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A numerical investigation on combustion and emission characteristics of a dual fuel engine at part load condition

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Highlights
- Flame structure in dual fuel engines depends on operating conditions.
- At part load, diesel liquid drops evaporate lately and far from injector nozzles.
- At part load, UHC is remained in the most remote areas from diesel fuel injector.
- Enlargement of diesel combustion region could ignite lean methane/air mixture.

Abstract
Dual fuel engines are more attractive due to lower emission levels in comparison with conventional diesel engines particularly at full loads. But it is required to study dual fuel combustion process with more details at part loads due to the poor performance and high CO and UHC emissions at these conditions. In the present study, numerical modeling of OM-355 dual fuel (injection of diesel pilot fuel to premixed mixture of air and methane) engine has been performed by using KIVA-3V code at part and full loads. Sub-models of the code were modified to simulate the fuel spray atomization, combustion and pollutants emissions processes, accurately. Results indicate that in-cylinder pressure, heat release rate and exhaust emissions predictions are in good agreement with experiments at all loads. Results show that a lean premixed natural gas mixture is ignited slowly. The slow progress of combustion process at part load, leads the heat release to be drawn more toward the expansion stroke which causes incomplete combustion, and consequently high amounts of UHC and CO will be emitted. It is found that at part loads, areas that are influenced by diesel diffusion flames are ignited and premixed natural gas flame could not be propagated properly. Hence development of diesel diffusion flame is required to burn lean natural gas mixture. But at full load, in addition to the diesel diffusion flames, premixed natural gas flame could be propagated suitably. Also, at part load because of low gas temperature in the environment of diesel spray and low diesel fuel temperature, diesel liquid droplets evaporate lately which are far from injector nozzles. Hence, it causes diesel diffusion flame from spray of each injector nozzles to be developed distinctly. It can be deduced that the flame structure is affected by operating conditions. Finally the effect of increasing the diesel fuel quantity on improving methane combustion is studied. The studied strategy could help to improving natural gas combustion due to enlarge the size of diesel combustion region.

1. Introduction

The compression ignition engine of the dual fuel type is a respectable alternative for conventional diesel engine. The dual fuel engine has many advantages over conventional diesel engine include economical, technical and environmental benefits. Dual fuel engine has been employed in a wide range of applications to utilize various gaseous fuel resources meanwhile exhaust gas emissions are minimized without excessive increase in the engine cost compared to that of conventional diesel engines [1]. Dual fuel engines emit low amounts of carbon dioxide due to the low C/H proportion of methane [2,3]. Also dual fuel engines have a notable potential to reduce Nitrogen Oxides (NOx) and Particulate Matter (PM) emissions. PM emissions could be reduced with the
substitution of a large quantity of diesel fuel with natural gas and NO\textsubscript{e} emissions of a dual fuel engine depend on the parameters of the diesel injection [3]. On the other hand, the low cost and easily converting possibility of the conventional diesel engines to dual fuel mode is the other benefit [4]. As the gaseous fuel is mixed with intake air in inlet manifold, the mixture formation is modified greatly, and then, inside the cylinder, the mixture undergoes a multi-point ignition due to combustion of a pilot diesel fuel spray. Then, flame propagation occurs throughout the premixed natural gas and air mixture. Thus, dual fuel operation with natural gas fuel can yield a high thermal efficiency, almost comparable to the same engine operating on diesel fuel at higher loads. However, dual fuel engines suffer from lower performance parameters, higher Carbon Monoxide (CO) and Unburned Hydrocarbon (UHC) emissions and consequently higher amount of chemical availability of unburned fuels at part loads. The main reason for this poor part load performance is due to the presence of very lean mixtures and poor flame propagation in the lean mixture [1,5]. The lean premixed natural gas mixtures are hard to ignite and slow to burn [1].

