1D COMBUSTION SIMULATION OF H2 IC ENGINE

M.Tech. Thesis

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DEPARTMENT OF MECHANICAL ENGINEERING INDIAN INSTITUTE OF TECHNOLOGY INDORE MAY 2024

1D COMBUSTION SIMULATION OF H2 IC ENGINE

A THESIS

Submitted in partial fulfillment of the requirements for the award of the degree of Master of Technology

> *by* **Gaurav Kumar**



DEPARTMENT OF MECHANICAL ENGINEERING INDIAN INSTITUTE OF TECHNOLOGY INDORE MAY 2024



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CANDIDATE'S DECLARATION

I hereby certify that the work which is being presented in the thesis entitled 1D COMBUSTION SIMULATION OF H2 IC ENGINE in the partial fulfilment of the requirements for the award of the degree of MASTER OF TECHNOLOGY and submitted in the DISCIPLINE OF THERMAL ENERGY SYSTEMS (MECHANICAL ENGINEERING, Indian Institute of Technology Indore, is an authentic record of my own work carried out during the time period from July 2022 to May 2024. Thesis submission under the supervision of Dr Ankur Miglani, Associate Professor, IIT Indore and Mr. Hardik Narendrabhai Lakhlani, Deputy General Manager, VECV.

The matter presented in this thesis has not been submitted by me for the award of any other degree of this or any other institute.

04-06-2024

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This is to certify that the above statement made by the candidate is correct to the best of my/our knowledge.

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Convener. DPGC Date:04-06-2024

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-Gaurav Kumar

Dedicated to my family for their love, care, and blessing

Abstract

This thesis presents an in-depth investigation into the 1D combustion simulation of a hydrogen (H2) internal combustion (IC) engine using Cruise-M software. The primary objective was to analyze the combustion characteristics of an IC engine fueled by hydrogen, an important alternative fuel in sustainable energy contexts. The study involved developing a 1D H2 IC engine combustion model using Cruise-M software, a well-established tool for engine performance analysis and simulation. Various parameters such as ignition timing (duration and start of combustion), pressure ratio , air-fuel ratio, and amount of air and fuel. were examined to optimize the engine's performance and emissions.

The research methodology comprised a thorough literature review, data collection, model development, simulation runs, and subsequent analysis of results. Validation of the developed model was achieved by comparing simulation results with experimental data. The effects of different operating conditions and design parameters on combustion efficiency, power output, and emissions were extensively explored. The key findings contribute significantly to understanding hydrogen-fueled IC engine combustion dynamics and offer valuable insights for optimizing engine design and operation. The study also underscores the potential of Cruise-M software in simulating and analyzing intricate combustion processes in internal combustion engines.

This thesis contributes to ongoing research in sustainable energy systems by focusing on hydrogen as a clean and efficient fuel for internal combustion engines, with practical implications for the automotive and power generation industries

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Nomenclature and Abbreviations

1D	1- Dimension			
ICE	Internal Combustion Engine			
PFI	Port Fuel Injection			
DFI	Direct Fuel Injection			
MFB	Mass Fraction Burned			
HRR	Heat Release rate			
a	Efficiency factor			
m	Shape factor			
IMEP	Indicated Mean Effective Pressure			
SOC	Start of Combustion			
DOC	Duration of Combustion			
RoHR	Rate of Heat Release			
EGR	Exhaust Gas recirculation			
HIL	Hardware-in-Loop			

Chapter 1

Introduction

1.1 Background Overview

The transition to sustainable energy sources is imperative as the global community faces increasing concerns over climate change and the volatility of petroleum prices. The transportation sector, responsible for about 25% of global CO2 emissions, predominantly uses fossil fuels, contributing significantly to greenhouse gas emissions and pollution. As populations and incomes rise, the demand for transportation grows, further escalating energy consumption and emissions. In this context, hydrogen (H2) emerges as a promising alternative fuel due to its clean combustion properties and high energy content. Hydrogen internal combustion engines (H2 ICEs) offer a viable solution by potentially reducing CO2 emissions significantly while leveraging existing combustion engine technology.

Hydrogen's primary combustion byproduct is water vapor, which drastically reduces CO2 and other harmful emissions compared to traditional fuels like gasoline and diesel. Additionally, hydrogen boasts a high energy content per unit mass, potentially leading to higher engine efficiencies. Its wide flammability range and high flame speed can enhance the combustion process, improving overall engine performance.

