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Parametric investigation of hydrogen-diesel combustion for a marine medium-speed dual fuel engine

Simulation Technologies, Digital Twins and Complex System Simulation

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ABSTRACT

Zero carbon fuels are expected to catalyse the decarbonisation of the maritime industry with hydrogen being considered a long-term solution. However, hydrogen combustion limitations must be addressed for marine engines, to accommodate the use of higher hydrogen energy fractions whilst maintaining knock-free conditions, minimise unburnt hydrogen, and reduce NOx emissions. Although hydrogen port injection can become an attractive solution to retrofit marine engines, studies in the pertinent literature are limited. This study aims to investigate a marine dual fuel engine operating with hydrogen as secondary fuel with 20% hydrogen energy fraction. A large marine four-stroke engine with nominal power output of 10.5 MW at 500 rpm is investigated considering hydrogen port injection. A CFD model is set up in CONVERGE for both the diesel and the diesel-hydrogen operating modes to investigate the effects of on the engine performance, emissions, and combustion characteristics. This model is validated against experimental data for the diesel mode and reported data for a smaller engine operating with diesel and hydrogen. The mesh characteristics are selected to compromise between the prediction error and computational effort. Case studies with varying in-cylinder temperature at inlet valve close are considered to identify the envelope for stable combustion. The results provide guidance to optimise the investigated engine settings considering the contradictory objectives of high efficiency, low NOx emissions and knock-free operation. This study contributes to the identification of efficient and reliable combustion conditions for diesel-hydrogen dual fuel marine engines.

1. INTRODUCTION

Hydrogen has emerged as a potential zero-carbon fuel, which can support the maritime sector to achieve the net-zero goals set by the International Maritime Organisation's (IMO) for the next 25 years [1]. Previous studies discussed hydrogen-fuelled engines feasibility, concluding that hydrogen-based operations could be economically viable when carbon taxation schemes come into effect [2]. Yet, adapting hydrogen for use in marine compression ignition engines poses significant challenges, mainly due to its high auto-ignition temperature, which demands high compression ratios [3]. Injecting hydrogen along with a high reactivity fuel, such as diesel, could overcome these issues [4]. Typically, diesel is injected near the top dead centre (TDC), while hydrogen can be injected either in the inlet ports or directly into the cylinders. The hydrogen injection strategy and settings (pressures and timings) affect the combustion stability as well as the engine performance and emissions [5].

Köse and Ciniviz [6] and De Morais et al. [7] reported that hydrogen port injection increases exhaust gas temperature and nitrogen oxides (NOx) emissions. Zhou et al. [8] and Talibi et al. [9] revealed the hydrogen injection led to increased in-cylinder pressure and temperature. Jamrozik et al. [10] concluded that the hydrogen higher burn rate leads to local maxima in the heat release rate, and shorter ignition delays due to hydrogen high laminar flame velocity. Li et al. [11] and Liu et al. [12] revealed that direct hydrogen injection at appropriated timing can mitigate issues like pre-ignition and knocking.

Despite these research efforts, hydrogen combustion and use in marine engines, especially for port injection and dual hydrogen–diesel engines, remain challenging. Given its potential for retrofitting, hydrogen port injection in marine engines could become an attractive solution for decarbonising the maritime industry [13].

This study aims at numerically quantifying the operating envelope, as well as the performance and emissions characteristics of a dual-fuel marine engine, operating with 20% hydrogen by using CFD modelling.

2. INVESTIGATED ENGINE

A large marine four-stroke engine is modelled. The main particulars of this engine are listed in Table 1. Further details of the engine are reported in Karvounis et al. [14].

Table 1. Marine engine characteristics.

Parameter	**Value**
Engine type	Wärtsilä L46C
Brake Power at MCR (kW)	10,500
Speed at MCR (r/min)	500
Cylinders Number (–)	9
Compression Ratio	14.0:1
Bore / Stroke (mm)	460 / 580
Diesel Start of Injection	6°CA BTDC
Diesel Injection Pressure (bar)	1,200
Hydrogen Energy Fraction (%)	20
Nozzle angle (deg)	67.5
Spray Cone Angle (deg)	17.5
Nozzle Diameter (mm)	0.78

3. METHODOLOGY

The followed methodology for developing the CFD models considers the seven steps described in detail by Karvounis and Theotokatos [15]. Step 1 defines engine input parameters considering the investigated engine characteristics. Step 2 includes the development of a CFD model for the diesel mode in CONVERGE. The initial and boundary conditions of this model are provided in Table 2 whereas the employed sub-models are listed in Table 3. Step 3 deals with a grid sensitivity study to compromise between accuracy and computational effort. Step 4 focuses on the CFD model validation for the diesel mode against experimental data. The derived results for the in-cylinder pressure and heat release rate (HRR) in 90% load are presented in Figure 1.