Karim et al. showed that with very lean mixture and small pilot quantities, the flames initiated by pilot fuel are unable to develop throughout the combustion chamber [6,7]. Tao concluded experimentally that Nitric Oxide (NO) emissions in dual fuel engines is much less than conventional diesel engines. Also, it was shown that late combustion and low temperature burning of gas result in low NO in dual fuel engines at all conditions [7,8]. Micklow and Gong studied performance and emission characteristics of a dual fuel engine at part load conditions using KIVA-3V code. Results showed that 40% of methane remained unburned near the cylinder wall [9]. Kusaka et al. used KIVA-3V code coupled with Chemkin-II for modeling of a dual fuel engine at part load conditions. They detailed chemical kinetics including 173 reactions and 43 species. Results showed that combustion of premixed mixture of natural gas and air is very slow, so natural gas burns incompletely [10]. They also investigated dual fuel engines at 2/5 load condition by using a multi-dimensional model combined with the detailed chemical kinetics including 290 reactions and 57 species. In this study, the effect of premixed charge concentration on combustion was examined. At 2/5 load due to the low concentration of the gaseous fuel in the mixture, combustion occurs incompletely which cause to decrease the thermal efficiency and to increase the UHC. When four cylinder dual fuel engine operates with two cylinder, combustion occurs completely due to high concentration of gaseous fuel in the mixture [11]. Reitz et al. investigated combustion of a dual fuel engine by using a multi-dimensional Computational Fluid Dynamic (CFD) model with KIVA-3V code. They represented that the characteristic-time model could predict engine combustion, performance and emission characteristics very well for cases with natural gas up to 90 percent (10 percent diesel pilot quantity). If the energy supplied by the diesel fuel is less than about 10%, a flame propagation model such a Spark Ignition (SI) engine should be used for natural gas combustion [12]. Liu et al. studied the dual fuel engine combustion with numerical and experimental methods. A 3D-CFD model based on KIVA was developed. The simulation includes a reduced detailed chemical kinetics for the diesel fuel and detailed chemical kinetics for the gaseous fuel component. They concluded that dual fuel engine combustion may be an effective approach to utilize gaseous fuel–air mixtures of low energy density and to achieve stable combustion, a minimum absolute quantity of diesel pilot is needed [13]. Hosseinizadeh et al. concluded that in dual fuel engine without hot Exhaust Gas Recirculation (EGR), because of the incomplete combustion at part load condition, chemical availability of unburned fuel is too much. In this condition, 28% of total input chemical availability is exhausted to the atmosphere [14]. Puduppakkam et al. studied the use of a five-component gasoline surrogate and a one-component diesel surrogate by using a multi-dimensional CFD model coupled with detailed chemical kinetics to simulate Homogeneous Charge Compression Ignition (HCCI) and Reactivity Charge Compression Ignition (RCCI) dual fuel engine operation. The results showed that the model predicted the combustion and emissions very well. Also the model represented that the most-reactive fuel component, n-heptane (component in both diesel and gasoline surrogates) is consumed at a much faster rate than other less-reactive gasoline surrogate components such as iso-octane and toluene [15]. Maghbouli et al. investigated the combustion process in the diesel and dual fuel engine with utilizing a 3D-CFD model coupled with chemical kinetics including 57 reactions and 42 species. They showed that by shifting the diesel combustion to the dual fuel combustion mode, the ignition delay time is increased [16]. Maghbouli et al. studied the combustion process under knocking conditions in dual fuel engines. They
showed that end-gas knock was occurred near cylinder walls in piston bowl corner of OM-355 engine [17]. Wurzenberger et al. offered a simulation model for dual fuel operated engines. The model concentrates on a computationally optimized method to comply with real-time constrains. Three different species transport modeling depth are offered. A thermodynamic highly accurate 6-species approach, a lumped 3-species and a lumped 1-species transport approach are investigated. They concluded that in comparison with experiments, the 6-species approach showed very good results [18]. Xu et al. investigated diesel–methanol dual fuel combustion and they expressed that with increasing the methanol fraction, the ignition delay is affected by the coupling of the diesel and methanol fuel chemical reactions and by changes in the in-cylinder temperature [19]. Rakopoulos et al. studied experimentally the effect of properties of various common bio-fuels on the DI diesel engine. They represented that, with increasing proportion of all bio-fuels in the blends, significant reduction of smoke is observed. With exemption of the vegetable oil blends, all the other bio-fuels diesel fuel blends illustrate a decrease of CO emissions [20,21].