Hydrogen can be produced from renewable sources, further promoting environmental sustainability. Utilizing hydrogen in ICEs leverages existing technologies and infrastructure, facilitating a smoother transition from fossil fuels to cleaner alternatives.

This project focuses on optimizing hydrogen-fuelled ICE performance through detailed 1D combustion simulations using the Cruise-M software. By simulating and refining parameters such as combustion duration, fuel amount, and pressure ratios, the project aims to achieve optimal torque and efficiency. This approach offers a cost-effective, safe, and time-efficient pathway to developing environmentally friendly transportation solutions.

1.2 Overview of current project

This thesis focuses on the simulation and optimization of a hydrogen internal combustion engine (H2 ICE) using the Cruise-M software. The project aims to create a detailed one-dimensional (1D) combustion model that can accurately predict the performance of an H2 ICE. This involves providing key input parameters such as the duration and start of combustion, the amount of fuel, lambda (air-fuel equivalence ratio), and pressure ratio. Additionally, specific shape parameters, 'a' and 'm', are determined to define the combustion characteristics. The simulation employs a two-zone Vibe combustion model, which offers a more precise representation of the combustion process by dividing the combustion chamber into two zones: the burned and unburned regions.

The primary goal of this project is twofold: firstly, to develop a simulation model that closely replicates test bed results, ensuring its accuracy and reliability; and secondly, to optimize the model to achieve a torque range of 450 to 600 Nm. This optimization process involves iterative adjustments to the input parameters to enhance engine performance. Key performance indicators such as torque, power, peak combustion pressure, peak temperature, and various component temperatures are analysed. Furthermore, the rate of heat release (ROHR) curve is examined to gain deeper insights into the combustion process and to optimize the thermal efficiency of the engine.

The selection of the Vibe dual-zone combustion model is pivotal to this study. This model is known for its capability to provide a detailed and accurate representation of the combustion dynamics by considering the differences in temperature and composition between the burned and unburned gases. By accurately modeling these differences, the Vibe dualzone approach allows for precise calculations of combustion dynamics, which are crucial for predicting engine performance and improving efficiency.

In the initial phase of the project, the simulation model is calibrated to match the test bed results. This calibration process involves adjusting the input parameters to ensure that the simulation accurately reflects the physical engine's performance metrics. Once the model is validated against these real-world results, the optimization phase begins. Finally 600 Nm Torque was achieved. This involves exploring various combinations of input parameters and analysing their impact on engine performance.

One of the significant advantages of using computer simulations in this research is the ability to perform rigorous testing without the risk of human injury. By utilizing detailed computer models, harsh testing scenarios can be simulated and analysed safely. Additionally, computer simulations can significantly reduce both the cost and time associated with engine development. Physical testing requires extensive resources, including materials, labour, and time. In contrast, simulations can be run quickly and repeatedly, allowing for rapid iteration and refinement of the engine model.

The importance of this study lies in its potential to advance the development of hydrogen-fuelled internal combustion engines. By providing a detailed simulation framework, this project enhances the understanding of hydrogen combustion and its practical application in ICEs. The insights gained from this study can inform the design and development of more efficient and environmentally friendly H2 ICEs, paving the way for their widespread implementation in the automotive industry.

In summary, this thesis represents a critical step towards optimizing hydrogen-fuelled internal combustion engines through detailed simulation and analysis using the AVL Cruise-M software. The project aims to refine the performance parameters of H2 ICEs, contributing to the development of

sustainable and high-efficiency transportation technologies. By achieving a balance between power, efficiency, and environmental impact, this study aligns with global efforts to transition towards cleaner energy sources and reduce the carbon footprint of the transportation sector. Through rigorous simulation and optimization, this research aims to demonstrate the viability and advantages of hydrogen as a sustainable fuel for internal combustion engines, offering a pathway to more environmentally friendly transportation solutions.

1.3 Difference between Hydrogen and conventional fuel properties.

1. Chemical Composition and Energy Content Hydrogen (H2):

Hydrogen (H2):

- **Composition:** Pure hydrogen gas (H2).
- Energy Content: High energy content per unit mass (~120 MJ/kg).
- **Combustion Products:** Produces only water vapor (H2O), resulting in zero CO2 emissions.

Conventional Fuels (Gasoline and Diesel):

- **Composition:** Hydrocarbons (mixtures of hydrogen and carbon atoms).
- Energy Content: Lower energy content per unit mass (Gasoline: ~44 MJ/kg, Diesel: ~45 MJ/kg).
- **Combustion Products:** Generates CO2, CO, NOx, hydrocarbons, and particulates, which contribute to pollution and greenhouse gas emissions.

