



Combustion Characteristics and Control of Marine Hydrogen-Diesel Dual-Fuel Engines with Port Fuel Injection

By

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The Universe is a Hydrogen Sonata.

Abstract

Driven by the IMO's greenhouse gas reduction strategy, maritime decarbonisation has become imperative. Hydrogen-Diesel dual-fuel (HDDF) engines offer a promising route to reducing CO₂ emissions from large-bore, medium-speed marine engines. However, port-fuel-injected (PFI) hydrogen presents unresolved combustion and emission challenges, including incomplete combustion, rapid heat release, and mixture inhomogeneity.

This study systematically investigates HDDF combustion and develops effective control strategies. The CFD model was verified through grid sensitivity analysis and validated against experimental data under diesel-only and dual-fuel conditions.

Firstly, the diesel injection strategy was optimised to enhance flame propagation, reducing the unburnt hydrogen fraction from 50% to 1% and thereby improving hydrogen combustion completeness.

Then, the combustion and emission characteristics at different hydrogen substitution ratios (HSRs) were investigated. Compared with diesel operation, 30% HSR improves indicated thermal efficiency (ITE) by 2.96% but increases NO_x emission by 3.11 g/kWh. To suppress unstable combustion at 90% and 95% HSRs, direct water injection (DWI) enables knock-free operation. At the recommended DWI control points, ITE increases by 1.43% and 1.39%, while NO_x emissions decrease by 6.01 g/kWh and 6.45 g/kWh, respectively.

Furthermore, the effects of hydrogen-air mixture inhomogeneity were investigated. Hydrogen stratification was found to govern local reactivity and combustion behaviour. An inverted Gaussian distribution achieved the highest ITE (48.9%) but caused unstable combustion, whereas a homogeneous mixture provided a balanced compromise between efficiency (48.0% ITE) and emissions.

Finally, to recover low-load performance, an increased compression ratio was combined with diesel split injection. At 60% HSR, this strategy achieved a hydrogen combustion efficiency of 96.5% and an ITE of 53.9%, representing a 3.0% improvement over diesel operation while reducing NO_x emissions by 1.59 g/kWh.

Overall, this study clarifies the combustion behaviour of marine HDDF engines and proposes practical control strategies for achieving stable, efficient, and cleaner Hydrogen-Diesel combustion.

Keywords: Decarbonisation; Marine diesel engine; Hydrogen-diesel dual-fuel; Computational fluid dynamics (CFD); Combustion characteristics; Dual-fuel control strategies.

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Abbreviation & Symbols List

Abbreviation	Description
AHRR	Apparent heat release rate
AMR	Adaptive mesh refinement
ATDC	After top dead centre
BTDC	Before top dead centre
BTE	Brake thermal efficiency
BSFC	Brake-specific fuel consumption
CA	Crank angle
CA10	Crank angle of 10% mass fraction burned
CA50	Crank angle of 50% mass fraction burned
CA90	Crank angle of 90% mass fraction burned
CCS	Carbon capture and storage
CR	Compression ratio
DI	Direct injection
DNV	Det Norske Veritas
DOE	Design of experiments
DWI	Direct water injection
EGR	Exhaust gas recirculation
EOC	End of combustion
EVO	Exhaust valve opening
FAT	Factory acceptance testing
GHG	Greenhouse gas

HC	Hydrocarbons
HDDF	Hydrogen-Diesel dual-fuel
HE	Hydrogen embrittlement
HO ₂	Hydroperoxyl
HPDI	High-pressure direct injection
HRR	Heat release rate
HSR	Hydrogen substitution ratio
IMEP	Indicated mean effective pressure
IMO	International Maritime Organization
ITE	Indicated thermal efficiency
IVC	Intake valve closing
KI	Knock intensity
KH–RT	Kelvin–Helmholtz Rayleigh–Taylor
LHV	Lower heating value
LNG	Liquefied natural gas
LPDI	Low-pressure direct injection
MEPC	Marine Environment Protection Committee
MH	Metal hydride
NO _x	Nitrogen oxides
NSC	Nagle–Strickland–Constable
NZF	Net-zero framework
PFI	Port fuel injection
PRR	Pressure rise rate

PWI	Port water injection
RI	Ringling intensity
RMSE	Root mean square error
SCR	Selective catalytic reduction
SOC	Start of combustion
SOI	Start of injection
SI	Spark ignition
TAT	Type approval testing
TDC	Top dead centre
TJI	Turbulent jet ignition
TKE	Turbulent kinetic energy
UDF	User-defined function
VCR	Variable compression ratio
W/F	Water-to-fuel ratio
WI	Water injection

Symbol	Description
γ	specific heat ratio
P	cylinder pressure
V	cylinder volume
θ	crank angle
ρ	density
m_{source}	mass source representing phase change

τ	viscous stress tensor
F_{source}	momentum source from spray drag and wall interactions
E	total energy per unit of mass
k	thermal conductivity
Q_c	heat release from combustion
Q_w	heat release from wall
Y_i	mass fraction of species i
ω_i	net reaction rate
R	specific gas constant
T	temperature
$v'_{m,i}$	stoichiometric coefficients of the reactants
$v''_{m,i}$	stoichiometric coefficients of the products
M	total number of species
q_i	progress rate
$[X_M]$	molar concentration of species m
$k_{i,f}$	forward rate constants of reaction i
$k_{i,r}$	reverse rate constants of reaction i
r_{KH}	breakup droplet
Λ_{KH}	wavelength
Δt	time interval
N_p	number of parcels
k	turbulent kinetic energy
μ_t	turbulent viscosity

μ_m	mixture viscosity
C_p	specific heat capacity
F	function defining the flow regime
T_f	fluid temperature
T_w	wall temperature
Pr_m	mixture Prandtl number
n_i	normal vector component
α	thermal diffusivity
A_f	rate constant
E_f	activation energy
m_{soot}	mass of soot
d_{soot}	diameter of soot
ρ_{soot}	density of soot
M_C	mole mass of carbon
p_{O_2}	partial pressure of oxygen
$p_{\max}$	maximum pressure
$T_{\max}$	maximum cylinder temperature
$P_{\max}$	maximum cylinder pressure
β	empirically scaling coefficient which relates the oscillations
$\dot{Q}_{\text{diesel}}^*(\theta)$	instantaneous diesel heat release rate
$\dot{Q}_{\text{tot}}(\theta)$	total heat release rate
$M_{H_2}^{\max}$	maximum hydrogen mass fraction
σ	standard deviation of the distribution

Chapter 1 Introduction

This chapter provides an overview of the thesis. It begins by introducing the background of shipping decarbonisation, including maritime greenhouse gas emission regulations and the physical and chemical properties of key zero-carbon fuels. It then presents the aims, objectives, and novelties of the study. Finally, the structure of the thesis is outlined.

1.1 Background

1.1.1 Marine greenhouse gas (GHG) regulations

Shipping accounts for over 80% of global trade, serving as a cornerstone of international transportation [1]. To date, internal combustion engines remain the prime movers for most international ships due to their advantages in economy, efficiency and reliability [2]. Furthermore, in the coming decades, internal combustion engines are expected to continue their dominance in ship propulsion [3]. However, despite these advantages, the maritime sector is also a significant contributor to greenhouse gas (GHG) emissions. Recent reports indicate that global GHG emissions have reached 53.0 Gt CO₂-equivalent per year [4]. The International Maritime Organization (IMO) has estimated that the maritime sector accounts for approximately 2.9% of the global GHG emissions [5]. The 2015 Paris Agreement, a landmark accord, called for significant reductions in greenhouse gas (GHG) emissions. Its principal goal is to "limit the increase in global average temperature to well below 2°C above pre-industrial levels" while striving to "restrict the temperature rise to within 1.5°C above pre-industrial levels" [6]. To support the Paris Agreement, the International Maritime Organization (IMO) has introduced a series of measures aimed at controlling greenhouse gas (GHG) emissions from shipping. The IMO's initial GHG strategy, adopted in 2018, outlines a plan to reduce the GHG emissions from shipping by at least 50% by 2050, compared to 2008 levels [7]. Furthermore, in July 2023, the 80th session of the International Maritime Organization's (IMO) Marine Environment Protection Committee (MEPC) adopted the 2023 IMO Strategy on the Reduction of GHG Emissions from Shipping. As shown in Fig. 1.1, this revised strategy emphasizes a commitment to significantly reduce GHG emissions from international shipping, with a target of achieving at least a 70% reduction by 2040 compared to 2008 levels. The final objective is to achieve net-zero GHG emissions in the maritime sector by 2050. Subsequently, in April 2025, the IMO further approved a Net-Zero Framework

(NZF), which establishes the mandatory fuel standard and GHG emissions pricing for the maritime sector [8].

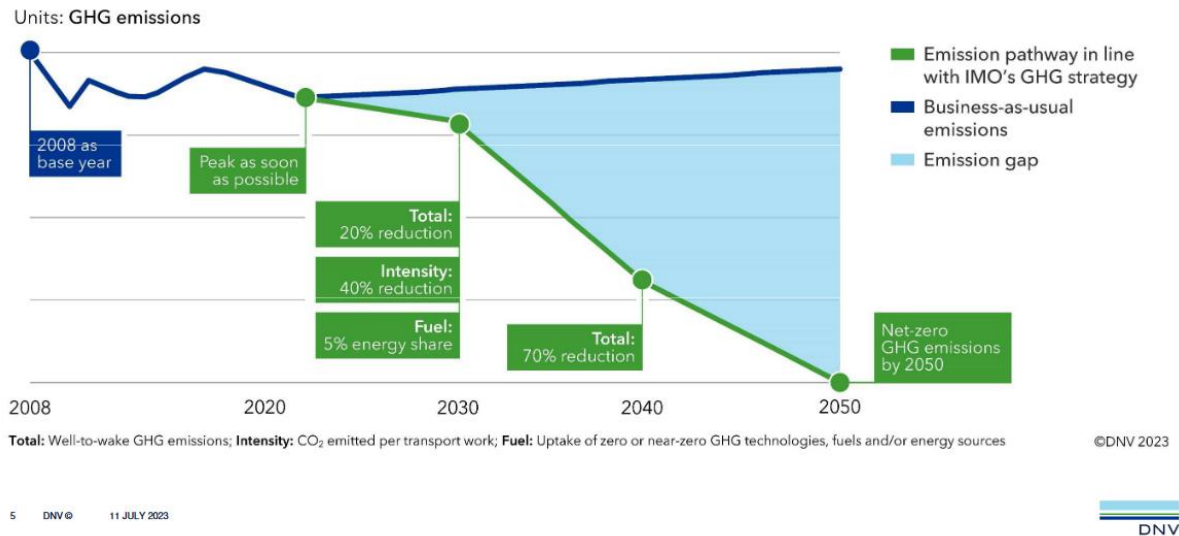


Fig. 1.1 The revised 2023 IMO GHG strategy target illustration [9].

To clarify the concept of “net-zero GHG emissions” in shipping, Lloyd’s Register [10] provided a detailed classification in 2023. According to this definition, zero GHG emissions in the shipping sector can be categorized into three types: (1) Absolute-zero emissions, where no GHG emissions are generated throughout the entire lifecycle of a ship; (2) Net-zero emissions, where the anthropogenic GHG emissions released over the ship’s lifecycle are offset by anthropogenic GHG removals; and (3) Near-zero emissions, where GHG emissions are reduced by more than 80% compared to low-sulfur fuel oil.

Therefore, to achieve the IMO’s 2050 net-zero target, it is essential to replace current diesel-fuelled engines with engines powered by low/zero carbon alternative fuels [11–17].

1.1.2 Zero-carbon marine fuels

According to DNV’s vision for the maritime sector [18], promising alternative fuels include hydrogen, ammonia, methanol, liquefied natural gas (LNG), and liquefied petroleum gas (LPG). Based on differences in carbon footprints, alternative fuels can be classified into three categories [19], often represented by three distinct colors: (1) Grey/brown fuels: These refer to traditional fossil fuels primarily extracted from geological reserves and are associated with high carbon

emissions. (2) Blue fuels: These are derived from traditional fossil fuels used as feedstock, with carbon capture and storage (CCS) technology applied during the production process. (3) Green fuels: These refer to carbon-neutral fuels produced exclusively from renewable energy sources, such as solar, wind or hydropower. Until now, most marine fuels have remained traditional grey or brown fuels. The maritime sector has increasingly focused on blue and green fuels to achieve net-zero Well-to-Wake GHG emissions [20]. However, achieving the target of absolute-zero GHG emissions requires the adoption of exclusively carbon-free fuels, such as ammonia and hydrogen [21–26]. Table 1.1 presents a detailed comparative analysis of the thermodynamic and chemical properties of hydrogen, ammonia and other alternative or traditional fuels.

Table 1.1 Thermodynamic and chemical properties of hydrogen, ammonia and other alternative or traditional fuels [27–32].

Property	Hydrogen	Ammonia	Diesel	Gasoline	LNG	Methane
Minimum ignition energy (mJ)	0.02	17	0.24	0.24	0.29	0.28
Representative density (kg/m ³)	0.09	0.73	845	745	452	0.7
Lower Heating Value (MJ/kg)	120	18.6	42.5	44	50	50
Autoignition Temperature (°C)	585	651	210	280	540	540
Laminar Flame Speed (cm/s)	265	7	86	58	40	40
Flammability Limit (% in air)	4-75	15-28	0.6-7.5	1.4-7.6	5-15	5-15
Stoichiometric Air-Fuel Ratio	34	4.3	14.5	14.7	17.1	17
Octane Number	>100	130	25-40	85-100	>120	107
Minimum quenching distance (mm)	0.64	2.5	0.65-1.5	2.0	1.5	2.03

1.1.2.1 Ammonia

Ammonia has garnered significant attention as a potential marine fuel due to its carbon-free composition and well-established industrial production [33–35]. Ammonia is relatively easy to store due to its liquefied temperature of $-33.34\text{ }^{\circ}\text{C}$ at atmospheric pressure. However, its toxic and corrosive nature necessitates specialized storage materials and equipment to ensure safe handling [36–38].

From the combustion properties, ammonia offers several advantages [39–41]. First, it has a high-octane number of approximately 130, significantly higher than that of diesel (25–40), which helps ensure a low tendency for knocking [42]. Consequently, when used in compression ignition engines, a relatively high compression ratio is required [43]. Second, ammonia has a high energy density [44]. As a carbon-free fuel, liquefied ammonia has an energy density of 13.6 GJ/m^3 , comparable to that of methanol (11.4 GJ/m^3), which is carbon-based [45].

When ammonia is used as a fuel, the following disadvantages need to be addressed. The autoignition temperature of ammonia is high ($651\text{ }^{\circ}\text{C}$), and its minimum ignition energy is elevated (17 mJ), making it challenging to use as a single fuel [46], particularly in compression-ignition engines where self-ignition is driven by compression. Besides, the laminar flame speed of ammonia ($\sim 7\text{ cm/s}$) is relatively slow, which may negatively affect combustion efficiency and reduce engine output power [47,48].

1.1.2.2 Hydrogen

Among the alternative fuels, hydrogen is a kind of zero-carbon fuel, which is also widely regarded as the ‘ultimate fuel’ [49]. This is because it has a high heating value while its combustion reaction produces only water and not any carbon oxides (CO and CO_2) nor hydrocarbons (HC). Looking at the combustion properties, hydrogen exhibits several special features compared with traditional fossil fuels: Firstly, hydrogen has a significantly smaller ignition energy of only 0.02 mJ, an order of magnitude lower than diesel's 0.24 mJ. This makes it more likely to undergo early ignition due to hot spots [50]. Additionally, hydrogen exhibits a wider flammability limit, which means it is easier to achieve lean combustion [51]. Its laminar flame speed is also faster, at 265 cm/s, compared to diesel's 86 cm/s under similar conditions. This means there could be knocking in the cylinder if a large percentage of hydrogen is added [52]. However, this speed decreases rapidly under lean combustion scenarios [53]. Another distinctive feature of hydrogen is its smaller

minimum quenching distance, compared to other gaseous fuels, which heightens the risk of backfire into the intake port [54]. Lastly, hydrogen's high auto-ignition temperature of 858 K makes it hard to achieve compression ignition [55]. Consequently, it can be inferred that hydrogen internal combustion engines can realize lean combustion but may face abnormal combustion problems like early ignition, knocking or backfire.

1.1.3 Commercialization of zero-carbon fuel marine engines

With the growing interest in zero-carbon marine fuels, the design and development of zero-carbon fuel marine engines is underway. Both two-stroke and four-stroke marine engines powered by ammonia or hydrogen are being tested by engine manufacturers.

1.1.3.1 Ammonia marine engines

Wärtsilä has announced the world's first ammonia-powered four-stroke marine engine “Wärtsilä 25 Ammonia” [56], as shown in Fig. 1.2. Subsequently, IHI Power Systems launched its four-stroke ammonia dual-fuel engine “6L28ADF” with 95% ammonia energy fraction in 2024 [57]. In parallel, Everllence has finished the single-cylinder test in 2023 and the full-scale test in 2024 of a 95% ammonia substitution two-stroke marine engine and will submit the developed engine to shipyard by 2026 [58]. Most recently, WinGD has finished both Type Approval Testing (TAT) and Factory Acceptance Testing (FAT) of its 52-bore ammonia-powered two stroke marine engine in January 2026.

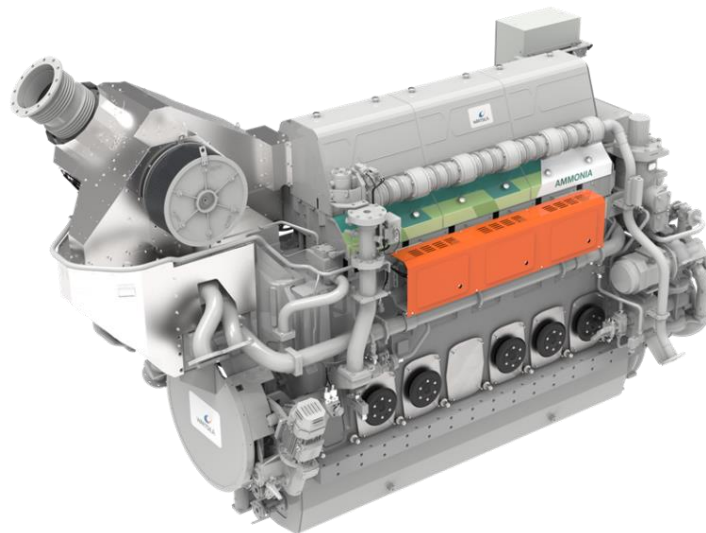


Fig. 1.2 World's first ammonia marine engine “Wärtsilä 25 Ammonia” [59].

1.1.3.2 Hydrogen marine engines

Compared to the ammonia marine engine, the commercialization of its hydrogen counterpart remains in a relatively nascent stage. In 2021, MAN introduced a 25 vol% hydrogen engine and subsequently declared that a pure hydrogen engine is their next step [60]. Meanwhile, Wärtsilä has not only successfully tested the performance of engines running on a 60 vol% hydrogen blend but also plans to have pure hydrogen engines by 2026 [61]. Besides, MITSUI E&S Co. Ltd has already successfully tested a 500 mm bore marine two-stroke low-speed engine running with hydrogen at 100% load, as shown in Fig. 1.3. It is the world's first hydrogen combustion trial in a large marine engine and realized a reduction of GHG emission of 95% [62]. It is evident that marine hydrogen engines are progressively moving towards commercialization. As this process advances, there will be a gradual increase in the substitution rate of hydrogen, as well as the development and transition from medium-speed engines to low-speed engines.

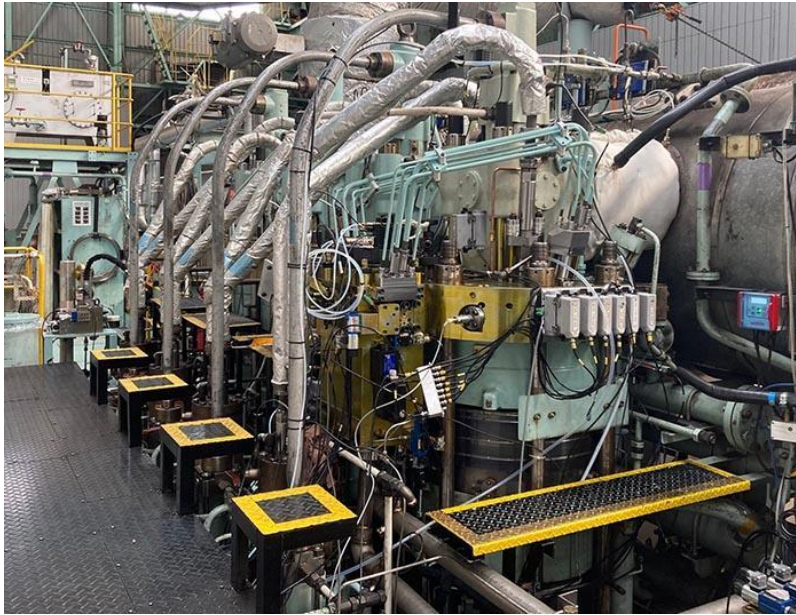


Fig. 1.3 The hydrogen two-stroke engine test by MITSUI E&S Co. Ltd [62].

1.2 Aim and Objectives

The aim of this study is to reveal the combustion and emission characteristics of Hydrogen-Diesel dual-fuel engines and to investigate combustion control strategies to address key combustion challenges, thereby optimising engine performance and emissions. The specific objectives related to the aim above are provided as follows:

1. To review the current state-of-the-art research on Hydrogen-Diesel dual-fuel engines, identify the major challenges associated with Hydrogen-Diesel combustion in marine engines, and highlight the research gaps.
2. To develop a computational fluid dynamics (CFD) model for a marine Hydrogen-Diesel dual-fuel engine with hydrogen port fuel injection (PFI) and validate the model by comparing the simulation results with experimental data under both diesel-only and Hydrogen-Diesel dual-fuel operating conditions.
3. To investigate the impact of diesel injection strategies on hydrogen-air mixture combustion and evaluate the potential for improving hydrogen combustion efficiency.
4. To investigate the effects of hydrogen substitution ratio on combustion and emissions in marine Hydrogen-Diesel dual-fuel engines and identify combustion control strategies that enable stable operation at high hydrogen substitution levels.
5. To investigate the impact of PFI hydrogen induction on mixture inhomogeneity in the combustion chamber and its effects on dual-fuel combustion and emissions, thereby providing insights for CFD modelling of PFI dual-fuel engines.
6. To investigate strategies for enhancing hydrogen combustion efficiency and improving engine performance under low-load conditions without increasing intake air temperature, while maintaining controlled emission levels through optimisation of engine operating parameters.

1.3 Novelty and Contribution

This study investigates the combustion characteristics and control strategies of PFI Hydrogen-Diesel dual-fuel marine engines via a validated CFD model. The key novelties and contributions are summarised as follows:

1. The influence of diesel injection control parameters on hydrogen combustion completeness and flame propagation characteristics in Hydrogen-Diesel dual-fuel engines is revealed.
2. The stability limits of hydrogen substitution ratio for stable combustion in Hydrogen-Diesel dual-fuel engines are identified. By applying in-cylinder water injection, knocking-free

combustion is achieved at a hydrogen substitution ratio of 95%, while nitrogen oxides (NO_x) emissions are effectively controlled.

3. A user-defined function (UDF) based CFD approach was developed to prescribe representative inhomogeneous hydrogen-air distributions, enabling investigation of PFI-induced mixture inhomogeneity beyond the conventional homogeneous-mixture assumption.

4. The influence of PFI-induced hydrogen-air mixture inhomogeneity on combustion and emissions in Hydrogen-Diesel dual-fuel engines is revealed for the first time, providing insights for intake control strategies and CFD modelling approaches for PFI dual-fuel combustion.

5. Under low-load conditions, increasing the compression ratio and adopting split diesel injection can mitigate performance deterioration in Hydrogen-Diesel dual-fuel operation, achieving comparable indicated thermal efficiency of diesel operation with modest emission reductions.

1.4 Thesis Outline

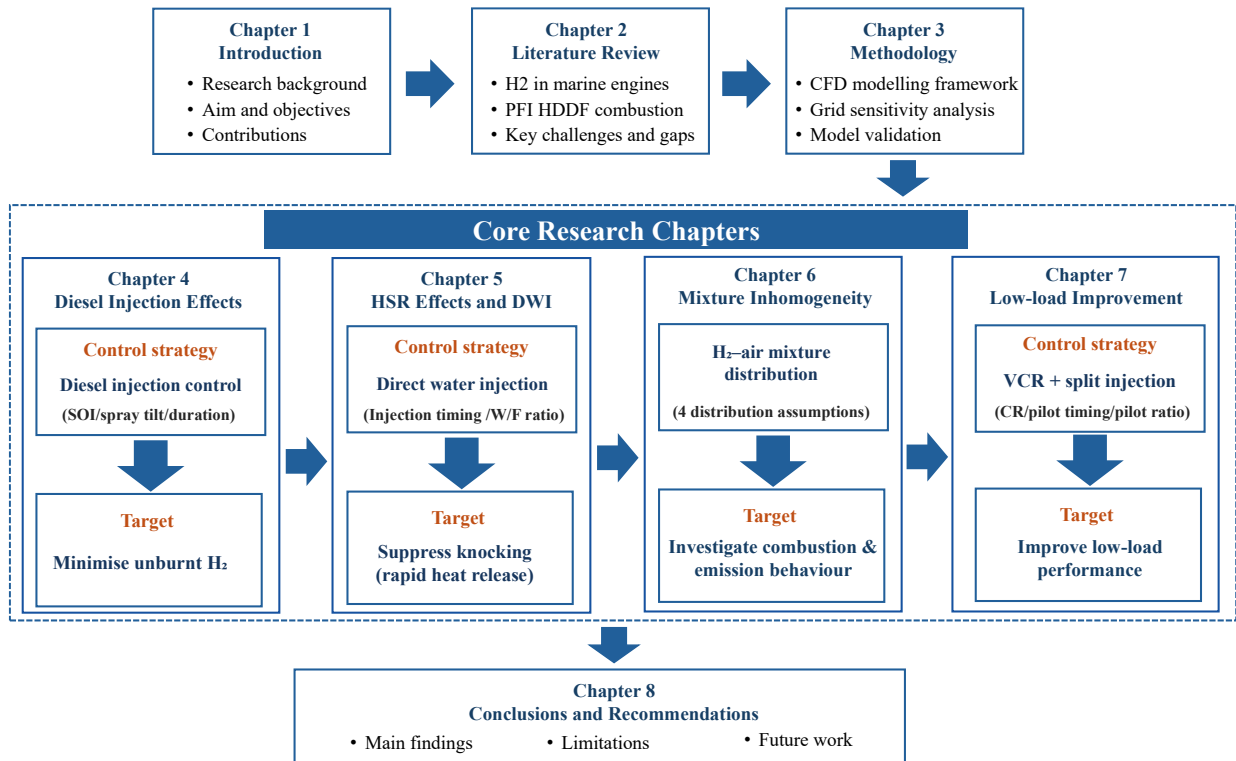


Fig. 1.4 Schematic diagram of the thesis structure.

As shown in Fig. 1.4, the thesis is structured as follows: Chapter 1 introduces the research background, aim and objectives, and the main novelty and contributions of the study. It also provides an overview of the thesis structure. Chapter 2 gives a literature review of the background of hydrogen-diesel dual-fuel engine and introduces the combustion challenges that remain to be solved. The research gaps are identified in this chapter; Chapter 3 introduces the numerical methodology of developing the CFD model of the hydrogen-diesel dual-fuel engine. The adopted sub-models and detailed information are included; Chapter 4 presents the results and analysis of how diesel injection parameters influence the fraction of unburnt hydrogen and the propagation of flames within the mixture under low-temperature intake conditions; Chapter 5 investigates the effects of hydrogen substitution ratio on combustion and emissions and demonstrates that stable combustion at high hydrogen substitution ratios can be achieved through in-cylinder water injection; Chapter 6 demonstrates the effects of PFI-induced hydrogen-air mixture inhomogeneity within the cylinder on combustion and emissions; Chapter 7 demonstrates the results of improving low-load engine performance by increasing the compression ratio and implementing split diesel injection; Chapter 8 summarizes the main findings of the thesis, discusses the limitations of the study, and outlines directions for future research.

Chapter 2 Literature Review

This chapter reviews the existing literature on Hydrogen-Diesel dual-fuel engines. The literature reviewed in this chapter was mostly identified through database of Scopus, Web of Science, ScienceDirect and Google Scholar. Search keywords included combinations of “marine hydrogen engine”, “hydrogen-powered ship”, “hydrogen safety”, “hydrogen-diesel dual-fuel engine”, “hydrogen direct injection”, “hydrogen port fuel injection”, “hydrogen substitution”, “low-load”, “knocking control”, “water injection”, “inhomogeneous hydrogen”. Recent publications within the past ten years were reviewed, while earlier publications were included if they provided landmark findings. The review begins by addressing the safety issues associated with the marine application of hydrogen. An introduction to engine combustion modelling approaches is then presented. Subsequently, recent studies on hydrogen-fuelled engines, including both pure hydrogen engines and Hydrogen-Diesel dual-fuel engines, are reviewed in detail. The chapter also compares the two main hydrogen supply strategies, namely direct injection and port fuel injection. The combustion challenges associated with port fuel injection are then discussed, and the chapter concludes by identifying the research gaps in port fuel injection Hydrogen-Diesel dual-fuel engines.

2.1 Hydrogen powered ships and safety issues

Hydrogen is attracting growing interest in maritime sector as a promising zero-carbon energy carrier [63]. Hydrogen-powered ships employ hydrogen engine or hydrogen fuel cell as power source according to the route and power demand. Hydrogen is usually stored onboard in compressed gas phase or liquid phase. However, many safety issues have to be addressed before widespread applications. The safety risks associated with hydrogen marine applications arise not only from the intrinsic properties of hydrogen, but also from the specific onboard operating conditions and scenarios, including confined spaces, limited natural ventilation, high-temperature equipment, and the close integration of fuel storage, supply, and propulsion systems.

2.1.1 Hydrogen powered ships

Hydrogen-powered ships are primarily powered by two kinds of technologies: hydrogen internal combustion engines (H_2 ICE) and hydrogen fuel cells (H_2 FC) [64–67]. The main properties and suitable application of H_2 ICE and H_2 FC are summarised in Table 2.1. In hydrogen-fuelled

compression ignition (CI) engines, due to the high auto-ignition temperature (858 K) of hydrogen, diesel fuel is usually employed as highly reactive pilot fuel to ignite hydrogen. The advantages of hydrogen-fuelled engines lie in good reliability, high power density, and the ease of retrofitting from conventional diesel engines [68]. Hence, hydrogen-fuelled engines are more suitable for long-range, high-power demand applications such as ocean-going vessels [69]. Notably, the limitation of hydrogen substitution ratio and high NO_x emissions remain critical challenges for hydrogen-fuelled engines [70,71]. In contrast, hydrogen fuel cells have higher energy conversion efficiency by directly converting the chemical energy into electricity through electrochemical reactions. Moreover, hydrogen fuel cells consume hydrogen as the only fuel, offering greater CO₂ reduction potential [72]. The fuel cells applied in marine propulsion are primarily solid oxide fuel cell (SOFC) and polymer electrolyte membrane fuel cell (PEMFC) [73]. SOFCs operate at high temperature (500-1,000°C) and offer good electrical efficiency (approximately 60%) [74]. In addition, SOFCs exhibit good fuel flexibility, can utilize hydrogen or hydrogen-carrier fuels such as ammonia, methanol or LNG as fuel. Due to the slow start-up and poor transient response, SOFCs are more suitable for steady load operation or auxiliary power [75]. PEMFCs, in contrast, operate at lower temperatures (<120°C) and require high-purity hydrogen as fuel. Their low operating temperature, fast start-up, and rapid load response make them particularly suitable for short-sea vessels, ferries, and fixed-route ships [76,77].

Table 2.1 Comparison of hydrogen power technologies for marine applications [78–82].

Technology	Main advantages	Limitations	Suitable applications
H ₂ ICE	High power density; easy retrofit; good reliability	NO _x emissions; knock/backfire risk; substitution ratio limitation	Large ships, ocean-going vessels, retrofits
H ₂ SOFC	High efficiency; near-zero local emissions; good for steady load	Slow start-up; poor transient response; high temperature durability issues	Auxiliary power, steady-load propulsion, future long-range ships
H ₂ PEMFC	Most mature FC option; fast response; zero local emissions	Needs high-purity H ₂ ; costly; limited by H ₂ storage	Ferries, inland ships, coastal vessels, fixed routes

Hydrogen-powered ship originated in 2000, marked by the launch of hydrogen-powered vessel “Hydra” produced in Germany [83]. As shown in Fig. 2.1, this ship is powered by a 6.8 kW hydrogen fuel cell and hydrogen is stored in a metal-hydride (MH) hydrogen storage tank. The

launch of “Hydra” represents the first-time application of hydrogen-powered ships. Subsequently, in 2008, “Alsterwasser” is served as the first commercial hydrogen-powered passenger ship in Hamburg, exhibiting the system reliability and operation feasibility of hydrogen fuel cell power system [84]. In recent years, the most representative hydrogen powered ship is “MF Hydra”, which integrates the liquid hydrogen storage, fuel cell generator and ferry services. The operation of “MF Hydra” is the milestone for the long-term operation of hydrogen powered ships [85].



Fig. 2.1 The world’s first hydrogen-powered ship “Hydra” [86].



Fig. 2.2 The world’s first hydrogen engine powered tugboat “Hydrotug 1” [87].

Fuel cell systems are better suited for short-range, fixed-route vessels due to their high efficiency and near-zero emissions but are constrained by low power density and limited scalability. In

contrast, hydrogen engines offer higher power density, wider power range, and greater compatibility with existing propulsion systems, making them more suitable for long-range, high-power applications despite challenges in NO_x emissions and combustion control [88]. The ferry “Hydroville” was built in 2017, which adopts hydrogen-diesel dual-fuel engine as power, showing the feasibility of hydrogen engine marine application. As shown in Fig. 2.2, the company extended the technology to tugboats, which is named as “Hydrotug 1”, demonstrating the potential for hydrogen-diesel dual-fuel engines in high-power workboats [89].

Currently, fuel cell-powered ships exhibit a higher level of technical maturity than hydrogen engine-powered ships. However, hydrogen engines offer lower retrofitting costs and greater operational reliability. Therefore, fuel cell systems are currently more suitable for near-term deployment in small-scale and short-range vessels, whereas hydrogen engines may represent a more practical option for large-scale marine applications and the retrofit of existing ships.

2.1.2 Safety considerations

The onboard hydrogen power system consists of hydrogen storage tank, hydrogen supply system, hydrogen prime mover, which is systematic and complicated [90]. Moreover, the special properties of hydrogen introduce significant safety challenges. Although hydrogen safety is not directly investigated in this thesis, reducing unburnt hydrogen is also relevant to safe operation, as residual hydrogen entering the exhaust system may introduce potential hazards within the exhaust ducts or near exhaust outlets under unfavourable dispersion conditions. This section provides an overview of the main safety concerns and the relevant strategies for hydrogen marine applications.

2.1.2.1 Leakage and ventilation

Hydrogen’s buoyancy and diffusivity are high, leakage from the storage tanks or supply system can result in its accumulation at the top of enclosed spaces, rapidly forming an explosive gas mixture [91]. Ryu et al. [92] reported the hydrogen accumulation at the ceiling and in the corners and spaces of the equipment. Guan et al. [93] investigated the hydrogen leakage and diffusion in the engine room of a hydrogen fuel cell powered ship, finding that smaller hydrogen pipe diameter helps improve the safety level of hydrogen system and reduces the explosion possibility of flammable cloud. Their results also indicate that top ventilation can reduce hydrogen accumulation risks. Similarly, Li et al. [94] found that in a hydrogen fuel cell powered ship, once hydrogen

leakage happens, the accumulation around the wall and corners in fuel cell room is the richest and detectors are recommended to install nearby. Xie et al. [95] reported that low ventilation rate increases the diffusion area of hydrogen and thereby high ventilation rate is needed for safety consideration. Hence, proper ventilation arrangement is of significance for the design of hydrogen-powered ships.

2.1.2.2 Fire and explosion risks

Due to its low minimum ignition energy and wide flammability and explosion limits, hydrogen presents potential fire and explosion hazards [96]. Moreover, compared to open spaces, hydrogen appears to rise rapidly due to buoyancy in the air [97], the confined spaces onboard may facilitate hydrogen accumulation, thereby further increasing the associated risks. Several studies have investigated the fire and explosion scenarios of hydrogen-powered ships. Yuan et al. [98] evaluated the effectiveness of water mist on suppressing hydrogen jet fire in a hydrogen fuel cell powered ship, finding that 30 μm size water mist can effectively reduce the temperature of fire field and control the hydrogen jet fire development. Liu et al. [99] investigated the explosion characteristics of hydrogen leakage in a marine engine room, showing that the explosion process and the dynamic evolution of relevant physical field parameters are strongly influenced by equipment layout and spatial confinement. In their subsequent study [100], the results show that increasing the ventilation rate can reduce the size of the hydrogen cloud, thereby effectively suppressing explosion overpressure, high-temperature regions, and flame propagation. Mao et al. [101] reported that in the hydrogen explosion scenario of a fuel cell powered ship, the bow compartment is the least affected place and recommend for temporary shelter.

2.1.2.3 Storage challenges

Hydrogen atoms can penetrate the lattice of metallic material, reducing its plasticity, which is called Hydrogen embrittlement (HE) phenomenon [102], as shown in Fig. 2.3. Hydrogen embrittlement can cause brittle fractures or microscopic cracking. The gaseous phase hydrogen storage enables onboard hydrogen storage with 200 to 700 bars high pressure but requires large storage volume. The liquid phase storage can reduce needed space but the extremely low temperature of liquid hydrogen storage ($-253\text{ }^{\circ}\text{C}$) also reduces the performance of metal [103]. Moreover, the harsh sea conditions accumulate stress load and cause fatigue damage to hydrogen storage tanks. These pose challenges to onboard storage of hydrogen [104].

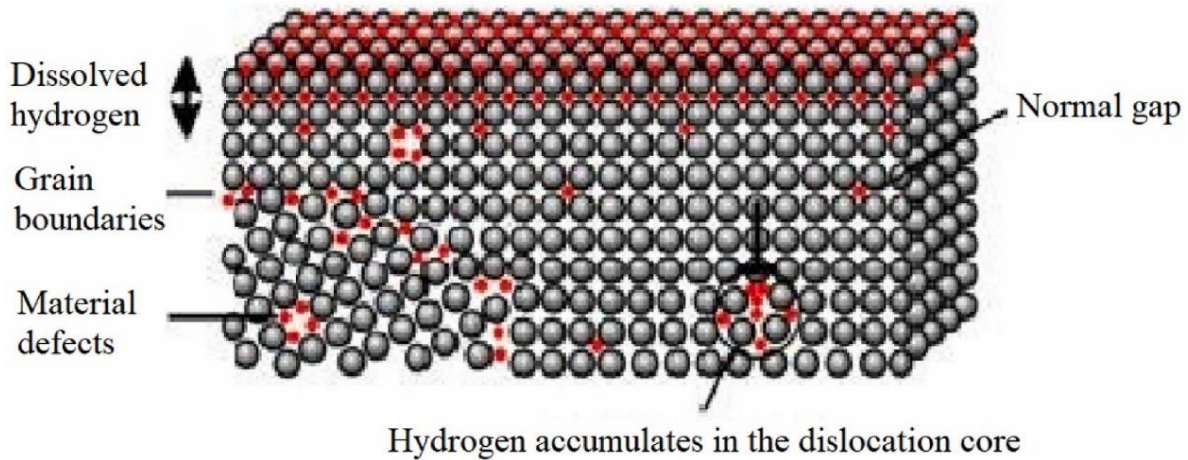


Fig. 2.3 Illustration of hydrogen embrittlement phenomenon [105].

2.2 Engine combustion modelling

Combustion modelling plays an important role in simulating and predicting the performance and emissions of internal combustion engines, particularly for dual-fuel engines [106–108]. Engine combustion models consist of a series of mathematical equations that describe the physical and chemical processes occurring within the cylinder, including fluid dynamics, heat transfer and thermodynamics, which are numerically solved to obtain the temporal evolution of key parameters in the combustion chamber.

Based on the development of engine simulation techniques and the increasing complexity of modelling approaches, combustion models can generally be classified into the following four categories: (1) Simple heat release rate model. (2) Zero-dimensional combustion model. (3) Quasi-dimensional combustion model. (4) Multi-dimensional (CFD) combustion model [109].

2.2.1 Simple heat release rate model

The heat release rate model analyses the combustion process in internal combustion engines by determining the amount of heat released from the fuel, using experimental measured cylinder pressure data. Based on the first law of thermodynamics, as shown in Eq. 2.1, the apparent heat release rate (AHRR) can be calculated from the pressure and volume variations with respect to crank angle.

$$AHRR = \frac{\gamma}{\gamma - 1} P \frac{dV}{d\theta} + \frac{1}{\gamma - 1} V \frac{dP}{d\theta} \quad (2.1)$$

where γ is the specific heat ratio, P is the cylinder pressure, V is the cylinder volume, and θ is the crank angle.

Due to its simplicity and straightforward application, this model remains applicable for performance studies. However, this approach requires cylinder pressure measurements at each operating condition to determine the heat release characteristics, which imposes demanding experimental requirements. Consequently, its application in engine process models remains relatively limited.

2.2.2 Zero-dimensional combustion model

The zero-dimensional combustion model, also referred to as the single-zone model, assumes that all thermodynamic properties within the cylinder are spatially uniform and vary only with time. Under this assumption, the entire cylinder is treated as a single homogeneous zone. The zero-dimensional model simplifies the complex physical and chemical processes occurring during combustion and therefore does not require detailed modelling of in-cylinder flow and combustion phenomena. Instead, the combustion process is typically represented by simple mathematical functions or combinations of empirical functions. These functions directly relate the heat release rate to combustion parameters, allowing the model to reproduce the heat release profile over a wide operating range through parameter calibration. The model parameters generally lack direct physical meaning and are determined by fitting to experimental data. At present, the most widely used zero-dimensional model is the Wiebe function [110].

Due to the computational efficiency, zero-dimensional models are widely used in engine performance simulations and parametric optimisation studies when detailed predictions of in-cylinder combustion processes are not required [111]. However, since pollutant formation is strongly influenced by the spatial distribution of in-cylinder parameters, zero-dimensional models are inadequate for accurately predicting emissions. Consequently, quasi-dimensional models were developed from the 1970s onwards to improve the prediction of emissions such as NO_x and HC, in response to increasingly stringent pollution concerns.

2.2.3 Quasi-dimensional combustion model

The quasi-dimensional model, which is also called multi-zone model, is positioned between the zero-dimensional model and multidimensional (CFD) model according to accuracy and complexity level. Compared with zero-dimensional models, quasi-dimensional models consider more detailed combustion processes, including fuel spray development and temperature distribution within the cylinder. In this approach, the combustion zone is divided into several independent zones, each of which is treated as a zero-dimensional control volume. The instantaneous fuel injection rate is introduced as an input parameter, and the temperature and gas composition within the cylinder are predicted by modelling the chemical reactions associated with fuel oxidation. Currently, the most widely used quasi-dimensional combustion models include the gas-jet combustion model proposed by Cummins Inc. and the droplet evaporation model proposed by Hiroyasu at Hiroshima University [112].

The quasi-dimensional model can be regarded as an extension of the zero-dimensional model, as it also employs crank angle as the only independent variable. Although quasi-dimensional models offer relatively low computational cost and enable the prediction of exhaust emissions, they still have limitations in accurately representing combustion chamber geometry and the influence of in-cylinder flow on the combustion process. Consequently, more detailed investigation of engine combustion requires the development of more advanced multi-dimensional (CFD) models.

2.2.4 Multi-dimensional (CFD) combustion model

Multi-dimensional models represent the most detailed and accurate combustion modelling approach currently, although they also require significantly higher computational resources. In these models, the combustion chamber is discretised into numerous computational cells to resolve the three-dimensional spatial distribution of in-cylinder processes. For each cell, the governing equations of mass, momentum, and energy conservation are solved to simulate the evolution of flow, combustion, and thermodynamic states within the cylinder. Within a multi-dimensional model, the governing conservation equations and submodels describing turbulence, heat transfer, and chemical reactions are solved numerically under specified boundary conditions. This allows the spatial and temporal evolution of thermodynamic parameters throughout the computational domain to be obtained accurately.

The aforementioned combustion models each have their own advantages and are suitable for different simulation purposes. In the present study, a multi-dimensional computational fluid dynamics (CFD) model was adopted to analyse the combustion characteristics and emissions of a Hydrogen-Diesel dual-fuel engine in detail.

2.3 Hydrogen-Diesel dual-fuel engines

The use of hydrogen as a substitute for conventional fossil fuels in internal combustion engines can significantly reduce carbon dioxide emissions, attracting widespread attention [113,114]. Research on hydrogen engines originates in the 1970s, when Furuhami et al. [115] first investigated the application of hydrogen in an automotive engine. They further conducted the road test successfully of the hydrogen-powered car, as shown in Fig. 2.4, marking the feasibility of hydrogen engine technology. Since then, extensive studies [116–120] have been conducted on hydrogen automotive engines, particularly spark-ignition engines, due to the favorable combustion characteristics of hydrogen.



Fig. 2.4 The hydrogen engine car road test by Furuhami et al. [121] in 1975.

For marine engines, most of them are compression-ignition diesel engines [122], in which diesel fuel is injected directly into the cylinder at high pressure and ignited by compression. However, owing to the high auto-ignition temperature of hydrogen (858K), achieving compression ignition with pure hydrogen is challenging [123]. Consequently, the Hydrogen-Diesel dual-fuel (HDDF) engines, in which highly reactive diesel fuel is used as a pilot to ignite hydrogen in the cylinder, are widely regarded as a practical approach for utilizing hydrogen in marine engines [124,125]. As shown in Fig. 2.5, there are mainly two kinds of hydrogen supply methods in HDDF engines: direct injection (DI) and port fuel injection (PFI) [126,127]. DI involves injecting hydrogen directly into the cylinder, while PFI involves sending hydrogen into the intake manifold, allowing the hydrogen-air mixture to enter the cylinder afterwards [128].

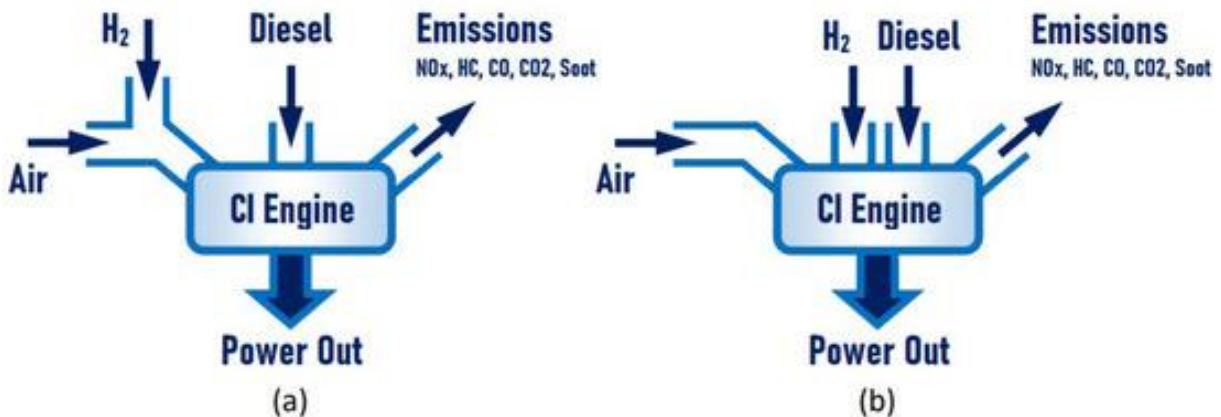


Fig. 2.5 Schematic diagrams of Hydrogen-Diesel dual-fuel engine with (a) port fuel injection (PFI), and (b) direct injection (DI) of hydrogen [129] .

Furthermore, hydrogen blending with natural gas has long been considered a practical pathway for introducing hydrogen into marine engines [130]. Compared with pure hydrogen combustion, the presence of natural gas can moderate the rapid combustion characteristics of hydrogen and provide more controllable combustion behaviour. However, natural gas remains a carbon-containing fuel, limiting its potential for deep carbon reduction, while methane slip introduces an additional emission challenge [131]. Consequently, the present study focuses on hydrogen-diesel dual-fuel combustion rather than hydrogen–natural gas blending, with the aim of achieving greater carbon-reduction potential and investigating combustion control strategies for high hydrogen substitution ratios.

2.3.1 DI Hydrogen-Diesel dual-fuel engines

The DI mode has received widespread attention in recent years due to its advantage in preventing backfire and maintaining volumetric efficiency [132,133]. DI mode can be further divided into the Low-Pressure Direct injection (LPDI) and High-Pressure Direct injection (HPDI) according to injection pressure. LPDI, with rail pressure lower than 50 bar [134], involves injecting hydrogen earlier, leading to premixed combustion without reducing volumetric efficiency [135]. Nevertheless, the early injection of LPDI may lead to the risk of premature ignition and knocking. In contrast, HPDI, of which the rail pressure can reach 300 bar, conducts hydrogen injection close to top dead centre (TDC) to realize non-premixed combustion.

Liu et al. [136] experimentally studied the performance and emissions of a high-pressure (20 MPa) DI Hydrogen-Diesel dual-fuel engine, noting that controlling the hydrogen injection timing can switch the combustion mode. The results show that at an early hydrogen injection timing, the combustion exhibits premixed characteristics while a late hydrogen injection timing leads to mixing-controlled combustion behaviour. Furthermore, a considerable indicated efficiency of 47% was achieved at 50% hydrogen energetic ratio and hydrogen injection timing of 40 °CA before top dead centre (BTDC). In a follow-up study [137], at 90% hydrogen energetic ratio, the optimal hydrogen injection timing (40 °CA BTDC) reduced the CO₂ by 85.9% and increased the indicated mean effective pressure (IMEP) by 13.3% compared to conventional diesel operation. They further extended this work by examining the effects of staged hydrogen injection [138]. The results indicated that advancing the timing of the first hydrogen injection promoted a more homogeneous hydrogen-air mixture, whereas the degree of hydrogen stratification was primarily governed by the timing of the second injection. Ramsay et al. [139] numerically tested the combustion performance of a high-pressure (25 MPa) hydrogen DI Hydrogen-Diesel dual-fuel engine with high hydrogen energetic fraction, observing the engine performance improvement under high load and performance degradation at low load. Treacy et al. [140] studied the effect of hydrogen DI pressure and start of injection (SOI) in an HPDI hydrogen heavy-duty engine, demonstrating maximum thermal efficiency of 54.9% at highest rail pressure (295 bar) and SOI of -7 °CA after top dead centre (ATDC). The above studies have primarily investigated direct injection in engines with small cylinder bores (≤ 150 mm), focusing mainly on the effects of injection parameters on combustion and emission characteristics.

Owing to the trend towards low-carbon shipping, research on hydrogen direct injection in large-bore marine engines has also begun to emerge. Qu et al. [141] analyzed hydrogen direct injection control in a large-bore (340 mm) marine low-speed two-stroke hydrogen/diesel engine, demonstrating that appropriate injection angles and injection timing are critical to balancing mixture homogeneity and hydrogen slip level. In their subsequent study [67], diesel direct injection and pre-chamber ignition strategies were compared in a hydrogen direct injection low-speed engine, showing that optimal pilot diesel fractions were 3% and 1%, respectively, and that pre-chamber ignition significantly enhanced lean-burn stability. Building on this work, optimisation of the passive turbulent jet ignition (TJI) pre-chamber design was conducted [142]. The optimised TJI pre-chamber configuration significantly improves the combustion performance of low-speed marine hydrogen engines, achieving approximately 85% of the diesel engine power output, an indicated thermal efficiency (ITE) of around 50%, and NO_x emissions well below IMO Tier III limits.

Although hydrogen direct injection offers several advantages, it faces several challenges, including high-pressure injection control, sealing difficulties, and hydrogen embrittlement. In addition, converting conventional diesel engines requires costly and complex modifications, meaning that its practical application remains some way off.

2.3.2 PFI Hydrogen-Diesel dual-fuel engines

The PFI (Port Fuel Injection) mode is easier to implement due to the relative ease of retrofitting conventional diesel engines [143], although it may lead to a reduction in engine output power because of decreased volumetric efficiency. Consequently, numerous studies have been conducted on the combustion characteristics and combustion control of hydrogen-diesel dual-fuel engines operating with PFI mode.

Yilmaz and Gumus [144] investigated the effect of hydrogen addition in the intake air for a diesel engine, finding that hydrogen addition increases the cylinder peak pressure, engine efficiency and reduce carbon-based emissions. Li et al. [145] examined effects of hydrogen substitution ratio (HSR) and diesel injection timing on a hydrogen-diesel dual-fuel engine at 20% and 40% load. The result shows that increasing HSR advances the peak pressure phase and effectively reduce carbon-related emissions, while advancing diesel injection timing improves brake thermal efficiency but increases NO_x emissions. Dimitriou et al. [146] evaluated the performance and

emissions of a PFI HDDF engine, and reported that, at medium load, NO_x emissions increased to four times compared to the conventional diesel operation. Kakran et al. [147] compared the engine performance of PFI HDDF mode with conventional diesel mode, identifying that the addition of hydrogen improved brake thermal efficiency (BTE) and reduced brake-specific fuel consumption (BSFC), though it also resulted in a reduction in volumetric efficiency. Abuelnour et al. [148] studied the effect of hydrogen addition and exhaust gas recirculation (EGR) in a hydrogen-diesel dual-fuel engine, indicating that increasing hydrogen fraction improves engine efficiency and significantly reduces CO and soot emissions, while increasing NO_x emissions, which can be effectively mitigated through EGR.

Overall, hydrogen addition via the PFI can improve engine efficiency and effectively reduce carbon-based emissions. However, the resulting increase in in-cylinder combustion temperature leads to higher NO_x emissions.

2.4 Combustion challenges in PFI HDDF engines

PFI Hydrogen-Diesel dual-fuel engines can effectively reduce carbon-related emissions and improve engine performance. However, owing to the unique combustion characteristics of hydrogen, the PFI mode still poses several challenges for combustion control, as discussed below.

2.4.1 Incomplete combustion and performance degradation

In hydrogen/diesel dual-fuel engines, the emission of unburnt hydrogen in the cylinder presents a significant challenge. This is typically caused by insufficient in-cylinder reactivity resulting from low intake air temperature or low engine load. This issue not only degrades engine performance but also raises potential safety concerns. Hydrogen has a very low ignition energy (~ 0.02 mJ) and a wide flammability range (4–75 vol%), with a lower explosive limit of about 4 vol% [149,150]. If accumulated in decks, the unburnt hydrogen can pose a safety hazard.

Several studies have reported incomplete hydrogen combustion or performance deterioration in Hydrogen-Diesel dual-fuel engines. Experimental studies conducted by Liew et al. [151] showed that adding hydrogen to a heavy-duty diesel engine results in a much lower hydrogen combustion efficiency at 70% engine load compared to diesel. Incomplete combustion becomes more pronounced at low hydrogen addition levels. Gatts et al. [152] experimentally tested the H₂

emissions characteristics of an H₂/diesel dual-fuel heavy-duty engine and found that hydrogen combustion efficiency is heavily influenced by engine load, with higher loads reducing unburnt hydrogen emissions. Under low-load conditions, the hydrogen located outside the diesel spray fails to participate in the main combustion process and therefore remains partially unburnt. Zhou et al. [153] observed reduction in maximum power, BTE and BSFC at low load in a hydrogen-diesel dual-fuel engine due to the low hydrogen combustion efficiency.

To mitigate the performance deterioration associated with incomplete hydrogen combustion under low-load conditions, Dimitriou et al. [154] adopted EGR in combination with advanced diesel injection timing. The results indicated that a high EGR rate elevated the intake charge temperature and enhanced in-cylinder reactivity, thereby improving hydrogen combustion efficiency at low load, while advancing SOI further improved efficiency but at the expense of increased NO_x emissions.

2.4.2 Substitution ratio limitation

As a result of hydrogen's high flame speed and rapid heat release characteristics, the PFI mode hydrogen addition can lead to knocking (excessively high pressure rise rates) in the engine, constraining the hydrogen substitution ratio (HSR), which is defined on an energy basis as the fraction of the total fuel chemical energy supplied by hydrogen. Szwaja and Grab-Rogalinski [155] reported that adding 5% of hydrogen in a compression ignition diesel engine shortens the diesel ignition delay and reduces the pressure rise rate, improving engine durability. However, higher hydrogen fraction (17%) increases the tendency for knocking.

Numerous studies indicate that reducing the compression ratio or adopting water injection (WI) can effectively increase the hydrogen substitution rate. Sharma et al. [71] found that in an HDDF engine, there is a clear trade-off relationship between compression ratio and maximum hydrogen substitution ratio. When compression ratio is reduced from 19.5 to 14.5, the maximum knocking-free HSR increased from 20% to 45%. Similarly, Chintala and Subramanian [156] reported that for compression ratio of 19.5, 16.5 and 15.4, the corresponding knocking limited maximum hydrogen substitution ratio is 19%, 59% and 63%, respectively. In their subsequent study [157], it was found that when the compression ratio was 19.5, the maximum hydrogen substitution ratio without knock was limited to 18.8%. By applying a combined strategy of in-cylinder water injection and reducing the compression ratio to 16.5, the hydrogen substitution ratio could be

increased to 79%. However, the reduction of the compression ratio may sacrifice thermal efficiency. Solely applying water injection appears to be a more practical approach to addressing the knocking issue and improve hydrogen substitution ratio. To comprehensively understand the effect of water injection on hydrogen dual-fuel engines and other types of engines, the relevant literature is summarized in Table 2.2.

Table 2.2 Literature review on water injection in engines.

