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Published in: Fuel

Link to article, DOI: 10.1016/j.fuel.2021.122651

Publication date: 2022

Document Version Publisher's PDF, also known as Version of record

Link back to DTU Orbit

A numerical study of the influence of pilot fuel injection timing on combustion and emission formation under two-stroke dual-fuel marine engine-like conditions

Arash Nemati, Jiun Cai Ong, Kar Mun Pang, Stefan Mayer, Jens Honoré Walther

Keywords: Marine engine, Dual-fuel, HPDI, Injection strategies, Engine load, CFD

Abstract

Stricter regulations imposed on emissions are motivating the scientific community to consider studying alternative fuels to achieve low emission, high efficient dual-fuel (DF) marine engines. In this context, three dimensional computational fluid dynamic (CFD) simulations are performed to study the combustion and emission formation under two-stroke, dual-fuel marine engine-like conditions. The DF engine configuration consists of a pilot diesel fuel and a high-pressure, direct injection (HPDI) of natural gas (NG). The simulation results are validated under both high load (high charge density) and low load (low charge density) operating conditions. Detailed analysis of the flame development and emission formation are performed. The interaction between the pilot diesel jets and the methane flame jets is studied. Based on the results, the further methane jets penetration in the low load case leads to better air–fuel mixing and a higher combustion intensity than that in the high load. Effects of the pilot fuel injection timing on combustion and emission formation and the governing mechanisms are also investigated in detail. Results indicate that the intense combustion of the accumulated methane expands the methane flame towards the piston when the pilot injection timing is retarded. The NO formation is lower in the high load case with higher charge density due to the lower combustion intensity. Also, retarding the pilot injection timing decreases the NO formation.

1. Introduction

Large two-stroke marine engines are the main source of propulsion in the shipping industry. The commonly used fuel in these engines is heavy fuel oil (HFO) which contains sulfur as an impurity. This leads to the formation of sulfur oxides (SO₂) and sulfuric acid (H₂SO₄) [1,2]. More stringent regulations imposed by the International Maritime Organization (IMO) on SO₂ has led ship builders to seek alternative fuels (e.g. methane) which does not contain sulfur and is cheaper than low sulfur diesel [3]. Therefore, in recent years, the use of alternative fuels in the marine engines have gained a strong interest in the industrial and research communities.

Natural gas (NG), which mainly comprises of methane, is one of the promising alternative fuels for marine engines. NG produces lower emissions (SO₂ and PM) and greenhouse gases after combustion due to having a lower carbon-to-hydrogen ratio [4]. There are two different types of dual-fuel (DF) diesel/NG marine engines based on their combustion principles. The first type is the premixed lean combustion, in which the premixed NG–air mixture is ignited by a pilot diesel fuel and the combustion mode is based on the Otto cycle [5]. The premixed lean combustion has the capability of significant NOₓ reduction. However, these engines may generate higher amounts of unburned hydrocarbon (UHC) emissions [6]. On the other hand, there is another type of DF engine known as the pilot-ignited, high pressure direct injection (HPDI) dual-fuel NG engine. In these engines, both the pilot diesel fuel and NG are directly injected into the in-cylinder region at high injection pressures, close to TDC. The pilot diesel and NG are injected at an angle such that the resulting flame jets come into contact. The pilot-ignited HPDI NG engines present a higher control on the combustion with controlling the injection strategies of diesel and NG fuels, separately. The combustion process initiates from the ignition of the pilot diesel fuel. The diesel flame jets then penetrate to the unburned NG cloud. The NG cloud is subsequently ignited by the high temperature diesel flames. Both the pilot diesel and NG undergo the non-premixed or diffusion combustion. It is important to note that the interaction between the pilot diesel fuel and NG jets has a major effect on the combustion of the pilot-ignited HPDI NG engines.

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https://doi.org/10.1016/j.fuel.2021.122651

Received 20 September 2021; Received in revised form 5 November 2021; Accepted 16 November 2021

Available online 21 December 2021

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Dual-fuel combustion concept is studied experimentally in small size engines. Fink et al. [7] performed experimental studies on pilot-ignited HPDI dual-fuel combustion of a NG jet in a rapid compression expansion machine. They concluded that variation of angle between methane and diesel jets causes significant impact on the combustion process. In separate works, dual-fuel combustion of diesel/methane was studied experimentally in a light duty compression ignition engine [8, 9]. Results of these studies revealed that when the engine operates in dual-fuel mode, a remarkable reduction of soot particles can be obtained. Furthermore, the use of two-pulse injections has positive effects on the methane oxidation at high loads, and was necessary to keep the combustion stability and noise within the limits at partial loads. Faghani et al. [10] conducted an experimental and numerical study on the injection parameters in a four-stroke heavy duty HPDI diesel/NG dual-fuel engine. They used a small diesel pilot injection (5–10% of the fuel energy) to ignite the direct injected gas jet. They studied the effect of late post injection of gas and concluded that it results in significant PM reductions with only small effects on other emissions and engine performance.

