

Analysis and Optimization of Diesel Injection Strategy to Minimize Unburned Hydrogen in a Hydrogen–Diesel Dual-Fuel Medium-Speed Marine Engine

Peilin Zhou¹, Binteng Gu¹ and Ning Chen²

Received: 13 April 2025 / Accepted: 04 September 2025
© The Author(s) 2026

Abstract

To advance shipping decarbonization, hydrogen is increasingly recognized as a viable zero-carbon fuel. Currently, a hydrogen/diesel dual-fuel medium-speed engine represents an optimal prime mover for ships. However, challenges such as the large cylinder dimensions of marine medium-speed engines and the low temperatures at the combustion chamber walls can hinder efficient flame propagation, leading to the emission of unburnt hydrogen. This not only diminishes the engine's mechanical output but also poses significant safety risks. To address these issues, this study employs computational fluid dynamics (CFD) modelling to explore optimal diesel injection strategies that minimize unburnt hydrogen emissions in such engines. Specifically, this research examines the impacts of the diesel injection start angle, spray tilt angle, and injection duration on hydrogen combustion efficiency. The findings reveal that fine-tuning injection parameters substantially lower the fraction of unburned hydrogen. Adjusting the injection timing from 9.5°CA BTDC to 49.5°CA BTDC decreases the unburnt hydrogen fraction from 50% to 3%. Furthermore, modifying the spray tilt angle from 75.5° to 55.5° further decreases it to 2%, while shortening the injection duration from 35°CA to 34°CA achieves the lowest unburnt hydrogen fraction at just 1%. These results underscore the effectiveness of diesel injection strategies in optimizing the combustion in hydrogen/diesel dual-fuel marine medium-speed engines, offering a pathway for similar applications in the sector.

Keywords Hydrogen/diesel dual-fuel; Marine medium-speed engine; Diesel injection strategy; Computational fluid dynamics (CFD); Unburnt hydrogen emission

1 Introduction

Shipping accounts for approximately 80% of global freight transportation (UNCTAD, 2021). Internal combustion engines (ICEs) are the predominant power source for ships, comprising over 95% of ship main engines, with expectations of maintaining this dominance for the next two to three decades (DNV, 2021). This widespread use raises significant environmental concerns, as marine inter-

nal combustion engines are major contributors to annual greenhouse gas emissions, exacerbating the greenhouse effect and atmospheric pollution (Olmer et al., 2017). In response, the 80 th session of the International Maritime Organization's (IMO) Marine Environmental Protection Committee (MEPC), held in July 2023, adopted the 2023 IMO Strategy on Reduction of GHG Emissions from Ships. This pivotal strategy commits to reducing GHG emissions from international shipping by at least 70% by 2040 compared to 2008 levels, with the ultimate goal of achieving net-zero GHG emissions in the maritime sector by around 2050 (International Maritime Organization, 2023). To support these objectives, DNV advocates for the adoption of more environmentally friendly, low-carbon, or zero-carbon alternative fuels for marine internal combustion engines. These alternatives include methanol, LNG, LPG, biofuels, ammonia, and hydrogen (DNV, 2019).

Among the alternative fuels, hydrogen is notably considered a zero-carbon fuel and often referred to as the 'ultimate fuel' (Cho et al., 2016). This designation stems from its high heating value and the fact that its combustion only produces water, without emitting carbon oxides (CO and CO₂) or hydrocarbons (HC) (Khairallah, 2015). Research

Article Highlights

- Reduce unburned hydrogen emissions by optimizing the diesel injection strategy.
- Examine the sensitivity of injection start, spray tilt angle, and injection duration.
- Achieve a reduction in unburned hydrogen emissions from 50% to 1% with the optimal strategy.

✉ Binteng Gu
binteng.gu@strath.ac.uk

¹ Department of Naval Architecture, Ocean and Marine Engineering, University of Strathclyde, 100 Montrose Street, Glasgow G4 0LZ, UK

² School of Energy and Power, Jiangsu University of Science and Technology, Zhenjiang 212003, China

on hydrogen engines dates back to the 1970s, marking the initial efforts to incorporate hydrogen into automobile engines. These early studies primarily addressed the abnormal combustion phenomena and characteristics of hydrogen-oxygen engines, setting a crucial foundation for further research in this domain. Building on this foundation, later research has extensively explored the distinctive chemical properties of hydrogen that influence its combustion behavior and engine performance. When compared to traditional fossil fuels, hydrogen displays several unique properties: Firstly, hydrogen's ignition energy is significantly lower, only 0.02 mJ, which is an order of magnitude less than diesel's 0.24 mJ. This attribute increases the likelihood of premature ignition due to hot spots (Wang et al., 2020). Furthermore, hydrogen has a wider flammability limit, facilitating easier achievement of lean combustion (Du et al., 2024). Its laminar flame speed is also higher, at 265 cm/s compared to diesel's 86 cm/s under similar conditions, which increases the risk of knocking if a substantial proportion of hydrogen is used (Gomes Antunes et al., 2009). However, this speed diminishes significantly under lean combustion conditions (Verhelst and Wallner, 2009). Another distinctive characteristic of hydrogen is its smaller minimum quenching distance relative to other gaseous fuels, which increases the risk of backfiring into the intake port (Gao et al., 2022). Lastly, the high auto-ignition temperature of hydrogen, at 858 K, complicates achieving compression ignition (Jabbar, 2020). Consequently, while hydrogen internal combustion engines can achieve lean combustion, they may encounter challenges related to abnormal combustion phenomena such as early ignition, knocking, or backfire.

In more recent years, the focus has shifted towards developing methods to control and prevent abnormal combustion in hydrogen engines. Additionally, the combustion characteristics and performance of hydrogen engines have emerged as pivotal areas of cutting-edge research. Sharma and Dhar (2018) explored the balance required to mitigate knocking in a hydrogen/diesel dual-fuel engine, identifying a trade-off between the hydrogen substitution rate and the compression ratio. Duan et al. (2023) conducted studies on the combustion characteristics of a direct injection turbocharged hydrogen engine under various operating conditions, achieving a peak thermal efficiency of 37.7%. Liu et al. (2022) successfully modified a single-cylinder diesel engine to facilitate hydrogen/diesel dual-fuel direct injection (H_2 DDI) operation with up to 90% hydrogen energy fraction, which resulted in high thermal efficiency and reduced emissions. Hanafi Gharehlar et al. (2024) numerically investigated the performance of a hydrogen/diesel Reactivity Controlled Compression Ignition (RCCI) engine at low loads, noting a 2% increase in output power compared to a natural gas/diesel engine. These studies collectively show the substantial potential of hydrogen/diesel

dual-fuel engines to achieve optimal performance while minimizing emissions, highlighting their significance in advancing hydrogen technology.

Although hydrogen engines have been studied for several decades, the research and development of hydrogen-powered marine engines remain in the early stages. Leading marine engine manufacturers such as MAN and Wärtsilä have made significant progress in this field. MAN has reported the successful operation of an engine running on a 25 vol% hydrogen blend, with plans underway to test engines operating on pure hydrogen (MAN Energy Solutions, 2023). Similarly, Wärtsilä has tested an engine with a 60 vol% hydrogen blend and aims to commercialize pure hydrogen engines by 2026 (Wärtsilä, 2023). In addition, MITSUI E & S Co., Ltd. has successfully conducted pure hydrogen combustion in a 500 mm-bore two-stroke low-speed marine engine, achieving a 95% reduction in greenhouse gas emissions (Mitsui Engineering & Shipbuilding, 2024). These developments indicate that the commercialization of hydrogen-fueled marine engines is approaching reality.

