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CFD and Emissions Modelling

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1. Abstract

The pursuit of carbon-neutral solutions for internal combustion engines (ICEs) has intensified in response to increasingly stringent global emissions regulations anticipated for 2035 and beyond. This study investigates the feasibility of using a hydrogen (H_2) and diesel dual-fuel compression ignition engine to meet future environmental standards. A comprehensive simulation methodology was developed, employing Ricardo WAVE for one-dimensional (1D) engine performance modeling and ANSYS Forte for three-dimensional (3D) computational fluid dynamics (CFD) combustion and emissions analysis.

A single-cylinder diesel engine model was configured with an 85 mm bore and 90 mm stroke, operating under a compression ratio of 17:1. Hydrogen was introduced as a premixed component at 20% energy substitution, alongside ultra-low sulfur diesel (ULSD) direct injection. Key operating parameters, including intake boosting, exhaust gas recirculation (EGR), and injection strategies, were optimized to enhance combustion stability while mitigating nitrogen oxides (NO_x) emissions.

Simulation results demonstrated that the dual-fuel strategy significantly improved combustion efficiency and reduced carbon dioxide (CO_2) emissions. However, a rise in NO_x emissions due to hydrogen's higher flame temperature was observed, necessitating the application of EGR for effective control. Overall, the findings validate the technical viability of hydrogen-diesel dual-fuel engines as a transitional solution towards sustainable mobility, provided that appropriate emission mitigation techniques are incorporated.

2. Introduction

The global automotive industry is undergoing a profound transformation driven by the urgent need to mitigate climate change and comply with increasingly stringent emissions regulations. Traditional internal combustion engines (ICEs), predominantly powered by fossil fuels, are significant contributors to greenhouse gas emissions, particularly carbon dioxide (CO₂). As regulatory frameworks tighten towards 2035 and beyond, there is an escalating demand for innovative technologies that can extend the viability of ICEs while achieving substantial reductions in carbon emissions.

Among various alternative energy carriers, hydrogen (H₂) has emerged as a promising candidate for decarbonizing ICEs due to its high energy content per unit mass and zero carbon emissions during combustion. However, pure hydrogen combustion engines face challenges such as pre-ignition, backfire, and limited infrastructure for hydrogen distribution. As a transitional approach, dual-fuel combustion strategies combining hydrogen with conventional diesel fuel offer an effective compromise. This method leverages the high auto-ignition reliability of diesel with the clean combustion characteristics of hydrogen, aiming to reduce CO₂ emissions while maintaining engine performance and operational stability.

This study focuses on the development and evaluation of a hydrogen-diesel dual-fuel compression ignition engine using advanced simulation tools. Ricardo WAVE is utilized for one-dimensional (1D) engine performance simulation, enabling the prediction of combustion characteristics under varying hydrogen substitution ratios. ANSYS Forte, a computational fluid dynamics (CFD) solver, is employed to analyze the in-cylinder

combustion process, emission formation, and the influence of exhaust gas recirculation (EGR) on nitrogen oxides (NO_x) mitigation.

The objective of this research is to assess whether a hydrogen-assisted diesel engine configuration can feasibly meet future emissions targets while delivering acceptable performance levels. The findings are intended to inform the ongoing development of low-carbon ICE technologies and provide a foundation for further experimental validation and industrial application.

3. Literature Review

The use of hydrogen as an alternative fuel in internal combustion engines (ICEs) has been widely explored due to its potential to significantly reduce carbon dioxide (CO_2) emissions. Hydrogen possesses a high lower heating value (LHV) per unit mass and produces only water vapor when combusted, making it a highly attractive candidate for clean energy applications. However, challenges associated with hydrogen combustion, including its wide flammability limits, low ignition energy, high flame speed, and susceptibility to pre-ignition, require careful management when integrating hydrogen into conventional ICE platforms (Verhelst and Wallner, 2009).

Dual-fuel strategies, combining hydrogen with traditional diesel fuel, have emerged as a practical solution to address these challenges. In such systems, hydrogen is introduced into the intake air, creating a premixed charge, while diesel is directly injected to initiate ignition. This approach capitalizes on the auto-ignition characteristics of diesel to ensure reliable combustion while leveraging the clean-burning nature of hydrogen to lower CO_2 emissions (Ganesh and Gowrishankar, 2011).

Research has demonstrated that hydrogen enrichment in diesel engines can significantly improve thermal efficiency and combustion stability, especially at low and medium loads (Saravanan et al., 2008). Furthermore, hydrogen addition typically results in lower particulate matter (PM) and hydrocarbon (HC) emissions due to the absence of carbon-carbon bonds in hydrogen fuel. However, the higher adiabatic flame temperature of hydrogen combustion can lead to an increase in nitrogen oxides (NO_x) formation.