WI of H₂ dual-fuel engines				
Reference	Engine details	H ₂ control (HSR/mode)	WI control (mode/duration/pressure)	Key findings
Serrano et al. [158]	HDDF engine, Nc=4, Bore=76 mm	0-74%/PFI	PWI/Var./N/A	Higher HSR increases NOx emissions, while a higher WI rate reduces NOx emissions.
Rueda-Vázquez et al. [159]	HDDF engine, Nc=4, Bore=83.1 mm	0-82%/PFI	PWI/Var./N/A	Combining WI with reduced CR and SOI effectively lowers NOx emissions, achieving over 35% efficiency.
Chintala et al. [160]	HDDF engine, Nc=1, Bore=102 mm	0-39%/PFI	PWI/Var./2 bar	Without WI, the engine's HSR is limited to 20%. However, as the WI amount increases, the HSR rises to a maximum of 39%.
Chintala et al. [161]	HDDF engine, Nc=1, Bore=102 mm	0-36%/PFI	PWI/Var./2 bar	WI maximizes the HSR, achieving comparable energy efficiency and lower NOx emissions than conventional diesel operation.
Wu et al. [162]	SI H ₂ -NG engine, Nc= 6, Bore=126 mm	0-10.5%/PFI	DI/10° CA/150 bar	A WI timing of -150 °CA enhances overall performance by reducing knock intensity (KI) and NOx emissions and increasing thermal efficiency and power output.
WI of Other Engines				
Reference	Engine details	WI control (mode/duration/pressure)		Key findings
Lius et al. [163]	Methanol SI engine, Nc= 6, Bore=127 mm	DI/0-5 ms/160 bar		DWI effectively suppresses knocking and reduces NOx, but combustion efficiency is reduced.
Mishra et al. [164]	HCCI gasoline engine, Nc= 1, Bore=86 mm	DI/13 °CA/40 bar		At a WIT of 60 °CA BTDC, the HRR and MRPR are minimized, and water vapor exhibits better distribution than other cases.
Sun et al. [165]	Marine two-stroke diesel engine, Nc= 6, Bore=350 mm	DI/N/A/180 bar		As water injection increased, in-cylinder pressure, temperature, indicated power, and NOx emissions decreased, while injection temperature had minimal effect on combustion and emissions.
Chen et al. [166]	Diesel engine, Nc=4, Bore=83.1 mm	PWI/Var./7 bar		The optimal WI timing is around -108 °CA ATDC with a wide range under single fuel injection, while for double fuel injection, it is 8–20 °CA before the first diesel injection with a narrower range.
Sehili et al. [167]	NG-H ₂ /diesel dual-fuel engine, Nc=1, Bore=95.5 mm	DI/6 °CA/250 bar		Pre-knock water injection is effective in mitigating abnormal combustion while maintaining engine performance.

Zembi et al. [168]	DISI engine, Nc=4, Bore=79 mm	PWI/20.4 °CA/3.5 bar	WI leads to an uneven distribution of the air-fuel mixture in the combustion chamber, increasing soot production.
Wei et al. [169]	Natural gas engine, Nc=6, Bore=130 mm	PWI/Var./Var.	WI timing and pressure are crucial in SI engines, with timing having a greater impact on combustion and emissions.
Liu et al. [170]	Hybrid gasoline engine, Nc=1, Bore=76 mm	DI/N/A/200 bar	Neither early nor late injection effectively suppresses knocking, and the KI value declines as WFR increases.

Abbreviations: CR, compression ratio; DI, direct injection; DISI, direct-injection spark-ignition; DWI, direct water injection; HCCI, homogeneous charge compression ignition; HRR, heat release rate; HSR, hydrogen substitution ratio; KI, knock intensity; MRPR, maximum rate of pressure rise; Nc, number of cylinders; NG, natural gas; PFI, port fuel injection; PWI, port water injection; SI, spark ignition; W/F, water-to-fuel ratio; WI, water injection; WIT, water injection timing; Var., variable; N/A, not available.

2.4.3 Inhomogeneous mixture

For hydrogen PFI dual-fuel engines, the assumption of homogeneous in-cylinder hydrogen-air mixture at the inlet valve closing is commonly adopted in CFD studies [55,148,171,172]. In reality, the port injection strategy significantly affects the hydrogen mixture homogeneity, whereas complete homogeneity is challenging to achieve [173]. Several studies have demonstrated that the inhomogeneity of hydrogen-air mixture can strongly influence flame propagation and combustion stability. Sheng et al. [174] studied non-homogeneous premixed hydrogen-air combustion in an obstructed channel, revealing that spatial hydrogen-air inhomogeneity promotes flame acceleration localised in hydrogen-rich regions, thereby enhancing the combustion instability. Wang and Wen [175] highlighted that, in an obstructed channel, the hydrogen-air inhomogeneity accelerates combustion and promotes detonation tendency. Lu et al. [176] compared the combustion between homogeneous and stratified hydrogen-air mixture in a lean-burn hydrogen DI engine, demonstrating that increasing mixture stratification leads to faster and more concentrated combustion. Ki et al. [177] experimentally investigated the hydrogen combustion under stratified conditions, finding that the local equivalence ratio at ignition location critically governs the hydrogen combustion characteristics.

2.5 Research Gaps

Based on the literature review, the current research gaps are identified as follows:

1. Hydrogen-Diesel dual-fuel engines suffer from incomplete hydrogen combustion, which becomes more pronounced under low-load conditions. However, effective solutions to this issue remain limited.
2. The effects of hydrogen port fuel injection (PFI) on combustion behaviour and emissions in marine engines remain insufficiently understood. In addition, the upper limit of hydrogen substitution ratio for stable combustion remains to be determined.
3. High hydrogen substitution ratios can lead to combustion instability. Existing control strategies often compromise engine performance and remain limited in enabling hydrogen substitution ratios of 90% or higher.
4. The introduction of hydrogen through PFI can lead to inhomogeneous hydrogen-air mixture formation within the cylinder. However, the impact of this mixture inhomogeneity on combustion and emissions in Hydrogen-Diesel dual-fuel engines remains unclear.

Chapter 3 Research Methodology

This chapter introduces the methodology of this study, including the CFD modelling framework, grid sensitivity test and validation against experimental data. Firstly, the engine modelling framework is presented, introducing the governing equations and several sub-models of the in-cylinder flow, injection and spray, evaporation, heat transfer, turbulence, combustion and emissions. Then, the grid sensitivity test results are given to prove the numerical convergence of the model. Finally, the model is validated against the experimental data of diesel operation and literature reported dual-fuel operation to verify the prediction accuracy of the CFD model.

3.1 Modelling framework

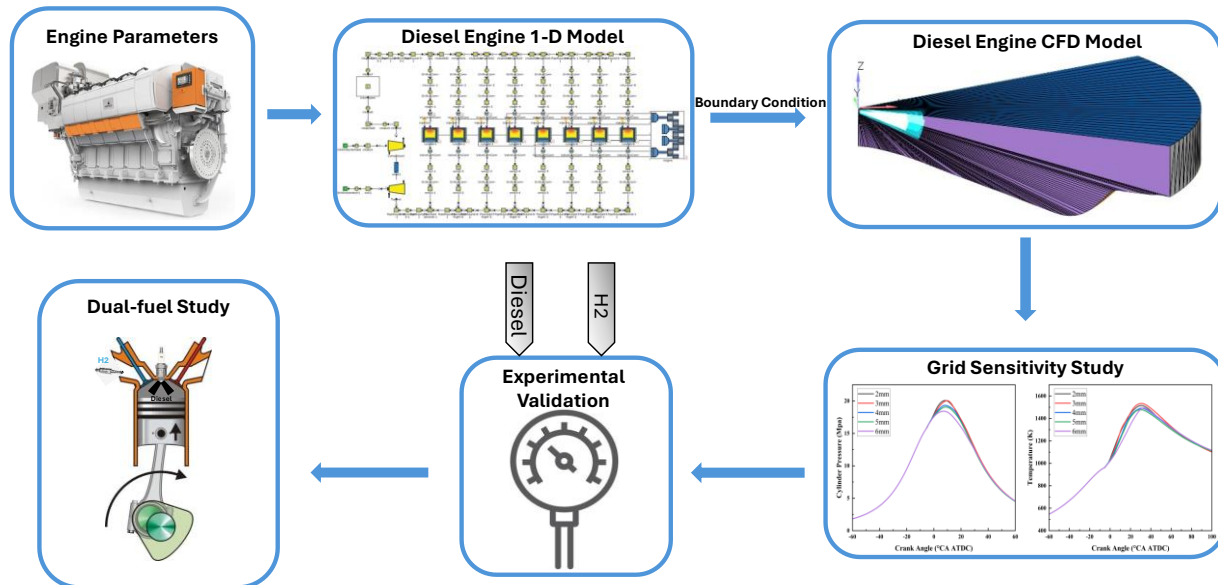


Fig. 3.1 The engine CFD modelling framework.

In this study, the engine CFD model is developed using the internal combustion engine CFD software CONVERGE V3.1. An 8-cylinder four-stroke marine medium-speed diesel engine with 4 MW rated power output at 750 r/min is considered for the full load analysis. Due to the lack of low load data, another 9-cylinder marine medium-speed engine with a rated power of 10.5 MW at 500 r/min is modelled for low load investigation. Fig. 3.1 illustrates the computational fluid dynamics (CFD) modelling framework adopted in this study. A one-dimensional (1D) engine model of the 4 MW rated power engine was developed in GT-POWER based on the engine

specifications and available experimental data. The measured in-cylinder pressure was analysed using the cylinder pressure analysis function in GT-POWER to derive the corresponding burn rate [178]. The resulting burn rate profile was then applied to reproduce the experimental engine operating condition. Similarly, the 1D engine model of the 10.5 MW rated power engine was developed by Tsitsilonis et al. [179] in a MATLAB environment. In the CFD model, the boundary and initial conditions are obtained through the 1D engine model.

Then, a grid sensitivity study was performed to ensure the numerical reliability of the CFD model. To achieve the trade-off between computational efficiency and accuracy, a converged grid setting is chosen for further simulation. Subsequently, the model was validated against experimental data under both conventional diesel and dual-fuel (diesel-hydrogen) combustion modes. The diesel mode is validated against the bench test data for the target engine, while the hydrogen-diesel dual-fuel mode data is validated through the literature reported light-duty engine data. Upon validation, a systematic investigation focusing on engine dual-fuel combustion characteristics and control strategies was conducted.

3.2 CFD sub-models

In the CFD model, the in-cylinder flow is governed by the Navier–Stokes equations, with the ideal gas equation of state employed to describe the thermodynamic behaviour of the gas mixture. The sub-models selected for simulating in-cylinder behaviour of combustion, droplet breakup, collision, turbulence, heat transfer and emissions are summarized in Table 3.1.

The SAGE model, which integrates detailed chemical reactions, is employed to simulate combustion. An experimentally validated hydrogen/n-heptane combustion mechanism, which includes 49 species and 174 reactions, was selected. It has been widely acknowledged that spray droplet size plays an important role in ignition and combustion behaviour. To capture the atomization and breakup behaviour of the diesel spray, the Kelvin–Helmholtz Rayleigh–Taylor (KH-RT) model was employed. The droplets collisions are modelled according to no-time-counter (NTC) model. The in-cylinder turbulence was modelled by the Re-Normalization Group (RNG) $k-\epsilon$ model. The O’Rourke and Amsden model was applied to calculate wall heat transfer. The extended Zeldovich mechanism, which describes the formation of thermal NO, was employed to model NO_x emissions. The Hiroyasu-NSC model, which describes soot formation and oxidation,

was employed as soot model. The detailed description and information of sub-models are presented in the subsequent paragraphs.

Table 3.1 Summary of sub-models and configurations in the CFD simulation.

Models	Name and details
Combustion model	SAGE: Two adaptive zones; Relative tolerance: 0.0001; Absolute tolerance: 10^{-14}
Reaction Mechanism	Hydrogen/n-heptane combustion mechanism consisting of 49 species and 174 reactions developed by Qu et al. [141].
Droplet breakup model	KH-RT: size constant: 0.60; velocity constant: 0.188 Mass diffusivity constants of C_7H_{16} : $D_0 = 5.94 \times 10^{-6}$, $n_0 = 1.6$
Collision model	The NTC collision
Turbulence model	RNG k- ϵ
Wall heat transfer model	O'Rourke and Amsden
NOx model	Extended Zeldovich: Thermal NOx model; Mass scaling factor to convert NO to NOx: 1.533
Soot formation model	Hiroyasu-NSC

3.2.1 Governing equations

In CONVERGE v3.1, the in-cylinder fluid dynamics are governed by the Navier-Stokes equations. The equations of mass, momentum, energy and species conservation are listed as follows:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = m_{source} \quad (3.1)$$

$$\frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho u u) = -\nabla p + \nabla \cdot \tau + \rho g + F_{source} \quad (3.2)$$

$$\frac{\partial (\rho E)}{\partial t} + \nabla \cdot [u(\rho E + p)] = \nabla \cdot (k \nabla T + \tau \cdot u) + \dot{Q}_c + \dot{Q}_w \quad (3.3)$$

$$\frac{\partial(\rho Y_i)}{\partial t} + \nabla \cdot (\rho u Y_i) = \nabla \cdot (D_i \nabla Y_i) + \dot{\omega}_i \quad (3.4)$$

Where ρ is the density, u is the velocity vector, m_{source} is the mass source representing phase change, ignition etc. p is the pressure, τ is the viscous stress tensor, F_{source} is the momentum source from spray drag and wall interactions, E is the total energy per unit of mass, k is the thermal conductivity, Q_c , Q_w represent the heat release from combustion, and wall respectively. Y_i is the mass fraction of species i , and ω_i is the net reaction rate.

The in-cylinder flow can be considered as compressible transient turbulent flow. In the simulations, the gas mixture can be considered ideal gas because of the high-temperature and low-density condition during combustion. At this condition, except the molecular collisions, intermolecular forces can be negligible because the kinetic energy magnitude is much larger than potential energy. Hence, the ideal gas state equation is used to govern the state of in-cylinder gases, as follows:

$$pV = mRT \quad (3.5)$$

Where, p is the pressure; V is the volume; m is the mass; R is the specific gas constant; T is the temperature.

3.2.2 SAGE combustion model

The SAGE combustion model, which solves detailed chemical reactions [180], is employed in the CFD model to accurately predict dual-fuel combustion. The SAGE solver computes the reaction rates of individual elementary reactions, while the CFD solver resolves the transport equations for mass, momentum, energy, and species. A multi-step chemical reaction mechanism can be written as:

$$\sum_{m=1}^M v'_{m,i} x_m \leftrightarrow \sum_{m=1}^M v''_{m,i} x_m \quad (3.6)$$

where $v'_{m,i}$ and $v''_{m,i}$ represent the stoichiometric coefficients of the reactants and products, respectively, for species m and reaction i ; and x_m is the chemical symbol for species m .

The net production rate of species can be calculated by:

$$\dot{\omega}_m = \sum_{i=1}^I v_{m,i} q_i \text{ for } m = 1, 2, \dots, M \quad (3.7)$$

where $v_{m,i} = v''_{m,i} - v'_{m,i}$, M is the total number of species, q_i represents the progress rate and can be calculated by:

$$q_i = k_{i,f} \prod_{m=1}^M [X_m]^{v'_{m,i}} - k_{i,r} \prod_{m=1}^M [X_m]^{v''_{m,i}} \quad (3.8)$$

In which, $[X_m]$ represents the molar concentration of species m , and $k_{i,f}$ and $k_{i,r}$ are the forward and reverse rate constants of reaction i , respectively.

3.2.3 Reaction mechanism

A hydrogen/n-heptane mechanism developed by Qu et al. [141], which includes 49 species and 174 reactions, is employed in this study. In this mechanism, N-heptane (C_7H_{16}) is chosen to represent diesel fuel due to its similar combustion characteristics but less computational cost. The chemical mechanism was optimised from the mechanism by Liu et al. [181] using genetic algorithm. This updated mechanism enhances the computational accuracy of the study by refining the reaction rate constants for C7 species from Liu's original model. The mechanism has been validated through rapid compression machine (RCM) experiments, demonstrating its ability to accurately predict the ignition delay time of hydrogen/n-heptane mixtures.

3.2.4 Breakup model

In this study, the Kelvin–Helmholtz Rayleigh–Taylor (KH-RT) model is employed to simulate the liquid droplet breakup behaviour. The illustration of KH-RT model is presented in Fig. 3.2. When fuel is injected from injector with high pressure, there is significant velocity difference between liquid and its surroundings gas phase. Hence, shear force is generated at the surface of the liquid jet, leading to the surface wave, which is known as KH instability. With the development of these waves, the surface of the liquid jet is going to be gradually unstable, forming droplet at wave crests. In the KH model, the radius of the breakup droplet (r_{KH}) is proportional to the wavelength (Λ_{KH}) of the KH wave with the maximum growth rate, can be calculated by:

$$r_{KH} = B_0 \Lambda_{KH} \quad (3.9)$$

The rate of parent droplet radius changing over time can be calculated by:

$$\frac{dr_p}{dt} = \frac{r_p - r_{KH}}{\tau_{KH}} \quad (3.10)$$

where τ_{KH} is the time of KH breakup and can be calculated by:

$$\tau_{KH} = \frac{3.788 B_1 r_p}{\Omega_{KH} \Lambda_{KH}} \quad (3.11)$$

where Ω_{KH} is the maximum growth rate of the KH wave.

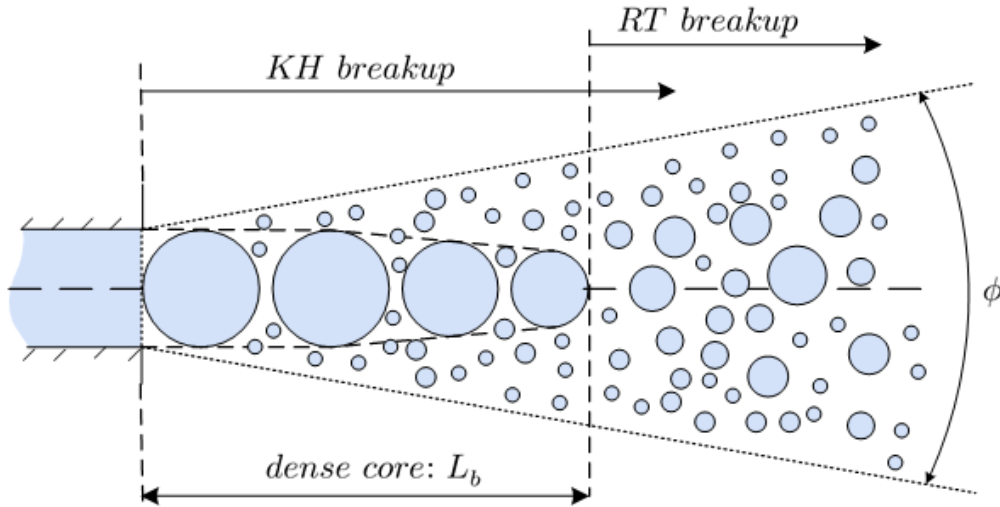


Fig. 3.2 The illustration of the breakup model mechanism [182].

The escaped droplet will be decelerated under the resistance force of surrounding gas. Because the density of the droplet is much larger than the surrounding gas, the surface of the droplet will form interactions, which is RT wave. With the enhancing of the interactions, the surface of the droplet will be gradually unstable, which is known as RT instability. Subsequently, smaller droplets will be formed by droplet breakup. The broken-up droplets radius in RT breakup process can be calculated by:

$$r_{RT} = \frac{1}{2} C_{RT} \Lambda_{RT} \quad (3.12)$$

where Λ_{RT} is the wavelength of the RT wave with the maximum growth rate.

The changing rate of the parent droplet can be represented by:

$$\frac{dr_p}{dt} = \frac{r_p - r_{RT}}{\tau_{RT}} \quad (3.13)$$

Where τ_{RT} can be calculated by:

$$\tau_{RT} = \frac{C_\tau}{\Omega_{RT}} \quad (3.14)$$

Where Ω_{RT} is the maximum value of RT wave.

During the breakup process, KH model and RT model dominate the different stages, respectively. The KH instability controls the initial breakup process while the RT instability becomes gradually significant in the later stage [183].

In the KH–RT model of this CFD model, the size constant is set to 0.60 and the velocity constant is set to 0.188. The mass diffusivity parameters for C_7H_{16} are specified as $D_0 = 5.94 \times 10^{-6}$ and $n_0 = 1.6$, which were determined through a sensitivity analysis [184].

3.2.5 Droplet collision model

In simulating the spray process, the interactive collision of droplet is significant to droplet size distribution and spray structure. The no-time-counter (NTC) model is employed in this study to simulate the droplet collision behaviour [185]. This model is based on Monte Carlo calculations, determining droplet collision events within each computational time step using random sampling. This method can avoid the explicit tracking of each droplet, effectively reducing the computational cost.

If a computational cell contains N droplets, with the collision cross-section defined as $\sigma_{ij} = \pi(r_i + r_j)^2$, the expected number of collisions within a time interval Δt can be obtained by summing the collision probabilities of all possible droplet pairs, as follows:

$$M_{\text{coll}} = \frac{1}{2} \sum_{i=1}^{\sqrt{M_{\text{cand}}}} q_i \sum_{j=1}^{\sqrt{M_{\text{cand}}}} \left(\frac{V_{i,j} q_j \sigma_{i,j}}{(V q \sigma)_{\text{max}}} \right) \quad (3.15)$$

where M_{cand} can be expressed by:

$$M_{\text{cand}} = \frac{(N_p^2 (q V \sigma) \Delta t)}{2V} \quad (3.16)$$

where N_p denotes the number of parcels in the cell and q represents the number of droplets contained in each parcel. The factor of one-half arises from symmetry considerations. This formulation represents the final expression of the NTC method when applied to parcels containing different numbers of droplets.

3.2.6 Turbulence model

Owing to the good numerical stability and relatively low computational cost, the in-cylinder turbulence is resolved by Reynolds-Averaged Navier–Stokes (RANS) k – ε model [186]. In this model, the transient flow variation can be divided into average and fluctuating components, introducing Reynolds' stress into momentum equations. The RANS momentum equation can be expressed as:

$$\frac{\partial(\rho \bar{u}_i)}{\partial t} + \frac{\partial(\rho \bar{u}_i \bar{u}_j)}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \right] - \frac{\partial}{\partial x_j} (\rho \bar{u}_i' u_j') \quad (3.17)$$

where the last item is RANS stress, and it can be represented by Boussinesq hypothesis as follows:

$$-\rho \bar{u}_i' u_j' = \mu_t \left(\frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \frac{2}{3} \rho k \delta_{ij} \quad (3.18)$$

where k is the turbulent kinetic energy and μ_t represents the turbulent viscosity.

The Re-Normalization Group (RNG) k – ε model is introduced to resolve turbulent viscosity, describing the turbulent kinetic energy k and its dissipation rate ε by resolving transport equations. The transport equations of k and ε can be expressed as:

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho k u_j)}{\partial x_j} = P_k - \rho \varepsilon + \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] \quad (3.19)$$

$$\frac{\partial(\rho\varepsilon)}{\partial t} + \frac{\partial(\rho\varepsilon u_j)}{\partial x_j} = C_{1\varepsilon} \frac{\varepsilon}{k} P_k - C_{2\varepsilon} \rho \frac{\varepsilon^2}{k} - R_\varepsilon + \frac{\partial}{\partial x_j} \left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon} \right) \frac{\partial \varepsilon}{\partial x_j} \right] \quad (3.20)$$

where R_ε represents the additional strain-dependent correction term in the RNG k- ε model.

The turbulent viscosity μ_t can be calculated by:

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \quad (3.21)$$

3.2.7 Wall heat transfer model

The O'Rourke and Amsden heat transfer model [187] is employed in the CFD model to simulate the heat transfer behaviour of cylinder boundaries. It can be given by the following equation:

$$k \frac{\partial T}{\partial x_i} = \frac{\mu_m C_p F (T_f - T_w)}{\text{Pr}_m y} n_i \quad (3.22)$$

Where k is thermal conductivity, μ_m is mixture viscosity, C_p is specific heat capacity, F is a function defining the flow regime, T_f is fluid temperature, T_w is wall temperature, Pr_m mixture Prandtl number, y is distance from the wall, n_i is the normal vector component.

This model calculates the wall heat flux in Fourier law with the near-wall temperature gradient estimated from the local fluid-wall temperature difference and mixture transport properties.

The thermal diffusivity α can be expressed as:

$$\alpha = \frac{k}{\rho c_p} \quad (3.23)$$

Where k is thermal conductivity, C_p is specific heat capacity, ρ is density.

This means that the thermal diffusivity of gas or hydrogen fuel has been considered in the O'Rourke and Amsden heat transfer model through the gas thermal conductivity. Therefore, the adoption of this heat transfer model is sufficient for hydrogen-enriched combustion.

3.2.8 NO_x model

In this study, the NO_x model used is the Extended Zeldovich model [188]. This means that all NO_x calculated in this study comes from thermal NO. Extended Zeldovich mechanism is as follows:



In which, NO_x mass = NO mass × Mass scaling factor (1.533). This thermal NO_x is highly affected by temperature.

3.2.9 Soot model

During the dual-fuel combustion process, the soot formation and oxidation are significant to the emission characteristics. In this study, the Hiroyasu–NSC model is employed to describe the soot formation process [189]. This model considers the variation of soot into two competitive processes of soot formation and oxidation. Its net variation rate can be represented as:

$$\frac{dm_{\text{soot}}}{dt} = \left(\frac{dm_{\text{soot}}}{dt} \right)_{\text{formation}} - \left(\frac{dm_{\text{soot}}}{dt} \right)_{\text{oxidation}} \quad (3.24)$$

The soot formation is calculated by Hiroyasu empirical model [190], and the formation rate can be expressed by:

$$\left(\frac{dm_{\text{soot}}}{dt} \right)_{\text{formation}} = A_f m_{\text{fuel}} p^{0.5} \exp \left(-\frac{E_f}{RT} \right) \quad (3.25)$$

where m_{fuel} is the evaporated fuel mass, p is the local pressure, T is temperature, A_f and E_f are the rate constant and activation energy.

The soot oxidation process is modelled by Nagle–Strickland-Constable (NSC) model [191]. This model takes into account the presence of different active sites on the surface of soot particles, classifying them into highly active A sites and less active B sites, and uses the distribution of these sites to describe the rate of the oxidation reaction.

The soot oxidation rate can be expressed by:

$$\left(\frac{dm_{\text{soot}}}{dt}\right)_{\text{oxidation}} = \frac{6M_C}{\rho_{\text{soot}} d_{\text{soot}}} m_{\text{soot}} K_{O_2} \quad (3.26)$$

where m_{soot} is the mass of soot, d_{soot} is the diameter of soot, ρ_{soot} is the density of soot, M_C is the mole mass of carbon.

The oxidation coefficient K_{O_2} can be expressed as:

$$K_{O_2} = \left(\frac{k_A p_{O_2}}{1 + k_Z p_{O_2}}\right) x_A + k_B p_{O_2} (1 - x_A) \quad (3.27)$$

where p_{O_2} is the partial pressure of oxygen, k_A , k_B and k_Z are the constant of reaction rate.

3.3 Modelling of 320-mm bore marine engine

In this study, a 320-mm bore marine medium speed engine with 4 MW rated output power is selected for the full load (100%) investigations. The engine geometrical characteristics and main parameters are presented in Table 3.2.

Table 3.2 The key parameters of the investigated 320-mm bore marine engine

Parameters	Value
Engine type	Four-stroke CI engine
Cylinder number	8
Rated power/(kW)	4,000
Rated speed/(rpm)	750
Bore/(mm)	320
Stroke/(mm)	420
Compression ratio	14.5:1
Simulated cycle period	IVC – EVO -167 ° CA ATDC-131° CA ATDC

Due to inherent symmetry in-cylinder a sector (60°) geometry is chosen to be simulated in order to increase the computational efficiency of the simulations. The simulations take place between the intake valve closing (IVC) (167 °CA BTDC) and exhaust valve opening (EVO) (131 °CA

ATDC). During the simulation, the intake and exhaust valves are fully closed, and the in-cylinder domain is treated as a closed system.

The CFD boundary conditions for the diesel operation are derived from 1D modelling. Table 3.3 includes the boundary and initial conditions for the diesel operation of the marine engine. During the dual-fuel operation, several modifications were required in engine initial conditions to accommodate the hydrogen fuel properties according to the previous study of the author [171].

Table 3.3 Boundary and initial conditions for CFD simulation of the investigated 320-mm bore marine engine diesel mode.

Boundary Conditions	Value
Piston temperature (K)	550
Cylinder head temperature (K)	520
Cylinder wall temperature (K)	430
Initial Conditions	
Pressure at the IVC (bar)	4.1
Temperature at the IVC (K)	360
Viscosity ratio	62.02
Length scale (m)	17,183
Liquid diesel spray temperature (K)	341

3.3.1 Grid sensitivity test

A grid sensitivity test has been conducted to achieve the balance between computational efficiency and accuracy. The grid strategy involves larger base grid size with local fixed embedding refinement and Adaptive Mesh Refinement (AMR). One-level fixed refinement was applied to the piston and cylinder head, whereas the diesel spray region was refined with two-levels to enhance spatial resolution in the spray development zone. The base grid sizes varying from 6 mm to 2 mm were tested under the same refinement strategy. Fig. 3.3 presents the in-cylinder pressure and

temperature of varying grid sizes. As the grid size decreases, the results are approaching convergence. From the results, the Pmax difference between 3mm and 4 mm grid is 0.723 MPa, which is still large. Furthermore, the difference between 2 mm and 3 mm grid results is relatively small, with a relative error of 0.1% for peak pressure and 1.2% for peak temperature. The root mean square error (RMSE) between 2 mm and 3 mm grid is 0.07 MPa for pressure and 8.22 K for temperature, demonstrating grid independence. Consequently, the 3mm base grid was selected for further validation and study, which can achieve the trade-off between accuracy and computational cost.

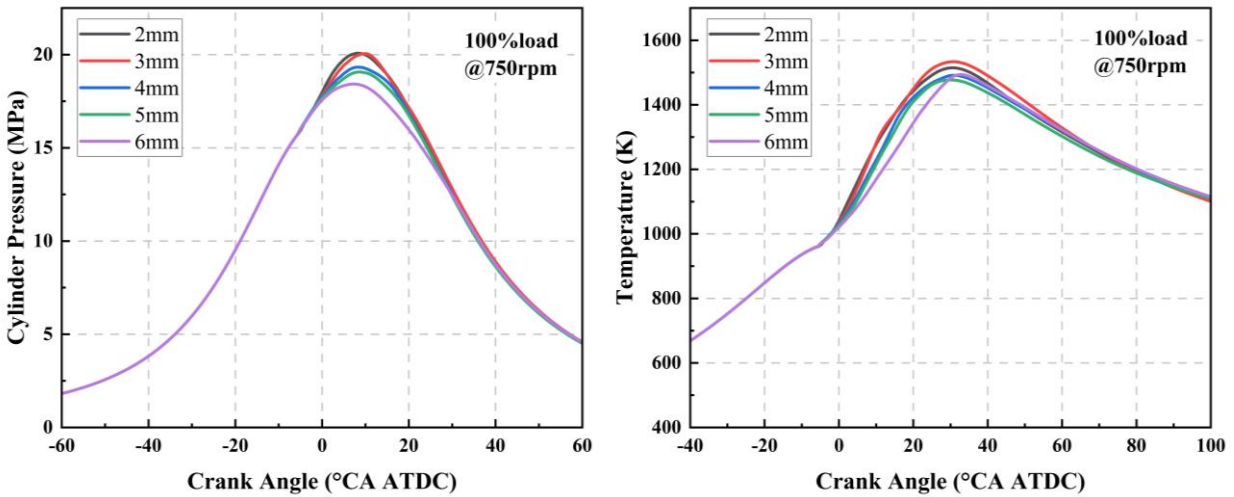


Fig. 3.3 Grid sensitivity test on in-cylinder pressure and temperature of 320-mm bore engine.

3.3.2 Diesel operation validation

The comparison between experimental test data and simulation results for the marine medium speed engine diesel-only mode at 75% and 100% load are shown in Fig. 3.4. As shown, the simulation results of maximum pressure ($p_{\max}$) and power output exhibit good agreement with the experimental measurements. At 75% load, the maximum relative errors are 1.98% for peak pressure and 4.09% for output power. At 100% load, the relative errors are 0.25% for peak pressure and 3.4% for power, which indicates higher accuracy compared to the 75% load case. The close agreement between the simulation and experimental results demonstrates the prediction reliability of the developed CFD model for diesel-only combustion in the marine medium-speed engine.

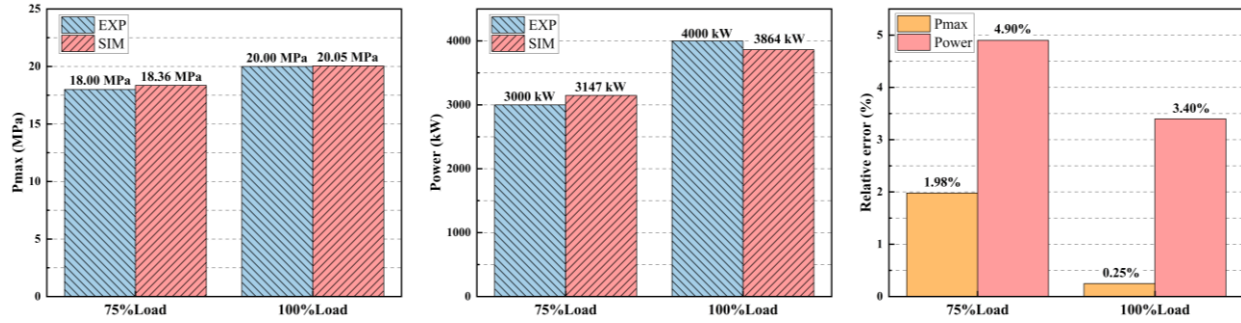


Fig. 3.4 Comparison of peak pressure (p_{max}) and power between simulation and experimental data for the 320-mm bore marine engine diesel-only mode at 75% and 100% load.

3.4 Modelling of 460-mm bore marine engine

Due to the lack of low load experimental data of 320-mm bore engine, another 9-cylinder 460-mm bore marine medium-speed engine with a rated power of 10.5 MW at 500 r/min is modelled for low load investigation. The main geometric and operating parameters are summarised in Table 3.4. A 1D engine model [179] was first developed based on the engine specifications to determine the boundary and initial conditions for the CFD model. The corresponding boundary and initial conditions for diesel and dual-fuel modes under low-load operation are presented in Table 3.5.

Table 3.4 The main parameters of the 460-mm bore marine engine.

Parameter	Value
Engine type	Wärtsilä 9L46C
Rated power/(kW)	10,500
Rated speed/(rpm)	500
Cylinder number	9
Bore/(mm)	460
Stroke/(mm)	580
Compression ratio	14.0:1
Nozzle angle/(deg)	67.5
Spray cone angle/(deg)	17.5
Nozzle diameter/(mm)	0.78
Simulated cycle period	IVC – EVO -135 °CA ATDC – 135 °CA ATDC

Table 3.5 Boundary and initial conditions for CFD simulation of the 460-mm bore marine engine diesel and dual-fuel mode at low load.

Boundary Conditions	Value
Piston temperature (K)	550
Cylinder head temperature (K)	520
Cylinder wall temperature (K)	430
Initial Conditions	
Pressure at the IVC (bar)	2.04
Temperature at the IVC (K)	330
Viscosity ratio	62.02
Length scale (m)	17,183
Liquid diesel spray temperature (K)	341

3.4.1 Grid sensitivity test

A grid sensitivity study was performed for the developed CFD model to ensure grid convergence while maintaining computational efficiency. Table 3.6 presents the configurations used in the grid sensitivity study, including four base grid sizes and various adaptive mesh refinement (AMR) strategies. Fig. 3.5 presents the results of different grid resolutions, including (a) cylinder pressure and heat release rate, (b) spatial distributions of NO_x and temperature, and (c) convergence metrics. As shown in Fig. 3.5 (a), the cylinder pressure and heat release rate progressively converge from G1 to G4, approaching experimental cylinder pressure. The difference between G3 and G4 becomes negligible. Fig. 3.5 (b) presents the NO_x and temperature distributions at 15°CA ATDC for different grid configurations. While G1 and G2 still exhibit noticeable deviations from G4, the spatial distributions of G3 and G4 are largely consistent. This trend is further confirmed in Fig. 3.5 (c), where both the relative error of peak pressure and Root Mean Square Error (RMSE) between the simulated and experimental cylinder pressures decrease from G1 to G4. Although G4 yields slightly lower errors than G3, the computational time increases significantly from 9.5 h (G3) to 23

h (G4) when performed on 40 Intel cores using Intel MPI. Considering the balance between computational accuracy and efficiency, the G3 grid configuration is selected for subsequent simulations.

Table 3.6 Grid settings for sensitivity study.

Parameter	Grid 1	Grid 2	Grid 3	Grid 4
Base grid size (mm)	12	10	8	6
Max AMR embedding level of velocity	3	3	4	4
Max AMR embedding level of temperature	3	3	4	4
Maximum total cell number	10,900	18,838	36,800	87,216

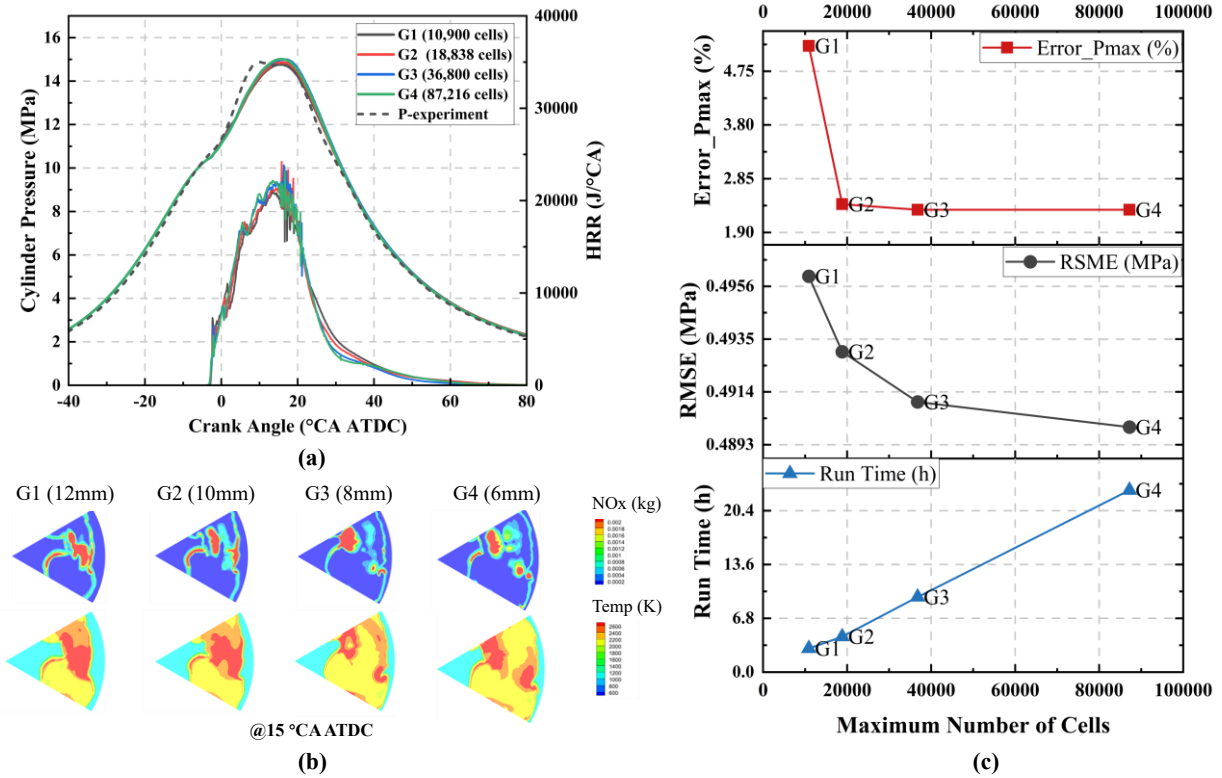


Fig. 3.5 Grid sensitivity study results of (a) cylinder pressure and heat release rate; (b) NOx and temperature spatial distribution; and (c) grid convergence metrics.

3.4.2 Diesel operation validation

Fig. 3.6 illustrates the comparison between experimental and simulated cylinder pressure and heat release rate of target 460-mm bore engine diesel operation at low (30%), medium (50%) and high (90%) loads. The experimental heat release rate is represented by apparent heat release rate (AHRR), calculated by Eq. 3.28 from measured cylinder pressure.

$$AHRR = \frac{\gamma}{\gamma - 1} P \frac{dV}{d\theta} + \frac{1}{\gamma - 1} V \frac{dP}{d\theta} \quad (3.28)$$

where γ is the specific heat ratio, P is the cylinder pressure, V is the cylinder volume, and θ is the crank angle.

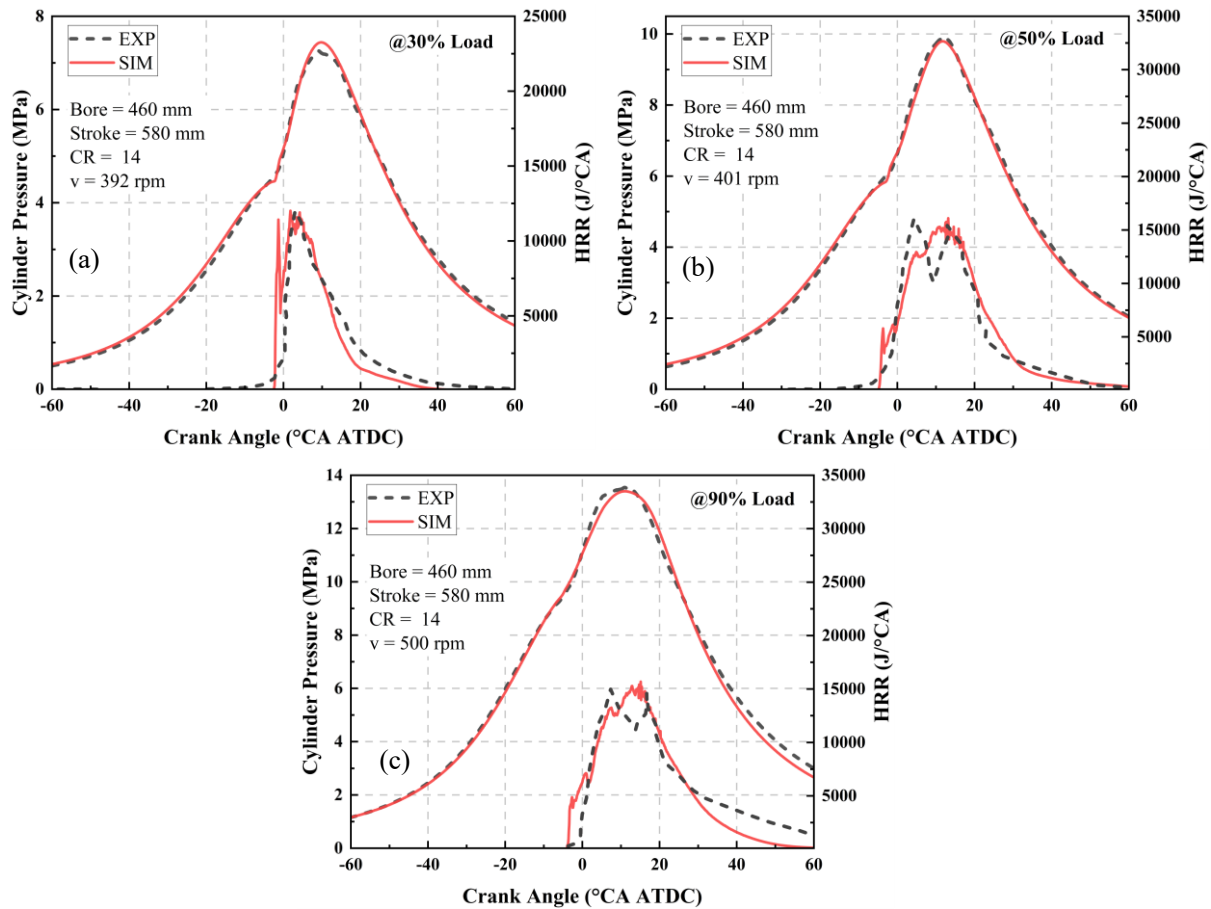


Fig. 3.6 The comparison of experimental and simulated cylinder pressure and heat release rate of investigated engine diesel mode at 30%, 50% and 90% loads.

As shown in Fig. 3.6, the cylinder pressure and heat release rate under all tested load conditions show good agreement between the experimental and simulated results. The relative errors in peak cylinder pressure and indicated power are both within 5%, indicating that the CFD model provides reliable predictive capability under diesel operation.

To further validate the CFD model, the comparison between CFD prediction and manufacturer's shop trials of diesel operation are listed in Table 3.7. The results show that at 50%, 75% and 100% loads, the relative errors are 3.7%, 3.4% and 0.1% for engine output power, 0.3%, 2.6% and 0.5% for peak pressure, and 8.5%, 8.7% and 2.3% for NO emissions.

Table 3.7 Comparison between simulated and measured data at shop trial test points of diesel operation.

Load (%)	Peak Pressure (MPa)			Indicated Power Output (kW)			NO Emissions (ppm)		
	Measured	CFD	Error (%)	Measured	CFD	Error (%)	Measured	CFD	Error (%)
50	13.5	13.54	0.3	4,725	4,900	3.7	9,679	10,500	8.5
75	15.6	16.0	2.6	7,088	6,850	3.4	9,296	10,100	8.7
100	20.5	20.4	0.5	9,450	9,440	0.1	9,179	9,390	2.3

3.5 Dual-fuel operation validation

Given the limited experimental data for marine-scale hydrogen PFI engines, the dual-fuel mode was validated against experimental data from a 115-mm bore light-duty Hydrogen-Diesel dual-fuel engine reported by Tsujimura and Suzuki [192]. This engine employs hydrogen PFI injection, consistent with the configuration used in the investigated marine engine. Fig. 3.7 compares the experimental and simulated in-cylinder pressure, heat release rate (HRR), and unburnt hydrogen fraction at HSR levels ranging from 0% to 24% under dual-fuel operation. Overall, the CFD model predicts the general cylinder pressure tendency, the two-stage heat release phase and peak value, and the unburnt hydrogen fraction with good consistency. At HSR of 0%, 14% and 24%, the RMSE for cylinder pressure is 0.116 MPa, 0.158 MPa and 0.178 MPa, respectively. The corresponding RMSE for HRR were 33.6 J/°CA, 38.1 J/°CA and 33.8 J/°CA respectively. The results indicate that the CFD model maintains consistent predictive accuracy across the investigated HSR range.

However, some discrepancies remain, mainly associated with ignition delay and combustion phasing. The predicted ignition delay is slightly larger than the experimental data and increases with higher HSR. This leads to the predicted first HRR peak to be sharper. Moreover, the second HRR peak appears approximately 5–6°CA earlier than in the experiment, resulting in an advanced second pressure peak. These differences suggest a slight overpredicted fuel consumption rate in the CFD simulation. With respect to hydrogen combustion efficiency, experimental measurements show that the unburnt hydrogen fractions at 14% and 24% HSR values are 27% and 30%, respectively, while the simulation predicts 31% and 33%. Although a slight overestimation is observed, the deviation remains within an acceptable range, demonstrating that the model well captures combustion efficiency of hydrogen under dual-fuel operation.

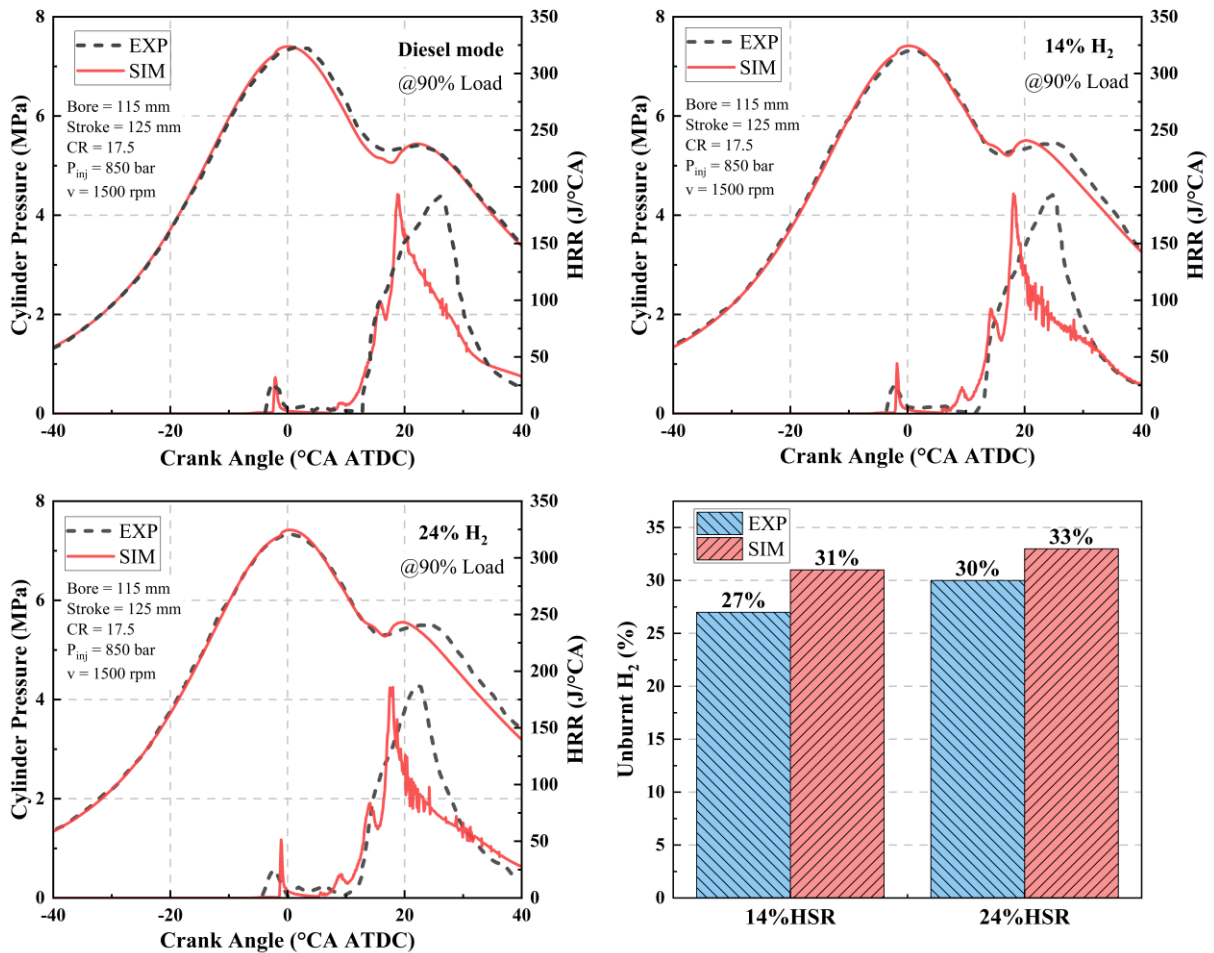


Fig. 3.7 Validation of in-cylinder pressure, HRR, and unburnt hydrogen fraction for light-duty Hydrogen-Diesel dual-fuel operation using data from Tsujimura and Suzuki [192].

The discrepancies between experimental and simulated cylinder pressure and HRR profiles can largely be attributed to modelling simplifications. Variations in piston bowl geometry between the simulated and experimental engines affect in-cylinder turbulence behaviour and local mixing processes. In addition, the adoption of a reduced chemical reaction mechanism influences reaction rate predictions, as detailed chemical kinetics is of significance in predicting ignition and combustion development. Employing a more comprehensive mechanism could further improve predictive accuracy. Another contributing factor is the in-cylinder distribution pattern of the hydrogen-air mixture. In the experiments, hydrogen is introduced through the intake valve, which may result in local stratification. In contrast, the simulations assume fully homogeneous hydrogen distribution within the cylinder, neglecting potential inhomogeneities. This assumption can influence flame propagation behaviour and heat release characteristics [193].

Across all investigated HSR conditions, deviations in peak pressure and power output are within 10%, which is generally considered acceptable for CFD-based combustion modelling [194]. Overall, the developed CFD model exhibits good capability of predicting hydrogen-diesel dual-fuel combustion behaviour.

Chapter 4 Effects of diesel injection on unburnt hydrogen emissions

This chapter focuses on the challenge of unburnt hydrogen emissions in Hydrogen-Diesel dual-fuel engines and explores the potential of diesel injection control to reduce unburnt hydrogen. To examine this issue under high-load conditions, the investigated case is set at 100% engine load with a hydrogen substitution ratio of 50%. The temperature at intake valve closing (IVC) is set to 320 K to represent low-temperature intake-air conditions.

The hydrogen substitution ratio (HSR) can be defined by Eq.4.1:

$$HSR = \frac{m_{H_2} \times LHV_{H_2}}{m_{H_2} \times LHV_{H_2} + m_{diesel} \times LHV_{diesel}} \times 100\% \quad (4.1)$$

where m_{H_2} and m_{diesel} are the mass of hydrogen and diesel, respectively; LHV_{H_2} and LHV_{diesel} are the lower heating values of hydrogen and diesel, respectively.

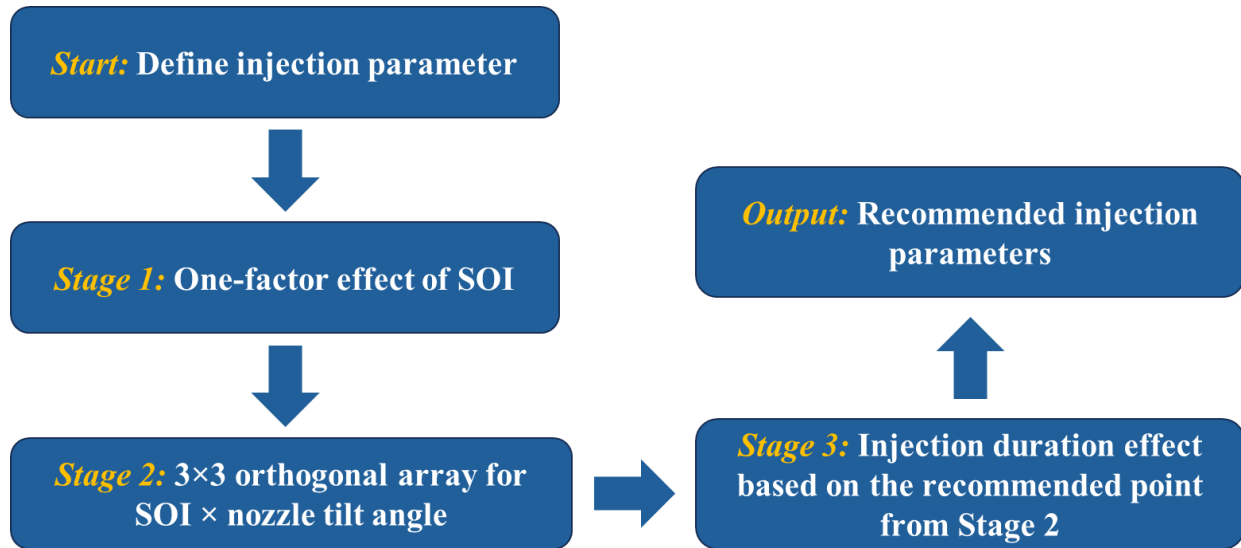


Fig. 4.1 Investigation flowchart of diesel injection effect on unburnt hydrogen emissions.

The investigation follows the flowchart presented in Fig. 4.1. Firstly, the injection parameters which may influence the mixing process are selected, including start of injection (SOI), spray tilt angle and injection duration based on literature investigation. Then, at stage 1, the effect of SOI was examined as earlier injection promotes diesel mixing. At stage 2, the coupled effect of SOI

and spray tilt angle was investigated by a 3×3 orthogonal array design of experiments (DOEs). At stage 3, the effect of injection duration was further tested at the recommended SOI and spray tilt angle obtained from stage 2. Finally, a diesel injection control point of SOI, spray tilt angle and injection duration was recommended.

To test the unburnt H₂ proportion, the residual percentage of hydrogen is defined by Eq.4.2:

$$\text{Residual Percentage of Hydrogen} = \frac{m_{H_2,Ub}}{m_{H_2}} \times 100\% \quad (4.2)$$

Where m_{H_2} is the total mass of hydrogen fuel supplied and $m_{H_2,Ub}$ is the mass of unburnt hydrogen at EVO moment.

This chapter focuses on the fuel-air interaction, combustion flow, and unburnt hydrogen fraction. The safety implications, NO_x emissions, efficiency trade-offs, and global performance parameters are not exhibited and discussed in this chapter. The combustion characteristics, performance, and emissions of Hydrogen-Diesel dual-fuel engines will be presented in the following chapters.

4.1 Effect of diesel start of injection (SOI) on residual hydrogen

Table 4.1 The injection settings of SOI effect study.

Case	SOI (°CA BTDC)	Tilt Angle (°)	Injection Duration (°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

To enhance the mixing of diesel with the H₂/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 H₂/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°CA) are studied. The injection settings are listed in Table 4.1.

Fig. 4.2 shows the percentage of residual hydrogen in the cylinder after combustion is completed, with the SOI of diesel varying from 9.5°CA to 69.5°CA BTDC. End of combustion (EOC) is defined as the crank angle when 95% of total cumulative heat release has occurred (CA95). When the SOI is set at 9.5°CA BTDC, with 50% of the hydrogen remaining unburnt at the moment the exhaust valve opens. As the SOI advances, the percentage of hydrogen initially decreases, reaching a minimum of 3% at 49.5°CA BTDC, before experiencing a slight increase. This trend suggests that earlier diesel injection allows for better fuel penetration into the hydrogen/air mixture, enhancing hydrogen ignition through diesel combustion.