In hydrogen/diesel dual-fuel engines, the emission of unburnt hydrogen within the cylinder after combustion represents a significant challenge, impacting not only energy conversion efficiency but also the safety of ship engine rooms and decks. Accumulated hydrogen poses significant safety risks, including the potential for explosions, which can lead to substantial economic losses and seriously threaten the lives of crew members (Xie et al., 2024; Yuan et al., 2020). Liew et al. (2010) investigated the effects of hydrogen addition on the combustion in a heavy-duty diesel engine, finding that at 70% engine load, hydrogen's combustion efficiency significantly lagged behind that of diesel. Gatts et al. (2010) conducted experimental tests on the hydrogen emissions characteristics of a hydrogen/diesel dual-fuel heavy-duty engine, revealing that hydrogen combustion efficiency is profoundly affected by the engine load, with increased load serving as a remedy for reducing unburnt hydrogen. Dimitriou et al. (2019) assessed a hydrogen/diesel dual-fuel engine under low-load conditions and discovered that combustion efficiency at most tested points was approximately 90%. These findings underscore the issue of unburnt hydrogen emissions and suggest that operating at higher loads reduces these emissions due to richer H_2 /air mixtures supporting the initiation and propagation of multiple turbulent flames. However, these studies primarily focus on engines with small cylinder bores. The situation differs substantially in marine medium-speed engines, which have larger cylinder sizes. Even at high load and high hydrogen substitution ratios, unburnt hydrogen remains a problem. The larger cylinder dimensions and the relatively lower temperatures of the combustion chamber walls, cooled by the engine's cooling system, increase the likelihood of flame extinguish-

ment before reaching the hydrogen farther from the ignition source.

Fuel injection control plays a crucial role in fuel–air mixing. Qu et al. (2022) investigated the impact of hydrogen injection on mixture homogeneity in a pure hydrogen marine engine and found that turbulence intensity and penetration distance are key factors influencing mixture quality. In a subsequent numerical study, Qu et al. (2024) examined the effect of direct hydrogen injection in a low-speed marine engine, concluding that early hydrogen injection promotes the formation of a more homogeneous mixture but increases the silp risk of hydrogen silp.

It can be concluded that, it is critical that the diesel injection assists in igniting most of the hydrogen, especially near the combustion chamber walls. This study explores the optimal diesel injection strategy to reduce unburned hydrogen emissions in a hydrogen/diesel dual-fuel marine medium-speed engine, using computational fluid dynamics (CFD) simulation. The conditions tested included 100% engine load with a hydrogen substitution ratio of 50%. The study examined the impact of diesel Start of Injection (SOI), spray tilt angle, and injection duration, individually and in combination. Results demonstrate that an optimized diesel injection strategy significantly reduces the fraction of unburned hydrogen, offering valuable insights for fuel injection control and safety design in similar engines.

2 Model and validation

2.1 Computational model

This research utilizes the I.C. engine computational fluid dynamics (CFD) program Converge v3.1 to simulate a four-stroke, medium-speed marine diesel engine, which serves as the prototype for the modified hydrogen/diesel dual-fuel engine under study. This engine is suitable for

deck carriers, bulk carriers under 20 000 DWT, chemical tankers, product oil tankers, and as the main engine for container ships with a capacity of up to 1 100 TEU. Figure 1 illustrates the CFD modelling framework adopted in this study. Table 2 details the primary parameters of this medium-speed marine diesel engine, which features an injector equipped with 12 orifices. To enhance the efficiency of the simulation, a sector model of 60° with two orifices is employed, with a 30° angle between the orifices. The simulation focuses exclusively on the closed part of the engine cycle, commencing from the intake valve closure (IVC) at 167°CA before the top dead centre (BTDC) and concluding at the exhaust valve opening (EVO) at 131°CA after top dead centre (ATDC). The boundary and initial conditions are obtained through the 1D engine model, and values are presented in Table 2. As illustrated in Figure 2, hydrogen is introduced into the engine through port fuel injection (PFI). At the moment of IVC, hydrogen is assumed to be uniformly distributed within the cylinder. This setup provides a detailed framework for analyzing the combustion dynamics and emissions characteristics of the hydrogen/diesel dual-fuel configuration under simulated operational conditions.

Table 1 The main parameters of the medium-speed engine

Parameters	Value
Engine type	Four-stroke, CI engine
Rated output (kW)	4000
Rated speed (r/min)	750
Bore (mm)	320
Stroke (mm)	420
Compression ratio	14.5
Connecting rod length (mm)	950

In this numerical model, the atomization and breakup process of diesel is modelled by the Kelvin-Helmholtz and

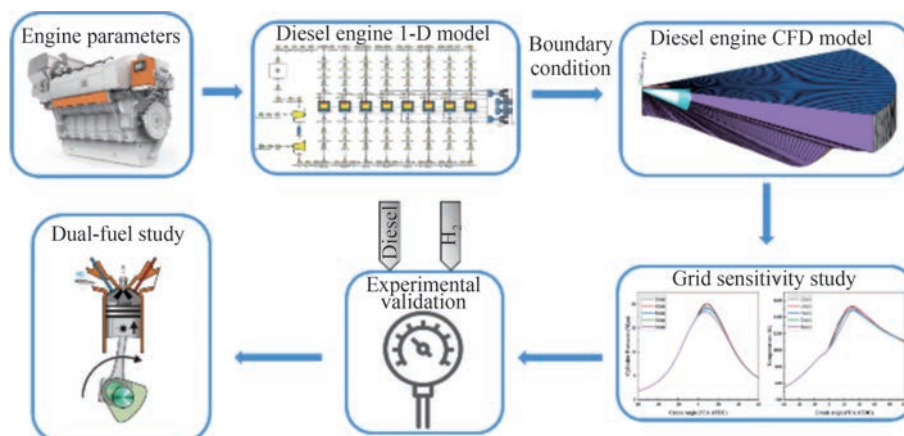
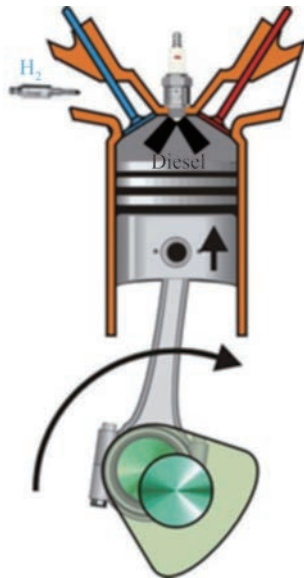


Figure 1 Numerical model methodology framework

Table 2 Boundary and initial conditions for CFD simulation of the investigated marine engine

Boundary Conditions	Value
Piston temperature (K)	550
Cylinder head temperature (K)	520
Cylinder wall temperature (K)	430
Initial Conditions	Value
Pressure at the IVC (bar)	4.1
Temperature at the IVC (K)	320

**Figure 2** The schematic diagram of PFI hydrogen-diesel dual-fuel engine

Rayleigh-Taylor (KH-RT) model (Beale and Reitz, 1999) and NTC collision model (Schmidt and Rutland, 2000). The combustion model is the SAGE model (Senecal et al., 2003), in which the detailed chemical mechanism is performed. The Re-Normalization Group (RNG) $k-\epsilon$ (kappa-epsilon) turbulence model based on Reynolds Averaged Navier-Stokes (RANS) (Han and Reitz, 1995) is used to model the turbulence effects in the fluid flow. The wall heat transfer model is the O'Rourke and Amsden wall heat transfer model (O'Rourke and Amsden, 1996; Anthony Amsden, 1999).

