Numerical Analysis of the Effects of Direct Dual Fuel Injection on the Compression Ignition Engine

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ABSTRACT: In this work, the influence of direct dual fuel injection on a compression ignition engine fueled with gasoline and diesel has been investigated. To do this, closed cycle combustion simulations have been performed. Gasoline has been supplied through port injection and early direct and late direct injection to achieve fuel stratification and emission reduction. Simulations have been done for various start of injection (SOI) timings of diesel fuel. A detailed discussion on a low temperature heat release (LTHR) mechanism has been done. Results revealed that the maximum gross indicated thermal efficiency (GITE) of 39% is obtained for port injection of gasoline mode. Direct dual fuel combustion (type 2) (DDC2) mode shows approximately 2% and 38% less GITE and oxides of nitrogen (NOx), respectively, and 40% more soot as compared to the port injection gasoline mode. DDC2 mode shows lower oxides of carbon and hydrocarbon emissions as compared to other dual fuel modes. More than 99% of combustion efficiency and less maximum pressure rise rate have been noticed in the DDC2 case. Strong LTHR and high temperature premixed combustion region have been found in advanced SOI timing cases (in DDC2). In-cylinder contours for the DDC2 case show that diesel and gasoline fuels combusted successively cause less in-cylinder temperature than that for the conventional dual fuel combustion case.

1. INTRODUCTION

Compression ignition (CI) engines are majorly used in the stationary prime movers and heavy vehicles because of their higher fuel conversion efficiency and durability. The heterogeneous combustion nature of CI combustion leads to more oxides of nitrogen (NOx) and soot emissions. Different operating and mixing strategies have been used to reduce the harmful emissions and to enhance the engine efficiency. High exhaust gas recirculation (EGR), early and late injection timing, and dual fuel supply are used to achieve lower exhaust emissions. Reactivity-controlled CI (RCCI) combustion mode has been shown to be more advantageous among different combustion strategies under low temperature combustion (LTC).\(^1\) RCCI mode uses dissimilar fuel reactivity to achieve an LTC strategy and to reduce NOx and soot emissions simultaneously. Usually, in RCCI mode, low reactivity fuel (LRF) is injected near the intake port to form a premixed charge and the high reactivity fuel (HRF) is directly injected into the cylinder to initiate combustion. Dual fuel combustion refers to use of two fuels in order to get defined engine outcomes. RCCI mode comes under the roof of LTC by changing the reactivity of fuels. Combustion phasing and flame propagation of RCCI combustion depend on the reactivity gradient and its spatial distribution as well as mass ratio of both fuels.\(^2\) Xu et al.\(^3\) studied the effect of the gasoline substitution ratio (GSR) (37–66%), start of injection (SOI, in degree) timing of diesel (−50 to 0 after top dead center, aTDC), and EGR valve opening (0–70%) on the engine characteristics. About 70, 48, and 67% reduction of combustion duration (CD), NOx, and soot, respectively, were reported while increasing the GSR. During the injection timing sweep, an increasing and a reducing trend in NOx was observed, and soot follows the opposite trend of the NOx trend.
Figure 1. Different fuel spray strategies: (a) CDFC, (b) DDC0, and (c) DDC1 and DDC2.

NOx and soot emissions and shorter combustion phasing were reported with EGR sweep. It was concluded that 66% GSR, −30 to −15 SOI, and 30% EGR valve opening show better engine outputs. However, knock intensity, hydrocarbon (HC), CO, and soot morphology were not discussed. Lee et al. reported that RCCI mode combustion (70% GSR) depicted 28% longer ignition delay (ID) period, 15% higher thermal efficiency, and 96% lower NOx than that of conventional diesel combustion (CDC) mode. Benajes et al. reported the influence of direct injection (DI) of the gasoline/diesel (70:30; 50:50) mixture in RCCI mode combustion. Different direct fuel (diesel) injection timing ranging between −60 and −20 SOI and EGR substitution effect were also analyzed. Results suggest that gasoline mixing reduces the HRF reactivity, thereby increasing the LRF reactivity gradients. This mode significantly reduces both CO and HC emissions and increases NOx emissions due to high combustion temperature. However, 50:50 diesel and gasoline mixture mode has worse combustion phasing because of early and rapid combustion reactions. It was concluded that the 70:30 mixture (40% EGR and 60% GSR) provides ultralow NOx and smoke emissions. Martin et al. investigated different combustion modes in between the CDC and RCCI modes. These combustion modes were accomplished by late DI fuel, early DI fuel, manifold port injection, and a combination of them. Premixed dual fuel combustion produces improvements on NOx, soot, and thermal efficiency similar to RCCI but without the high peak pressure and rate of pressure rise.