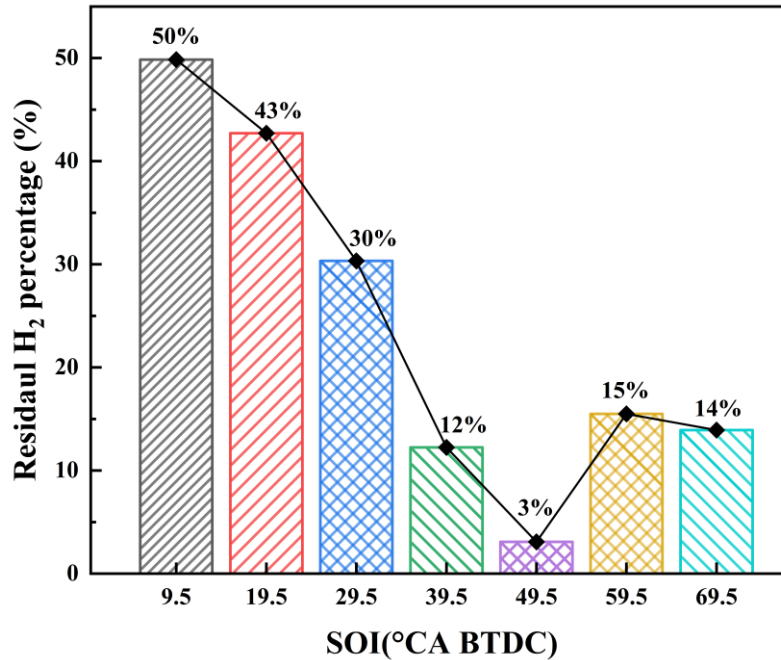


Fig. 4.2 Residual hydrogen percentage at different diesel SOI timings.

The in-cylinder flow field, which greatly impacts the mixing of fuel and air, is significantly affected by the advancement of diesel SOI. To comprehensively quantify the mixing capability of the in-cylinder flow field, three key parameters have been chosen: the swirl ratio, turbulent kinetic energy (TKE), and the magnitude of vorticity.

The swirl ratio, which is defined as the ratio of angular momentum to radial momentum in the cylinder flow field [195], describes the rotational flow characteristics of the flow field. A certain

amount of swirl is created by intake air in diesel engines to promote fuel/air mixing. Fig. 4.3 illustrates the evolution of swirl ratio with crank angle under different SOI conditions. The graph shows that as SOI advances, the in-cylinder swirl ratio initially drops slightly before increasing, reaching its highest near TDC. This behaviour can be attributed to the momentum of the injected diesel, which has a radial component rather than an angular one, temporarily reducing the swirl ratio during the injection duration. However, once combustion begins, the swirl ratio rises rapidly due to combustion propagating along the radial direction of the cylinder, which diminishes radial momentum. Besides, the swirl ratio for SOI = 49.5°CA BTDC remains sufficiently high before combustion, explaining why hydrogen combustion is more efficient compared to SOI = 59.5°CA and 69.5° CA BTDC.

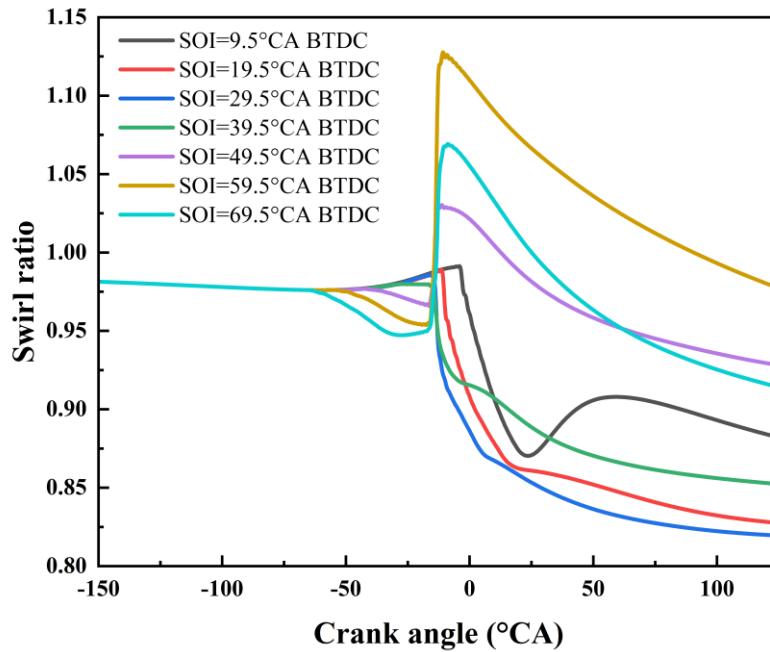


Fig. 4.3 Swirl ratio under different diesel SOI timings.

TKE is an indicator of the in-cylinder turbulence intensity, reflecting the potential for irregular motion and enhanced fuel-air mixing. The magnitude of vorticity represents the rotational strength of the flow field, and it strongly correlates with TKE. Hence, the magnitude of vorticity can also serve as an indicator of fuel-air mixing potential. Fig. 4.4 illustrates the in-cylinder TKE and the magnitude of vorticity under different diesel SOI. As the diesel SOI advances, the general trends of TKE and vorticity magnitude are pushed ahead resultantly. This is because the high-pressure diesel injection serves as the primary source of turbulence, generating numerous eddies that

contribute to an increase in vorticity. Once the injection ends, TKE gradually diminishes. The reason hydrogen combustion is most efficient at $\text{SOI} = 49.5^\circ\text{CA}$ BTDC is that, at the moment of ignition, TKE remains high, resulting in a more effective mixing of hydrogen and diesel and enhanced turbulent flame development. The strong turbulence facilitates more intense interactions between diesel and the hydrogen/air mixture, leading to more complete combustion. Subsequently, TKE rises dramatically as combustion itself generates additional turbulence, creating a feedback loop where turbulence intensity and combustion mutually enhance one another interdependently. At last, with the end of the combustion, the TKE and the magnitude of vorticity diminish eventually.

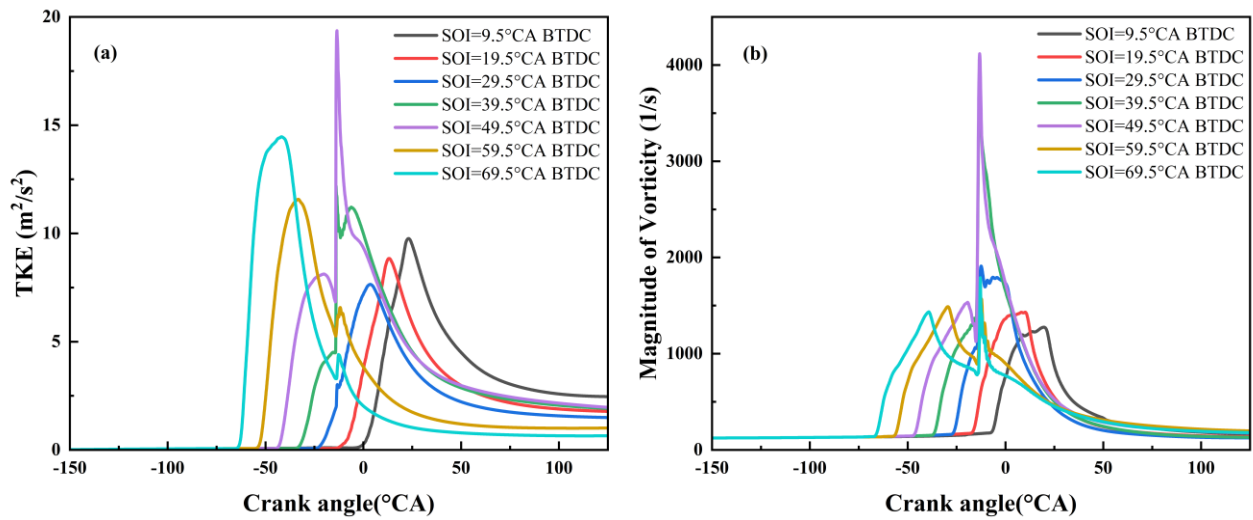


Fig. 4.4 Variation of TKE (left) and magnitude of vorticity (right) with crank angle for different diesel SOI.

Fig. 4.5 presents the equivalence ratio measured at SOC as the SOI advances. The figure shows that regions with high equivalence ratios are concentrated near the diesel spray, reflecting the distribution of diesel fuel. At $\text{SOI} = 9.5^\circ\text{CA}$, 19.5°CA , and 29.5°CA BTDC, due to the injection occurring too close to TDC, causing ignition before the diesel spray can fully expand. As a result, the diesel remains primarily concentrated near the cylinder head. Conversely, at $\text{SOI} = 59.5^\circ\text{CA}$ and 69.5°CA BTDC, the injection occurs very early, causing most of the diesel spray to be injected and accumulated around the cylinder wall. The optimal case appears at $\text{SOI} = 39.5^\circ\text{CA}$ and 49.5°CA BTDC, where the diesel spray can fully expand. Among these, $\text{SOI} = 49.5^\circ\text{CA}$ BTDC demonstrates better mixing due to its earlier injection timing. This evidence proves that, before

combustion, the $\text{SOI} = 49.5^\circ\text{CA BTDC}$ case achieves the best fuel-air mixing among all tested conditions.

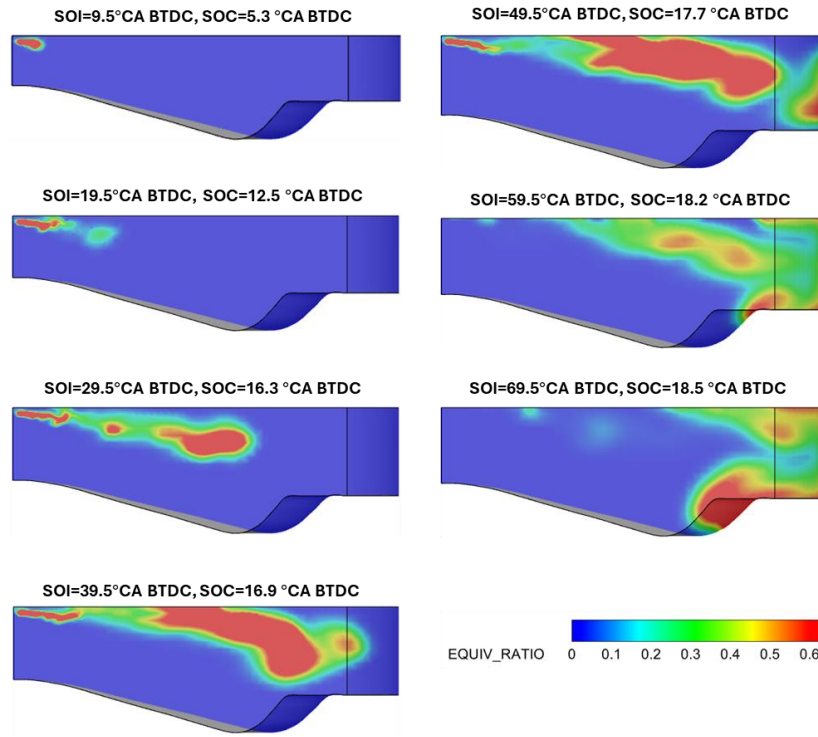


Fig. 4.5 Equivalence ratio distribution at the start of combustion (SOC) for different SOI timings.

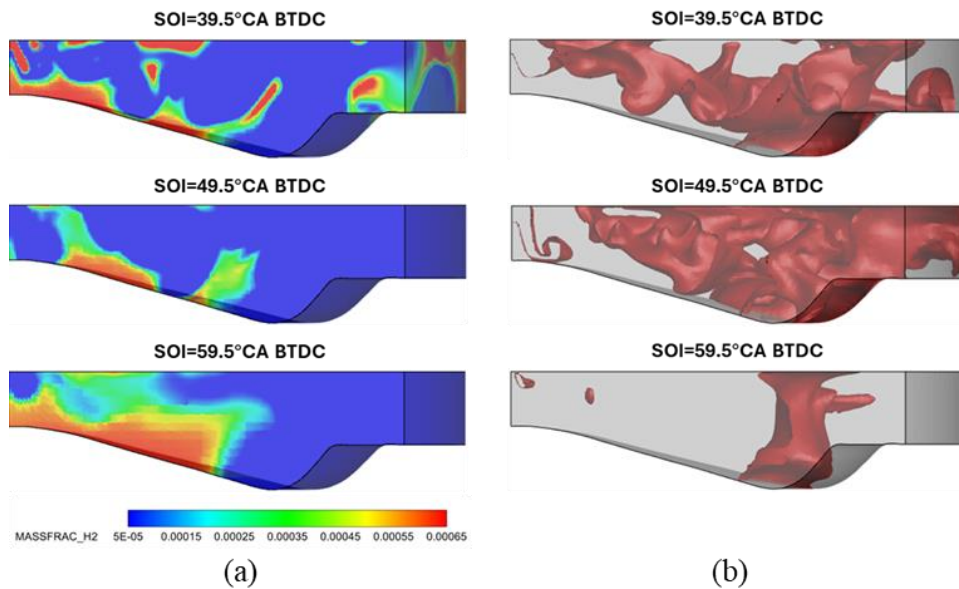


Fig. 4.6 In-cylinder conditions at TDC for different SOI cases: (a) unburnt H_2 mass fraction, (b) $1,500\text{ K}$ isothermal surface.

Due to the early injection of diesel and rapid heat release of hydrogen, combustion is nearly complete by TDC. Fig. 4.6 (a) presents the unburnt hydrogen mass fraction at TDC for different SOI cases, showing that unburnt hydrogen accumulates around the inner rim of the piston's upper edge. Fig. 4.6 (b) displays the 1,500K isothermal surface at TDC for different SOI conditions, revealing that the isothermal surface closely mirrors the distribution of the unburnt hydrogen gas. This occurs because the flame is quenched as it tries to reach the hydrogen near the combustion chamber wall. The primary reasons are the lower temperature of the combustion chamber wall and the significant distance between the diesel spray and the combustion chamber wall.

4.2 Coupled effect of SOI and spray tilt angle

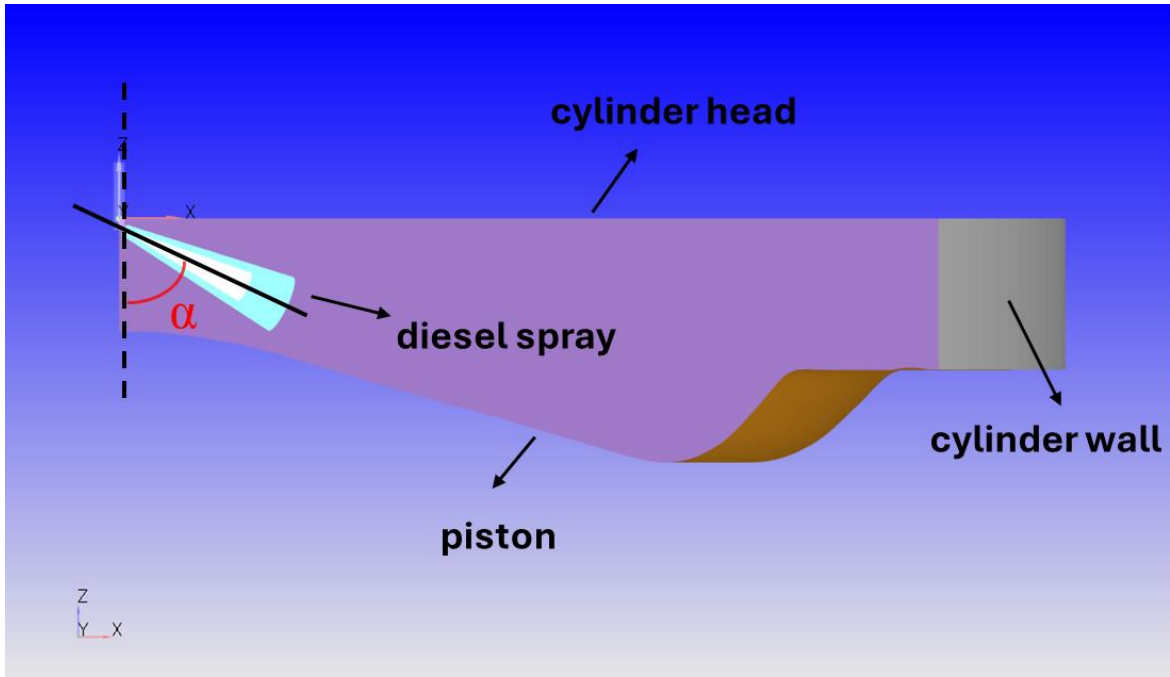


Fig. 4.7 Schematic diagram of spray tilt angle, α .

In Section 4.1, it was observed that unburnt hydrogen accumulates at the inner rim of the piston's upper surface. To further ignite the remaining unburnt hydrogen, the inferable method is to direct the diesel spray to its neighbourhood region. Without increasing the injection pressure, changing the spray tilt angle α , as shown in Fig. 4.7, can alter the trajectory of the diesel spray. The original spray tilt angle is set to 75.5° . The presence of curved ridges in the combustion chamber helps diffuse the diesel spray, utilizing the momentum of the diesel and the reaction force from the cylinder wall to improve mixing. Additionally, the timing of the SOI influences whether the diesel

spray reaches these curved ridges. To explore the combined effect of SOI and spray tilt angle, a series of 3×3 orthogonal experiments is designed, as listed in Table 4.2. A total of nine cases are considered, with three different SOIs (39.5°CA, 49.5°CA, 59.5°CA BTDC) and spray tilt angles (55.5°, 65.5°, 75.5°). Based on the observations from the previous section, where SOI= 49.5°CA BTDC left the least hydrogen unburnt, therefore, the SOI values of 39.5°CA and 59.5°CA BTDC are also chosen to assess whether there is a more optimal condition. Additionally, the spray tilt angle is decreased from the previous 75.5° to 65.5° or 55.5°, as the equivalence ratio distribution in Fig. 4.5 suggests that reducing the tilt angle may direct the spray toward the curved ridge more effectively.

Table 4.2 Nine orthogonal experimental cases considered.

Case	SOI (°CA BTDC)	α (°)
1	39.5	75.5
2	39.5	65.5
3	39.5	55.5
4	49.5	75.5
5	49.5	65.5
6	49.5	55.5
7	59.5	75.5
8	59.5	65.5
9	59.5	55.5

Fig. 4.8 depicts the residual percentage of hydrogen in the cylinder, highlighting the combined effects of SOI and spray tilt angle. As shown, at SOI = 39.5°CA BTDC, reducing the spray tilt angle initially increases the residual hydrogen percentage by 2%, followed by a 3% decrease, showing a trend similar to that observed at SOI = 49.5°CA BTDC. At SOI = 59.5°CA BTDC, the residual hydrogen percentage initially decreases by 4%, then remains constant. Notably, even if the spray tilt angle changes, the hydrogen residual percentage at SOI = 49.5°CA BTDC remains the lowest, confirming the findings from the previous section. The lowest residual hydrogen

percentage is observed at $\text{SOI} = 49.5^\circ\text{CA BTDC}$ and a spray tilt angle of 55.5° , reducing the previous best value of 3% to 2%. This improvement suggests that reducing the spray tilt angle enhances hydrogen consumption, likely due to the influence of the cylinder wall's force, which alters the movement of the diesel spray.

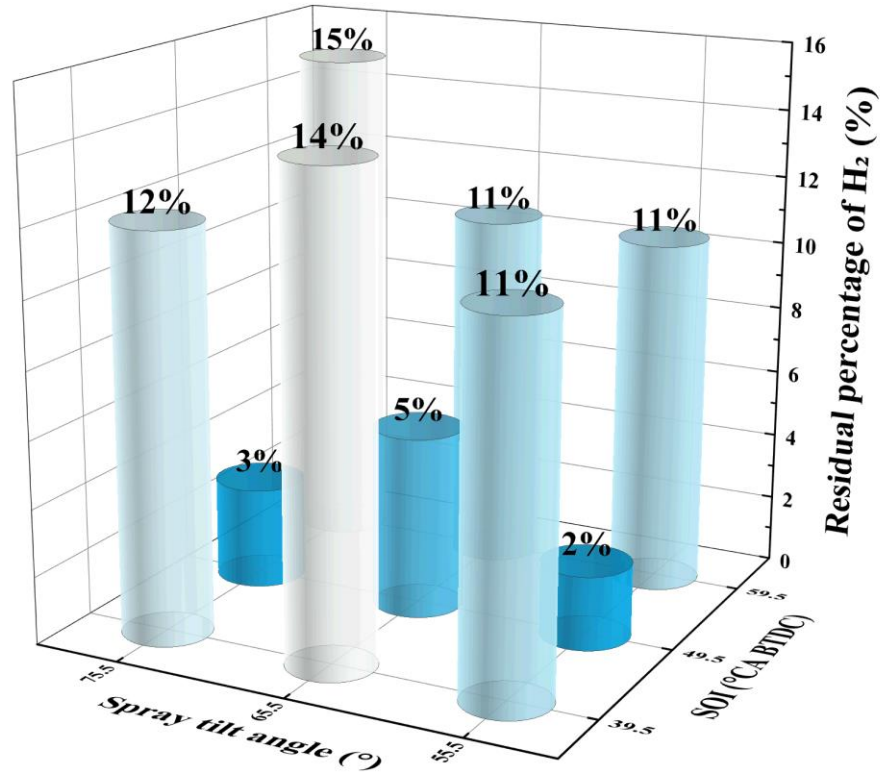


Fig. 4.8 Combined effect of SOI and spray tilt angle on the residual percentage of H_2 .

Fig. 4.9 shows the hydrogen consumption process from -15° to 2°CA for case 6, which displays minimal unburnt H_2 . The combustion of hydrogen starts from the concave depression of the piston bowl and subsequently spreads towards the cylinder head. A small amount of hydrogen remains near the middle and outer regions near the cylinder head by the end of the process.

This phenomenon coincides with the evaporation and ignition of the diesel spray. When low-temperature fuel is injected into the high-temperature air environment, the diesel spray penetrates further, causing a significant amount of air/hydrogen to mix with the diesel. As the diesel heats up and evaporates, it forms an outer sheath of vapour/air and hydrogen mixture, which surrounds the front and outer region of the diesel spray. Consequently, the downstream portion of the diesel spray creates a well-mixed zone of gaseous diesel and the air/hydrogen mixture. Premixed combustion

of diesel then begins in this well-mixed zone due to the optimal mixing of diesel and air. Following this, the combustion diffusion process begins and gradually progresses towards the inner part of the combustion chamber, as the premixed combustion intensifies its interaction with the cylinder wall, generating complex turbulent vortices.

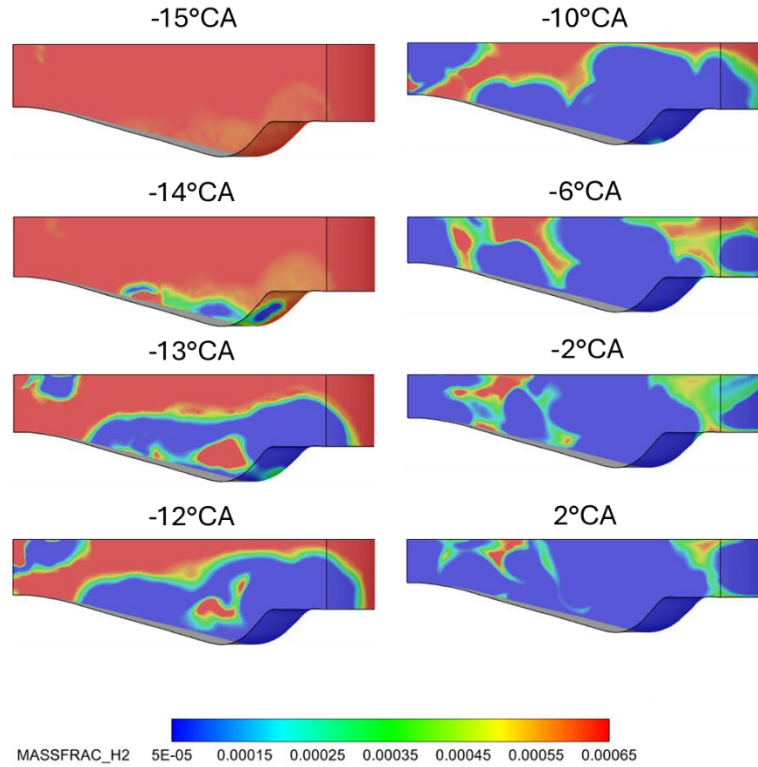


Fig. 4.9 Hydrogen consumption process at different crank angles (CA) in Case 6.

Equivalence ratio distribution can show the process of diesel injection and consumption clearly. Fig. 4.10 illustrates the equivalence ratio distribution after the diesel injection for case 6, clearly showing the diesel/air mixture dynamics. It can be observed that at -30°CA and -20°CA , the diesel is initially injected directly into the piston's curved ridge. As the crank angle progresses, the diesel gradually moves towards the centre of the piston. Between -16°CA and -15°CA , the green band area expands, indicating the onset of premixed combustion, which begins to consume the diesel in this region. At -13°CA , the diesel-rich region grows larger as diesel is injected onto the cylinder wall, forming wall jets that distribute near the impingement point, where the high-temperature piston surface generates significant diesel vapor. Following this, due to the diffusion combustion turbulence, the diesel mixture spreads towards the upper and inner areas near the cylinder head,

aided by the reflection force of the cylinder wall. Additionally, the turbulence generated by the diesel spray head during premixed combustion further promotes the diffusion process.

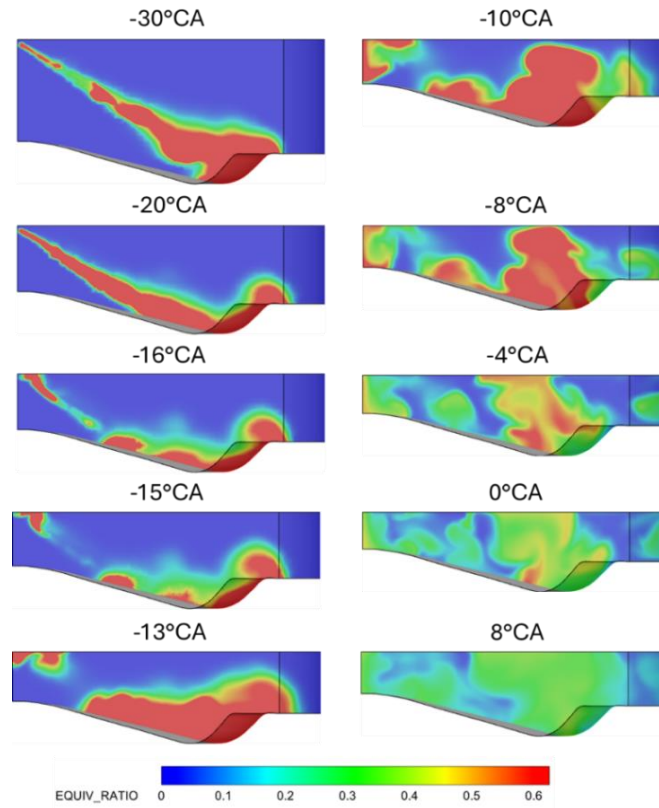


Fig. 4.10 Post-SOI equivalence ratio distribution (Case 6)

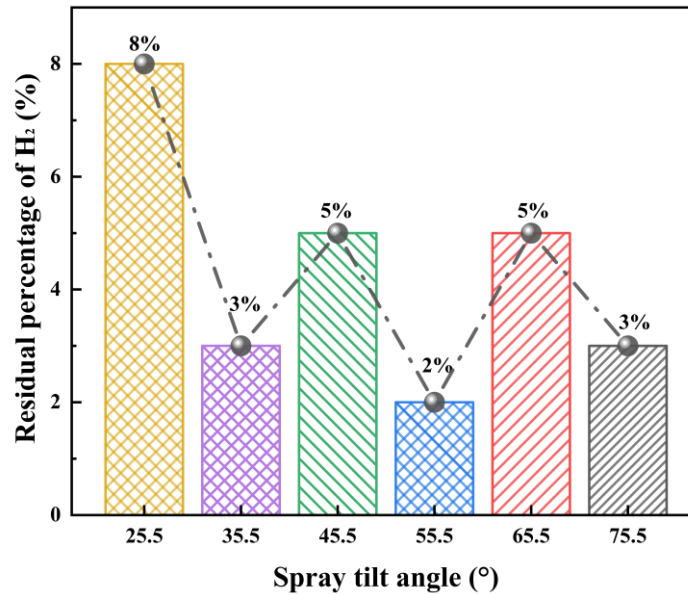


Fig. 4.11 H₂ residual percentage for different spray tilt angles (SOI = 49.5°CA BTDC)

As observed in the previous sections, an SOI of 49.5°CA BTDC was identified as the optimal timing for diesel injection, as it results in the least amount of unburnt hydrogen in the cylinder. However, only 3 different spray tilt angles - 55.5°, 65.5°, and 75.5° - are tested, which may not provide a comprehensive conclusion. To explore the possibility of further improvement, additional cases with smaller spray tilt angles of 45.5°, 35.5°, and 25.5° were investigated. Fig. 4.11 shows that the case with a 55.5° tilt angle continues to yield the lowest hydrogen residual (2%) in the cylinder, despite testing smaller angles. Therefore, the subsequent optimisation of injection will be based on this case. This outcome may be attributed to variations in spray-wall impingement locations under different spray tilt angle conditions, which can have a significant impact on subsequent combustion behaviour and fuel diffusion.

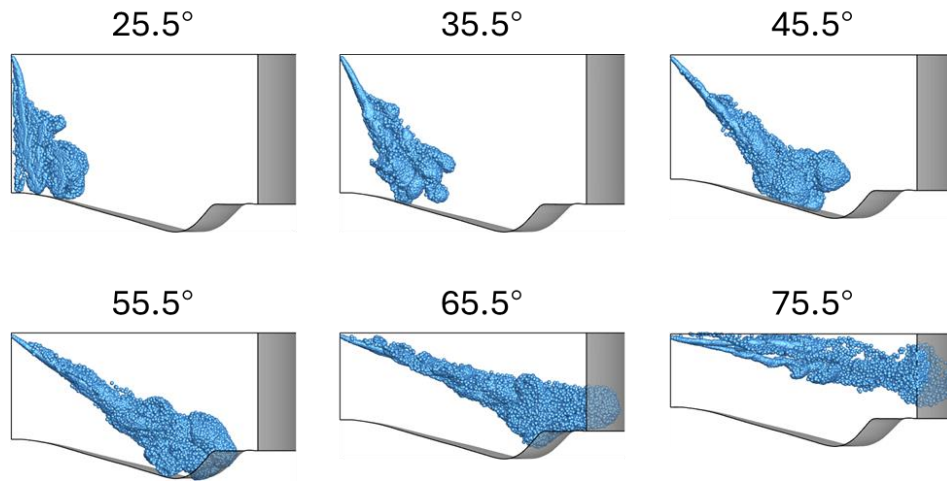


Fig. 4.12 Schematic diagram showing spray-wall impingement locations under different spray tilt angle conditions.

Due to the high-pressure nature of diesel injection, the spray exhibits a significant penetration distance, making spray-wall impingement inevitable. Fig. 4.12 shows how spray-wall impingement locations vary with different spray tilt angles. As the spray tilt angle increases, the impingement locations shift progressively from the centre of the piston crown to the crown bottom, then to the curved ridge of the piston crown, and finally to the cylinder wall. In terms of spray morphology, an increase in tilt angle causes the diesel spray, at the moment of wall impingement, to transition from a short and wide shape at lower angles (e.g., 25.5°) to a narrower and more elongated form at higher angles (e.g., 75.5°). At a tilt angle of 25.5°, the spray is nearly vertical, leading to earlier wall impingement during the compression stroke. As the tilt angle increases, the

vertical velocity component of the spray decreases, delaying the compression stroke. This extended development time provides the rationale for the elongation of the diesel spray and, subsequently, the spray penetration.

Referring to Fig. 4.11, the minimum residual hydrogen fraction is observed when the spray tilt angle is 55.5° . This occurs because, under this configuration, the diesel spray impinges the wall precisely at the inner edge of the curved ridge, with the midline of the high-pressure diesel spray nearly perpendicular to the plane of the curved ridge's inner edge. This orientation enhances the wall jet effect generated by interactive forces, along with the force generated by the upward movement of the piston and the turbulence generated by diffusion combustion, causing the diesel spray to expand around and disperse towards the flame non-propagation zone at the cylinder top. Additionally, the interaction with the high-temperature piston surface enhances the vaporization effect because the curved surface enlarges the contact area by the wall jet effect. The resulting increase in diesel vapour, along with better diesel spray penetration, explains why the combustion of hydrogen at a spray tilt angle of 55.5° is more complete compared to other angles.

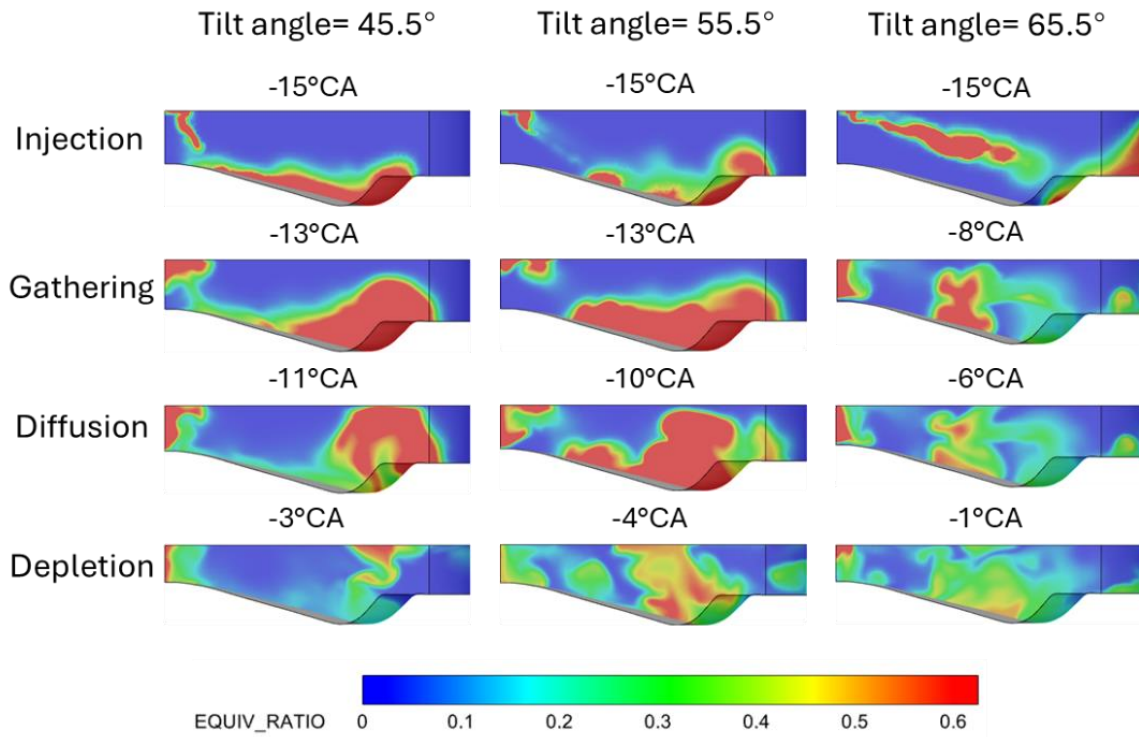


Fig. 4.13 Equivalence ratio distribution evolution process for varying spray tilt angles (SOI = 49.5°).

When the tilt angle is less than 55.5° , the penetration distance is limited, reducing coverage and vapour formation. Conversely, at angles greater than 55.5° , part of the spray strikes the relatively cooler cylinder wall rather than the hotter piston head, weakening vaporization despite the increased penetration distance. Ultimately, the location of spray-wall impingement plays a crucial role in determining the evaporation rate and the fuel distribution within the combustion chamber. The turbulence generated during diffusion combustion transports diesel vapour throughout the cylinder, and the specific locations it reaches influence flame propagation, and, in turn, the overall completeness of hydrogen combustion within the cylinder.

Fig. 4.13 illustrates the equivalence ratio distribution evolution process for various spray tilt angles at an SOI of 49.5°CA BTDC. The evolution process can be categorised into four distinct stages: the injection, the gathering, the diffusion, and the depletion - each represented by a column in the diagram.

- At a spray tilt angle of 45.5° , the diesel is injected toward the bottom of the piston bowl at -15°CA and accumulates there by -13°CA . Then, the diffusion combustion turbulence, along with the reflection force from the piston bowl bottom wall, pushes the diesel vapour upward vertically at -11°CA . The diesel is consumed completely by -3°CA .
- At a tilt angle of 55.5° , the diesel is injected into the outer sidewall of the piston bowl at -15°CA and forms a wall jet by -13°CA . As a result, the diesel vapour region becomes wider. Subsequent diffusion combustion, turbulence, and the reflection force from the sidewall of the piston bowl drive the vapour inward at approximately a 45° angle – vertical to the outer sidewall of the piston bowl – by -10°CA . Eventually, the combustion completes by -4°CA .
- With a tilt angle of 65.5° , the diesel is injected at the corner, between the cylinder wall and piston, at -15°CA . After the injection is finished, part of the diesel gathers at the inner sidewall of the piston bowl at -8°CA . Reflection and turbulence then push the vapor outward at a 45° angle – vertical to the inner sidewall of the piston bowl – at -8°CA , most of the diesel is consumed by -1°CA .

In summary, the spray tilt angle decides the diesel's accumulation zone, while the geometry and orientation of the wall at that zone govern both the quantity of diesel gathered and the direction of its diffusion.

4.3 Effect of injection duration

By keeping the diesel SOI and total fuel injection quantity constant, altering the duration of injection inherently affects the injection pressure and the end timing of injection. These changes influence the air-fuel mixing condition within the cylinder. The description of investigated cases is summarized in Table 4.3.

Table 4.3 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

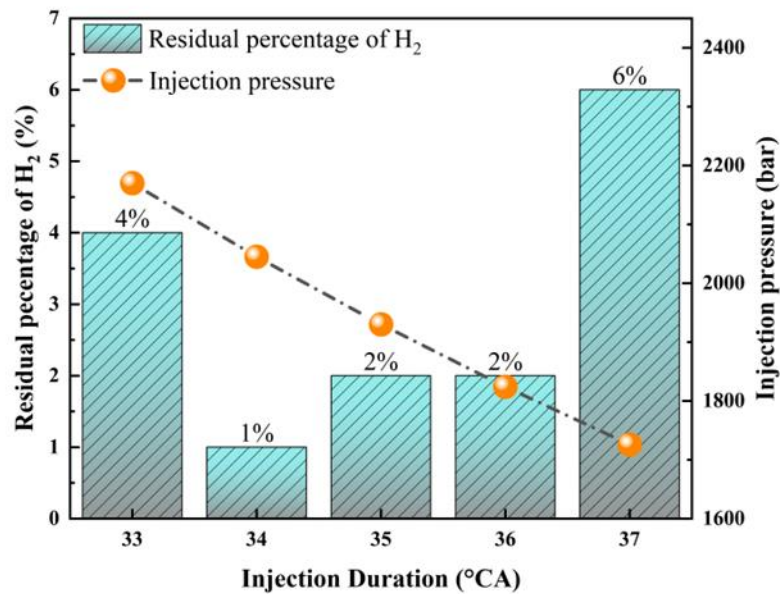


Fig. 4.14 H₂ residual percentage under different injection durations.

Fig. 4.14 depicts the residual H₂ under different injection durations, all under the previously optimised conditions of SOI = 49.5°CA BTDC and spray tilt angle = 55.5°CA. The injection

pressure decreases linearly as the duration of injection is prolonged because the injected fuel quantity remains constant.

As the injection duration increases, the residual percentage of H_2 initially decreases from 4% to a minimum of 1% at 34°CA , before slightly rising to 2% and remaining unchanged at 36°CA . At 37°CA , a sharp increase to 6% is observed. The injection duration of 34°CA yields the lowest unburnt H_2 fraction (1%), improving upon the previous best of 2%. This demonstrates that optimizing the injection duration can significantly lower the residual percentage of H_2 .

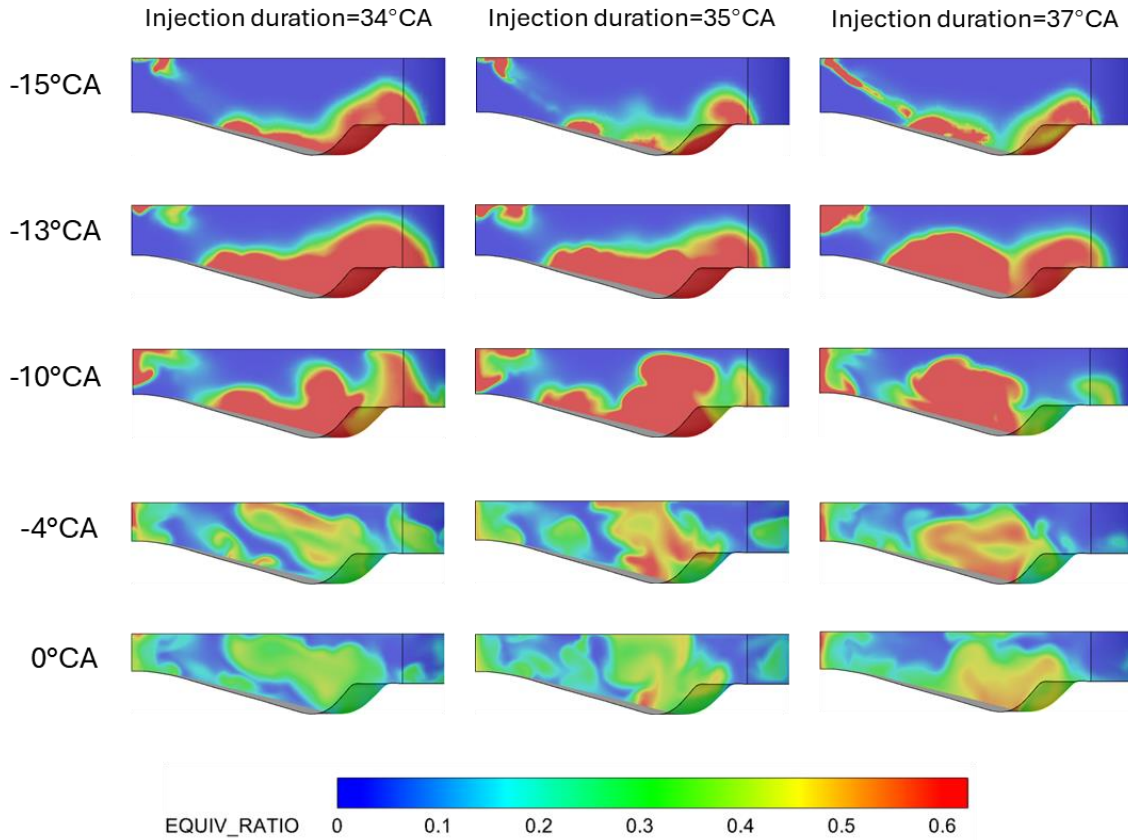


Fig. 4.15 Equivalence ratio distribution over time for different injection durations.

Fig. 4.15 illustrates the evolution of equivalence ratio distribution under different injection durations, focusing on the key stages of gathering and diffusion, as defined earlier (injection, gathering, diffusion, and depletion). When the injection duration is 34°CA , diesel first accumulates around the piston bowl between -15°CA and -13°CA , followed by the diffusion starting at -10°CA . At -4°CA , the diffusion direction is predominantly inward. For injection durations of 35°CA and

37°C A, the evolution process is similar to the 34°C A case; however, the primary locations of diesel vapor diffusion differ at -10°C A. In the 34°C A case, the diesel vapour cloud is concentrated near the outer sidewall of the piston wall. In the 35°C A case, the cloud shifts slightly lower, while in the 37°C A case, the cloud moves significantly inward, gathering along the inner sidewall of the piston bowl. These differences in the main diffusion of the diesel vapour cloud's locations influence the subsequent diffusion directions. For example, the 34°C A case exhibits a more horizontal inward diffusion path – allowing the flame to propagate further toward the cylinder centre, improving the combustion of hydrogen in regions typically harder to ignite. In contrast, the injection duration of 37°C A shows a more vertical diffusion trajectory, which is less effective in targeting the central flame non-propagation zone of the cylinder, explaining the higher H₂ residual percentage observed.

In summary, changes in injection duration and the resulting injection pressure shift the aggregation location of the main diesel vapour cloud. Coupled with the piston's complex geometry, this shift alters the diffusion direction of the vapor cloud, ultimately influencing whether hydrogen in difficult-to-reach areas is successfully ignited and consumed.

4.4 Critical discussion

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

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 unburnt. 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 unburnt 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, 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 application of precise diesel fuel control strategies may lead to increased upfront investment, particularly in engine hardware and control systems.

4. *Safety impact:* Although hydrogen is not a direct greenhouse gas, its release into the atmosphere may have indirect climate effects. More importantly from an onboard safety perspective, hydrogen leakage into confined or semi-enclosed spaces on 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.

4.5 Summary

In this chapter, numerical investigations were conducted to explore the optimal diesel injection strategies to realize the potential of more complete H_2 combustion in a hydrogen/diesel dual-fuel marine medium-speed engine. The injection parameters, including SOI, spray tilt angle, and injection duration, were analysed individually and jointly to reduce the residual proportion of hydrogen. The main findings of the chapter are as follows:

1. *Optimal SOI Timing:* The early injection strategy can effectively reduce the unburnt H_2 proportion. However, the SOI cannot be too early. When $SOI = 49.5^\circ CA$ BTDC, the unburnt H_2 percentage is lowest; it reduces from 50% to 3% compared to the original $SOI = 9.5^\circ CA$ BTDC. Part of H_2 is left unburnt because the flame quenches before it can reach the distant low-temperature combustion chamber wall.

2. *Effect of Spray Tilt Angle:* Changing the spray tilt angle can further reduce the unburnt H_2 proportion. When the spray tilt angle is altered, the optimal SOI remains unchanged. When the tilt angle decreases from 75.5° to 55.5° , the unburnt H_2 percentage drops from 3% to 2%, resulting in a 33.3% improvement. The optimal SOI remains at $49.5^\circ CA$ BTDC. This is attributed to the

positive influence on diesel diffusion combustion brought by the better spray-wall impingement location. This positive impact is reflected in the diesel vapor diffusion directions.

3. *Spray-Wall Interaction & Diffusion Dynamics*: The spray tilt angle influences where diesel gathers and in which direction it diffuses after injection. At 55.5° , the diesel spray forms an efficient wall jet, directing vapor inward and upward, helping flames reach the central flame non-propagation zone to consume trapped hydrogen more effectively.

4. *Injection Duration Effect*: Altering the duration of injection can facilitate a more complete combustion of H_2 . The best performance was achieved at $34^\circ CA$ duration, where unburnt H_2 was reduced to just 1%—lower than the previous best of 2%, resulting in a 50% improvement, effectively enhancing the energy conversion efficiency. The impact of altering the duration of injection on diesel diffusion is reflected in the position of the primary diesel diffusion cloud. A strategic position will direct diesel diffusion towards the far end of the ignition source, thereby igniting hydrogen that is more challenging to ignite.

5. *Equivalence Ratio Distribution Analysis*: The evolution of equivalence ratio distribution revealed that diesel vapor cloud behaviour and interaction with piston geometry significantly influence the completeness of hydrogen combustion. Proper alignment of spray direction with piston bowl contours enhances vaporization and flame propagation.

In summary, optimizing diesel injection strategies can effectively reduce the fraction of unburnt hydrogen, thereby increasing fuel conversion efficiency and lowering safety risks for ships. This provides a viable solution for the utilization of hydrogen in marine medium-speed engines. However, the hydrogen substitution effect on combustion and emission characteristics haven't been sufficiently understood. Hence, the following chapter will focus on this issue.

Chapter 5 Knocking suppression via direct water injection at high HSRs

The combustion and emission characteristics of hydrogen substitution remain insufficiently understood and operation with high hydrogen substitution ratio faces knocking risks. This chapter therefore explores the combustion and emission characteristics under hydrogen substitution and the feasibility of achieving stable dual-fuel combustion at high hydrogen substitution ratios through in-cylinder direct water injection. Two knocking-free strategies are investigated: low hydrogen substitution ratios (0–40%) without water injection and high hydrogen substitution ratios (90 and 95%) with water injection.

5.1 Water injection modelling and parameter definition

5.1.1 Water injection modelling

Table 5.1 The main parameters of water injection modelling.

Water injection parameter	Value
Orifices number	6
Orifice diameter (mm)	1.2
Spray cone angle (°)	10
Spray tilt angle (°)	45
Injection duration (°CA)	30
Injection pressure (bar)	250
Temperature (K)	300

In this chapter, the in-cylinder direct water injection is adopted, whereas the main parameters are presented in Table 5.1. The direct water injection schematic is shown in Fig. 5.1. For each cylinder, there are 12 diesel orifices and 6 water orifices for injection. Since this is a 60° sector model, the water injection orifice is located between the two diesel orifices. The water spray is oriented at a tilt angle of 45°, for which previous direct water injection studies have reported favourable in-

cylinder water distribution [164]. The injection pressure for water was set to 250 bar, within the 200–400 bar range reported for marine direct water injection systems by Wärtsilä [196], to provide sufficient atomization and spray penetration within the cylinder. The injection duration was specified as 30° crank angle, considering injection durations of approximately $20\text{--}40^\circ\text{CA}$ adopted in previous water injection studies on hydrogen-fuelled engines [197]. This duration allows the water spray to develop fully and interact effectively with the in-cylinder flow field, while maintaining sufficient time separation from the subsequent diesel injection.

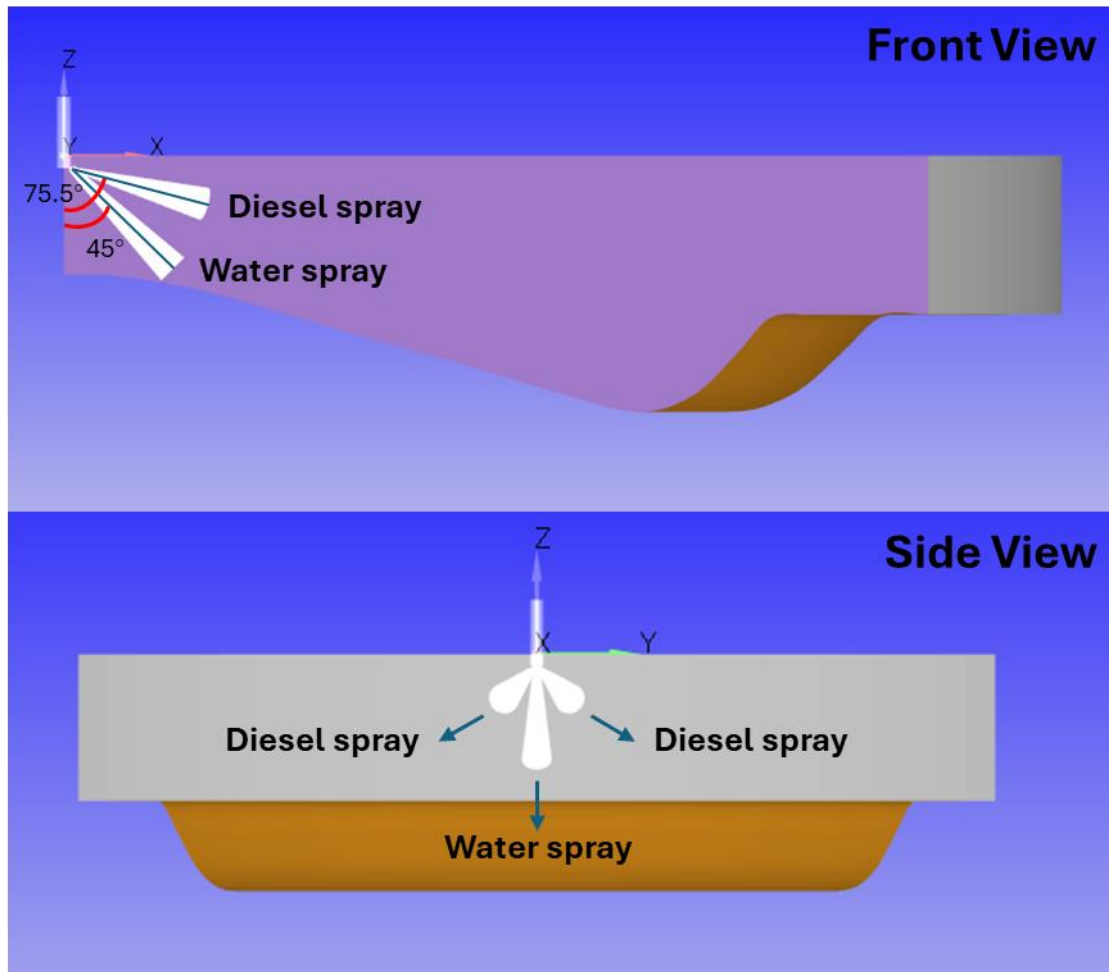


Fig. 5.1 The schematic diagram of in-cylinder direct water injection.

5.1.2 Parameter definition

In this study, knocking is defined as excessively rapid heat release resulting from overly rapid combustion. To quantify knocking and determine the maximum HRR that avoids knocking, the

concept of Ringing Intensity (RI) has been introduced. The RI is calculated by using the equation given below [198]:

$$RI = \frac{\sqrt{\gamma R T_{\max}}}{2\gamma P_{\max}} \left[\beta \left(\frac{dP}{dt} \right)_{\max} \right]^2 \quad (5.1)$$

In which, γ is the ratio of specific heat, R is the gas constant, $T_{\max}$ is the maximum cylinder temperature, $P_{\max}$ represents the maximum cylinder pressure, β is an empirically scaling coefficient which relates the oscillations and the rise rate of pressure (in this study β is set as 0.05, a value that has been widely adopted in relevant studies [199,200]), $\left(\frac{dP}{dt} \right)$ is cylinder pressure rise rate.

In four-stroke marine medium-speed engines, the upper limit of Ringing Intensity (RI) is typically within the range of 4–5 MW/m². Exceeding this threshold leads to an increase in the intensity of roar combustion, which can eventually cause knocking. Following Han et al. [201] and Karvounis et al. [202], an operational limit of 4 MW/m² is adopted as the threshold in this study.

Water-to-Fuel Ratio (W/F) is defined to measure the mass of water injection. The W/F is calculated by the equation below:

$$W/F = \frac{m_{\text{water}}}{m_{\text{fuel-eqv}}} \quad (5.2)$$

where m_{water} is the mass of injected water and $m_{\text{fuel-eqv}}$ is the equivalent fuel mass calculated by Eq.5.3.

$$m_{\text{fuel-eqv}} = \frac{m_{H_2} \times LHV_{H_2} + m_{\text{diesel}} \times LHV_{\text{diesel}}}{LHV_{\text{diesel}}} \quad (5.3)$$

Indicated thermal efficiency (ITE) is defined as the ratio of the indicated work output to the total chemical energy supplied by hydrogen and diesel, as shown in Eq.5.4.

$$ITE = \frac{W_i}{m_{H_2} LHV_{H_2} + m_{\text{diesel}} LHV_{\text{diesel}}} \quad (5.4)$$

where m_{H_2} and m_{diesel} are the mass of hydrogen and diesel, respectively; LHV_{H_2} and LHV_{diesel} are the lower heating values of hydrogen and diesel, respectively.

5.2 Case studies description

Previous study by the author [171] has shown that the initial temperature significantly affects the combustion efficiency of hydrogen. Therefore, to ensure that most hydrogen can be burned, the following case studies use an initial temperature of 370 K.

5.2.1 Low HSRs without water injection

To investigate the effects of hydrogen substitution, a series of cases were conducted with hydrogen substitution ratios (HSRs) ranging from 0% to 40%. This study aims to identify the maximum hydrogen substitution ratio that can be achieved without inducing engine knocking, in the absence of any knocking-suppressing measures such as water injection.

5.2.2 High HSRs with water injection

Due to hydrogen's rapid heat release characteristics, the hydrogen substitution ratio (HSR) is typically limited. The application of water injection at an HSR greater than 90% has been rarely investigated. In this study, the effect of water injection on the suppression of engine knocking under high HSR conditions is comprehensively considered.

As shown in the design of experiments (DOE) matrix in Fig. 5.2, a set of 30 ($2 \times 5 \times 3$) DOEs was developed, incorporating three critical factors: hydrogen substitution ratio (HSR), water injection (WI) timing, and water-to-fuel (W/F) ratio. To evaluate whether high hydrogen substitution ratios (HSRs) can achieve stable combustion through the suppression of detonation by water injection (WI), HSR levels of 90% and 95% were selected to represent high HSRs. Furthermore, since stable combustion is typically easier to achieve when WI is completed prior to diesel injection, the WI timing was chosen within the range of -40 to -160 °CA ATDC, in increments of 30 °CA. This range covers the entire interval from the intake valve closing (IVC) to the start of diesel injection (SOI). Additionally, three levels of the water-to-fuel (W/F) ratio (1.5, 2, and 2.5) were selected to represent low, medium, and high water injection mass levels. This range is commonly employed in diesel-hydrogen dual-fuel water injection systems. The summary of water injection factors are their values are listed in Table 5.2.