Numerous works have also been carried out on the pilot-ignited HPDI NG low speed two-stroke marine engines. The MAN ME-GI engine and the development of this engine from the first tests are described in [3]. The ME-GI engine is a two-stroke pilot-ignited HPDI NG engine. An electronically controlled two-stroke low speed marine diesel research engine, 4T50ME-X was retrofitted to gas operation to perform the engine tests [3]. The ME-GI engine was based on a diesel-type combustion process of a gas jet that is injected into the combustion chamber with high pressure between 150 and 315 bar depending on engine load. Engine fuel efficiency was essentially unchanged when changing from oil to gas given comparable engine operating conditions. The methane slip and unburned methane was generally measured to be very low in this engine [3]. In a more recent experimental study, Hult et al. [11] conducted an optical experimental study on a pilot-ignited HPDI NG MAN 4T50ME-X test engine. Therein, only one diesel injector and one NG injector were used such that cameras could be installed to capture the flame development. They used the space carving method to estimate a three-dimensional flame contour to calculate flame length and lift-off length [11]. They compared the flames from pilot-ignited HPDI NG engine and a conventional diesel engine and concluded that the flame development was similar for two flames because the NG injection rate was calibrated to achieve a similar combustion rate as that in the diesel engine mode. However, the lift-off length for the NG flame was longer than that of the diesel flame. The information about flame formation and development was limited in this experimental setup as the flame penetrated inwards the combustion chamber and could only be captured for a limited time (around 4.5 ms) by cameras.

Experimental studies on the pilot-ignited HPDI NG engine are limited and there is only limited information about the detailed local flame and emission formation inside these engines. Hence, the fundamental knowledge about the flame formation and development as well as emission formation is not available for such large marine engines. Therefore, three-dimensional (3D) computational fluid dynamic (CFD) modeling can be considered as a considerable complement in gaining more insights. Lucchini et al. [12], developed a tabulated kinetics method and successfully simulated the dual-fuel combustion under the pilot-ignited HPDI NG marine engine-like conditions. In another study, Li et al. [4] investigated the influence of the NG injection profile on the combustion process in a pilot-ignited HPDI NG marine engine using CFD tools. Five different profiles: trapezoid (the base case), wedge, slope, triangle, and rectangle shapes are numerically studied. It was concluded that the NG injection profile had a significant effect on the combustion and emissions and the wedge and trapezoid shapes showed a good balance between the emissions and the output power of the engine. In addition to these, Yang et al. [13] investigated the injection parameters in a two-stroke pilot-ignited HPDI NG marine engine by performing CFD simulations. Their results revealed that the lateral angle of the gas nozzle had a considerable effect on the NG combustion process and changing this angle from 0° to 30°, increased the closed cycle indicated pressure by 12%. It was also concluded that carbon monoxide (CO) and NOx emissions were 21% and 31% lower than those in the diesel engine counterpart, respectively.

In all of the aforementioned studies, the interaction between the diesel flame and NG jets is not studied in engines. Furthermore, detailed information about the combustion phases and emission formation is not available. Considering these shortcomings in the literature, the main objectives of this CFD work are (1) to perform simulation and validation of the dual-fuel combustion in a two-stroke pilot-ignited HPDI NG engine under marine engine-like conditions, (2) to study the formation of diesel and methane (methane is considered as surrogate for NG) flames, and (3) to carry out investigation of diesel injection timing on the combustion and formation of emissions. These aims are achieved by coupling an Unsteady Reynolds-averaged Navier–Stokes (URANS) simulation with a finite-rate chemistry.

The paper is organized as follows. In the next section, the test engine specifications used in experimental test are presented. It is followed by the descriptions of the numerical methods. In the results section, the model setup is first validated under two operating conditions. The formation of diesel and methane flames is then presented. In addition to this, the effects of pilot diesel injection timing on combustion, methane flame development and emission formation are studied. Conclusions from this study are outlined in the last section.