Premixed mode of LRF supplied engine operations has some limitations like higher HC and carbon monoxide (CO) emissions and cycle-to-cycle fluctuations. Because of the uniform charge formation, inefficient burning of the charge occurs near the walls and crevices. Many researchers claim that these issues could be reduced by DI of LRF into the cylinder. Direct dual fuel injection is one of the promising ways to control the mixing charge process in a dual fuel engine. Li et al. conducted a comparison study for different dual fuel combustion modes. The benefits of the direct dual fuel combustion (intelligent charge CI, ICCI) over RCCI mode combustion were reported. In ICCI, a portion of gasoline is injected directly into the cylinder at −280 SOI to form premixed air−fuel charge. Then, at compression stroke, diesel and gasoline are alternatively injected to create arbitrary stratification of charge. As compared to RCCI mode, almost similar NOx and soot emissions with 1.5% higher thermal efficiency have been reported in ICCI mode. ICCI mode shows better combustion efficiency up to 8 bar indicated mean effective pressure (IMEP) and for higher IMEP cases RCCI mode produces higher combustion efficiency. Saccullo et al. investigated the effect of diesel and methanol fuels in direct dual fuel combustion. To achieve better combustion phasing, fuel 1 (diesel) was injected at −12 SOI and fuel 2 (diesel or methanol) injected at −6° SOI was reported. As compared to diesel−diesel case, diesel−methanol case displays 19 and 98% lower NOx and soot emissions respectively, and 13% higher in-cylinder pressure with comparably lower thermal efficiency. Long et al. reported the effects of direct dual fuel combustion on CI engine. In this study, 10% ethanol−90% gasoline has been taken as LRF and diesel is used as HRF. HRF injection timing was changed from −26 to −11 SOI and the LRF SOI changes from −90 to −45 SOI. It was concluded that direct dual fuel injection strategy can efficiently and robustly control the combustion phasing and emissions of premixed combustion mode operation. A higher value of LRF injection pressure (600−900 bar) can produce more lean uniform distribution of fuel, which increases the HC and CO emissions. Ning et al. investigated the effects of injection timing on methanol/diesel dual DI engines. Methanol injection timing changed from −60 to −30 SOI. Diesel injection timing and methanol injection duration were adjusted to keep the engine load. Diesel and methanol injection pressures were maintained at 1000 and 120 bar, respectively. Increase in BTE, coefficient of variance of IMEP (COV_{IMEP}), HC, NOx, and reduction in CO and soot were observed during methanol substitution sweep. Yang et al. reported the effects of injection timing of HRF and LRF on the DI of methane and diesel dual fuel combustion. Decreases in COV_{IMEP} were observed with retarded injection timing of LRF. During the port fuel injection, some of the fuel is pushed out through intake port because of the late intake valve closing which causes the charge formation in the valve port and combustion deck. In the case of use of alcoholic fuels, its corrosive property damages the intake path and valve stem. Generally, exhaust gas temperature (EGT) of the gasoline port injection (GPI) engine is about 300−400 °C whereas it is around 600 °C for the gasoline DI (GDI) engine which assists catalytic converter operations. GDI produces more torque over a wide range of speeds as compared to the GPI case. Garcia et al. stated that high HC and CO emission levels combined with the low EGT during RCCI could present a challenge for the present exhaust after-treatment technologies.

Hence, DI of LRF has predominant benefits as compared to the port fuel injection case. Moreover, the RCCI mode engine is limited to medium loads and medium GSR, beyond which it shows more cycle-to-cycle variations. The reactivity gradient and its spatial distribution of dual fuel mixture dominate the engine performance characteristics. The different degree of charge mixture will be obtained by adjusting the relative chronology of the HRF and LRF. To get charge stratification, injection characteristics (injection pressure, timing, and orientation of spray plume) of LRF become more significant. Initially, experimental work has been conducted in conventional dual fuel combustion (CDFC) mode, and the CDFC mode outcomes are validated by the numerical simulations.
Then, numerical work has been performed for different DI of LRF cases. Different orientations of LRF spray plume with respect to HRF spray plume have been analyzed. Finally, a simulation work has been performed to analyze the effects of SOI of HRF on the engine performance. To achieve this, a full cylinder model has been used along with two fuel injectors. Finally, a low temperature heat release (LTHR) mechanism and soot modeling analysis have been performed.