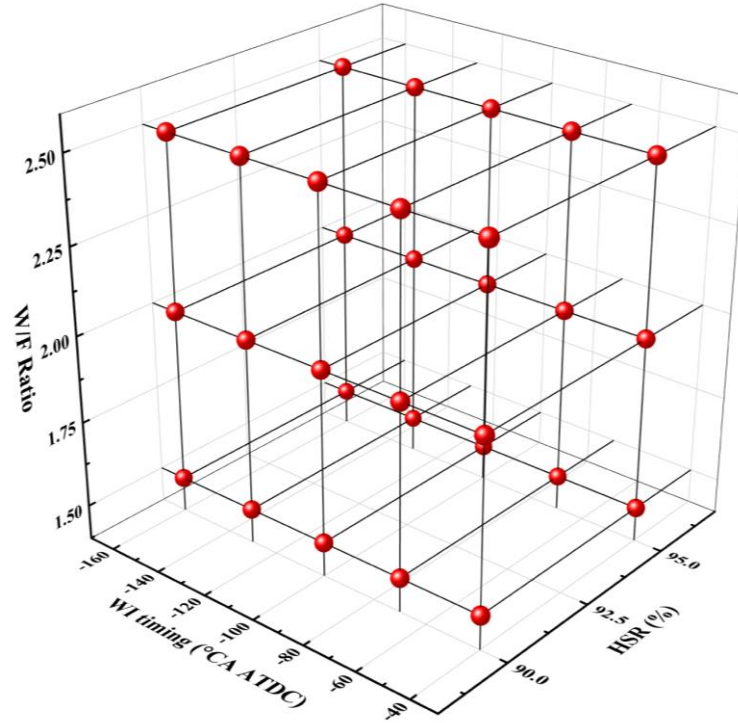


Fig. 5.2 The DOEs matrix of water injection factors.

Table 5.2 Summary of water injection control factors and values.

Factor	Unit	Values
WI timing	°CA ATDC	-160, -130, -100, -70, -40
W/F ratio	-	1.5, 2.0, 2.5
HSR	%	90, 95

5.3 Hydrogen substitution ratio effect (0-40%)

5.3.1 Combustion characteristics

Fig. 5.3 shows the calculated cylinder pressure and heat release rate (HRR) of pure-diesel mode and hydrogen/diesel dual-fuel mode with HSR ranging from 0 to 40%. It can be seen from Fig. 5.3 (a) that as HSR increases, the cylinder peak pressure gradually rises. This is because the hydrogen burning velocity is an order of magnitude higher than diesel, resulting in rapid combustion, yielding increased peak pressure. For 40% HSR, hydrogen premixed combustion yields intensive

and concentrated heat release, resulting in unstable operation. Additionally, the maximum rate of pressure rise (PRR_{max}) increases with HSR, as shown in Fig. 5.4. Notably, the pressure rise rate (PRR) shows a significant and substantial increase from 30% HSR. This can be attributed to the faster flame propagation and increased combustion concentration, which lead to a higher heat release rate per crank angle and result in a steeper pressure rise curve. At HSRs of 30% and above, the hydrogen proportion becomes sufficient to significantly alter the overall combustion process, leading to a noticeable increase in PRR_{max} .

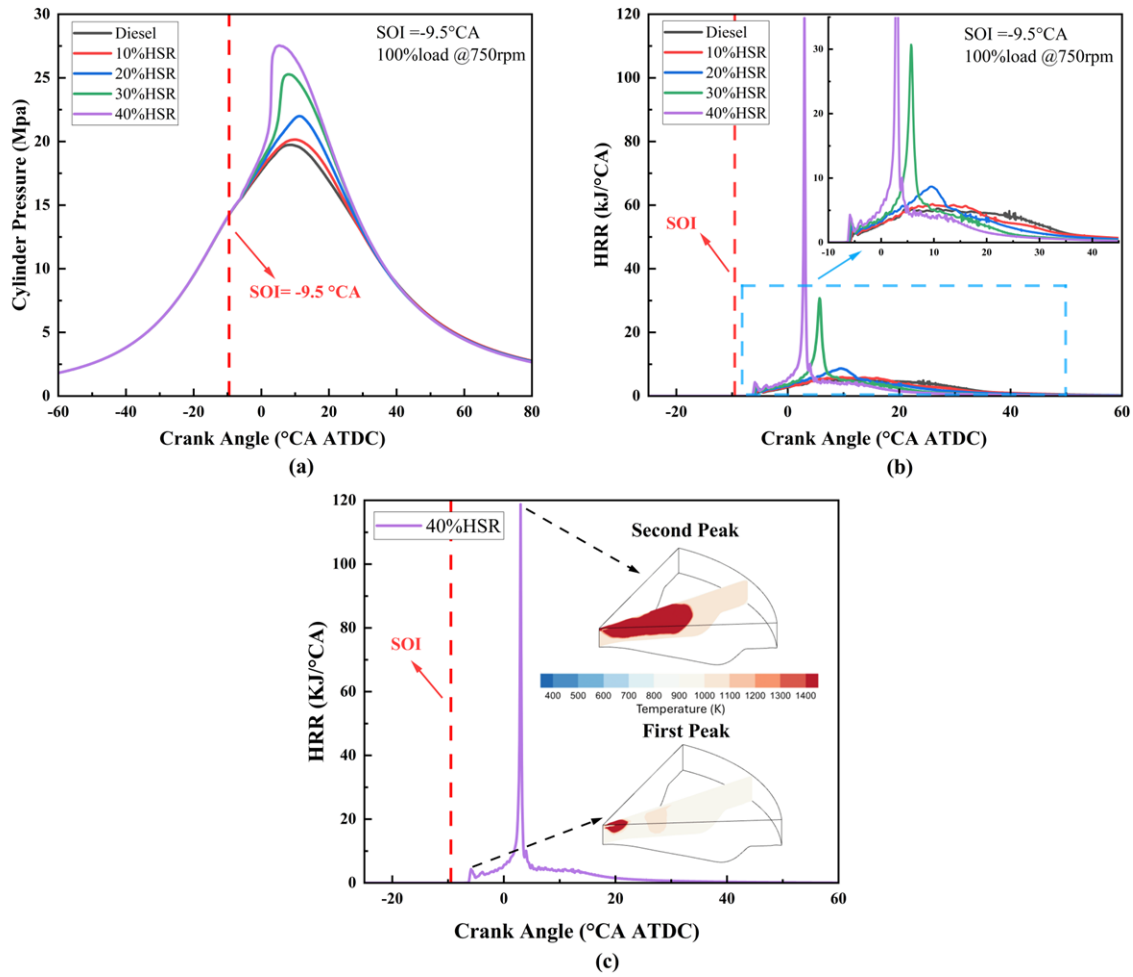


Fig. 5.3 Cylinder pressure and heat release rate with HSR varying from 0% to 40%.

As illustrated in Fig. 5.3 (b), the HRRs exhibit a two-peak shape from pure diesel mode to dual-fuel mode, with the first peak being notably shorter. Diesel combustion is characterised by a small premixed part pertinent to the air-fuel mixture formed between the start of injection and the start of combustion, and a diffusive part. Conversely, in the dual-fuel operation, hydrogen has formed

a homogeneous mixture with air in the cylinder, and hence, as HSR increases, the combustion is premixed-dominated.

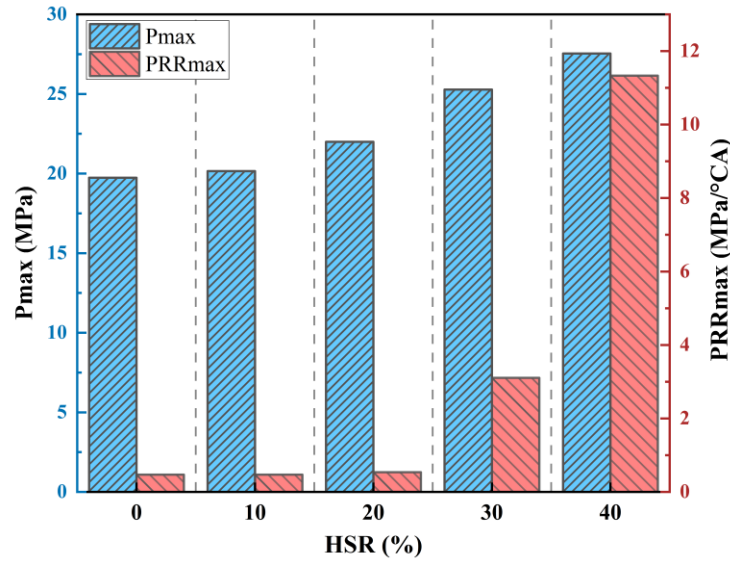


Fig. 5.4 Peak in-cylinder pressure and maximum pressure rising rate with varying HSR.

According to Karim's dual-fuel theory [203], the heat release process of dual-fuel engine combustion can be divided into three overlappable stages: (I) the combustion of pilot fuel; (II) The combustion of pilot fuel and gaseous fuel near the ignition point; (III) Turbulent flame propagation in gaseous fuel-air mixtures. Combined with Fig. 5.3 (c), which illustrates the temperature distribution at two HRR peaks at 40% HSR, it can be concluded that: In dual-fuel mode, the diesel fuel is initially ignited at the tip of the diesel spray, where it is well mixed, forming the first HRR peak. This is evident in the temperature contour, where the high-temperature zone appears near the diesel spray. This peak resembles the premixed combustion stage observed in conventional diesel combustion. Subsequently, the diesel continues to burn, driving the surrounding hydrogen-air mixture to combust. This process leads to the formation of the second peak, as shown in the temperature contour, where the high-temperature zone appears both in the diesel spray and in the surrounding hydrogen. It can be attributed to the combined effects of diesel diffusion combustion and hydrogen combustion. Most of the hydrogen was consumed at this period, which can be reflected in Fig. 5.5. After the main combustion stage, there is still a stage of combustion which is usually known as 'tail combustion'. This is because some diesel fuel not fully involved in the main combustion continues to oxidize slowly alongside the hydrogen-air mixture in localized areas of

the cylinder or near the cylinder walls. As a result, the heat release rate exhibits a relatively gentle decay trend.

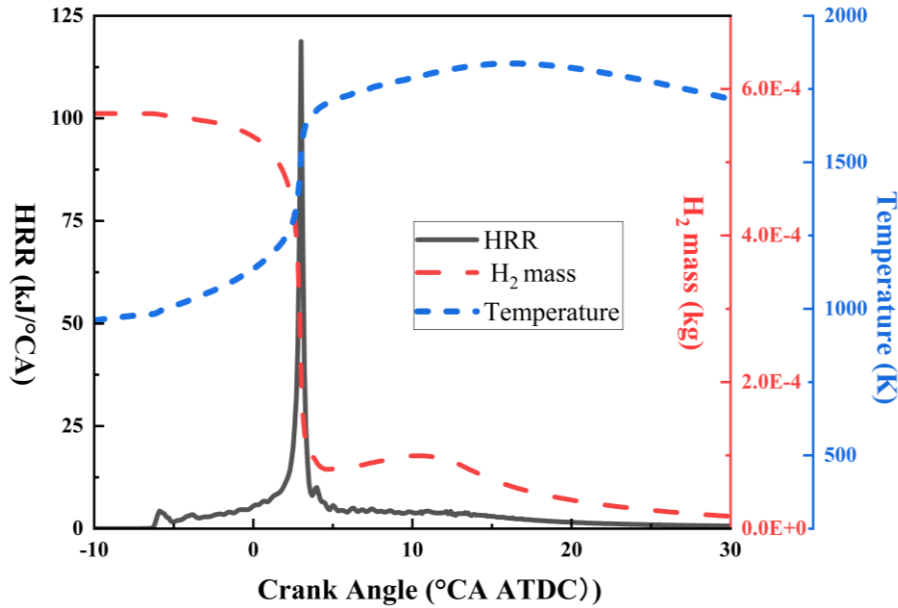


Fig. 5.5 The HRR, H₂ mass and in-cylinder temperature of 40% HSR case.

With the rise of HSR, the first peak slightly advances, and its peak value increases gradually. The reason is that as more hydrogen is introduced into the cylinder, the hydrogen's high diffusivity and shorter ignition delay enhance the evaporation and the homogeneity of diesel fuel at ignition delay period [63]. With the increase in HSR, the second peak occurs at an earlier crank angle, and its amplitude grows substantially, although the overall duration of the peak shortens. The reason is that, in lean hydrogen-air mixture, the flame speed of hydrogen increases with higher equivalence ratio, accelerating the heat release process.

Fig. 5.6 presents the ignition delay, Crank angle of 50% mass fraction burned (CA50) and combustion duration under varying HSR conditions. As shown, the ignition delay decreases gradually with increasing HSR, following a linear trend. This occurs mainly because, under relatively high temperatures, hydrogen can partially decompose to generate free radicals, which accelerate the chain reaction of diesel molecules, thereby shortening the overall reaction pathway and leading to earlier ignition. Meanwhile, the CA50 advances as HSR increases, owing to higher reactivity and faster laminar flame speed of hydrogen, which makes the combustion process shorter. Additionally, the diesel injection duration gradually shortens at higher HSR levels, further contributing to an accelerated combustion phase. Regarding the combustion duration, it initially

exhibits a slight increase before dropping sharply as HSR continues to rise. This phenomenon is attributed to the low hydrogen/air ratio at around 10% HSR, which is insufficient for robust diesel-hydrogen coupling combustion. Once the HSR exceeds 10%, however, the high reactivity and rapid combustion characteristics of hydrogen yield high heat release, resulting in combustion duration reduction.

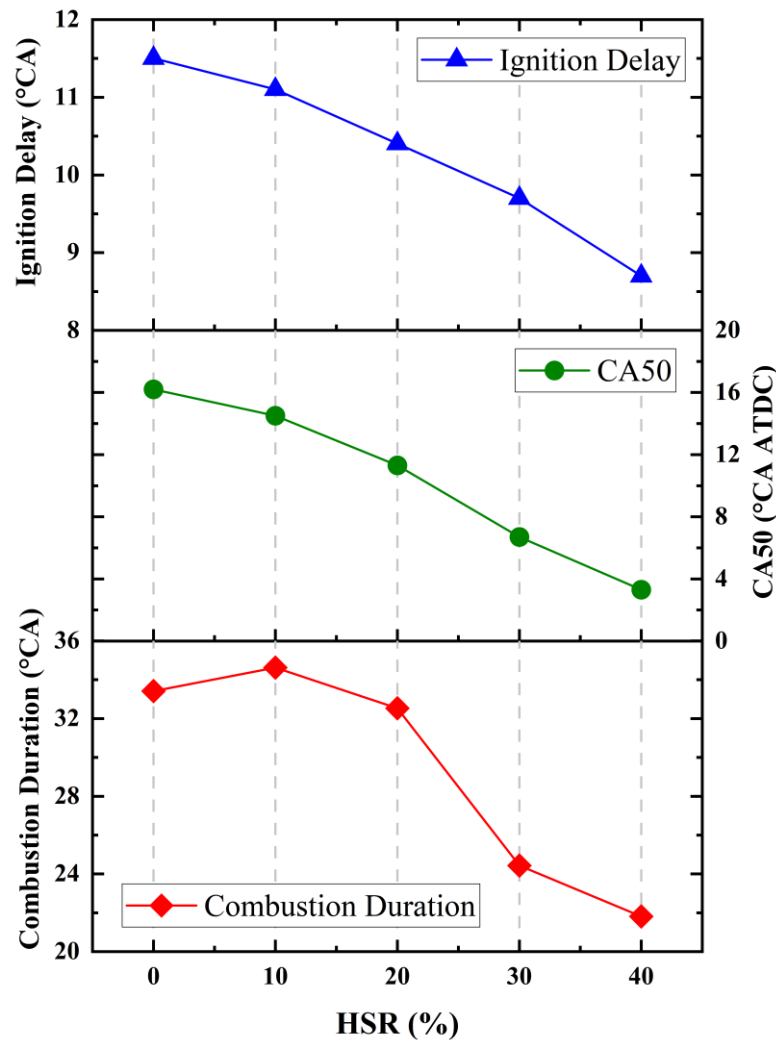


Fig. 5.6 Effect of HSRs on Ignition Delay, CA50, and Combustion Duration.

5.3.2 Engine performance

The heat release and flame propagation speed of hydrogen are significantly higher than those of conventional fuels. Consequently, with the increasing of HSR, the likelihood of knocking in the cylinder increases.

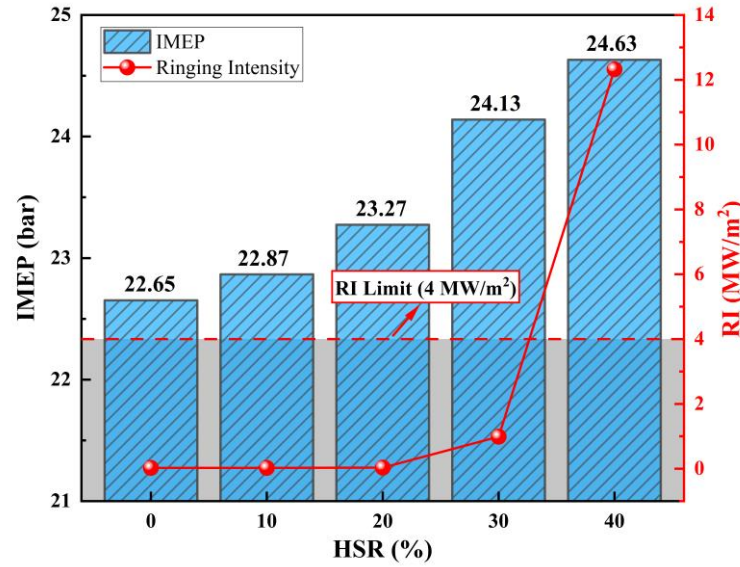


Fig. 5.7 IMEP and Ringing Intensity (RI) with varying HSR.

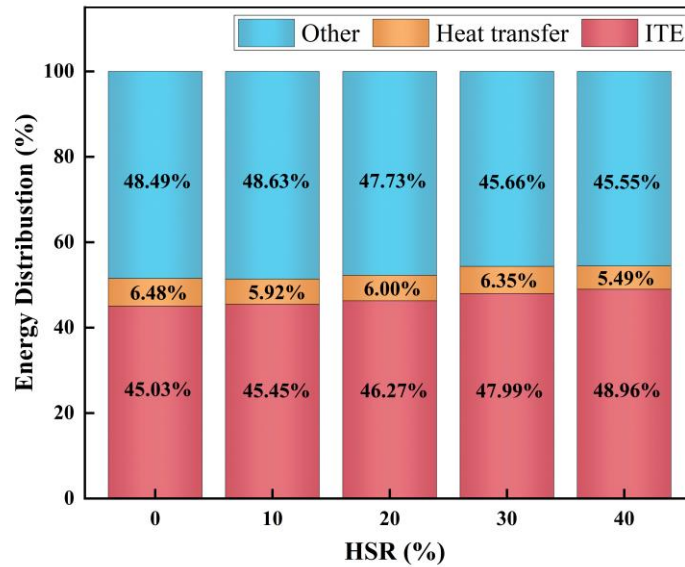


Fig. 5.8 The energy distribution under different HSR conditions.

Fig. 5.7 presents the Indicated Mean Effective Pressure (IMEP) and Ringing Intensity (RI) of HSR over a range of 0% to 40%. As HSR increases from 0% to 40%, the IMEP increases from 22.65 MPa to 24.63 MPa, showing a steady increasing trend. This is because the high reactivity and rapid heat release intensify the combustion process, yielding elevated peak cylinder pressure. Furthermore, hydrogen's wide flammability range and faster flame propagation promote a more complete combustion in a shorter duration. Concurrently, the RI exhibits an increasing trend,

remaining relatively stable at low and medium HSR levels but rising sharply beyond 30%, exceeding the 4 MW/m² operational limitation, reaching 12 MW/m² at 40% HSR. Mixture homogeneity plays a pivotal role in the reaction dynamics, and the greater the concentration of hydrogen, the faster the combustion process, yielding increased dP/dt .

In Fig. 5.8, the energy distribution at varying HSR conditions is depicted, including the indicated thermal efficiency (ITE), heat transfer, other energy that pertains to exhaust loss and incomplete combustion loss. ITE rises gradually from 45.03% to 48.96% as the HSR increases. This trend occurs because the introduction of hydrogen enhances the combustion process, as a result of faster combustion exhibited in the dual-fuel operation as opposed to the diesel one. Furthermore, the gradually shorter combustion duration shifts the process closer to constant volume combustion, thereby reducing irreversible losses. Heat transfer losses reduce from 6.48% for the diesel operation to 5.92, 5.49% for HSR of 10 and 40%, respectively. At HSRs from 20 to 30%, the heat transfer loss rises slightly from 6.00 to 6.35%. The heat transfer rates for 0 to 40% HSR cases are shown in Fig. 5.9. It shows that the nonlinear heat transfer reduction attributes to the combined effect of higher in-cylinder temperature, which enhance instant heat transfer, and shorter combustion duration, which limits the overall heat transfer period. As HSR increases, the proportion of 'Other' losses decreases from 48.49% to 45.55%, due to improved thermal efficiency and reduced exhaust energy dissipation.

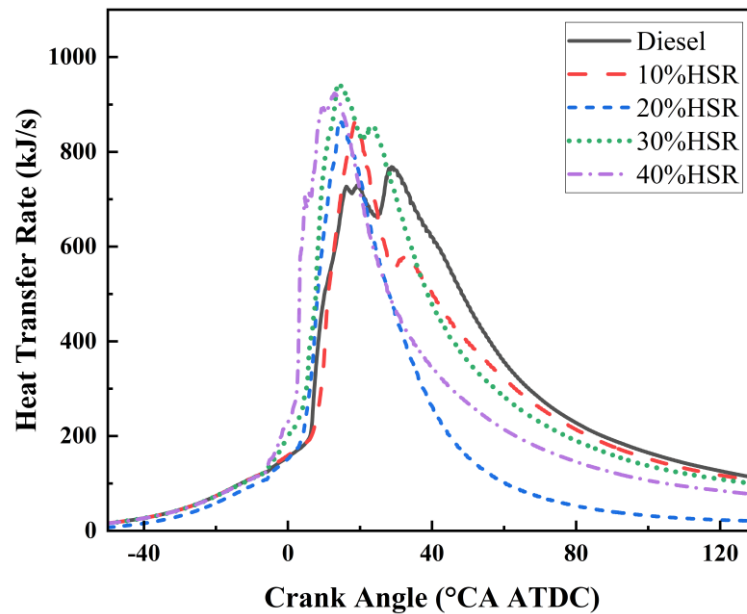


Fig. 5.9 Wall heat transfer rate of HSR varies from 0 to 40%.

5.3.3 Emission characteristics

To investigate the effects of hydrogen substitution on engine emissions, Fig. 5.10 presents the variation in NO_x and soot emissions as the HSR increases from 0% to 40%. As shown, NO_x emissions initially decrease and then rise with increasing HSR. From 0% to 20% HSR, the combustion process shifts from conventional high-temperature diffusion combustion toward a partially premixed mode initiated by diesel ignition. As a result, the in-cylinder temperature distribution becomes more uniform, and peak temperatures are slightly lower than in pure diesel operation, causing NO_x emissions to drop. However, once the HSR reaches or exceeds 30%, the further increase in hydrogen accelerates and intensifies the combustion process, leading to significantly higher average and peak in-cylinder temperatures, and consequently a notable surge in NO_x emissions. Overall, soot decreases with the increase of HSR except at 20% HSR, where a slight rebound occurs. The rebound is due to the hydrogen replacement effect for oxygen and thereby forming fuel-rich zone in spray, as shown in Fig. 5.12. Besides, the in-cylinder temperature is not significantly higher to provide an enhanced oxidation, leaving the residual soot mass high. At 40% HSR, the reduction of diesel fraction and the stronger oxidation brought by higher temperature minimize the soot mass, which is reflected in Fig. 5.13 and Fig. 5.14.

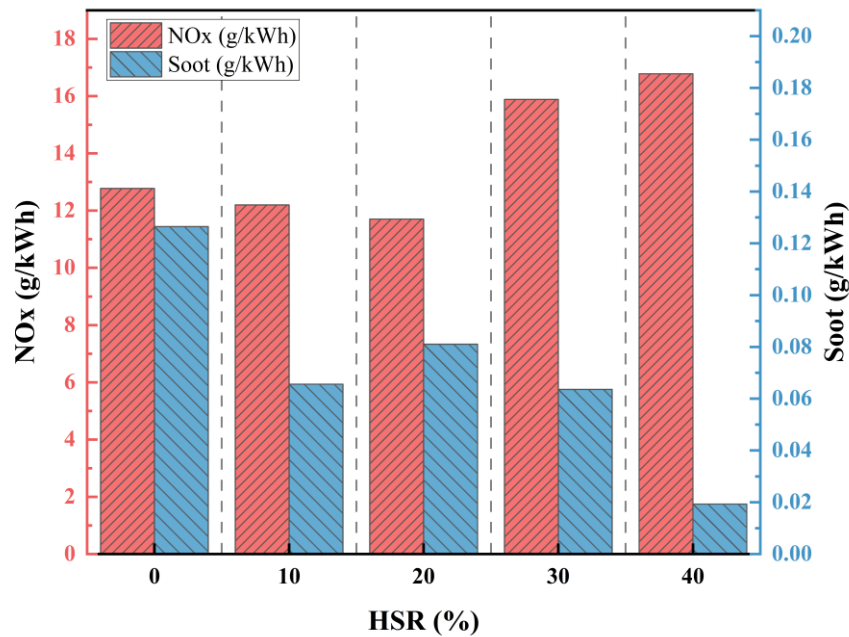


Fig. 5.10 NO_x and Soot emissions with varying HSR.

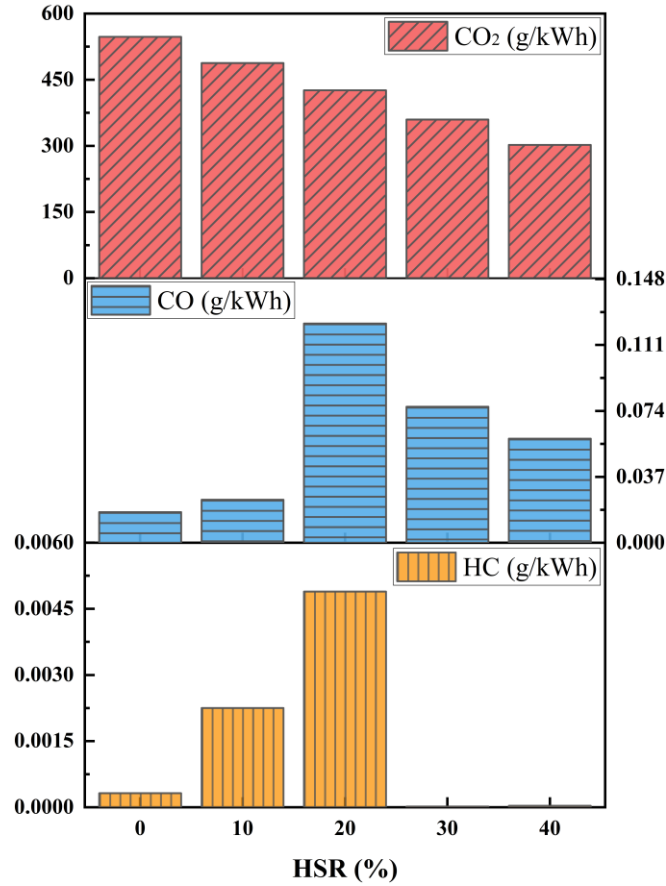


Fig. 5.11 CO₂, CO and HC emissions with varying HSR.

The emissions of most concern when using hydrogen as an alternative fuel are carbon oxides. Fig. 5.11 illustrates the CO₂, CO, and HC emissions as the HSR increases from 0% to 40%. As shown in the figure, the CO₂ concentration exhibits an overall decreasing trend with increasing HSR. This decline occurs because higher HSR reduces the amount of diesel fuel injected, thereby lowering the overall carbon content in the cylinder. In contrast, CO and HC emissions first increase and then decline, peaking at an HSR of around 20%. The initial rise is because hydrogen replaces part of the intake air there, reducing the oxygen local concentration. As shown in Fig. 5.12, 20%HSR case exhibits higher equivalence ratio in spray tip region at peak HRR moment. Meanwhile, the in-cylinder temperature, which is shown in Fig. 5.13, is not significantly higher than diesel mode, oxidation merely mildly strengthens. Once the HSR reaches 40%, however, the significantly higher in-cylinder temperature, drives more effective oxidation of CO and HC, making their residual mass lower, which is reflected in Fig. 5.13 and Fig. 5.15.

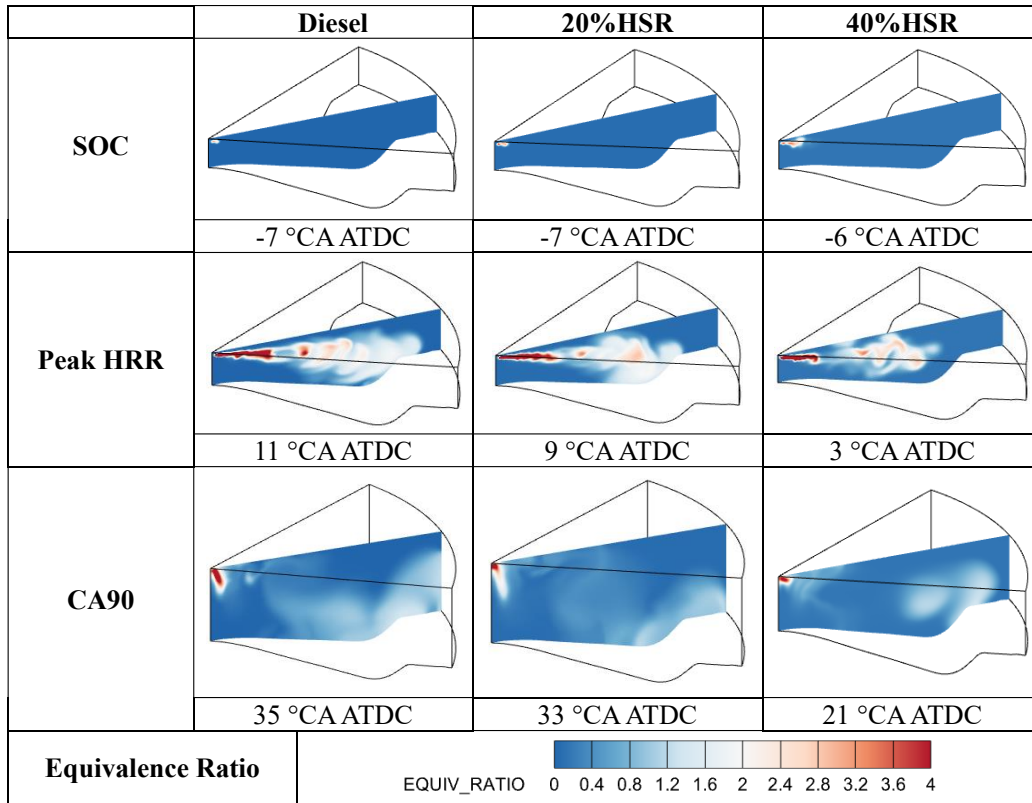


Fig. 5.12 The equivalence ratio distribution of diesel, 20% and 40%HSR cases.

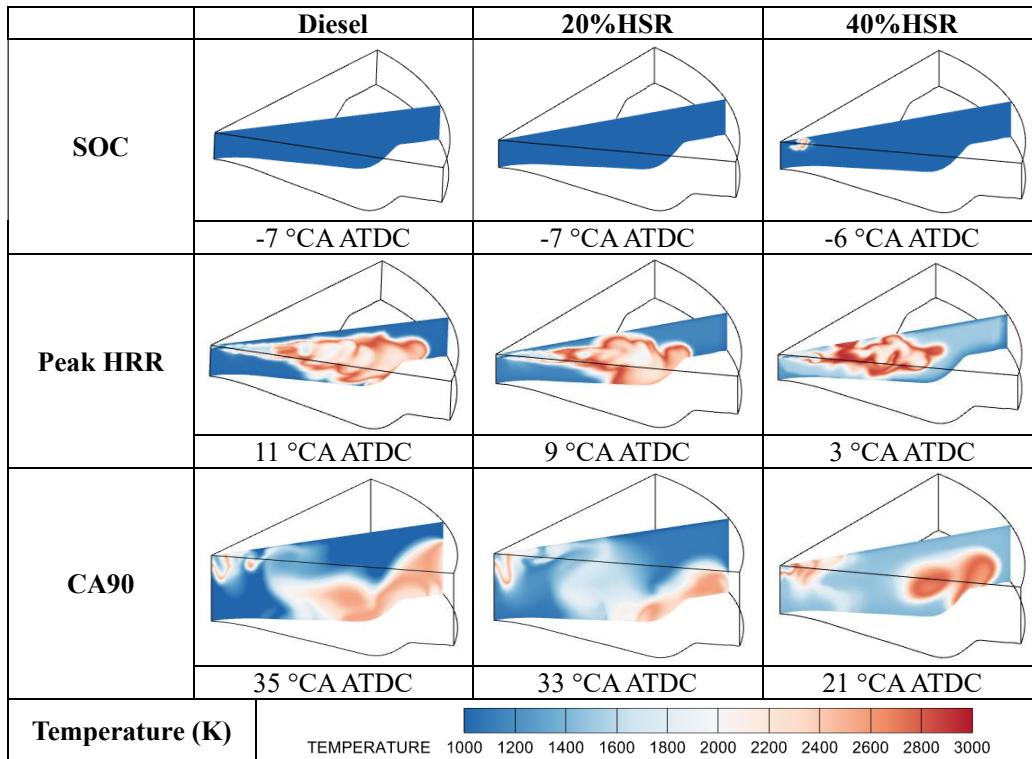


Fig. 5.13 The temperature distribution of diesel, 20%HSR and 40%HSR cases.

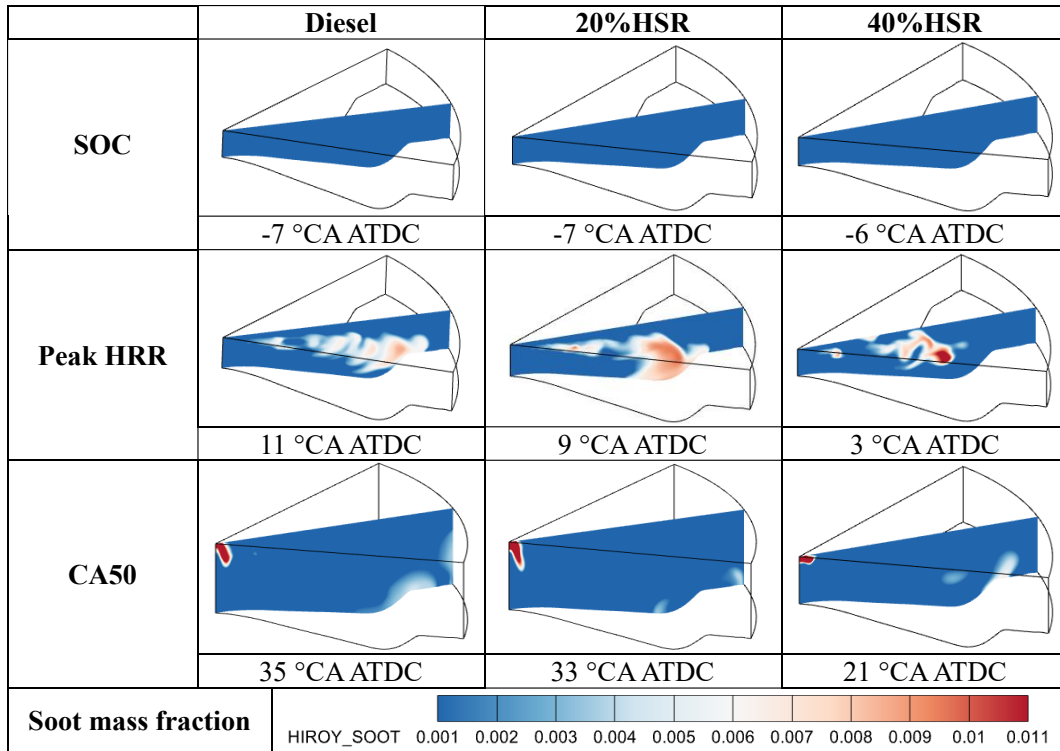


Fig. 5.14 The soot distribution of diesel, 20%HSR and 40%HSR cases.

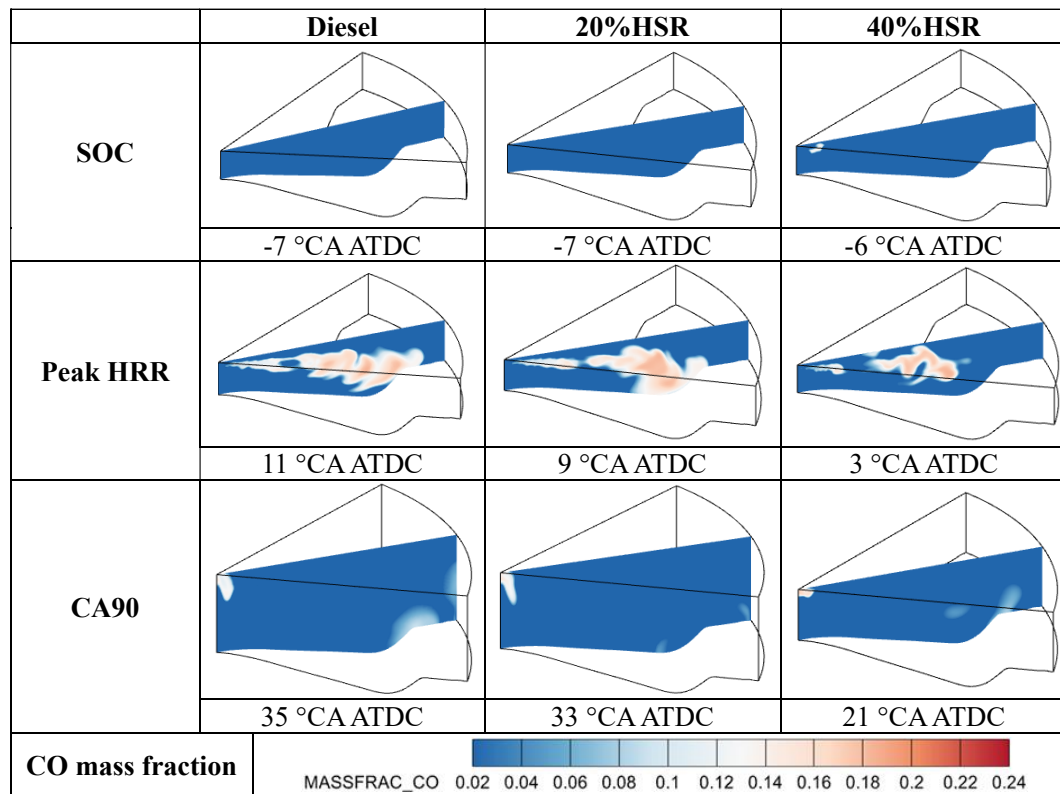


Fig. 5.15 The CO distribution of diesel, 20%HSR and 40%HSR cases.

5.4 DI water injection effect on high (90% and 95%) HSR conditions

5.4.1 The effect of WI on combustion and performance

The cylinder pressure and heat release rate profiles provide direct insight into the effectiveness of water injection (WI) in suppressing knocking. Fig. 5.16 and Fig. 5.17 present the in-cylinder pressure and heat release rate for various WI timings at W/F ratios of 1.5, 2.0, and 2.5 under hydrogen substitution ratios (HSR) of 90% and 95%, respectively. As shown in Fig. 5.16a and b (HSR = 90%, W/F = 1.5), advancing the WI timing leads to a delay in the second heat release peak, which becomes progressively broader and lower, indicating effective suppression of premixed combustion. However, when the WI timing is excessively early (-160°CA), the heat release becomes more advanced and sharper again. This phenomenon is attributed to the fact that moderate WI advancement allows sufficient time for water vapor to mix uniformly with the in-cylinder charge, thereby enhancing suppression.

In contrast, the excessively early water injection causes water to evaporate during the compression stroke, resulting in a leaner distribution at SOC and thus a limited knocking suppression contribution. The above explanation can be supported by Fig. 5.18. Regarding in-cylinder pressure, a similar trend is observed: as WI timing advances, the post-TDC pressure rise becomes more gradual and delayed. Nevertheless, at -160°CA , the pressure profile becomes steep again due to reduced vapor-phase dispersion and earlier combustion onset. A comparable pattern is observed at W/F = 2.0 (Fig. 5.16c and d). Compared to W/F = 1.5, the heat release profiles at all WI timings are generally flatter and broader, reflecting improved suppression due to the increased water mass. This is also reflected in the pressure traces, which remain relatively low and smooth across all WI timings. For W/F = 2.5 (Fig. 5.16e and f), the inflection point in the heat release trend shifts to an earlier WI timing of -130°CA . Beyond this point (i.e., -130°CA and -160°CA), the heat release becomes increasingly steep and concentrated, suggesting a degradation in suppression. This indicates that, at higher W/F ratios, advancing WI timing excessively causes greater premature evaporation, which reduces the effectiveness of knocking suppression more significantly.

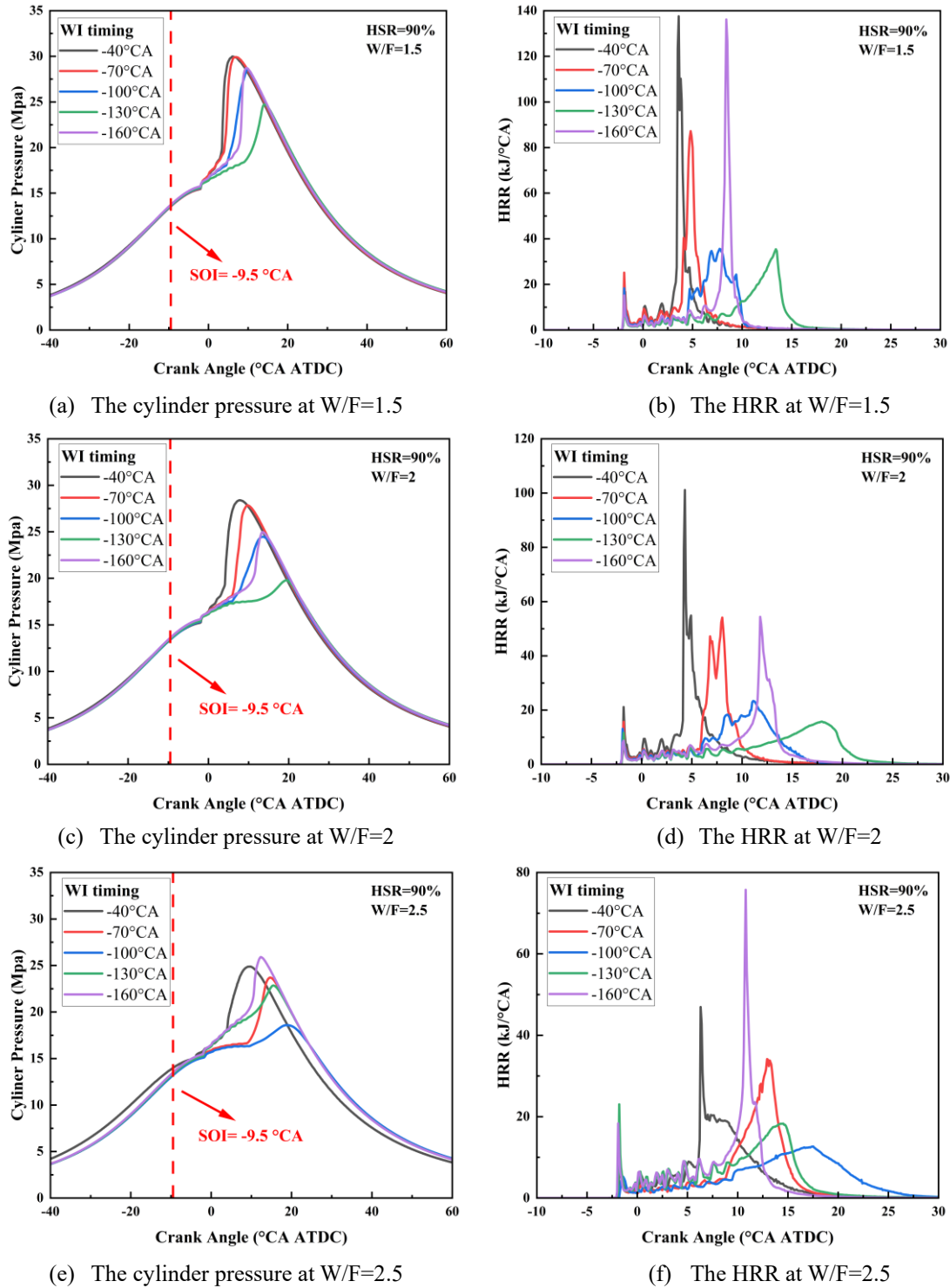
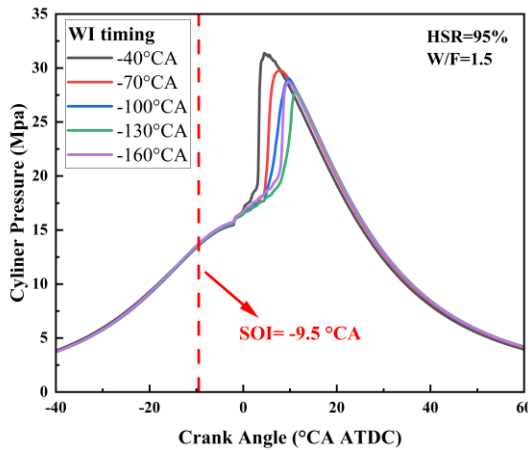


Fig. 5.16 WI timing effect on cylinder pressure and heat release rate at HSR=90%.

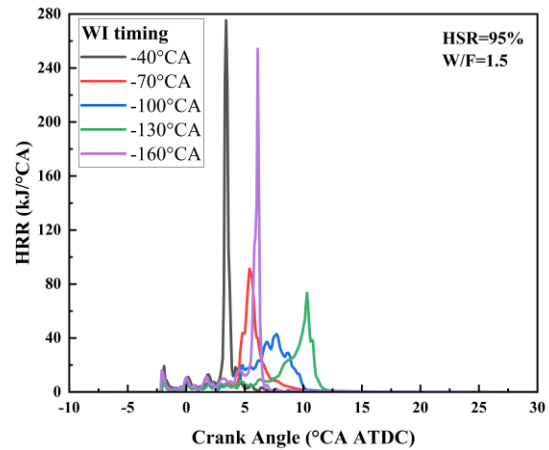
When comparing HSR = 95% to HSR = 90%, the pressure and heat release rate (HRR) exhibit similar trends at W/F = 1.5, as illustrated in Fig. 5.17(a) and (b). However, under HSR = 95%, the HRR profile becomes narrower and peaks at a higher value, which corresponds to an increase in

in-cylinder pressure. This phenomenon is attributed to the higher laminar flame speed associated with higher hydrogen content in the fuel mixture, which intensifies the rapid heat release during combustion.

For the condition of $HSR = 95\%$ and $W/F = 2.0$ (Fig. 5.17c and d), advancing the WI timing causes the HRR peak to be delayed until $WI = -130^\circ\text{CA}$. This turning point appears earlier than in the corresponding $HSR = 90\%$ case, indicating a stronger sensitivity to water distribution. This is because a large amount of water injected too early tends to produce non-uniform vapor distribution, thereby reducing the suppression effect on premixed combustion. At $WI = -160^\circ\text{CA}$, the heat release occurs earliest and exhibits the highest and most concentrated peak, due to ineffective water dispersion. Notably, the heat release of $WI = -160^\circ\text{CA}$ at $W/F = 2$ is earlier than that of $W/F = 1.5$, which is unexpected. The reason is, as more water injected at $W/F = 2$, the turbulent kinetic energy (TKE) is higher at the end of compression stroke, as shown in Fig. 5.19. The higher TKE rises the higher turbulent flame speed once hydrogen is ignited, accelerating the flame propagation throughout the cylinder. Therefore, hydrogen is consumed more rapidly, and the main heat release occurs earlier. In the case of $HSR = 95\%$ and $W/F = 2.5$ (Fig. 5.17e and f), the overall variation of HRR and in-cylinder pressure with WI timing resembles that observed under $HSR = 90\%$. Notably, at $WI = -100^\circ\text{CA}$, both pressure and HRR show significant reductions. This is attributed to the strong suppression effect of a large, well-distributed water spray, which inhibits hydrogen ignition.



(a) The cylinder pressure at $W/F = 1.5$



(b) The HRR at $W/F = 1.5$

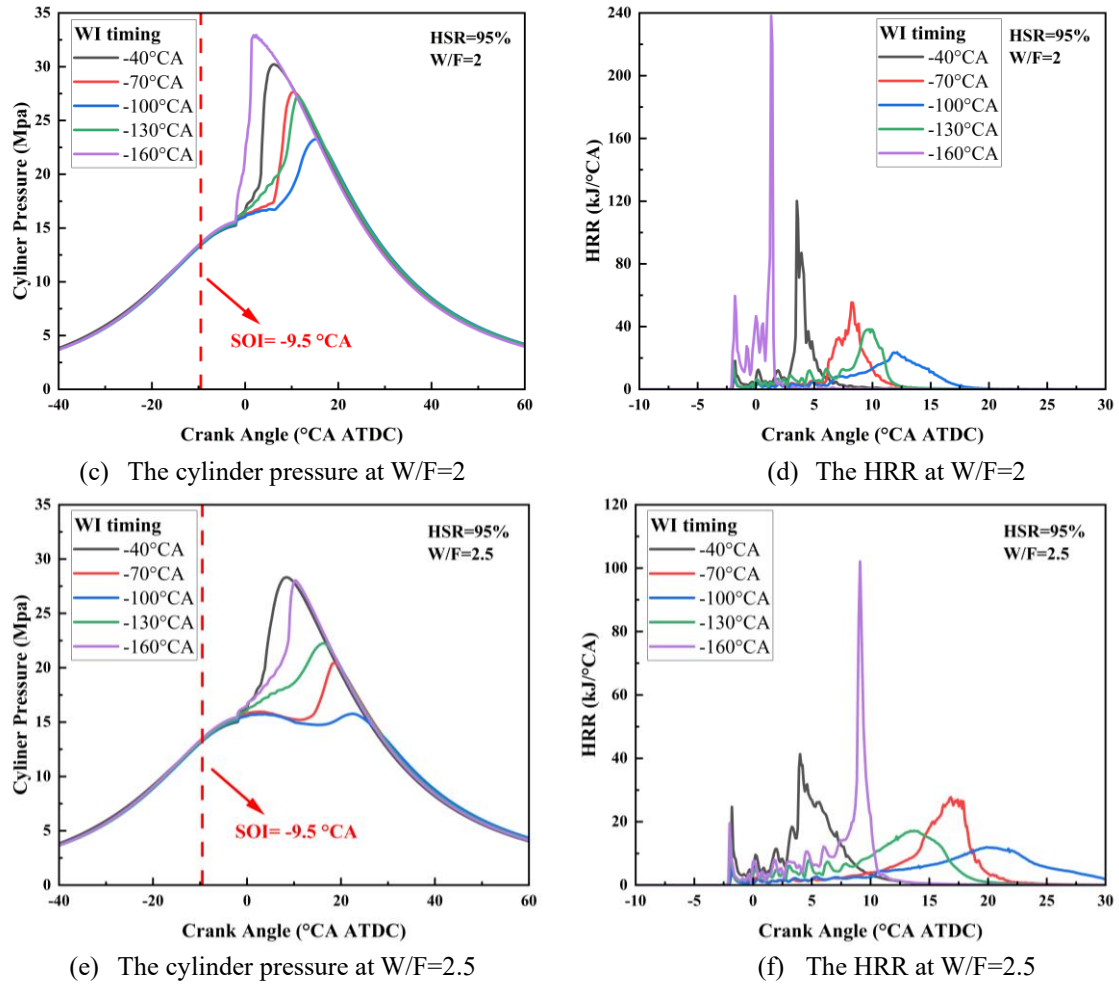


Fig. 5.17 WI timing effect on cylinder pressure and heat release rate at HSR=95%.

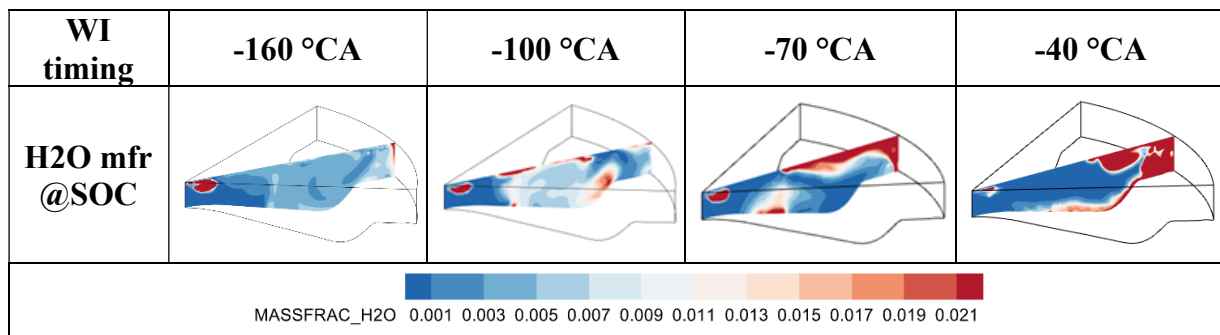


Fig. 5.18 The water distribution at start of combustion for varying water injection timing at 90%HSR and W/F=1.5 condition.

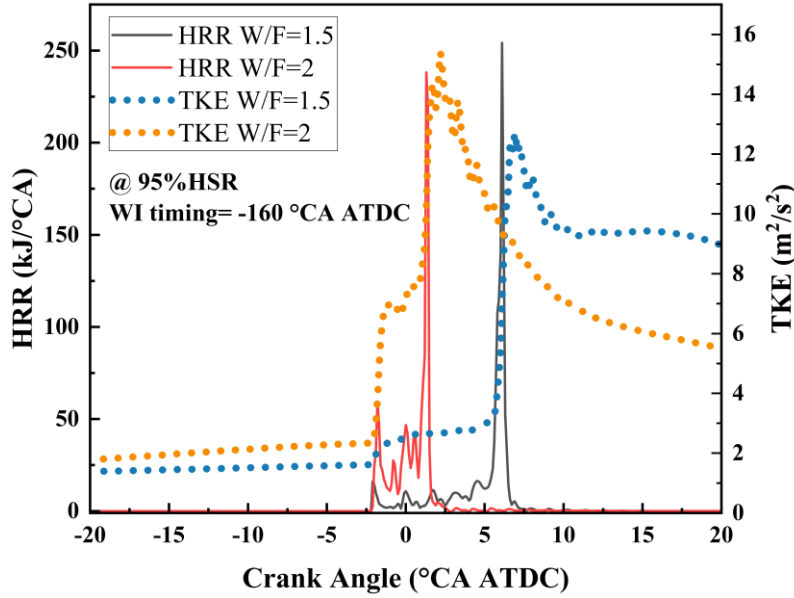


Fig. 5.19 The HRR and TKE of W/F=1.5 and 2.0 at 95% HSR, WI timing=-160 °CA ATDC condition.

Fig. 5.20 presents the effects of water injection (WI) timing and water-to-fuel (W/F) ratio on the maximum in-cylinder pressure (P_{max}) and maximum pressure rise rate (PRR_{max}) under hydrogen substitution ratios (HSR) of 90% and 95%, respectively. P_{max} and PRR_{max} serve as critical indicators for diagnosing knocking behaviour and evaluating its impact on engine performance and mechanical stress. At HSR = 90%, Fig. 5.20a shows that, for all W/F ratios (1.5, 2.0, 2.5), P_{max} initially decreases and then increases as the WI timing is delayed from -160 °CA to -40 °CA. This implies that WI should be neither excessively early nor overly delayed. Specifically, the lowest P_{max} is observed at -130 °CA for W/F = 1.5 and 2.0, and at -100 °CA for W/F = 2.5. For WI timing ≤ -130 °CA, W/F = 2.0 produces the lowest P_{max} among the three ratios, whereas for WI timing ≥ -100 °CA, increasing the W/F ratio leads to a further decrease in P_{max} . This suggests that, in addition to the adverse effects of premature injection (e.g., -130 °CA and -160 °CA), increasing the water amount enhances suppression of rapid heat release.

The trend of PRR_{max} shown in Fig. 5.20 (b) is broadly consistent with that of P_{max} , exhibiting a similar U-shaped profile. However, within the whole WI timing window, differences in PRR_{max} between various W/F ratios are more pronounced than P_{max} , indicating a stronger sensitivity of pressure rise suppression to injection quantity. Notably, the cases of W/F = 2.0 at -130 °CA and W/F = 2.5 at -100 °CA both yield P_{max} values approaching those of the pure diesel mode (~ 20

MPa), while also achieving the lowest PRRmax among all HSR = 90% cases, suggesting these are optimal operating conditions.