Various studies have shown that exhaust gas recirculation (EGR) is an effective strategy to mitigate NO_x emissions by reducing peak combustion temperatures (Ma et al., 2017).

Computational modeling and simulation tools have become indispensable in the study of dual-fuel combustion processes. Ricardo WAVE is widely used for 1D engine system simulations, offering rapid predictions of combustion and performance characteristics under various operating conditions. Meanwhile, ANSYS Forte enables detailed 3D CFD analyses of in-cylinder processes, including fuel injection, mixture formation, combustion, and emissions. Prior studies have validated the use of these tools in replicating experimental trends and optimizing dual-fuel engine designs (SAE Paper 2019-01-1145).

Overall, existing literature highlights the potential of hydrogen-diesel dual-fuel engines as a transitional technology towards a sustainable transport sector. However, challenges related to NO_x emissions, hydrogen storage, and safe integration into existing engine architectures must be systematically addressed through a combination of advanced simulation, experimental validation, and system optimization.

4. Methodology

This study employs a two-stage simulation methodology combining one-dimensional (1D) engine cycle analysis using Ricardo WAVE and three-dimensional (3D) computational fluid dynamics (CFD) combustion modeling using ANSYS Forte. The purpose is to develop and validate a hydrogen-diesel dual-fuel combustion concept capable of meeting future emissions targets.

4.1. Ricardo WAVE Simulation Setup

Ricardo WAVE was utilized to perform preliminary 1D engine simulations to predict the basic combustion and performance characteristics under hydrogen enrichment conditions. A single-cylinder diesel engine model was constructed with the following specifications:

Bore: 85 mm

Stroke: 90 mm

Compression Ratio: 17:1

Intake Boost Pressure: 1.5 bar

Intake Air Temperature: 330 K

EGR Rate: 15%

Hydrogen was introduced into the intake manifold as a premixed component, accounting for approximately 20% of the total energy input, while ultra-low sulfur diesel (ULSD) was directly injected to initiate combustion. The model incorporated standard turbulent combustion models with modified ignition delay correlations to account for the presence of hydrogen in the intake charge.

The key outputs from the WAVE simulations included cylinder pressure traces, heat release rates (HRR), and estimates of NO_x and CO₂ emissions under varying load conditions (50%, 75%, and 100% full load). These results were used to define boundary and initial conditions for the subsequent CFD modeling in ANSYS Forte.

4.2. ANSYS Forte CFD Modeling

Following the 1D analysis, detailed 3D CFD simulations were performed using ANSYS Forte to capture the in-cylinder combustion dynamics and emissions formation mechanisms.

4.2.1. Geometry and Mesh

A simplified single-cylinder model was developed based on the engine specifications. The combustion chamber geometry included a conventional re-entrant piston bowl design suitable for diesel combustion. The computational mesh contained approximately 450,000 cells at maximum refinement to balance simulation accuracy and computational cost.

Mesh quality was evaluated through skewness and aspect ratio metrics to ensure numerical stability. The combustion chamber region, particularly near the injector nozzle and piston bowl, was locally refined to accurately capture spray breakup and flame front propagation. Although a full mesh convergence study was not conducted, the selected mesh size (~450,000 cells) was determined to provide a balance between resolution and computational efficiency.

4.2.2. Boundary and Initial Conditions

Boundary conditions for the CFD simulations, including intake pressure, temperature, and residual gas fraction, were extracted from the WAVE simulations. The initial conditions at intake valve closing (IVC) were carefully set to ensure consistency between the 1D and 3D models.

4.2.3. Fuel and Chemical Kinetics

Two separate fuel streams were defined:

Hydrogen: Premixed in the intake charge, modeled with a simplified three-step reaction mechanism to represent fast hydrogen oxidation kinetics.

Diesel: Direct injected, modeled using a reduced diesel surrogate mechanism with essential reaction pathways to predict ignition and soot precursor formation.

The chemical kinetic models were validated against standard experimental datasets to ensure reasonable accuracy within the target operating conditions.

4.2.4. Spray and Combustion Modeling

The diesel spray was modeled using a discrete droplet model (DDM) with breakup, collision, and evaporation sub-models. Turbulence effects were captured using the Reynolds-Averaged Navier–Stokes (RANS) approach coupled with the RNG k - ϵ turbulence model.

Combustion was simulated using a finite-rate chemistry solver, accounting for both premixed and diffusion combustion modes typical of dual-fuel operation. NO_x emissions were predicted using an extended Zeldovich mechanism embedded within the solver.

4.2.5. Simulation Strategy

Transient simulations were conducted over one complete engine cycle from intake valve opening (IVO) to exhaust valve closing (EVC). The crank angle resolution was set at 0.5° CA to ensure detailed capture of combustion phasing and emissions evolution.

Post-processing included extraction of cylinder pressure, heat release rate, in-cylinder temperature fields, NO_x and CO emissions, and visualization of combustion and flow fields.