Table 3 The models used in the simulation

Models	Name
Droplet breakup model	KH-RT
Collision model	The NTC collision
Combustion model	SAGE
Turbulence model	RNG $k-\epsilon$
Wall heat transfer model	O'Rourke and Amsden

2.2 Chemical Kinetics

In this study, n-heptane is used as a representative for diesel fuel due to its similar combustion characteristics. Due to its simple molecular structure, n-heptane reduces the computational complexity in CFD simulations. However, it often leads to underestimation of ignition delay times and soot formation, limiting its accuracy in representing real diesel combustion behavior. The chemical mechanism employed to model the oxidation processes in the hydrogen/n-heptane mixture is a skeletal oxidation mechanism developed by Qu et al. (2024). This mechanism, which is an optimized version derived from the original framework (Liu et al., 2012) using a genetic algorithm, provides enhanced computational accuracy for this study. The optimization process involved updating the reaction rate constants of C7 species from Liu's mechanism and validating the updated mechanism through rapid compression machine experiments. These experiments demonstrated that the mechanism accurately predicts the ignition delay times for hydrogen/n-heptane mixtures. It is worth noting that the mechanism was validated against experimental data within the temperature range of 600 to 800 K. Therefore, its accuracy outside this range may be limited, potentially affecting the prediction of ignition delay. The selected chemical mechanism comprises 49 species and 174 reactions, facilitating a comprehensive analysis of the combustion processes within the dual-fuel engine under study.

2.3 Grid sensitivity test and model validation

In this study, a grid strategy that balances computational efficiency with simulation accuracy is adopted, crucial due to the large dimensions of marine engines. The grid settings used in the simulation are listed in Table 4. Utilizing an excessively small base grid size could lead to impractical simulation times. Thus, a combination of a larger base grid size with localized fixed embedding and Adaptive Mesh Refinement (AMR) is implemented. In regions characterized by diesel spray, a two-level fixed embedding refinement is applied to ensure detailed resolution where it is most needed. Similarly, the temperature and velocity fields within the simulation are refined using two-level AMR, allowing for dynamic adjustment of mesh resolution in response to changes in these critical parameters. Figure 3 illustrates how the cylinder pressure and temperature converge as the base grid size is adjusted from 6 mm to 2 mm while maintaining the same grid strategy. This convergence indicates that the simulation achieves grid independence, confirming the reliability of the results at various mesh scales. Notably, the accuracy between using base grid sizes of 2 mm and 3 mm is nearly identical. The variation in results between the 2 mm and 3 mm grid resolutions is minimal, with relative errors of 0.1% in peak

pressure and 1.2% in peak temperature. The calculated root mean square errors (RMSE) are 0.07 MPa for pressure and 8.22 K for temperature, demonstrating good grid independence. Consequently, a base grid size of 3 mm is selected for the subsequent simulations. This choice strikes an effective balance between computational load and the level of detail necessary to accurately capture the key phenomena in the hydrogen/diesel dual-fuel engine simulation.

Table 4 The grid settings used in the simulation

Setting	Value
Base grid size (mm)	3
Maximum total grids	866 000
Embedding level of Nozzle	2
Velocity AMR level	2
Temperature AMR level	2

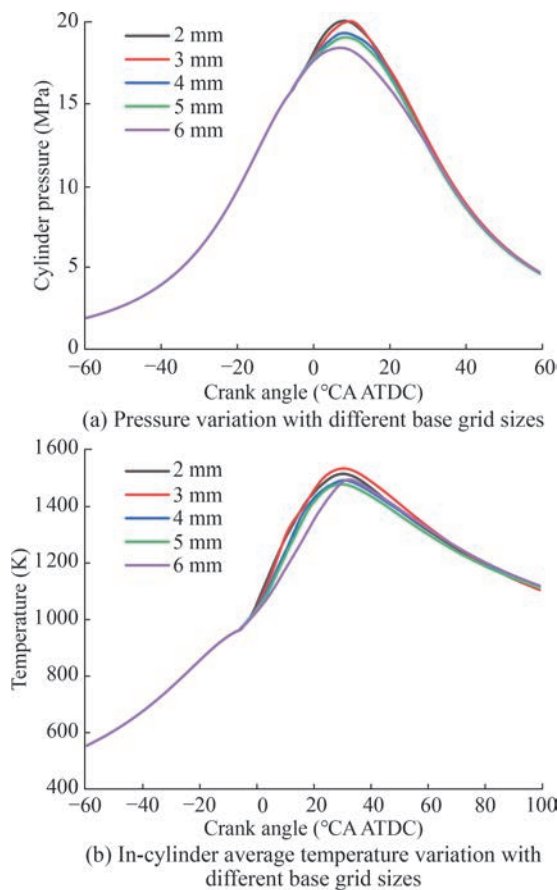


Figure 3 The cylinder pressure and temperature under different base grid sizes

Figure 4 presents a comparison between the simulated cylinder pressure of a diesel engine at 100% rated operating condition and the corresponding experimental data. The comparison indicates that the simulated values align closely with the experimental results, with the difference considered acceptable. Notably, the primary differences

occur around the start of combustion; however, these remain within a 3% relative error margin. This level of accuracy suggests that the simulation effectively captures the essential dynamics of the engine's performance under full-load conditions. The minor variations observed at the start of combustion are typical in such simulations due to slight deviations in modelling assumptions or initial conditions. Overall, the close agreement across the majority of the cycle confirms the precision of the simulation methodology employed in this study.

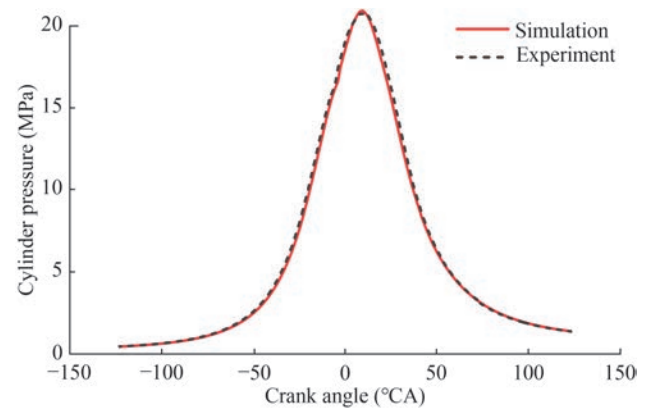


Figure 4 Comparison of measured and simulated in-cylinder pressure

2.4 Parameter definition

In order to investigate the effect at a high engine load with sufficient hydrogen addition. This study is based on the 100% engine load with a 50% hydrogen substitutional ratio. The hydrogen substitutional ratio can be defined by Eq. (1):

$$\text{Hydrogen Substitutional Ratio} = \frac{m_{H_2} \times \text{LHV}_{H_2}}{m_{H_2} \times \text{LHV}_{H_2} + m_{\text{diesel}} \times \text{LHV}_{\text{diesel}}} \times 100\% \quad (1)$$

where m_{H_2} is the mass of hydrogen and m_{diesel} is the mass of diesel.

