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Article

Enhancing Efficiency and Combustion in Methanol Dual-Fuel Compression Ignition Engines Through Hydrogen Enrichment: A Computational Assessment

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Abstract

Hydrogen enrichment of compression ignition (CI) engines has emerged as a promising strategy to simultaneously enhance thermal efficiency and reduce carbon-based emissions. This study numerically investigates how hydrogen enrichment affects engine performance and emissions in methanol-diesel dual-fuel CI engines, a combustion mode gaining increasing attention for replacing fossil diesel with sustainable fuels, particularly in hard-to-abate sectors such as maritime transport. The simulations are based on the Unsteady Reynolds-Averaged Navier–Stokes (URANS) equations, incorporating the RNG $k-\epsilon$ turbulence model, the Eddy Dissipation Concept (EDC) for turbulence–chemistry interaction, and the G-equation for turbulent premixed flame propagation. The numerical model is validated against experimental data for in-cylinder pressure and heat release rate at 45% methanol substitution ratio (by energy). The results indicate that increasing the hydrogen enrichment ratio (HER, defined on an energy basis) from 5% to 20% raises the Sauter Mean Diameter (SMD) of the diesel fuel from 20.2 μm to 28.0 μm (+38%), driven by the reduction in gas-phase density and weakened Weber-number-controlled droplet breakup efficiency as hydrogen displaces charge oxygen. Furthermore, hydrogen's elevated adiabatic flame temperature and superior mass diffusivity intensify combustion, raising peak in-cylinder pressure from 75.2 to 79.1 bar (+5.2%), amplifying the peak heat release rate from 129 to 211 J/°CA (+63.6%), and elevating maximum in-cylinder temperature from 1542 to 1735 K (+193 K). These thermodynamic gains translate directly into a 6% improvement in indicated thermal efficiency and a 14% reduction in indicated specific fuel consumption (accounting for hydrogen, methanol, and diesel) at HER 20%. On the emissions front, CO₂ declines by 24% in direct proportion to the carbon-containing fuel mass displaced by hydrogen substitution, while NO_x surges 3.52-fold through intensified Zeldovich thermal pathways. These findings establish hydrogen-enriched methanol–diesel dual-fuel combustion as a viable pathway toward high-efficiency, low-carbon CI engine operation, provided that targeted NO_x mitigation strategies, such as exhaust gas recirculation (EGR) or optimized injection timing, are concurrently applied.

Keywords: CFD; spray development; hydrogen enrichment; methanol; dual fuel CI engine

Nomenclature

Abbreviation / Symbol	Definition
CA50	Crank angle at 50% mass fraction burned
CFD	Computational Fluid Dynamics
CI	Compression Ignition
DMC	Discrete Multi-Component vaporization model
EDC	Eddy Dissipation Concept
EGR	Exhaust Gas Recirculation
HER	Hydrogen Enrichment Ratio (energy basis, %)
HRR	Heat Release Rate (J/°CA)
ISFC	Indicated Specific Fuel Consumption
IVC	Intake Valve Closing
KH-RT	Kelvin-Helmholtz / Rayleigh-Taylor model
LHV	Lower Heating Value
MSR	Methanol Substitution Ratio (energy basis, %)
RCCI	Reactivity Controlled Compression Ignition
RNG k-ε	Renormalization Group k-epsilon (turbulence model)
SMD	Sauter Mean Diameter (μm)
TDC	Top Dead Centre
URANS	Unsteady Reynolds-Averaged Navier-Stokes
We	Weber number (dimensionless)

1. Introduction

The ongoing global energy crisis, caused by the trade-off between rising energy demands and the growing urgency of mitigating climate change, has intensified the need for sustainable solutions [1]. In hard-to-abate sectors such as maritime shipping, and heavy-duty road transport, where full electrification remains technically and economically challenging in the near term, low-carbon fuels integrated into advanced combustion concepts represent the most viable transition pathway [2–4]. Among candidate fuels, methanol has gained significant attention because of its low carbon content, high octane number, inherent oxygen content, and compatibility with existing compression ignition (CI) infrastructure [5–8]. Methanol is liquid at standard temperature and pressure, miscible with water, and can be produced from renewable feedstocks via green synthesis routes rendering it one of the most scalable carbon-neutral hydrogen carriers [9,10]. It is also considered a promising e-fuel. Using methanol as a blending fuel for diesel is one of the simplest and most cost-effective methods [11]. Extensive experimental and numerical research has confirmed that methanol-diesel dual-fuel CI operation consistently reduces exhaust emissions and improves thermal efficiency relative to neat diesel, with performance strongly dependent on the methanol substitution ratio and injection strategy [13–17]. However, a high substitution ratio tends to extend the ignition delay [17]. Compared to diesel, methanol can be operated under lean conditions due to its higher laminar flame velocity [18].

Hydrogen is an additional compelling fuel candidate owing to its high specific energy (120 MJ/kg), wide flammability range (4-75 vol%), near-zero carbon footprint and superior laminar flame speed [19][20]. Conventionally, hydrogen is produced via natural gas steam reforming [21] or coal partial oxidation [22], but progress towards green production (including water electrolysis powered by renewables and photo-electrochemical splitting) is accelerating [23]. A particularly relevant production route for engine applications is on-board catalytic steam reforming of part of the

methanol, which uses engine exhaust heat to generate a hydrogen-rich reformat gas [24]. This approach is thermodynamically advantageous because it recovers otherwise wasted exhaust enthalpy, avoids the safety concerns and volume penalties of hydrogen storage, and does not introduce an independent third fuel: the hydrogen originates directly from part of the methanol already carried on board. Consequently, in the combustion system studied here, the premixed charge entering the cylinder consists of hydrogen-methanol- air, where hydrogen is a reformat derivative of methanol rather than separately sourced fuel. This distinction is important for lifecycle assessment and practical implementation, as it preserves a two-tank fuel architecture while enabling hydrogen enrichment benefits. In fact, on-board methanol reforming has recently been reported as a promising technique to improve overall engine efficiency while mitigating some drawbacks associated with the direct use of methanol, such as its cooling effect under cold engine conditions [25][26].

When hydrogen is added to CI engines under conventional diesel combustion (CDC), significant reductions in CO and particulate matter are observed, accompanied by improvements in thermal efficiency [27][28]. However, the temperature peaks associated with hydrogen's high adiabatic flame temperature consistently increases NO_x emissions [29][30]. The benefits are strongly influenced by factors such as injection timing, EGR rate, and hydrogen fraction [31].