2. Numerical modeling

2.1. Engine specifications

The inputs for the CFD simulations are carried out based on the 4T50ME-X research engine located at MAN Energy Solutions, Denmark. Two operating conditions with different charge densities are considered in the present study. For brevity, the low load (LL) represents the case with low charge density; while high load (HL) represents the case with high charge density. Details of the engine specifications are presented in Table 1. It should be highlighted that the simulated operating conditions are not representatives of the real engine operation. The start of injection timing and duration as well as the injected fuel mass and diesel/NG ratio were all adjusted to conveniently perform detailed optical measurements of the combustion process [11]. Diesel and NG are delivered by two separate injectors placed on the cylinder cover. An illustration of these injectors in the experimental setup by Hult et al. [11] can be found in Fig. 1. It should be highlighted that the positions of the diesel and NG injectors were deliberately arranged in the optical experimental tests in [11] in order to capture the flame development by cameras (cf. Fig. 1). In this study, the injectors are rotated to be in the positions and directions similar to those in the real engine operation. Therefore, the validation of the numerical setup is first performed based on the experimental setup shown in [11]. Upon validation, all subsequent numerical simulations are carried out based on the rotated injectors (cf. Fig. 2). The liquid fuel is marine gas oil, which has similar properties to diesel fuel. NG with the methane (CH4) content of around 97% is used as the gaseous fuel [11]. Diesel and methane start of injection (SOI) are provided in Table 1 for the LL and HL cases.

2.2. Numerical simulation models

3-D CFD simulations in the present study are performed using the Siemens Star-CCM+ version 15.06.008-R8. The turbulent flow is modeled using the Unsteady Reynolds Averaged Navier–Stokes (URANS) method with the k-ω Shear Stress Transport (SST) model [14]. For the diesel spray, the Rosin–Rammler is utilized to model the initial droplet size distribution, while the Reitz–Diwakar model [15] is applied to simulate the secondary breakup. In this study, n-heptane is considered
3.1. Validation of numerical model under low and high engine load conditions

For model evaluation, the in-cylinder pressure and heat release rate (HRR) are compared against the experimental data (cf. Fig. 5). A reasonable agreement is achieved between the predicted in-cylinder pressure and the measurement. The deviation in the absolute value of the peak pressure and the associated timing in terms of CAD are 0.5% and 0.3% for the LL case and 2.1% and 0.4% for the HL case. The HRR profiles are derived based on their respective pressure curves [25]. The sudden rise in pressure, which corresponds to a steep increase in HRR, is attributed by the diesel auto-ignition and premixed combustion of methane. Such steep rise in pressure or HRR may be due to the absence of turbulence chemistry interaction model. Similar trend is observed in engine combustion simulations where well-stirred reactor model is used [26]. Furthermore, during calculation of the experimental HRR, the experimental pressure data is filtered and averaged to avoid large fluctuations which also may lead to deviation between the numerical and experimental HRR. Nevertheless, the magnitude and trend are well captured by the numerical simulations at both the high and low load cases with high and low charge densities.

A typical combustion process in a pilot-ignited HPDI NG engine consists of five stages [27]: (1) ignition of pilot diesel fuel, (2) pilot diesel fuel flame penetration, (3) premixed combustion of the methane gas, (4) mixing-controlled combustion of the methane gas, and (5) post oxidation of the diesel and methane fuels. The first and second stages are identical to the normal diesel combustion as described by Heywood [28]. The premixed combustion of methane gas (stage 3) releases a considerable amount of heat, which leads to the increase in the in-cylinder pressure. This is evident in Fig. 5 after the methane SOI. The combustion intensity of the premixed combustion stage is related to the interaction between flame with the unburned methane gas and amount of unburned methane gas. Therefore, the pilot diesel injection timing is expected to have a significant influence on this combustion phase. The associated results and discussion on the effects of pilot diesel injection timing on the flame and emissions can be found in Section 3.3.

The effect of in-cylinder charge density on the methane flame length is next evaluated. It should be highlighted that the current test cases are different from those reported by Hult et al. [11] for methane as the surrogate fuel for the pilot diesel fuel. The liquid properties of the diesel fuel are represented by tetradeane (C_{14}H_{30}) considering the similarity of thermo-physical properties of C_{14}H_{30} with diesel fuel [16,17]. Natural gas is represented by methane as methane is the main component of natural gas [11]. Different walls of the combustion chamber including piston, liner, cover, and valve are shown in Fig. 2. The wall temperatures of piston, liner, and cover are fixed at 673 K, while the wall temperature of the bottom of the valve is set to 850 K. The mass flow rates for both the diesel and methane injections deduced from the experiment. To consider the scavenging flow effects on the combustion, a tangential velocity with a solid body rotation profile is initiated at 120 crank angle degrees (CAD) after bottom dead center (ABDC) which is the start of the simulation. The initial axial velocity is set using a linear velocity profile, starting from zero in the vicinity of the exhaust valve and increasing to be the same value as the piston velocity near the piston [18]. A no-slip condition is applied at each wall boundary and the all y+ wall treatment is used as the wall model. The mesh resolution of the combustion chamber is set to 0.005xD (D is the cylinder diameter). The mesh in the vicinity of the diesel and methane injector exits is further refined to 0.0025xD and 0.00125xD, respectively. Such refinement is carried out to capture the air-fuel mixing and flame penetration accurately. The time step size is set to 1 μs in this study.

