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The influence of varying hydrogen-methane-diesel mixture ratio on the combustion characteristics and emissions of a direct injection diesel engine

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ABSTRACT

The influence of diesel enrichment with hydrogen and methane (H₂/CH₄) blend in a direct injection compression ignition (DICI) engine were computationally studied. Numerical results by using ANSYS FLUENT software are obtained for 40%, 50% and 60% diesel (by mass) with remaining fraction by various blend of H₂/CH₄ (0%/100%, 30%/70%, 50%/50%, 70%/30% and 100%/0%). Combustion analysis are presented as pressure and temperature behavior as well as rate of heat release. Increasing diesel fraction reduces peak cylinder pressure but shorten ignition delay. Methane-only presence in diesel mix increases ignition delay but as hydrogen content builds up, ignition delay is shorten and peak pressure increase linearly and significantly. Similarly, in-cylinder temperature increases with gaseous fuel presence and directly influenced by hydrogen portion. Highest in-cylinder pressure and temperature are found with hydrogen-diesel mix at 40% diesel. Heat release rate (HRR) is highly influence by gas fuel presence. Peak HRR increases with decreasing diesel fraction but the behavior is less predictable compared to pressure and temperature behavior. Elevated combustion temperature due to increasing hydrogen percentage in the mixture is proportionally evidence in NO formation. While increasing diesel fraction suppresses NO formation, increasing hydrogen content linearly increase NO. Formation of CO is mainly dominated by methane content but increasing hydrogen fraction reduces CO to the level similar to diesel only operation. Formation of NO at different mixture ratio were spatially illustrated showing direct relation to higher temperature spots. Based on the pressure and HRR analysis, it can be inferred that in all fractions of diesel, the mixture of 70% hydrogen and 30% methane yield optimal balance between combustion, resulting cylinder work and emission characteristics. However, to maintain low combustion temperature, higher diesel content are preferable in order to gain higher thermal efficiency by avoiding excessive heat loss.

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1. Introduction

Ground transportation is the main consumer of diesel and gasoline fuels and is a significant contributor to environmental pollution [1]. Diesel is particularly used in compression ignition (CI) engine with benefit from higher fuel efficiency and lower emissions of carbon dioxide (CO_2) compared to gasoline. However, particulate matter (PM) and nitric oxides (NOx) emissions pose

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http://dx.doi.org/10.1016/j.fuel.2016.11.010 0016-2361/© 2016 Elsevier Ltd. All rights reserved. significant challenge to diesel combustion [2]. Among others, selective catalytic reduction (SCR) as well as diesel particulate filter (DPF) have been installed so engines can meet ever stringent emission regulations. Unfortunately, the dependence on costly metal catalysts and high expenses of post-treatment devices limited their use. Other compromised strategies including "dual-fuel diesel engine" have been developed [3]. A comparative study on an engine powered with both pure diesel and biodiesel revealed that the torque and power outputs of biodiesel fuel driven engine are usually lower than those operate with pure diesel [4].

Natural gas (NG) is capable to forming suitable blends to operate with diesel in CI engines. The high knock resistance, thus high octane number of NG (RON > 120) allows engines to operate at

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higher compression ratio leading to higher thermal efficiency. Converting any diesel or petrol engine to bi-fuel or dual-fuel with NG operation require minimal mechanical alterations and clearly evident itself in the steady rise of natural gas vehicles resulting from conversion into CNG engines [5–16]. Studies on the operational features of diesel-NG dual-fuel single-cylinder diesel engine discovered the diesel-NG dual-fuel operation results in longer ignition delay than diesel-only operation [17,18]. In-cylinder pressure and maximum heat release rate are lower at part loads as NG contents increased. Conversely, they are enhanced at high load. The use of diesel-NG dual-fuel engine displayed remarkable increase of CO, HC and PM emissions [19]. However, CO emission can be reduced through the intake of pre-heated air and enhanced quantity of pilot diesel fuel as well as a slight decrease of NO emission is noticed [20]. When a dual-fuel (NG-diesel) engine is operated at various compression ratio and engine speed, increased thermal efficiency and reduced CO emission were discovered at increased compression ratio and elevated engine speed, but thermal efficiency appeared poor at low engine load [21].

Hydrogen is proven to be very efficient and clean fuel [1]. It possesses high specific energy, low ignition energy requirement, superior flame speed and broad flammability range. However, engine run solely with hydrogen requires expensive hydrogen generation which limits its use. Blending hydrogen with other fuels seems to be more practical to gain its advantages. An investigation on the combustion behavior of a diesel-hydrogen engine revealed optimal peak in-cylinder pressure enhancement at 70% load, which is prerequisite for safer and durable engine performances [22]. Also peak heat release rate coupled with CO and smoke emissions reduction were recorded [23]. The combustion efficiency is determined to be relatively lower with high fraction of hydrogen. The efficiency of hydrogen combustion is found to depend on the engine load and it is suggested that in order to obtain superior energy conversion efficiency, hydrogen should be inserted at higher load [24]. Increasing hydrogen content reduces emissions of HC, CO, CO₂ and PM almost linearly [22,25]. On the other hand, NOx emission is decreased at lower part loads but increased at high loads [26]. High combustion temperature which enhanced NOx formation due to high combustion rate of hydrogen is the reason. Thermal efficiency of an engine is decided by its load, speed and the amount of incorporated hydrogen [27]. Increasing hydrogen content tend to reduce thermal efficiency while increase specific fuel consumption [28].