Several studies have examined hydrogen enrichment in dual-fuel CI engines. Yahyaei et al. [32] showed that 12% hydrogen enrichment in a biodiesel/natural gas dual-fuel engine reduced unburned hydrocarbons by 40%, lowered carbon monoxide, shortened the ignition delay from 10.5 to 9.3 CAD, and increased thermal efficiency. Bayramoğlu et al. [33] demonstrated that hydrogen addition improved the energy and exergy efficiency of a biodiesel-diesel-hydrogen engine, with the highest thermal and exergy efficiencies reaching 30.5% and 28.5% respectively, particularly at intermediate engine load. Fakhari et al. [34] studied the effects of hydrogen enrichment in ammonia/diesel combustion within a Reactivity Controlled Compression Ignition (RCCI) engine. The findings showed that hydrogen enrichment improved combustion efficiency and enhanced the indicated mean effective pressure, while simultaneously decreasing NO_x, CO, HC, unburnt ammonia, and N₂O emissions. Ahmadi et al. [35] numerically investigated the effects of hydrogen addition under CDC and RCCI combustion in a Caterpillar 3401 heavy-duty diesel engine. The results indicated that hydrogen addition in RCCI combustion improved combustion efficiency and reduced emissions, except for NO_x. However, adding hydrogen to diesel led to knock when it contributed more than 60% of the total energy.

While methanol–diesel dual-fuel CI combustion has been investigated, and hydrogen enrichment has been documented in dual-fuel CI systems based on diesel, biodiesel, natural gas, and ammonia, the specific effects of adding hydrogen to a methanol–diesel dual-fuel configuration have not yet been explored. This gap is noteworthy given the potential benefits when hydrogen is supplied by an onboard methanol reformer. In fact, methanol reforming requires lower exhaust temperatures than those needed for natural gas or ammonia reforming, thereby enabling operation over a wider engine map. Moreover, this approach could help mitigate drawbacks associated with the cooling effect of port-fuel methanol injection, particularly at low engine loads. In addition, methanol substitution reduces the energy density (by mass) of the mixture relative to neat diesel operation owing to methanol's low LHV; hydrogen enrichment is therefore investigated as a targeted strategy to recover this energy deficit while preserving the carbon reduction benefits of the methanol-diesel system. Adding hydrogen to this charge creates a fundamentally different interaction. In the methanol-diesel baseline, the premixed charge already contains methanol, a fuel with an inherent oxygen content and a higher laminar flame speed. Adding hydrogen to this already oxygen-bearing, fast-burning mixture amplifies a reactivity level that does not exist in conventional diesel engines, producing interactions in spray atomization, equivalence ratio distribution, and reaction zone topology that differ qualitatively from those observed when hydrogen is added to a pure diesel charge. The combined effects of hydrogen enrichment on spray atomization, reaction zone distribution, engine performance, and emissions in this specific methanol-diesel engine constitute the principal knowledge gap addressed by the present work. The objective of this study is to investigate,

via three-dimensional URANS-based CFD simulations, the effects of hydrogen enrichment ratio (HER= 5, 10, 15, 20 on an energy basis) on: i) diesel spray atomization and vaporization characteristics; ii) OH radical distribution and flame propagation topology; iii) in-cylinder pressure, heat release rate, and peak temperature; iv) engine performance and emissions. The hydrogen is treated as premixed with the incoming methanol-air charge prior to the intake valve closing. The findings are intended to provide quantitative guidance for the design of high-efficiency, low-carbon dual-fuel CI engines in maritime and heavy-duty applications.

2. Numerical setup

2.1. Flow and Combustion Modelling

The numerical study is performed using ANSYS Forte 2023 R2 under academic license. The physical configuration is based on a single-cylinder AVL 580 engine [11,20], whose specifications are summarized in Table 1. The fuel delivery architecture comprises two injection events: a pilot injection delivering 15% of the total fuel mass through a common-rail direct injector, followed by a main injection of the remaining 85%. Methanol is supplied via port fuel injection, premixed with the intake air. Hydrogen is introduced as a premixed component in the intake charge. It is important to note that the numerical model was first validated against experimental data at a methanol substitution ratio of 45% by energy; hydrogen was subsequently introduced parametrically across four enrichment levels (HER = 5, 10, 15, and 20) while keeping the diesel and methanol flow rates unchanged. A high-pressure cooled EGR system is incorporated at 7.5% EGR ratio across all cases. The computational domain is a 45° sector of the full cylinder geometry, encompassing the cylinder volume and piston bowl (Figure 1). Featuring eight holes, the injector operates within a domain assumed to be axisymmetric. The analysis is restricted to the period when both valves remain closed, extending from 148° BTDC (IVC) to 130 ATDC (EVO). Initial and boundary conditions are listed in Table 2.

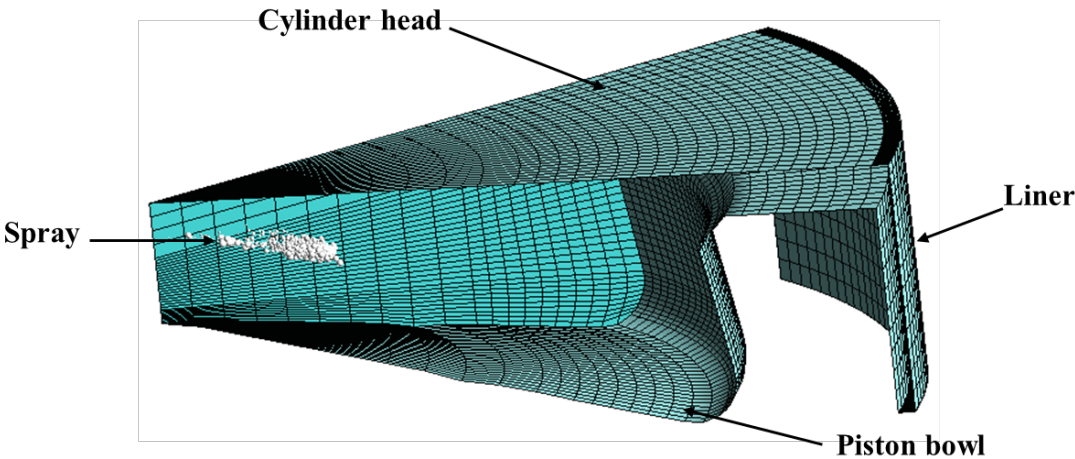


Figure 1. Computational model.

Table 1. Engine specifications.

Parameters	Value
Number of cylinders	1
Bore x stroke [mm]	106.5x 127
Connecting rod length [mm]	203
Displacement volume [L]	1.13
Compression ratio [-]	15.84
Diesel fuel injection type	Direct injection

Methanol injection type	Port injection
Hydrogen delivery	Premixed with intake charge

Table 2. Initial and boundary conditions.

Initial and boundary conditions	Specific conditions
Temperature of the combustion chamber at IVC [K]	400
Pressure inside the combustion chamber at IVC [bar]	1.3
Turbulent kinetic energy [m ² /s ²]	17
Turbulence length scale [m]	0.005
Temperatures of Cylinder Head, Piston, and Liner Wall [K]	400

The flow field is modeled using the Unsteady Reynolds-Averaged Navier-Stokes (URANS) framework, where the continuity, momentum, energy, and species transport equations are ensemble-averaged over turbulent fluctuations. The pressure-velocity coupling is solved with the SIMPLE algorithm, which iterates between extrapolated pressure fields and velocity/temperature corrections until convergence is achieved at each crank-angle time step. This iterative correction is necessary because the pressure at the new time level depends on both velocity and acceleration fields derived from that same pressure. Figure 2 depicts the methodology used in the numerical simulation.