2. DUAL DIRECT INJECTION

During CDFC mode, diesel is injected into the premixed charge to initiate the combustion. Figure 1a shows the single diesel spray plume for CDFC mode operation. For later cases, simulations alone have been performed for different direct dual fuel (injection) combustion (DDC) to reduce the time, experimental work, and expenditure. Initially, LRF and HRF spray plumes are kept at different spray plume positions, thereby increasing the air entrainment effect and charge homogeneity. In this spray pattern, the angle between the LRF and HRF is 60° (z axis). Here, both injectors have been placed at the center of the cylinder and closer to each other, as shown in Figure 1b. Unfortunately, this mode could not produce better results as compared to the CDFC case. Then, the spray plume position (injector clocking; circumferential rotation of the injector\textsuperscript{16}) of LRF changed to coincide with the spray angle of HRF, as shown in Figure 1c. Generally, injection pressure of gasoline in the GDI engine ranges from 50 to 500 bar.\textsuperscript{17} However, published papers\textsuperscript{18−20} suggest the use of 150 and 130 bar injection pressures based on the fuel property and exhaust emissions. Based on the literature study, SOI of LRF has been set at −50 SOI and the injection pressure has been set as 130 bar. HRF injection timing has been changed in order to get the desired combustion phasing similar to the earlier CDFC case. The SOI has been changed from −23 to −15 SOI. The amount of LRF and HRF fuel supply has been taken from −25 SOI gasoline/diesel CDFC case, and it has been fixed to all gasoline/diesel trials. Another direct dual fuel injection strategy (DDC2) has been tried to overcome the drawbacks associated with the earlier direct dual fuel injection (DDC1) strategy. In this strategy, SOI of gasoline occurs after the SOI of diesel fuel. After a number of trials, it has been found that SOI of gasoline after 2 CAD of SOI of diesel shows better results. Figure 2 (left) shows the computational domain at TDC with a grid in a vertical cross section along the spray axis. The evolution of the number of computational cells against the crank angle is shown in Figure 2 (right). To reduce the complications and for the ease of comparisons, the same technical specification of the diesel injector has been used for the direct LRF injector.

3. RESULTS AND DISCUSSION

Figure 3 (left) shows the pressure and HRR of DI of gasoline and diesel combustion (DDC1). This type of fuel injection strategy produces stratification charge CIC\textsuperscript{21} combustion and thereby reduces the unburned fuel emissions. Similar to earlier CDFC cases, the advanced SOI case shows higher in-cylinder pressure and temperature. Retarded SOI (−15 and −17) cases show less maximum pressure rise rate (MPRR) as compared to...
advanced SOI (−21 and −23) cases. Advance SOI timing cases show a longer ID period because the fuel is injected at a low temperature charge. This situation leads to more air–fuel mixture formation before the oxidation reactions, resulting in a rapid combustion process. Moreover, longer CD has been observed for retarded SOI cases, and it can be observed from the HRR graph (note: HRR values obtained from pressure trace values). DDC2 cases (Figure 3, right) show similar in-cylinder pressure increase with SOI as compared to DDC1 cases. However, the pressure curve follows different patterns for both DDC1 and DDC2 cases. The pressure rise follows an almost convex pattern in DDC1 and concave pattern in DDC2 mode.

It is noted that both NOx and soot emissions increased with SOI advance in DDC1 mode because of the higher combustion temperature and higher equivalence ratio (Figure 4, left). In the DDC2 test set, SOI of diesel has been varied from −21 to −29 SOI, and the results are shown in Figure 4. However, increase in NOx and reduction in soot trends have been observed with SOI advance for both CDFC and DDC2 modes. Similar outcomes were reported by Sindhu et al. HC and CO emissions are higher in both DDC1 and DDC2 modes, as compared to port-injected gasoline CDFC mode. Approximately, 2 and 38% lower gross indicated thermal efficiency (GITE) and carbon dioxide have been observed, respectively, in DDC1 mode as compared to the CDFC mode. DDC2 mode shows better combustion and emission performances as compared to the DDC1 strategy. About 38% lower NOx and 40% higher soot emissions have been observed in dual fuel injection cases as compared to the earlier CDFC case. In addition, about 60% rise in HC and 60% fall in CO emissions have been observed along with significant reduction in GITE.