2.3. Chemical mechanism

A skeletal n-heptane mechanism (Seidel mechanism [19]) consisting of 56 species and 128 reactions is utilized to simulate the oxidation of methane and n-heptane in the present work. A sub-mechanism is added to simulate the thermal NO_x formation. Prior to the CFD calculation, zero-dimensional (0-D) homogeneous reactor calculations are conducted to evaluate the performance of the Seidel mechanism. The 0-D homogeneous reactor simulations are conducted for pure n-heptane and pure methane fuels using the ANSYS CHEMKIN-PRO software [20]. Fig. 3 presents the Seidel mechanism performance in predicting the pure n-heptane fuel ignition delay times. The associated results are compared with the shock tube experimental data [21] and Zhang detailed n-heptane mechanism [22] for different operating conditions. The ignition delay time (IDT) is defined as the time where the mixture temperature increases to 400 K above the initial temperature. The in-cylinder pressure is approximately 90 bar for the low load operating condition and 120 bar for the high load operating condition at the diesel SOI timing and there is no experimental data for such high pressures. Therefore, the performance of the Seidel mechanism at 90 bar and 120 bar is only compared with the Zhang detailed n-heptane mechanism [22]. As depicted in Fig. 3, the Seidel mechanism predicts the IDTs reasonably well at both low and high pressures.

The performance of the Seidel mechanism in predicting the pure methane IDT is presented and compared with the detailed methane mechanism by Hashemi et al. [23] in Fig. 4. The comparison is carried out at 90 bar and 120 bar. Two different equivalence ratios (ϕ_{CH}_4=1 and ϕ_{CH}_4=3) are considered. As it is shown in Fig. 4, a good agreement between the Seidel mechanism and the detailed Hashemi mechanism [23] is obtained. Fig. 4c shows the predictions of the laminar flame speeds (LFS) in methane-air mixtures at ambient pressures of 1 atm and 20 atm. The initial unburned methane fuel temperature is set to 300 K. The Seidel mechanism shows comparable LFS prediction to the measurement by Rozenchan et al. [24] and the detailed methane mechanism by Hashemi et al. [23].

Table 1

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Low load (LL)</th>
<th>High load (HL)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore [mm]</td>
<td>500</td>
<td>78</td>
</tr>
<tr>
<td>Stroke [mm]</td>
<td>2200</td>
<td>2010</td>
</tr>
<tr>
<td>Connecting rod [mm]</td>
<td>2885</td>
<td>190</td>
</tr>
<tr>
<td>Engine speed [rpm]</td>
<td>78</td>
<td>120</td>
</tr>
<tr>
<td>Diesel SOI [CAD ABDC]</td>
<td>179.0</td>
<td>178.0</td>
</tr>
<tr>
<td>Methane SOI [CAD ABDC]</td>
<td>181.0</td>
<td>180.0</td>
</tr>
</tbody>
</table>

Fig. 1. A simplified schematic diagram of the experimental setup. A full schematic diagram and experimental setup is available in [11] (cf. Figures 2 and 3 in [11]).

Fig. 3 presents the Seidel mechanism performance in predicting the oxidation of methane and n-heptane fuels using the ANSYS CHEMKIN-PRO software [20].
flame length. Hence, there is no experimental methane flame length data available for model validation. In addition to that, there is no clear definition on the flame length in CFD calculation to ensure a fair comparison between measured and calculated flame lengths. A qualitative evaluation can however be made, instead of a quantitative one. Hult et al. [11] compared the diesel flame length at different in-cylinder charge densities (high and low loads). At a lower charge density (low load), the diesel flame length appears to be longer. Such effect is expected to remain the same for other fuel types such as methane. Since methane jet penetration can be associated to methane flame length, the methane jet penetration from our non-reacting engine case is represented here. In this work, the methane jet penetration is consistently defined as the longest distance of the methane jets from the methane injector in the non-reacting cases. Fig. 6 shows that the current model is capable to capture the qualitative changes of methane jet penetration with respect to the variation of in-cylinder charge densities in high and low loads. Further discussion about methane flame development under different operating conditions can be found in Section 3.3.2.

