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RESEARCH NOTE

Toward an Improvement of Natural Gas-diesel Dual Fuel Engine Operation at Part Load Condition by Detail CFD Simulation

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ABSTRACT

Natural gas-diesel dual fuel combustion is a beneficial strategy for achieving high efficient and low emissions operation in compression ignition engines, especially in genset application heavy duty diesel engine at rated power. This study aims to investigate a dual fuel engine performance and emissions using premixed natural gas and early direct injection of diesel fuel. Due to the different reactivities of natural gas and diesel fuels, the mentioned dual fuel combustion is based on reactivity controlled compression igniton (RCCI) which is introduced whitin the cylinder. A six-cylinder direct injection (DI) diesel engine was properly modified to run on dual-fuel mode. Based on experimental study, comparative results are given for various operating modes; conventional diesel mode, convential dual-fuel mode, and RCCI mode; revealing the effect of combustion mode on performance and emission characteristics in a compression ignition engine. The results show that the conventional dual fuel combustion reduces nitrogen oxides (NOx) emissions but suffers from higher carbon monoxide (CO) and unburned hydrocarbon (HC) emissions in compared to conventional diesel mode at part load condition. Results of detailed assessment of different dual fuel modes with CFD model coupled with chemical kinetic mechanism reaveled that RCCI strategy led to higher combustion efficiency as well as lower HC and CO emissions compared to conventional dual fuel combustion at part load condition.

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1. INTRODUCTION

The direct injection compression ignition (DICI) engines have been widely used in mass transportation and genset application, largely due to high efficiency and durability compared to spark ignition (SI) engines. Despite the fact that diesel engines fulfill the daily increasing power demand, high emission amounts have been challenges for diesel engines [1]. In diesel engines, emissions are formed mainly through the heterogeneous mixture within the cylinder and its production rate increases exponentially with increasing temperature [2].

Conventional dual fuel combustion with alternative fuel is a promising way to overcome this challenge [3, 4]. In this method, a premixed charge of air and fuel e.g., Natural gas (NG) is imported into the cylinder and ignited by pilot diesel fuel injection.NGis a low reactivity fuel with high octane number that has a clean burning in compared to liquid alternative fuels like diesel due to chemical composition [5]. But, the main reported drawback of mentioned strategy is partial burning and incomplete combustion as well as high amount of HC and CO emissions at part load condition [6].

Also, low temperature combustion (LTC) is the newest proposed solution to reach low exhaust emissions in diesel engines [7]. Recently, various premixed LTC strategies are defined to avoid high in-cylinder temperature as well as locally rich mixture by prolonging ignition delay [8]. LTC has the capability to simultaneously reduce harmful emissions and from the other side, maintaining thermal efficiency by reduction of heat loss in diesel engines [9]. The premixed combustion is a strategy to reach LTC condition. The premixed charge can be achieved by fuel injection

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through intake port fuel or direct injections early in the intake and compression strokes [10]. The main challenges to the use of premixed LTC regimes are that combustion phasing control becomes more difficult; because these methods are governed by chemical kinetics, the operating range for these systems is generally confined to a relatively smaller range in compared with conventional diesel combustion (CDC) [11-13]. The new LTC which has been introduced is reactivity controlled compression ignition (RCCI) concept with high and low reactivity fuels [14].

Based on the aforementioned benefits of dual fuel and LTC strategies in compression ignition (CI) engines, it is worthy to investigate the behavior of NG-diesel dual fuel combustion under part load condition with considering LTC mode. The current study aims to explore the potential of early injection of diesel fuel in a dual fuel engine with EGR as LTC strategy to enhance combustion and emissions at part load condition. This kind of combustion is known as a partially premixed dual fuel combustion or RCCI. Firstly, combustion analysis is presented in conventional diesel and dual fuel mode based on experimental study. Also, in order to focus insight into combustion process in dual fuel mode, the numerical investigation is conducted using a three dimensional CFD model coupled with a chemical kinetic mechanism which was developed based on experimental study in conventional dual fuel and RCCI.

2. EXPERIMENTAL SETUP

An inline six-cylinder 13L diesel engine equipped with a common-rail direct injection system and cooled EGR was used to produce experimental data for the NG substitution investigation and CFD model validation. Its main characteristics are summarized in Table 1.

The low and high reactivity fuels employed in this work are NG and ultra low sulfur diesel (ULSD), respectively. The engine was coupled to a 560 kW alternating current dynamometer (HS001779, ABB Innovasys). The NG and diesel fuel flow meter (CMF025M319NRAUEZZZ, Micro Motion) and the air flow meter (14241-7962637, ABB) were used to measure required flow ratesEngine-out and tailpipe gaseous emissions were measured with an emission analyzer (MEXA 7500 DEGR, Horiba).