2. Flammability and Ignition

Hydrogen:

- Flammability Range: Wide range (4-75% in air), enabling various air-fuel mixtures.
- Minimum Ignition Energy: Very low (~0.02 mJ), making

hydrogen highly ignitable.

• **Flame Speed:** High flame speed (up to 2.65 m/s), improving combustion efficiency but increasing pre-ignition and knock risk.

Conventional Fuels:

- Flammability Range: Narrower range (Gasoline: 1.4-7.6% in air, Diesel: 0.6-5.5% in air).
- **Minimum Ignition Energy:** Higher (Gasoline and Diesel: ~0.25 mJ), reducing accidental ignition risk.
- Flame Speed: Lower flame speed (Gasoline: ~0.37 m/s, Diesel: ~0.30 m/s), resulting in smoother but less efficient combustion.

3. Combustion Characteristics

Hydrogen:

- **Quenching Distance:** Short distance (0.64 mm), making it harder to extinguish flames and increasing backfire risk.
- **Combustion Temperature:** High temperature, which can elevate NOx emissions if not managed properly.
- Lean Operation: Supports stable operation with lean mixtures, enhancing thermal efficiency and reducing fuel use.

Conventional Fuels:

- Quenching Distance: Longer distance (Gasoline: ~2.0 mm), aiding in flame control within the combustion chamber.
- **Combustion Temperature:** High but manageable temperatures that contribute to NOx emissions.
- Lean Operation: Limited ability for lean operation without sacrificing performance and stability.

4. Storage and Handling

Hydrogen:

- **Storage:** Requires high-pressure tanks (350-700 bar) or cryogenic storage at -253°C, posing storage and transport challenges.
- **Handling:** Hydrogen's small molecular size increases leakage risk and material permeability issues.

Conventional Fuels:

- **Storage:** Stored at ambient conditions in liquid form, simplifying handling and transportation.
- **Handling:** Well-established infrastructure for safe handling and distribution, with fewer leakage risks.

5. Environmental Impact

Hydrogen:

- **Emissions:** Only produces water vapor, leading to zero carbon emissions if sourced from renewable energy.
- **Production:** Can be generated through electrolysis using renewable energy, significantly reducing the carbon footprint.

Conventional Fuels:

- **Emissions:** Significant CO2 and pollutant emissions, contributing to global warming and air pollution.
- **Production:** Extraction, refining, and distribution have substantial environmental and ecological impacts.

6. Engine Performance

Hydrogen:

- Efficiency: Higher potential efficiency due to superior combustion characteristics and higher energy content.
- Adaptability: Existing internal combustion engines can be adapted to use hydrogen, though significant redesign may be necessary.

Conventional Fuels:

- Efficiency: Lower efficiency compared to hydrogen, but welloptimized performance and reliability in current engines.
- Adaptability: Perfectly suited to existing engine designs with extensive optimization for performance.

Conclusion

Hydrogen is a promising alternative to conventional fuels in internal combustion engines, offering high energy content, cleaner combustion, and

potential for renewable production. However, challenges in storage, handling, and engine adaptation need to be addressed to maximize hydrogen's advantages. Conventional fuels, while more straightforward to use with current infrastructure, significantly contribute to environmental pollution and face increasing regulatory pressures to reduce emissions.

Parameter	Diesel	Gasoline	Methane	H2
Density [kg/m3]	830	730-780	0.72	0.089 71
Stoichiometric	14.5	14.7	17.2	34.3
Lower heating value [MJ/kg]	42.5	43.5	50	120
Boiling temperature"[[C]	180-360	25-215	-162	-253
Ignition limits IV [X]	0.5-1.3	0.4-1.4	0.7-2.1	0.14-10
Minimum ignition	0.24	0.24	0.29	0.02
Self-ignition temperature [°C]	~250	~250	595	585
Specific heat		1.389	1.354	1.401
Laminar flame speed IV, [cm/s]	40-80	40-80	40	200
Quenching		2	2.03	0.64
Carbon content [Mass-%]	86	86	75	0

Table 1.1: Tabular Form of H2 vs Diesel vs Methane vs Gasoline

1.4 Injection strategies: Port Vs Direct Injection

1. Port Fuel Injection (PFI):



Figure 1.1: Port Fuel Injection

Injection Location: Injects hydrogen into the intake manifold, mixing it with air before entering the combustion chamber.