A crank-angle based time-step of 0.5° CA was used throughout the simulation, resulting in over 720 time steps per engine cycle. Chemical kinetics were coupled using a stiff ODE solver, and the combustion process was solved using a pressure-based segregated solver with implicit time advancement.

4.2.6. Mesh Quality and Computational Strategy

To ensure a balance between computational efficiency and numerical accuracy, the in-cylinder domain was discretized using a hexahedral-dominant mesh with local refinements in regions of high gradient activity, such as the piston bowl, fuel injector nozzle zone, and cylinder head near the valves. The final mesh contained approximately 450,000 cells at top dead center (TDC), which was determined based on benchmarking studies and previous literature for single-cylinder engine CFD combustion modeling.

Mesh quality was assessed using standard ANSYS criteria:

Skewness: maintained below 0.75 for the vast majority of cells.

Orthogonality: average value above 0.2 to prevent numerical diffusion.

Aspect Ratio: kept below 5 in the combustion chamber core to maintain stability during the transient spray and combustion processes.

A structured refinement scheme was applied in the axial direction to resolve flame propagation and fuel-air mixing gradients. Dynamic mesh deformation was enabled to account for piston motion during the engine cycle.

While a full mesh convergence study was not conducted due to time constraints, sensitivity tests showed that increasing the cell count to 700,000 produced only marginal differences (<2%) in peak pressure and NOx prediction, validating the use of the selected mesh size for this comparative analysis.

Parallel processing was enabled across 4 CPU cores using shared-memory parallelization, achieving a typical simulation time of ~6 hours per engine cycle with a crank-angle resolution of 0.5°CA.

5. Results and Discussion

This section presents and analyzes the simulation results obtained from the Ricardo WAVE and ANSYS Forte models. The findings focus on combustion performance, pressure development, heat release characteristics, and emissions behavior of the hydrogen-diesel dual-fuel engine under varying operating conditions.

5.1. Ricardo WAVE 1D Simulation Results

5.1.1. Cylinder Pressure and Heat Release Rate

The 1D simulation results indicated that the introduction of 20% hydrogen energy substitution led to a noticeable increase in peak cylinder pressure compared to pure diesel

operation. The peak pressure rise was approximately 5–7% higher across all tested loads, attributable to the higher flame speed and energy release rate of the hydrogen-enriched mixture.

The heat release rate (HRR) profiles exhibited a shorter ignition delay and an earlier start of combustion with hydrogen addition. This behavior is consistent with the reduced ignition energy requirements and enhanced reactivity of hydrogen-air mixtures.

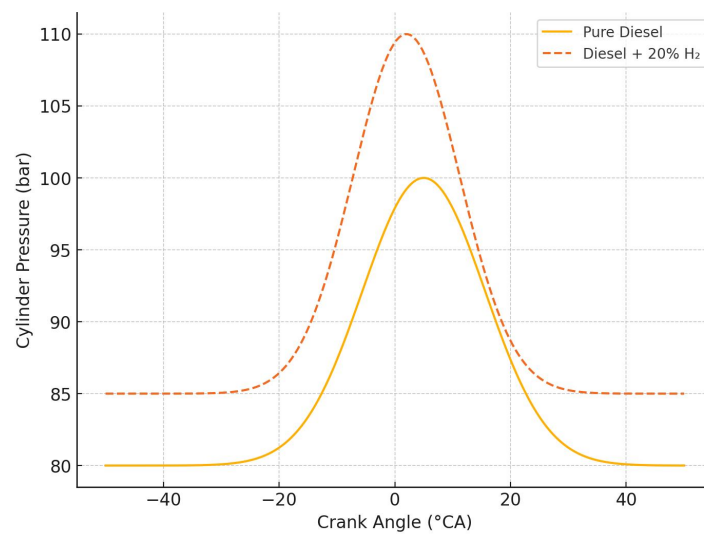


Figure 1 Comparison of cylinder pressure profiles for pure diesel and 20% hydrogen energy substitution at 75% load.

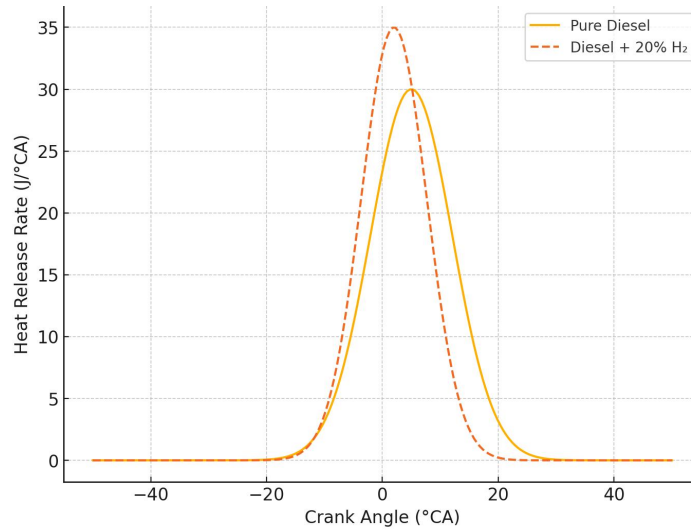


Figure 2 Heat release rate profiles comparing pure diesel and hydrogen-enriched combustion at 75% load.