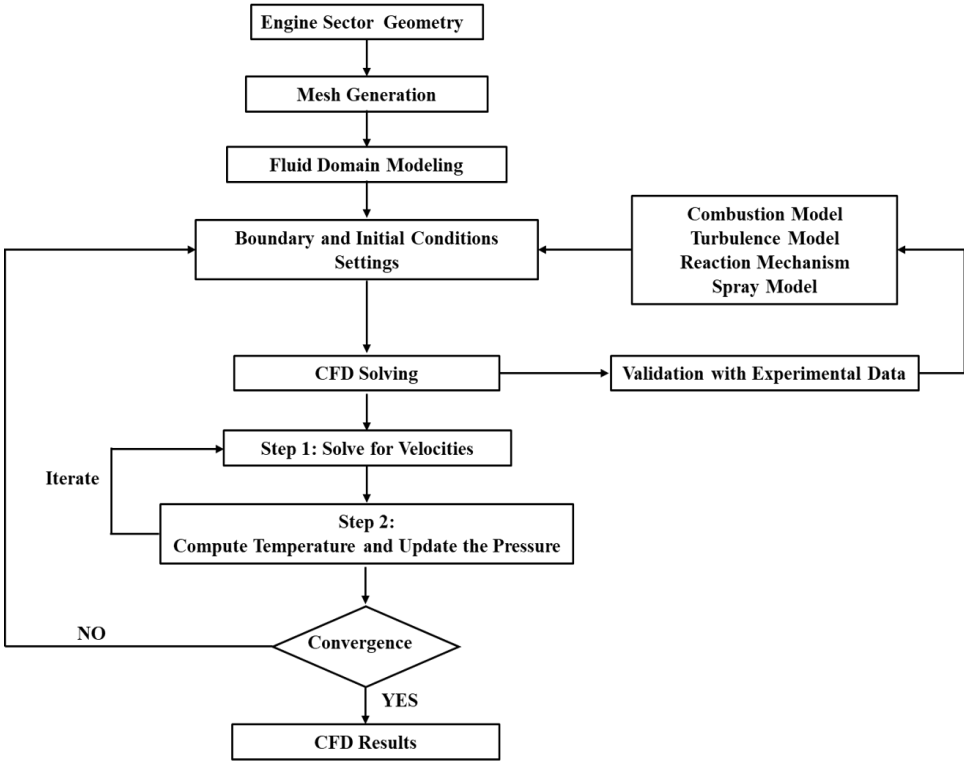


Figure 2. Numerical simulation methodology.

Turbulence is modelled using the Renormalization Group $k-\epsilon$ (RNG $k-\epsilon$) model, which is preferred over the standard $k-\epsilon$ formulation for engine in-cylinder flows due to its improved capability for handling high strain rates [36]. Ignition kernel growth is modelled using the discrete particle approach of Tan and Reitz [37], in which the flame front is tracked as a Lagrangian particle. Once ignition is established, the turbulent flame surface density is determined from particle concentration within each computational cell, and flame propagation is governed by the G-equation model [39–41]. The G-equation partitions the flow domain into burned and unburned regions via a level-set scalar G , with $G = 0$ defining the instantaneous flame surface. The local turbulent flame speed is coupled to the laminar flame speed through the Peters [38] framework, which distinguishes corrugated-flamelet and this-reaction zone regimes depending on the ratio of the Kolmogorov length

scale to the laminar flame thickness. The laminar flame speed is computed using the Gülder correlation [42,43]:

$$S_{L,ref}^0 = \omega \varphi^\eta e^{-\xi(\varphi-\sigma)^2} \quad (1)$$

here ω , η , ξ , and σ are empirical parameters derived from experimental data in [42,43]. The turbulent flame speed within the G-equation is evaluated as:

$$\frac{S_T^0}{S_L^0} = 1 + I_p \left\{ -\frac{a_4 b_3^2 l_l}{2 b_1 l_F} + \left[\left(\frac{a_4 b_3^2 l_l}{2 b_1 l_F} \right)^2 + a_4 b_3^2 \frac{u' l_l}{S_L^0 l_F} \right]^{1/2} \right\} \quad (2)$$

where I_p represents a progress variable, l_l and l_F refer to the turbulence integral length scale and the laminar flame thickness, respectively, and constants b_1 , b_3 , and a_4 , are calibrated by Peters [38]. The turbulence-chemistry interaction is modelled using the Eddy Dissipation Concept (EDC), implemented in ANSYS Forte through the Turbulence Chemistry Interaction (TCI) model linked to ANSYS Chemkin-Pro solver [44,45]. The effective species production rate accounts for the fact that chemical reactions occur in fine-scale turbulent structures, introducing a mixing time scale τ_{mix} that competes with the chemical time scale τ_{chem}

$$\tau_{eff} = \tau_{chem} + \tau_{mix} \quad (3)$$

$$\tilde{\omega}_{k,eff} \Delta t = \tilde{Y}_k^{n+1} - \tilde{Y}_k^n = \frac{\tau_{chem} \tilde{\omega}_k \Delta t}{\tau_{eff}} = \frac{\tau_{chem} (\tilde{Y}_k^{kin} - \tilde{Y}_k^n)}{\tau_{chem} + \tau_{mix}} \quad (4)$$

where $\tilde{Y}_k^n$ and $\tilde{Y}_k^{n+1}$ represent the species mass fraction at the current and next time steps, respectively, and $\tilde{Y}_k^{kin}$ denotes the species mass fraction predicted by chemical kinetics.

A detailed reaction mechanism comprising 425 species and 3128 reactions is employed. n-heptane has been used as diesel fuel surrogate. It is sourced from the ANSYS Model Fuel Library. The validation of this mechanism has been demonstrated under constant pressure conditions across a range of fuel mixtures [44]. The Kelvin-Helmholtz-Rayleigh-Taylor (KH-RT) hybrid model is employed to simulate spray atomization and droplet breakup within the solid-cone. Within the breakup length from the nozzle exit, the KH model is employed to describe primary breakup, while the RT model accounts for secondary breakup [45]. Additionally, spray droplet vaporization is represented using the Discrete Multi-Component (DMC) vaporization approach. It tracks individual fuel droplets throughout the evaporation process and enables coupling with the reaction kinetics of specific fuel components. This model assumes spherical liquid fuel droplets and analyzes only cold flow physical parameters, excluding chemical reactions [46].

2.2. Mesh Sensitivity Analysis

The mesh dependency analysis is performed under specified operating conditions. The operating conditions include an engine speed of 1600 rpm and an indicated mean effective pressure (IMEP) of 5.2 bar. These analyses ensure consistency and reliability in assessing numerical accuracy. Three mesh densities were assessed: 25000, 50000, and 100000 cells (Figure 3). The 50000 cells mesh was selected as the optimal compromise between solution fidelity and computational cost. The 25000 cells mesh produces acceptable results but marginally under-resolves the spray-flame interaction zone near TDC. In contrast, the 100000 cells mesh slightly underpredict the in-cylinder pressure throughout the compression and combustion phases, a behavior consistent with numerical diffusion associated with excessively small cell sizes in conjunction with the employed spray-turbulence coupling scheme, a known phenomenon in URANS-based engine CFD when the grid resolution exceeds the turbulence model's valid range. The mesh of 50000 cells closely reproduces the experimental pressure trace, particularly near TDC where combustion is most sensitive to spatial resolution.