Figure 4 (right) shows the combustion parameters for different test trials based on simulation results. Combustion efficiency loss (CEL) depicts the successful burning of fuel molecules, and it has been calculated based on cumulative heat release and energy supplied (simulation). It has been noted that combustion efficiency (1-CEL) increases with advancing of SOI timing of HRF. Yousefi et al.25 stated that advancing of fuel injection timing and fuel injection pressure enhanced the air–fuel mixing process, which improves the combustion efficiency. About 38.5 and 78% reduction of CEL has been noticed for DDC1 and CDFC cases, respectively, during the HRF injection timing sweep. More than 99% of combustion efficiency has been predicted for DDC2 cases, and this value is almost equal to CDC.24 EGT plays an important role in soot oxidation and efficiency of the exhaust after-treatment system.26 DDC2 mode displays approximately 10 °C more EGT as compared with CDFC and DDC1 modes. Reduced EGT trends have been noticed with advancing of HRF injection timing because of the reduction of the diffusion combustion phase. DDC2 mode has a less premixed (uncontrolled) combustion phase and more diffusion (controlled) combustion phase, as compared with DDC1 and CDFC because of the successive injection of LRF. MPRR depicts an increasing trend with advancing of injection timing. As the HRF injection timing is advanced, the charge temperature is not sufficient to ignite the fuel. As a result, more HRF fuel gets accumulated during the ID period and is prone to a rapid combustion process, which increases the rate of pressure rise.27 CDFC mode shows high MPRR values as compared to other test modes because of the better LRF and HRF mixing and combustion. In DDC2, diesel is combusted first and then gasoline is combusted, which reduces the cumulative burning nature of LRF and HRF, thereby minimizing the MPRR. In DDC2, about 68% increase in MPRR has been observed for −29 SOI as compared to −21 SOI because of shift of combustion phasing toward the top dead center. While considering engine safety and noise reduction, MPRR should be maintained below 5 bar/CAD; hence, DDC2 mode is more safer than CDFC mode. DDC1 mode has a minute increasing trend of CD with advancing of injection timing. However, both CDFC and DDC2 modes...
follow a decreasing trend with SOI of HRF. As discussed earlier, advanced SOI timing provides longer ID, which reduces the CD, and similar outcomes have been reported by Teoh et al.\textsuperscript{29} The spatial distribution of HRF merges with LRF spray plume. However, LRF is injected earlier which reduces the LRF entrainment effect in-line with retardation of HRF. Hence, advance SOI timing of HRF increases the percentage of burning of LRF as compared to late SOI timing of HRF. Therefore, CD increases with SOI timing of HRF in DDC1 cases and the complementary higher unburned HC and CO emissions have been predicted for late SOI timing cases. Li et al.\textsuperscript{30} reported that longer ID was observed for advance SOI of HRF in CDFC mode. Moreover, the ID period increases (at $-35$ SOI) with augmentation of the LRF substitution ratio with respect to HRF. However, it shows significant reduction in the ID period with the LRF substitution ratio for the late SOI case ($-17$ SOI). Generally, longer ID results in shorter CD because of the higher premixed combustion phasing, which causes more NOx emissions and MPRR.\textsuperscript{31} Both CDFC and DDC1 modes adhere to the earlier statement; however, DDC2 mode follows a different trend. It can be observed that the ID period decreases up to $-21$ SOI and increases for later SOI cases. Finally, a longer ID period has been observed for DDC2 mode because of early SOI timings, but this mode also produces longer CD because of subsequent injection of HRF and LRF.