To measure the unburnt H_2 fraction, the residual percentage of hydrogen is defined by Eq. (2):

$$\text{Residual Percentage of Hydrogen} = \frac{m_{H_2, \text{Ub}}}{m_{H_2}} \times 100\% \quad (2)$$

where m_{H_2} is the total mass of hydrogen fuel and $m_{H_2, \text{Ub}}$ is the mass of unburnt hydrogen after combustion.

3 Results and discussion

3.1 Research on the SOI of diesel

In a port fuel-injected (PFI) hydrogen/diesel dual-fuel

engine, it is assumed that the gaseous H_2 is distributed homogeneously within the cylinder at the moment of intake valve closure. The cylinder dimensions of a marine medium-speed engine are considerably larger than those typical of small engines. The extensive distance from the ignition source to the combustion chamber walls, coupled with the low-temperature impact of these walls, poses challenges to effective flame propagation. Consequently, conventional diesel injection timing may not ensure comprehensive flame distribution throughout the cylinder. This is attributed to the inability of the flame initiated by the diesel to reach every area within the cylinder and ignite the uniformly distributed hydrogen, potentially resulting in a 'dead zone' where the H_2 /air mixture fails to encounter the flame. As a result, this hydrogen may remain unburnt.

To enhance the mixing of diesel with the H_2 /air mixture, the adoption of an early injection strategy should be considered. This approach entails injecting diesel earlier, thus allowing more time and space for the diesel to integrate with the H_2 /air mixture during the initial stage of the compression stroke. To study the effect of early injection, cases with varying SOIs but same tilt angle (75.5°) and injection duration ($35^\circ CA$) are studied. The injection settings are listed in Table 5. Figure 5 illustrates the percentage of residual hydrogen in the cylinder after combustion with the Start of Injection (SOI) of diesel varying from $9.5^\circ CA$ to $69.5^\circ CA$ before Top Dead Center (BTDC). The original SOI setting at $9.5^\circ CA$ BTDC demonstrates bad combustion efficiency, with 50% of the hydrogen remaining unburnt at EVO. As diesel SOI advances, the initial percentage of hydrogen left in the cylinder decreases, reaching a minimum of 3% at $49.5^\circ CA$ BTDC, before showing a slight rise. The reason behind this is that earlier diesel injection furnishes extended duration for the diesel to penetrate the hydrogen/air mix, enhancing the likelihood of igniting a larger quantity of hydrogen.

Table 5 The injection settings of SOI effect study

Case	SOI ($^\circ CA$ BTDC)	Tilt angle ($^\circ$)	Injection duration ($^\circ CA$)
1	9.5	75.5	35
2	19.5	75.5	35
3	29.5	75.5	35
4	39.5	75.5	35
5	49.5	75.5	35
6	59.5	75.5	35
7	69.5	75.5	35

Figure 6 displays the equivalence ratio immediately prior to ignition as the SOI progresses. The figure highlights a region of high equivalence ratio adjacent to the diesel spray, indicative of the concentration of diesel fuel vapor.

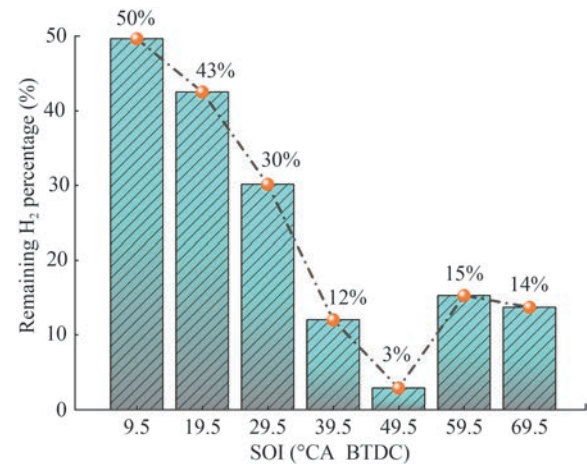


Figure 5 Unburnt H_2 percentage of different diesel SOI

- **Late injection (9.5° , 19.5° and 29.5° BTDC):** Combustion begins before the spray can spread; the rich zone stays tightly clustered near the cylinder centreline just below the head.

- **Intermediate injection (39.5° BTDC):** Extra premixing time pushes vapor toward mid-radius, but the cloud still leans toward the upper bowl.

- **Optimal injection (49.5° BTDC):** Residence time and momentum balance best; the spray fans across the bowl, yielding the most uniform fuel–gas mixture of all cases.

- **Very early injection (59.5° , 69.5° BTDC):** Excess lead time drives the spray against the cylinder wall, so fuel pools at the periphery and the core remains lean.

This configuration at $49.5^\circ CA$ BTDC is demonstrated to facilitate the most effective mixing of fuel and gas prior to combustion among the evaluated scenarios.

Due to early diesel injection and the rapid combustion rate from hydrogen, combustion is largely complete by the time the piston reaches top dead center (TDC). Figure 7(a) illustrates the unburnt hydrogen mass fraction at TDC for different SOI timings. The unburnt hydrogen predominantly accumulates around the inner rim of the piston's upper edge. Figure 7(b) illustrates the 1500 K isothermal surface at TDC of different SOIs. As shown in the diagram, the isothermal surface exactly complements the shape of the unburnt hydrogen gas. This accumulation occurs because the flame extinguishes as it attempts to reach the hydrogen near the combustion chamber walls. The low temperature of the combustion chamber walls and the large distance from the diesel spray to these walls together contribute to this phenomenon.

3.2 Research on the coupling effect of SOI and spray tilt angle

From Section 3.1, we observed that unburnt hydrogen tends to accumulate at the inner rim of the piston's upper surface. To effectively ignite this residual hydrogen, one