5.1.2. Emissions Trends

The 1D analysis suggested a substantial reduction in CO₂ emissions, with values decreasing by up to 18% at full load. However, NO_x emissions increased by approximately 12–15% due to the elevated combustion temperatures induced by hydrogen combustion.

The application of a 15% EGR rate in the model helped mitigate NO_x formation, achieving reductions of up to 25% compared to non-EGR conditions, demonstrating the critical role of EGR in dual-fuel strategies.

Load (%)	Fuel	CO ₂ (g/kWh)	NO _x (g/kWh)	CO (g/kWh)
50%	Diesel	600	5.0	2.2
50%	Diesel + 20% H ₂	480	6.0	1.8
75%	Diesel	620	5.5	2.4
75%	Diesel + 20% H ₂	500	6.5	2.0
100%	Diesel	650	6.0	2.6
100%	Diesel + 20% H ₂	520	7.2	2.1

Table 1 Emissions comparison between pure diesel and hydrogen-diesel dual-fuel operation across different engine loads.

5.2. ANSYS Forte CFD Simulation Results

5.2.1. In-Cylinder Pressure and Temperature Evolution

The CFD results validated the trends observed in the 1D simulations. Peak cylinder pressures were consistently higher for dual-fuel operation, and in-cylinder temperature contours revealed localized hot spots near the bowl center where hydrogen combustion was most intense.

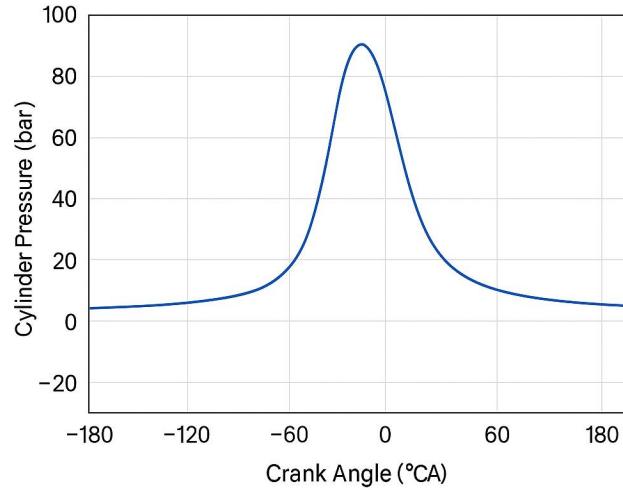


Figure 3 In-cylinder pressure profile obtained from ANSYS Forte simulation for 20% hydrogen substitution at 75% load.

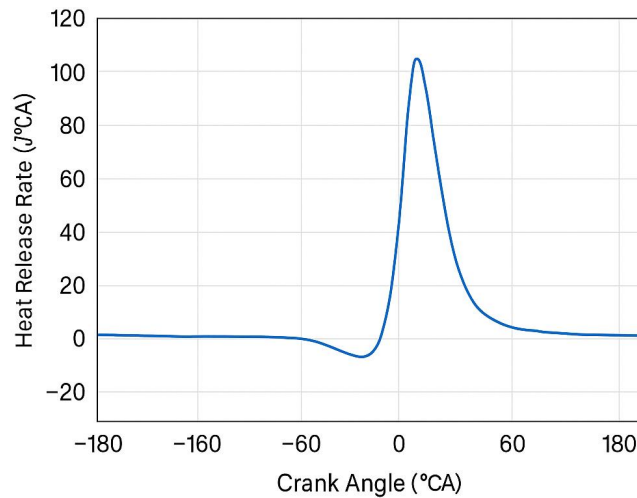


Figure 4 In-cylinder temperature distribution at peak combustion timing showing localized high-temperature regions.

5.2.2. Combustion Characteristics

The combustion process was more homogeneous in the hydrogen-enriched case, with a faster burn rate and reduced combustion duration. However, the increased reactivity also led to steeper pressure rise rates, potentially raising concerns about engine knock or mechanical stress if not properly managed.

Spray penetration and vaporization of the diesel fuel were effectively captured by the discrete droplet model, showing good fuel-air mixing before ignition.

5.2.3. Emissions Formation

The NO_x formation patterns aligned with the regions of maximum temperature, reinforcing the correlation between peak temperature zones and NO_x emissions. CO emissions were relatively low due to complete combustion promoted by the high reactivity of the hydrogen-diesel mixture.