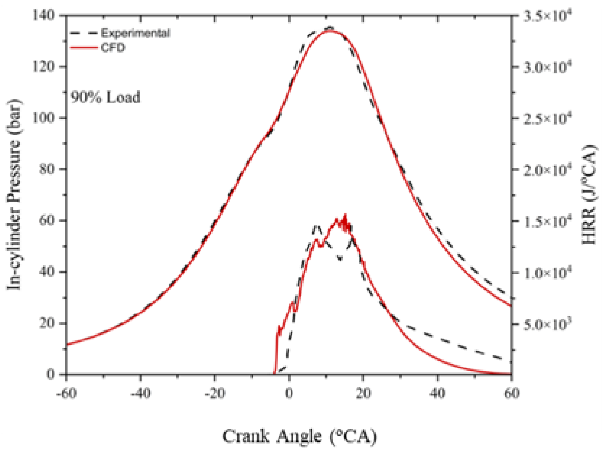

Figure 1. In-cylinder pressure and heat release rate for diesel operation at 90% load (CFD results and measured data).

Step 5 deals with the CFD model extension for the dual fuel (DF) mode. This model employs the same solver, grid, and settings. It is considered that the hydrogen is injected in the intake port and a homogeneous hydrogen–air mixture is formed at the inlet valve close, whereas the diesel fuel is injected in-cylinder to start the combustion. The study considers 20% hydrogen energy fraction (HEF). Step 6 deals with the parametric investigation considering several values of the temperature at the inlet valve close (IVC). Step 7 discusses the results to reveal the hydrogen combustion characteristics in the investigated marine diesel engine.

The CFD models are developed based on the following assumptions:

- Homogenous air–hydrogen mixture.
- Diesel fuel direct injection in-cylinder considering a trapezoidal injection pulse.
- Ideal gas state representing the in-cylinder working medium thermodynamic behaviour.
- Identical behaviour of all engine cylinders, hence the single cylinder model represents the whole engine.

The root mean square error (RMSE) is calculated to quantify the variation between the CFD results and measured values. The in-cylinder pressure RMSE was found 3 bar, which is deemed acceptable. The maximum in-cylinder pressure error was found around 0.1%, whereas the crank angle at maximum pressure for the CFD results was found retarded by 2ºCA compared to the measurements.

To validate the dual diesel-hydrogen combustion model, a smaller engine for which experimental data was reported was simulated. The pertinent results are not presented for brevity. The estimated error metrics provide evidence on the CFD models adequacy for the investigated case studies.

Table 2. CFD model boundary and initial conditions for the diesel mode.

Boundary Conditions	**Value**
Cylinder head Temperature (K)	500
Cylinder liner Temperature (K)	400
Piston Temperature (K)	520
Initial Conditions	
Temperature at the IVC* (K)	360
Pressure at the IVC (bar)	2.8
Turbulent kinetic energy (m^2/s^2)	62.02
Turbulent dissipation (m^2/s^3)	17,183
Diesel fuel temperature at nozzle (K)	340

*IVC: inlet valve close

Table 3. Employed Sub-models.

Mechanisms	**Model**
Turbulence model	RANS k-ε
Droplet breakup model	KH-RT
Spray/Wall model	Han
Droplets collision model	NTC
NO_x mechanism	Extended Zeldovich
Reaction mechanism	Andrae and Head

4. GRID SENSITIVITY STUDY

A grid sensitivity analysis is performed to evaluate the trade-off between error and computational time for both the diesel and dual fuel modes. The employed grids include a base element size of 8 mm, which progressively refined through adaptive mesh refinement (AMR) to 2 mm, 1 mm, and 0.5 mm for Grids 2, 3, and 4, respectively. Grid 1 represents the base grid without AMR, maintaining an 8 mm cell size. These meshes characteristics are listed in Table 4.