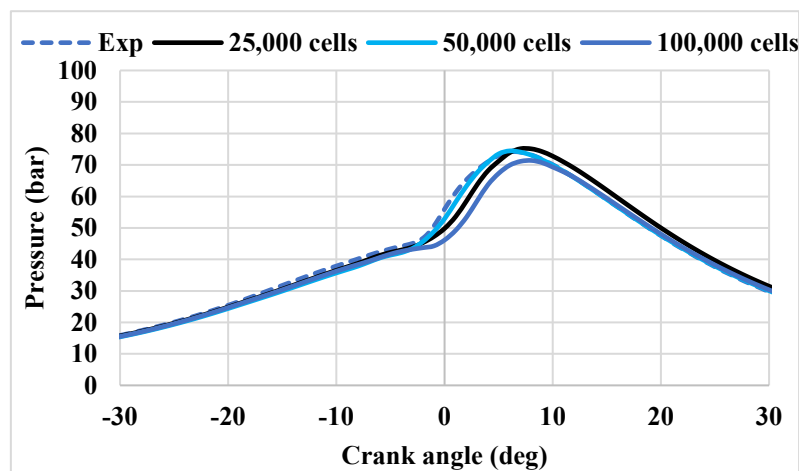


Figure 3. Effect of mesh resolution on cylinder pressure.

2.3. Validation and Cases Study

Figure 4 presents the numerical validation of in-cylinder pressure and Heat Release Rate (HRR) for methanol-diesel dual-fuel combustion. In this configuration, diesel is directly injected into the combustion chamber, while methanol is supplied via port fuel injection. The validation corresponds to a methanol substitution ratio of 45%. The numerical validation is carried out using the experimental data from Domínguez et al. [47]. The simulation results show good agreement with experimental data, accurately capturing the compression phase and peak pressure. Overall, these results suggest that the model reliably predicts combustion behavior. The HRR trend is also well predicted. However, a slight overestimation is observed in the HRR peak, suggesting a more intense energy release in the simulation compared to the experiment. Despite this, the results confirm that the CFD model reliably reproduces the key combustion characteristics of methanol-diesel operation, validating its applicability for further analysis.

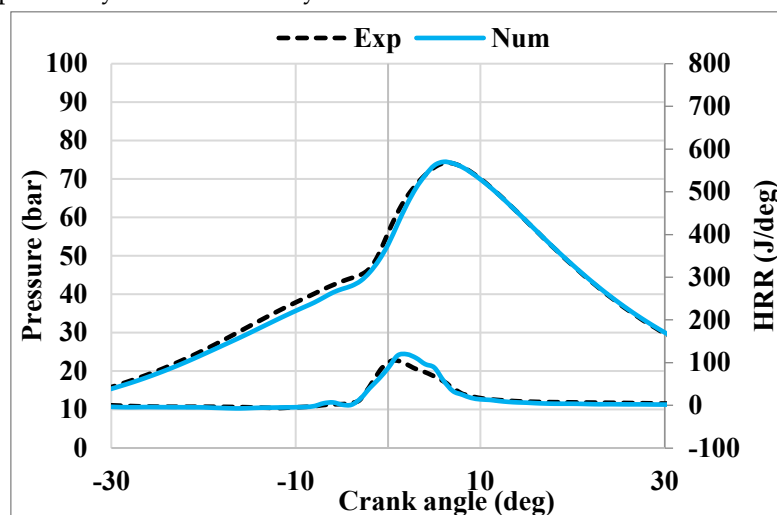


Figure 4. Numerical validation of the in-cylinder pressure and heat release rate.

Following the validated numerical framework established in [12], in which the model was assessed across three methanol substitution ratios (MSR 35, MSR 45, and MSR 55). The MSR 45 case is selected as the baseline configuration for the present study. Hydrogen enrichment is subsequently introduced parametrically at four energy ratios. The diesel and methanol mass flow rates are held constant across all cases (Table 3), with hydrogen supplementing the baseline fuel blend as an additional energy contributor, so that the total energy input rises with HER. This approach ensures that any changes in combustion characteristics, engine performance, and emissions can be directly

attributed to the hydrogen enrichment ratio. Four hydrogen enrichment ratio (HER) are investigated: HER 05, HER 10, HER 15, and HER 20, defined on an energy basis as [48]:

$$\text{HER} = \frac{m_H \text{LHV}_H}{m_D \text{LHV}_D + m_M \text{LHV}_M} 100\% \quad (5)$$

where m_D is the mass flow rate of diesel (kg/h), m_M is the measured mass flow rate of methanol (kg/h), m_H is the mass flow rate of hydrogen (kg/h) LHV_D and LHV_M refer to the lower heating value of diesel and methanol, respectively.

Table 3. Operating variables for different HERs.

Operating variables	HER 05	HER 10	HER 15	HER 20
$\dot{m}_{air}$ [g/s]	7.9	7.9	7.9	7.9
$\dot{m}_{diesel}$ [g/s]	0.21	0.21	0.21	0.21
$\dot{m}_{Methanol}$ [g/s]	0.367	0.367	0.367	0.367
$\dot{m}_{Hydrogen}$ [g/s]	0.00687	0.0137	0.0206	0.0276
EGR [%]	7.5			
Start of pilot injection BTDC [CAD]	30	30	30	30
End of pilot injection BTDC [CAD]	27.9	27.9	27.9	27.9
Start of main injection BTDC [CAD]	20	20	20	20
End of main injection BTDC [CAD]	16	16	16	16

3. Results and Discussion

3.1. Spray Characteristics

Figure 5.a illustrates the total vapor mass of the heptane spray as a function of engine crank angle. As the HER increases ($0 \leq \text{HER} \leq 20$), there is no significant change in the peak total vapor mass. This is explained by the fact that the injected diesel quantity remains constant. At HER 15 and HER 20, a marginal prolongation of late-cycle vapor is observed, indicating a longer combustion duration. The vapor penetration length refers to the distance from the nozzle exit to the point where 99.9% of the injected liquid fuel has vaporized. It is determined by accumulating the mass of fuel vapor in each cell, starting from the nozzle hole. In Figure 5.b, the decline in vapor penetration length to zero confirms that the entire diesel has burned. For HER 10, the vaporization process takes less time. As HER increases from HER 10 to HER 15, the peak vapor penetration length increases from 77.6 mm to 95.9 mm. After reaching the peak, the vapor penetration length drops rapidly to zero. Additionally at HER 15, the peak occurs at a later crank angle compared to HER 10, indicating a longer combustion duration. However, the vapor penetration length continues to increase, reaching approximately 100 mm at HER 20 at 130° CA, with vaporization persisting throughout the entire cycle. This behavior can be explained by the local equivalence ratio fields: as HER increases, the premixed charge becomes progressively fuel-rich, reducing the oxygen availability that drives oxidation-coupled vaporization. As a result, a portion of the diesel remains unburned. Similar observations were recorded by Kokjohn [49] under natural gas/diesel dual-fuel mode and various engine loads. As later explained in Section 3.3, ignition delay remains largely unaffected by hydrogen addition; therefore, the longer vapor penetration observed at higher HER is primarily linked to the extended combustion duration rather than a prolonged ignition delay.