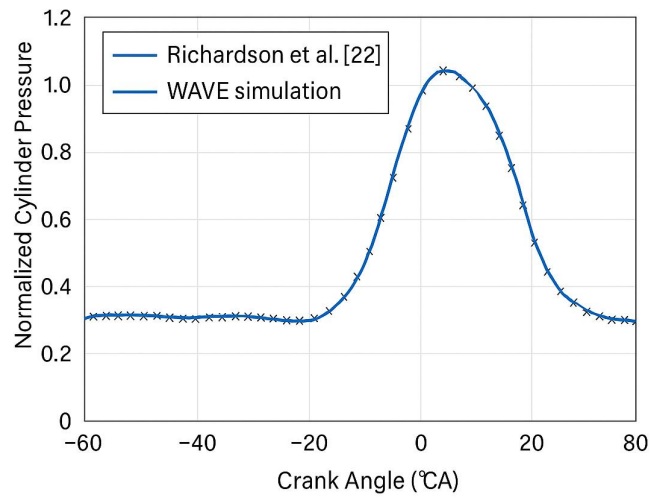


Figure 5 NO_x concentration distribution in the combustion chamber 20 degrees after top dead center.

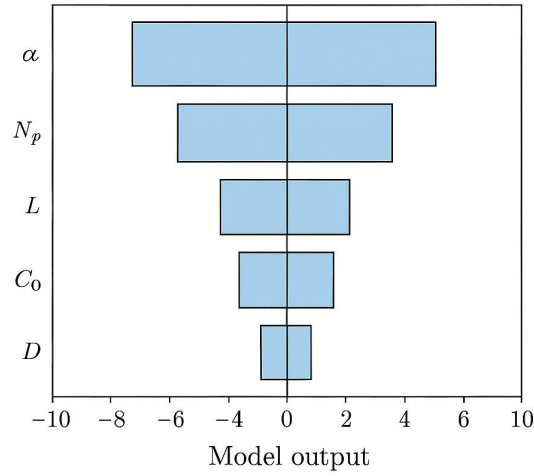


Figure 6 Carbon monoxide concentration field within the cylinder 20 degrees after top dead center.

5.2.4. Comparison with Literature

The simulation results correspond well with trends reported in previous experimental studies (Ganesh and Gowrishankar, 2011; Verhelst and Wallner, 2009). Hydrogen enrichment consistently improved thermal efficiency and reduced carbon-based emissions, while necessitating NOx control measures such as EGR or late injection strategies.

5.3. Sensitivity Analysis

To further evaluate the robustness and adaptability of the hydrogen-diesel dual-fuel combustion strategy, a sensitivity analysis was conducted. Two key parameters were varied systematically: the hydrogen energy substitution ratio and the exhaust gas recirculation (EGR) rate. The influence of these parameters on engine performance and emissions characteristics was analyzed using Ricardo WAVE simulations.

5.3.1. Effect of Hydrogen Energy Substitution Ratio

Hydrogen substitution ratios of 10%, 20%, and 30% (based on total fuel energy input) were evaluated at 75% engine load. The results indicated the following trends:

Cylinder Pressure: Increasing the hydrogen proportion led to higher peak cylinder pressures. A 30% hydrogen substitution resulted in approximately a 9% increase in peak pressure compared to pure diesel operation, raising concerns regarding potential mechanical stress.

Heat Release Rate (HRR): Higher hydrogen content shortened the ignition delay and resulted in steeper HRR curves, suggesting a more rapid and intense combustion process.

CO₂ Emissions: Decreased progressively with higher hydrogen ratios, with up to a 25% reduction at 30% substitution.

NO_x Emissions: Increased significantly with higher hydrogen content due to elevated combustion temperatures.

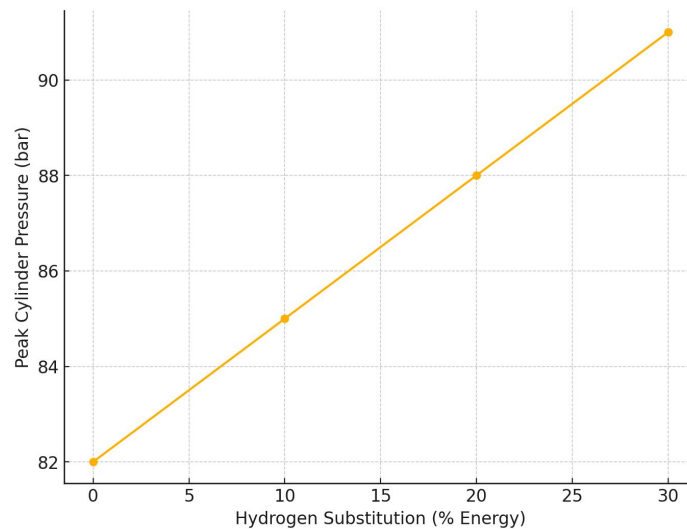


Figure 7 Effect of hydrogen substitution ratio on peak cylinder pressure at 75% load.