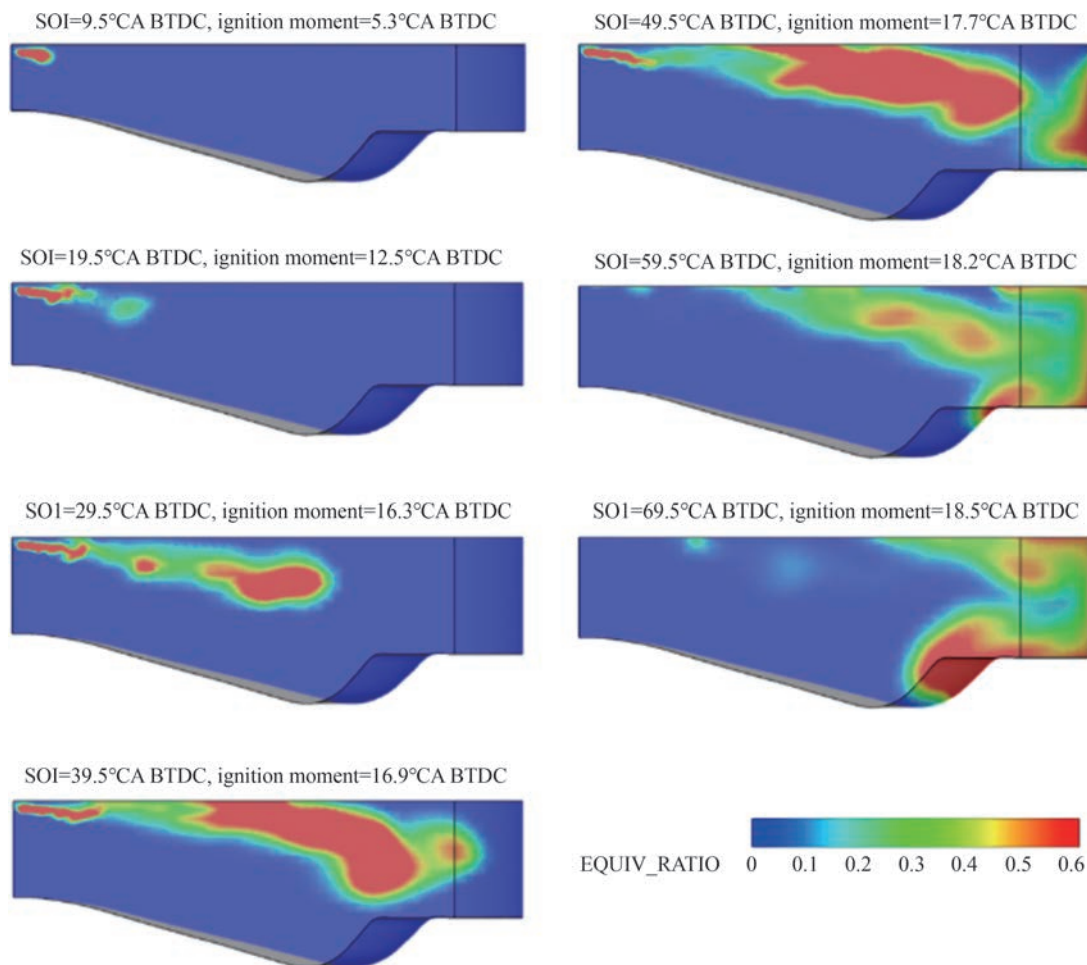


Figure 6 The equivalence ratio at the moment before ignition with different SOI

viable strategy involves redirecting the diesel spray towards this area. An adjustment to the spray tilt angle α , as depicted in Figure 8, could change the trajectory of the diesel spray without the need to increase injection pressure. Originally, the spray tilt angle was set at 75.5° . The combustion chamber's curved ridges help diffuse the diesel spray, utilizing both the momentum of the diesel and the reaction force from the cylinder wall to enhance mixing. The SOI also affects whether the diesel spray effectively reaches the curved ridge. To examine the combined influence of SOI and spray tilt angle, a set of 3×3 orthogonal experiments is designed, as shown in Table 6. These experiments vary by three different SOIs and spray tilt angles. Based on earlier observations where SOI at 49.5° CA BTDC resulted in minimal unburnt hydrogen, additional SOIs at 39.5° and 59.5° CA BTDC are included to explore potentially more optimal settings. Furthermore, the spray tilt angle is adjusted to 65.5° or 55.5° . This change is based on analysis from Figure 6, suggesting that a reduced tilt angle might better direct the spray towards the curved ridge, potentially improving the combustion of hydrogen.

Figure 9 illustrates the residual percentage of H_2 in the

cylinder, elucidating the combined effects of SOI and spray tilt angle. The data indicate that at an SOI of 39.5° CA BTDC, the residual percentage of H_2 initially increases by 2% and subsequently decreases by 3%, a pattern similar to that observed at SOI= 49.5° CA BTDC. At an SOI of 59.5° CA BTDC, there is an initial 4% reduction in the residual H_2 percentage, which then stabilizes regardless of further changes in the spray tilt angle. Consistent with earlier findings, the lowest residual H_2 percentage occurs at an SOI of 49.5° CA BTDC, particularly at a spray tilt angle of 55.5° . This configuration reduces the residual H_2 from the previously best 3% to 2%. The improvement suggests that a decrease in the spray tilt angle enhances H_2 consumption, likely due to altered diesel motion influenced by the cylinder wall's force effect.

The distribution of the equivalence ratio provides a clear visualization of the diesel injection process and subsequent fuel consumption. Figure 10 illustrates this distribution following diesel injection in Case 6, effectively showcasing the diesel/air mix dynamics. Initially, as observed in the subgraphs for -30° CA and -20° CA, diesel is injected directly onto the piston's curved ridge. As the

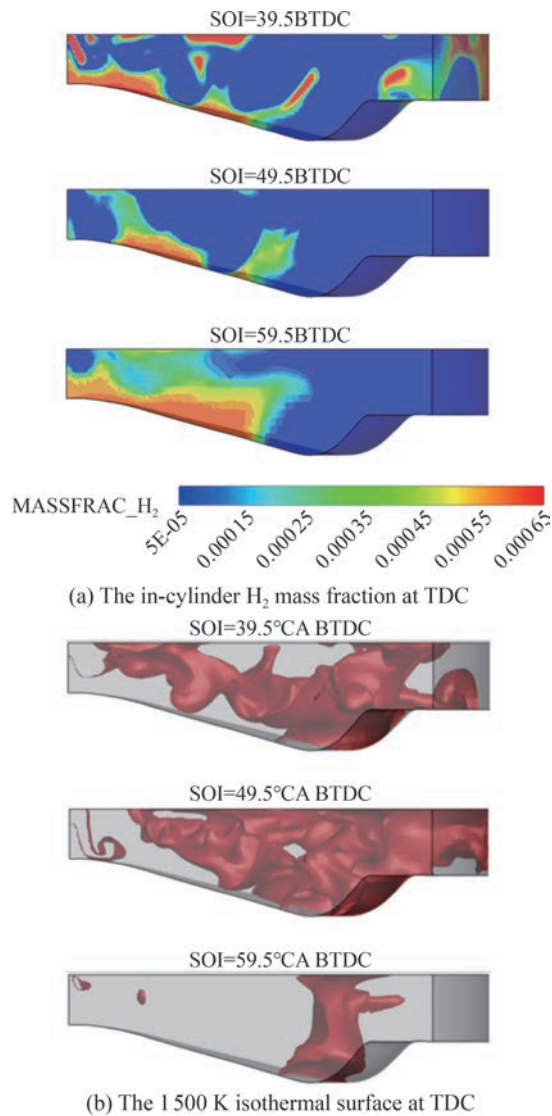


Figure 7 The in-cylinder state at TDC

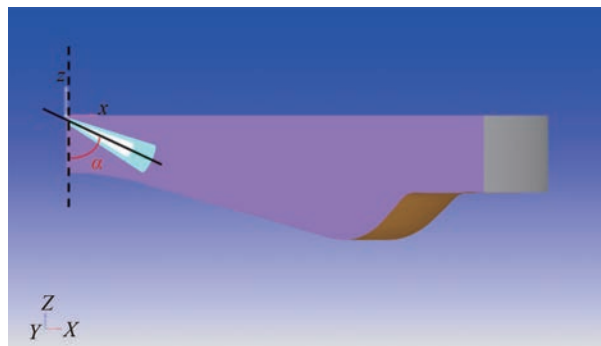


Figure 8 Schematic diagram of spray tilt angle

crank angle (CA) progresses, the diesel migrates towards a more central position within the piston.