Advantages:

- Simpler and less expensive conversion on existing engines.
- Lower cost due to lower pressure injectors.
- Cooling effect reduces knocking risk.
- Easier maintenance with less complexity.
- Reduced NOx emissions due to lower combustion temperatures.

Disadvantages:

- Less precise air-fuel mixture control.
- Potentially lower thermal efficiency as hydrogen is not injected directly into the combustion chamber.

2. Direct Fuel Injection (DFI):



Figure 1.2: Direct Fuel Injection

Injection Location: Injects hydrogen directly into the combustion chamber.

Advantages:

- Better control over the air-fuel mixture, improving combustion efficiency.
- Potentially higher thermal efficiency.
- Can deliver more power due to high-pressure injection directly where it combusts.

Disadvantages:

- More complex and costly conversion due to high-pressure injectors and extensive modifications.
- More difficult and expensive maintenance.
- Higher pressure increases wear and tear on engine components

1.5 Advantages of Port Fuel Injection (PFI) Hydrogen ICE Conversion:

Converting a conventional internal combustion engine (ICE) to use hydrogen as a fuel can be approached in two primary ways: port fuel injection (PFI) and direct fuel injection (DFI). Each method has its advantages and challenges. Below are the advantages of converting a conventional ICE to a port fuel injection hydrogen ICE over a direct hydrogen ICE.

- 1. Simpler Design and Implementation:
 - Ease of Conversion: PFI systems are generally easier to implement because they modify the existing fuel injection system less extensively. The injectors are placed in the intake

manifold, which is less complex than directly injecting into the combustion chamber.

 Lower Cost: The conversion to PFI hydrogen ICE typically involves lower costs compared to DFI. This is because PFI systems use lower pressure injectors and require fewer modifications to the engine block and head.

2. Component Compatibility:

- Existing Components: Many components of the conventional ICE, such as the intake manifold and fuel rails, can often be reused with PFI. This reduces the need for new parts and simplifies the conversion process.
- Fuel Injector Durability: PFI systems use lower pressure injectors which are generally more durable and less expensive than the high-pressure injectors required for DFI systems.

3. Maintenance and Reliability:

- Easier Maintenance: PFI systems are simpler and easier to maintain due to their lower complexity. This means regular maintenance is more straightforward, reducing downtime and costs.
- Reduced Wear and Tear: PFI systems tend to exert less stress on components compared to DFI systems, leading to potentially longer engine life and fewer breakdowns.
- 4. Thermal Management:
 - **Cooling Effect:** In PFI systems, hydrogen is injected into the intake manifold where it can cool the intake air through evaporation. This helps to manage the temperature within the engine and reduce the risk of knocking.

• Lower Thermal Stress: The cooling effect can also reduce thermal stress on engine components, potentially extending their lifespan.

5. Control and Tuning:

- Simpler Engine Control: The control systems for PFI are generally less complex. This makes tuning the engine for optimal performance and emissions easier compared to DFI systems.
- Flexible Fuel Delivery: PFI systems allow for more straightforward adjustment of the air-fuel mixture, which can be beneficial for achieving different performance and efficiency goals.

6. Emissions:

• Lower NOx Emissions: PFI systems typically result in lower combustion temperatures compared to DFI, which can help reduce NOx emissions. This is beneficial for meeting stringent emission standards without the need for complex aftertreatment systems.

Summary

Converting a conventional ICE to a port fuel injection hydrogen ICE offers several advantages, including simpler design and implementation, lower costs, compatibility with existing components, easier maintenance, improved thermal management, and potentially lower emissions. While direct fuel injection has its own set of benefits, the overall ease and costeffectiveness of PFI make it an attractive option for those looking to transition to hydrogen fuel without extensive modifications to their existing engine setup.

1.6 Brief Literature Review

Hydrogen internal combustion engines (H2ICEs) hold great promise for reducing greenhouse gas emissions and dependence on fossil fuels. However, the accurate simulation of hydrogen combustion in these engines presents several research gaps that must be addressed to fully leverage this technology. Current combustion models often simplify the complex chemical reactions involved in hydrogen combustion. The simplification leads to inaccuracies in predicting the combustion characteristics, such as flame speed, ignition delay, and the formation of NOx. Improved simulation techniques that can accurately predict and mitigate these issues are essential for reliable engine operation. Many simulation models are developed and validated using limited experimental data, often from controlled environments. There is a gap in integrating extensive real-world operational data to validate and refine these models, ensuring their robustness under varied driving conditions. Hydrogen combustion leads to different thermal profiles compared to conventional fuels. Detailed studies on the thermal behavior of engine components and the development of advanced cooling strategies are necessary to prevent overheating and improve engine durability. While hydrogen combustion primarily emits water vapor, the formation of NOx due to high combustion temperatures remains a concern. Advanced models that can accurately predict NOx formation and assist in developing effective mitigation strategies are needed. Addressing these research gaps will significantly enhance the accuracy and reliability of H2ICE combustion simulations, facilitating the development of more efficient and environmentally friendly hydrogen-powered engines. Hydrogen Internal Combustion Engine (H2 ICE) technology holds immense potential for sustainable transportation solutions. However, there's a critical research gap in the development of 1D simulation tools tailored specifically for H2 ICE engines. This report highlights key areas requiring attention in this domain.