The Sauter Mean Diameter (SMD) represents the droplet size with an equivalent volume-to-surface area ratio as the overall spray. It serves as a key parameter for evaluating spray distribution quality. A smaller SMD improves liquid fuel vaporization, resulting in enhanced and faster mixing. Figure 5.c shows that as the HER increases from 5% to 20%, the Sauter mean diameter also tends to increase, rising from 20.2 μm to 28 μm (+38%). This trend is governed by the reduction in gas-phase

density as hydrogen, with its low molecular weight, displaces a portion of the denser charge gas [20]. The Weber number driving KH instability-based primary breakup scales as:

$$We = \frac{(\rho_g (\Delta u)^2 d)}{\sigma} \quad (6)$$

where ρ_g is the gas-phase density, Δu is the relative velocity between liquid jet and surrounding gas, d is the droplet diameter, and σ is the liquid surface tension. Since injection pressure and therefore initial jet momentum are held constant across all HER cases, and heptane surface tension is unchanged, the reduction in Weber number is driven entirely the decrease in ρ_g . A lower Weber number reduces the aerodynamic drag force destabilizing the liquid jet surface, weakening KH primary breakup and producing larger primary droplets. The RT secondary breakup mechanism is similarly weakened by reduced gas-phase density, reinforcing the SMD increase. Additionally, hydrogen addition modifies the kinematic viscosity of the charge gas mixture: although hydrogen's dynamic viscosity is lower than that of air, the substantial reduction in mixture density results in a net increase in kinematic viscosity, which further dampens the aerodynamic instabilities governing droplet disintegration and contributes to the observed SMD increase. As a result, higher HER cases produce sprays with larger droplets, reduced surface-to-volume ratios, slower evaporation mass transfer, and delayed atomization. The environment surrounding diesel droplets is responsible for evaporating the spray. Although the injected diesel quantity remains constant, the addition of hydrogen alters the in-cylinder ambient conditions. The resulting decrease in oxygen availability and changes in gas-phase density reduce the efficiency of droplet breakup and vaporization.

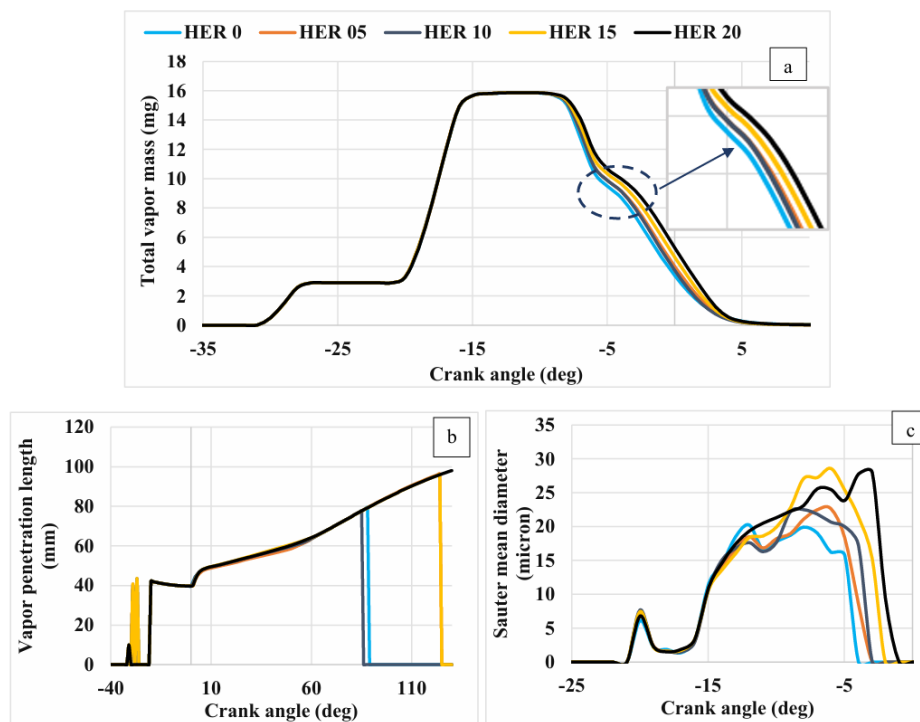


Figure 5. Spray characteristics; a) Vapor mass, b) Vapor penetration length, and c) Sauter mean diameter, for different HER values.

3.2. Flame Propagation Pattern

A qualitative study of OH radical and temperature contours is presented, with plots at two selected timeframes: 23° and 33° After Start Of Injection (ASOI), as shown in Figure 6. The OH radical is a key oxidation intermediate whose concentration serves as a reliable indicator of heat-releasing reaction zones in hydrocarbon flames. The spatial extent of elevated OH concentration expands progressively with HER, indicating a broader and more volumetrically distributed reaction zone. This is attributed to hydrogen’s mass diffusivity (roughly 4× that of hydrocarbons), which promotes rapid radial diffusion of the premixed hydrogen-methanol-air mixture. Ignition consistently occurs at the periphery of the spray plume, where the local equivalence ratio is near stoichiometric controlled diesel ignition that persists across all HER levels. The temperature contours confirm that peak temperatures are localized in the post-flame region adjacent to the diesel spray axis, with the hot zone expanding and intensifying larger fractions of the bowl volume, reflecting the combined effect of higher HRR, faster flame propagation, and reduced heat capacity of the hydrogen-enriched charge.

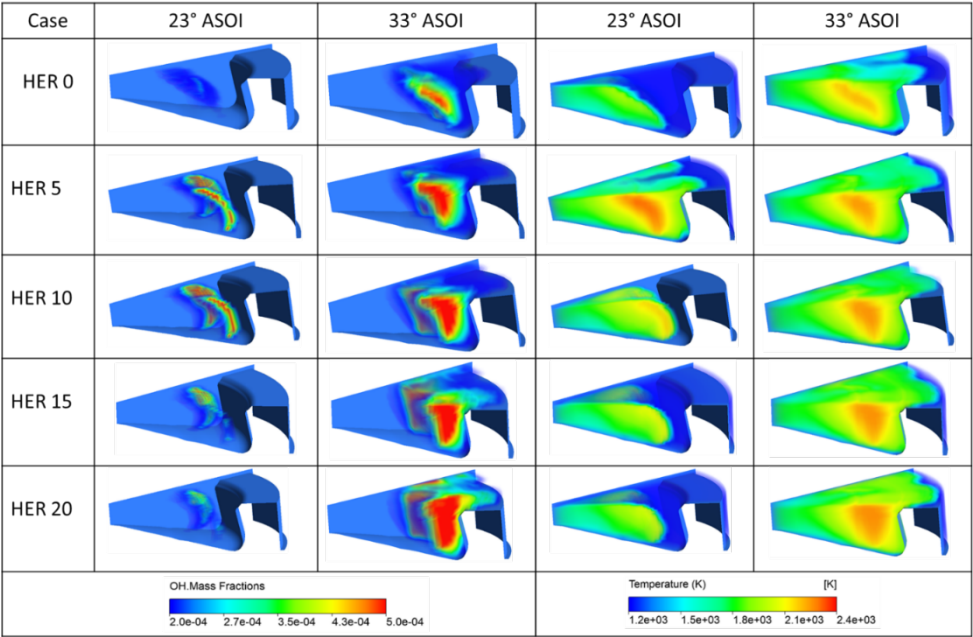


Figure 6. Spatial contours of OH radical and temperature for various HERs.