The ignition processes of spark-ignition engine containing NGhydrogen blend as fuel are extensively analyzed and certain limitations associated with the efficiency and emissions are removed [29]. Ignition delay reduction has been achieved with adjustment of partial oxygen pressure in air [30]. This influences the normal diesel combustion. Hydrogen is use to expand methane leanlimit of and also enhance the combustion rate [31]. Increasing hydrogen fraction in a hydrogen-methane engine linearly enhances the laminar flame speed of the mixture [32]. The advantage of mixing hydrogen with was also found to shorten ignition delay [33].

Lately, the notion of tri-fuel engines is introduced to extend the performance of conventional dual-fuel engines. Theoretical and experimental investigation on a diesel engine performance mixed with LPG-hydrogen has been carried out, showing significant efficiency improvement particularly at low and part loads when hydrogen is introduced to the LPG-diesel mix [34]. Blending of hydrogen with methane is thought as alternative route for combustion improvement which could lead to higher flexibility of diesel engine operations. However, in the hydrogen-diesel combustion, combustion instability were found at high engine loads with some knocking effect due to inherit hydrogen properties (high diffusivity, low energy required for ignition and superior

burning rate). Addition of methane makes combustion of hydrogen more stable by avoiding unusual ignition. Nevertheless, methane presence reduces the combustion temperature of hydrogen and suppresses NOx emission [35]. A study on various energy content ratio of hydrogen-methane-diesel blend on the performance on a Cl engine revealed that medium ratio of gas fuel in the mix is more beneficial [36].

Despite the introduction of several alternative fuels, petroleumbased fuel still remains economic and practical. However, rapid industrialization and motorization of modern world poses serious concern regarding these conventional fuels mainly for two reasons: non-renewability and also environmental worsening. Intensive efforts must be dedicated to lessen the use of fossil fuels in transport vehicle. In this view, we computationally investigated the effect of tri-fuel direct injection CI engine operation with hydrogen-methane mix with diesel in a broader mixture ratio range. The focus were on the combustion and emission characteristics. From the previous works described in the preceding paragraphs, the benefits of adding methane and hydrogen onboard vehicle in terms of reducing emissions and long-term fossil fuel sustainability can surpass the concerns of adding weight, volume and cost to vehicles provided that the system is calibrated accordingly. This tri-fuel application is more practical with heavy duty engines and vehicles.

2. Numerical model setup

The investigation was performed using ANSYS-Fluent 14.5. The geometry of the combustion chamber was prepared in ANSYS-Design Modular. The mathematical model in CFD starts with construction of computational domain. The simulation starts at 53°CA ABDC and ends at 53°CA BBDC (IVC \rightarrow EVO) i.e. only part of compression and expansion strokes were considered. Computational domain consists of combustion chamber geometry without any valves or ports. The injector is inclined at 15° to vertical. This non-uniformity required a full 360° model. The combustion chamber is bowl-in-piston type. Table 1 summarizes key parameters of the engine under investigation. The cylinder is divided into two zones: zone 1 consists of clearance volume and swept volume and zone 2 have piston bowl volume. Zone 1 is meshed with quad-mesh while zone 2 which is meshed with tri-mesh. The meshed domain consist of 80,020 elements.

In FLUENT, the mixing and transport of chemical species are simulated by solving the equations of conservation which include diffusion, convection and reaction sources of every individual species. Reactions occurring was used to model multi chemical reactions. Finite-Rate/Eddy-Dissipation model was used to simulate the turbulent species transport combustion [37]. 1-step and 4-step chemical reactions were adopted in combustion process. In the 1-step reaction, combustion of 5 species (CH_4 , CO_2 , H_2O , O_2 and N_2) refer to Westbrook and Dryer global chemical kinetics scheme, while in the 4-step reaction, combustion of 7 species

Table 1

Key parameters of the single-cylinder Yanmar L100AE-D engine.

Engine parameter	Value	Unit
Bore	86	mm
Stroke	70	mm
Displacement volume	406	cm ³
Compression ratio	19.3:1	-
Intake valve open-IVO	20	BTDC
Intake valve close-IVC	53	ABDC
Exhaust valve open-EVO	53	BBDC
Exhaust valve close-EVC	20	ATDC
Maximum power output (3600 rpm)	7.4	kW

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