Existing 1D simulation models primarily cater to conventional internal combustion engines fuelled by hydrocarbons. Adapting these models to

accurately represent the combustion characteristics and thermodynamic properties of hydrogen is essential for reliable H2 ICE simulation. Current models often fail to account for hydrogen's unique combustion behaviour, such as its wide flammability range and fast flame speed, leading to inaccuracies in predicting engine performance and emissions.

Secondly, the integration of advanced control strategies and emission reduction technologies, such as exhaust gas recirculation (EGR) or leanburn combustion, poses additional challenges for 1D simulation tools. These tools must be capable of simulating the complex interactions between various engine subsystems and control parameters while accurately predicting the impact on performance and emissions.

Furthermore, there's a lack of comprehensive validation datasets specific to H2 ICE engines for benchmarking and validating 1D simulation models. Establishing standardized validation procedures and datasets tailored to hydrogen combustion is crucial for ensuring the accuracy and reliability of simulation results.

In conclusion, the development of advanced 1D simulation tools tailored for H2 ICE engines is essential for optimizing their design and performance while minimizing environmental impact. Addressing the identified research gaps will pave the way for more efficient and reliable hydrogen-powered transportation systems

- 1. Chapter 1: Provides an overview. It includes a concise review of relevant literature and outlines the objectives of the study.
- 2. Chapter 2: An extensive literature review is conducted to provide a detailed understanding of how different researches have been done.
- 3. Chapter 3: Methodology

- 4. Chapter 4: Provides a comprehensive elaboration of the results obtained from the experimental investigations, offering detailed insights and analysis.
- 5. Chapter 5: It delves into the conclusions drawn from our current simulations. This chapter also explores the potential for future research in this area.

Chapter 2

Detailed Literature Review

2.1 Detailed Review

The search for alternative fuels is driven by fluctuating petroleum prices and environmental concerns. The transport sector, responsible for 25% of global CO2 emissions, is one of the few industrial sectors where emissions are still growing, with a projected increase of 50% by 2030 and 80% by 2050. The transport sector's contribution to global CO2 emissions increased by 68% from 1990 to 2013, with road transport accounting for threequarters of these emissions. International travel and trade have significantly increased emissions from marine and aviation sectors, which grew by 64% and 90% respectively from 1990 to 2013. To address this, the rapid introduction of current and emerging technologies that can substantially reduce CO2 emissions is essential.

High-pressure hydrogen storage is favoured due to its straightforward design, low energy requirements for compression, and quick refilling capabilities. Storage pressures typically range from 350 to 700 bar. Tanks are often constructed from carbon fiber-resin composites with high-density polyethylene or aluminium liners. For example, a 350bar tank designed to carry 5.6 kg of hydrogen consists of 53% carbon fiber by weight and 81% hydrogen by volume. Hydrogen's physical and chemical properties make it an attractive fuel. Hydrogen molecules are small, light, and mobile, with low density under atmospheric conditions. The wide flammability range ($\lambda = 10$ to 0.14) allows for varied engine power outputs. Hydrogen's small quenching distance (0.64 mm) and high flame speed enhance combustion efficiency but also increase susceptibility to backfire. Its low boiling point (-253°C) complicates liquid storage. Despite these challenges, hydrogen's high specific heat ratio and low ignition energy make it suitable for lean operation, potentially offering higher thermal efficiency compared to

gasoline engines. Hydrogen has several attractive properties. Its small molecular size and low density at atmospheric conditions enable a wide flammability range, allowing stable combustion under highly dilute conditions. Hydrogen's small quenching distance and high flame speed enhance combustion efficiency but increase the risk of backfire, as the hydrogen-air mixture can more easily pass through small gaps compared to gasoline-air mixtures.