Figure 7 depicts the local equivalence ratio and H₂ mass fraction contours for different HERs at various crank angles. At 23° ASOI, hydrogen is still present in substantial concentrations near the cylinder walls (yellow/red zones), where the premixed charge has not yet been consumed by the advancing flame. By 33° ASOI, the blue zones (near-zero H₂ mass fraction) confirm complete hydrogen consumption at the periphery, while elevated H₂ concentrations persist in the dense spray core where oxygen availability is locally suppressed. The coexistence of unreacted hydrogen in the spray core with fully burnt peripheral zones illustrates the sequential combustion mode: premixed peripheral hydrogen-methanol combustion occurs first, followed by diffusion-limited diesel spray combustion, a phasing that becomes more pronounced at higher HER.

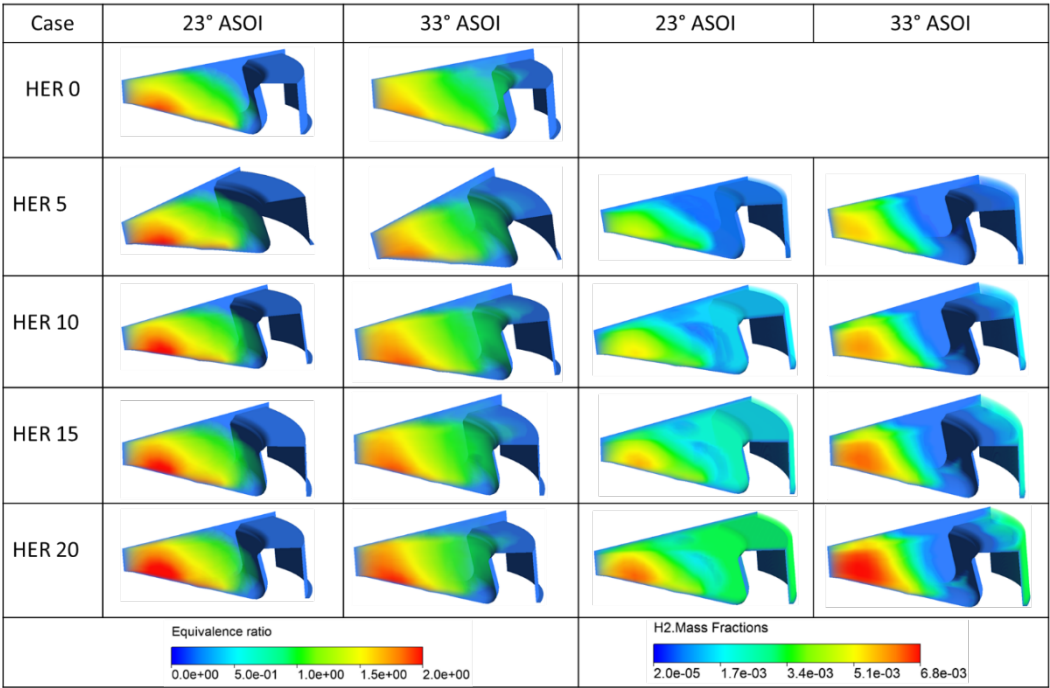


Figure 7. Spatial contours of equivalence ratio and H₂ mass fraction for various HERs.

3.3. In-Cylinder Combustion Pattern

The effect of varying hydrogen enrichment on in-cylinder pressure, heat release rate (HRR), and maximum in-cylinder temperature is illustrated in Figure 8. The enhanced in-cylinder pressure and HRR peaks reflect the combined contribution of a higher energy input and the combustion properties of hydrogen (high flame speed, elevated adiabatic flame temperature, and high diffusivity). The peak in-cylinder pressure increases from 75.2 bar at HER 0 to 79.1 bar at HER 20, representing 5.2% increase. The HER increases proportionally with HER, rising from 129 J/deg at HER 0 to 211 J/deg at HER 20 (+63.6%). The maximum temperature also shows an upward trend, increasing from 1542 K at HER 0 to 1735 K at HER 20, driven by hydrogen’s high adiabatic flame temperature [50,51]. Moreover, since the LHV of hydrogen is approximately three times that of diesel and six times that of methanol, both the peak pressure and maximum temperature increase as the ratio of hydrogen in the fuel mixture rises [50][51]. Similar results have been reported by Karagöz et al. [29] and Christodoulou and Megaritis [52] for hydrogen-supplemented diesel engines.

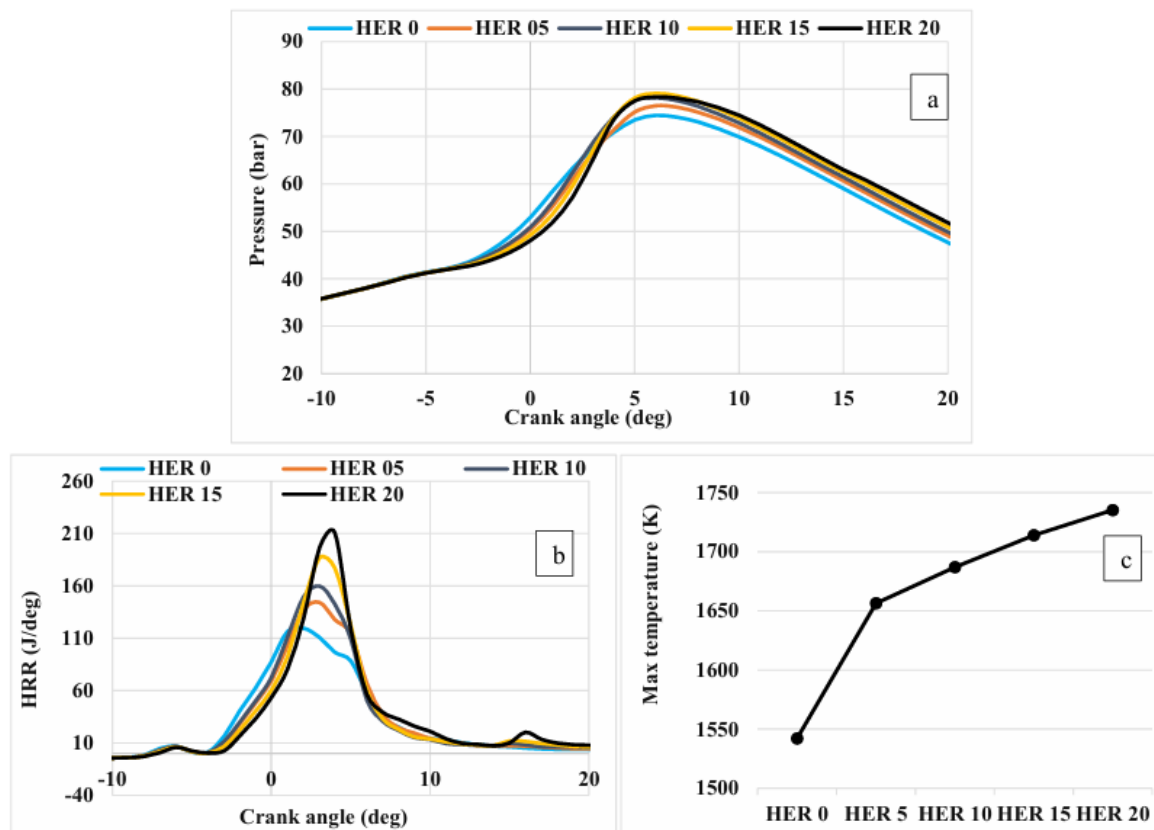


Figure 8. Effect of HER on: a) in cylinder pressure, b) heat release rate, and c) max temperature.