3.2. Diesel and methane flame development

In this section, a detailed examination of diesel and methane combustion is carried out. The iso-volume contours of temperature in Fig. 7 are used to represent the diesel flame. The Lagrangian particles are used to indicate the penetration of the diesel jets. The contours are shown at three different CADs in the initial stages of the diesel flame development. These results are presented only for the high load case as a similar trend is observed for the low load case. All of the diesel spray jets from the four nozzles are set to have the same mass flow rate, but at different injection directions. It can be seen in Fig. 7 that the first and the second diesel fuel jets penetrate relatively longer into the combustion chamber. Also, it is noted that the diesel ignition starts in the upper part of the jet as shown in Fig. 7 at 179.16 CAD ABDC. This may be attributed by the better air/fuel mixing by the swirling flow as discussed earlier.

Next, the interaction between the diesel flame and the methane jets is examined to understand the methane combustion in the premixed combustion phase of methane (cf. Fig. 8). To visualize this phenomenon, the iso-surface of methane mass fraction with a value of 0.01 colored by temperature is presented in Fig. 8. These contours are presented at 3 different CADs: 181.3 CAD ABDC which is around the first diesel flame–methane jets interaction, 181.8 CAD ABDC at which diesel flame–methane jets interaction continues, and 183.2 CAD ABDC at which the methane flame jets penetrate. In the first row, the iso-surface contours at 181.3 CAD ABDC are presented. The blue surface represents the cold injected methane, while the high temperature iso-surface is the methane produced in the decomposition process of the diesel fuel. The region of the cold methane jets heated by the diesel flame is indicated by a circle and arrow. This implies that the diesel flame has come into contact with methane jets at 181.3 CAD ABDC. The iso-surface contours at 181.3 CAD ABDC are presented. The blue surface represents the cold injected methane, while the high temperature iso-surface is the methane produced in the decomposition process of the diesel fuel. The region of the cold methane jets heated by the diesel flame is indicated by a circle and arrow. This implies that the diesel flame has come into contact with methane jets at 181.3 CAD ABDC. The iso-surface contours at 181.8 CAD ABDC demonstrate that a greater amount of methane fuel starts to burn. At 183.2 CAD ABDC, the methane formed in the pilot diesel combustion has diminished and the methane fuel close to the methane injector starts to burn. Yet, there remain some regions upstream methane jets (shown with arrow) that are not burned. It is worth mentioning that the methane jets from the holes which are in the same direction with in-cylinder flow burns faster

Fig. 2. Left: combustion chamber geometry including diesel and methane injectors and different walls of combustion chamber, right: cross section of computational grids.

Fig. 3. Calculated ignition delay times (IDT) for \(n\)-heptane using the Seidel [19] and Zhang mechanisms [22] as a function of temperature \((T)\). Measurement data is from shock tube experiment [21]. Test conditions are set to (a) \(P_{\text{am}} = 42\) bar, \(\phi_{C_7H_8} = 1\) and (b) \(P_{\text{am}} = 120\) bar, \(\phi_{C_7H_8} = 1\).
Fig. 4. Calculated ignition delay times (IDT) for methane using the Seidel mechanism (skeletal) [19] and the Hashemi mechanism (detailed) [23] as a function of temperature \(T\) at (a) \(P_{\text{am}} = 90\) bar and (b) \(P_{\text{am}} = 120\) bar (Solid and dashed lines represent \(\phi_{\text{CH}_4}\) of 1 and 3, respectively) as well as (c) laminar flame speed (LFS) of methane/air mixture at \(P_{\text{am}}\) of 1 atm (dashed lines) and 20 atm (solid lines). LFS measurements from Ref. [24].

In order to obtain a deeper insight into the formation of the methane flame and combustion, distribution of normalized methane (\(\text{CH}_4\)) mass and methyl radical (\(\text{CH}_3\)) mass are presented in Fig. 9 for different ranges of temperature and equivalence ratio. \(\text{CH}_3\) is presented as it is the first species in the decomposition chain of \(\text{CH}_4\). These species distribution are presented at the three same CADs as in Fig. 8. The local equivalence ratio \(\phi\) of the mixture that contains hydrocarbon fuels and C, H, and O elements can be defined as follow [25]:

\[
\phi = \frac{2X_C^0 + 0.5X_H^0}{X_O^0}
\]

where \(X_C^0\), \(X_H^0\), and \(X_O^0\) are the mole fractions of C, H, and O, respectively. Superscript 0 denotes the state before the onset of chemical reactions.