Despite its advantages, hydrogen's properties can lead to abnormal combustion phenomena such as backfire, pre-ignition, and knock. Backfire occurs when the air-hydrogen mixture ignites during the intake valve opening, while pre-ignition occurs during the compression stroke. Knock results from the spontaneous ignition of part of the charge, causing high-pressure oscillations and potential engine damage. Safety is a critical concern for hydrogen vehicles due to hydrogen's potential to ignite or explode, particularly in confined spaces. Detonation can occur when the flame front changes from laminar to turbulent, and hydrogen's high burning velocity increases this risk. Proper storage and fuel line design are essential to prevent leaks and maintain separation between hydrogen and air.

Shah Saud Alam1 and Christopher Depcik in the research paper focuses on adaptive Wiebe function parameters for port-fuel injected hydrogen-fuelled engines, crucial for UAV applications. Precise operational control is essential for utilizing hydrogen in internal combustion engines (ICEs), requiring a correlation between fuel burn rate and ICE operating parameters. Sensitivity analysis using linear regression enables the estimation of key parameters (a, m, θ d) with high accuracy. The study underscores the significance of Wiebe function parameters in simulating the combustion process for hydrogen-fuelled engines, offering a methodology applicable to other engine and fuel types.

Yeliana, C. Cooney, J. Worm, D. Michalek, J. Naber in the paper also addresses Wiebe function parameters for mass fraction burn calculation in ethanol-gasoline fueled SI engines. The function models combustion processes, providing insights into fuel burning rates and efficiencies, and highlights the importance of Mass Fraction Burn (MFB) and Heat Release Rate (HRR) in engine efficiency and emissions research. Various fitting methods, including least square methods and direct algebraic solutions, are compared to analyze the combustion process accurately. Experiments with different ethanol-gasoline blends determine Wiebe function parameters across various fuel compositions and compression ratios, emphasizing the importance of accurate parameter determination for combustion analysis.

Vincent Knop et. Al. did CFD modeling as mentioned ahead. Adapting 3D CFD models for hydrogen combustion involves modifications for low density and high laminar flame speed. The Extended Coherent Flame Model (ECFM) and modified Zeldovitch model are employed to predict NOx emissions, aiming to provide insights into combustion and pollutant formation in hydrogen-fuelled engines.

Klepatz et al. in the paper discusses the use of hydrogen as a carbon-free fuel in internal combustion engines, highlighting its potential for decarbonizing the transport sector .It mentions the challenges associated with using hydrogen in internal combustion engines, such as the flammability of hydrogen affecting ignition system requirements and combustion chamber design .The study emphasizes the importance of hydrogen delivery to the combustion chamber for engine performance, comparing multi-point injection (MPI) and direct injection (DI) methods. It notes that direct injection of hydrogen offers a 15% performance advantage over gasoline engines with port injection, emphasizing the significance of injection timing and strategy for optimized engine performance .The research focuses on analyzing thermodynamic and mechanical losses in a hydrogen direct-injection engine to compare efficiencies with MPI and Diesel compression-ignition operation, using a one-dimensional simulation model based on measured data from a commercial Diesel engine.Cylinder Pressure achieved in the study is shown below:



Figure 2.1: Comparison of the measured and simulated cylinder pressure for the four operation points

In the research article Bradley Thompson and Hwan-Sik Yoon addresses on the following, A Simulink-based 1D flow engine modeling framework for ICEs is developed, leveraging MATLAB/Simulink for automotive system simulations. A gas dynamics model integrated into the framework allows for a physically representative connection of engine components, validated through 1D flow simulation with commercial engine software. This framework advances engine modeling and simulation.

Federico Millo, et.al, in the research paper focuse on Port-fuel injection (PFI) systems that are pivotal for hydrogen-fueled ICE performance and emissions control, providing precise hydrogen supply control and leading to higher efficiencies and reduced emissions. Optimizing PFI involves intake system redesign, lean combustion effects, turbocharger selection, and

EGR path modifications. Advanced computational simulations and engine adjustments are critical for PFI system optimization in hydrogen combustion applications.

2.2 Current developments

Hydrogen combustion engines have been studied for years, with various automotive companies developing prototypes and commercial models. Toyota, Mazda, Ford, and BMW have all made significant advancements in hydrogen internal combustion engines (H2ICEs), focusing on dual-fuel systems, hybrid technology, and dedicated hydrogen vehicles to enhance performance and reduce emissions. These developments highlight the potential of hydrogen as a sustainable alternative fuel for the transport sector.