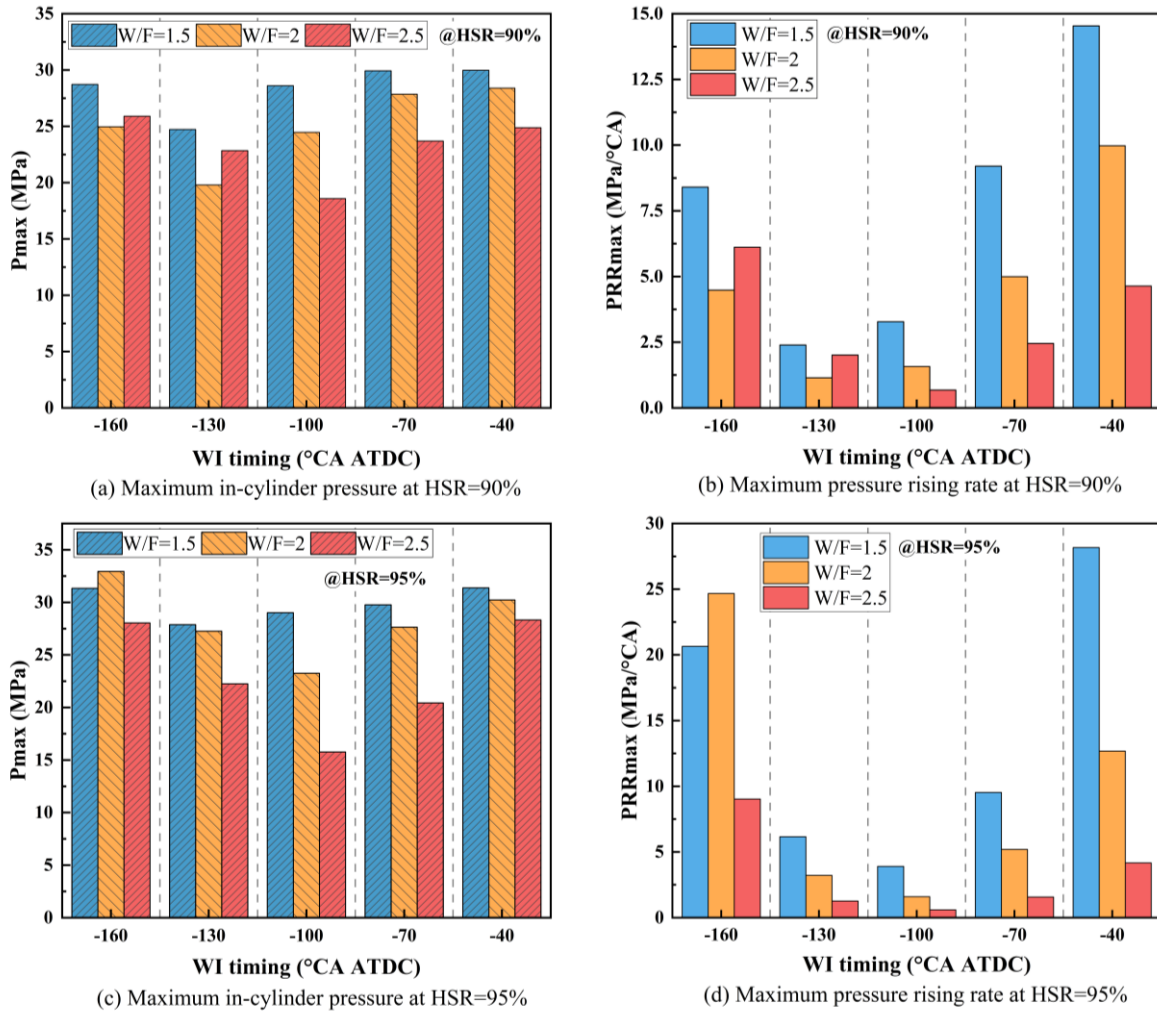


Fig. 5.20 The WI timing and W/F ratio effect on maximum in-cylinder pressure and maximum pressure rising rate at HSR=90% and 95%.

At HSR = 95% (Fig. 5.20 c), a similar trend is observed: Pmax decreases and then increases with WI timing for all W/F ratios. The minimum Pmax occurs at -130 °CA for W/F = 1.5 and at -100 °CA for W/F = 2.0. At -160 °CA, W/F = 2.0 shows the highest Pmax. For WI timing later than -130 °CA, increasing the W/F ratio consistently leads to lower Pmax values. PRRmax results (Fig. 5.20 d) also follow a similar pattern, where for each WI timing (except -160 °CA), PRRmax decreases with increasing W/F ratio. At -160 °CA, W/F = 2.0 shows the highest PRRmax, further confirming the adverse effect of premature injection. Interestingly, two cases (W/F = 2.5 at

-130°CA and -70°CA) exhibit P_{max} values comparable to pure diesel while achieving the lowest PRR_{max} under $\text{HSR} = 95\%$.

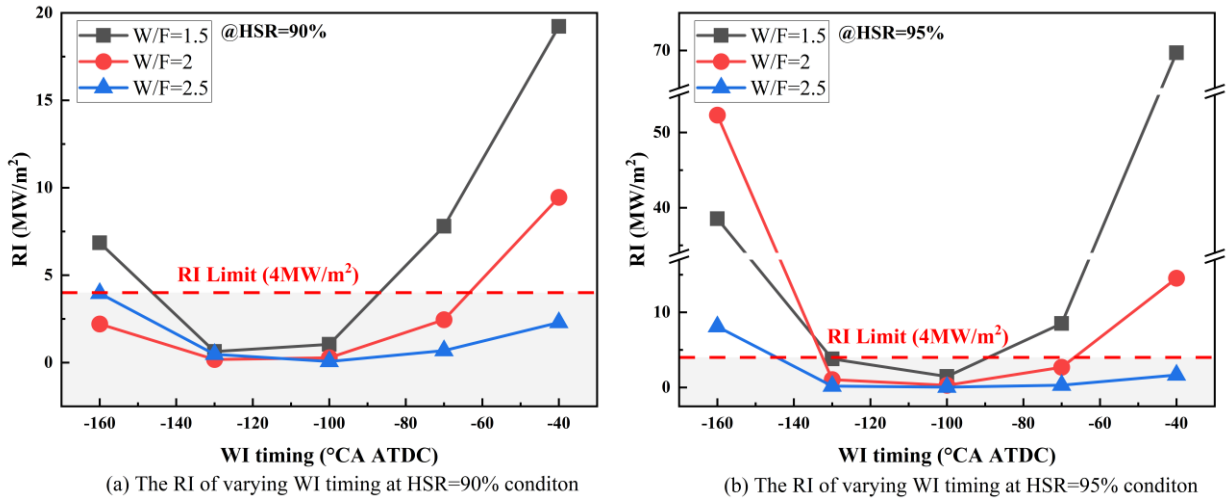


Fig. 5.21 The WI timing and W/F ratio effect on ringing intensity (RI) at $\text{HSR} = 90\%$ and 95% .

Ringing intensity (RI) is a widely used indicator for diagnosing the severity of engine knocking. Fig. 5.21 presents the variation of RI with different water injection (WI) timings and water-to-fuel (W/F) ratios under hydrogen substitution ratios (HSR) of 90% and 95% . A threshold value of 4 MW/m^2 is adopted, above which knocking is considered to occur. For both $\text{HSR} = 90\%$ and 95% , RI generally decreases initially and then increases with the delay of WI timing. Acceptable RI values are primarily observed when WI timing is within the range of -130°CA to -70°CA . This is because an appropriate WI timing promotes a more uniform distribution of water vapor within the cylinder. Under $\text{HSR} = 90\%$, several additional cases at $\text{W/F} = 2$ and 2.5 also fall below the RI threshold even outside this optimal timing range. This is because a larger W/F ratio can compensate for suboptimal WI timing by enhancing the overall knocking suppression effect. Notably, for all WI timings at $\text{W/F} = 2.5$ under $\text{HSR} = 95\%$, RI remains below the threshold, indicating effective knocking suppression of a large W/F ratio. However, RI values under $\text{HSR} = 95\%$ are generally higher than those under $\text{HSR} = 90\%$, suggesting increased knocking propensity at higher hydrogen substitution levels even with water injection. Consequently, higher W/F ratios and carefully optimised WI timings are essential to suppress knocking effectively under high HSR conditions. Additionally, except for the WI timing cases of -160°CA and -130°CA at $\text{HSR} = 90\%$, as the W/F ratio increases, RI becomes lower, which highlights the importance of sufficient water for controlling knocking.

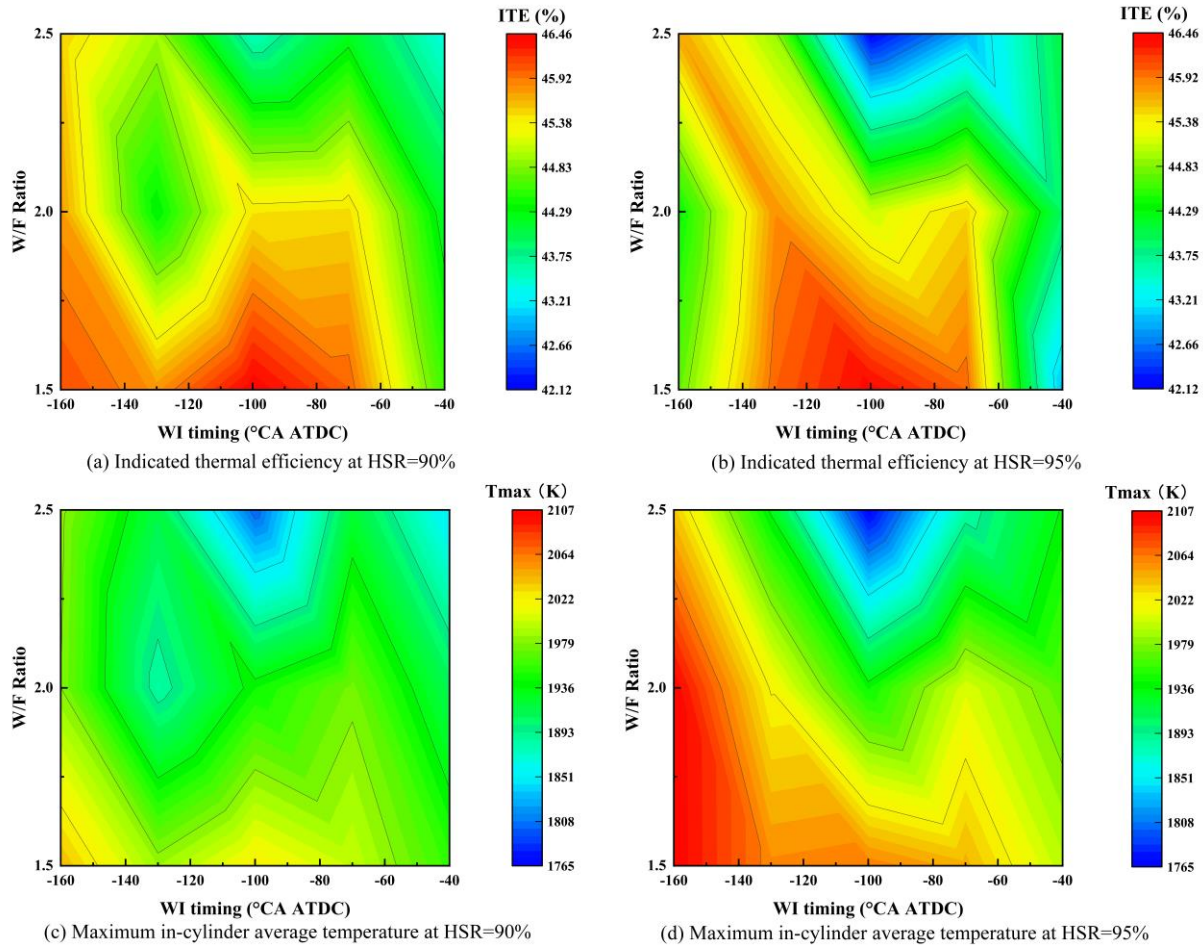


Fig. 5.22 The WI timing and W/F ratio effect on indicated thermal efficiency and maximum in-cylinder average temperature at HSR=90% and 95%.

Indicated thermal efficiency (ITE) is a key parameter in engine research, as it directly reflects the effectiveness of converting the chemical energy of fuel into indicated work. Fig. 5.22(a) and (b) show the combined effects of water injection (WI) timing and water-to-fuel (W/F) ratio on ITE under hydrogen substitution ratio (HSR) conditions of 90% and 95%. As illustrated, the maximum ITE exceeds 46% under both HSR levels. For HSR = 90%, the ITE ranges from 44.38% to 46.46%, with the highest values occurring at low W/F ratios (1.5–2.0) and early WI timings (–130 °CA to –100 °CA ATDC). Under HSR = 95%, the ITE varies between 42.12% and 46.42%. The optimal region shifts slightly later in WI timing, appearing between –130 °CA and –70 °CA, also at lower W/F ratios (1.5–2.0). Compared to HSR = 90%, the distribution of peak ITE values under HSR = 95% is shifted toward later injection and is generally lower. High ITE is observed when WI timing

effectively controls knocking under low W/F conditions (e.g., $W/F = 1.5$). This is primarily because of a well-controlled and moderately phased heat release. At this combustion phasing shortly after TDC, high in-cylinder pressure works effectively on downward piston, generating more expansion work ($\int p dV$). If the heat release is too early, the combustion will resist the piston's upward motion at the end of compression stroke. If the heat release is too late, the in-cylinder pressure is too low to generate sufficient expansion work. Furthermore, the limited amount of injected water minimizes heat absorption due to evaporation, thereby avoiding excessive charge cooling and maintaining high combustion efficiency. In contrast, a high W/F ratio combined with WI timing ($-100\text{ }^{\circ}\text{CA}$ to $-70\text{ }^{\circ}\text{CA}$) that effectively suppresses knocking leads to low ITE. This is primarily due to the excessive heat absorption during water evaporation and the dilution of the combustible mixture, both of which reduce the in-cylinder temperature and slow down the combustion process. This can be supported by Fig. 5.23, as the water evaporation delays the arrival of the second heat release peak. As a result, the combustion phasing shifts away from the optimal crank angle range, leading to lower indicated thermal efficiency. Overall, high ITE is more likely to be achieved at lower W/F ratios, which can be attributed to reduced heat absorption associated with less water evaporation.

Direct in-cylinder water injection suppresses engine knocking through its cooling effect. Therefore, the maximum average in-cylinder temperature can serve as an indicator of the overall heat load and cooling demand, providing a useful reference. Fig. 5.22 (c) and (d) depict the maximum average in-cylinder temperature under the combined effects of WI timing and the W/F ratio at HSR conditions of 90% and 95%. For the HSR=90% condition, the T_{max} range is between 1,800 and 2,044 K. The highest T_{max} region shows at low W/F ratio (1.5-2.0) and early-to-medium WI timing ($-160^{\circ}\sim -60\text{ }^{\circ}\text{CA ATDC}$) condition. For the HSR=95% condition, the T_{max} range is between 1,765 and 2,107 K. The highest T_{max} region is at low W/F ratio (1.5-2.0) and early WI timing ($-160\sim -130\text{ }^{\circ}\text{CA ATDC}$) conditions. For all the WI timings at HSR = 90% and 95% conditions, the T_{max} decreases with the increase in W/F ratio. This can be attributed to the heat absorption of added water.

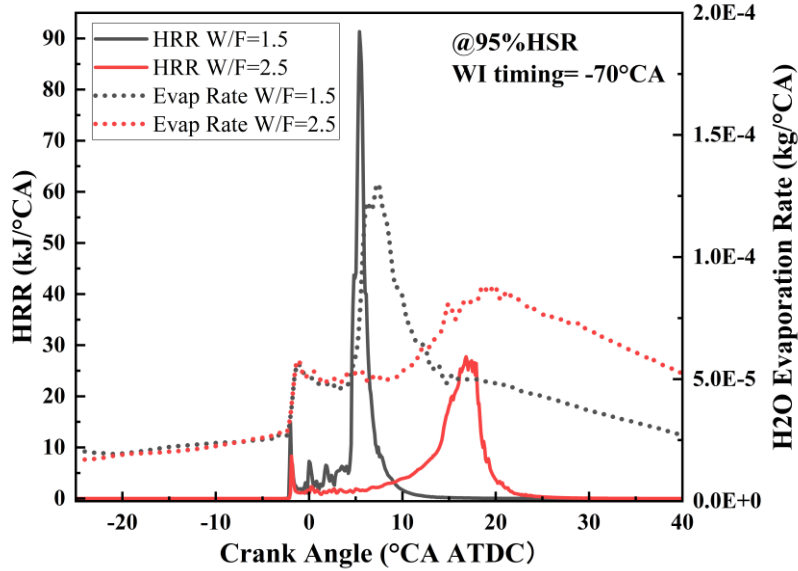


Fig. 5.23 Comparison of HRR, H₂O evaporation rate between W/F=1.5 and 2.5 at 95% HSR, WI timing=-70 °CA ATDC condition.

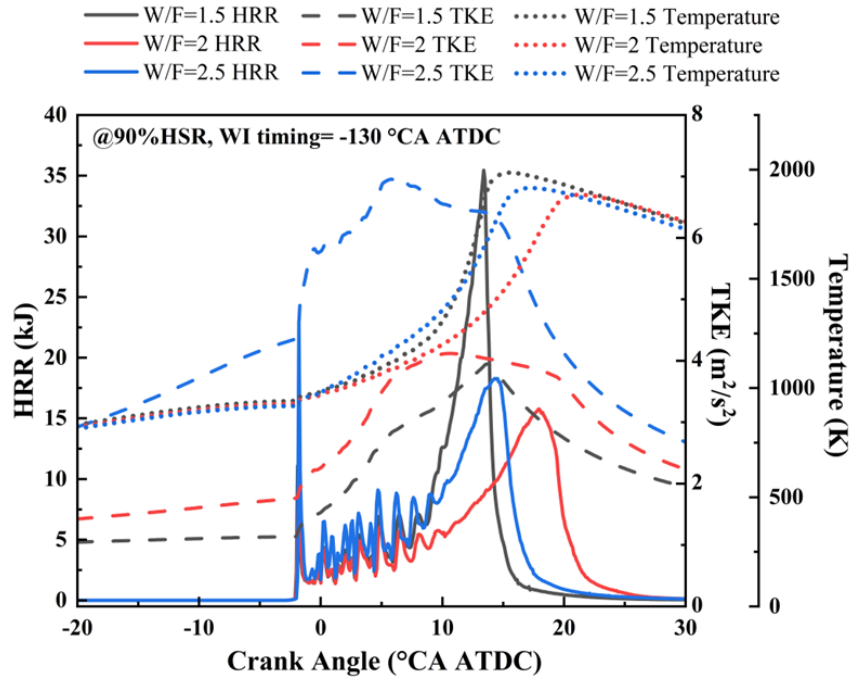


Fig. 5.24 The HRR, TKE and temperature variations of 90%HSR at WI timing=-160 °CA ATDC for W/F=1.5, 2, 2.5.

Comparing Fig. 5.22(c) with Fig. 5.22(a), at HSR = 90%, the trends of ITE and T_{max} are highly correlated where regions with higher T_{max} correspond to higher ITE. This indicates that moderate in-cylinder temperatures favor efficient combustion phasing and expansion work. It's worth noting

that at 90% HSR, with WI timing = -130°CA and $W/F = 2$, both the temperature and ITE are lower than those under $W/F=1.5$ and 2.5 conditions, which is unexpected. This phenomenon can be explained by Fig. 5.24. As shown, when $W/F=2.5$, the significantly higher TKE caused by the larger amount of water injection promotes earlier and more intense heat release than expected. In contrast, the $W/F = 2.0$ case exhibits much lower TKE, leading to the latest and mildest heat release. It leads to the lowest in-cylinder peak temperature of 1,884 K. Owing to the deviation of its heat release phase from the optimal combustion phasing, the expansion work is reduced, resulting in the lowest indicated thermal efficiency (ITE) of 44.30%. For $W/F = 1.5$, the minimal water injection results in the earliest and strongest heat release.

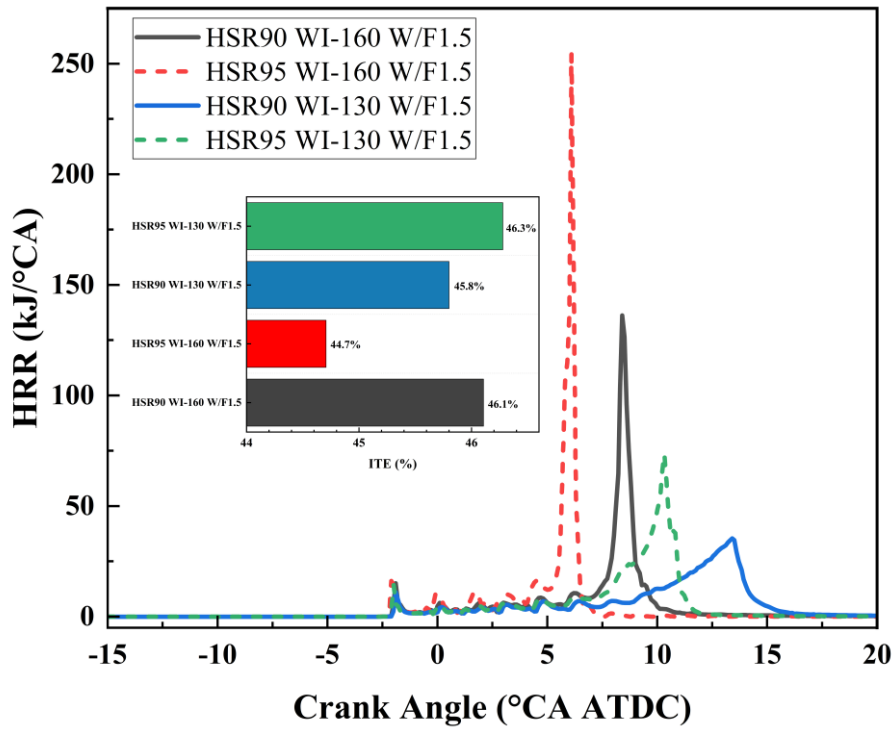


Fig. 5.25 The HRR and ITEs of early WI timings of $W/F=1.5$ at 90% and 95% HSR conditions.

As shown in Fig. 5.22(c) and (d), at HSR = 95%, the correlation between ITE and T_{max} is reduced. Notably, low W/F ratios and early WI timings result in high combustion temperatures, yet the ITE remains low. This phenomenon results from inadequate knock suppression, allowing combustion to initiate too early, ahead of the optimal expansion phase. Consequently, though in-cylinder temperatures increase, the efficiency of energy conversion declines. This can be supported by Fig. 5.25. It can be seen at 95% HSR condition, though the WI timing is the same with 90% HSR, the

combustion is earlier and faster. This results from more hydrogen addition. Hence, the WI timing = -160 °CA at 95% HSR condition case's HRR (too close to TDC) deviates the optimal combustion phase, resulting in lower expansion work ($\int p dV$). In contrast, the other three cases' HRR are later, making them near the optimal heat release phase. Therefore, the ITEs are higher.

5.4.2 The effect of WI on emissions

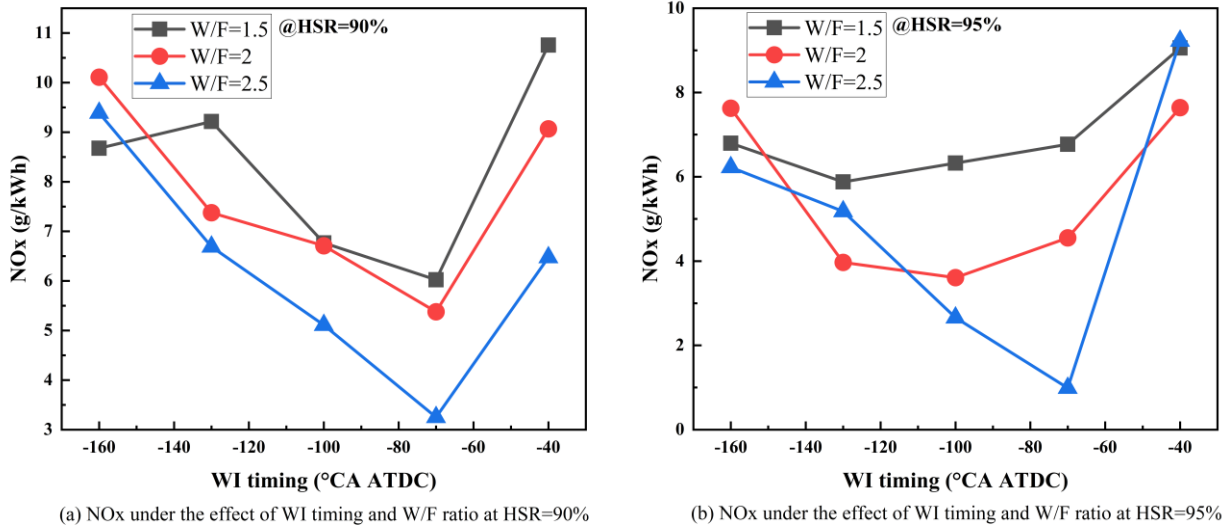


Fig. 5.26 The WI timing and W/F ratio effect on NOx emissions at HSR=90% and 95%.

Water injection (WI) helps control the in-cylinder temperature and thereby contributes to the reduction of NOx emissions. Fig. 5.26 presents the WI effects on NOx emissions at HSRs of 90% and 95%. As shown in Fig. 5.26(a), NOx emissions decrease and then increase with delayed WI timing for all W/F ratios. For all W/F ratios, the lowest NOx emissions are observed at a WI timing of -70 °CA. Similarly, for HSR = 95%, NOx emissions first decrease and then increase with delayed WI timing for all W/F ratios, as shown in Fig. 5.26(b). For W/F ratios of 1.5 and 2.0, the lowest NOx emissions occur at a WI timing of -100 °CA. For W/F = 2.5, the lowest NOx is observed at a WI timing of -70 °CA. Overall, for the same W/F ratio and WI timing, NOx emissions are lower under HSR = 95% than under HSR = 90%. This is attributed to the shorter overall combustion duration at HSR = 95%, which leads to a reduced high-temperature residence time and a shorter window for NOx formation. In contrast, at HSR = 90%, the presence of more diesel fuel promotes the formation of localized high-temperature and oxygen-rich zones that are favourable for NOx generation. For both HSR = 90% and 95%, NOx emissions decrease with

increasing W/F ratio. This is because, as more water is injected, its evaporation reduces the peak in-cylinder temperature. Since the formation of hot NO_x is highly temperature sensitive, this cooling effect directly limits NO_x production.

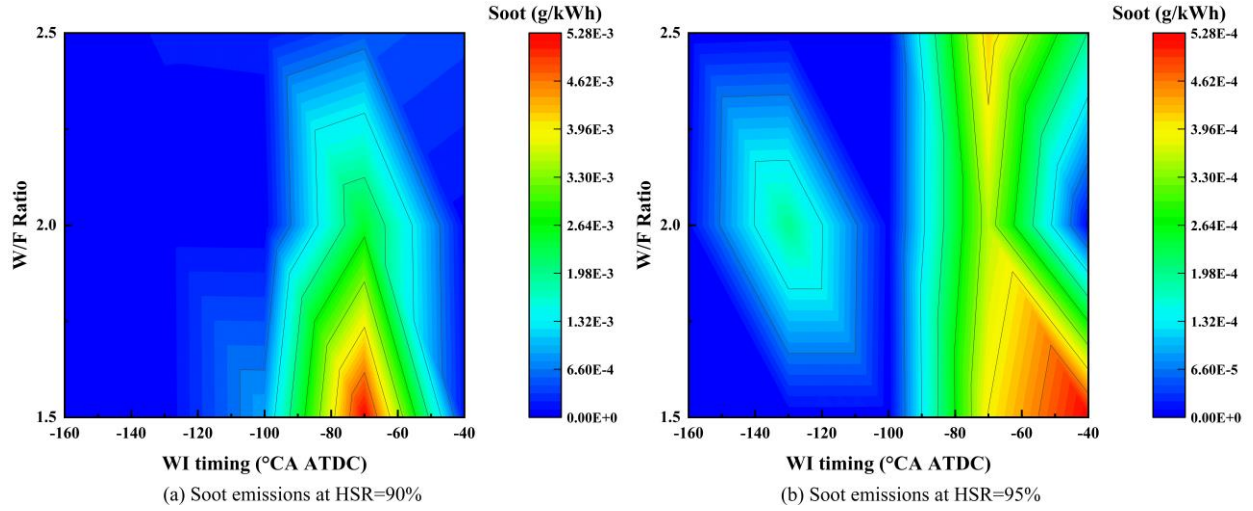


Fig. 5.27 The WI timing and W/F ratio effect on Soot emissions at HSR=90% and 95%.

Soot is primarily formed through the pyrolysis and incomplete combustion of partially oxidized fuel at high temperatures during the diesel engine combustion process. Water absorbs heat through evaporation and can influence fuel-air mixing and combustion chemistry, thereby affecting soot production.

Fig. 5.27 shows the soot emissions for HSR=90% and 95% conditions under the effect of W/F ratio and WI timing. It can be seen from Fig. 5.27 that the legend range of HSR=95% is one order of magnitude lower than 90%. This general trend is due to the small fuel-rich region and higher local oxygen ratio to the reduced diesel supply. This can be seen in Fig. 5.29 and Fig. 5.30. Comparing the 90% HSR, WI=−70 °CA, W/F=2.5 case with the 95% HSR, WI=−70 °CA, W/F=2.5 case, the latter case shows a lower equivalence ratio-rich region and less soot formation. From Fig. 5.27(a), the high soot region is at low W/F ratio (1.5 and 2.0) and late WI timing (−100 to −70 °CA ATDC). This is because limited water injection results in insufficient cooling, which can be reflected in Fig. 5.28, as 90%HSR, WI=−70 °CA, W/F=1.5 case shows higher in-cylinder temperature than the 90%HSR, WI=−70 °CA, W/F=1.5 case at selected moments.

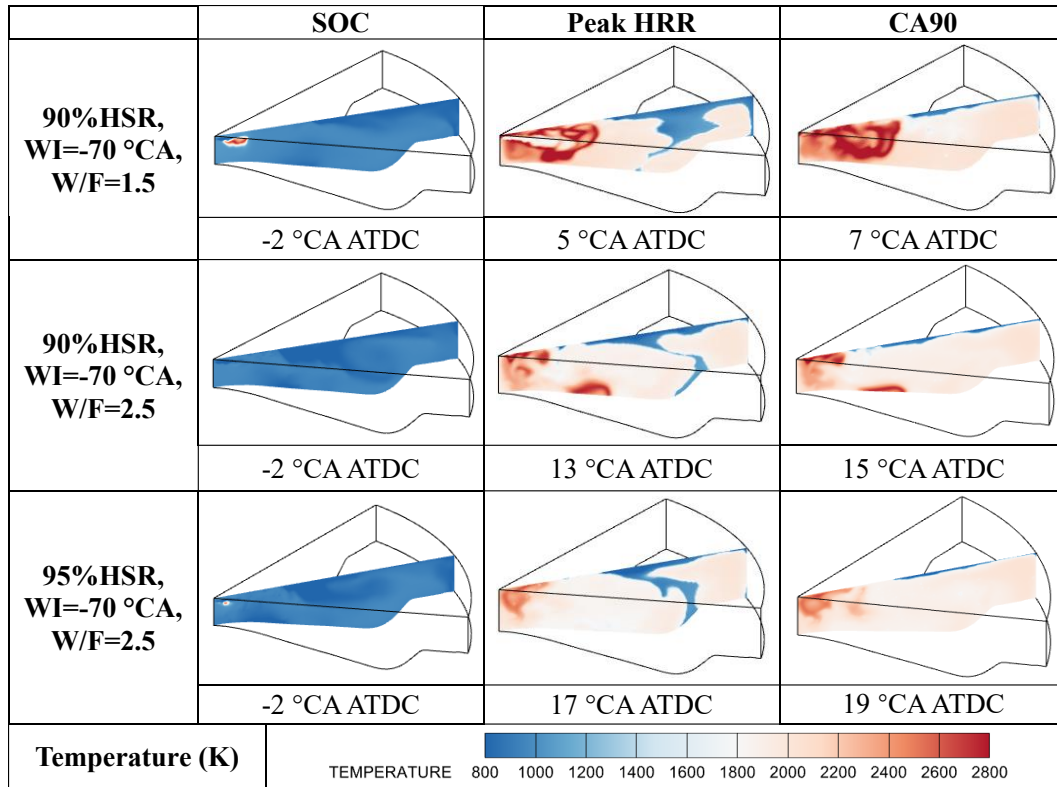


Fig. 5.28 The temperature distribution of representative cases.

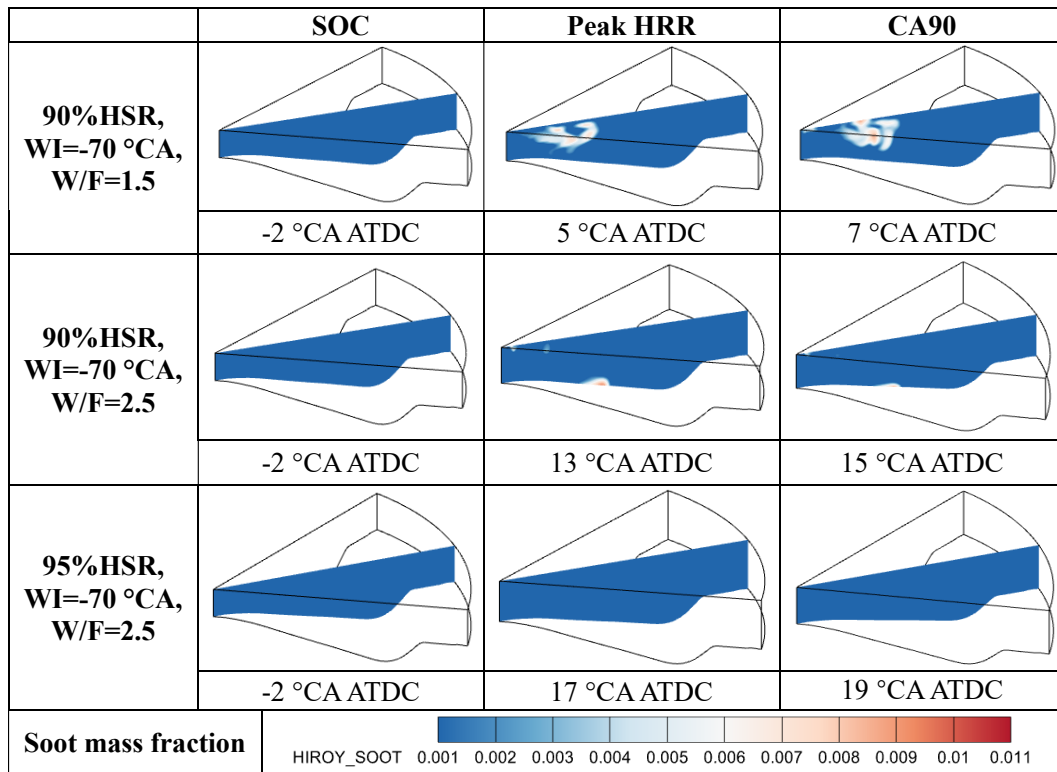


Fig. 5.29 The soot distribution of representative cases.

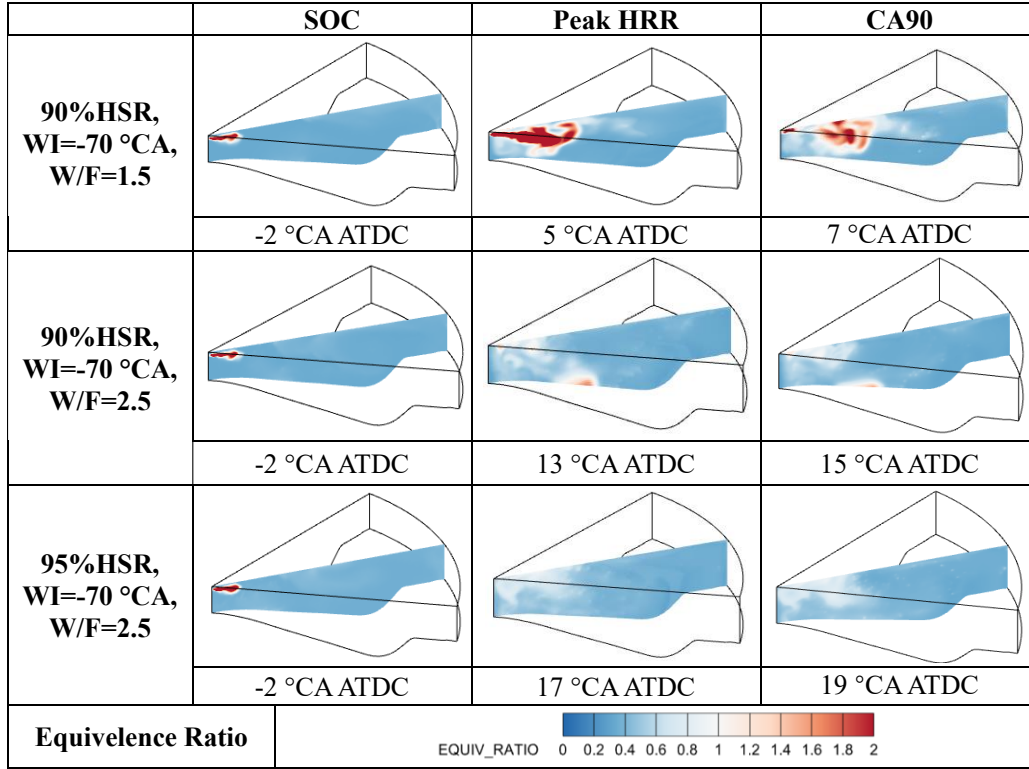


Fig. 5.30 The equivalence ratio distribution of representative cases.

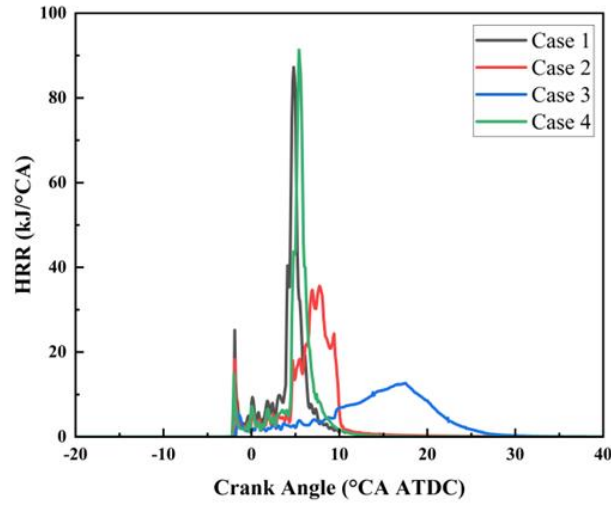
Meanwhile, late water injection brings local water concentration, which can be seen in Fig. 5.18. This inhibits soot oxidation and can be seen in Fig. 5.28 and Fig. 5.29. At HSR = 95%, the high-soot region spans a wider W/F range due to weaker oxidation capability. The weakened diesel diffusion combustion and reduced local oxygen availability contribute to this, which is reflected in the Fig. 5.28 and Fig. 5.30.

5.4.3 Spatial distribution analysis

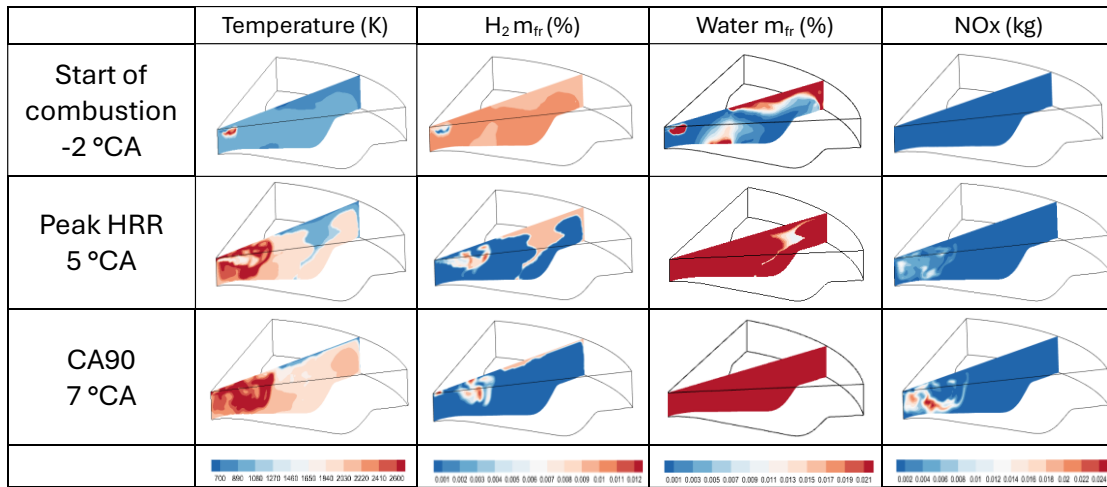
Table 5.3 The description of 4 representative cases.

Case No.	HSR (%)	WI SOI (°CA ATDC)	W/F Ratio	RI (MW/m ²)
1	90	-70	1.5	7.8
2	90	-100	1.5	1.0
3	90	-100	2.5	0.1
4	95	-70	1.5	8.5

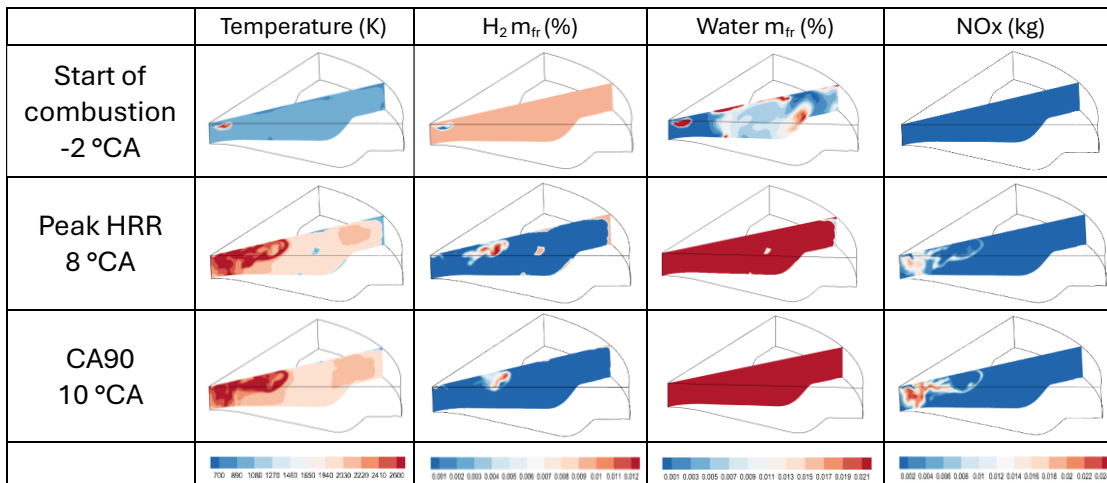
To further analyse the effect of water injection on combustion, four representative cases with varying control parameters are selected to present the spatial results, as shown in Table 5.3. Among these, two cases have RIs exceeding the knocking threshold, while the other two fall below it.



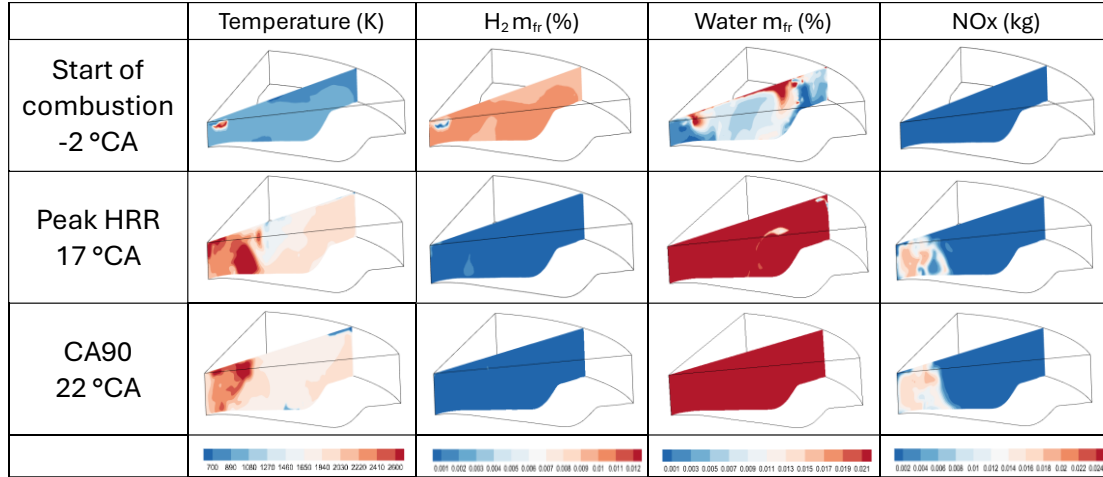
(a) The heat release rates of four representative cases



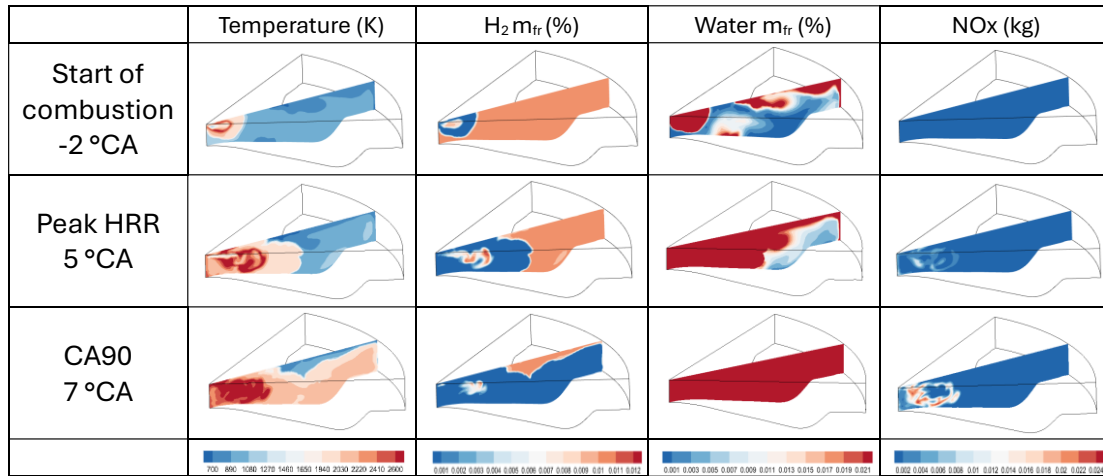
(b) Case 1 (HSR=90%, WI SOI=-70°CA, W/F=1.5)



(c) Case 2 (HSR=90%, WI SOI=-100°CA, W/F=1.5)



(d) Case 3 (HSR=90%, WI SOI=-100°CA, W/F=2.5)



(e) Case 4 (HSR=95%, WI SOI=-70°CA, W/F=1.5)

Fig. 5.31 Spatial distribution of in-cylinder temperature, hydrogen mass fraction and NOx emissions of the representative cases.

The HRRs of these 4 cases are compared in Fig. 5.31(a), showing heat release in Cases 1 and 4 is faster and more concentrated, whereas in Cases 2 and 3 it is slower and gentler. Fig. 5.31(b), (c), (d) and (e) illustrate the spatial distribution of in-cylinder temperature, hydrogen and water mass fraction and NOx emissions of the 4 representative cases at SOC, Peak HRR CA and CA90. In Case 1, combustion starts at -2 °CA with premixed combustion of diesel fuel, subsequently triggering hydrogen combustion around the spray region. A water-rich region is formed near the cylinder head and wall. As combustion progresses, at the peak HRR occurring at 5 °CA, more hydrogen participates in the reaction. The high-temperature region expands, and the surrounding hydrogen is consumed. However, due to the presence of a water-rich region near the cylinder head,

the hydrogen nearby remained unburnt. The combustion reaction of hydrogen ($2\text{H}_2 + \text{O}_2 \rightarrow 2\text{H}_2\text{O}$) produces more water in the cylinder. At this stage, a certain concentration of NO_x is formed near the diesel spray. By CA90, the high-temperature region has spread across the entire slice, with only a small amount of unburnt hydrogen remaining near the cylinder head due to the lower temperature in that area. Since most of the hydrogen has already been burnt, water generated from hydrogen combustion is distributed throughout the cylinder. The NO_x concentration increases and accumulates near the diesel spray, driven by the local temperature exceeding 2,500 K. Throughout the combustion process, the highest temperatures are consistently concentrated near the diesel spray, which corresponds to the central region of the combustion chamber.

At the SOC moment, Case 2 exhibits a more uniform temperature distribution than Case 1, which shows a low-temperature region near the cylinder head. This difference is attributed to the earlier water injection timing at -100°CA in Case 2, leading to a more homogeneous water distribution within the cylinder. The more uniform water distribution results in the full involvement of in-cylinder hydrogen in the combustion process, which can be seen at peak HRR moment (8°CA). In contrast, in Case 1, hydrogen remains unignited due to the presence of the water-rich region near the cylinder head. This more uniform distribution of water, especially in the central part of the slice, also contributes to the suppression of rapid hydrogen combustion, thereby reducing the RI to an acceptable level (1.0). In addition, due to the absence of water-rich zones in case 2, at both the peak HRR and CA90 moments, the in-cylinder temperature distribution is more uniform, and the NO_x generation is richer.

In Case 3, at the SOC moment (-2°CA), although a water-rich region exists near the cylinder head, the higher W/F ratio (2.5) leads to not only a uniform but also a high overall water concentration throughout the cylinder, which significantly slows down the burning velocity of hydrogen. Therefore, the peak HRR moment is delayed to 17°CA . In addition, the cooling effect induced by the high volume of injected water leads to lower temperatures in the high-temperature region of the cylinder, resulting in reduced NO_x concentrations at CA90 compared to Case 1 and 2.

Since Case 4 has a hydrogen substitution rate (HSR) of 95%, a higher hydrogen concentration is observed at the SOC moment (-2°CA) compared to the other cases. Due to the late timing of water injection at -70°CA , a water-rich region forms around the cylinder head and along the cylinder wall. Consequently, at the peak HRR moment (5°CA), a substantial amount of unburnt

hydrogen remains in the low-temperature, water-enriched zone. Even at the CA90 moment, unburnt hydrogen is still present in this region. Furthermore, because Case 4 has the highest HSR, it also exhibits the highest peak heat release rate, and knocking is not effectively suppressed due to the delayed water injection.

Overall, a WI timing of -70°CA results in an uneven moisture distribution within the cylinder, leading to the formation of a water-rich region near the cylinder head, which is less effective in suppressing rapid hydrogen combustion. In contrast, a more appropriate WI timing, such as -100°CA , allows for a greater amount of water injection, which can further decelerate the hydrogen combustion rate and reduce NO_x formation more effectively. However, a higher hydrogen content increases the peak exothermic rate and intensifies knocking severity.

5.5 Summary

This chapter explores the application of hydrogen fuel in marine medium-speed engines, highlighting the role of direct water injection in achieving high hydrogen substitution ratios. To achieve knocking-free combustion, two strategies were investigated: combustion with low hydrogen substitution rates (0–40%) without water injection, and high substitution rates (90% and 95%) combined with direct water injection. The combustion and emission characteristics under these conditions were analyzed. The main findings of this chapter are as follows:

1. As the HSR increases, the combustion process gradually shifts to being hydrogen-dominated, resulting in a more rapid heat release. This leads to elevated and advanced peak in-cylinder pressures, significantly increasing the tendency for knocking. In addition, the addition of hydrogen shortens the combustion duration, resulting in higher ITE. Without in-cylinder water injection, the maximum HSR for knocking-free combustion is limited to approximately 30%.
2. As the HSR increases, CO₂ emissions gradually decrease due to the carbon-free nature of the hydrogen. When the HSR exceeds 20%, NO_x emissions begin to rise as a result of increased combustion temperatures.
3. In cases of high HSRs (90% and 95%), in-cylinder water injection can effectively suppress knocking and maintain high ITE. However, its effectiveness depends on proper control of injection timing (-130°CA to -70°CA). Overly early water injection weakens knocking effectiveness due

to premature evaporation, while overly late water injection limits knocking suppression owing to non-uniform water distribution.

4. A higher water injection quantity can effectively reduce NO_x emissions by lowering the in-cylinder temperature. However, the enhanced evaporative cooling effect also leads to a decrease in indicated thermal efficiency.

5. At both 90% and 95% HSR, the recommended water injection control (1.5 W/F, -100°CA timing) results in higher ITE and lower NO_x emissions compared to the pure diesel mode.

This investigation provides valuable insights into achieving stable combustion of high hydrogen substitution ratios in marine engines. However, it has certain limitations. In particular, the assumption of a homogeneously premixed in-cylinder hydrogen-air mixture under PFI conditions is idealized and may not fully represent real engine behaviour. Next chapter will address this by considering the effects of hydrogen stratification and non-uniform distribution.

Chapter 6 Investigation of the effect of hydrogen-air mixture inhomogeneity

The previous chapter discussed the combustion and emission characteristics of low HSR operation and the stable operation of high HSR via water injection. However, the simulations are based on the fully homogeneous hydrogen-air distribution assumption, which is ideal. In realistic PFI process, the hydrogen mixes with air in the intake pipe and subsequently get charged into the cylinder, forming inevitable inhomogeneity. This chapter will introduce the effect of hydrogen-air mixture inhomogeneity on combustion behaviour and emission characteristics based on different hydrogen-air mixture inhomogeneous assumptions.

6.1 Parameter definition and analytical methods

In this chapter, a subtractive separation method [204,205], shown in Eq. 6.1 is applied to decouple the heat release rate of hydrogen and diesel. The key concept is to first calculate the instantaneous heat release rate of hydrogen from its instantaneous fuel consumption rate $\frac{dm_{H_2}}{d\theta}$ and its lower heating value LHV_{H_2} . Subsequently, the instantaneous diesel heat release rate $\dot{Q}_{\text{diesel}}^*(\theta)$ is obtained by subtracting the hydrogen contribution from the total HRR $\dot{Q}_{\text{tot}}(\theta)$.

$$\dot{Q}_{\text{diesel}}^*(\theta) = \dot{Q}_{\text{tot}}(\theta) - \left(\frac{dm_{H_2}}{d\theta} \right) LHV_{H_2} \quad (6.1)$$

The method assumes that thermo-chemical interactions between hydrogen and diesel are negligible. Although hydrogen oxidation involves a relatively simple reaction compared with diesel hydrocarbon oxidation, interactions between the two fuels may still affect their individual heat-release characteristics. In addition, a small amount of hydrogen may be formed through diesel thermal cracking. Therefore, the decoupled heat-release rates should be regarded as approximate contributions rather than strictly independent heat-release rates. Nevertheless, hydrogen combustion efficiency exceeds 97% for all cases investigated in this study and approaches complete combustion for some cases. Under this simplification, it provides an effective means for analysing the heat release characteristics of dual-fuel combustion.

In this chapter, knocking is defined as the rapid heat release accompanied by a sharp rise in in-cylinder pressure. Ringing Intensity (RI) is introduced in this study to quantify knocking tendency from an engineering perspective. RI is calculated as follows [198]:

$$RI = \frac{\sqrt{\gamma R T_{\max}}}{2\gamma P_{\max}} \left[\beta \left(\frac{dP}{dt} \right)_{\max} \right]^2 \quad (6.2)$$

where γ is the ratio of specific heat, R is the gas constant, $T_{\max}$ is the maximum cylinder temperature, $P_{\max}$ represents the maximum cylinder pressure, β is an empirically scaling coefficient which relates the oscillations and the rise rate of pressure (in this study β is set as 0.05), $\left(\frac{dP}{dt} \right)$ is cylinder pressure rise rate. Following previous studies [201,202,206], an RI threshold of 4 MW/m² is adopted, above which can be diagnosed as knocking.

6.2 Cases description

The in-cylinder homogeneity of the air-fuel mixture when the fuel is injected via port manifold, is challenging to quantify. Wang et al. [173] and Lee et al. [207] have reported a quasi-gaussian distribution of in-cylinder air-fuel mixture, where fuel is distributed according to the swirl direction without wall impingement. This distribution implies that the mixture concentration is relatively higher near the cylinder core and gradually decreases toward the exterior. Tabata et al. [208], Wang et al. [209] and Gammaidoni et al. [210] proposed that under specific conditions, such as high swirl or injection retardation (port injection but closer to intake valve opening) fuel can be concentrated closer to the combustion chamber walls, which is close to Inverted Gaussian distribution. Indicators of homogeneous mixture can be observed during the combustion process (such as increased premixed part of combustion).

To take into account of the inhomogeneous mixture in-cylinder, four hydrogen distributions are explored at the inlet valve closing moment as presented in Fig. 6.1 and explained in Table 6.1. The designed distributions are benchmarked with the homogeneous mixture assumption. In port-fuel-injection (PFI) hydrogen engines, the fuel is introduced upstream of the intake valves, allowing some degree of mixing with air before entering the combustion chamber. However, the in-cylinder distribution after intake valve closure is strongly influenced by complex aerodynamics, including swirl, tumble, and boundary-layer effects, and cannot be directly measured or precisely predicted

in every cycle. As a result, the exact hydrogen concentration field at IVC is uncertain and likely exhibits non-uniformities such as central enrichment, wall-biased accumulation, or layered structures depending on injection timing, flow dynamics, and chamber geometry. To capture the impact of these possible stratification scenarios on combustion, multiple in-cylinder distributions, such as Gaussian, Inverted Gaussian, Exponent Decay, and Double Gaussian, are considered. These distributions are selected to represent plausible extremes and intermediate states of mixing: the Gaussian captures centrally enriched zones that may occur when swirl and radial diffusion dominate; the Inverted Gaussian represents fuel accumulation near walls due to outward transport or wall-film retention; the Exponent Decay mimics strong radial gradients that could arise from partially mixed layers; and the Double Gaussian accounts for deformation of the injected cloud by combined swirl and tumble motions. By exploring this spectrum of distributions, the simulation framework can assess how in-cylinder stratification affects ignition timing, combustion propagation, heat release and emissions, providing a physically meaningful parametric study even in the absence of direct experimental measurements of hydrogen fields after IVC.

For all the defined cases, the diesel peak injection pressure is 1,600 bar, whereas the injection duration is 24.5 °CA. The hydrogen substitution ratio (HSR) utilised is 30% at 100% load engine condition. Such value lies within knocking limitations and is close to the validated values of 24%.

Table 6.1 Cases description with different distribution of H₂ in-cylinder.

No.	Distribution	Equation	Rationale
1	Homogeneous	-	Fully homogeneous air-hydrogen mixture in-cylinder. A very early PFI timing usually results in improved mixture homogeneity, although complete homogeneity can only be achieved under ideal conditions. This case serves as a baseline assumption and is explored for benchmarking purposes.