Table 4. Computational mesh characteristics

Parameter	**Grid 1**	**Grid 2**	**Grid 3**	**Grid 4**
Base element size (mm)	8	8	8	8
Final element size (mm)	8	2	1	0.5
Solution duration (h)	4	11	20	70
RMSE on p_{cyl}* (MPa)	0.288	0.244	0.215	0.214
Error on p_{max} (%)*	6.2	4.4	1.3	3.4
Adaptive mesh refinement	On: between 12ºCA BTDC and 135ºCA ATDC			
Number of Cores Used	40: Intel Cores IPM			

*for the diesel mode; RMSE: root mean square error; p_{cyl}: in-cylinder pressure for the closed cycle; p_{max}: maximum in-cylinder pressure

The in-cylinder pressure, mean temperature, and heat release rate (HRR) for each grid along with measured results for the diesel mode are illustrated in Figure 2.

Grids 3 and 4 exhibit only slight deviations in the maximum in-cylinder pressure and heat release rate. Grid 4 exhibits a slightly lower maximum in-cylinder temperature compared to Grid 3. Similar findings are obtained for the dual fuel mode. Based on these results, Grid 3 is identified to provide a compromise between computational efficiency and accuracy.

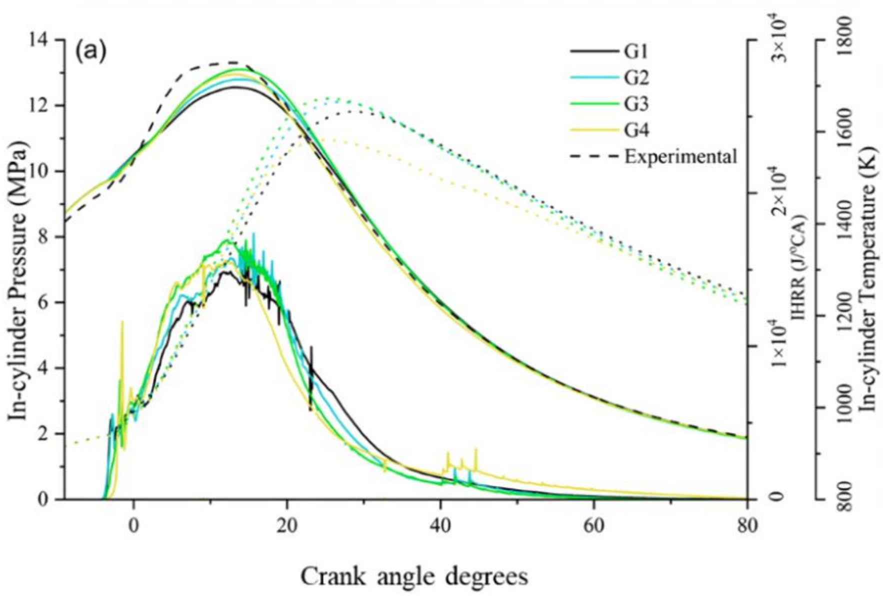

Figure 2. In-cylinder pressure, heat release rate and mean in-cylinder temperature variation for the selected grids in the diesel mode.

5. CASE STUDIES

The laminar flame velocity of hydrogen fuel is significantly higher compared to diesel, which leads in rapid combustion for high in-cylinder temperature and pressure conditions [16]. However, hydrogen ignition resistance is significant, hence an ignition source is needed to start the combustion [17]. This study considers 20% hydrogen energy fraction (HEF), with the hydrogen–air mixture being assumed homogenous at inlet valve close (IVC).

The initial temperature at IVC for the diesel mode is 300 K and varies up to 440 K to investigate its effect on hydrogen combustion. For higher in-cylinder temperature, the NOx emissions increase, hence it is intended to retain T_{IVC} as low as possible, while accounting for the unburned hydrogen limit of 3% [18]. Increasing the charging temperature is expected to reduce the air density and hence increased boost pressure is needed to provide the same charge mass. The considered T_{IVC} range and increment are provided in Table 5.

Table 5. Modelled cases initial temperature at Inlet Valve Closure (IVC).