Figure 5 (left) depicts the comparison of combustion species (OH, HCHO, and heptyl peroxy radicals) and combustion parameters for CDFC, DDC1, and DDC2 modes. For advanced SOI timing cases and charge condition, the combustion process is characterized by single-stage LTHR and followed by single-stage high temperature heat release (HTHR). The first stage is also named as cool flame reaction, and it occurs below the auto-ignition temperature of the fuel and a detailed report can be found in ref \textsuperscript{32}. Pan et al.\textsuperscript{33} reported that less than 10% of total HRR and 900–1100 K of temperature were observed during the cool flame. Similar outcomes have been observed in CDFC and DDC1 modes. The $\text{C}_7\text{H}_{15}\text{O}_2$ yields ketohydroperoxide and OH components during cool flame reactions. Then, ketohydroperoxide yields formaldehyde (HCHO) and OH radicals along with other species.\textsuperscript{34} CDFC mode depicts short and intense premixed combustion phasing after a small LTHR zone, and in addition, double HTHR peaks have been predicted. Clear cool flame reaction is observed for both DDC0 and DDC1 cases as compared to the CDFC case. However, no evidence of double HTHR peaks has been observed. Some form of LTHR has been noticed in the DDC2 case along with the double HTHR pattern. CDFC mode shows higher in-cylinder temperature as compared to other test cases because of the earlier combustion phasing. Both DDC0 and DDC1 cases show a similar temperature profile. However, significantly less in-cylinder temperature is noticed for DDC2 case because of the progressive combustion of HRF and LRF. Hence, it can be stated that DDC2 mode works under the LTC strategy.\textsuperscript{35} Aglave\textsuperscript{36} reported the low temperature oxidation mechanisms. At temperatures lower than about 900–1000 K, most important reaction is the addition of oxygen to alkyl radical to form alkylperoxy radical ($1-\text{C}_7\text{H}_{15}+\text{O}_2 \rightarrow 1-\text{C}_7\text{H}_{15}\text{O}_2$). Then $1-\text{C}_7\text{H}_{15}\text{O}_2$ (C$_7$H$_{15}$O$_2$ radical) undergoes isomerization to form alkenyl-hydroperoxide or undergoes further reactions with HO$_2$ to form hydrogen peroxide and few other radicals. Higher quantity of the alkylperoxy radical has been observed for the CDFC case as compared to direct dual fuel combustion cases. The cool flame reactions expedite the high temperature reactions because they produce more free radicals. The DDC2 case shows less alkylperoxy radicals during the cool flame reactions, resulting in lower HTHR as compared to the CDFC case. CDFC mode shows less HCHO species as compared to direct dual fuel combustion cases. CDFC shows a rapid increase of OH species during the premixed combustion of HRF. Then, it follows a progressive pattern because of the
initiation of LRF combustion. The production rate of OH species is very high in DDC1 because of the fuel stratification. Generally, OH species represents the high temperature combustion regions. In the CDFC case, the LRF is spread across the entire combustion chamber, and hence, the flame takes a certain time to consume it. Conversely, in DDC1 mode, the LRF has been involved in reactions once the HRF initiates the combustion process. Hence, the temperature and HRR show a rapid change as compared to the other two modes. DDC2 mode shows progressive combustion phasing resulting from HRF and LRF combustion. Double HRR peaks have been observed during HRF and LRF combustions in DDC2. This mode depicts the minimum in-cylinder temperature and a prolonged HRR as compared to DDC1 mode. SOI timing of HRF plays an important role on the location and quality of LTHR; hence, the effect of SOI has been analyzed. Figure 5 (right) illustrates the combustion parameters for DDC2 mode for different SOI timings. As discussed earlier, C_7H_15O_2 is an intermediate combustion radical which indicates the low temperature fuel oxidation. Increasing of the C_7H_15O_2 radical has been observed for advancing SOI timings and the complementary outcomes can be seen in the HRR curve. Double peaks in HRR (HTHR) have been observed for retarded SOI timing cases, but this phenomenon disappears with advanced SOI timings. A longer ID period has been noticed for advance SOI timings, and this situation is favorable for cool flame reactions. The relation between the LTHR and injection timing and its effects on HTHR have been reported by Cong et al.\(^3^7\) As discussed previously, in-cylinder temperature increases with advanced SOI timings. Formaldehyde (HCHO) is an intermediate combustion species and is generated during the low temperature oxidation condition and is mostly consumed during high temperature combustion. Cung et al.\(^3^8\) reported the production and consumption of HCHO during the combustion process. Generally, the OH radical (later than the HCHO radical) is present in the oxidation and burned gas regions during high temperature combustion.\(^3^9\) The OH radical has a significant impact on the NO formation and soot oxidation. The OH radical rapidly increases, while advancing the SOI timing, and this boosts the combustion reactions, resulting in higher HRR. This combustion situation increases the NO formation (N + OH \(\rightarrow\) NO + H) and soot oxidation (C_{soot} + OH \(\rightarrow\) CO + products).\(^4^0\)