2	Gaussian	$y_{H_2} = M_{H_2}^{max} e^{-\frac{(r-r_c)^2}{\sigma^2}}$ $M_{H_2}^{max} = 0.00829, \sigma = 0.16$	Represents a centrally enriched fuel zone resulting from an early to intermediate PFI timing and subsequent radial diffusion modelling partially premixed charge compression ignition (PPCI) cases where some mixing occurs before compression begins.
3	Inverted Gaussian	$y_{H_2} = M_{H_2}^{max} \left(1 - e^{-\frac{(r-r_c)^2}{\sigma^2}} \right)$ $M_{H_2}^{max} = 0.00506, \sigma = 0.16$	Reflects wall-concentrated hydrogen stratification due to late PFI timing with insufficient mixing time, swirl-induced outward transport, or wall-film deposition. It captures conditions in dual-fuel engines where hydrogen accumulates near cylinder walls, with leaner core region.
4	Exponent Decay	$y_{H_2} = M_{H_2}^{max} e^{-k(r-r_c)^2}$ $M_{H_2}^{max} = 0.00828, k = 6.25$	This distribution, generated by early-to-intermediate PFI timing, is Gaussian-like in shape but shows a sharper radial decay near the cylinder centre. It suits conditions where fuel is layered intentionally to control ignition timing and spatial burn progression.
5	Double Gaussian (elliptical)	$y_{H_2} = M_{H_2}^{max} \left[e^{-\frac{(r-r_{c1})^2}{\sigma_1^2}} + e^{-\frac{(r-r_{c2})^2}{\sigma_2^2}} \right]$ $M_{H_2}^{max} = 0.00977, \sigma_1 = 0.08, \sigma_2 = 0.12$	Under intermediate PFI timing, and before IVC, the swirl field stretches the port-injected H ₂ -air mixture into an elongated, elliptical cloud. Simultaneously, the tumble motion shears this cloud into two mirror-symmetric vortex bands. Within each band, the hydrogen concentration is highest at the core and decreases progressively toward the cylinder walls.

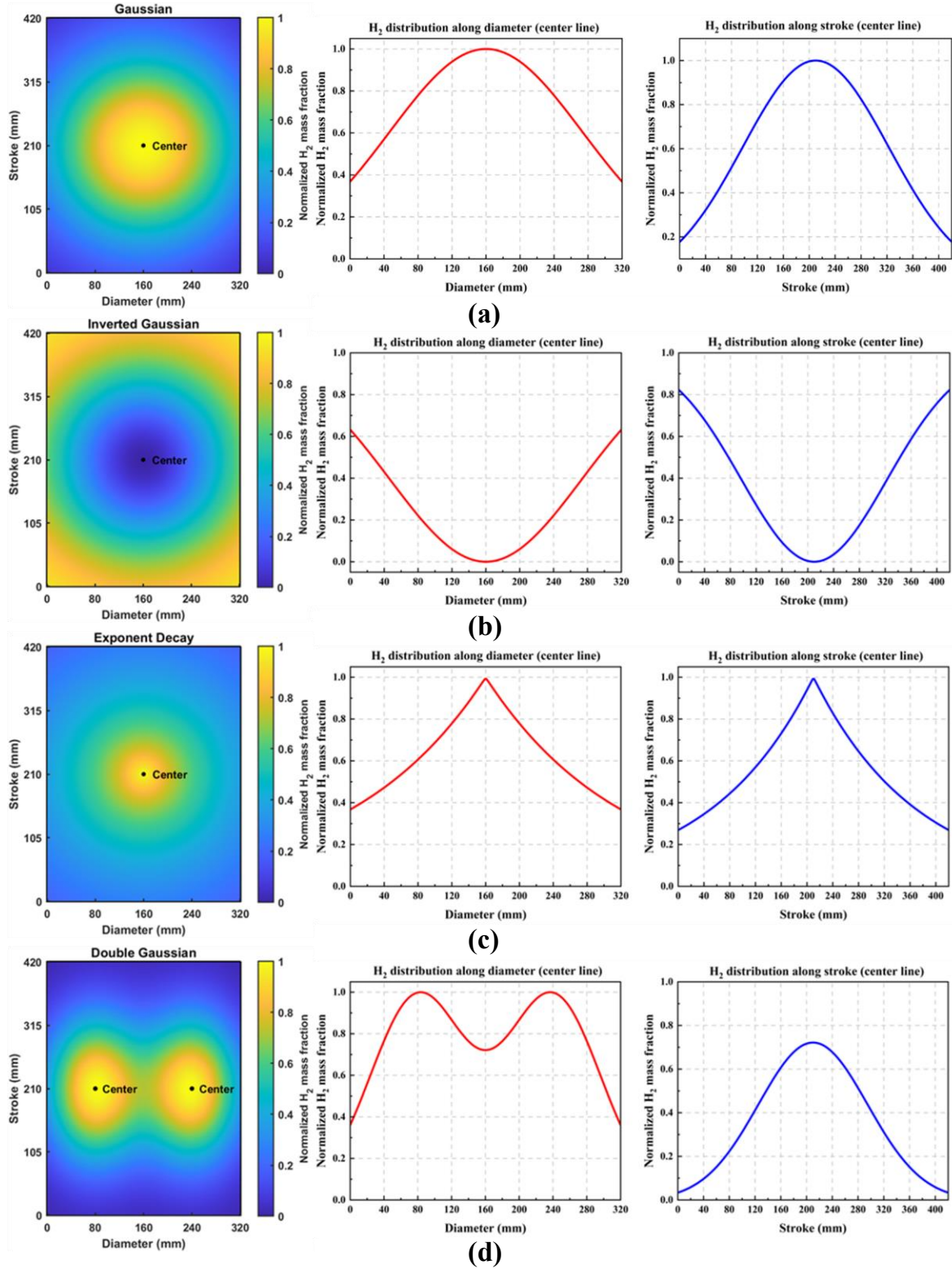


Fig. 6.1 Hydrogen distribution in-cylinder for (a) Gaussian, (b) Inverted Gaussian, (c) Exponent Decay and (d) Double Gaussian distributions.

In Table 6.1, $M_{H_2}^{max}$ is the maximum hydrogen mass fraction, k is the decay factor, $r-r_c$ is the distance from the cylinder centre, σ is the standard deviation of the distribution controlling the spread of the fuel concentration profile. In the above equations the degree of homogeneity is represented by σ and k . Increase in σ represents more uniform distribution, as mass of hydrogen is rising slower from the cylinder centre, whereas smaller σ represents sharper wall enrichment pertaining to stronger stratification. Conversely, for the decay factor k , high values represent reduced homogeneity.

6.3 Engine combustion characteristics

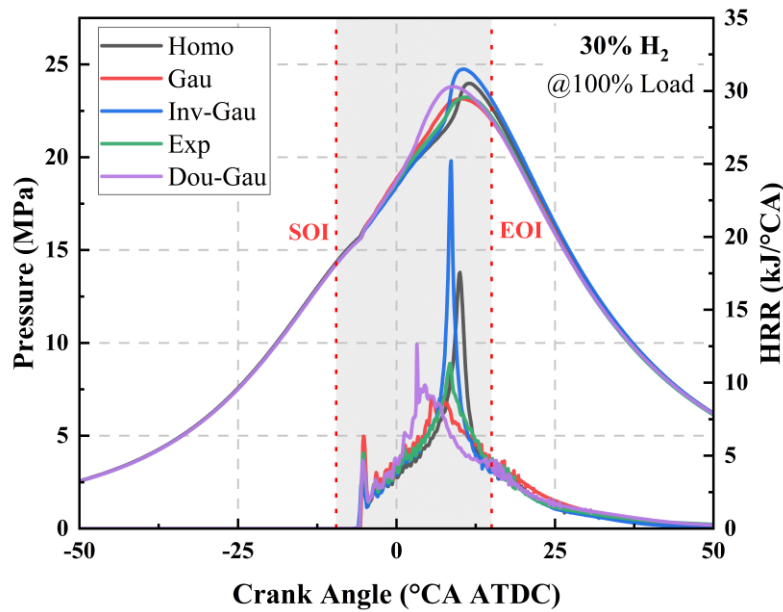


Fig. 6.2 In-cylinder pressure and heat release rate for the explored hydrogen-air mixture distributions.

Fig. 6.2 illustrates the in-cylinder pressure and heat release rate for the examined hydrogen-air mixture distributions. It is evident that the mixing of hydrogen-air significantly influences in-cylinder combustion behaviour. As shown in the figure, the start of combustion (SOC) is nearly identical across all cases, since ignition is mainly governed by the premixed diesel spray. Between the cases, Gaussian and Exponent Decay present higher first peak heat release of 6.3 kJ/°CA and 5.1 kJ/°CA, respectively. The reason is the richer hydrogen concentration around the spatial ignition position. For the second heat release peak, the Inverted Gaussian case exhibits the highest peak value of 25.2 kJ/°CA at 8.6 °CA ATDC, occurring later in the cycle because hydrogen is

concentrated near the chamber boundaries, where the flame front arrives at a later stage. Due to the shorter heat release, the Inverted Gaussian case also attains the highest peak-pressure, reaching 24.7 MPa. Compared to all other cases, the Homogeneous distribution exhibits a delayed peak heat release and peak pressure, occurring at 10°CA and 11.6°CA ATDC, respectively. To further investigate the mechanism of dual-fuel combustion and heat release characteristics under different mixture distributions, a heat release rate (HRR) decoupling analysis, together with a phase-based analysis of key combustion events (SOC, CA10, CA50, and CA90), was conducted for each case.

6.3.1 Homogeneous distribution

Fig. 6.3 (a) and (b) present the heat release decoupling analysis and dual-fuel combustion evolution under homogeneous distribution assumption. For the homogeneous hydrogen-air mixture, the premixed diesel located at the front edge of the spray is responsible for triggering ignition at 6.7 °CA BTDC. The first heat release peak is dominated by diesel combustion, showing a heat release rate of 3.6 kJ/°CA. As diesel combusts with a diffusive flame front, the in-cylinder conditions approach the auto-ignition threshold of hydrogen near top dead centre (TDC), after which hydrogen starts to burn in a premixed flame mode. Until 0.3 °CA ATDC, 10% of total heat release (CA10) is completed, which is mostly contributed by diesel combustion. Owing to its homogeneous distribution in the cylinder and significantly higher burning velocity compared with diesel [43], hydrogen exhibits a rapid heat release, with the peak heat release reaching 12.3 kJ/°CA for hydrogen and 17.6 kJ/°CA for dual-fuel at 10°CA ATDC. It is observed from the contours that at peak HRR the hydrogen located at central cylinder has been consumed, forming high-temperature region at 0.3 °CA ATDC. Due to the thermal cracking of long-chain hydrocarbons, additional hydrogen is formed in the central region where the initial hydrogen has been consumed. At 9.9 °CA ATDC, 50% heat release (CA50) is reached, contributed by both diesel and hydrogen combustion. By 26.5°CA ATDC, the flame front has propagated towards the cylinder boundaries and piston bowl as demonstrated by the high-temperature region around the combustion chamber boundaries. Results for fully premixed mixture are in alignment with the ones observed from the pertinent studies of Karvounis et al. [171,211]. The homogeneous distribution represents the ideal hydrogen premixed condition. From the result, it can be concluded that diesel combustion governs the overall combustion duration while hydrogen combustion is the reason for the HRR peak value.

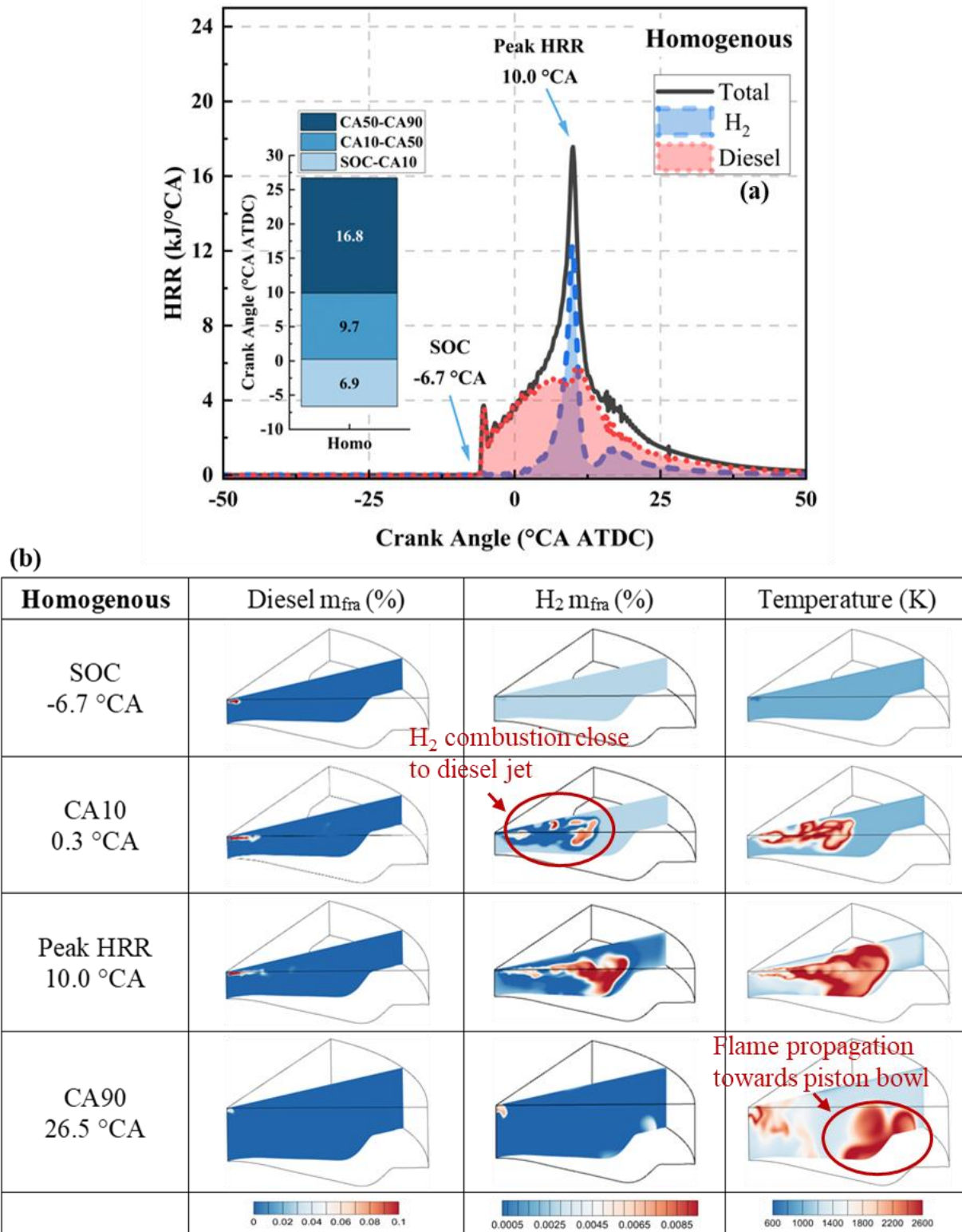


Fig. 6.3 Combustion analysis of hydrogen-diesel dual-fuel combustion under the homogeneous distribution assumption.

6.3.2 Gaussian distribution

The Gaussian distribution represents a centrally hydrogen-rich mixture that gradually decays towards the cylinder walls, corresponding to conditions formed by early or centrally focused port injection followed by radial diffusion.

Fig. 6.4 (a) and (b) present the decoupled heat release analysis and the evolution of dual-fuel combustion under the Gaussian distribution. Combustion is initiated at -6.6°CA ATDC, when diesel auto-ignition occurs and promptly induces the ignition of hydrogen in the adjacent hydrogen-rich region. This is reflected by the nearly simultaneous onset of heat release from both diesel and hydrogen. The simultaneous ignition is attributed to the penetration of the diesel spray front into a locally hydrogen-enriched zone close to the wall, where the high reactivity of the mixture, together with the heat released from diesel diffusion combustion near the spray jet, provides adequate conditions for hydrogen ignition.

The first heat release peak results from the coupled combustion of diesel and hydrogen, with diesel contributing the major portion. Consequently, CA10 is reached at -0.7°CA ATDC, only 5.9°CA after SOC, yielding shorter duration than in the homogeneous case (6.9°CA ATDC), indicating a faster early heat release phase. The peak HRR reaches $8.9\text{ kJ}/^{\circ}\text{CA}$ at 7.4°CA ATDC, while a hydrogen-related peak of $4.6\text{ kJ}/^{\circ}\text{CA}$ appears between 5 and 12.5°CA ATDC, corresponding to hydrogen combustion in the central region. Due to the stratified and sparse hydrogen distribution near the combustion chamber boundary, the hydrogen oxidation is limited, resulting in a significantly lower peak heat release ($4.6\text{ kJ}/^{\circ}\text{CA}$) compared with the homogeneous case ($12.3\text{ kJ}/^{\circ}\text{CA}$). The Gaussian distribution therefore exhibits a longer CA10–CA50 (10.2°CA ATDC) and CA50–CA90 (17.6°CA ATDC) durations, reflecting slower oxidation in the late stage. Between 12.5 and 20°CA ATDC post H_2 combustion occurs where the flame front reaches rich cylinder areas.

Overall, this hydrogen distribution alleviates ignition difficulties in locally lean regions and yields a milder heat release profile, effectively mitigating the knocking tendency associated with rapid hydrogen combustion.

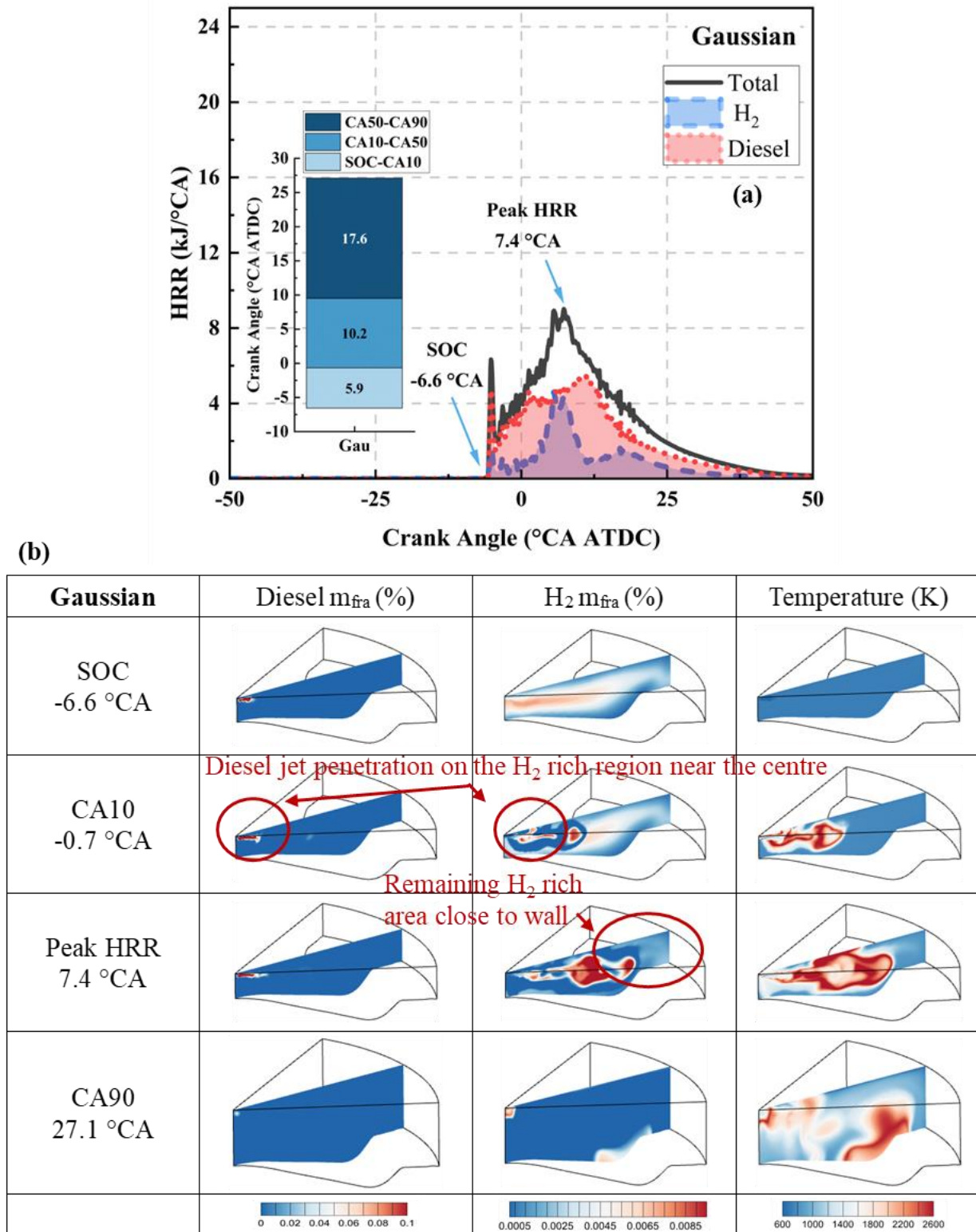


Fig. 6.4 Combustion analysis of hydrogen-diesel dual-fuel combustion under the Gaussian distribution assumption.

6.3.3 Inverted-Gaussian distribution

The Inverted-Gaussian hydrogen distribution in-cylinder implies wall impingement where hydrogen rich zones are observed close to the cylinder walls whereas the mixture turns leaner towards the centre. This distribution represents the outer layer enriched hydrogen distribution.

The decoupled HRR and the evolution of dual-fuel combustion are illustrated in Fig. 6.5 (a) and (b). As shown, the lean hydrogen-air mixture at the cylinder centre offers limited mixture reactivity, leading to a relatively delayed SOC (6.8°CA BTDC). The diffusive diesel flame propagates through the lean hydrogen-air mixture until TDC, when the hydrogen ignition conditions are achieved through both, richer hydrogen mixture and cylinder compression. Consequently, it can be observed that before TDC, nearly all the heat release is attributed to diesel combustion.

Due to the lean hydrogen region at the cylinder centre, the Inverted Gaussian case exhibits the longest SOC–CA10 duration (7.1°CA) among all the defined distributions. At peak HRR (8.6°CA ATDC), due to the combustion of hydrogen-rich layer around the combustion chamber, a highly concentrated hydrogen heat release peak ($19.1\text{ kJ}/^{\circ}\text{CA}$) occurs. The flame front observed is significantly larger than in the case of homogeneous combustion assumption, implying potential combustion instability. Coupled with diesel combustion, the total heat release reaches $25.2\text{ kJ}/^{\circ}\text{CA}$ potentially yielding unstable combustion conditions in-cylinder. Moreover, the Inverted Gaussian case exhibits the shortest CA10-CA50 (8.5°CA) and CA50-CA90 (14.3°CA) among all the explored distributions because of the concentrated heat release by boundary hydrogen-rich layer. The rapid heat release under Inverted Gaussian distribution aligns with the experimental results of Qiao et al. [212], which demonstrated that intensification of combustion is strongly governed by the spatial distribution of hydrogen inhomogeneity. The hydrogen post-combustion area is smaller as the greatest part of fuel has been consumed by 12°CA ATDC leaving a small H_2 -rich region at the bottom of the piston bowl. At 23.1°CA ATDC several areas in-cylinder present high temperature ($2,200 - 2,600\text{ K}$) implying potential knocking occurrence as the temperature field is not uniform.

Overall, the result shows that Inverted-Gaussian distribution led to rapid heat release and potentially causes unstable combustion. The detailed discussion of combustion stability will be expanded in the following section.

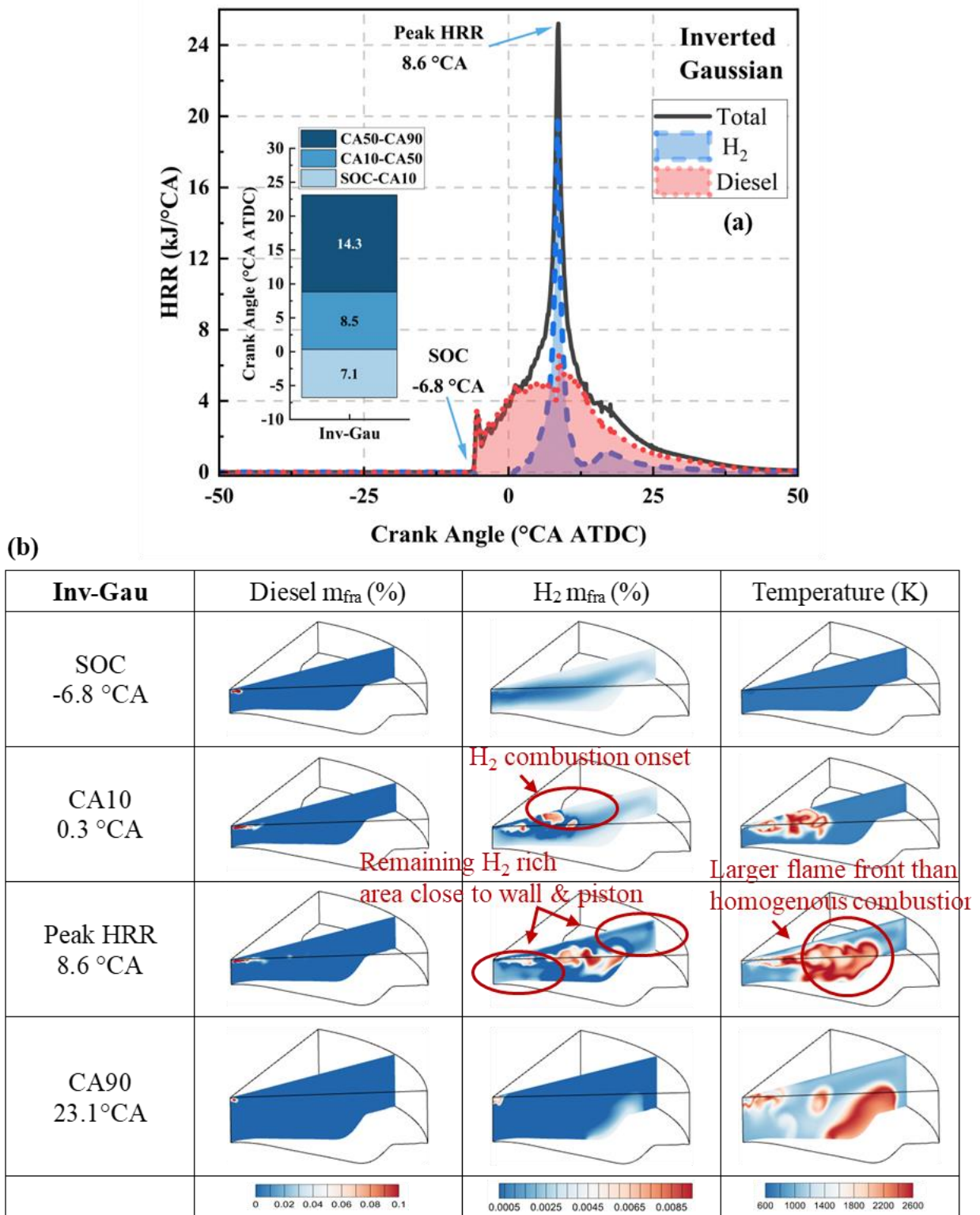


Fig. 6.5 Combustion analysis of hydrogen-diesel dual-fuel combustion under the Inverted Gaussian distribution assumption.

6.3.4 Exponent Decay distribution

The Exponent Decay distribution resembles the Gaussian distribution in exhibiting hydrogen enrichment at the cylinder centre, but its central richness is lower than that of Gaussian. Besides, its attenuation towards the cylinder periphery is more gradual. Consequently, the hydrogen-air mixture around the combustion chamber is richer than that in the Gaussian distribution.

Fig. 6.6 presents the combustion behaviour and the decoupled HRR analysis of Exponent Decay distribution. Due to the hydrogen enrichment at the cylinder centre, similar to the Gaussian distribution, the diesel-initiated combustion achieves earlier ignition in the locally rich hydrogen-air mixture, occurring at 6.6 °CA BTDC. Similarly to Gaussian distribution, hydrogen releases heat nearly simultaneously with diesel ignition, jointly forming the first heat release peak. Consequently, CA10 is reached 6.3 °CA after SOC, indicating a rapid early combustion phase. The Exponent Decay case exhibits a higher hydrogen heat release peak (6.4 kJ/°CA) at 8.4 °CA ATDC, which is higher than that of Gaussian (4.6 kJ/°CA). Such behaviour is observed as the flame has propagated towards the combustion chamber boundaries, where the hydrogen-air mixture is richer than that in the Gaussian distribution. The coupled hydrogen-diesel heat release at that moment is 11.3 kJ/°CA, higher than the 9.0 kJ/°CA value in the Gaussian case. Between the cases, the Exponent Decay one presents extended combustion duration with an amount of hydrogen remaining unburnt. From the perspective of diesel combustion, the HRR profile of Exponent Decay is similar to Gaussian distribution. The peak pressure for the two cases is around 23 MPa, with a 2 °CA phasing delay in the Exponent Decay case. Notably, the Exponent Decay distribution exhibits the longest combustion duration (SOC-CA90) among all cases (37.2 °CA).

Overall, although Exponent Decay distribution shares similar inner hydrogen-enriched pattern with the Gaussian distribution, the HRR profiles and combustion phases exhibit different characteristics. This indicates that hydrogen stratification degree influences dual-fuel combustion behaviour.

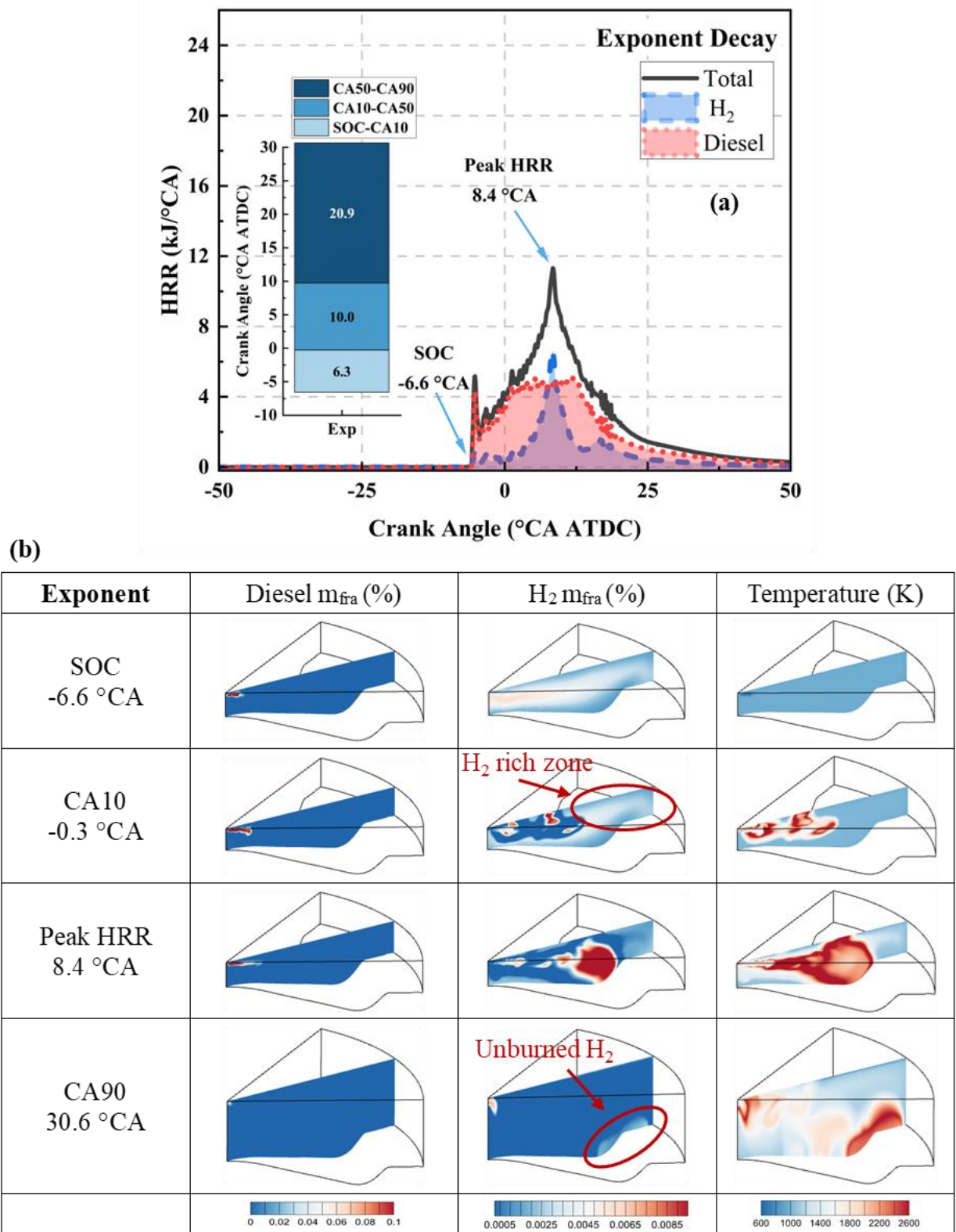


Fig. 6.6 Combustion analysis of hydrogen-diesel dual-fuel combustion under the Exponent Decay distribution assumption.

6.3.5 Double Gaussian distribution

The Double Gaussian distribution represents two hydrogen enrichment zones in cylinder with large central richness but a leaner hydrogen-air mixture near the cylinder head and piston compared with the Gaussian and Exponent Decay distributions. Fig. 6.7 (a) and (b) present the decoupled heat release analysis and the evolution of dual-fuel combustion under the Double Gaussian distribution.

The heat release characteristics demonstrate that diesel combustion initiates at 6.6 °CA BTDC, producing the sharp initial peak due to its short ignition delay and high cetane number. The hydrogen contribution, shaped by the Double Gaussian stratification, sustains combustion in two distinct phases. The hydrogen-rich region in the Double Gaussian case is the richest among all distributions. Therefore, the peak HRR position is the earliest, at 3.2 °CA, showing a peak value of 12.6 kJ/°CA. At 12.5 °CA, wall impingement is observed as the flame front reaches piston bowl and wall regions, where heat losses attenuate combustion.

In the Double Gaussian case, the main reactions occur at the periphery of the diesel jet and within the two hydrogen-rich zones in the cylinder. After 12.5°CA, the momentum from diesel injection promotes the radial dispersion of the flame front, while heat losses continue to suppress combustion near the wall. However, the former effect overrides the latter, resulting in a second, smaller peak heat release until 22 °CA ATDC. The peak in-cylinder pressure is shifted closer to TDC, occurring at 6°CA ATDC, compared with the fully homogeneous and Gaussian distributions. Due to the leanest hydrogen-air mixture around the combustion chamber boundaries, the Double Gaussian case exhibits the longest CA50-CA90 duration (21°CA).

Compared to other distributions, Double Gaussian distribution exhibits a more typical two-stage hydrogen heat release owing to its double-central pattern. Moreover, its peak HRR phase is the earliest among all the investigated distributions.

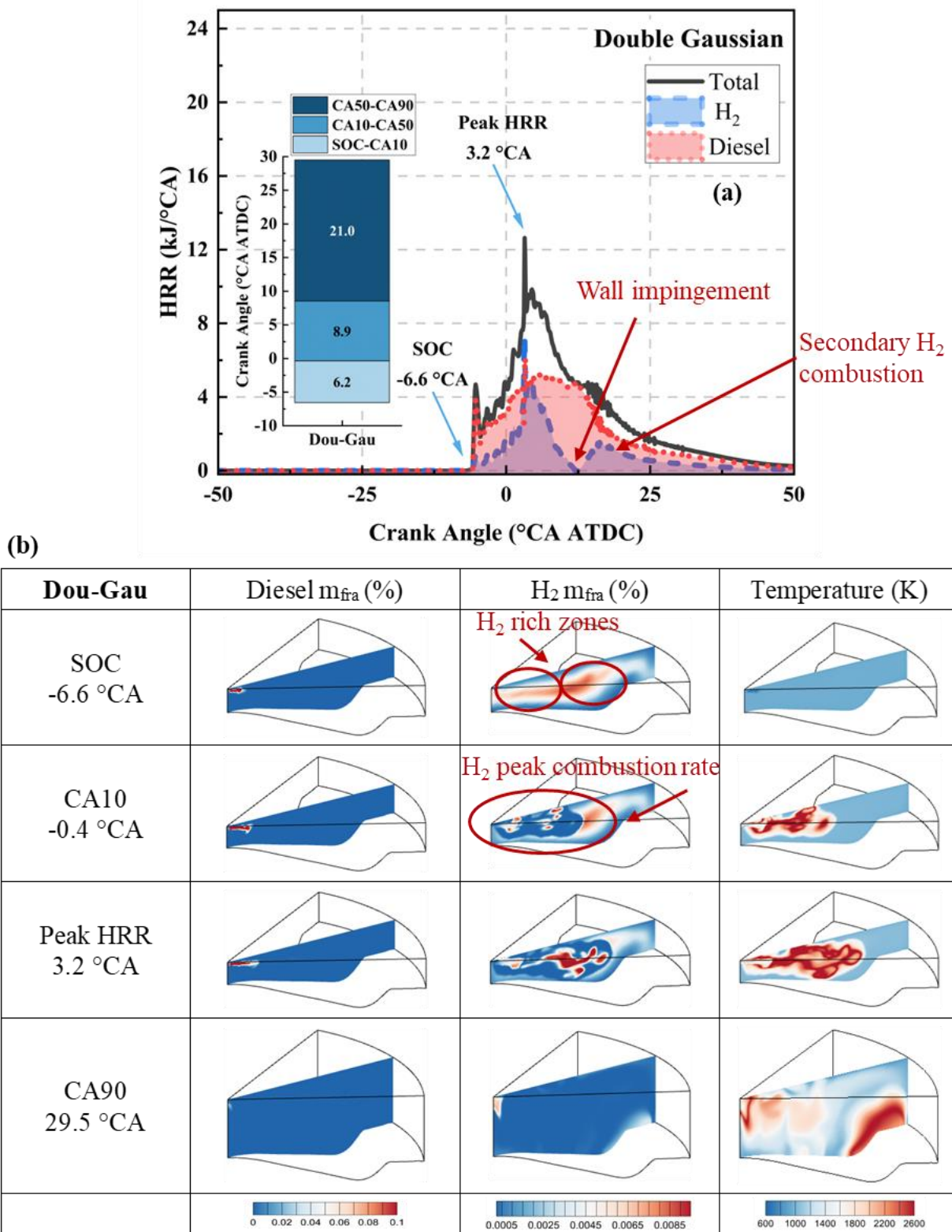


Fig. 6.7 Combustion analysis of hydrogen-diesel dual-fuel combustion under the Double Gaussian distribution assumption.

6.4 Engine performance

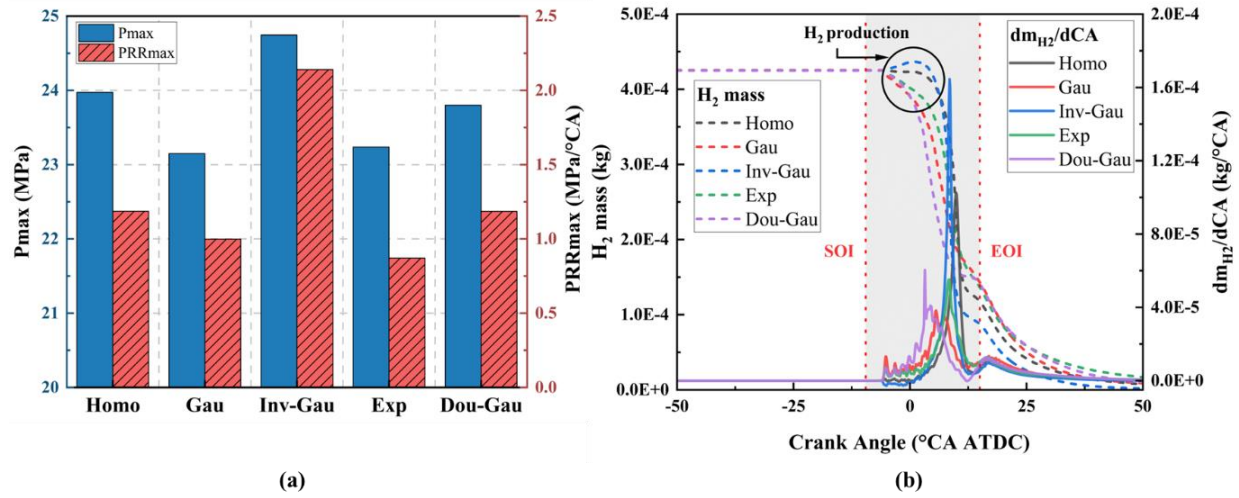


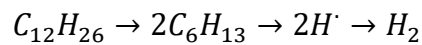
Fig. 6.8 (a) Maximum pressure and maximum rate of pressure rise and (b) hydrogen mass and rate of hydrogen consumption for the explored mixture distributions in-cylinder.

Fig. 6.8 (a) presents the maximum pressure in-cylinder (p_{max}) and the maximum pressure rise rate (PRR_{max}) for the different distribution cases. The latter serves as an indicator of unstable engine operation and values above 2 MPa/°CA should be avoided to ensure engine stability [213]. Among the examined cases, the Inverted Gaussian distribution yields the highest peak pressure and maximum pressure rise rate (24.7 MPa and 2.1 MPa/°CA, respectively). This is attributed to the increased in-cylinder hydrogen stratification, with most of the fuel concentrated near the cylinder walls, where locally rich zones combust rapidly during the late combustion phase. The maximum pressure rise rate exceeds the stability threshold, which may result in rough engine operation. Beyond the pressure rise rate (PRR), the Ringing Intensity (RI) was employed as an additional indicator to assess knocking tendency. The RI of the Inverted Gaussian calculated using Equation 6.2 is 0.46 MW/m², which is lower than the adopted threshold of 4 MW/m². However, the Inverted Gaussian case exhibits the highest RI among the investigated distributions. This suggests an increased tendency toward knock-prone combustion behaviour for the Inverted Gaussian under the same initial condition and hydrogen substitution ratio.

Homogeneous distribution assumption results in a 24.0 MPa maximum pressure with a 1.2 MPa/°CA PRR_{max} associated with stable combustion conditions that are secured due to hydrogen-air mixture uniformity in-cylinder. Gaussian, Exponent Decay and Double Gaussian

cases yield maximum pressure values of 23.1 MPa, 23.2 MPa and 23.8 MPa respectively whereas the PRR_{max} is 1.0, 0.9 and 1.2 MPa/°CA respectively. The small variations indicate that central hydrogen-rich mixture leads to milder combustion conditions with prolonged combustion duration. The combustion initiation from diesel diffusive spray ignites the rich regions of hydrogen simultaneously providing a stable flame front, whereas subsequent flame propagation to the other zones occurs gradually. Such progressive burning reduces the instantaneous heat release rate resulting in lower maximum pressure in-cylinder. Such behaviour is susceptible to reversed inhomogeneity, as observed in the case of Inverted Gaussian distribution, where the high temperature flame front reached the mixture later and resulted in instantaneous burning.

Fig. 6.8 (b) illustrates the in-cylinder hydrogen mass and the rate of hydrogen consumption during the combustion process for different mixture distribution assumptions. The mass of hydrogen in-cylinder indicates the hydrogen combustion efficiency for each homogeneity assumption. Different cases exhibit hydrogen reduction at different crank angles due to variations in the start of combustion (SOC) timing. For the homogeneous and Inverted Gaussian cases, it is evident that hydrogen formation occurs in-cylinder at approximately 5°CA ATDC. When diesel is injected into the highly compressed air-hydrogen mixture, atomization and vaporization take place, while the locally rich spray core reaches temperatures above 1,500 K. Under these conditions, long-chain hydrocarbons undergo thermal cracking, producing smaller hydrocarbon radicals and hydrogen, as represented by the following thermal pathway to H₂ formation [214].



The recombination of hydrogen radicals (H[·]) to form molecular hydrogen (H₂) is a highly temperature-dependent process, promoted by elevated in-cylinder temperatures. Notably, diesel thermal cracking is accompanied by heat absorption from the surrounding, as evidenced by the relatively low-temperature regions associated with hydrogen formation in Fig. 6.3 (b)–Fig. 6.7 (b). Fig. 6.9 presents the H radicals and in-cylinder temperature for different distributions. As shown, the H radicals and temperature increase rapidly after TDC, reaching their peak value between 10–20 °CA ATDC. After that, the radicals level drops down, indicating the recombination reaction of hydrogen. The Inverted Gaussian and homogeneous case exhibit a higher in-cylinder temperature and a faster H radical consumption compared with the other distributions. That's the reason why more hydrogen production is observed for these two cases in Fig. 6.8 (b).

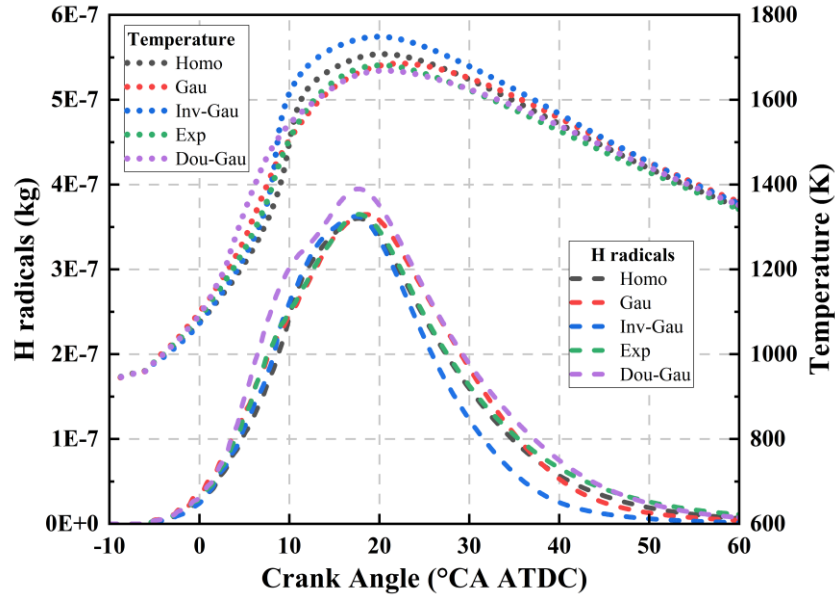


Fig. 6.9 H radicals and in-cylinder temperature variations under different inhomogeneous assumptions.

Hydrogen combustion efficiency is evaluated based on the unburnt hydrogen remaining at the end of the combustion process. According to the results, all cases exhibit adequate combustion efficiency ($m_{H_2_out}/m_{H_2_in} > 97\%$), whereas the homogeneous and Inverted Gaussian cases achieve nearly complete combustion ($m_{H_2_out}/m_{H_2_in} > 99.5\%$). The rapid hydrogen oxidation rate shortens the combustion duration in the homogeneous and Inverted Gaussian cases, with all hydrogen consumed by 27°CA ATDC. In contrast, the Gaussian, Exponent Decay, and Double Gaussian cases exhibit prolonged hydrogen combustion. Because the temperature rise in-cylinder is milder, no intermediate hydrogen formation is observed in these cases.

Fig. 6.10 (a) demonstrates the energy distribution for the explored mixture homogeneity assumptions. The total energy entering the cylinder is represented in three distinct bars highlighting the indicated thermal efficiency (red bar), the heat transfer losses that pertain to the cylinder walls, cylinder head and piston bowl (yellow bar) and other losses (blue bar) that mainly represent wasted exhaust gas energy, incomplete combustion loss and radiant heat dissipation. Wall heat transfer loss is identified as a critical energy loss component that significantly affects the indicated thermal efficiency. The detailed heat transfer from the boundaries, including the piston, cylinder wall, cylinder head, and total heat loss, is presented in Fig. 6.10 (b). Inverted Gaussian distribution presents higher indicated thermal efficiency (ITE), reaching 48.9%. This is attributed to the rapid

and concentrated heat release, which produces elevated in-cylinder temperatures within a short crank-angle duration, as well as the complete combustion of hydrogen. The Exponent Decay and Double Gaussian cases exhibit similar thermal efficiencies (47.3% and 47.7%, respectively), as a portion of the input fuel energy is lost due to incomplete hydrogen combustion. Compared to the homogeneous case, the Gaussian distribution exhibits a longer combustion duration but lower in-cylinder temperatures. The net outcome is smaller wall heat transfer losses, which can be seen in Fig. 6.10 (b). Nevertheless, the thermal efficiency improves only slightly (from 48.0% to 48.1%) because of incomplete hydrogen combustion. Overall, the air-hydrogen mixture in-cylinder affects the indicated thermal efficiency of the engine mainly through heat transfer and incomplete combustion losses variations.

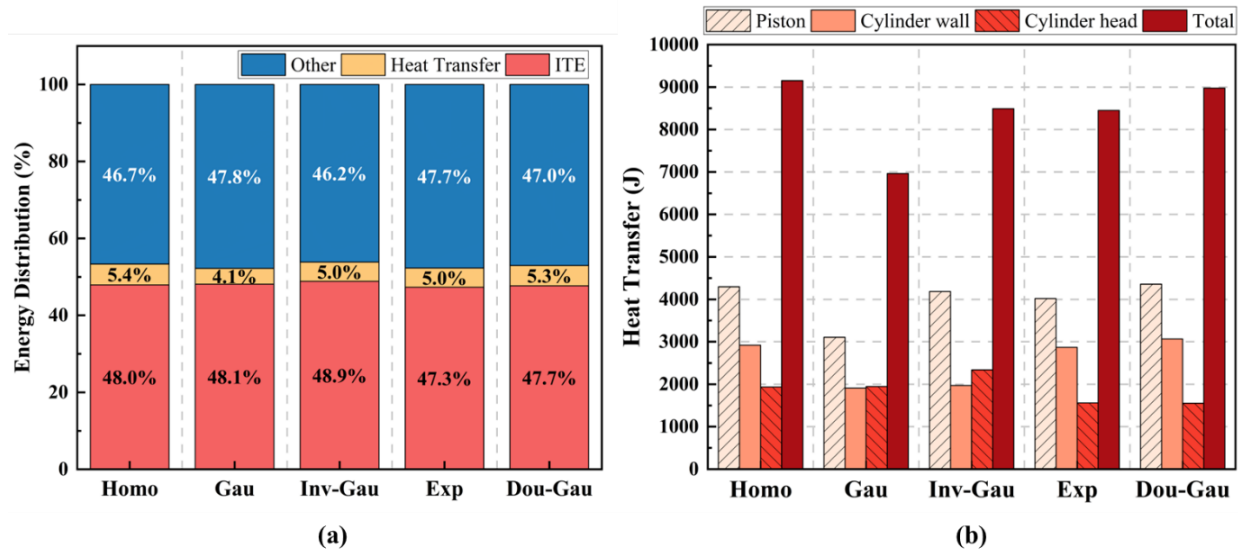


Fig. 6.10 Energy analysis for the explored mixture distributions in-cylinder. (a) Energy distribution analysis (b) heat transfer distribution.

According to Fig. 6.10 (a) it is observed that the heat transfer losses account for 5.4%, 4.1%, 5.0%, 5.0%, and 5.3% of the input fuel energy for the homogeneous, Gaussian, Inverted Gaussian, Exponent Decay, and Double Gaussian cases, respectively. All non-homogeneous cases exhibit slightly lower heat transfer losses compared with the fully homogeneous mixture. The total wall heat transfer loss of the homogeneous distribution is 9,152 J, the highest among all examined cases. This is attributed to the high in-cylinder temperatures and relatively long combustion duration. Compared with the Inverted Gaussian case, although higher temperatures are achieved, the much

shorter combustion duration contributes to its lower heat transfer loss (8,492 J). Owing to its moderate heat release and centrally confined combustion, the Gaussian case exhibits the lowest total wall heat transfer loss (6,965 J), with the smallest contributions from the piston (3,108 J) and cylinder wall (1,909 J). The Double Gaussian case exhibits 527 J higher wall heat transfer than the Exponent Decay case, primarily contributed by the piston and cylinder wall, due to its earlier heat-release peak near TDC (3.2°CA ATDC).

6.5 Engine regulated emissions

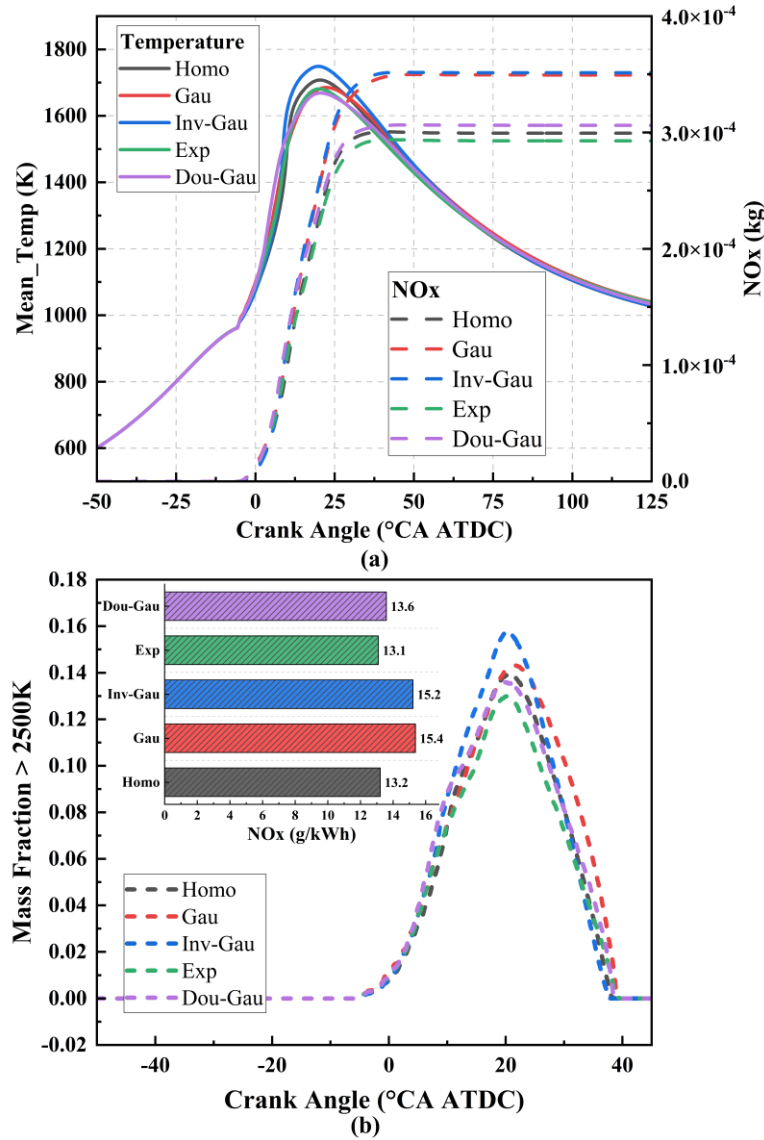


Fig. 6.11 NOx emissions for the examined cases. (a) mean in-cylinder temperature and NOx formation; (b) regulated NOx emissions and in-cylinder mass fraction above 2,500 K.

Fig. 6.11 illustrates the in-cylinder temperature, NO_x emissions and fraction of in-cylinder mixture exposed to temperatures above 2,500 K. Because NO_x formation increases exponentially with temperature, variations in the extent and distribution of high-temperature regions strongly influence the resulting NO_x emissions. The Inverted Gaussian case exhibits the highest peak in-cylinder temperature, reaching 1,749 K, due to the rapid and concentrated heat release of hydrogen combustion in the boundary-enriched region. The Inverted Gaussian case shows the largest mass fraction above 2,500 K between 12° and 24°CA ATDC, reaching a peak of 0.16 at 20°CA ATDC. The near-wall intensive combustion observed in Fig. 6.5 is shown by localized high-temperature regions, which strongly promote thermal NO formation via the extended Zeldovich mechanism. Based on the above analysis, the Inverted Gaussian case exhibits the highest total NO_x formation but the second-highest NO_x emissions (15.2 g/kWh), this is attributed to its greater indicated work output resulting from the complete hydrogen combustion. The Gaussian distribution produces nearly as much NO_x as the Inverted Gaussian case, owing to its high mass fraction above 2,500 K after 24°CA ATDC. However, its regulated NO_x emissions are 0.2 g/kWh higher, attributed to the lower hydrogen combustion efficiency. The regulated NO_x for Homogeneous, Exponent Decay and Double Gaussian case is relatively lower at 13.2, 13.1 and 13.6 g/kWh. It can be seen that, for these three distributions, the in-cylinder mass fraction above 2,500 K remains low, and the residence time of high-temperature gases is relatively short.

The regulated emissions, including CO, soot, and unburnt H₂, are presented in Fig. 6.12. Among all the cases, the Exponent Decay distribution exhibits the highest levels for all emission species, with 0.365 g/kWh of CO, 0.197 g/kWh of soot, and 0.191 g/kWh of H₂, indicating lower combustion efficiency. In contrast, the Inverted Gaussian distribution demonstrates complete combustion, with CO and soot emissions below 0.03 g/kWh and nearly zero H₂ emission. The Homogeneous case presents relatively high CO (0.281 g/kWh) and soot (0.099 g/kWh) but low hydrogen emissions (0.059 g/kWh), while the Gaussian case shows the lowest CO (0.015 g/kWh) and moderate soot (0.040 g/kWh) emissions but high hydrogen slip (0.148 g/kWh). Compared with the Gaussian distribution, the Double Gaussian case yields higher CO and soot emissions, while its hydrogen emission is slightly lower, at 0.135 g/kWh. Overall, the emission variations indicate that combustion completeness is strongly affected by the in-cylinder hydrogen distribution pattern.