Operating Mode	HEF (%)	Temperature at IVC (K)
Diesel	0	300
Dual Fuel	20	300–440 (10 K increment)

6. RESULTS

Figure 3 illustrates the T_{IVC} range for achieving stable combustion in 20% HEF; the regions of misfire and knocking are also illustrated. For T_{IVC} below 360 K, misfiring occurs due to the hydrogen high ignition energy and lean limit. Das et al. [19] also reports that hydrogen ignition is highly temperature-dependent, whereas lower intake temperature leads to unstable combustion and misfiring conditions.

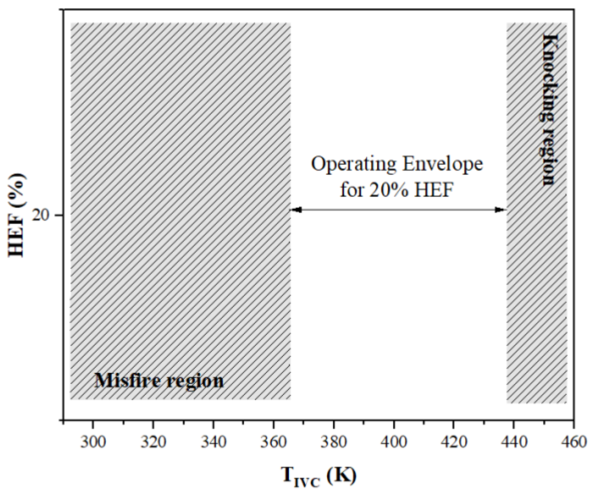

Figure 3. T_{IVC} range for stable combustion in 20% HEF.

For T_{IVC} exceeding 440 K, knocking conditions occur, characterised by the advanced autoignition of the hydrogen–air mixture followed by the fast flame propagation. Stable combustion conditions (without misfire or knocking) are obtained for T_{IVC} between 360 K and 440 K. This range ensures sufficient thermal energy for hydrogen ignition while avoiding excessive temperature areas that cause knock. However, retaining high T_{IVC} requires intake air heating systems, increasing the engine design complexity. Additionally, higher intake temperatures may require adjustments to engine cooling systems for addressing increased thermal loads. Furthermore, high temperatures favour NOx formation. Based on the preceding discussion, the selected T_{IVC} was 370 K.

Figure 4 presents the in-cylinder pressure, heat release rate and hydrogen mass for the diesel and DF modes for T_{IVC} of 300 K and 370 K.

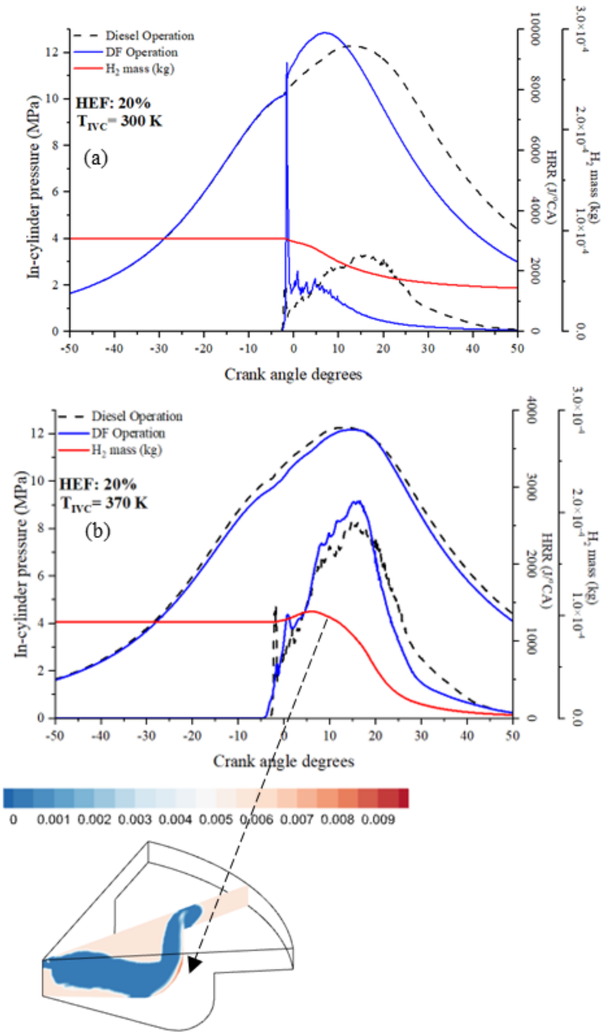

Figure 4. In-cylinder pressure, heat release rate and hydrogen mass for diesel and dual fuel modes for T_{IVC} of (a) 300 K and (b) 370 K.