Between -16°CA and -15°CA , the expansion of the green band area indicates the onset of premixed combustion, which rapidly consumes the localized diesel. By -13°CA ,

Table 6 Injection settings of orthogonal cases

Case	SOI ($^\circ\text{CA BTDC}$)	Tilt angle ($^\circ$)	Injection duration ($^\circ\text{CA}$)
1	39.5	75.5	35
2	39.5	65.5	35
3	39.5	55.5	35
4	49.5	75.5	35
5	49.5	65.5	35
6	49.5	55.5	35
7	59.5	75.5	35
8	59.5	65.5	35
9	59.5	55.5	35

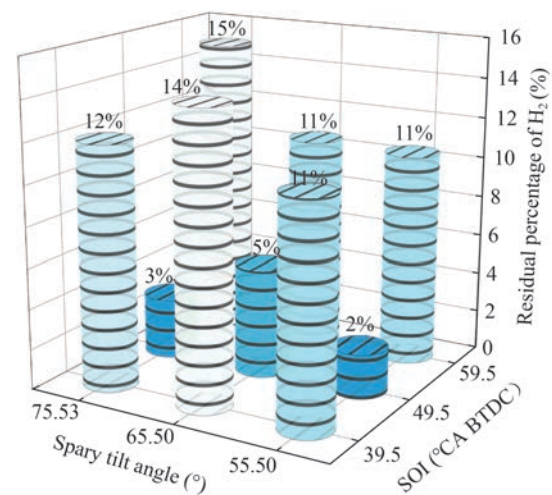


Figure 9 The combined effect of SOI and spray tilt angle on the residual percentage of H_2

the region enriched with diesel expands significantly as the fuel is injected towards the cylinder wall, creating wall jets that impinge upon the surface, leading to increased diesel vapor generation due to the high-temperature piston surface.

Subsequently, the diesel diffuses upwards and inwards towards the cylinder head, driven by the turbulence of diffusion combustion and the reflective forces of the cylinder wall. Additionally, the turbulence created by the diesel spray head during premixed combustion further aids in dispersing the diesel throughout the cylinder.

3.3 Research on the effect of injection duration

Under the conditions where the diesel SOI and the total fuel injection quantity remain constant, modifying the injection duration alters when the injection ends, affecting the air-fuel mixing within the cylinder. Based on the earlier settings of SOI at 49.5°CA BTDC and a spray tilt angle of 55.5°CA , cases of varying injection duration are tested as shown in Table 7.

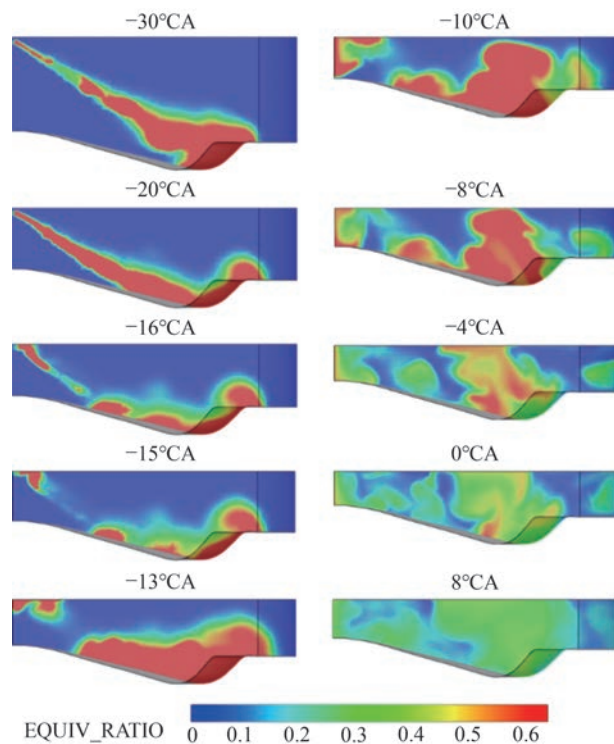


Figure 10 The equivalence ratio evolution of case 6

Table 7 The injection settings of injection duration effect

Case	SOI (°CA BTDC)	Tilt angle (°)	Injection duration (°CA)
1	49.5	55.5	33
2	49.5	55.5	34
3	49.5	55.5	35
4	49.5	55.5	36
5	49.5	55.5	37

Figure 11 illustrates the residual percentage of hydrogen under various injection durations. The injection pressure decreases linearly as the duration of injection prolongs because the total injected diesel mass remains constant. As injection duration increases, the residual percentage of hydrogen initially decreases from 4% to 1%, then rises slightly to stabilize at 2% when the injection duration is 36°CA. However, it sharply increases to 6% at an injection duration of 37°CA. The optimal result, with only 1% residual hydrogen, occurs at an injection duration of 34°CA. This outcome highlights that adjusting the injection duration effectively reduces the residual hydrogen percentage. Compared to the previous best result of 2%, the minimum unburned hydrogen fraction was halved to 1% by optimizing the injection duration.

Figure 12 displays the evolution of the equivalence ratio distribution for different injection durations, following the four stages of diesel behavior in the cylinder: ‘injection, gathering, diffusion, and depletion’. This figure primarily

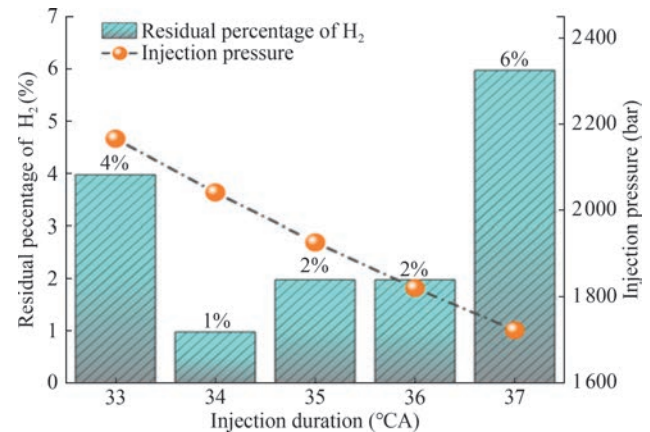


Figure 11 The residual percentage of H_2 under different injection durations

focuses on the gathering and diffusion stages.

- **34°CA:** Fuel gathers near the bowl rim from -15°CA to -13°CA , then diffuses inward toward the cylinder centre between -10°CA and -4°CA .

- **35°CA:** Fuel follows a similar timeline, but the main vapour cloud at -10°CA is located slightly lower on the outer bowl wall, leading to a more oblique diffusion path.

- **37°CA:** The primary cloud forms on the inner bowl wall at -10°CA and diffuses predominantly upward, resulting in a more vertical flame trajectory.

- **Impact on hydrogen burn-out:** The horizontal, inward diffusion at 34°CA promotes central flame travel and leaves only $\approx 1\%$ residual H_2 , whereas the altered paths at 35°CA and 37°CA reduce hydrogen entrainment.

3.4 Discussion

In the above parametric study, it was found that optimizing the injection parameters of diesel fuel can effectively reduce unburned hydrogen emissions. In this study, the following points need to be discussed:

- 1) *Underlying mechanism:* Hydrogen is premixed with intake air before entering the cylinder, forming a hydrogen–air mixture whose combustion reactivity is influenced by both the equivalence ratio and the initial in-cylinder temperature. In this study, the initial temperature is relatively low (320 K), which leads to reduced reactivity of the hydrogen–air mixture. Under such conditions, the flame kernel created by diesel ignition cannot propagate through the low-reactivity mixture, leaving part of the hydrogen unburned. Therefore, the hydrogen-combustion efficiency becomes highly sensitive to the diesel injection parameters that govern kernel size, location and residence time.