The ignition delay denotes the time between the start of injection and the start of ignition. It is defined as the moment when 10% of the fuel mass has burned. Figure 9.a illustrates the effect of HER on ignition delay, showing that the addition of hydrogen has a negligible impact on the ignition delay, reducing it by only 1° for HER 05, HER 10, HER 15, and HER 20, compared to HER 0. The near-constancy of ignition delay despite increasing HER reflects the dominant role of the heptane pilot fuel in controlling the onset of ignition: the pilot is directly injected into a hot compressed charge and undergoes auto-ignition driven by its own low-temperature chemistry, largely independently of the premixed hydrogen-methanol fraction. This is consistent with dual-fuel ignition behavior reported by Zou et al. [53].

Figure 9.b, shows that for $0 \leq \text{HER} \leq 10$, the combustion duration remains relatively unchanged. However, for $15 \leq \text{HER} \leq 20$, the combustion duration increases by approximately 2° CA and 3° CA, respectively, indicating a notable effect of hydrogen addition at higher ratios. The observed increase in combustion duration is primarily attributed to locally fuel-rich pockets that develop in the spray core as HER increases, where the equivalence ratio moves toward richer conditions, and reduced oxygen availability slows flame propagation (Section 3.2). Although hydrogen's high mass diffusivity enhances fuel-air mixing and typically promotes faster combustion, this effect is outweighed at high enrichment levels by the dominant influence of mixture richness. As shown in Section 3.1, higher HER levels additionally produce larger spray droplets and longer vapor penetration, both of which further contribute to a more distributed, longer-duration combustion process. The CA50 is the crank angle at which 50% of the mass fraction is burned, representing the center point of heat release. It is commonly used to optimize the combustion process, aiming to reduce fuel consumption and enhance engine performance [54]. Figure 9.c indicates that CA50 remains constant for $0 \leq \text{HER} \leq 10$. However, it increases for $15 \leq \text{HER} \leq 20$, indicating a shift of approximately 1° CA in combustion phasing as the hydrogen enrichment ratio rises. This is due to the extended combustion duration within this range of HER.

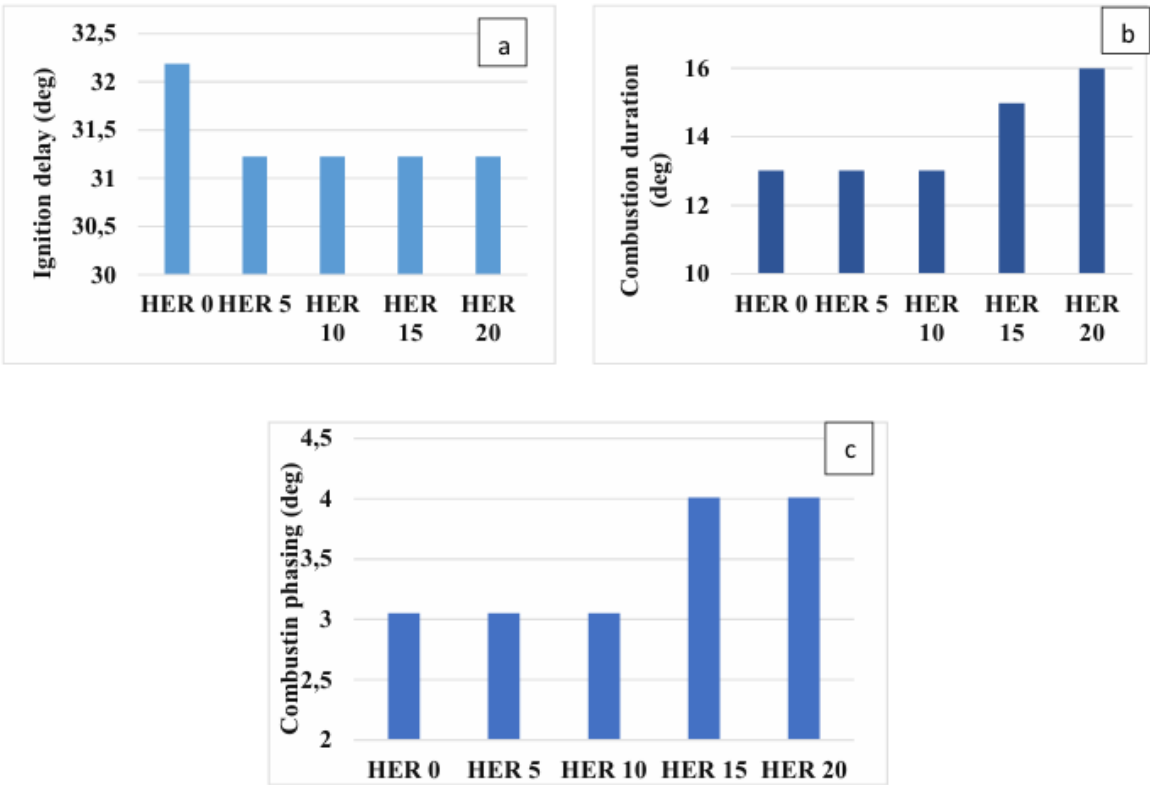


Figure 9. Impact of HER on a) Ignition delay b) combustion duration, and c) Combustion phasing CA50.

3.4. Engine Performance and Emissions

Figure 10 presents the normalized thermal efficiency and indicated specific fuel consumption (ISFC) relative to the baseline methanol-diesel case (HER 0), where normalization is performed with respect to the neat methanol-diesel operating point without hydrogen enrichment. It is found that hydrogen addition boosts thermal efficiency while reducing ISFC. The ISFC is computed as the ratio of total fuel mass flow rate (diesel + methanol + hydrogen) to indicated power output. It decreases across all HERs, from approximately 0.94 at HER 05 to 0.86 at HER 20. As noted above, since hydrogen is added the total energy input and IMEP both increase with HER. Therefore, the ISFC reduction reflects two compounding effects: hydrogen’s LHV (≈ 120 MJ/kg, approximately 2.8 $\times$ that of diesel and 6 $\times$ that of methanol) contributes a disproportionately large energy increment per unit mass added, while an actual improvement in fuel conversion efficiency also occurs, as evidenced by the indicated thermal efficiency which rises from +3.4% at HER 05 to +6.2% at HER 20. This efficiency gain is attributed to the reduction in flame quenching distance associated with hydrogen’s low Lewis number allows more complete combustion near the cylinder walls, recovering energy that would otherwise be lost as unburned hydrocarbons [55].