For the dual fuel mode and T_{IVC} of 300 K, incomplete combustion conditions occur resulting in considerable amount of unburnt hydrogen. The in-cylinder pressure increase is greater compared to diesel due to the premixed combustion of hydrogen. The HRR profile for dual fuel mode exhibits a high peak before the top dead centre (TDC), attributed to the premixed hydrogen combustion. This is followed by a phase associated with diesel diffusive combustion, which releases less heat compared to the diesel mode. The hydrogen mass remains constant before ignition, whereas gradually reduces from the start of combustion (SOC) associated with the hydrogen combustion. The lower in-cylinder temperature reduces the hydrogen reactivity resulting in lower combustion efficiency compared to the diesel mode. The advanced ignition, the faster flame propagation due to the premixed hydrogen combustion and the incomplete hydrogen combustion conditions results in lower engine thermal efficiency.

For the dual fuel mode and T_{IVC} of 370 K, the in-cylinder hydrogen mass variation supports that complete combustion is achieved. For the period 2–10°CA ATDC a small amount of hydrogen is produced (the hydrogen mass increases) attributed to the intermediate combustion reactions of the diesel fuel. The HRR for the diesel mode is characterised by the premixed and the diffusive parts. The DF mode is characterised by a shorter ignition delay. Pilot diesel ignition cause the combustion of the prepared mixture. The first peak of HRR just before the TDC is attributed to the diesel premixed combustion and a small part of hydrogen combustion in areas around the diesel jet. The produced flame propagates burning the hydrogen-air mixture.

Between 7 and 12°CA ATDC further HRR increase is observed, attributed to the hydrogen–air mixture combustion in other areas of the engine cylinder. The peak HRR is reached at 17°CA ATDC where the flame reaches the cylinder walls and quenches. For the DF mode, the combustion duration reduces (compared to the diesel mode) whereas the crank angle at the maximum pressure (p_{max}) is retarded by 1.6°CA, as inferred from the results presented in Table 6. This is attributed to the increased hydrogen laminar flame speed that is an order of magnitude higher than the one for diesel.

Table 6. Maximum rate of pressure rise, maximum pressure (p_{max}), CA at p_{max} and start of combustion (SOC) for the diesel and dual-fuel modes.

Parameter / Mode	Diesel	Dual Fuel (20% HEF)
$(dp/d\theta)_{max}$ (MPa/ºCA)	0.43	0.31
p_{max} (MPa)	12.3	12.2
CA at p_{max} (°CA ATDC)	13.3	14.9
SOC (°CA BTDC)	4.5	4.3

The fast hydrogen combustion and increased T_{IVC} cause higher in-cylinder temperature for the DF mode. This results in considerably higher NOx emissions (compared to the diesel mode). The indicated NOx emissions for the diesel and DF modes were calculated 8.5 g/kWh and 16.2 g/kWh, respectively.

Figure 5 (a and b) reveals that significant parts of the cylinder mass are exposed to temperature levels above 2500 K and 2700 K for the DF mode compared to the diesel mode. This favours the formation of thermal NOx, as the in-cylinder nitrogen (in the ambient air) has more time to react with the in-cylinder oxygen.

Figure 6 illustrates the in-cylinder spatial distributions of the temperature, NOx, as well as hydrogen and diesel mass fractions for the DF mode and T_{IVC} of 370 K. The indicated crank angle degrees correspond to the start of combustion (SOC) at 4.3°CA BTDC, the peak HRR at 17 °CA ATDC, and the point where 90% of combustion is completed at 28°CA ATDC. At SOC, the diesel fuel initiates combustion, accompanied by the onset of premixed hydrogen combustion close to the injector area.

For the period between the SOC and the peak HRR, diesel combustion and premixed hydrogen combustion occur simultaneously. The hydrogen use extends the premixed combustion phase duration, as it is deduced by the HRR curve between SOC and 3°CA ATDC. At 17°CA ATDC, the temperature distribution reveals the simultaneous combustion of diesel and hydrogen.