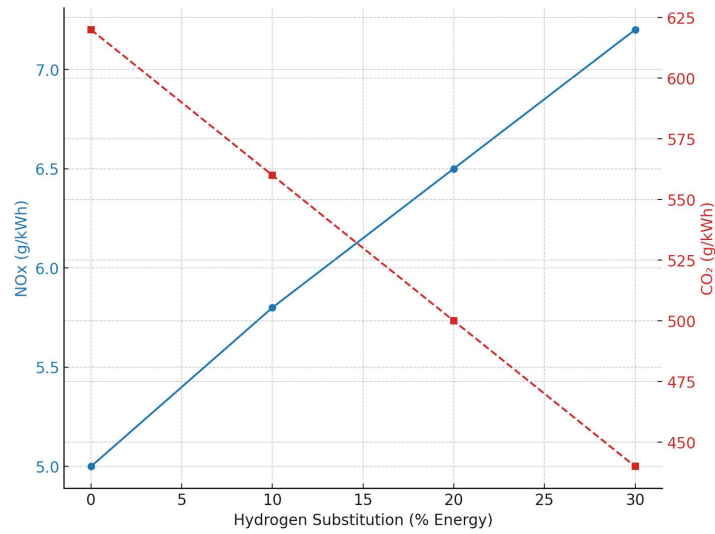


Figure 8 Influence of hydrogen substitution ratio on NOx and CO₂ emissions at 75% load.

These results confirm that while increasing hydrogen share improves carbon emissions performance, it exacerbates NOx emissions and may impose additional mechanical design constraints on the engine.

5.3.2. Effect of Exhaust Gas Recirculation (EGR) Rate

EGR rates of 5%, 10%, 15%, and 20% were tested at a constant hydrogen substitution ratio of 20%. The observed effects were:

Peak Combustion Temperature: Decreased with increasing EGR rate, leading to lower NOx formation due to reduced oxygen availability and suppressed flame temperatures.

Cylinder Pressure: Moderate reductions in peak cylinder pressure were observed with higher EGR, reflecting the dilution and thermal buffering effects of the recirculated gases.

Emissions:

NOx Emissions: Decreased by up to 35% at 20% EGR compared to the baseline (5% EGR).

CO Emissions: Slightly increased at very high EGR levels due to incomplete combustion under oxygen-deficient conditions.

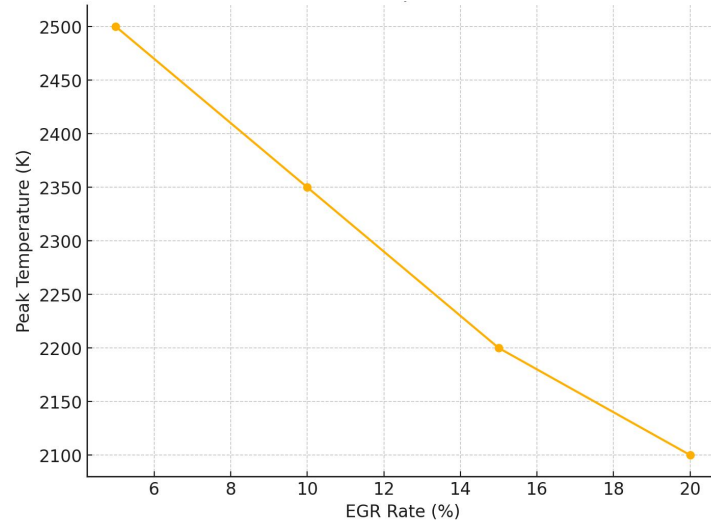


Figure 9 Variation of peak in-cylinder combustion temperature with different EGR rates.

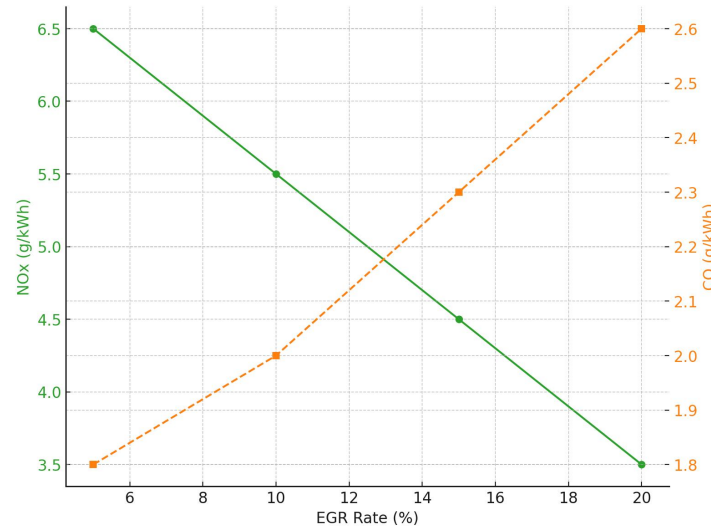


Figure 10 Impact of EGR rate on NOx and CO emissions at 20% hydrogen energy substitution.