TABLE 1. Engine specification

Characteristics	Values
Type	In-line 6 cylinder
Fuel	NG-Diesel
Engine Speed (rpm)	1500
Displacement (L)	12.4
Intake valve closing (CA bTDC)	150
Exhaust valve opening (CA aTDC)	144

3. COMPUTATIONAL APPROACH

In this study, AVL FIRE code was used as the numerical model for dual fuel engine with the specifications and operating conditions on Table 1.

For modeling the turbulent effects, the k-zeta-f model was selected. This model developed and introduced by Hanjalic et al. [15] for reaction flows within the internal combustion engine. Diesel fuel spray breakup has been simulated by Kelvin-Helmholtz and Rayleigh-Taylor (KH-RT) model [16, 17]. The Dukowicz model was choosen for accounting heat-up and evaporation of liquid droplets of injected diesel fuel [18]. As mentioned before, a multi-dimensional CFD model coupled with chemical kinetics was developed by the means of FIRE internal chemistry interpreter detailed chemistry solver based on CHEMKIN theory [19, 20]. FIRE internal chemistry interpreter, calculates the reaction rates for each elementary reaction while the CFD solves the transport equations. In this study, a reduced dual-fuel chemical mechanism for n-heptane and methane composed of 40 species and 130 reactions is used for detailed combustion chemistry calculations during engine cycle. This is based on pervious work by Nieman et al. [21]. The NOx formation chemistry is represented by 4 species and 12 reactions, which is the GRI NOx mechanism based on Zeldovich mechanism [22, 23].

4. RESULTS AND DISCUSSIONS

4. 1. Dual Fuel Combustion Assessment To demonstrate the effect of NG substitution and conventional dual fuel strategy on combustion characteristics and emissions at part load condition in mentioned diesel engine, the results of experimental study for in-cylinder pressure, HRR, and emissions e.g., NOx, HC, and CO are provided for two cases as conventional diesel and dual fuel cases. For both tests, engine load and speed is set at 500 Nm (as 25% of full load) and 1500 rpm. The operation condition of defined cases is summarized in Table 2. In this study, NG substitution is defined as the ratio of NG and diesel fuel energy share.

Figure 2 shows the in-cylinder pressure and HRR as combustion characteristics. The present work indicates that cylinder pressure of dual fuel combustion is lower comparatively to the conventional diesel combustion. The lower cylinder pressure observed under dual fuel combustion is the result of lower heat release rate.

TABLE 2. Operating conditions in diesel and dual fuel modes

Case	EGR (%)	SOI (CA bTDC)	NG substitution (%)
Diesel mode	0	8	0
Dual Fuel mode	0	17	71

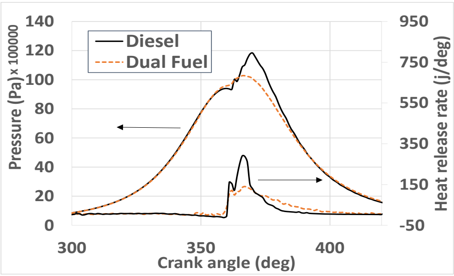

Figure 2. Pressure trace and heat release rate

This could be the consequence of reduction in injected diesel fuel as high reactivity fuel and slower combustion rate of the poor air-NG mixture within the cylinder compared to neat diesel combustion [24].

The specific emission amounts are directly calculated from the engine-out exhaust emissions divided by the fuel mass flow rate. Table 3 shows the results concerning various emissions, NOx, HC and CO as well as combustion efficiency in conventional diesel and dual fuel mode. As can be seen, the total NOx emission for dual fuel mode is lower than the conventional diesel mode. This is to be expected since NG combustion has lower temperature [25]. However, HC and CO emissions for dual fuel combustion are considerably higher in comparison to those corresponding to conventional diesel mode. This higher concentration is particularly the result of a low quality and slow heat release rate at part load in dual fuel mode that consequently results in poor combustion efficiency.

The results show that NG-diesel dual fuel mode suffers from the lack of high-efficiency combustion and high HC and CO emissions at part load engine condition. Whereas, it can be an efficient technique to reduce NOx emissions compared to conventional diesel case.