The LTHR plays a vital role in the combustion radical formations and shape of the HTHR profile. In order to determine the significant reactions that lead to low temperature ignition, all the elementary reactions have been analyzed. Figure 6 depicts qualitatively the changing trend of elementary species mass (kg/CAD) during low temperature ignition reaction. The reactions involved in the LTHR or before initiation of ignition are shown in Figure 6 (left: CDFC and right: DDC2 case at \(-23\) SOI). Negligible involvement of isooctane reaction species can be noted in LTHR formation as compared to \(n\)-heptane reaction species. Xu et al.\(^3^7\) reported that a longer ID period was observed for isooctane than that of \(n\)-heptane. The vital reaction species involved in the path from \(n\)C_7H_16 to low temperature ignition are shown in Figure 6 (\(n\)C_7H_16 to C_7H_11CO). The chemistry is chiefly dominated by the formation and oxidations of alkylperoxy radicals, particularly, oxidation of HCs at low to intermediate temperature.\(^4^2\) Guo and Wang\(^4^3\) reported that more than
90% of mass of the C7H15 (heptyl) radical will transform into the C7H16O radical, and moreover, it is an equilibrium reaction. It can be observed that an increase in the C7H15 radical mass is due to n-heptane and oxygen reaction. With an increase in the amount of C7H15, the conditions for forming C7H16O2 are more. Hence, more C7H16O2 radicals have been perceived in LTHR. The detailed forward and backward reaction of this mechanism can be found in ref 43. Oxidation of the C7H15 radical is an exothermic reaction, and the backward reaction of C7H15O2 is an endothermic reaction. This reaction slightly increases O2 (oxygen) mass fraction and absorbs some heat energy (drop in HRR). The O2 molecule has a significant effect on C7H16O2 production; hence, C7H16O2 production slows down for O2 dilution scenarios. Hence, conditions like EGR addition and more GSR cause comparatively less O2 presence, postponing the C7H15O2 and C7H15O2 production. In cool flame regime, the C7H15O2 (alkylperoxy or heptyl-peroxy) radical undergoes isomerization reaction to form C7H15OOH. The literature reports that isomerization toward C7H15OOH (alkylperoxy-alkyl) species formation results in enhanced overall reactivity. C7H15OOH decomposition reactions and the OH radical consuming reactions (by HCHO, HO2, etc.) cause slight reduction in temperature. Comparatively, slightly more species (in LTHR) concentration has been observed for the CDFC case, and the DDC2 case shows a smooth increase and decrease of combustion species trend against the crank angle for CDFC and DDC2 case. Probably because of this continuous change in radical species, the initial LTHR is sustained for a certain period of time or till the commencing of HTHR in te DDC2 case.

The effects of SOI timing in the low temperature reaction species for DDC2 mode are shown in Figure 7. As discussed earlier, the progress of LTHR regime improves with advanced SOI timing and the complementary reduction has been noticed in the oxygen mass. It can be clearly observed that advanced SOI cases show a clear LTHR peak, as compared to retarded SOI timing. As shown in Figure 4, a longer ID period was noticed for advanced SOI cases, and this longer ID enables more fuel accumulation inside the cylinder. Hence, the −27 case shows a smooth increase and decrease of the C7H16 profile than that of the −21 SOI case. Because of shorter ID, some of the C7H16 molecules start reaction to develop C7H15 radicals. The conversion time for the C7H16 molecule into C7H15 species takes less time for the −27 SOI case as compared to the −21 case. Net mass of the C7H15 radical depends on the competition between the oxidation of the C7H16 molecule and decomposition of C7H15O2 species. In the −29 SOI case, the C7H15 radical has a flat trend between the increasing trend. However, this trend could not be observed in the −27 SOI case, but a small flat trend is visible in a C7H15 decreasing slope in the −21 SOI case. No such trend has been noticed in the C7H15O2 radical and its magnitude decreases with retarded (late) SOI timings. The C7H16 molecule follows a smooth decrease trend; hence C7H15 would show an inceasent rise till its maximum point. The small flat trend (in C7H15) implies that as soon as C7H15 is formed, it is converted into the C7H15O2 radical. A small rise in C7H15 (after a flat trend) results from cumulative C7H15 production from the oxidation of the C7H16 molecule and decomposition of the C7H15O2 radical. A detailed description of this statement can be found in a published report by Vuilleumier. Then, the C7H15 radical undergoes different reaction processes and then forms the LTHR species C7H15CO radical. Details of the high temperature reactions in the n-heptane mechanism can be found in the literature.