2.3 Combustion Model

In computational modelling, reducing complex models to 0-D formulations enhances efficiency and reduces processing time, though at some cost to accuracy. Simplified analytical functions, such as those by Rassweiler-Withrow, Watson, Whitehouse-Way, and Wiebe, replace detailed chemical kinetics to predict fuel combustion. The Wiebe function, introduced in 1962, is particularly popular for its simplicity and effectiveness in predicting the mass fraction burned (MFB) profile based on crank angle or time, balancing computational efficiency with accurate combustion modelling.

The Wiebe function describes the heat release rate (HRR) during the combustion of fuel in an engine cylinder over time. Wiebe function is simple, popular, and ability to quickly predict Mass Fraction Burned as a function of crank angle or time.

$$Y_b = 1 - e^{-a \cdot \left(\frac{\theta - \theta_{ign}}{\Delta \theta_d}\right)^{m+1}}$$

 $\Delta \theta_d$ = Combustion Duration (° Crank Angle)

- a = Efficiency Factor in Wiebe Equation
- m =Form Factor or shape factor in Wiebe Equation
- θ =Instantaneous Crank Angle
- $\Delta \theta_{ign} =$ Ignition Crank Angle

Effects of vibe function parameters:

- For a less value of Efficiency factor i.e., a, fuel will burn slower.
- If m is less quicker light-off occurrence.
- For less Combustion duration

Chapter 3

Methodology:

3.1 Basic model for H2

A basic H2 model and three rpm cases were created. The software used for this modelling was Cruise-M. This Software includes the blocks that have all the required equations and fundamental laws. Software is used for designing 1D models. Diesel Model was already their, For hydrogen engine development whole model was created from the lowest level, complete cylinder block was created by adding all the properties and characteristics of engine that was same as Test Bed Facility at VECV. An air path followed by a cylindrical block was created. Air path includes the following blocks System boundaries, plenums, compressor, heat transfer elements, walls, Temperature boundaries, fuel Tank, shafts, Turbine, maps, etc. Plenums are used to create a chamber that offer a constant pressure volume spaces. At first, Only a single cylinder was created no dedicated four cylinders was created, number of represented cylinders were considered as 4.



Figure 3.2: Basic model

3.1.1 Four cases that were created are as follows:

Speed, Flow per second(kg/s) of Hydrogen, and Target pressure ratio was considered as input parameters and other parameters were considered as constant and result as observed.

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Active	Case	Speed (rpm)	Flow_per_second (kg / s)	Target_pressure_ratio ([-])
	1000	1000	33	1.3
	2000	2000	44	2.2
	3000	3000	44	2.5
0	4000	4000	44	3

Table 3.1: Parameters case setup table in Cruise-M Software.

3.2 Four Cylinder updated Cruise-M model:

The model was updated by adding intercooler and separate dedicated cylinder was created and then again model was tuned to achieve results similar to test Bed with in a accuracy of 10-20 % by Hit and Trial method and by the ranges of a and m that were selected by research papers. Results were observed and verified by matching with test bed. Direct injection was converted to port fuel injection in this model to match with The Test Bed specifications.



Figure 3.3: Updated model

3.2.1 Subsystem of Updated cylinder block

Now dedicated four cylinders were used as shown in figure. Firing order was 1-3-4-2. Cylinder subsystem showing combustion elements like walls, heat transfer elements, intake and exhaust port and port injector. Combustion model used was Two zone vibe (Wiebe) combustion. In that start of combustion and combustion duration was also the input parameters for the model.

3.2.2 Three cases that were created are as follows:

Speed, Flow per second(kg/s) of Hydrogen, air mass flow, start of combustion , combustion duration, Rail pressure and Target pressure ratio was considered as input parameters and other parameters were considered as constant and result as observed.

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Active	Case	Speed (rpm)	Target_pressure_ratio ([-])	H2_Flow (kg / h)	air_Mass_flow (kg / h)
0	Case 1	1200	2	0.925	56.
	Case 2	1400	2	1.2	77.
	Case 3	1600	2	1.5275	102.
		1000	-	15215	

Table 3.1(a): Parameters case setup table in Cruise-M Software(Updated

model).

air_Mass_flow (kg / h)	Combustion_duration	Start_of_combustion (deg)	Rail_Pressure (bar)
56.6	47	-6.5	6.9
77.5	48	-6	7.46
102.5	49	-6.5	8.81

Table 3.1(b): Parameters case setup table in Cruise-M Software (Updated

model).

3.3 Final Cruise-M model:

Final model is shown with all the labelling for better understanding. The figure 3.3 is also showing the air flow path.