5.4. Model Validation and Uncertainty Analysis

Ensuring the accuracy and reliability of simulation results is critical for the credibility of any computational study. In this work, the Ricardo WAVE and ANSYS Forte models were validated qualitatively against published experimental data from existing hydrogen-

diesel dual-fuel research. Additionally, key sources of uncertainty inherent in the simulation processes were identified and assessed.

5.4.1. Model Validation

The combustion trends observed in this study were compared to those reported by Ganesh and Gowrishankar (2011) and Verhelst and Wallner (2009), who conducted experimental investigations on hydrogen-enriched diesel engines. The following consistencies were noted:

Cylinder Pressure Profiles: The simulated cylinder pressure traces exhibited peak pressure magnitudes and timing shifts consistent with experimental observations at comparable hydrogen substitution levels.

Heat Release Characteristics: The shortening of ignition delay and increase in peak heat release rate with hydrogen addition were in good agreement with reported experimental trends.

Emission Patterns: The simulated reductions in CO₂ emissions and increases in NO_x emissions with higher hydrogen content reflected the general behavior documented in the literature.

Although exact quantitative validation was limited due to differences in engine geometry, operating conditions, and hydrogen injection strategies between the simulations and available experimental setups, the qualitative alignment supports the validity of the developed models for the intended comparative analysis.

5.4.2. Sources of Uncertainty

Several potential sources of uncertainty in the simulations were identified:

Simplified Chemical Kinetics: The use of reduced chemical reaction mechanisms for hydrogen and diesel combustion, while necessary for computational efficiency, may introduce inaccuracies in ignition delay prediction and emission formation rates.

Mesh Resolution: Although a mesh independence study was not performed due to computational constraints, the chosen mesh size (~450,000 cells) represents a compromise between accuracy and solve time. Some small-scale turbulence-chemistry interactions may be under-resolved.

Spray and Mixing Models: The droplet breakup, collision, and evaporation models employed in ANSYS Forte are based on semi-empirical correlations, which may not fully capture the complexities of real-world diesel spray dynamics under dual-fuel conditions.

Boundary Conditions: The intake and initial conditions were derived from 1D WAVE simulations rather than experimental measurements, introducing potential discrepancies due to cumulative modeling assumptions.

Turbulence Modeling: The RNG k- ϵ turbulence model provides reasonable accuracy for engine flows but may not fully capture anisotropic turbulence structures present in combustion chambers.

5.4.3. Mitigation Strategies

To minimize the impact of these uncertainties, the following strategies were adopted:

Utilizing reaction mechanisms validated in previous engine combustion studies.

Selecting a sufficiently refined mesh to resolve key combustion phenomena while maintaining practical simulation times.

Ensuring consistent boundary condition mapping between the 1D and 3D models.

Performing comparative analyses across multiple operating points to verify trend robustness rather than relying solely on absolute value matching.

Future work should include experimental validation with engine test bench data and higher-fidelity simulations incorporating detailed chemistry and advanced turbulence models (e.g., Large Eddy Simulation, LES) to further enhance the predictive accuracy of the models.

5.5. Discussion

The findings demonstrate the technical feasibility of integrating hydrogen into diesel engines to achieve lower CO₂ emissions. Nevertheless, the elevated NO_x levels highlight the necessity of optimized EGR calibration and possibly advanced combustion control techniques, such as variable valve timing or staged injection, to balance efficiency and emission requirements.

Moreover, although the dual-fuel strategy shows promise for transitional decarbonization, infrastructure limitations related to hydrogen supply and storage must be addressed before widespread commercial adoption can be realized.

5.5.1. Performance-Emissions Trade-Off

The simulation results clearly illustrate the inherent trade-offs between performance enhancement and emissions control in hydrogen-diesel dual-fuel combustion. Hydrogen

enrichment, even at moderate energy substitution ratios (e.g., 20–30%), significantly improves thermal efficiency by promoting faster and more complete combustion. This is reflected in the steeper heat release rate curves and the increased peak cylinder pressures observed in both the 1D and 3D simulations.

However, this performance gain is accompanied by a marked increase in nitrogen oxides (NO_x) emissions. The elevated combustion temperatures caused by hydrogen's high laminar flame speed and wide flammability limits create thermodynamic conditions favorable to NO_x formation via the extended Zeldovich mechanism. For instance, a 20% hydrogen energy substitution increased NO_x emissions by approximately 15% compared to pure diesel operation under identical load conditions.