From the previous brief survey, it can be concluded that dual fuel engines have limitations at some conditions. The most important limitation of dual fuel engines is related to part load conditions. By reference to previous studies on dual fuel engines although many studies were carried out in the recent years, but the dual fuel combustion process specially at part loads is still unclear and more CFD simulations are needed [3]. The CFD simulation is one of the best tools to investigate complex in-cylinder actions of engines. The contribution of the simulation results to engine design chiefly depend on the predictive capabilities and the reliability of the models [22]. In the present work, due to the lack of detailed and comprehensive study at part loads, combustion of dual fuel engines at part loads is studied. Multi-dimensional CFD model is used to simulate a dual fuel engine combustion process with modified KIVA-3V code.
In this study, suitable combustion and spray model added to KIVA-3V code to simulate part load condition properly. To achieve the mentioned scope, heat release rate, in cylinder pressure diagrams and emissions contours were plotted and then the methane burning and flames structure at part and full load are compared and discussed. Finally one of the suggested strategies is investigated to overcome part load disadvantages.

2. Model description

The KIVA-3V was used to simulate the closed part of the cycle in the present work. In this code governing equations are conservation of mass, momentum, energy, chemical components and the equation of state [23]. The governing equations are solved by finite volume modified method that called Arbitrary Lagrangian Eulerian (ALE) method [24]. Flowchart of 3D-CFD numerical modeling is presented in Fig. 1 [23].

Table 2

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<thead>
<tr>
<th>Simulation case</th>
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<td>1600</td>
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<tr>
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2.1. Breakup, evaporation, collision and turbulence models

In this simulation, the wave breakup model developed by Reitz [25] has been replaced instead of KIVA-3V original TAB model. In the wave model, the injected fuel is presumed as parcels of droplets that the size of these parcels is calculated from the fuel nozzle diameter and the numbers of parcels is calculated from fuel flow rate. Breakup and atomization processes are modeled by means of Kelvin–Helmholtz jet stability model. In this model, the fuel vapor distribution predicted well, because the new drops produced by high-pressure spray can be subdivided into smaller droplets at each timestep and the small product drops vaporize very rapidly [26]. The fuel drops breakup is derived from the result of a stability
Fig. 8. Methane and diesel concentration (g) contours for part load case 1 (left) and full load (right) conditions at several CADs.
analysis, and the mass of new droplets, which is formed due to breakup, is deducted from the parent drops. The radius of parent drops “a” alters by the subsequent rate equation:

\[
\frac{da}{dt} = \frac{(a - r)}{\tau}
\]

where “r” is the radius of the child drop radius (r ≤ a). The breakup time τ and the breakup drop radius r are determined by:

\[
\tau = \frac{3.726B_1a}{A\Omega}
\]

\[
r = B_0A
\]

where \(B_0A ≤ a\), and the surface wave length and growth rate \(A\) and \(\Omega\) are gained by utilizing jet stability analysis, and \(B_0\) and \(B_1\) are adaptable empiric coefficients that their quantities are 0.6 and 1.7, respectively [3,25,27]. Semi-empirical frossling model is used for calculating evaporation of diesel fuel droplets in which the effects of temperature, concentration and velocity on the droplet evaporation can be considered [23]. Droplet collision modeling is done with the O’Rourke model. This model considers tracking of droplets for estimating the number of collisions with using the Poisson distribution function [23]. RNG K-ε turbulent flow model is used for turbulence modeling. The model was derived using a very accurately statistical method and is similar to RNG model with this difference that the effect of rotation (Swirl) is considered in the combustion chamber [23].