4. 2. RCCI Combustion Assessment In this section, the possibility of dual fuel combustion improvement with partially premixed strategy was investigated. Four different dual fuel cases were experimentally explored with EGR. Diesel fuel SOI timing become advance from around TDC in conventional dual fuel mode to early injection at 35 CA bTDC in RCCI mode. To insight into combustion properties, numerically analysis conducted using CFD model. This is a well-known method for detailed

TABLE 3. Comparison of conventional diesel and dual fuel

Case	NOx (gr/kg-fuel)	HC (gr/kg-fuel)	CO (gr/kg-fuel)	Comb. eff. (%)
Conventional Diesel	53.46	14.18	13.90	94.58
Conventional Dual Fuel	24.83	192.11	104.47	72.12

investigation on combustion process in internal combustion engines [26].

Table 4 shows the defined cases for dual fuel combustion development. Cases 1 and 2 represent combustion and emissions in a conventional dual fuel mode due to late diesel fuel SOI timing. Whereas, other cases possibly have combustion condition in RCCI engine; which is discussed in next sections. The engine load for each case was held constant at 500 Nm (as 25% engine load) by adjusting the total fueling NG and diesel according to the desired substitution level.

Figures 3 and 4 indicate the comparison of the obtained results from the multi-dimensional CFD model with the experimental data of the different cases. It is observed that there is lowest cylinder pressure and HRR in case 1 compared to other cases.

TABLE 4. Selected engine operating conditions for validation

Case	EGR (%)	SOI (CA bTDC)	NG substitution (%)
1	33	8	83.13
2	36	19	80.11
3	36	31	79.14
4	36	35	80.17

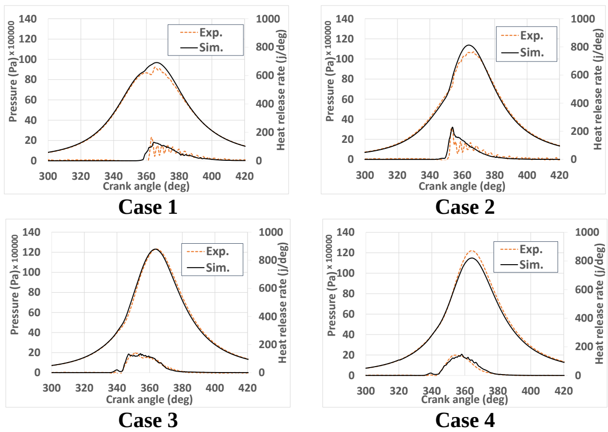

Figure 3. Cylinder pressure, HRR for different cases in Table 4

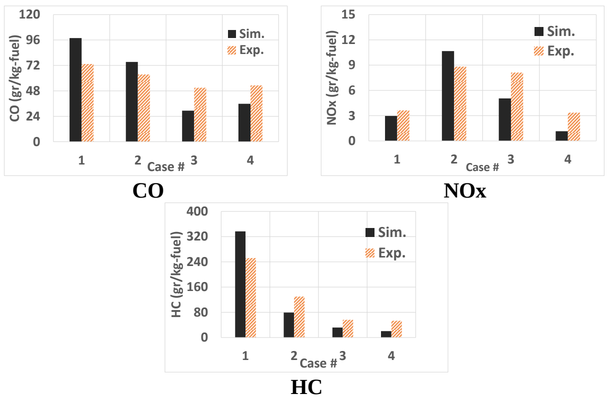

Figure 4. CO, NOx, and HC validation for cases in Table 4

This could be due to less time for mixing of diesel fuel as pilot fuel with air at late SOI timing and lower premixed combustion rate in expansion stroke in this case. Other possible reason is the lowest global reactivity with 83% NG substitution. However, reactivity gradient in different SOI timings could affect combustion features in other cases, which have almost equally NG substitution.

The numerical results demonstrate that the peak pressure location and magnitude predicted are in good agreement with the experimental data. Also, it can be seen that the calculated cylinder pressure traces in compression and expansion stroke are almost matches the corresponding experimental ones. As it can be seen in Figure 3, there is a slight over-prediction in pressure and HRR in cases 1 and 2. This issue can be regarded to inevitable inhomogeneity of the NG-air mixture in terms of fuel density, temperature and residual gases in experimental engine, which could notbe considered in simulation; which was the other reason for differences between experimental and numerical results within the combustion chamber. According to HRR curves, low temperature heat release (LTHR) around 20 CA bTDC and high temperature heat release (HTHR) can be significantly seen for SOI timing of 31 CA bTDC and 35 CA bTDC. Therefore, it was concluded that the heat release profile shows LTC mode and RCCI combustion in mentioned cases.