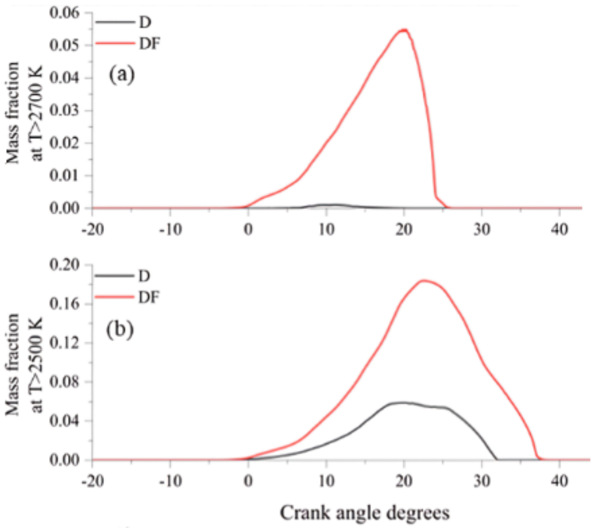

Figure 5. Mass fraction of in-cylinder mixture at temperature above (a) 2500 K and (b) 2700 K for diesel and dual fuel modes.

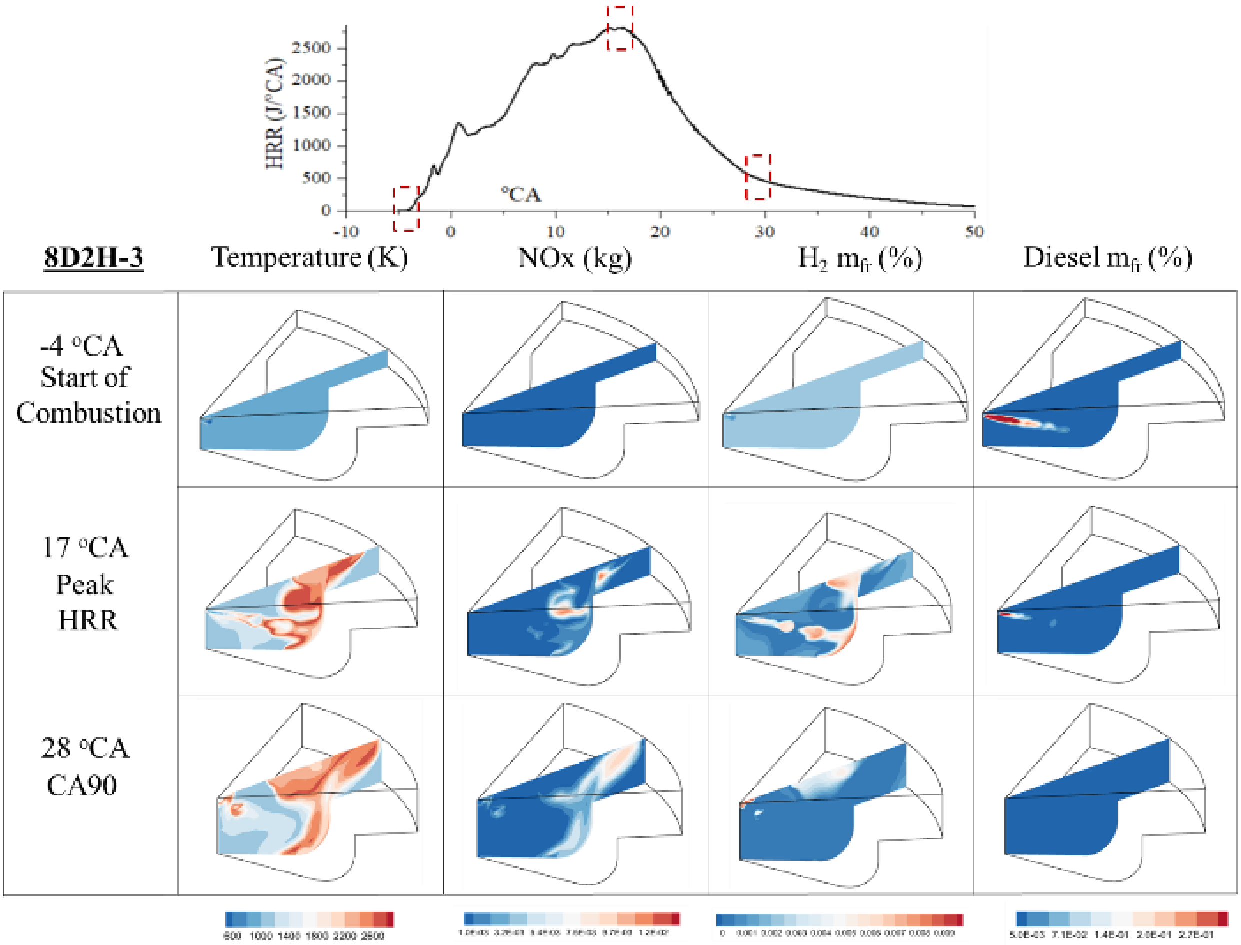

Figure 6. In-cylinder spatial distributions of temperature, NOx, hydrogen and diesel mass fractions at three crank angles for the DF mode and T_{IVC} of 370 K.

The flame front close to the cylinder head corresponds to the premixed hydrogen combustion, while diesel undergoes diffusive combustion, in the areas surrounding the jet. At this stage, the in-cylinder temperature exceeds 1800 K, initiating the formation of NO_x emissions. The homogeneous hydrogen–air mixture promotes rapid combustion, which results in increased in-cylinder temperature. The prolonged residence time at high temperatures contributes to the NOx formation. As combustion progresses, the peak temperature reduces, and the spatial temperature becomes more uniform throughout the cylinder.

7. DISCUSSION

This study provides insights on the hydrogen-diesel dual-fuel combustion for marine medium-speed engines. Hydrogen use leads to shorter ignition delays and higher combustion efficiency due to hydrogen increased laminar flame speed compared to diesel. However, it also highlights challenges, particularly the increased NOx emissions due to higher in-cylinder temperatures.

The findings of this study have implications for the future marine engines, particularly for addressing the IMO net-zero goals. The results indicate that stable hydrogen combustion conditions can be achieved for 20% hydrogen energy fraction. Hence, hydrogen systems could be retrofitted in existing marine diesel engines, thereby providing a pathway to reduce greenhouse gas emissions. Hydrogen port injection systems can be considered for retrofitting, thus accelerating the adoption of hydrogen technologies in the maritime sector. However, the industry must address practical challenges, such as hydrogen storage and the risks of pre-ignition or knocking associated with high hydrogen energy fractions.