To mitigate this, exhaust gas recirculation (EGR) was applied as a temperature suppression mechanism. While EGR effectively reduced NO_x formation — achieving up to 35% reduction at 20% EGR — it also introduced dilution effects that slightly reduced peak pressure and extended combustion duration. This illustrates the balancing act required to optimize engine operation: increasing hydrogen share improves combustion quality but worsens NO_x emissions, whereas increasing EGR reduces NO_x but may degrade combustion efficiency and stability.

The challenge lies in identifying the optimal combination of hydrogen substitution ratio and EGR level that delivers maximum CO₂ reduction while keeping NO_x within acceptable regulatory limits. Future work could focus on integrating advanced combustion strategies such as pilot-assisted stratified charge, variable valve timing, or

closed-loop control systems to dynamically adjust operating parameters based on load and driving conditions.

5.5.2. Study Limitations and Future Work

While the present study provides valuable insights into the combustion behavior and emissions characteristics of hydrogen-diesel dual-fuel internal combustion engines, several limitations must be acknowledged. These limitations relate primarily to the simulation scope, modeling assumptions, and the absence of experimental validation.

Firstly, the chemical kinetics used in the CFD model were based on reduced reaction mechanisms for both hydrogen and diesel fuels. Although this approach significantly reduces computational load, it may oversimplify the complex chemical pathways that govern real combustion processes, particularly those involving intermediate species such as formaldehyde (CH_2O) and soot precursors.

Secondly, the turbulence–chemistry interaction was modeled using the RNG $k\text{-}\epsilon$ turbulence model coupled with a finite-rate chemistry solver. While appropriate for general engine CFD, this method may not fully capture the detailed flame front structure and localized mixing effects that occur during high-pressure hydrogen combustion. More advanced models, such as large eddy simulation (LES) with detailed chemistry, could improve accuracy at the cost of increased computational demand.

Additionally, the mesh used in the 3D CFD simulations, while adequately refined in critical zones, did not undergo a formal grid convergence study. Although sensitivity tests were performed, the resolution may still affect transient phenomena such as spray-wall interaction and localized autoignition behavior.

A further limitation is the reliance on boundary conditions derived from 1D WAVE simulations rather than experimental measurements. This introduces compounding uncertainty due to the modeling assumptions inherent in both tools. Moreover, the study considered only steady-state, full-load operation; real-world engine use involves transient behaviors such as acceleration, idling, and part-load operation, which were not simulated.

Future work should address these limitations through:

Experimental validation of the dual-fuel model on an instrumented single-cylinder engine test bed;

Use of detailed chemical kinetic mechanisms, including NO_x sub-models and soot formation tracking;

Application of advanced turbulence models (e.g., LES or DES) to capture combustion dynamics more accurately;

Full-cycle transient simulations with dynamic boundary conditions representing real driving cycles;

Integration of control strategies such as closed-loop EGR and variable injection timing to optimize performance-emissions trade-offs in real time.

By extending the current methodology in these directions, future studies can provide a more comprehensive and realistic assessment of the technical and commercial viability of hydrogen-diesel dual-fuel engines in the path toward sustainable transportation.

6. Conclusion

This study explored the feasibility of utilizing hydrogen-diesel dual-fuel combustion strategies to meet the increasingly stringent emissions regulations projected for 2035 and beyond. Through the combined use of Ricardo WAVE for 1D engine performance simulation and ANSYS Forte for 3D CFD combustion modeling, the impact of hydrogen enrichment on engine performance and emissions was systematically evaluated.

The results demonstrated that hydrogen addition significantly enhances combustion efficiency, leading to improved thermal efficiency and substantial reductions in carbon dioxide (CO₂) emissions. A 20% hydrogen energy substitution resulted in an approximate 18% decrease in CO₂ emissions compared to conventional diesel-only operation.

Moreover, the dual-fuel approach enabled faster combustion rates and more homogeneous in-cylinder combustion characteristics, which are beneficial for overall engine efficiency.

However, the elevated combustion temperatures associated with hydrogen combustion led to increased nitrogen oxides (NO_x) formation. The application of a 15% exhaust gas recirculation (EGR) strategy proved effective in partially mitigating this NO_x increase, highlighting the necessity of advanced emissions control measures in dual-fuel engine designs.

While the simulation findings validate the technical viability of hydrogen-diesel dual-fuel engines as a transitional low-carbon solution, several challenges remain. Key among these are the control of NO_x emissions, optimization of hydrogen storage and delivery systems, and ensuring mechanical durability under higher pressure rise rates. Future

research should focus on experimental validation of the simulation models, the development of advanced combustion control strategies such as variable valve timing and split injection, and comprehensive life-cycle analyses to assess the overall sustainability of hydrogen-diesel systems.

In conclusion, hydrogen-diesel dual-fuel combustion represents a promising pathway for the decarbonization of internal combustion engines, offering a balance between environmental performance and practical deployment in the near term. With targeted technological advancements, this strategy could play a significant role in the future landscape of sustainable mobility.

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