Based on exhaust emissions in different cases, it could be observed from Figure 4 that the predicted trends of CO, HC, and NOx emissions are consistent with the measurements for various engine operation condition. The numerical results show that the emission is somewhat under-predicted or over-predicted by the model, but it is reasonable and the trend is well predicted. These error values may be due to simplified EGR modeling, and uncertainty in defining combustion chamber wall temperature as boundary conditions in the CFD model. In addition, it should be noticed that, the exact matching is not possible because one cylinder combustion process simulation is done, whereas the experimental values are averaged of all six cylinders [12]. An increase in NOx emission was observed up to case 2 condition, but then dropped in case 4. In addition, CO and HC emissions reduction occurs from case 1 to case 3 with partially premixed combustion, without significantly change in case 4 compared to case 3. It can be concluded that the combustion simulation model performed in this study are able to represent the real combustion process inside combustion chamber and validated results indicate good reliability of the mechanisms and models used in the present CFD model to predict combustion features. Therefore, the CFD model has the capability for further calculation.

In order to find the reasons for the different combustion features and emission characteristics in various cases, the detailed investigation was conducted by the results of CFD simulation. The combustion analysis was performed by means of parameters including combustion phasing (CA50), burn duration, temperature distribution in combustion chamber, emission mass fraction distribution within the cylinder (e.g., NOx, HC, CO), as well as combustion efficiency.

To demonstrate combustion behavior and in-cylinder conditions, Figure 5 represents the combustion phasing characteristics including CA50, which means the crank angle where 50% of total combustion heat is released as well as burn duration. Burn duration in different cases define based on the difference between CA90 (as the crank angle position in which the cumulated heat release has reached a value of 90%) and CA10 (as the crank angle position in which the cumulated heat release has reached a value of 10%). It is observed that the combustion phasing significantly shifts backwards to before TDC from cases 1 to 3. However, in case 4, the combustion phasing moved closer to TDC. It should be noted that, this trend has been shown previously for RCCI operation and other LTC strategies with a controlled heat release rate due to reactivity gradient. This can be associated with locally leaner and less reactivity stratification due to longer mixing times at ignition delay. Also, the results of burn duration comparison show that RCCI combustion reduces the burn duration compared to conventional dual fuel combustion. It could be the result of partially premixed combustion in LTC mode.

In order to further insight into combustion development and defining the reasons of various combustion phasing in different cases, in cylinder images from the simulation work are presented. Figure 6 represents cut planes coincident with the spray axis colored by temperature. It can be seen that the lower cylinder temperature can be seen at the end of compression stroke in case 1 which consequently resulting from lower global reactivity with higher NG blend ratio. Also, comparing different cases, high temperature regions are accumulated in piston bowl in cases 1 and 2. However, as illustrated, high temperature regions can be observed in outer parts of piston bowl in squish and near liner region in cases 3 and 4 at more advanced SOI timing.

This is closely associated with the high reactivity fuel distribution as ignition points in piston bowl region

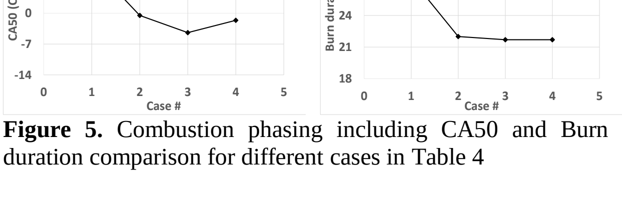

Figure 5. Combustion phasing including CA50 and Burn duration comparison for different cases in Table 4

at retard SOI timing (toward TDC) compared its distribution in squish region at earlier SOI timing because of diesel fuel jet target and longer mixing time. It can be found that combustion will propagate in the larger regions within the cylinder by advancing SOI timing due to high-reactivity fuel distribution in larger zones and consequently causes higher advanced HRR and cylinder pressure.

Figure 7 depicts the variation of combustion efficiency in different cases. The combustion efficiency reaches to more than 90% in cases with RCCI combustion condition. Case 1 with lower global reactivity has the minimum combustion efficiency. It is observed that, as the SOI is advanced with almost equally global reactivity in cases 2 to 4, combustion efficiency increases. It should be noted that combustion efficiency is affected by unreacted and partially reacted fuel in the combustion chamber (i.e., higher HC and CO). Therefore, efficient dual fuel combustion was achieved with proper global reactivity and high reactivity fuel distribution to prevent the incomplete combustion.