2.2. Combustion model

Combustion process in dual fuel engines consists of diesel and natural gas oxidations. Tetradecane (C_{14}H_{30}) and methane (CH_{4}) are utilized as diesel and natural gas fuels representatives, respectively. One step reaction has been presumed for diesel fuel with this chemical reaction [23,24]:

\[
2C_{14}H_{30} + 43O_2 \rightarrow 28CO_2 + 30H_2O
\]

In this modeling, combustion of natural gas is calculated by chemical reactions entirely and natural gas is supposed as 100% methane. Two step reactions are added to code from research work published by Micklow and Gong [9]. These two reactions include:

\[
CH_4 + 1.5O_2 \rightarrow CO + 2H_2O
\]
The reaction rates are given by Eqs. (13) and (14). Also six equilibrium reactions are considered in combustion process as follows [9,23,24]:

\[ \text{CO} + 0.5\text{O}_2 \rightarrow \text{CO}_2 \] (6)

\[ \text{H}_2 \rightarrow 2\text{H} \] (7)

\[ \text{O}_2 \rightarrow 2\text{O} \] (8)

\[ \text{N}_2 \rightarrow 2\text{N} \] (9)

\[ \text{O}_2 + \text{H}_2 \rightarrow 2\text{OH} \] (10)

\[ \text{O}_2 + 2\text{H}_2\text{O} \rightarrow 4\text{OH} \] (11)

\[ \text{O}_2 + 2\text{CO} \rightarrow 2\text{CO}_2 \] (12)

\[ \frac{d}{dt} \left[ \text{CH}_4 \right] = -2.8 \times 10^8 \left[ \text{CH}_4 \right]^{-0.3} \left[ \text{O}_2 \right]^{1.3} \times \exp \left( \frac{48.4}{RT} \right) \] (13)

\[ \frac{d}{dt} \left[ \text{CO} \right] = -3.98 \times 10^{14} \left[ \text{CO} \right]^{0.5} \left[ \text{H}_2\text{O} \right]^{0.5} \times \exp \left( \frac{40.0}{RT} \right) + 5.0 \times 10^4 \left[ \text{CO}_2 \right]^{1.0} \times \exp \left( \frac{40.0}{RT} \right) \] (14)

Since the contribution of NO formation is greater than Nitrogen Dioxide (NO₂), so NO formation mechanism is studied mainly [28]. Extended Zeldovich’s mechanism has been utilized for NO formation [23,24]. The combustion of diesel fuel in direct injection dual fuel engines occurs in chemically controlled and mixing controlled phases that should be implemented in combustion modeling. In this work, specific temperature is used as the threshold value for transition from ignition to combustion. The ignition delay time is supposed as a period when the cell temperature is less than 1100 K [12,29] and this phase is controlled chemically. The ignition model was used to consider low temperature combustion [29]. To simulate this phase of diesel combustion, RR1 equation was used as:

\[ \text{RR}_1 = A \exp \left( -\frac{E_a}{RT} \right) \left[ \text{C}_1\text{H}_{30} \right]^{a} \left[ \text{O}_2 \right]^{b} \] (15)

When diesel combustion is controlled by turbulent eddies, Eddy Dissipation model is used. The model was proposed by Magnussen and Hjertager [30]. In this model, Rate of the combustion is calculated at molecular scale by the eddy mixing rate of the fuel and oxygen separately. The rate of the fuel and oxygen are presented in Eqs. (16) and (17) for diffusion combustion. Fig. 2 shows the mentioned combustion model for diesel fuel. The second and third stages assume that each of the three combustion rates is lower, it controls the combustion [29].

\[ \text{RR}_2 = A \left( \text{C}_{\text{fuel}} \frac{E_a}{K} \right) \] (16)

\[ \text{RR}_3 = A \left( \text{C}_{\text{oxygen}} \frac{E_a}{K} \right) \] (17)

3. Engine specifications and geometry

3.1. Engine specifications and operating conditions

In this study, medium duty turbocharged OM-355 direct injection diesel engine converted to dual fuel mode is used as a dual fuel engine. The model has been validated using experimental data were carried out by Pirouzpanah et al. [31] in the diesel–gas research facility [32]. The specifications of the engine are summarized in Table 1. A schematic of the experimental setup presented in Fig. 3 [16]. Table 2 lists operating conditions of modeling cases under full and part loads operation.