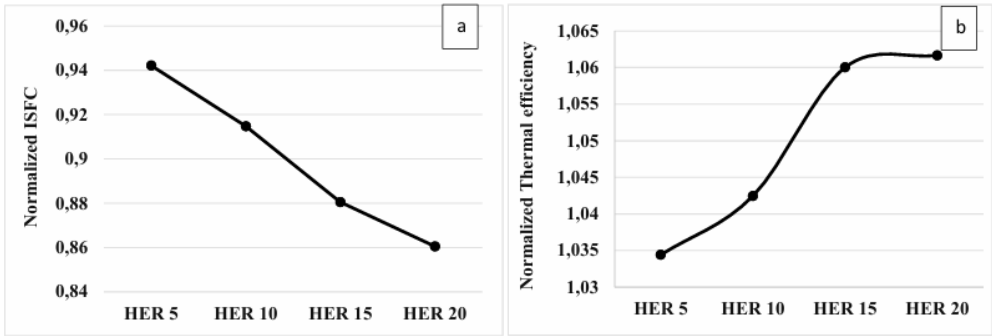


Figure 10. Normalized ISFC and normalized thermal efficiency.

The addition of hydrogen leads to a reduction in CO₂ emissions (Figure 11.a). Since the carbon-containing fuel inputs (diesel and methanol) are held constant across all HER cases, the total carbon input to the combustion chamber remains unchanged. However, as hydrogen is a carbon-free fuel, its addition increases the total power output without introducing additional CO₂, thereby reducing the specific CO₂ emissions per unit power output. At HER 05, CO₂ emissions decrease by 9.5%, while at higher enrichment ratios, such as HER 20, the reduction reaches 24%. Similar results were found by Ene et al. [56], who studied the effects of hydrogen addition on engine performance and pollutant emissions. Their experiments were conducted on an automotive diesel engine, operating at 2000 rpm and 70% load.

The effect of hydrogen enrichment on NO_x emissions is shown in Figure 11.b. For a 5% hydrogen enrichment (HER 05), the normalized NO_x emission is 2.05, representing approximately a twofold increase compared to the neat methanol-diesel mixture (0% hydrogen). A further rise in NO_x emissions is observed at HER 20, with the normalized NO_x reaching 3.52. This is mainly attributed to the increase of in-cylinder gas temperature (Figure 8.c), as the addition of hydrogen elevates the thermal conditions in the combustion chamber, promoting higher NO_x formation [57][58]. To mitigate NO_x penalty while preserving the efficiency gains, a coupled HER-EGR-injection timing parametric study is identified as the highest-priority direction for future work: increasing EGR from 7.5% to approximately 20-25% is estimated to reduce NO_x by 50-60%, and a further 15-25% reduction can be achieved through injection timing retardation of 3-5° CA at a modest efficiency penalty.

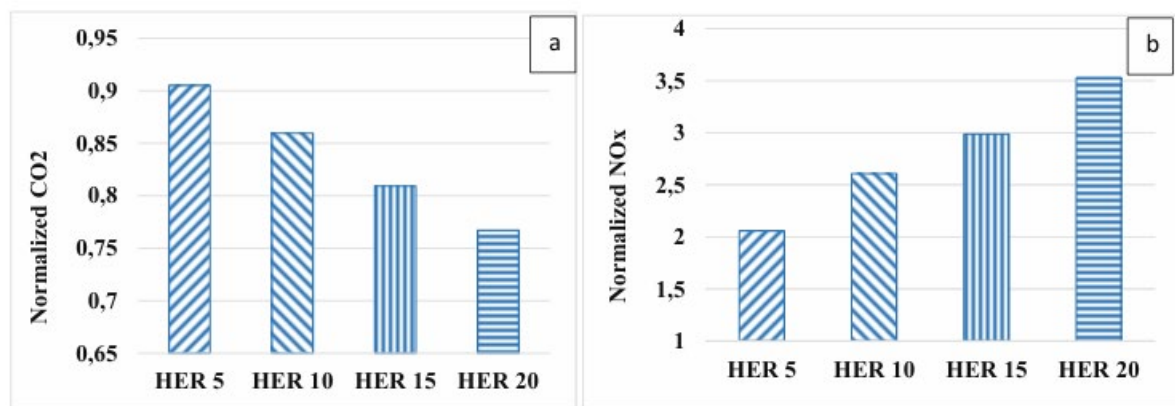


Figure 11. Normalized CO₂ and NO_x emissions.

4. Conclusions

This study examines the impact of hydrogen enrichment ratios on spray atomization, and the combustion performance of methanol-diesel dual-fuel combustion. The simulations are conducted using an Unsteady Reynolds-Averaged Navier-Stokes approach along with an Eulerian-Lagrangian framework. The G-equation is used to model turbulent flame evolution and establish a direct correlation with the laminar flame speed. The KH-RT model captures spray breakup, while turbulence is governed by the RNG k- ϵ model. A detailed reaction mechanism of 425 species and 3128 reactions is implemented. The numerical results are validated against experimental data, and the key findings are summarized as follows:

- Increasing the HER from 5% to 20%, raises the SMD of the diesel surrogate spray from 20.2 μm to 28 μm (+38%), indicating a reduction in the atomization of the fuel spray. This trend is due to the low density of hydrogen, which weakens Weber-number-driven KH aerodynamic breakup, resulting in the formation of larger droplets with reduced surface-to-volume ratios and slower evaporation rate. Despite this spray-side degradation, the combustion-enhancing properties of hydrogen dominate the overall engine response.

- The peak in-cylinder pressure, HRR, and maximum temperature all increase as the ratio of hydrogen increases, driven by both higher total energy input and hydrogen's elevated adiabatic temperature and faster flame speed. The HRR peak amplification of 63.6% at HER 20 indicates a transition towards premixed-dominated combustion, with the diesel pilot serving primarily as a combustion initiator for hydrogen-methanol premixed charge.
- Hydrogen-enriched methanol-diesel mixtures promote combustion efficiency by up to +6.2% at HER 20, with a corresponding ISFC reduction. The gain reflects the proportionally larger increase in indicated power relative to total fuel mass consumption, driven by hydrogen's high flame speed, high diffusivity, and reduced quenching losses.
- CO₂ decreases by 24% at HER 20 since the carbon-containing fuel inputs (diesel and methanol) are held constant while hydrogen, being a carbon-free fuel, increases the power output without introducing additional carbon, thereby reducing the CO₂ formation per unit power output. NO_x surges 3.52-fold, driven by the temperature sensitivity of the Zeldovich mechanism and the 193 K elevation in peak cylinder temperature.

Overall, hydrogen-enriched methanol-diesel dual-fuel combustion represents a pathway toward high-efficiency, low-carbon CI engine operation. Future work should quantify the coupled effect of EGR rate and HER on the NO_x-efficiency trade-off and extend the analysis to multi-cycle operation to assess cycle-to-cycle variability.

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