IS THC and IS NO<sub>x</sub> emissions of reformate RCCI compared with conventional dual-fuel RCCI

### Conclusions:

“Single-fuel” RCCI was investigated experimentally using reformate fuel mixtures generated from a CPOX reformation process of diesel fuel. Their combustion characteristics were compared with conventional gasoline-diesel RCCI and natural gas-diesel RCCI. A CFD model was also developed and validated against the experimental results. The model’s ability to capture the physical trends was tested by studying the effect of the start of injection in both the CFD simulations and the experiment. The CFD model was then used to validate the approximation of reformate species required for experimental testing. From this detailed analysis of the results, the following conclusions can be drawn:

1. “Single-fuel” RCCI using the direct injection of diesel with diesel’s reformate mixtures as the premixed fuel shows high thermal efficiencies, low emissions, and good controllability. The efficiency was at least equal to, if not better than, conventional RCCI (gasoline-diesel and natural gas-diesel). IS-NO<sub>x</sub> and IS-THC emissions of reformate RCCI were better than conventional RCCI. However, IS-CO and IS-CO<sub>2</sub> were slightly higher than conventional RCCI, due to the unfavorable H/C ratio of diesel (the parent fuel of the reformate).
2. The high concentration of diluents in the reformate mixture displaces incoming air and acts as built-in EGR. Since the reformate fuel displaces a large fraction of intake air, the intake pressure needs to be elevated to counteract the oxygen deficiency.
3. The reactivity of the reformate mixture is lower than gasoline but higher than natural gas. Since the high reactivity fuel in all four cases is diesel, the reactivity separation follows the same trend as the octane rating of the premixed fuel. Therefore, the combustion behavior of reformate RCCI was between, but similar to, the two conventional RCCI fuel pairs.
4. Either from the CFD simulations results, or from experimentally testing the two different reformate fuel compositions, it can be concluded that single-fuel RCCI with onboard fuel reforming is not overly sensitive to the specific composition CPOX reformate. Small adjustments to conventional control parameters (including start of injection timing, blend ratio, and EGR) can be used to compensate for differences in the reformate composition.

**Acknowledgement:**

The authors wish to gratefully acknowledge the financial support of the Department of Energy under award number DE-EE0007216.

**Appendix:**

Uncertainties in experimental data measurements and instruments are unavoidable. Based on a detailed uncertainty analysis, the uncertainty of the indicated thermal efficiency was calculated. Since the actual indicated thermal efficiency is calculated from the gross IMEP, mass of low reactivity and high reactivity fuels, and combustion efficiency, their uncertainties were used as the factors to calculate the uncertainty of ITE. The following values were calculated and tabulated:

Table A.1: Calculated uncertainty values in the combustion characteristics.

Low reactivity fuel	Uncertainty in				
	IMEPg (bar)	PFI fuel (g)	DI fuel (g)	Combustion efficiency (%)	Thermal efficiency (%)
DR1	±0.14	±3e-4	±7e-4	±2.1	±1.5
DR2	±0.13	±2e-4	±6e-4	±1.9	±1.4
Gasoline	±0.04	±12e-4	±10e-4	±0.3	±2.0
CNG	±0.09	±2.2e-5	±2e-4	±2.1	±1.1

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