3.2. Engine computational mesh

In this simulation, the full circle combustion chamber was meshed by the ANSYS ICEM CFD software. Three type of computational grid is generated as showed in Fig. 4. The grid independence test is conducted on the in-cylinder pressure results. Fig. 5 shows predicted in-cylinder pressure results by three computational grids for part load case 1. As it can be seen, maximum in-cylinder pressure values predicted by mesh type 1 is very low in comparison with mesh type 2, 3 and experiments. Therefore due to the proximity of the maximum cylinder pressure values with the experimental values and because of low computation time, the mesh type 2 with 19,679 cells was selected as a suitable computational grid.

4. Results and discussion

In this section, the most important results of the numerical outputs will be discussed. As shown in Fig. 6, there are good agreements
between experimental data and numerical results especially at ignition and peak pressure times in all operating conditions. At part loads, it can be seen some differences between measured and predicted pressure data during the combustion and expansion phases. The reason for this trend could be the low-efficiency of heat transfer model [33]. Also heat release rate at full load and part load conditions are shown in Fig. 6. Vital effective parameters on the ignition delay time are in-cylinder temperature, pressure and methane concentration near the diesel fuel spray [7,34]. It can be understood that the combustion process at full load starts earlier than part load owing to higher in-cylinder temperature and pressure. Slow progress of combustion process at part load leads heat release to be drawn more toward the low temperature expansion stroke. The main pollutant emissions of dual fuel engines are UHC, CO and NOx. Table 3 shows the predicted and measured emissions results which are in good agreement with each other at full load and part load conditions.

Fig. 7 illustrates the predicted CO, NO and UHC emissions at all conditions. As shown in Fig. 7 at part loads, CO and UHC emissions are higher in comparison with the full load condition. But NO emissions at part loads is lower in comparison with full load condition.

Fig. 8 shows the methane and diesel concentration contours for part load case 1 and full load conditions at several crank angle degrees (CAD). It is seen that at part load, mixture of the methane and air is very lean and combustion rate of the lean mixture is slow. Slow progress of combustion process leads the combustion to be drawn more toward the low temperature at expansion stroke which causes incomplete combustion. Hence less fuel will be burn at part load condition in comparison with full load. It can be seen that at part load, because of slow combustion speed of very lean
methane/air mixture, remarkable amount of the unburned methane is remained in the most remote areas from diesel fuel injector such as the bottom of the piston bowl and in four directions where diesel fuel is not injected. As it is clear from contours, at part load only areas that are influenced by diesel diffusion flames could be ignited, and premixed methane/air flame could not be propagated suitably. But at full load, in addition to diesel diffusion flame, premixed methane/air flame could be propagated, properly. Hence development of diesel diffusion flame is needed to burn lean natural gas/air mixture entirely at part load condition.

Fig. 9 indicates the difference between flame structures in both of examined cases. As it can be seen, at part load, premixed methane/air flame propagated in the path of the diesel spray.

Fig. 10 illustrates diesel fuel droplets size, penetration and gas temperature at $-11\text{ CAD After Top Dead Center (ATDC)}$ for part load case 1 and full load. It can be implied that liquid drops quantity at part load is more than full load. It is due to low gas temperature and low diesel fuel temperature of part load that could evaporate fewer droplets. Also based on Dent [35] empirical equation with decreasing the gas temperature of the combustion chamber, depth of the spray penetration is increased. It is found that at part load because of low gas temperature in environment of diesel spray and low diesel fuel temperature, diesel liquid droplets evaporate lately and far from injector nozzles, so it causes that diesel diffusion flame from spray of each injector nozzles developed distinctly. Finally it can be concluded that the flame structure is affected by operating conditions.