5. CONCLUSION

In the present work, firstly, three combustion concepts including conventional diesel, NG-diesel dual fuel, and NG-diesel RCCI were experimentally compared in combustion properties and exhaust emissions characteristics in a six cylinder engine at part load condition. In order to further insight into RCCI combustion, a detailed multi-dimensional CFD model coupled with chemical mechanism was developed. After CFD model validation against the results of experimental work, the impacts of RCCI strategy on combustion parameters and exhaust emission were investigated compared to conventional dual fuel combustion. The conclusion of study can be summarized as follows:

In a conventional NG-diesel dual fuel combustion at part load engine, incomplete combustion would be seen with lower cylinder pressure and HRR in compared to conventional diesel mode due to lower global reactivity of NG fuel as main fuel. So this combustion causes higher HC and CO emissions together with lower NOx emission compared to diesel combustion.

In RCCI combustion with early diesel fuel injection and EGR, cylinder pressure and HRR increase in compared to conventional dual fuel combustion with late diesel fuel injection. In very early injection in studied RCCI mode (i.e., 35 CA bTDC), more time is available for the diesel fuel to mix with the premixed NG-air mixture, local reactivity is reduced and combustion phasing is retarded.

Conventional dual fuel combustion can result in considerably increasing CO and HC emissions due to incomplete combustion and lower combustion efficiency as a main drawback in investigated operation condition at part load. However, by advancing diesel fuel SOI timing, RCCI operation achieved in SOI timing at 31 CA bTDC with simultaneously reduction of exhaust emissions including CO, HC, and NOx as well as increment of combustion efficiency more than 90%. It happens due to staged combustion of diesel fuel and NG in RCCI combustion with proper global reactivity and local reactivity distribution, which can results in uniform progress of low temperature combustion within the whole of cylinder to prevent the incomplete combustion.

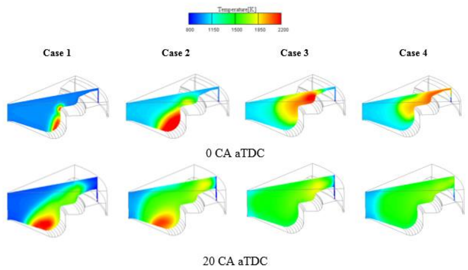

Figure 6. Cut planes coincident with the spray axis colored by temperature for different cases in Table 4 at twoCAs

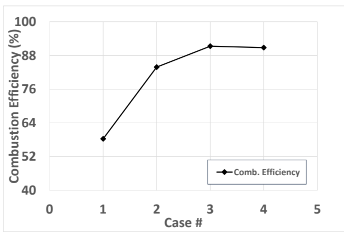

Figure 7. Combustion efficiency for cases in Table 4

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چکیده

احتراق دوگانه سوز گاز طبیعی- دیزل راهبرد موثری در جهت دستیابی به عملکرد با بازده بالا و آلایندگی پایین در موتورهای اشتعال تراکمی، بویژه در کاربری سنگین نیروگاهی در بار و توان نامی موتور می‌باشد. **هدف از** تحقیق حاضر، بررسی عملکرد و آلایندگی یک موتور دوگانه سوز مرسوم با بکارگیری مخلوط پیش آمیخته سوخت گاز طبیعی و تزریق زودهنگام سوخت دیزل است. بدلیل واکنش پذیریهای متفاوت سوخت گاز طبیعی و دیزل، احتراق دوگانه سوز ذکر شده برپایه اشتعال تراکمی با واکنش پذیری کنترل شده در داخل سیلندر است که تحت عنوان RCCI معرفی می‌گردد. به این منظور، یک موتور شش سیلندر تزریق مستقیم جهت بررسی عملکرد در حالت دوگانه سوز آماده سازی شده است. برپایه مطالعه تجربی، نتایج مقایسه‌ای برای حالات مختلف عملکردی شامل دیزلی مرسوم، دوگانه سوز مرسوم و RCCI ارائه شده است که نشان دهنده تاثیر نوع احتراقهای مذکور بر عملکرد و آلایندگی در یک موتور اشتعال تراکمی می‌باشند. نتایج نشان می‌دهند که احتراق دوگانه سوز مرسوم میزان انتشار آلاینده اکسیدهای ازت را در مقایسه با احتراق دیزلی مرسوم در بارهای پایین موتور کاهش داده، اما منجر به تولید مقادیر زیاد آلاینده‌های مونواکسید کربن و هیدروکربنهای نسوخته می‌گردد. نتایج ارزیابی حالات مختلف احتراق دوگانه سوز به همراه یک مدل CFD کوپل شده با مکانیزم سینتیک شیمیایی نشان می‌دهد که راهبرد RCCI منجر به بازده احتراقی بالاتر و انتشار هیدروکربن نسوخته و مونواکسید کربن کمتر در مقایسه با حالت دوگانه سوز مرسوم در بارهای پایین می‌گردد.

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