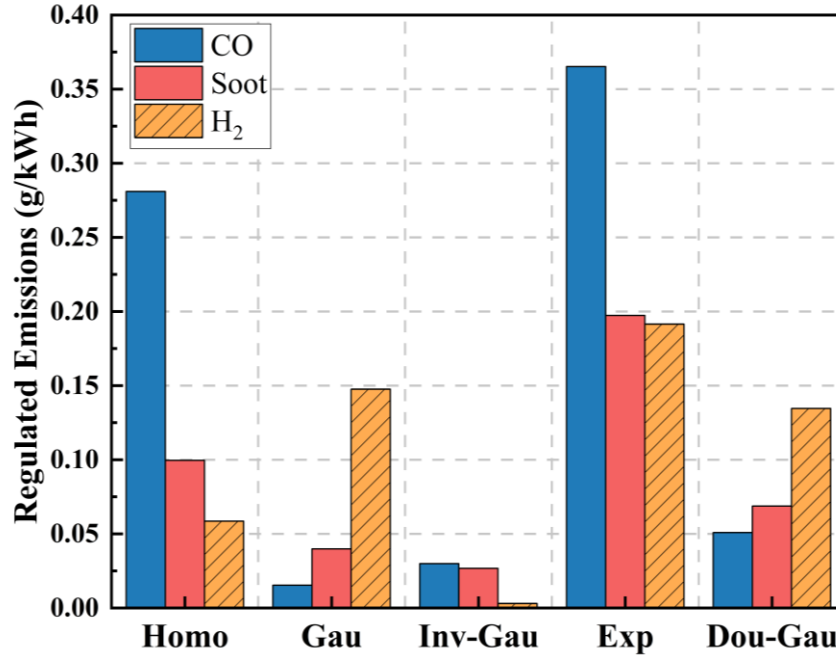
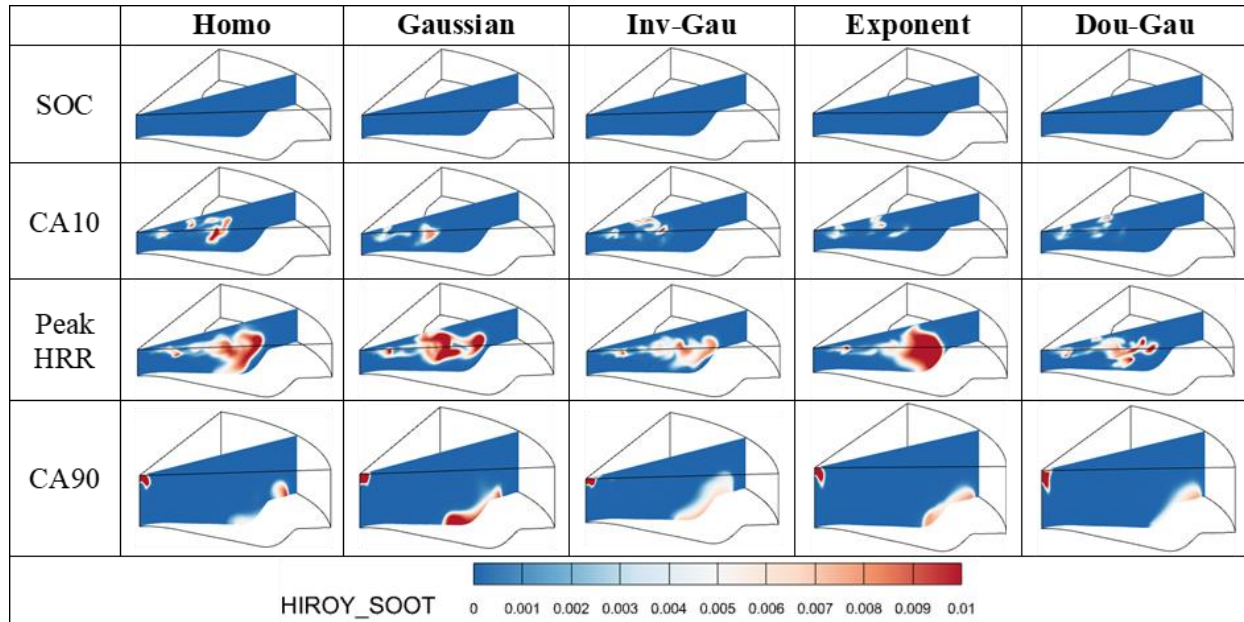
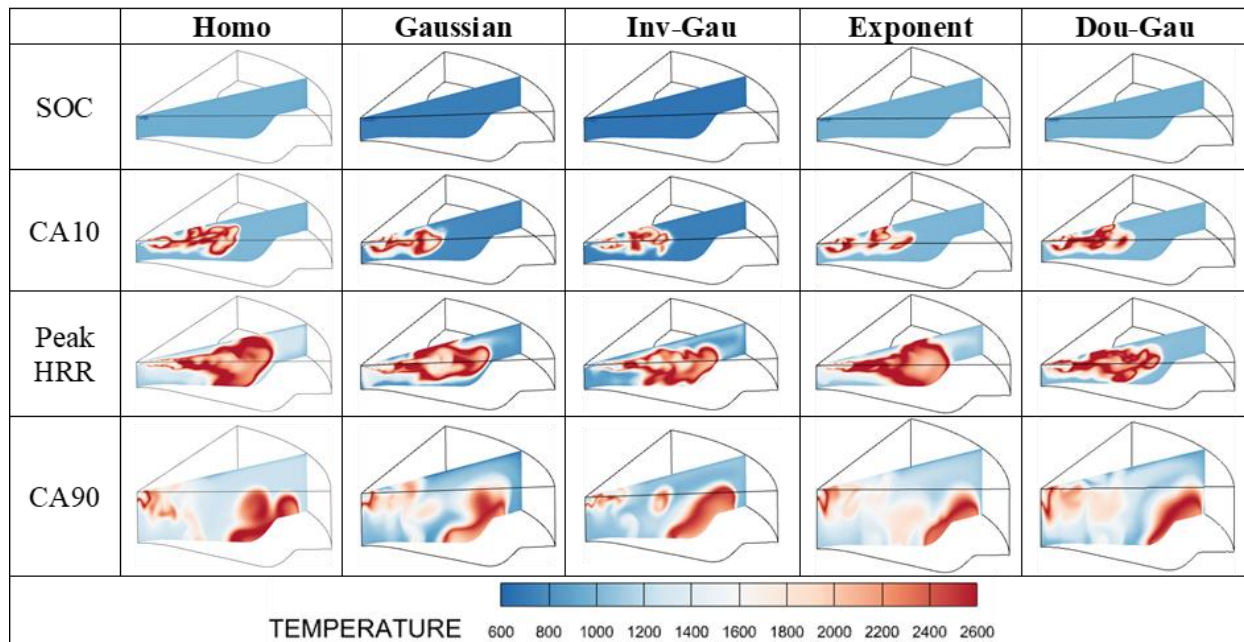


Fig. 6.12 Regulated CO, Soot and H₂ emissions for examined cases.

Fig. 6.13 illustrates the evolution of soot and temperature distributions for the explored cases at representative crank angles. Soot is a product of incomplete diesel combustion, typically formed in regions with high temperature and insufficient oxygen availability [215]. In general, comparing the soot and temperature distributions, high soot concentrations are observed in relatively cooler regions, between 1,600–2,200 K, on the inner side of high-temperature zones, suggesting the soot formation temperature window. For all cases, soot formation reaches its maximum at peak HRR, where diesel and hydrogen combustion consumes the available in-cylinder oxygen. The Exponent Decay case displays a wide soot-enriched region at 8.4°CA ATDC, consistent with its highest soot emission in Fig. 6.12. This is attributed to the combined effects of locally diesel-rich combustion and the soot formation temperature window of 1,600–2,200 K. Although soot oxidation occurs at a later stage, a substantial amount of soot remains at the end of combustion. Conversely, the Inverted Gaussian case shows limited soot formation at 8.6°CA ATDC due to weaker oxygen competition from hydrogen, resulting in the lowest soot emission. Both the Homogeneous and Gaussian cases produce noticeable soot during the peak HRR phase. However, the Gaussian case undergoes stronger late-stage oxidation, reducing soot emissions to less than half those of the Homogeneous case. The Double Gaussian case exhibits moderate soot accumulation (0.069 g/kWh) at 3.2°CA ATDC.



(a)

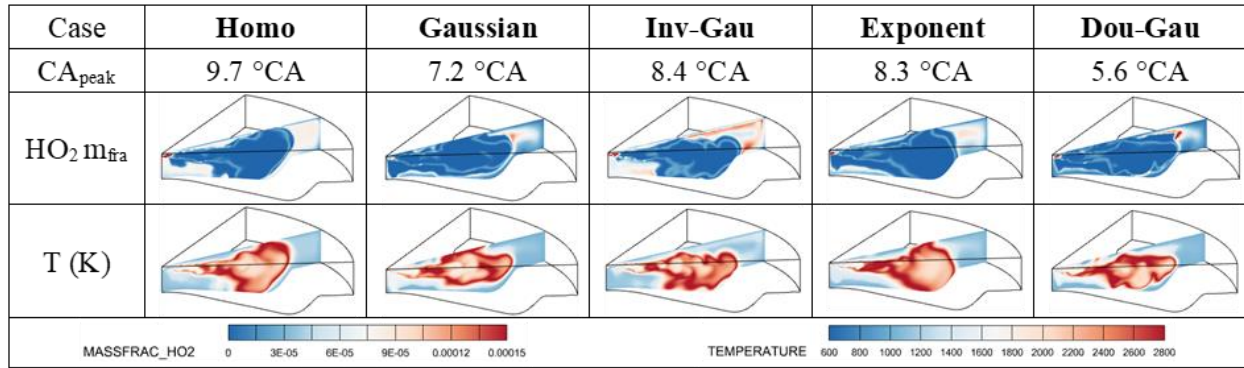
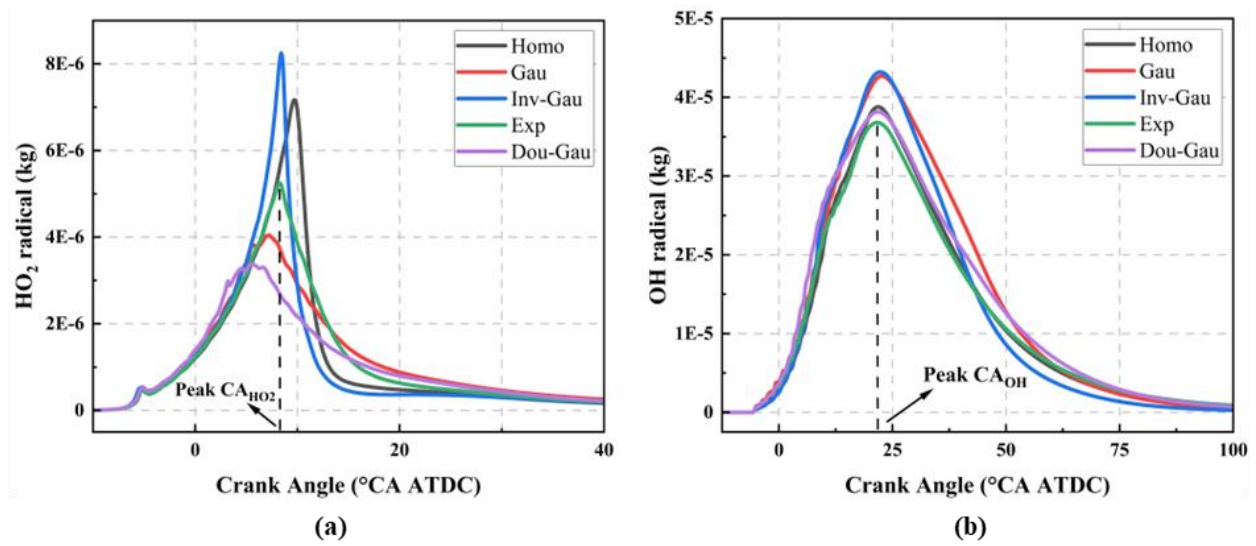


(b)

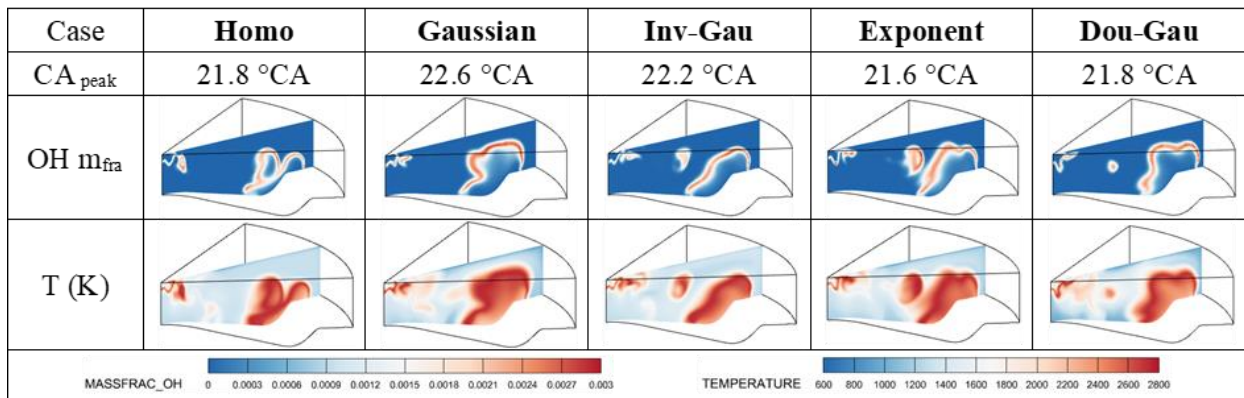
Fig. 6.13 Soot formation and temperature evolution for the investigated cases at SOC, CA10, peak HRR, and CA90.

During hydrogen combustion, Hydroperoxyl (HO_2) radicals are important intermediate species, representing the low-temperature (800–1,100 K) chain reaction activity [216]. It indicates the potential for achieving more complete combustion [217]. To illustrate the intensity of low-temperature reactions, Fig. 6.14 (a) and (c) compare the in-cylinder HO_2 level and spatial distribution at the peak HO_2 crank angle. In all cases, HO_2 accumulates in the low-temperature region before the main combustion develops and is subsequently consumed as the temperature rises. The HO_2 -rich regions generally align with the unburnt hydrogen zones, indicating the preparatory activation of hydrogen prior to oxidation. For the Double Gaussian case, the HO_2 peak occurs earliest at 5.6°CA ATDC and exhibits the lowest intensity, indicating limited reaction potential for this case. This is because hydrogen is largely consumed at the early stage, leaving limited residual hydrogen available for subsequent oxidation. In contrast, the Inverted Gaussian and Homogeneous cases exhibit higher reaction potential, with a larger proportion of hydrogen remaining unburnt at the peak HO_2 moment. For these two distribution patterns, the hydrogen concentration in the central region of the cylinder is relatively lean.

OH radicals, shown in Fig. 6.14 (b) and (d), reflect high-temperature oxidation intensity and are concentrated along the flame front [218]. The OH peak crank angle is nearly identical for all cases (around 22°CA ATDC), since the high-temperature oxidation is governed mainly by diesel combustion, which follows a similar combustion profile across cases. At the OH peak, strong oxidation occurs along the high-temperature flame front near the piston surface. The Inverted Gaussian and Gaussian cases show the highest OH peaks, with darker red bands in the central region, indicating relatively stronger combustion intensity. The Inverted Gaussian case exhibits the highest HO_2 and OH peaks, reflecting both strong low-temperature activation and intense high-temperature oxidation, thereby resulting in the most complete combustion. In contrast, limited HO_2 formation in the Gaussian case restricts oxidation propagation, leading to locally intense but spatially confined combustion and higher unburnt hydrogen emissions. The Exponent Decay case exhibits a moderate HO_2 level but the lowest OH concentration, confirming incomplete oxidation and explaining its elevated CO and soot, emissions.



(c)



(d)

Fig. 6.14 (a) and (b) Temporal variations of HO₂ and OH radicals for explored cases; (c) and (d) The spatial distribution of HO₂ and OH radical for the explored cases.

6.6 Critical discussion

A comprehensive comparison of key combustion and emission parameters (ITE, Peak HRR CA, PRRmax, NOx, soot, and unburnt H₂) for the explored hydrogen distributions is presented in Fig. 6.15. This discussion focuses on comparing the combustion and emission characteristics of the prescribed CFD distribution cases and does not aim to determine an optimal hydrogen distribution. As shown, the homogeneous distribution, as the benchmark case, exhibits the latest peak HRR crank angle of 10.0°CA ATDC, indicating that inhomogeneous hydrogen distributions advance the hydrogen combustion phase. Although the Inverted Gaussian case exhibits the highest ITE and the lowest soot and unburnt hydrogen emissions, the relatively high PRRmax may lead to rough operation and potential combustion instability. Conversely, the Exponent Decay case, due to its mild combustion intensity, results in the highest soot and unburnt hydrogen emissions. Moreover, its ITE and NOx are the lowest among all cases. The Double Gaussian case shows the earliest peak HRR crank angle, suggesting that its combustion is concentrated in the early stage.

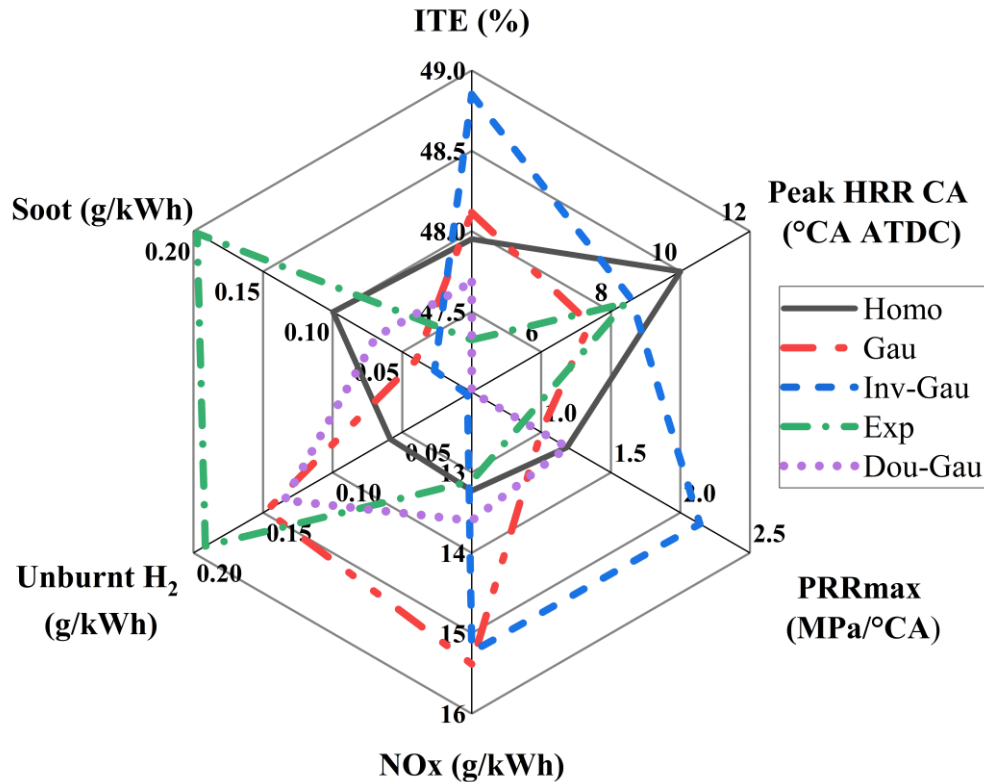


Fig. 6.15 Radar chart comparison of key combustion and emission parameters under different hydrogen distributions.

6.7 Summary

This chapter investigates the effects of inhomogeneous premixed hydrogen distributions on hydrogen-diesel dual-fuel combustion and emission characteristics under a 30% hydrogen substitution ratio (HSR) of port fuel injection (PFI). Through a UDF definition, four patterns of in-cylinder hydrogen inhomogeneous distribution were explored and benchmarked with the homogeneous combustion assumption. The main findings of this chapter are as follows:

1. Different hydrogen distribution patterns strongly influence the dual-fuel heat release behaviour, primarily through their impact on hydrogen combustion. In contrast, the difference in the decoupled diesel heat release profile is relatively limited.
2. For all the inhomogeneous distributions, the peak heat release rate (HRR) occurs at an earlier crank angle compared to the homogeneous benchmark, suggesting that inhomogeneity advances the hydrogen combustion phase. For CFD simulations that adopt homogeneous assumptions, a delayed heat release is predicted compared to the inhomogeneous condition. Among these cases, the Double Gaussian distribution exhibits the earliest peak HRR, appearing at 3.2° CA ATDC, earlier than any other cases.
3. The Inverted Gaussian distribution demonstrates the highest indicated thermal efficiency of 48.9% and the most complete dual-fuel combustion. However, it shows a maximum pressure rise rate of $2.1 \text{ MPa}/^{\circ}\text{CA}$, exceeding the stable threshold, indicating that an exterior-rich hydrogen distribution may induce unstable combustion and potential knocking tendency.
4. Although the Gaussian, Exponent Decay, and Double Gaussian cases share a similar centre-rich hydrogen distribution pattern, they exhibit distinct combustion characteristics due to their different degrees of stratification.
5. The homogeneous distribution, used as the benchmark case, exhibits an ITE of 48.0% together with relatively moderate emission levels. This case provides a reference for assessing the sensitivity of combustion and emissions to the assumed inhomogeneous hydrogen distributions.

This chapter sheds light on inhomogeneous premixed hydrogen combustion behaviour and provides guidance for PFI control in marine diesel engines under port-fuel injection conditions.

Chapter 7 Investigation of low-load performance improvement strategies

The previous chapters investigate the engine combustion and emissions behaviour under high load conditions. However, engine low-load performance of hydrogen-diesel dual-fuel operation usually degrades, mainly due to hydrogen incomplete combustion caused by insufficient in-cylinder reactivity. Few studies have discussed the control strategies to recover engine performance, especially in high HSR conditions. This chapter gives a systematic investigation of the control strategies to improve the low-load performance of engine dual-fuel operation. The effects of compression ratio, diesel injection timing, and diesel split injection control were examined both individually and in combination at 20% load. Due to the lack of low-load operation data of 320 mm-bore engine, this chapter conducts investigation based on the 460 mm-bore engine.

7.1 Case study description

Marine medium-speed engines may operate at low loads during manoeuvring, port operations and other low-power-demand conditions, as well as during generator-set operation owing to variations in onboard electrical demand [219]. Under such conditions, reduced in-cylinder temperature and reactivity can lead to incomplete hydrogen combustion and deterioration in engine performance. Therefore, a 20% load condition was selected in this study as a representative low-load case to investigate hydrogen combustion deterioration and the corresponding control strategies.

To systematically investigate combustion control strategies for performance improvement under low-load (20% load) condition, a stepwise parametric investigation framework was adopted, which is illustrated by Fig. 7.1. This study considers a variable compression ratio engine, with the compression ratio varied from 14 to 19 and adjusted according to engine load and hydrogen substitution ratio. The parametric investigation was conducted under the constraints of maintaining the indicated thermal efficiency (ITE) of the diesel baseline and NO_x emissions not exceeding the baseline. In the first stage, the compression ratio (CR = 14, 16.5, and 19) was varied at hydrogen substitution ratios (HSR) of 20%, 40%, and 60%, while the diesel start of injection (SOI) was fixed at -7°CA ATDC, corresponding to diesel operation. This resulted in 9 simulation cases. In the second stage, the influence of injection timing was evaluated by varying the SOI (-4° , -7° , and $-$

10°C_A ATDC) at the same HSR levels, while maintaining a fixed compression ratio of 14, consistent with the baseline diesel configuration. This stage also comprised 9 cases. Subsequently, a coupled analysis was performed to examine the interaction effects of CR and SOI. A full-factorial CR–SOI–HSR design ($3 \times 3 \times 3$) was established, resulting in a total of 27 cases. Among these, 18 cases had already been resolved in the previous single-variable investigations, and 9 additional simulations were conducted to complete the full matrix.

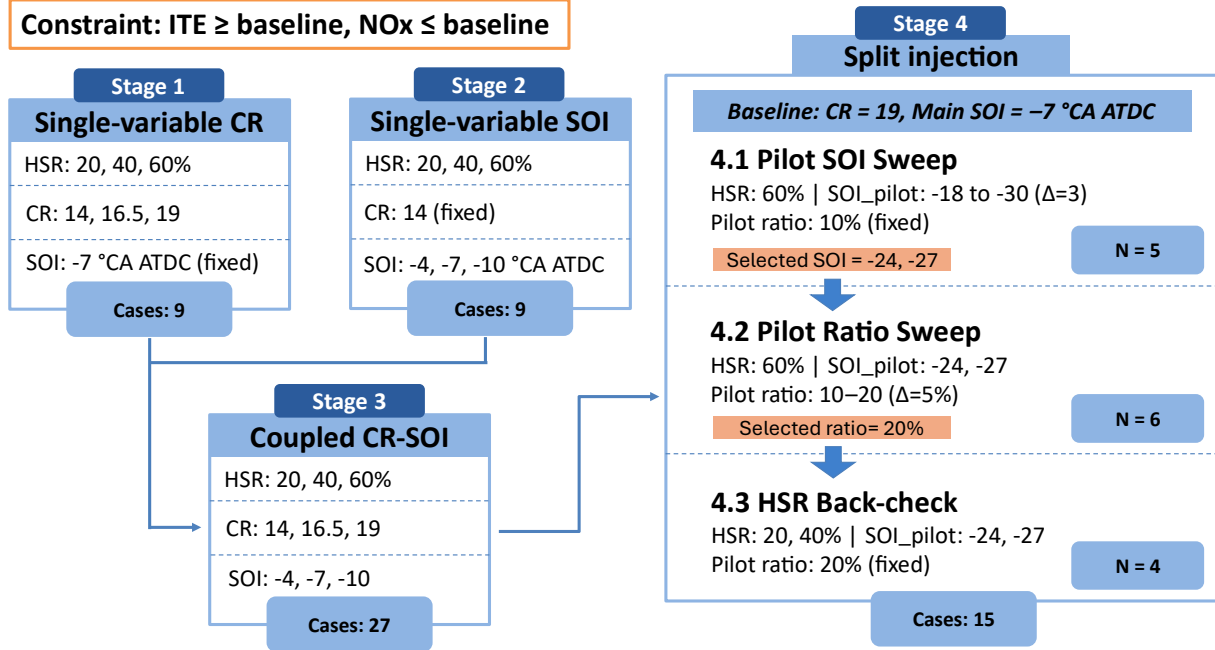


Fig. 7.1 Stepwise parametric investigation framework of low load combustion control strategy.

Based on the outcomes of the coupled analysis, a split injection strategy was further investigated under high compression ratio conditions to enhance in-cylinder premixing reactivity and achieve additional combustion enhancement. The split injection investigation focused on 60%HSR conditions, where combustion behaviour is mainly governed by premixed hydrogen combustion.

A pilot SOI sweep was first conducted, in which pilot diesel fraction was fixed at 10%, and the pilot injection timing ranged from -18° to -30°C_A ATDC with an interval of 3°C_A, resulting in 5 cases. Subsequently, a pilot energy ratio sweep was performed at selected pilot SOI conditions to evaluate the influence of pilot fraction (10%, 15%, and 20%). Finally, additional simulations were conducted at HSR levels of 20% and 40% to assess the applicability of the split injection strategy across different substitution ratios.

7.2 Effect of compression ratio

Fig. 7.2 presents the effect of varied compression ratio on H_2 combustion efficiency, indicated thermal efficiency, regulated NO_x and CO at varying HSR. As shown in Fig. 7.2 (a), at CR of 14, hydrogen combustion efficiency remains low under all three HSR, and progressively decreases as HSR increases. At HSR = 60%, the combustion efficiency is limited to 36.3%, indicating that the original compression ratio is insufficient for high HSR combustion at low load. This behaviour can be explained by insufficient in-cylinder reactivity due to low intake temperatures at low loads. With increasing HSR, the combustion process becomes increasingly hydrogen-dominated, further amplifying the sensitivity to reactivity. As the compression ratio is elevated from 14 to 16.5 and further to 19, hydrogen combustion efficiency improves consistently across all HSR conditions. At CR = 19, the combustion efficiency exceeds 59% for all substitution ratios, reaching a maximum of 64% at HSR = 20%. The rate of combustion efficiency improvement from CR = 14 to 16.5 is comparable among the three HSR conditions. However, when the compression ratio increases from 16.5 to 19, the combustion efficiency enhancement at HSR = 60% becomes markedly more pronounced than at lower substitution ratios. This trend suggests that hydrogen combustion efficiency exhibits increased sensitivity to elevated compression ratios under high hydrogen substitution conditions. This is because the increased compression ratio elevates the cylinder temperature at top dead centre (TDC), and hydrogen combustion efficiency is temperature-sensitive, the effect of compression heating becomes more effective under hydrogen-dominant conditions.

As shown in Fig. 7.2 (b), at CR = 14, ITE decreases progressively with increasing hydrogen substitution ratio (HSR), remaining below the diesel operation value of 50.9%. This reduction is mainly associated with incomplete hydrogen oxidation under low-load conditions, which limits effective heat release. For all investigated HSR levels, ITE increases with rising compression ratio. Nevertheless, the overall trend persists whereby higher hydrogen substitution ratios correspond to lower ITE. Similar to combustion efficiency, for HSR levels of 20% and 40%, the improvement in ITE exhibits a nearly linear response to compression ratio increase. At HSR = 60%, the enhancement becomes more pronounced when the compression ratio elevates from 16.5 to 19. At CR = 19, the ITE at 20% HSR approaches the diesel baseline, reaching 49.7%. This can be attributed to improved hydrogen combustion efficiency and the high laminar flame speed of

hydrogen that promotes rapid heat release [206]. However, at 40% and 60% HSR, the corresponding ITE values remain limited to 44.8% and 41.3%, respectively. These results suggest that compression ratio elevation alone is insufficient to fully recover engine efficiency at medium-to-high hydrogen substitution ratios during low-load operation.

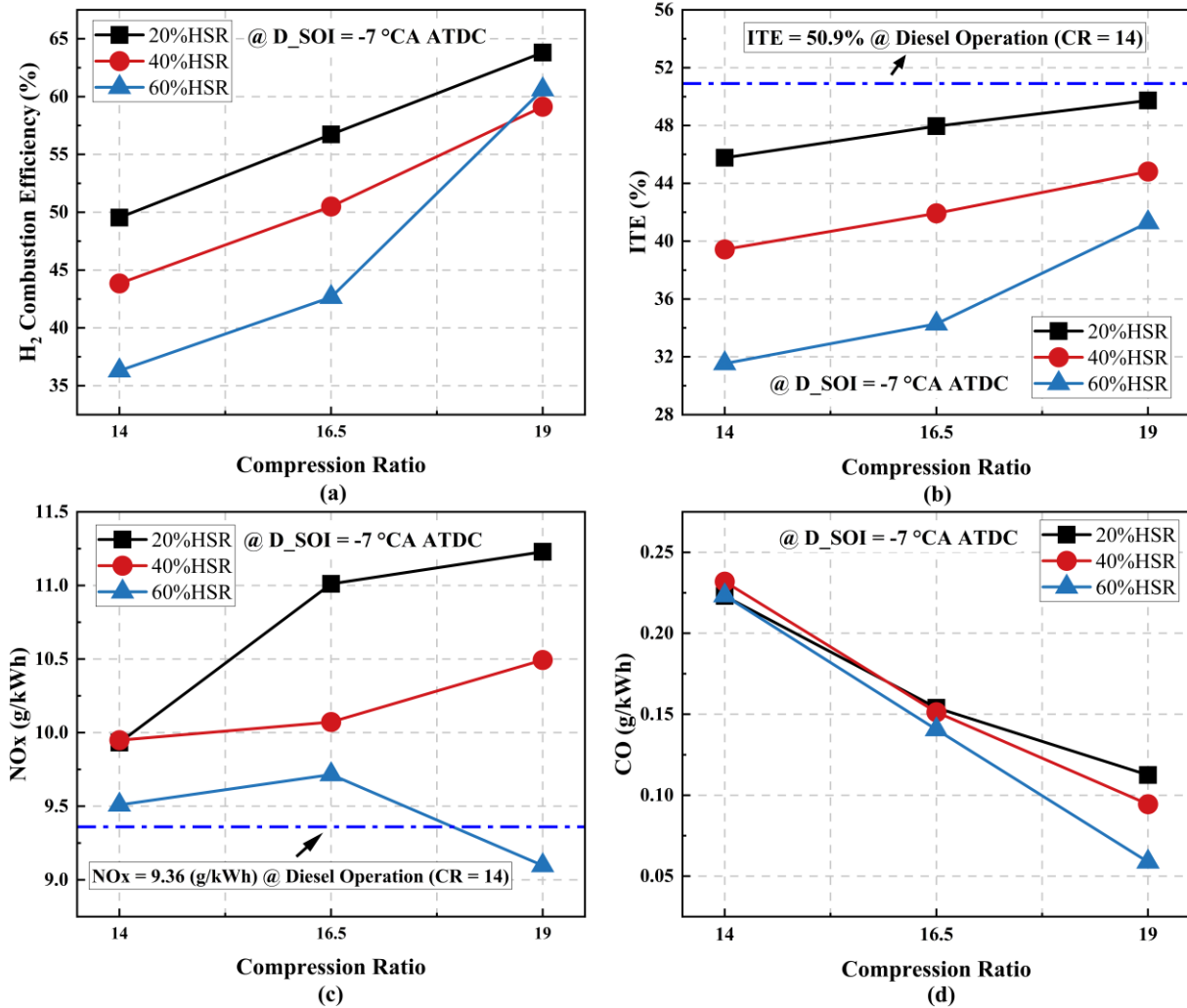


Fig. 7.2 Effect of compression ratio on (a) hydrogen combustion efficiency, (b) indicated thermal efficiency, (c) regulated NO_x and (d) regulated CO at different HSR (20–60%).

As shown in Fig. 7.2 (c), regulated NO_x emissions increase under all HSR conditions when the compression ratio rises from 14 to 16.5. This behaviour can be explained by the elevated in-cylinder temperatures associated with the higher compression ratio, which promotes thermal NO formation. Although indicated power also increases over this range, the improvement is relatively limited, resulting in higher NO_x emissions when expressed on a work-specific basis. However,

when the compression ratio further elevates from 16.5 to 19, NO_x emissions continue to rise for the 20% and 40% HSR cases, whereas a decrease is observed at 60% HSR. This trend arises from the substantial improvement in indicated work output at 60% HSR. Although the NO_x formation still increases, the gain in indicated work is proportionally larger, resulting in a decreased work-specific NO_x emission (g/kWh). Notably, at CR = 19, the regulated NO_x emission for the 60% HSR case becomes lower than that of the diesel baseline. As shown in Fig. 7.2 (d), the regulated CO level decreases as the compression ratio increases under all HSR conditions. This can be attributed to the elevated in-cylinder temperatures caused by the elevated compression ratios, which enhance the oxidation of CO to CO₂. Moreover, the reduction in CO becomes more pronounced at higher HSR levels, as the lower diesel fuel fraction decreases the carbon availability.

Fig. 7.3 illustrates the varied compression ratio effect on combustion process and spatial distribution under 60% HSR. As shown in Fig. 7.3 (a) and (b), with increasing compression ratio, the start of combustion (SOC) advances slightly, the first HRR peak occurs earlier, and its peak value gradually decreases. This is because the elevated in-cylinder temperature shortens the ignition delay, allowing the premixed diesel fuel to reach the ignition condition earlier. Meanwhile, the shortened ignition delay limits the amount of premixed diesel accumulated before ignition; consequently, the first HRR peak associated with premixed combustion becomes weaker. In contrast, the second HRR peak increases with increasing compression ratio, and the heat release during the late combustion stage also rises. This is attributed to the higher in-cylinder temperature, which enhances mixture reactivity and enables a larger fraction of hydrogen to participate in combustion during the diesel diffusion combustion stage. Fig. 7.3 (c) presents the effect of varying compression ratios on the in-cylinder temperature and hydrogen mass fraction distributions at HSR = 60%. The selected crank angles of 10°CA ATDC and 20°CA ATDC represent the main combustion stage and the further development stage, respectively. At 10°CA ATDC, the temperature in the low-temperature region increases with increasing compression ratio, providing more favorable thermal conditions for hydrogen oxidation. Consequently, at CR = 19, the hydrogen mass fraction within the cylinder is noticeably lower than that observed at the other two compression ratios. As combustion develops further to 20°CA ATDC, the high-temperature region becomes more uniformly distributed with increasing compression ratio, indicating more effective flame propagation under higher compression conditions. Correspondingly, under the CR = 19

condition, the remaining hydrogen within the cylinder is significantly reduced, suggesting more complete hydrogen oxidation.

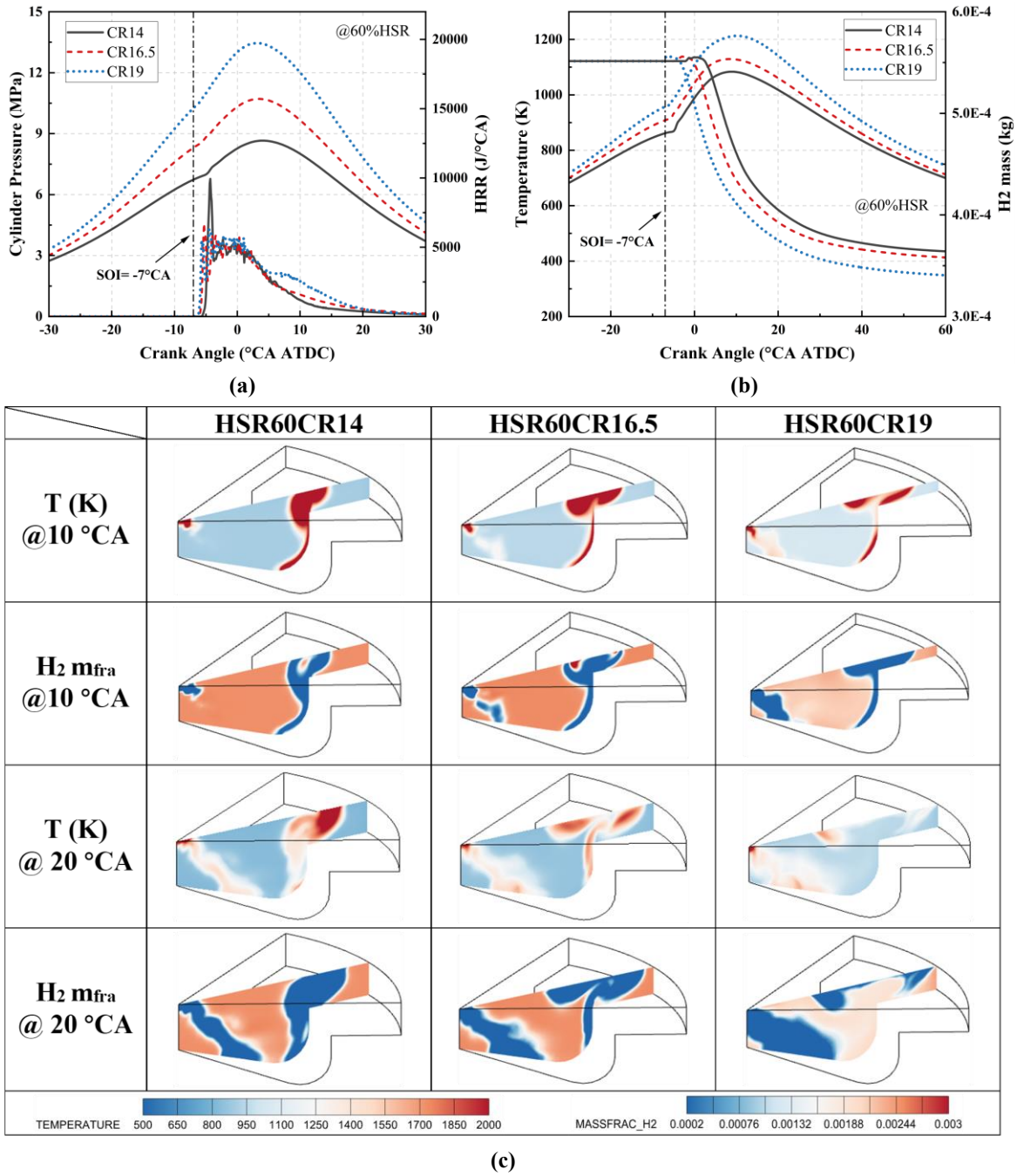


Fig. 7.3 Effects of compression ratio on (a) cylinder pressure and HRR, (b) in-cylinder temperature and hydrogen consumption, and (c) temperature and H₂ mass fraction distributions at 10°CA and 20°CA ATDC (HSR = 60%).

Overall, increasing the compression ratio enhances hydrogen combustion efficiency through the compression heating effect under all HSR conditions and improves ITE and diesel combustion completeness, with more pronounced benefits observed at higher HSR levels.

7.3 Effect of diesel SOI

Fig. 7.4 illustrates the effects of different diesel SOI timings on cylinder pressure and HRR under various HSR, with the compression ratio fixed at 14. Under all HSR conditions, advancing the diesel SOI results in an overall earlier combustion phase and a stronger first peak in the HRR. Moreover, advancing the SOI shifts the overall heat release earlier and leads to earlier and higher peak cylinder pressures for all HSR cases. For a given SOI, increasing the hydrogen substitution ratio results in a gradual rise in the first HRR peak, which corresponds to the premixed diesel combustion together with the surrounding entrained hydrogen-air mixture [203]. At higher HSR, hydrogen contributes a larger fraction of the released energy and increasingly dominates the early combustion process. The high flame speed of hydrogen results in a more rapid and concentrated heat release, thereby resulting in a sharper first HRR peak.

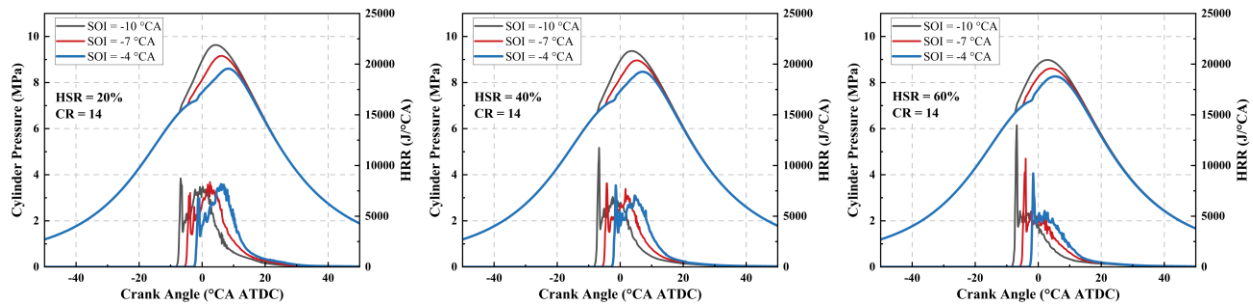


Fig. 7.4 Effect of diesel SOI on cylinder pressure and HRR at different HSR (20–60%) under CR=14.

Fig. 7.5 illustrates the effects of different SOI timings on the in-cylinder average temperature, hydrogen mass consumption, and diesel spray distribution at SOC under HSR = 60% and CR = 14. As SOI is advanced, SOC occurs progressively earlier, and the diesel spray at SOC penetrates further and covers a wider region of the cylinder. This indicates that the diesel fuel is distributed over a larger in-cylinder volume. After the start of combustion, this broader spray distribution promotes the oxidation of the surrounding hydrogen-air mixture, leading to a stronger initial heat release. This explains the gradual increase in the first HRR peak observed in Fig. 7.4 as the SOI is

advanced. In addition, an earlier SOI results in greater heat release before TDC, which elevates the average in-cylinder temperature and promotes more intense oxidation, thereby improving hydrogen combustion efficiency. Notably, small amounts of hydrogen are generated after SOC, which is attributed to the thermal cracking reaction of long-chain hydrocarbons under high-temperature conditions [220]. This reaction pathway can be expressed as:

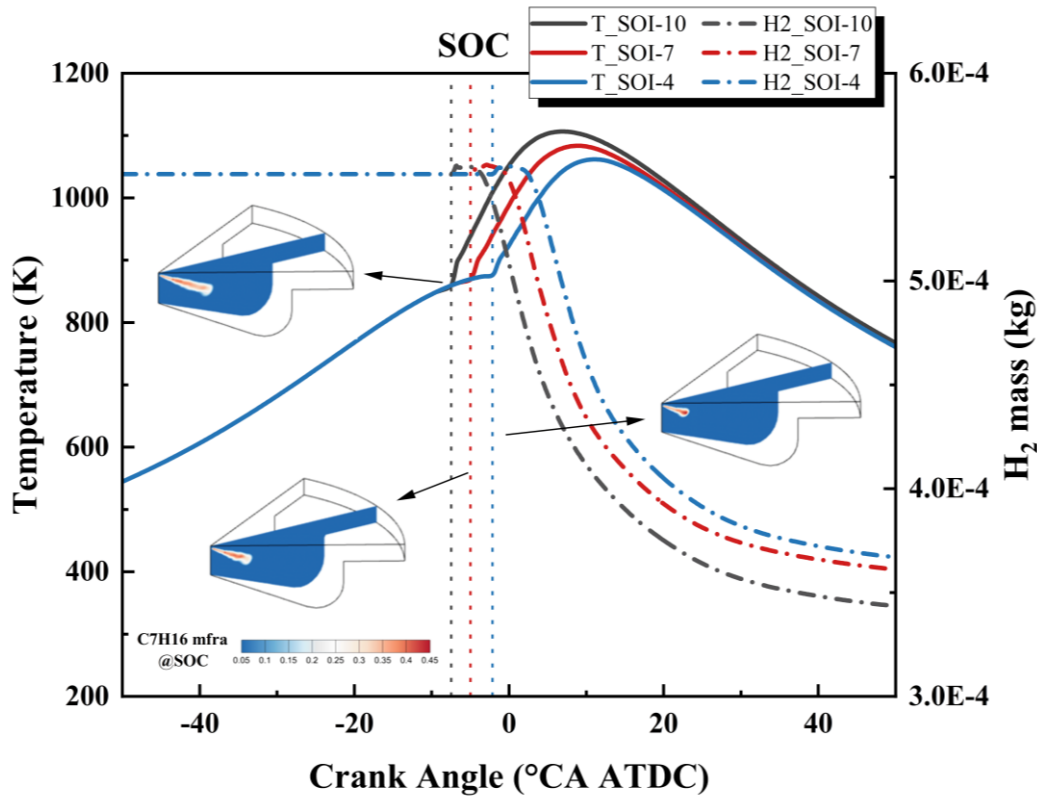
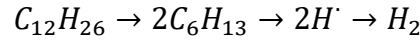


Fig. 7.5 In-cylinder temperature, H₂ mass consumption and diesel spray distribution at SOC under different SOI timings (HSR = 60%, CR = 14).

Fig. 7.6 illustrates the effect of diesel SOI on hydrogen combustion efficiency, indicated thermal efficiency (ITE), regulated NO_x emissions, and CO emissions at different hydrogen substitution ratios (HSRs) with the compression ratio fixed at 14. As shown in Fig. 7.6 (a), advancing the diesel SOI improves hydrogen combustion efficiency under all HSR conditions, with a similar magnitude of improvement observed across the different HSRs. This is because advancing the diesel injection elevated the in-cylinder temperature. However, even when SOI is advanced to $-10^{\circ}\text{CA ATDC}$,

hydrogen combustion efficiency remains relatively low, reaching only 51%, 46%, and 39% for HSRs of 20%, 40%, and 60%, respectively. As shown in Fig. 7.6 (b), advancing the diesel SOI improves ITE under all HSR conditions, primarily due to the enhancement in combustion efficiency. When the SOI is advanced from -4°CA to -10°CA ATDC, the ITE increases by 0.4%, 1.1%, and 1.3% for HSRs of 20%, 40%, and 60%, respectively, indicating a progressively stronger effect at higher HSR. This is because the higher hydrogen substitution ratio corresponds to a larger increase in the mass of hydrogen consumed during combustion. It can be observed that the ITE at $\text{SOI} = -10^{\circ}\text{CA}$ ATDC remains significantly lower than the diesel-mode value of 50.9% under all HSR conditions. In particular, at 60% HSR the ITE exhibits only 32.1%.

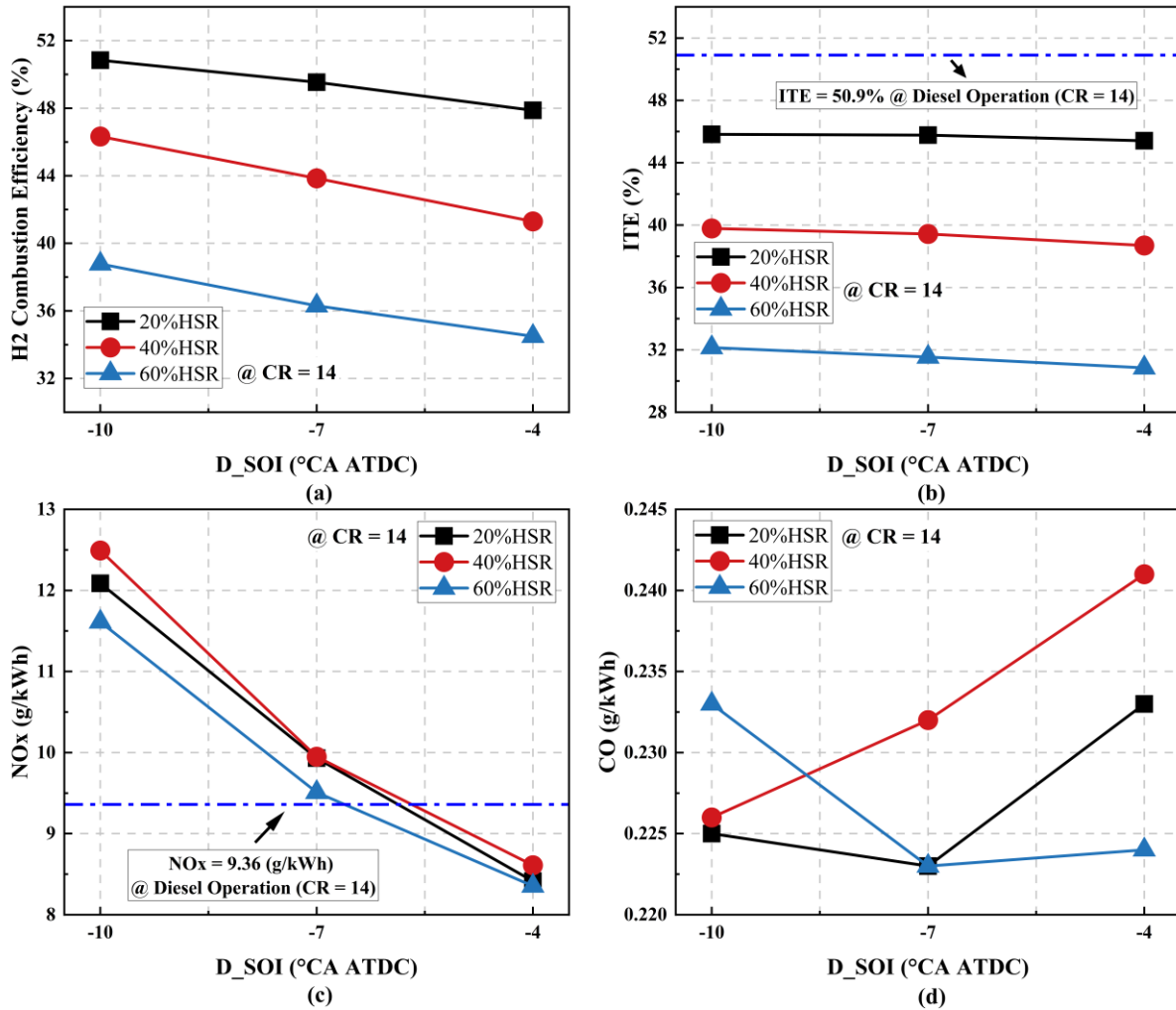


Fig. 7.6 Effect of diesel SOI on (a) hydrogen combustion efficiency, (b) indicated thermal efficiency, (c) regulated NO_x and (d) regulated CO at different HSR (20–60%).

As shown in Fig. 7.6 (c), NO_x gradually increases under all HSR conditions with the SOI advancing. This trend is because earlier diesel SOI raises the maximum in-cylinder temperature [154,221]. When the SOI is set to -7°CA and -10°CA , NO_x emissions at all HSR conditions exceed the diesel baseline. Fig. 7.6 (d) illustrates the effect of SOI on CO emissions under different HSR conditions. Overall, SOI exhibits only a slight influence on CO emissions, with the maximum variation under all HSR conditions examined remaining below 0.02 g/kWh. This indicates that SOI has only a limited effect on the oxidation process of pilot diesel and the subsequent conversion of CO.

Overall, advancing the SOI provides limited potential for enhancing hydrogen combustion efficiency and improving ITE, while simultaneously increasing NO_x emissions.

7.4 Coupled effect of compression ratio and SOI

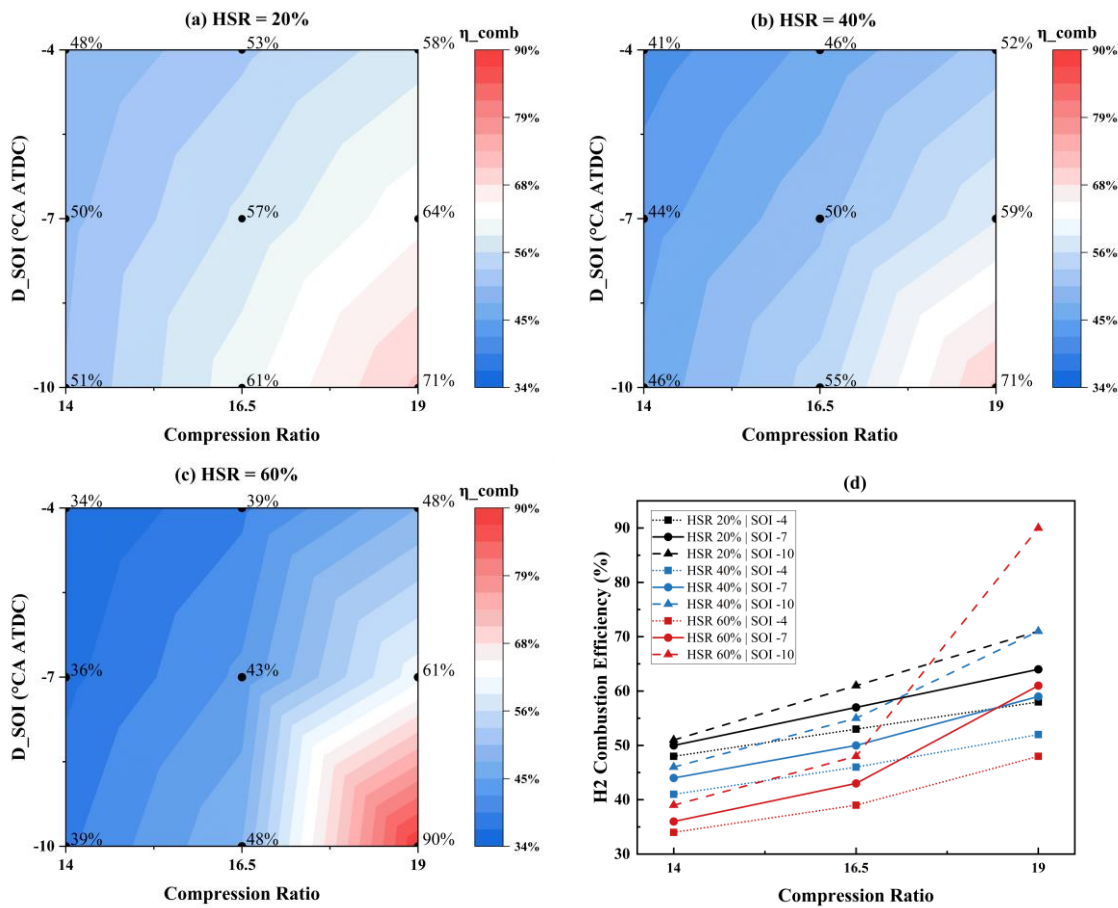


Fig. 7.7 Combined effect of compression ratio and diesel SOI on hydrogen combustion efficiency under various HSR conditions.

As the individual effects of compression ratio and SOI on low-load performance improvement are limited, a combined strategy of both parameters was therefore investigated. Fig. 7.7 illustrates the combined effect of compression ratio and SOI on hydrogen combustion efficiency under 20%, 40% and 60% HSR conditions. As shown, increasing the compression ratio together with advancing the diesel SOI improves hydrogen combustion efficiency across all HSRs, and the improvement becomes increasingly pronounced as HSR increases.

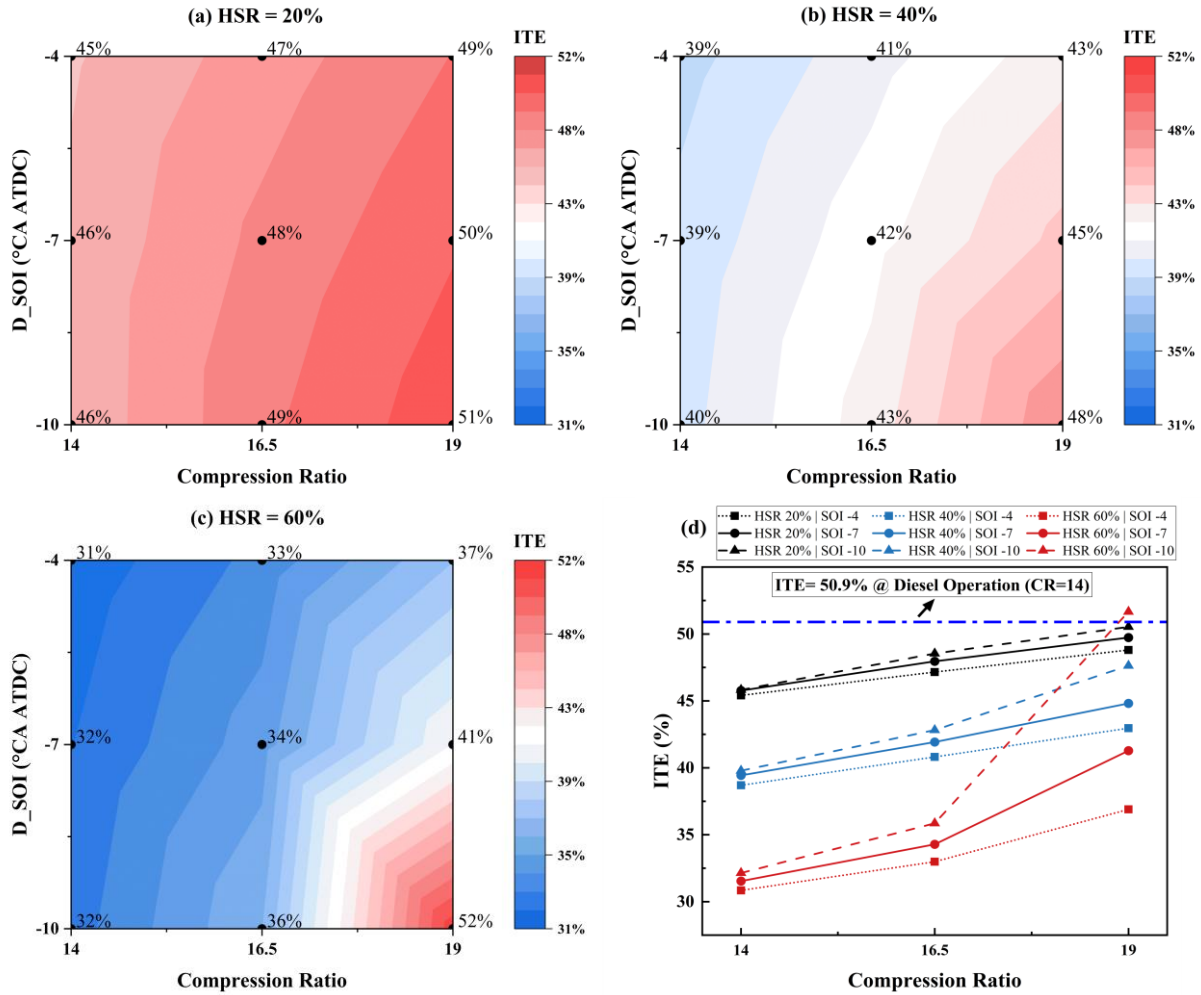


Fig. 7.8 Combined effect of compression ratio and diesel SOI on indicated thermal efficiency (ITE) under various HSR conditions.