However, the hydrogen use results in increased NOx emissions, which are associated with the higher in-cylinder temperature due to the faster hydrogen combustion and the requirement for increased T_{IVC}. To curtail NOx emissions, future studies could investigate the EGR use that lowers the in-cylinder reactivity, optimised injection timings, as well as concepts and designs with variable compression ratio and pre-chamber.

8. CONCLUSIONS

This study aimed at quantifying the performance of a dual fuel marine engine operating with 20% hydrogen energy fraction. A CFD model was developed for both the diesel and dual fuel modes. The model was validated with experimental data for the diesel mode and reported data for a smaller engine operating with diesel–hydrogen. The main findings are summarised as follows.

- Using hydrogen in dual-fuel marine engines results in shorter ignition delays and combustion duration due to hydrogen higher laminar flame speed compared to diesel.
- For the DF mode, higher mass of the in-cylinder mixture remains above the NOx cut-off temperature for a longer period, favouring the nitrogen oxidation to NOx
- The use of hydrogen leads to significantly increased NOx emissions due to the higher in-cylinder temperature, highlighting the need for effective emissions control strategies.
- 20% HEF only slightly impacts the in-cylinder pressure, whereas the exhibited ignition delay resulted in retarding the crank angle of the peak pressure.
- The homogeneous hydrogen–air mixture results in rapid combustion, while the progression of combustion results in more uniform temperature throughout the cylinder. This uniformity further contributes to NO_x emissions, particularly in the near-wall regions with higher temperatures.

The results provide insights for the hydrogen use as alternative fuel in retrofitted marine diesel engines. The study limitations are associated with the unavailability of experimental data from marine engines to validate the CFD models for the hydrogen-diesel mode. Future studies will investigate effective NOx emissions reduction techniques such as EGR, injection advancing, split injection strategies and engine design modifications.

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