- 2) *Potential challenges:* SOI has a significant influence on the unburned hydrogen fraction. However, implementing an early injection strategy in practice often leads to increased NO_x emissions. Therefore, it is necessary to couple this approach with an appropriate aftertreatment system,

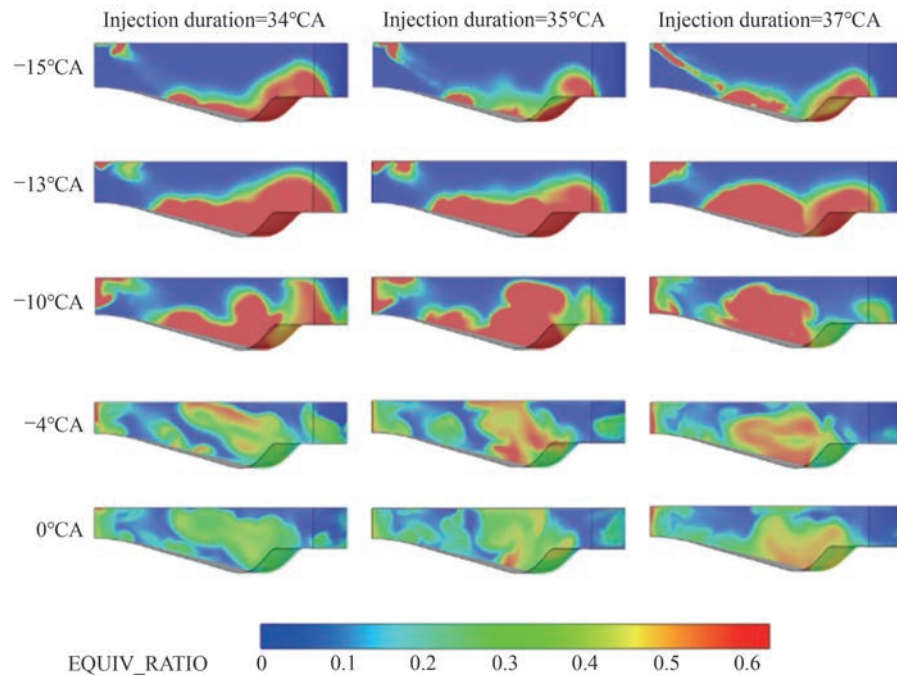


Figure 12 The equivalence ratio distribution evolution process for different injection duration

such as selective catalytic reduction (SCR), or adopt complementary strategies to effectively control NO_x emissions.

3) *Economic impact*: Controlling the unburnt hydrogen emissions can improve fuel conversion efficiency, reduce fuel consumption and the operating costs of shipowners. However, the applying of precise diesel fuel control strategies may lead to increased upfront investment, particularly in engine hardware and control systems.

4) *Environmental impact*: Although hydrogen itself is not a greenhouse gas and does not directly contribute to the greenhouse effect, its release into confined or semi-enclosed areas on board ships can lead to localized accumulation. Such accumulation poses significant safety risks due to hydrogen's low ignition energy and high diffusivity, which may endanger both crew members and onboard equipment. From an environmental and operational safety perspective, managing hydrogen emissions is therefore crucial, not only to maintain safe working conditions but also to ensure compliance with maritime regulations.

4 Conclusions

In this study, numerical simulations were carried out to identify the optimal diesel injection strategy for enhancing hydrogen combustion in a hydrogen/diesel dual-fuel marine medium-speed engine. Key injection parameters including SOI, spray tilt angle, and injection duration were analyzed both individually or collectively to minimize residual hydrogen levels. The principal findings of this study are summarized as follows:

1) *Optimal SOI Timing*: Early diesel injection effectively reduces the unburnt hydrogen fraction. The optimal SOI found was 49.5°CA BTDC, where the unburnt hydrogen percentage decreased dramatically from 50% to 3%, as compared to the baseline SOI of 9.5°CA BTDC. However, injecting too early results in part of the hydrogen being left unburnt due to flame quenching before reaching the cooler, distanced combustion chamber walls.

2) *Effect of Spray Tilt Angle*: Modifying the spray tilt angle further lowers the unburnt hydrogen fraction. When the angle is reduced from 75.5° to 55.5° , the unburnt hydrogen percentage decreases from 3% to 2%, a 33.3% improvement. The optimal SOI remains at 49.5°CA BTDC, with improved outcomes attributed to better diesel spray-wall impingement which favorably influences the direction of diesel vapor diffusion.

3) *Injection Duration Effect*: Adjusting the injection duration can also lead to more complete hydrogen combustion. Reducing the injection duration from 35°CA to 34°CA leads to a decrease in unburned hydrogen from 2% to 1%, achieving a 50% improvement. This change affects the position of the primary diesel diffusion cloud, strategically enhancing diesel diffusion towards areas further from the ignition source, thus facilitating the ignition of hard-to-reach hydrogen.

In conclusion, optimizing diesel injection strategies can significantly reduce the fraction of unburned hydrogen, thereby increasing fuel conversion efficiency and reducing safety risks aboard ships. These findings support the potential for hydrogen use in marine medium-speed engines. In future research, the combined optimization of multiple diesel injection strategies and engine cylinder geometry could

be explored to further reduce unburned hydrogen emissions. Additionally, the impact of higher hydrogen substitution ratios should be investigated to better understand their influence on combustion behavior.

Abbreviation

AMR	Adaptive mesh refinement
ATDC	After top dead center
BTDC	Before top dead center
CA	Crank angle
CFD	Computational fluid dynamics
CI	Compression ignition
CO	Carbon monoxide
CO ₂	Carbon dioxide
DNV	Det norske veritas
EVO	Exhaust valve opening
GHG	Greenhouse gas
HC	Hydrocarbons
H ₂	Hydrogen
H ₂ DDI	Hydrogen/diesel dual-fuel direct injection
ICE	Internal combustion engine
IMO	International maritime organization
IVC	Intake valve closing
KH-RT	Kelvin-helmholtz rayleigh-taylor
MEPC	Marine environment protection committee
NTC	No time counter
PFI	Port fuel injection
RANS	Reynolds averaged Navier–Stokes
RCCI	Reactivity controlled compression ignition
RNG k - ϵ	Re-normalization croup kappa-epsilon
RMSE	Root mean square error
SAE	Society of automotive engineers
SAGE	Standardized agile general engine
SOI	Start of injection
TDC	Top dead center

Acknowledgement Supported by SAFeCRAFT project jointly funded by Horizon Europe 101138411-SAFeCRAFT, and UKRI: 10110519. The CFD simulations were performed on the ARCHIE-WeSt High Performance Computer (<https://www.archie-west.ac.uk>) based at the University of Strathclyde.

Competing interests Peilin Zhou is an editorial board member for the Journal of Marine Science and Application and was not involved in the editorial review, or the decision to publish this article. All authors declare that there are no other competing interests.

Open Access This article is licensed under a Creative Commons Attribution 4.0 International License, which permits use, sharing, adaptation, distribution and reproduction in any medium or format,

as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons licence, and indicate if changes were made. The images or other third party material in this article are included in the article's Creative Commons licence, unless indicated otherwise in a credit line to the material. If material is not included in the article's Creative Commons licence and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder. To view a copy of this licence, visit <http://creativecommons.org/licenses/by/4.0/>.