As it is shown in Fig. 9a, there is a certain amount of newly injected methane with temperatures of less than 500 K. At 181.3 CAD ABDC, most of the methane has a temperature of less than 1000 K, indicating that the methane jets has not ignited yet (cf. the blue surface in Fig. 8, at 181.3 CAD). The small amount of methane with temperatures higher than 1000K are the products of diesel fuel combustion and also the methane fuel heated by the pilot fuel flames (cf. Fig. 8, top
and compared for the various pilot fuel injection timings at both the 3.3.1. In-cylinder pressure and HRR

The diesel SOI is retarded by 3 CADs relative to the base case for both high and low loads. Cases with different pilot injection timings are studied next. The diesel flame has developed into the inner region of the methane jets which is too rich to combust. Based on the equivalence ratio plots (Fig. 9b and 9c), the low normalized CH₄ mass at this CAD is located at the equivalence mass fraction is also presented in the Figs. 12 c and d, the maximum amount of unburned CH₄ located at the equivalence ratios around 2 to 4 and the trend is similar for all presented CADs. It is worth mentioning that the normalized CH₄ mass moves to higher values of ϕ at 183.3 CAD ABDC (cf. Fig. 9d). This implies that the flame has developed into the inner region of the methane jets which is a fuel-richer region.

3.3. Effects of pilot diesel fuel injection timing under high and low loads

In this section, the diesel pilot fuel injection timing is varied to first study its effects on the premixed combustion of the methane. The associated effects on later stages of the combustion ((4) mixing-controlled combustion of methane (5) post oxidation) as well as emission formation are studied next. The diesel SOI is retarded by 3 CADs relative to the base case for both high and low loads. Cases with different pilot injection timings are presented in Table 2. D3 represent cases where the pilot injection timing are retarded by 3 CAD, while D0 represent the base cases.

3.3.1. In-cylinder pressure and HRR

The average in-cylinder pressure and HRR profiles are presented and compared for the various pilot fuel injection timings at both the high and low engine loads in Fig. 10. The start of combustion is directly related to the pilot fuel injection timing. The peak HRR of the pilot fuel combustion which is the first peak in the HRR profile is indicated by the green arrows for different cases. The magnitude of the first HRR peak is almost the same for different pilot fuel injection timings at each load conditions. This is attributed by the comparable in-cylinder conditions for the base and retarded cases at their respective pilot SOI. The second HRR peak in Fig. 10 (indicated by the orange arrows) corresponds to the methane gas combustion. The first and second peaks for the retarded pilot fuel injection cases (HL - D3 and LL - D3) are close to each other in terms of CADs. In the retarded cases, there is already a great amount of unburned methane prior to diesel combustion. The methane combustion starts almost after the pilot fuel injection in the retarded pilot injection timing cases. The combustion of the great amount of relatively well-mixed methane–air leads to a higher heat release in the retarded cases and higher second HRR peaks than base cases. After the high peak, the HRR levels off and drops to the same level as that in the base case counterpart, suggesting that the mixing-controlled combustion of methane is not highly affected by the pilot diesel injection timing. Based on Fig. 10, the HRR magnitude is higher in the low load cases than that in their high load counterparts.

In the experiments, the amount of both diesel and methane fuels are comparable at both high and low loads. Therefore, it is possible to compare the HRR of the high and low load cases. The higher HRR for the low load cases may be attributed by the lower charge density than that in the high load cases. Fuel jets penetrate further (cf. Fig. 6) and wider in the lower charge density condition, leading to better air-fuel mixing and a higher HRR in the low load operating condition.

Table 2

<table>
<thead>
<tr>
<th>Case</th>
<th>Diesel injection timing</th>
<th>Methane injection timing</th>
</tr>
</thead>
<tbody>
<tr>
<td>LL D0 (base)</td>
<td>179.0</td>
<td>181.0</td>
</tr>
<tr>
<td>LL D3</td>
<td>182.0</td>
<td>181.0</td>
</tr>
<tr>
<td>HL D0 (base)</td>
<td>178.5</td>
<td>180.5</td>
</tr>
<tr>
<td>HL D3</td>
<td>181.5</td>
<td>180.5</td>
</tr>
</tbody>
</table>

3.3.2. Flame development and flame–wall interaction

In this section, the flame development and flame–wall interaction during the mixing-controlled phase (stage 4) of methane combustion are studied. It is worth mentioning that in the experimental study, it was not possible to record the flame development after a specific time as the flame turned inwards the cylinder. The current CFD simulation allows the investigation of the development of flame and species for the whole combustion process. Varying the pilot fuel injection timing influences the local stratification of the methane fuel. The local distribution of equivalence ratio and temperature are presented on a cross-sectional plane passing through one of the methane injector holes in Fig. 11. The contours are presented only for the high load as a similar trend is observed under the low load. Fig. 11 depicts that, for the base case (HL - D0), methane jets penetrate further in the injection direction. On the other hand, for the retarded case (HL - D3), methane is distributed towards the piston. In the HL - D3 case, as the diesel flame reaches the methane jets, there exists a big cloud of unburned methane prior to the diesel combustion. The intense combustion of the methane, which starts from the top of methane jets, propagates downwards, thus expanding the flame and methane gas towards the piston. This observation is found to has an effect on the flame–wall interaction, which will be discussed next.