Fig. 11 shows equivalence ratio and temperature contours for part load case 1 and full load conditions before combustion process and Fig. 12 displays CO concentration contours for part load case 1 and full load conditions at several CADs. Formation of CO is affected by fuel oxidation mechanism. Shape of the CO concentration contours at both loads shows that with diesel fuel injection and start of combustion, CO is formed at fuel-rich zones of the flame path. Owing to the presence of richer mixture at full load, the amount of CO formation at full load is more than part load at the primary CADs. Then at full load because of the suitable flame propagation and fast progress of combustion process in depth of combustion chamber at the subsequent CADs, CO could be oxidized more. At part load, CO concentration at fuel-rich zones of the flame path is high and the produced CO could not be oxidized further. Carbon monoxide is not only considered as undesirable pollutants but also it could waste chemical energy.

To overcome part load disadvantages, any plan to enlarge the size of diesel combustion region or increase the flammability limits of premixed natural gas could be beneficial [6,7]. Increasing diesel fuel quantity [7] and injection pressure, advancing diesel fuel injection [7,36], multiple injection [9], restricting intake air quantity [7], increasing the number of diesel fuel injector nozzles [7], optimizing intake charge temperature and pressure [36] and EGR [1] could improve low load combustion of dual fuel engines. In this research the effect of increasing the diesel fuel quantity at part load conditions, to overcome the mentioned drawbacks, is studied.

Fig. 13 illustrates the effect of increasing the diesel fuel quantity on improving methane combustion. In addition to 12% diesel fuel of base line (part load case 1), the second quantity of diesel fuel value is considered to be 20%. It should be noted that total input energy, fluid flow and thermodynamic initial conditions are kept constant. It is seen that with increasing the amount of diesel fuel at part load condition, diffusion flame penetration of diesel fuel increased. Hence very lean methane/air mixture that influenced by diesel diffusion flames could be ignited properly and propagated rapidly.
5. Conclusions

In this investigation, combustion process of OM-355 dual fuel engine was modeled using KIVA-3V code at the closed part of the cycle. Sub-models of the code are modified to simulate combustion process, accurately. Some important characteristics of the combustion and emission at part load were investigated and compared with full load. Hence, the main conclusions are drawn as below:

1. The combustion process increment at full load starts earlier than part load condition owing to sufficient methane concentration and the rapid growth of flame. Hence ignition delay and combustion duration time at part load is longer than full load condition.

2. At part load condition, because of low combustion speed of very lean methane/air mixture and incomplete combustion, methane could not be burned completely. Then significant amount of the unburned methane is remained in the most remote areas from diesel fuel injector such as the bottom of the piston bowl and four directions where diesel fuel is not injected.

3. At part load only areas that are influenced by diesel diffusion flames could be ignited and premixed methane/air flame could not be propagated suitably. But at full load in addition to diesel diffusion flame, premixed methane/air flame could be propagated properly. Hence, development of diesel diffusion flame is needed to burn lean natural gas air mixture at part load condition.

4. It is found that at part load because of low gas temperature in surrounding of diesel spray and low diesel fuel temperature, diesel liquid droplets vaporate lately and far from injector nozzles. Therefore, it causes diesel diffusion flame from spray of each injector nozzles to be developed, distinctly. This mentioned fact is the cause of flame structure differences at both conditions.

5. CO is formed at fuel-rich zones of the flame path. Owing to the presence of the mixture rich mixture at full load, the amount of CO formation at full load is more than part load at the primary CADs. But at the subsequent CADs because of the suitable flame penetration and fast progress of combustion process at full load, CO could be oxidized more and to be decreased to low values in comparison with part load.

6. To overcome part load disadvantages, increasing diesel fuel quantity was investigated. At part load condition, by increasing the amount of diesel fuel quantity, with the assumption of constant input energy, diffusion flame penetration of diesel fuel is increased. Hence very lean methane/air mixture could be ignited suitably and propagated quickly due to enlarge the size of diesel combustion region.

References