References

- Anthony Amsden L (1999) A block-structured KIVA program for engines with vertical or canted valves. Los Alamos National Laboratory (LANL), Los Alamos
- Beale JC, Reitz RD (1999) Modeling spray atomization with the Kelvin-Helmholtz-Rayleigh-Taylor hybrid model. *Atomization and Sprays* 9(6): 623–650. <https://doi.org/10.1615/AtomizSpr.v9.i6.40>
- Cho ES, Ruminski AM, Aloni S, Liu YS, Guo J, Urban JJ (2016) Graphene oxide/metal nanocrystal multilaminates as the atomic limit for safe and selective hydrogen storage. *Nat Commun* 7: 10804
- Dimitriou P, Tsujimura T, Suzuki Y (2019) Low-load hydrogen-diesel dual-fuel engine operation – A combustion efficiency improvement approach. *International Journal of Hydrogen Energy* 44(31): 17048–17060
- DNV (2019) Assessment of selected alternative fuels and technologies in shipping. DNV. Available from <https://www.dnv.com/maritime/publications/alternative-fuel-assessment-download.html> [Accessed on April 25, 2024]. Greenhouse gas emissions from global shipping
- DNV (2021) The role of combustion engines in decarbonization: Seeking fuel solutions. DNV. Available from <https://www.dnv.com/expert-story/maritime-impact/The-role-of-combustion-engines-in-decarbonization-seeking-fuel-solutions.html> [Accessed on May 15, 2024]
- Du H, Chai WS, Wei H, Zhou L (2024) Status and challenges for realizing low emission with hydrogen ultra-lean combustion. *International Journal of Hydrogen Energy* 57: 1419–1436
- Duan Y, Sun B, Li Q, Wu X, Hu T, Luo Q (2023) Combustion characteristics of a turbocharged direct-injection hydrogen engine. *Energy Conversion and Management* 291: 117267. <https://doi.org/10.1016/j.enconman.2023.117267>
- Gatts T, Li H, Liew C, Liu S, Spencer T, Wayne S, Clark N (2010) An experimental investigation of H₂ emissions of a 2004 heavy-duty diesel engine supplemented with H₂. *International Journal of Hydrogen Energy* 35(20): 11349–11356
- Gao J, Wang X, Song P, Tian G, Ma C (2022) Review of the backfire occurrences and control strategies for port hydrogen injection internal combustion engines. *Fuel* 307: 121553. <https://doi.org/10.1016/j.fuel.2021.121553>
- Gomes Antunes JM, Mikalsen R, Roskilly AP (2009) An experimental study of a direct injection compression ignition hydrogen engine. *International Journal of Hydrogen Energy* 34(15): 6516–6522
- Han Z, Reitz RD (1995) Turbulence modeling of internal combustion engines using RNG k - ϵ models. *Combustion Science and Technology* 106(4–6): 267–295
- Hanafi Gharehlar H, Ebrahimi M, Hosseinzadeh M, Hosseini S (2024) Hydrogen/diesel RCCI engine performance assessment at low load. *International Journal of Hydrogen Energy* 58: 200–209
- International Maritime Organization (2023) Marine Environment

- Protection Committee (MEPC 80). International Maritime Organization. Available from <https://www.imo.org/en/MediaCentre/MeetingSummaries/Pages/MEPC-80.aspx> [Accessed on April 25, 2024]
- Jabbar, AI (2020) Combustion and emission characteristics of IC engines fueled by hydrogen and hydrogen/diesel mixtures and multi-objective optimization of operating parameters. PhD thesis, Missouri University of Science and Technology, Rolla. https://scholarsmine.mst.edu/doctoral_dissertations/2916
- Khairallah HA (2015) Combustion and pollutant characteristics of IC engines fueled with hydrogen and diesel/hydrogen mixtures using 3D computations with detailed chemical kinetics. PhD thesis, Missouri University of Science and Technology, Rolla. https://scholarsmine.mst.edu/doctoral_dissertations/2410
- Liew C, Li H, Nuszowski J, Liu S, Gatts T, Atkinson R, Clark N (2010) An experimental investigation of the combustion process of a heavy-duty diesel engine enriched with H₂. *International Journal of Hydrogen Energy* 35(20): 11357-11365
- Liu X, Seberry G, Kook S, Chan QN, Hawkes ER (2022) Direct injection of hydrogen main fuel and diesel pilot fuel in a retrofitted single-cylinder compression ignition engine. *International Journal of Hydrogen Energy* 47(84): 35864-35876
- Liu Y, Jia M, Xie M, Pang B (2012) Enhancement on a skeletal kinetic model for primary reference fuel oxidation by using a semidecoupling methodology. *Energy & Fuels* 26(12): 7069-7083
- MAN Energy Solutions (2023) MAN to investigate engine concepts for maritime hydrogen applications. Retrieved from <https://www.man-es.com/company/press-releases/press-details/2023/10/12/man-to-investigate-engine-concepts-for-maritime-hydrogen-applications> [Accessed April 25, 2024]
- Mitsui Engineering & Shipbuilding (2024) World's first successful hydrogen combustion operation with a large marine engine. Retrieved from https://www.mes.co.jp/english/press/2024/0307_002400.html [Accessed April 25, 2024]
- Olmer N, Comer B, Roy B, Mao X, Rutherford D (2017) Greenhouse gas emissions from global shipping, 2013-2015 Detailed Methodology. International Council on Clean Transportation: Washington, DC, USA, 1-38
- O'Rourke P, Amsden A (1996) A particle numerical model for wall film dynamics in port-injected engines. *SAE Transactions*, 2000-2013
- Qu W, Fang Y, Song M, Wang Z, Xia Y, Lu Y, Feng L (2024) Hydrogen injection optimization of a low-speed two-stroke marine hydrogen/diesel engine. *Fuel* 366: 131352. <https://doi.org/10.1016/j.fuel.2024.131352>
- Qu W, Fang Y, Wang Z, Sun H, Feng L (2022) Optimization of injection system for a medium-speed four-stroke spark-ignition marine hydrogen engine. *International Journal of Hydrogen Energy* 47(44): 19289-19297. <https://doi.org/10.1016/j.ijhydene.2022.04.096>
- Senecal P, Pomraning E, Richards K, Briggs T, Choi C, McDavid R, Patterson M (2003) Multi-dimensional modeling of direct-injection diesel spray liquid length and flame lift-off length using CFD and parallel detailed chemistry. *SAE Transactions*, 1331-1351
- Schmidt DP, Rutland CJ (2000) A new droplet collision algorithm. *Journal of Computational Physics* 164(1): 62-80
- Sharma P, Dhar A (2018) Compression ratio influence on combustion and emissions characteristic of hydrogen diesel dual fuel CI engine: Numerical Study. *Fuel* 222: 852-858
- UNCTAD (2021) Review of maritime transport 2021. UNCTAD. Available from <https://unctad.org/publication/review-maritime-transport-2021> [Accessed on May 15, 2024]
- Verhelst S, Wallner T (2009) Hydrogen-fueled internal combustion engines. *Progress in Energy and Combustion Science* 35(6): 490-527
- Wärtsilä (2023) Hydrogen test. Wärtsilä Energy. Retrieved from <https://www.wartsila.com/energy/sustainable-fuels/hydrogen-test> [Accessed April 25, 2024]
- Wang X, Sun B, Luo Q, Bao L, Su J, Liu J, Li X (2020) Visualization research on hydrogen jet characteristics of an outward-opening injector for direct injection hydrogen engines. *Fuel* 280: 118710. <https://doi.org/10.1016/j.fuel.2020.118710>
- Xie Y, Liu J, Qin J, Xu Z, Zhu J, Liu G, Yuan H (2024) Numerical simulation of hydrogen leakage and diffusion in a ship engine room. *International Journal of Hydrogen Energy* 55: 42-54
- Yuan Y, Wang J, Yan X, Shen B, Long T (2020) A review of multi-energy hybrid power system for ships. *Renewable and Sustainable Energy Reviews* 132: 110081. <https://doi.org/10.1016/j.rser.2020.110081>