The high temperature combustion phasing plays an important role in engine efficiency and emissions formation. Figure 8 illustrates the high temperature combustion (HTC) species trend against the crank angle for CDFC and DDC2 modes at −23 SOI timing. Rise in in-cylinder gas temperature happens in two stages for the CDFC case, but it is in a single stage for the DDC2 case. Double peaks in H2O and HCHO species have been observed for the CDFC case, and the DDC2 case shows a single peak. Formaldehyde (H2CO or HCHO) is produced/decomposed from the oxygenated HC's that are products of ketohydro-peroxide (7KET) decomposition. In addition to HCHO, a considerable amount of hydroperoxide (H2O2) is also formed. H2O2 plays a significant role in the second stage of C7H16 ignition. H2O2 is developed
mainly by combination of hydroperoxyl (HO₂) radicals that are developed during the first stage of ignition. Also, formyl (HCO) radicals are formed from HCHO and HO₂ reactions. Oxidation of HCHO and other radicals continues to develop HO₂ radicals, which continue to maintain the pool of H₂O₂.52 H₂O₂ simultaneously decomposes into OH radicals. OH radical population rises mainly from the H₂O₂ decomposition. The peak of OH regime indicates the end of the premixed (uncontrolled) combustion phasing, when CO and HC are consumed. CO is a partially oxidized species, and it is mainly produced from oxidation and decomposition of HCO. Moreover, a large portion of CO is oxidized as the temperature reaches its maximum. In CDFC, CO follows the two-stage rise because of the premixed and diffusion combustion regions. However, the final CO emission value is nearly the same for both cases. More HC species have been observed in the DDC2 case as compared to the CDFC case because of the rich air−fuel regime. Formation of NO is rapid in regions of peak OH concentration, and only a small portion of NO is transformed into other N₂O₅ species. Rapid changes in OH radicals’ trend is observed during the combustion phasing. Note that the stages of combustion mentioned in Figure 8I−V are first-stage pre-ignition, first-stage ignition (premixed combustion), second-stage pre-ignition, second-stage ignition (diffusion combustion), and late combustion (after burning), respectively. DDC2 mode shows dominant first-stage pre-ignition regime, lower
Understanding the soot formation and oxidation is quite difficult. Detailed soot evolution mechanisms can be found in previous articles. Figure 9 depicts the soot evolution processes for CDFC and DDC2 for the $-25$ SOI case. More soot formation and oxidation have been detected for the DDC2 case, as compared to the CDFC case. Dominant nucleation mode is observed for the CDFC case because of the higher in-cylinder temperature. More condensation particles have been noticed in the DDC2 case, as compared to the CDFC case. Soot formation ends around 5 CAD for CDFC and around 15 CAD for the DDC2 case. Similarly, a longer soot oxidation process has been noticed for DDC2 because of the late cycle combustion temperature.

Figure 10 shows the primary particle diameter ($D_p$) and soot particle distribution for CDFC and CCD2 cases for $-25$ SOI timing at 144 CAD (end of simulation). The $D_p$ after combustion has been observed as 17 nm (nanometre) and 28 nm for CDFC and DDC2 cases, respectively. Both modes show almost similar nucleation particles ($D_p < 50$ nm), but higher agglomeration mode particles ($D_p > 50$ nm) have been observed in the DDC2 case. Generally, agglomerated soot particles are preferred over nucleation mode particles because they can be trapped easily in a diesel particulate filter (DPF) and it reduces the complications of DPF design.54

Figure 11 shows the in-cylinder temperature contour for different dual fuel cases ($-23$ SOI). As discussed earlier, sector geometry has been used for CDFC mode analysis and full cylinder geometry has been used for direct dual fuel injection cases. In the CDFC case, high temperature regions were observed in the HRF zone and medium temperature regions were observed in the LRF zone. High temperature regions have been observed in almost the entire piston bowl area in the DDC0 case because of the LRF fuel stratification. Both HRF and LRF combusted almost at the same crank angle range which results in strong high temperature regions during the DDC1 case. In the DDC2 case, HRF combusted initially and LRF combusted successively, resulting in lower high temperature regions. Finally, based on this work, DDC2 mode shows better combustion and emission performances in the $-27$ SOI case. (Figure 12).