For each HSR, the effect of compression ratio is stronger than that of SOI, as indicated by the steeper variation in combustion efficiency along the compression-ratio direction. This suggests that enhancing in-cylinder reactivity through compression heating plays a more dominant role than

combustion phasing adjustment by SOI. In particular, at HSR = 60% and SOI = -10°CA , increasing the compression ratio from 16.5 to 19 raises the hydrogen combustion efficiency significantly from about 48% to 90%, which is pronounced. This indicates that the increased compression ratio enables the mixture to overcome the low-reactivity limit and enter an efficient combustion window. This further suggests that, under low-load and high-HSR conditions, insufficient in-cylinder reactivity is the main factor limiting hydrogen combustion.

Fig. 7.8 illustrates the combined effect of compression ratio and SOI on ITE under different HSR conditions. At 20% HSR, ITE remains relatively high over all the points investigated. The combined control strategy (CR=19, SOI= -10°CA) provides 4.7% ITE improvement from original setting (CR=14, SOI= -7°CA). As HSR increases, however, increasing the compression ratio together with advancing SOI becomes increasingly effective in improving ITE, as reflected by the steeper ITE variation and denser contour lines at higher HSR levels. This indicates that at high HSR conditions, insufficient in-cylinder reactivity becomes a more critical limitation to hydrogen oxidation. Therefore, increasing the compression ratio and advancing SOI enhance hydrogen combustion efficiency, thereby leading to a more remarkable increase in ITE. As shown in Fig. 7.8 (d), when the compression ratio is increased from 16.5 to 19 at HSR = 60%, ITE rises markedly from 35.9% to 51.7%, representing the only case that exceeds the diesel baseline of 50.9% ITE.

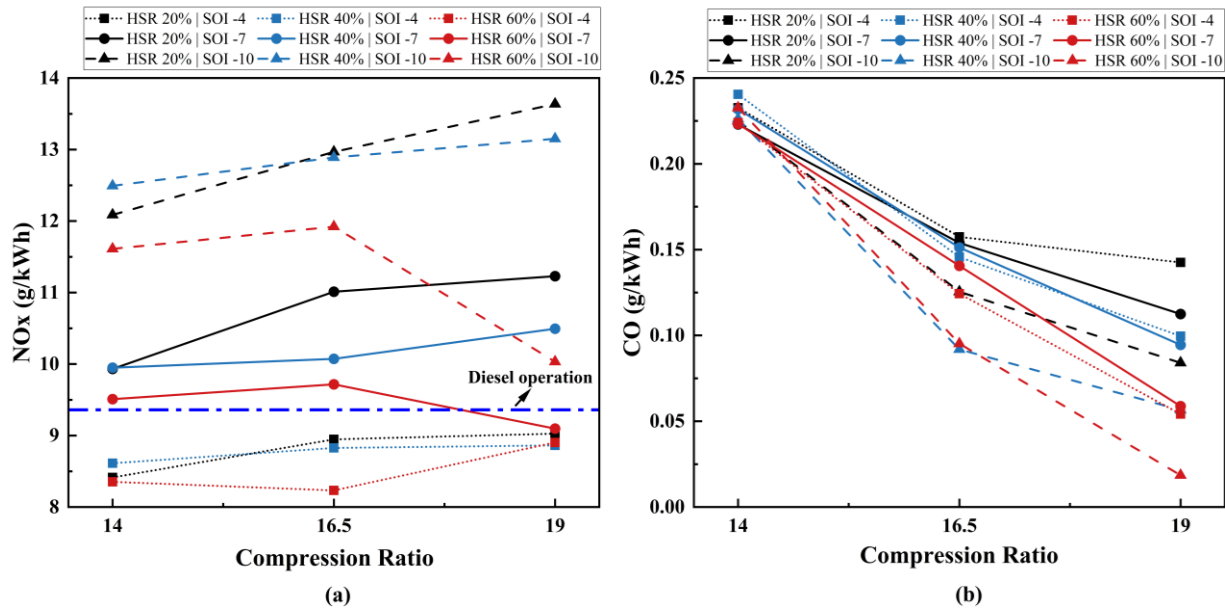


Fig. 7.9 Combined effects of compression ratio and SOI on (a) NOx emissions and (b) CO emissions under different HSR conditions.

Fig. 7.9 illustrates the combined effect of compression ratio and SOI on regulated NO_x and CO emissions under different HSR conditions. As shown in Fig. 7.9 (a), for HSR levels of 20% and 40%, regulated NO_x emissions increase gradually with increasing compression ratio. This behaviour is primarily driven by the elevated in-cylinder temperatures at higher compression ratios, which enhance thermal NO_x formation. In contrast, at 60% HSR, regulated NO_x emissions first rise and then drop with increasing compression ratio for SOI values of -7 and -10 °CA ATDC. This behaviour is because the remarkable improvement in hydrogen combustion efficiency at higher compression ratios significantly increases the indicated power output, thereby reducing the regulated NO_x expressed in g/kWh. Overall, SOI exhibits a stronger influence on NO_x emissions than compression ratio. At SOI = -4 °CA ATDC, NO_x emissions remain below the diesel baseline across all compression ratios and HSR conditions. When SOI is -7 °CA ATDC, only the 60% HSR case at CR = 19 is lower than the diesel baseline.

As shown in Fig. 7.9 (b), CO emissions decrease with increasing compression ratio under all HSR and SOI conditions. This trend is mainly attributed to the elevated in-cylinder temperature and enhanced oxidation process of CO to CO₂ at higher compression. In addition, the regulated CO values at SOI = -10 °CA ATDC generally remain at the lower end of the graph, indicating that advancing diesel SOI also contributes to more complete combustion.

Among all the investigated conditions, the improvement in hydrogen combustion efficiency from CR16.5 to CR19 at HSR = 60% and SOI = -10 °CA ATDC is the most pronounced, increasing from 48% to 90%. Therefore, these two representative cases are selected to further analyze the underlying combustion mechanism. Fig. 7.10 compares the combustion process of the CR16.5 and CR19 cases. As shown in Fig. 7.10 (a), when the compression ratio increases from 16.5 to 19, the first heat release rate (HRR) peak decreases, while the heat release during the later stage of the main combustion (5°CA – 20°CA ATDC) increases significantly. The comparison of hydrogen consumption indicates that this additional heat release mainly originates from the additional oxidation of hydrogen. The temperature and hydrogen distributions presented in Fig. 7.10 (c) and (d) provide further information about this behaviour. At TDC, the in-cylinder temperature in the CR19 case is slightly higher than that in the CR16.5 case. At this stage, hydrogen consumption has just begun, and therefore no significant difference in hydrogen distribution is observed. At 5°CA ATDC, the hydrogen concentration in the CR19 case already shows a lower level relative to the

CR16.5 case. Over the subsequent 10°CA ATDC, hydrogen in the CR19 case continues to be consumed, and by 20°CA ATDC a small quantity of hydrogen remains in the cylinder. In contrast, in the CR16.5 case a considerable amount of hydrogen remains distributed outside the high-temperature region and doesn't participate in combustion. This is mainly due to the lower overall in-cylinder temperature, as can be seen from Fig. 7.10 (c), at 5, 10, 20 °CA ATDC, the overall temperature in CR19 case is relatively higher.

As shown in Fig. 7.10 (b), when the compression ratio increases from 16.5 to 19, the average in-cylinder temperature difference at the SOC moment is approximately 45 K. The higher temperature increases the overall reactivity of the mixture and enhances the subsequent combustion process, which contributes to the significant improvement in hydrogen combustion efficiency observed in the CR19 case. Owing to the higher temperature at SOC and the larger amount of hydrogen participating in combustion, the subsequent temperature rise in the CR19 case is both greater in magnitude and sustained for a longer duration, leading to increased NO_x formation. However, despite the higher NO_x production, the regulated NO_x of the CR19 case (10.03 g/kWh) is lower than that of the CR16.5 case (11.92 g/kWh), mainly due to the substantial increase in total indicated work. A comparison with Fig. 7.10 (e) further shows that NO_x formation is concentrated in the high-temperature regions. At TDC, 5°CA ATDC and 10°CA ATDC, the NO_x isosurface distributions of the two cases are similar, as the temperature difference between them remains relatively small. At 20°CA ATDC, however, the longer combustion duration in the CR19 case leads to a further increase in in-cylinder temperature, resulting in a more extensive NO_x distribution and higher concentration. This indicates that combustion propagates over a wider region within the cylinder.

Overall, increasing the compression ratio together with advancing the SOI improves hydrogen combustion efficiency across different HSR levels. This combined strategy is more effective under high HSR conditions. At a compression ratio of 19 and an SOI of -10°CA ATDC, HSR 60% condition achieves 90% hydrogen combustion efficiency while maintaining an indicated thermal efficiency of 51.7% comparable to diesel operation (50.9%) with the expense of 0.67 g/kWh NO_x increase. However, the hydrogen combustion efficiency of 20% and 40% HSR is limited to 71%.

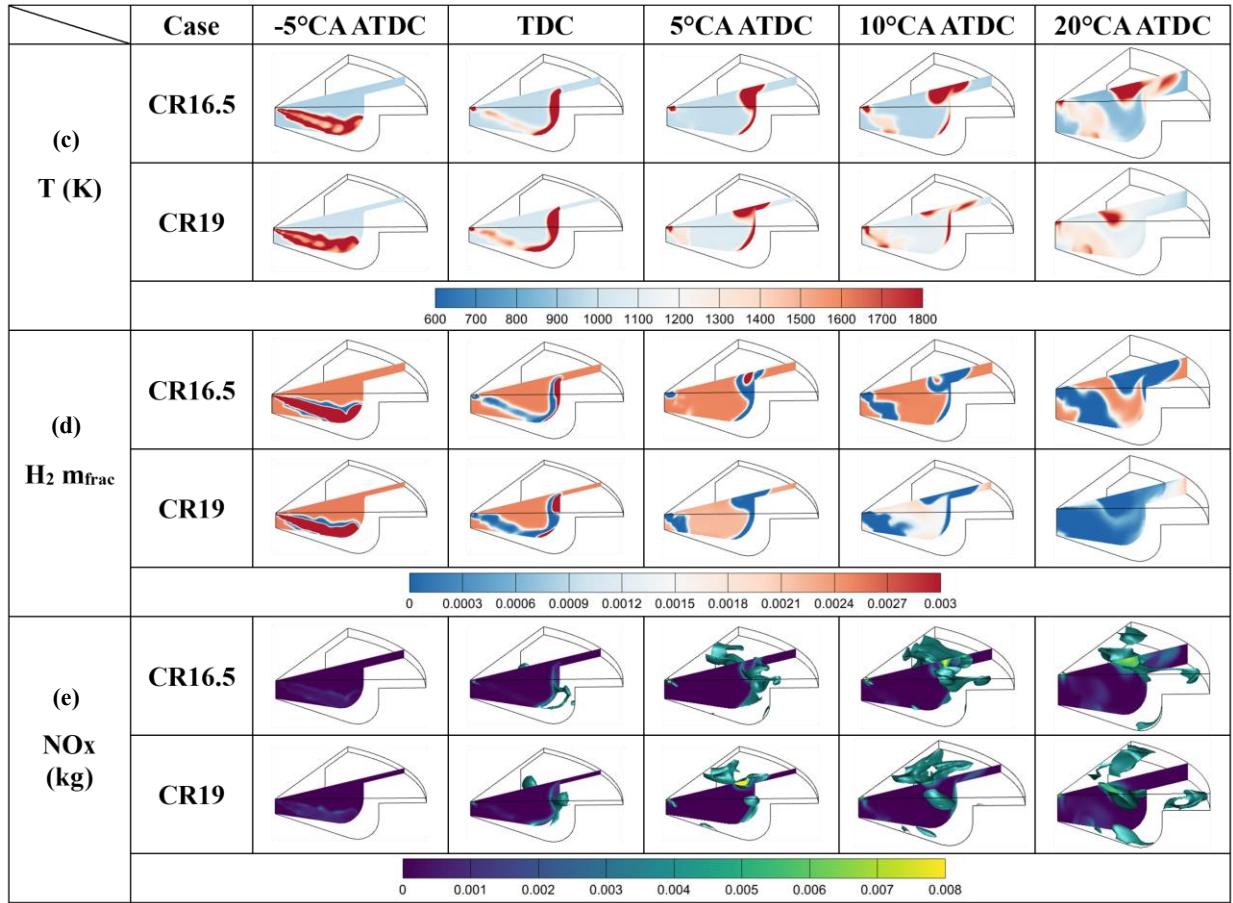
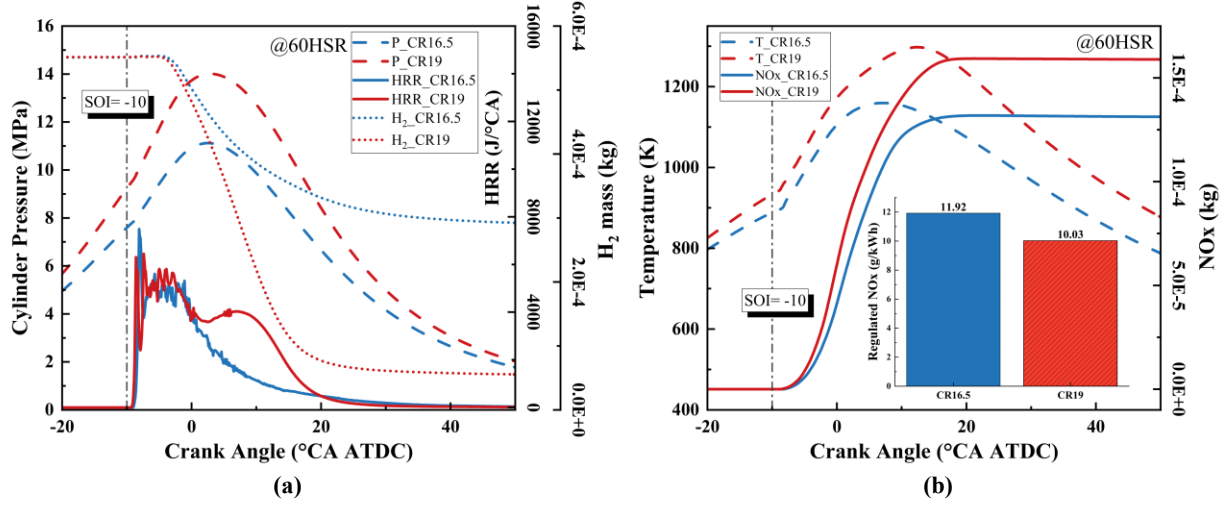


Fig. 7.10 Comparative analysis of the CR16.5 and CR19 cases at HSR = 60% and SOI = -10°C AATDC: (a) cylinder pressure, heat release rate and hydrogen consumption; (b) in-cylinder temperature, NOx formation and regulated NOx; (c) temperature distribution; (d) hydrogen mass fraction distribution; and (e) NOx mass distribution and the NOx = 0.004 isosurface.

7.5 Effect of split injection

As the combined strategy of increasing compression ratio and advancing SOI yields limited performance improvement, further investigation was conducted to evaluate the potential of diesel split injection to enhance hydrogen combustion efficiency and engine performance without penalizing emissions. Since increasing compression ratio has been prove effective, in this section the compression ratio is fixed at 19. The effects of pilot start of injection (SOI_pilot) and pilot ratio (fraction of the total diesel mass allocated to the pilot injection) are investigated sequentially.

7.5.1 Effect of pilot SOI

The effect of pilot SOI is investigated in this section, with the pilot ratio fixed at 10% and main SOI set to -7°CA ATDC . Fig. 7.11 illustrates the effects of the pilot SOI on hydrogen combustion efficiency, ITE, regulated NOx, and CO. As the pilot SOI is advanced, combustion efficiency gradually increases from 70.3% to 84.1%. The combustion efficiency at all pilot SOI settings investigated is higher than the 61% achieved by single injection (SOI=-7, CR=19). Similarly, ITE increases gradually from 44.3% to 49.6%, higher than the 41.3% ITE for single injection. This occurs because pilot injection enhances the reactivity of the premixed charge within the cylinder. Furthermore, as SOI advances, diesel premixing becomes more effective, facilitating more efficient flame propagation and thereby increasing hydrogen oxidation during the main combustion process. However, all the investigated pilot SOI conditions result in ITE being lower than the diesel operation (50.9%), indicating limited improvement.

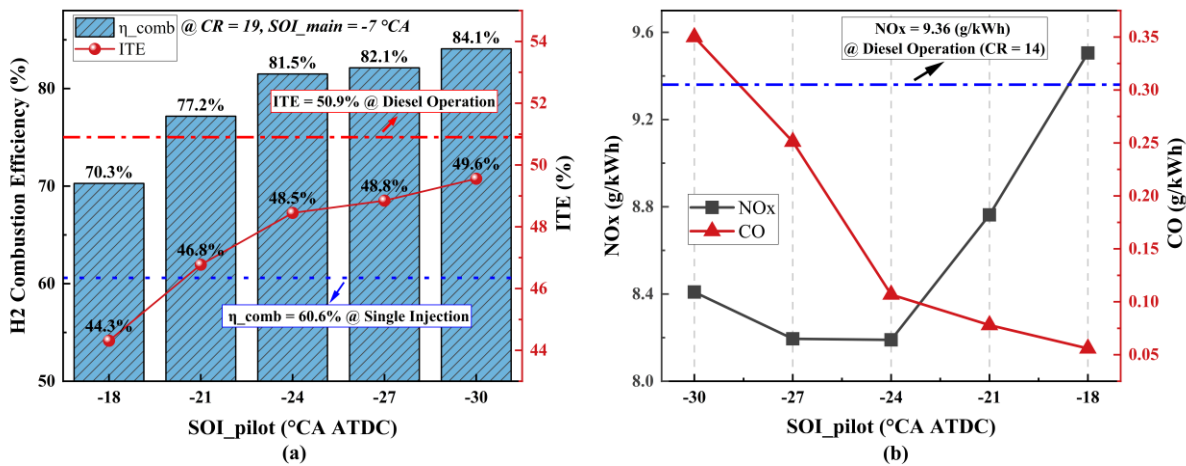


Fig. 7.11 Effect of pilot SOI on (a) hydrogen combustion efficiency and ITE, and (b) regulated NOx and CO emissions.

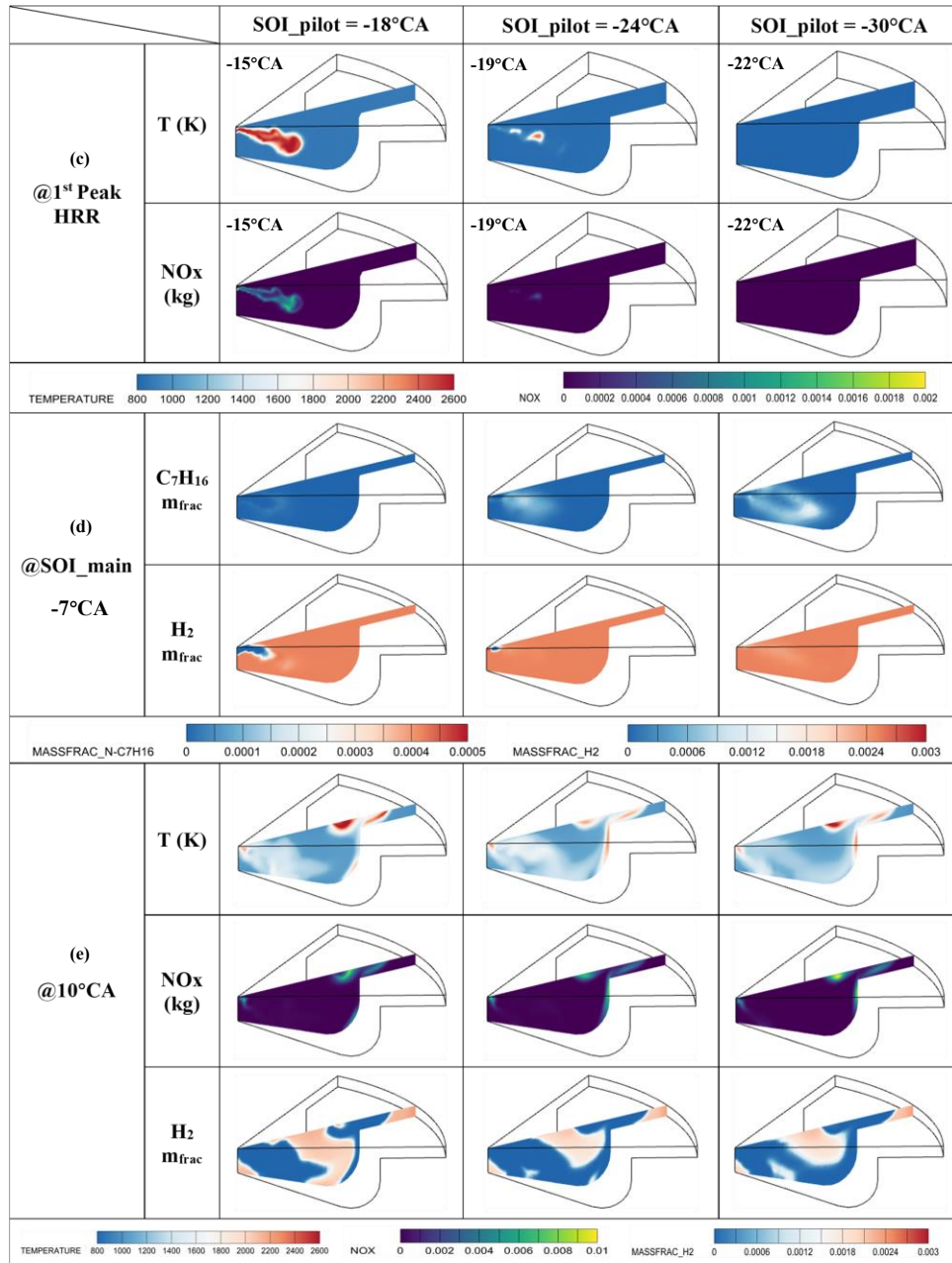
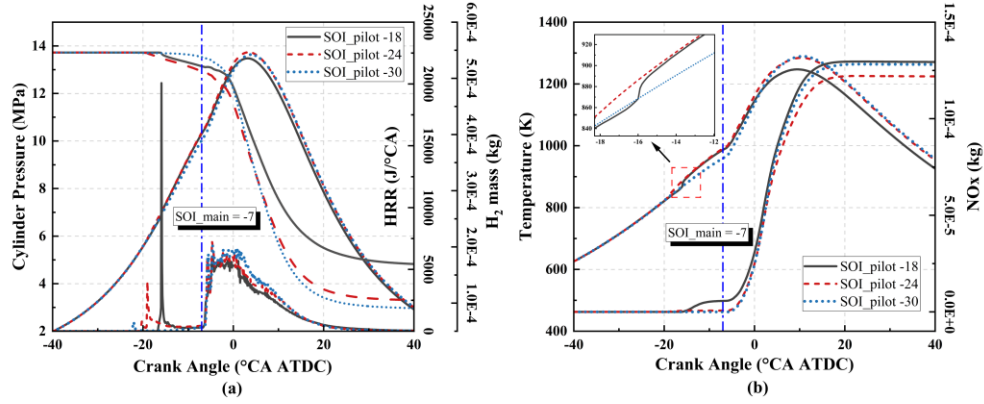


Fig. 7.12 Comparative analysis of pilot injection timing ($\text{SOI}_{\text{pilot}} = -18, -24$ and -30 °CA ATDC) on: (a) cylinder pressure, heat release rate (HRR), and H_2 consumption; (b) in-cylinder average temperature and NO_x formation; (c) spatial distributions of temperature and NO_x at the first HRR peak; (d) spatial distributions of C_7H_{16} and H_2 at SOI_{main} ; (e) spatial distributions of temperature, NO_x , and H_2 at 10 °CA.

As shown in Fig. 7.11 (b), advancing the pilot SOI initially reduces the regulated NO_x emissions, reaching a minimum of 8.19 g/kWh at -24 °CA ATDC. Further advancement of the pilot SOI leads to a slight increase in NO_x . Except for the case at -18 °CA ATDC, all investigated pilot SOI conditions exhibit lower NO_x levels than the diesel-only operation, demonstrating the effectiveness of split injection in NO_x mitigation. In contrast, advancing the pilot SOI results in a gradual increase in regulated CO emissions, from approximately 0.05 to 0.35 g/kWh, indicating deteriorated diesel combustion completeness.

Fig. 7.12 presents a comparative analysis of combustion characteristics under different pilot injection timings ($\text{SOI}_{\text{pilot}} = -18, -24$ and -30 °CA ATDC). As illustrated in Fig. 7.12 (a), advancing the pilot SOI leads to a gradual weakening of the first HRR peak, transitioning from a pronounced peak at -18 °CA to a much weaker one at -30 °CA. This is because when the pilot injection occurs closer to TDC, the higher in-cylinder reactivity triggers the diesel premixed combustion with surrounding hydrogen easily, and the initial combustion is more intensive due to better reactivity. This can be reflected by Fig. 7.12 (d), at the SOI_{main} timing, partial hydrogen consumption is already evident for $\text{SOI}_{\text{pilot}} = -18$ °CA, indicating that the heat released from the early-stage diesel combustion promotes the oxidation of the surrounding hydrogen

At the timing of the first HRR peak (Fig. 7.12 (c)), ignition of the diesel spray is clearly observed for the case with $\text{SOI}_{\text{pilot}} = -18$ °CA, leading to local high-temperature regions and the formation of a certain amount of NO_x . This is consistent with the trend in Fig. 7.12 (b), where a sharp increase in in-cylinder temperature is observed between -20 and -10 °CA ATDC, accompanied by early-stage NO_x formation.

At the SOI_{main} timing (Fig. 7.12 (d)), advancing $\text{SOI}_{\text{pilot}}$ results in a more extensive and widely distributed C_7H_{16} field, primarily because earlier injection provides additional time for

spray dispersion and premixing. Moreover, an earlier SOI_{pilot} reduces early diesel oxidation, preserving a larger fraction of the diesel spray prior to the main injection.

Following the SOI_{main} timing (-7 to 20 °CA ATDC), the main combustion phase becomes increasingly pronounced as SOI_{pilot} is advanced (Fig. 7.12 (a)), which is mainly attributed to enhanced hydrogen oxidation. Correspondingly, the peak in-cylinder temperature increases with advancing SOI_{pilot} (Fig. 7.12 (b)). However, as shown in Fig. 7.12 (e), the case with SOI_{pilot} = -24 °CA exhibits a relatively uniform temperature distribution at 10 °CA ATDC, without significant localised high-temperature regions, resulting in lower NO_x formation compared to the other cases. In terms of hydrogen distribution, hydrogen consumption at SOI_{pilot} = -24 °CA is significantly improved compared to -18 °CA, while showing only marginal differences relative to -30 °CA.

In general, the pilot SOI of -24 and -27 °CA ATDC shows a trade-off between combustion efficiency and emissions. The pilot SOI of -24 °CA achieves the lowest NO_x emissions, while -27 °CA provides higher combustion efficiency with only a limited NO_x penalty. Therefore, these two pilot SOIs are selected for the subsequent study of pilot ratio.

7.5.2 Effect of pilot ratio

Previous study has shown that increasing the pilot ratio of split injection can enhance the combustion efficiency of gaseous fuels in dual fuel engines [222]. Therefore, the effect of pilot ratio was investigated at the selected pilot SOIs of -24 °CA and -27 °CA.

As shown in Fig. 7.13, for both selected pilot SOIs, hydrogen combustion efficiency increases with increasing pilot ratio, exceeding 96% at a pilot ratio of 20% in both cases. Correspondingly, the indicated thermal efficiency (ITE) also increases gradually. At pilot ratios of 15% and 20%, the ITE surpasses the diesel baseline of 50.9%, showing satisfactory improvement. At a pilot SOI of -24 °CA, NO_x emissions decrease progressively with increasing pilot ratio. In contrast, at -27 °CA, NO_x emissions initially increase and then decrease as the pilot ratio increases. For CO emissions, a monotonic decrease is observed with increasing pilot ratio for both pilot SOI conditions.

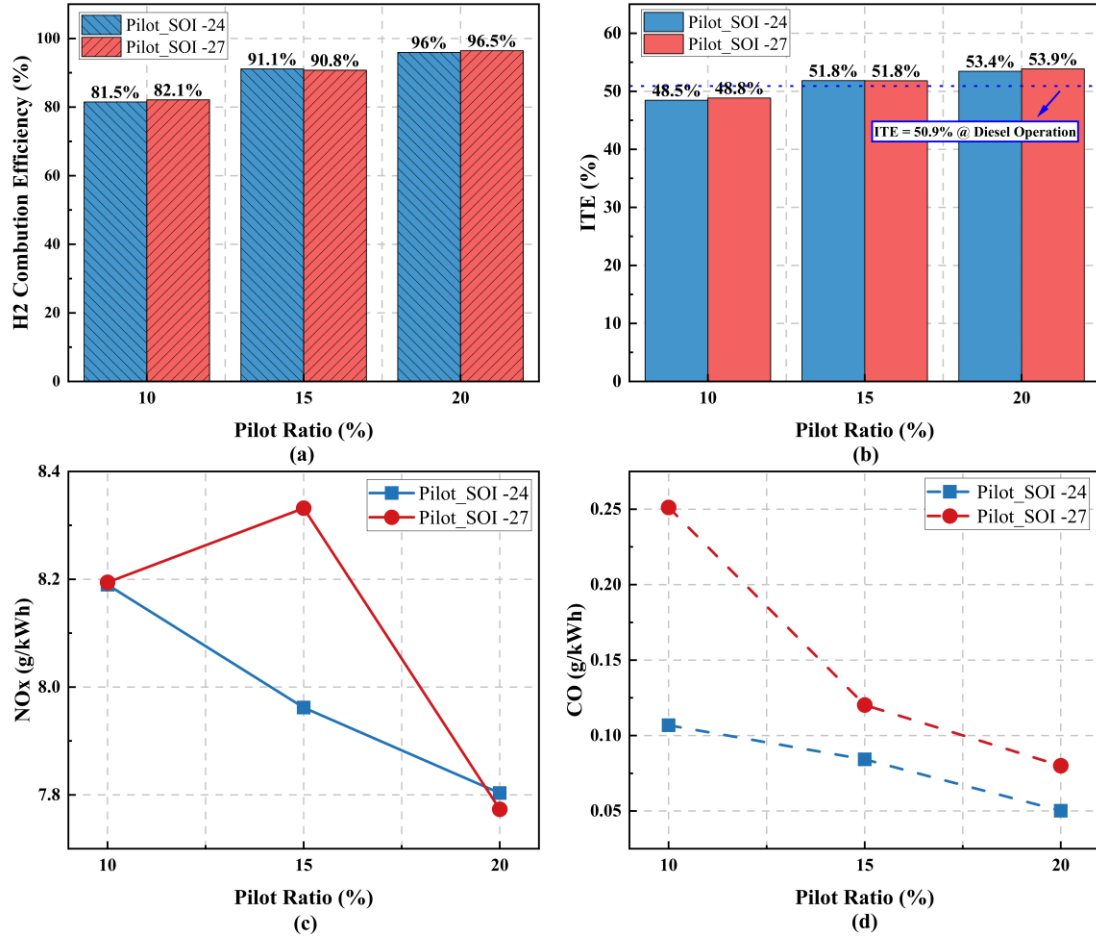


Fig. 7.13 Effect of pilot ratio on hydrogen combustion efficiency, indicated thermal efficiency, regulated NO_x and CO emissions at pilot SOI = -24 and -27°C A ATDC.

Fig. 7.14 presents a comparative analysis of the combustion behaviour for pilot ratios of 10%, 15% and 20% (at SOI_{pilot} = -27 °CA ATDC). As shown in Fig. 7.14 (a), increasing the pilot ratio progressively strengthens the early HRR peak from -25 to -10 °CA associated with pilot injection. This early-stage heat release is attributed to the combustion of pilot diesel together with the surrounding hydrogen, indicating that a portion of hydrogen is already involved in the reaction prior to the main injection. This behaviour is further supported by the hydrogen distribution at the SOI_{main} timing (Fig. 7.14 (c)), where the cases with 15% and 20% pilot ratios exhibit partial hydrogen consumption near the cylinder head. In contrast, only limited differences are observed in the spatial distribution of C₇H₁₆ at this timing, suggesting that the influence of pilot ratio is not primarily associated with a significant change in diesel distribution, but rather with the enhanced early-stage combustion intensity. The stronger pilot combustion at higher pilot ratios leads to

partial consumption of diesel fuel and promotes the formation of a more reactive in-cylinder environment.

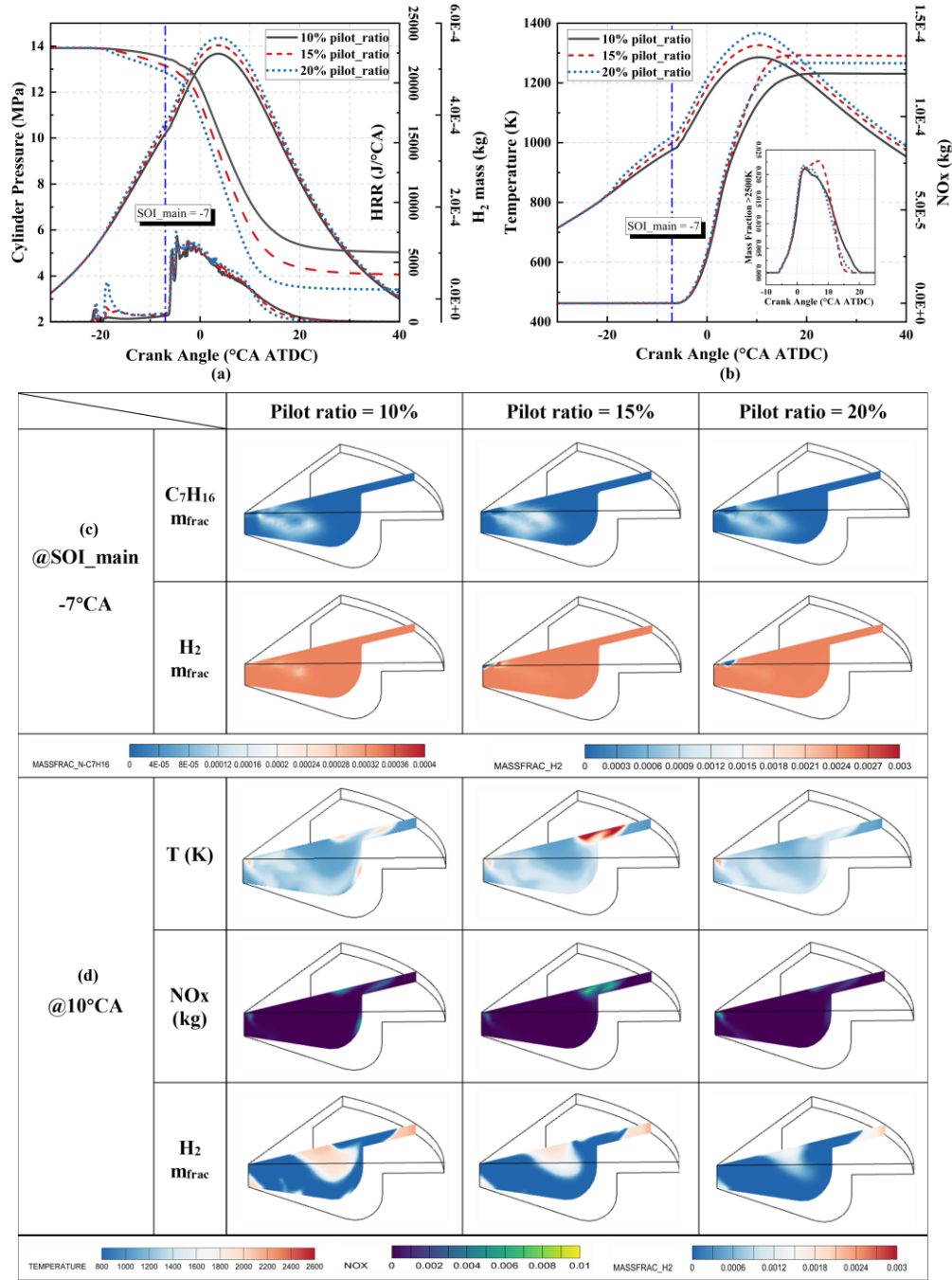


Fig. 7.14 Comparative analysis of pilot ratio = 10%, 15% and 20% (pilot SOI = -27°CA ATDC) on: (a) cylinder pressure, heat release rate (HRR), and H₂ consumption; (b) in-cylinder average temperature, NOx formation and mass fraction > 2,500K; (c) spatial distributions of C₇H₁₆ and H₂ at SOI_main; (d) spatial distributions of temperature, NOx, and H₂ at 10 °CA.

As shown in Fig. 7.14 (b), the enhanced early heat release results in a higher average in-cylinder temperature at the SOI_{main} timing for higher pilot ratios. This more favourable thermal condition facilitates subsequent hydrogen oxidation during the main combustion stage, as reflected in the faster hydrogen consumption in Fig. 7.14 (a) and (d). For the case with a 20% pilot ratio, only a small amount of residual hydrogen remains near the cylinder head and cylinder wall at 10 °CA ATDC, indicating more complete hydrogen oxidation.

Despite the gradual increase in average in-cylinder temperature with increasing pilot ratio, the total NO_x formation is highest at the 15% pilot ratio. This is attributed to the more localised high-temperature regions in this case. As shown in Fig. 7.14 (d), the 15% pilot ratio exhibits a concentrated high-temperature zone, which promotes intensified NO_x formation. In contrast, the temperature distributions for the 10% and 20% cases are relatively more uniform, leading to comparatively lower NO_x formation. This observation is consistent with Fig. 7.14 (b), where the 15% pilot ratio shows the highest mass fraction of regions exceeding 2,500 K within 5–15 °CA ATDC, which is a key factor contributing to enhanced thermal NO_x formation.

7.6 Critical discussion

As high compression ratio and split injection strategy were shown to demonstrate significant performance improvements at 60% HSR, while effectively controlling NO_x emissions, the recommended control point (CR = 19, SOI_{pilot} = -27 °CA, pilot ratio = 20%) was further applied to 20% and 40% HSR conditions to evaluate its overall effectiveness.

Fig. 7.15 compares the baseline and optimised cases under 20%, 40%, and 60% HSR conditions. As shown, hydrogen combustion efficiency is substantially improved under all HSR conditions following optimisation, exceeding 80% in all cases. The highest hydrogen combustion efficiency is achieved at 60% HSR, reaching 96.5%. Correspondingly, the indicated thermal efficiency (ITE) is also significantly enhanced under all HSR conditions, reaching 51.2%, 51.4% and 53.9% for 20%, 40% and 60% HSR, respectively. All HSRs exceed the diesel baseline ITE of 50.9%.

In terms of NO_x emissions, the optimised control strategy effectively reduces NO_x at 60% HSR, with emissions falling well below both the diesel baseline and the IMO Tier II limit. However, for the 20% and 40% HSR cases, NO_x emissions remain elevated and exceed the Tier II threshold. This indicates tailored control is required for lower HSRs.

These results demonstrate that elevated compression ratio combined with diesel split injection is highly effective in enhancing hydrogen combustion efficiency and overall engine performance at low loads. Nevertheless, the same control strategy does not ensure acceptable NO_x emissions at lower HSR levels, indicating that additional optimisation or tailored control strategies are required for low HSR conditions to achieve a well-balanced trade-off between ITE and emissions.

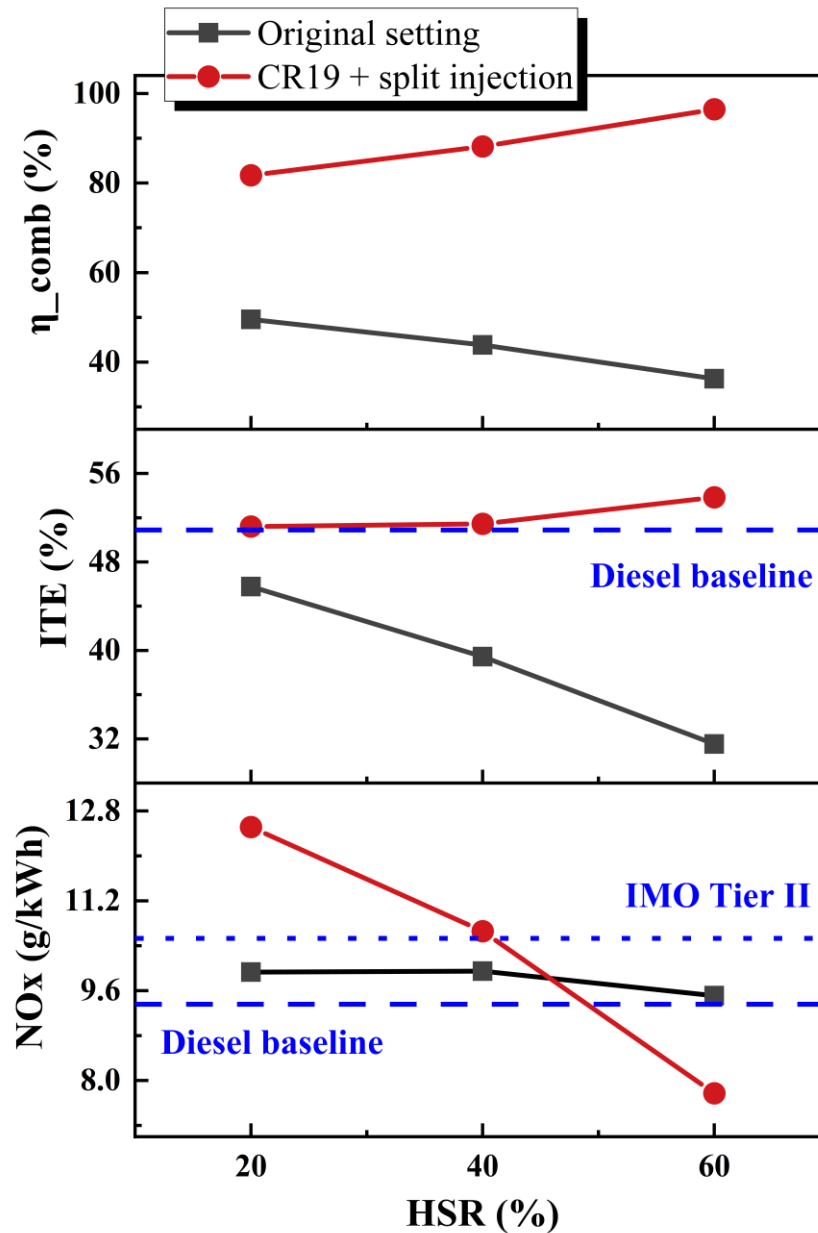


Fig. 7.15 Comparison of hydrogen combustion efficiency, ITE and NO_x between original and optimised strategies for 20%, 40% and 60% HSR.

7.7 Summary

This chapter investigates the control strategies to enhance low-load performance of Hydrogen-Diesel dual-fuel marine engines, where incomplete hydrogen combustion caused by insufficient in-cylinder reactivity. Various control strategies were examined individually and in combination at 20% load, including elevating compression ratio, advancing diesel SOI, adopting diesel split injection. The main findings are summarised as follows:

1. Low-load engine performance is strongly limited by incomplete hydrogen combustion. Hydrogen combustion efficiency decreases with increasing hydrogen substitution ratio (HSR), falling to 36.3% at 60% HSR under the initial settings, which leads to substantial deterioration in overall engine performance.
2. Increasing the compression ratio improves hydrogen combustion efficiency by enhancing the in-cylinder temperature and reactivity, with the strongest effect observed at 60% HSR. However, compression ratio increase alone is insufficient to recover engine performance to the diesel baseline.
3. Advancing diesel SOI promotes hydrogen combustion by improving the in-cylinder conditions for subsequent hydrogen oxidation. Nevertheless, this strategy is accompanied by a pronounced NO_x penalty.
4. The combined strategy of elevated compression ratio and advanced diesel SOI at 60% HSR enables an ITE comparable to the diesel baseline, but with a NO_x increase of 0.67 g/kWh. However, its effectiveness at lower HSRs is limited, while the associated NO_x penalty becomes more severe.
5. Under 60% HSR conditions, by maintaining a high compression ratio (CR=19) and adopting a split injection strategy, hydrogen combustion efficiency of up to 96.5% and ITE of 53.9% were achieved at the recommended control point. This corresponds to a 3.0% increase in ITE compared to the diesel baseline, while simultaneously reducing NO_x emissions by 1.59 g/kWh.

Overall, the results demonstrate that elevated compression ratio combined with diesel split injection is an effective approach for overcoming low-load performance degradation in Hydrogen-Diesel dual-fuel marine engines, particularly at high HSR. However, NO_x emissions remain elevated at lower HSRs, indicating that the optimal control strategy is HSR-dependent.

Chapter 8 Conclusions and recommendations

This study aims to investigate the combustion characteristics and the control strategies of stable and efficient combustion of hydrogen-diesel dual-fuel marine engines. The literature review in Chapter 2 identified the key research gaps associated with incomplete hydrogen combustion, HSR limitations, unstable combustion at high HSRs, hydrogen-air mixture inhomogeneity and low-load performance deterioration, while Chapter 3 established and validated the CFD framework for the subsequent investigations. These challenges were systematically investigated in Chapters 4–7 in accordance with the research objectives defined in Chapter 1. The main conclusions are summarised below in relation to these research objectives and research gaps, followed by the limitations of the present study and recommendations for engine design and future work.

8.1 Conclusions

1. Low intake air temperature leads to insufficient in-cylinder reactivity, causing incomplete hydrogen combustion and a high residual hydrogen fraction. Advancing diesel injection timing can enhance local reactivity and promote flame propagation, thereby reducing the unburnt hydrogen fraction. However, this strategy also leads to a significant increase in NO_x formation. Diesel spray tilt angle and injection duration strongly influence the in-cylinder mixing and the spatial distribution of diesel ignition sources, showing potential for improving hydrogen combustion efficiency. These findings address the research objective of evaluating diesel injection strategies for improving hydrogen combustion completeness and the research gap associated with incomplete hydrogen combustion.
2. HSR is limited by unstable combustion caused by the large premixed hydrogen fraction and the high laminar flame speed of hydrogen. With increasing HSR, dual-fuel combustion gradually shifts towards hydrogen-dominant combustion, characterised by rapid heat release, increased peak pressure, and higher pressure rise rates. As a result, the in-cylinder temperature increases, leading to a pronounced NO_x penalty and a narrower stable operating range at high HSRs. These findings clarify the mechanisms associated with the HSR limitation identified in the literature review.
3. In-cylinder water injection can stabilise the excessively rapid heat release under high-HSR conditions through evaporative cooling, dilution, and increased mixture heat capacity. By adopting

appropriate water injection strategies, NO_x emissions can be reduced due to the lower in-cylinder temperature. However, water injection timing and water-to-fuel ratio are critical parameters, as excessive or improperly timed water injection may deteriorate ITE. Therefore, direct water injection provides an effective trade-off between knock suppression, NO_x control, and thermal efficiency at high HSRs. Together, Conclusions 2 and 3 address the research objective of investigating HSR effects and identifying control strategies for stable combustion at high HSRs, as well as the associated research gaps concerning HSR limitation and high-HSR combustion instability.

4. PFI-induced hydrogen-air mixture inhomogeneity significantly influences the combustion and emission characteristics of Hydrogen-Diesel dual-fuel combustion. The externally hydrogen-rich distribution pattern, represented by the inverted Gaussian distribution, results in the highest ITE but also causes unstable combustion due to intensive heat release. The centrally hydrogen-rich distribution patterns exhibit distinct combustion behaviours depending on the stratification level. In contrast, the homogeneous assumption provides a more balanced performance–emission compromise, suggesting that mixture distribution caused by PFI control should be carefully considered in CFD modelling and intake control strategies for PFI HDDF engines. These findings address the research objective and research gap concerning PFI-induced hydrogen-air mixture inhomogeneity and its effects on combustion and emissions.

5. Under low-load conditions, engine performance deteriorates mainly due to incomplete hydrogen combustion caused by insufficient in-cylinder temperature and reactivity. This deterioration becomes more severe at high HSRs, where the reduced diesel pilot quantity is insufficient to support complete hydrogen oxidation. Individual strategies, including increasing the compression ratio or advancing diesel injection timing, can improve hydrogen combustion but are insufficient to fully recover diesel-baseline performance without emission penalties. The combination of elevated compression ratio and advanced diesel injection timing enables diesel-comparable ITE, but at the expense of increased NO_x emissions.

6. The combined strategy of high compression ratio and diesel split injection effectively enhances in-cylinder reactivity and improves the spatial and temporal distribution of ignition sources. Under 60% HSR conditions, the recommended strategy achieves a hydrogen combustion efficiency of 96.5% and an ITE of 53.9%, corresponding to a 3.0% improvement over the diesel baseline, while

reducing NO_x emissions by 1.59 g/kWh. These results demonstrate that elevated compression ratio combined with diesel split injection is an effective approach for mitigating low-load performance degradation in marine PFI Hydrogen-Diesel dual-fuel engines, although the optimal control strategy remains HSR-dependent. Together, Conclusions 5 and 6 address the research objective of improving hydrogen combustion efficiency and engine performance under low-load conditions while maintaining emissions level.

Overall, the contribution of this thesis lies in clarifying the mechanisms governing incomplete hydrogen combustion, hydrogen substitution ratio limitations and high-HSR combustion instability, PFI-induced mixture inhomogeneity and low-load performance deterioration, together with identifying corresponding combustion control strategies. These findings provide practical guidance for the combustion control of marine PFI hydrogen-diesel dual-fuel engines. However, the specific quantitative improvements, operating limits and recommended control parameters reported in this study were obtained under the investigated engine configurations and specific operating conditions and may vary for other engines and operating conditions.

8.2 Limitations

Although this study provides a systematic numerical investigation of the combustion and emission characteristics and control strategies of Hydrogen-Diesel dual-fuel (HDDF) marine engines, several limitations should be acknowledged.

First, the present work is primarily based on CFD simulations. Due to the limited availability of experimental data for hydrogen combustion in large-bore marine engines, the validation of dual-fuel operation was conducted using experimental data from a small-bore hydrogen-diesel dual-fuel engine. Although this validation provides a useful basis for assessing the predictive capability of the numerical model, scale effects associated with cylinder size, combustion chamber geometry, in-cylinder flow, and heat transfer may introduce uncertainties when extending the model to marine-scale engines. In addition, direct experimental validation of large-bore marine engines operating at high hydrogen substitution ratios remains unavailable, and a systematic uncertainty analysis was not conducted in the present study. Therefore, the predicted trends and relative changes between different control strategies are considered more reliable than the specific quantitative values. Further experimental validation, particularly for large-bore marine engines

operating at high HSRs, together with systematic uncertainty analysis, should be conducted to improve confidence in the quantitative predictions. Second, although the effects of in-cylinder hydrogen-air mixture inhomogeneity on combustion and emissions were investigated, the hydrogen distribution patterns considered in this study were based on idealized assumptions. These prescribed distributions allowed the influence of mixture stratification to be systematically examined; however, they may not fully represent the actual mixture formation process caused by hydrogen port fuel injection, intake flow, valve motion, and in-cylinder turbulence. Future work should therefore couple intake-port hydrogen injection modelling with in-cylinder combustion simulations to obtain more realistic hydrogen-air distribution fields. Finally, uncertainties remain in several sub-models used for Hydrogen-Diesel dual-fuel combustion, particularly the wall heat transfer model under hydrogen-rich conditions. Owing to the high thermal diffusivity and distinct combustion characteristics of hydrogen, the near-wall temperature field and heat transfer behaviour may differ from those in conventional diesel combustion. These effects may not be fully captured by existing empirical wall heat transfer models. Therefore, more advanced hydrogen-specific heat transfer sub-models should be developed and validated to improve the accuracy of future CFD predictions.

8.3 Recommendations for engine design and control

Based on the findings of this thesis, the following recommendations are given for the design and control of marine PFI hydrogen-diesel dual-fuel engines:

1. Diesel injection control should be optimised to improve hydrogen combustion completeness. During the calibration of hydrogen-diesel dual-fuel marine engines, the SOI, tilt angle and injection duration of the diesel injectors are key calibration parameters, as these factors influence the mixing and combustion processes.
2. Direct water injection can be adopted to suppress excessively rapid heat release at high HSRs. Water injection timing and water-to-fuel ratio should be jointly controlled to suppress rapid heat release and reduce NO_x emissions while avoiding excessive deterioration in engine thermal efficiency.
3. Hydrogen-air mixture distribution control should be considered in the design of PFI systems. The results demonstrate that mixture inhomogeneity can significantly affect local reactivity,

combustion behaviour and emissions. Therefore, intake and hydrogen injection control strategies should avoid forming unfavourable mixture distributions and promote stable combustion.

4. Variable compression ratio technology combined with diesel split injection is recommended for improving low-load operation. The compression ratio and diesel injection control strategy should be adjusted according to engine load and HSR rather than keeping a fixed setting over the entire operating range.

8.4 Recommendations for future research

Future research will address the unsolved but significant problems of the present study. The following research directions are therefore presented:

1. Future research may benefit from exploring ternary combustion, such as introducing ammonia to moderate hydrogen's rapid burning velocity. However, foundational experimental data will be essential to validate and ensure the accuracy of combustion simulations for such ternary mixtures.
2. This research was conducted on four-stroke marine engines. However, the development of large-bore low-speed two-stroke engines powered by hydrogen is of importance. Future research should be conducted on the application of hydrogen in two-stroke engines, considering pre-chamber ignition and pilot diesel ignition methods.
3. The performance and emissions of hydrogen-diesel dual-fuel operation are influenced by several control and design parameters. Therefore, to achieve efficient operation under various operating conditions, future research could explore the use of data-driven surrogate models for multi-objective optimization.
4. Under extreme sea conditions, such as operations in polar regions or rough seas, the transient performance of marine engines is significantly compromised. Consequently, it is essential to develop a one-dimensional model of a hydrogen-diesel dual-fuel engine to investigate these transient fluctuations and explore effective control strategies.
5. A comprehensive assessment of life-cycle costs and carbon emissions for both diesel and hydrogen-diesel dual-fuel engines provides the necessary foundation for determining retrofitting viability. This topic needs to be further discussed based on the gradually lower price of hydrogen fuel.

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Research Output

Journal papers:

- [1] **Gu, B.***, Karvounis, P., Zhou, P., Theotokatos, G., Chen, N., & Liu, Y. (2026). Numerical investigation of the effect of inhomogeneous hydrogen-air mixture on PFI marine dual-fuel engine performance and emissions. *Fuel*, 418, 138739.
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- [11] Sun, M., Wang, S.*, Deng, W., **Gu, B.**, Han, G., Yuan, Z., Chen, H., & Sun, Y. (2024). Innovative multi-tagline anti-swing and positioning system: Dynamic analysis and experimental validation for slender-beam payloads in offshore environments. *Ocean Engineering*, 313, 119461.
- [12] Liu, Y.*, Zhou, P., Wang, H., **Gu, B.**, & Yang, L. (2026). Pressure–composition design-space optimization of H₂-He-Ne working fluids for 20–100 K shipboard LH₂ cold-energy recovery. *International Journal of Hydrogen Energy*, 247, 155803.
- [13] Liu, Y.*, Zhou, P., Wang, H., **Gu, B.**, & Yang, L. (2026). Architecture Evaluation and Screening of an LH₂ Cold Energy and Low-Grade Heat Recovery System for Marine Liquid Hydrogen Fuel Utilisation. *Applied Thermal Engineering*, Under review.
- [14] Karvounis, P.*, Jeon, J., Theotokatos, G., Patil, C., **Gu, B.**, & Zhou, P. (2026). Multi-objective optimisation of novel variable compression ratio marine engine operating with methanol using CFD. *International Journal of Hydrogen Energy*, Under review.

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- [15] Zhou, P., **Gu, B.***, & Chen, N. (2024). Study on the diesel injection strategy to reduce unburned hydrogen in a hydrogen/diesel dual-fuel marine medium-speed engine. In *the 2024 Innovation & Cooperation in Naval Architecture & Marine Engineering Conference (ICNAME 2024)*, Harbin, China, August 2024.
- [16] Karvounis, P.*, Theotokatos, G., **Gu, B.**, & Zhou, P. (2025). Numerical investigation of marine dual-fuel engine operating with 60% premixed hydrogen fuel using LES. In *the 12th European Combustion Meeting (ECM)*, Edinburgh, UK, April 2025.
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