Figs. 12a and b illustrate the temperature contours for different pilot injection timings. CH₄ mass fraction is also presented in the Figs. 12c and d at the same CADs to visually separate the location of diesel and methane flames. Fig. 13 depicts the normalized volume of the high temperature region beside walls by the volume of combustion chamber at TDC (Vwall/Vchamber). The high temperature region is defined as the cells at a distance of 5 mm from the wall with a temperature higher than 1000 K. Fig. 13a depicts the high temperature region by the valve, cover, and liner surfaces, while Fig. 13b illustrates the high temperature region by the piston surface. The separation of the surfaces is carried out to clarify the direction of flame development. As shown in Figs. 12 and 13, at 185 CAD ABDC, the diesel flame reaches the liner in the HL - D0 case. The location of diesel flame–liner wall interaction is specified by arrow in Fig. 12a at 185 CAD ABDC. As it can be seen in Fig. 12c, there is no CH₄ in the location of diesel flame–liner wall interaction.
Fig. 7. Spatial distribution of high temperature ($T$) region which presents the formation of diesel flame. The values lower than the 1000 K are clipped from the contours. The diesel fuel particles are represented by blue Lagrangian particles. The outlines show the cylinder liner and methane injector. Arrows show the swirl direction. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Fig. 8. The iso-surface of methane mass fraction with a value of 0.01 colored by temperature ($T$) to show diesel flame-methane jets interaction and methane flame in the premixed combustion phase from side view (left column) and top view (right column). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

at 185 CAD ABDC which suggests that the flame specified in Fig. 12a with the arrow belongs to the diesel combustion. Based on Figs. 12b and 13, there is no high temperature region beside the valve, cover, and liner walls in the HL-D3 case. On the other hand, the methane
flame propagation towards the piston in the HL - D3 case leads to a higher flame–wall interaction on the piston than that of in the base case (HL - D0). It may be expected that the diesel flame in the HL - D3 case reaches the liner at 188 CAD ABDC similar to that in the HL - D0 case, as there is a 3 CAD time interval between these two cases. However, it can be observed that the diesel flame in the HL - D3 case does not penetrate through the cold methane jets, and therefore there is no considerable flame impingement on the valve, liner and cover wall regions in the HL - D3 at 188 CAD ABDC (cf. the specified location on the temperature contours in Figs. 12a and b with blue arrows). The intense flame of the premixed methane has a high interaction on the piston in the HL - D3 case at 188 CAD ABDC due to the propagation of the methane flame towards the piston.

At 191 and 194 CAD ABDC, the methane flame for the HL - D3 case reaches the valve, liner, and cover surfaces but with a weaker interaction on these surfaces than in the HL - D0 case. For the later CADs such as 197 CAD, the methane flames for both the cases reach the wall and flame–wall interaction is similar for both of the base and retarded cases. Based on the results, it can be concluded that in the base case at the initial stages of the combustion between 185 to 197...
Fig. 11. Local distribution of equivalence ratio ($\phi$) and temperature ($T$) for different pilot fuel injection timings on a plane passes through the third nozzle hole of the methane injector in the high load case with (a) base and (b) retarded pilot fuel injection timings. Arrows indicate the methane penetration direction.

Fig. 12. Temperature ($T$) contours at various CADs illustrating flame-wall interaction at different pilot injection timings in the high load operating condition: (a) base and (b) retarded pilot fuel injection timings. Mass fraction of CH$_3$ in the high load operating condition: (c) base and (d) retarded pilot fuel injection timings. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)
CAD ABDC, the main flame–wall interaction occurs at the vicinity of the valve, cover, and liner surfaces as the diesel flame penetrates through the methane jets. On the other hand, in the retarded case the main flame–wall interaction occurs on the piston due to the formation of a large methane flame zone at the piston surface.

3.3.3. Emission formation

In this section, the effects of the pilot fuel injection timing on the emission formation under both the high and low load conditions are investigated.

Unburned hydrocarbons (UHC) and soot is a common problem in small scale engines as demonstrated in [8–10]. In the present low speed pilot-ignited HPDI NG engine, the amount of soot emission at the exhaust valve opening (EVO) is negligible because methane combustion generally produces low levels of soot. At the same time, soot has a long time for oxidation before EVO. Therefore, the soot results are not reported in this study. It is reported that the measured methane slip and unburned methane is lower than 0.2 g/kwh in low speed pilot-ignited HPDI MAN ME-GI engine [3]. Therefore, the results of unburned methane and methane slip are not presented in this study.