4. CONCLUSIONS

In this study, the effects of diesel fuel injection timing on a direct dual fuel injection CI engine fueled with gasoline and diesel have been investigated. Modeling has been done for direct dual fuel injection to reduce the difficulties associated with the port injection strategy. The direct dual fuel injection strategy (DDC2) shows that the NOx and CO emissions were reduced by 38 and 60%, respectively, as compared to the CDFC counterpart. DDC2 mode shows lower in-cylinder temperature, NOx, and CO emissions than other dual fuel
cases. Relatively, higher quantity of LTC species has been observed in the DDC2 case as compared to the CDFC case. Advanced SOI timing shows stronger LTHR as compared to retarded SOI timing in the DDC2 mode. Double HTHR peaks have been observed in the CDFC case during the SOI timing sweep. In DDC2 mode, double HTHR peaks have been noticed for retarded SOI cases and a single HTHR peak for advanced SOI cases. More agglomerated soot particles in DDC2 mode have been observed as compared to CDFC mode in the −25 SOI case. From temperature contours, minor high temperature and major low temperature regions have been observed for the DDC2 case.

5. METHOD AND VALIDATION

The experimental work has been conducted on a single cylinder CI, light duty, DI, naturally aspirated, and variable compression ratio engine. Detailed test engine specifications are given in Table 1. An electronic injection system has been used to supply both LRF and HRF fuels. The experiments have been conducted at 1500 rpm with 80% engine load. This study analyzes the effects of HRF injection timing and fuel stratification. The tail pipe emissions have been measured with the help of an AVL MDS 418 gas analyser. Air metrics TAS-5.0 has been used to measure the exhaust gas particulate matter that was collected on a Whatman glass fibre filter paper. In this work, closed cycle combustion simulations have been performed using CONVERGE, a computational fluid dynamics tool for multiphase reacting flows has been used. For faster computations, a 120° sector grid has been used in accordance with the three-hole injector for CDFC mode cases. More details about the modeling approach can be found in the authors’ previous article. As discussed earlier, for CDFC combustion, LRF is supplied during the intake stroke and has been assumed to be homogeneous at the start of simulations, and hence, the simulation is initiated with gaseous species mass fraction. The HRF is injected directly into the cylinder and is represented using relevant discrete phase spray models. A kinetic scheme developed for gasoline/diesel involving 73 species 296 reactions has been used to model gasoline/diesel combustion. Isooctane and n-heptane have been used as surrogates to represent the physical and combustion properties of gasoline and diesel, respectively. Soot and NOx have been modeled using a modified version of the Hiroyasu soot model and thermal NOx model. Injection timings for different engine simulation cases are presented in Table 2.

Table 2. Fuel Injection Timing of Different Cases

| Case   | SOI for HRF (CAD) | SOI for LRF (CAD) | LRF and HRF clocking angle difference (deg) | LRF spray objective |
|--------|------------------|------------------|-------------------------------------------|---------------------|
| CDFC   | −25 to −19       | −380             | N/A                                       | homogeneity         |
| DDC0   | −23              | −50              | 60                                        | heavy stratification|
| DDC1   | −23 to −15       | −50              | 0                                         | heavy stratification|
| DDC2   | −29 to −21       | SOI of HRF−2     | 0                                         | rich burn           |

Initially, simulations have been performed to validate the CDFC combustion mode operations. Engine experiments have been done for different SOIs of diesel of CDFC mode operation. During this operation, SOI of diesel varies from −25 to −19 aTDC. Figure 12 shows the combustion characteristics of experimental and simulation results. A good agreement between simulations and experiments can be seen. Two HRR peaks corresponding to premixed and diffusion combustion can be observed. Kokjohn et al. reported that SOI timing of diesel (ignition source) should be kept in −45 to −30 aTDC to get an effective RCCI combustion. Nevertheless, in this study, it is difficult to shift the SOI of diesel earlier than −25 aTDC without changing of other operating parameters. The engine is operated with dual fuel, but the nature of combustion is closer to CDC. Hence, this dual HRR peak combustion nature (Figure 12) mode has been referred to as the CDFC engine in this paper.

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Notes

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