The average in-cylinder temperature ($\bar{T}$) and average NO mass fraction ($\bar{Y}_{NO}$) are presented in Fig. 14. The maximum value of $\bar{T}$ occurs almost at the same CAD for all pilot fuel injection timings for each load (cf. Fig. 14a). This implies that the mixing-controlled phase of methane
combustion does not change considerably with the variation of the diesel injection timing. In the NO emission production, the main factors are temperature, reaction time, as well as concentrations of oxygen, OH and O. Based on Fig. 14b, the $\bar{Y}_{NO}$ levels appear to be higher in the low load case than those in the high load. As it is mentioned before in Section 3.3.1, with the same amount of fuel, the combustion intensity is higher in the low load case than that in the high load case. This is due to further propagation and wider distribution of methane (because of the lower charge density) and longer IDT of methane in the low load than that in the high load which lead to better air–fuel mixing. This leads to a higher temperature and higher concentrations of radicals (OH and O) that result in a higher NO formation under the low load condition. For the base and retarded pilot injection timings, the average NO under the low load is 85% and 65% higher than their respective high load counterpart.

The base pilot fuel injection timing cases have a higher net NO emission according to Fig. 14b. This is likely due to the later start of the combustion in the retarded case, which resulted in a lower $\bar{T}$ at the start of combustion than that in the base case. Fig. 15 depicts the NO and CH$_4$ distribution. It can be clearly seen that the instantaneous NO distribution in the retarded case is less than that in the base case. One will notice the presence of empty pockets in the NO distribution (as indicated by the arrows). It is speculated to be due to the cold methane jet which lowers the local temperature around its vicinity. Furthermore, it could be also due to the low oxygen content locally. These collectively inhibit the formation of NO.

4. Conclusion

Three dimensional computational fluid dynamic (CFD) simulations are performed to study the combustion and emission formation under two-stroke, dual-fuel (DF) marine engine-like conditions. The non-premixed DF engine configuration is considered here, at which operates using a high-pressure, direct injection (HPDI) of methane. A skeletal mechanism consisting of 56 species and 128 reactions is used. The numerical results under high and low load operating conditions with high and low charge densities are compared against the experimental data of the test engine. Reasonable agreement is observed for the predicted pressure and heat release rate (HRR) profiles. The main findings are as follows:

- The diesel spray jets from the nozzle holes which are aligned with the swirl direction, penetrate longer into the combustion chamber and ignite relatively earlier than the other diesel spray jets.

- Methane flame initiates at the location when the diesel flame comes into contact with the methane jets. Thereafter, the flame develops first around the outer region of the jet before burning towards the inner, fuel-richer region.

- The methane jets penetrate further into the chamber in the low load case due to lower charge density. This longer penetration leads to better air–fuel mixing, higher combustion intensity and HRR in the main premixed and mixing-controlled combustion phases.

- The injection timing of the pilot diesel fuel has a major effect on the early stages of combustion such as the premixed combustion phase of methane under the investigated operating conditions. It is found that the intense combustion of methane in the retarded pilot diesel injection timing expands the flame downwards towards the piston surface leading to a stronger flame interaction. On the other hand, in the base case with an early diesel injection timing, the diesel flame penetrates through the methane jets and impinges onto the liner wall.

- The net amount of NO emission is lower in the retarded pilot injection timing due to lower combustion chamber temperature. Similar observation are obtained for different charge densities under the present investigated operating conditions.

CRediT authorship contribution statement

Arash Nemati: Conceptualization, Methodology, Validation, Writing – original draft. Jiun Cai Ong: Conceptualization, Supervision, Writing – review. Kar Mun Pang: Conceptualization, Supervision, Writing – review & editing. Stefan Mayer: Writing – review & editing. Jens Honoré Walther: Supervision, Writing – review & editing.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgments

The authors gratefully acknowledge the financial support from the Independent Research Fund Denmark (DDF) and MAN Energy Solutions under the grant number 8022-00143B. The authors also would like to thank MAN Energy Solutions, Denmark for sharing the experimental data. The computations were performed using the Niflheim cluster at Department of Physics at the Technical University of Denmark (DTU). The authors acknowledged PRACE for awarding us access to Joliot-Curie at GENCI@CEA, France.
Fig. 15. Spatial distribution of CH$_4$ and NO in the high low load case for (a) base pilot injection timing and (b) retarded pilot injection timing. The outlines show the cylinder liner and methane injector.

References