Figure 3.7: Final model

3.4 Further Steps

Finally, model was finalized after the results of peak combustion pressure was matched with 450Nm torque curve data. All the data was recorded and analyzed thoroughly.

Speed(rpm)	Target Torque(Nm)	Power(Kw)	Power(hp)
1000	500	52	70
1200	600	75	101
1400	600	87	118
1600	600	100	135
1800	600	113	152
2000	570	119	160
2200	550	127	170
2400	534	134	180

Table 3.2: Target Torque

- At first to increase torque for a specific speed, fuel and air amount was increased respectively, when it reaches till saturation (no further torque was increasing), then duration of combustion was decreased (i.e., in degree angle), after it, start of combustion was done advanced, then at last Pressure ratio of turbocharger was increased to 2.25 from 2 for achieving maximum Torque curve(600Nm).
- Work has been done on a lambda of 2.1. Lambda is the ratio of actual air fuel ratio to stoichiometric air fuel ratio.
- Stoichiometric Air Fuel ratio for complete combustion of Hydrogen ICE is 34.3:1.
- Input parameters for final model are Fuel and air quantity by keeping lambda 2.1, start of combustion, duration of combustion, Target pressure ratio, speed, and rail pressure.
- Air flow and h2 flow were increased by some multiplier keeping lambda 2.1 constant.

Finally, for achieving 600Nm torque, input parameters were modified to get required torque, and impact on different components was observed and recorded.

3.5 Summary of Methodology

- At first a H2 1D Cruise M model was created.
- Then, 3 rpms case setup were made for (1200, 1400, 1600) rpms, it is simulated and result was observed.
- Further Model was updated, different required changes were made and then a and m parameters of vibe combustion was selected.
- A cycle of all rpms was also created but that was not able to provide results, and it was also difficult to find out that issue. Then separately all rpms were simulated.
- After it, more rpms cases were created (1000, 1200, 1400, 1600, 1800, 2000, 2200, 2400) rpms and then simulated results were matched with test bed data. This experiment was for 450 Nm torque.
- At last, for achieving 600Nm torque, input parameters were modified to get required torque, and impact on different components was observed and recorded.

Chapter 4

Results and discussion

This section includes results of every stages of project. Basic model and updated results are just for display purpose so that every stage could be understood and actual results will be from final model.

4.1 Results of Basic model



Table 4.1: Input Parameters of Basic model

Results:

Peak combustion pressure 62,113,121,133 bar for 1000, 2000, 3000, 4000 rpms. Other results are:



Figure 4.1: Rate of Heat Release(J/deg)



Figure 4.2: Power (kW)



Figure 4.3: Torque(Nm)

4.2 Results of Updated model

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Active	Case	Speed (rpm)	Target_pressure_ratio ([-])	H2_Flow (kg / h)	air_Mass_flow (kg / h)
0	Case 1	1200	2	0.925	56.6
	Case 2	1400	2	1.2	77.5
	Case 3	1600	2	1.5275	102.5

Table 4.2(a): Parameters case setup table in Cruise-M Software (Updated

model).

air_Mass_flow (kg / h)	Combustion_duration	Start_of_combustion (deg)	Rail_Pressure (bar)
56.6	47	-6.5	6.9
77.5	48	-6	7.46
102.5	49	-6.5	8.81

Table 4.2 (b): Parameters case setup table in Cruise-M Software(Updated model).

Results:

Peak combustion pressure is 100, 103, 101 bar for 1200, 1400, and 1600 rpms. Other results are:



Figure 4.4: Rate of Heat Release(J/deg)



Figure 4.5: Power (kW)



Figure 4.6: Torque (Nm)

As we can say that there were the improvement in the Updated model as compared from Basic Model. Now Finally we have our final model, all results of this will be displayed in detail, results are shown as a comparison of 450 Nm torque curve and 600 Nm Torque Curve.

4.3 Final Model

Case setup (Input parameters) for achieving 450 Nm and 600Nm Torque curve:

normal1000-2400 rpm 4501	MM					
Parameter group 1						
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Active Case	air_Mass_flow (kg / h)	Start_of_combustion (deg)	Target_pressure_ratio [[-])	Speed (rpm)	Rail_Pressure (bar)	Combustion_duration (deg)
Case1000	44.29	-63	2	1000	5.81	87
Case 1200	66.62	-6.5	2	1200	69	47
Case 1400	86.43	ę	2	1400	7,46	48
Case 1600	110.02	-6.5	2	1600	8.81	69
Case 1800	131.83	-6.5	2	1800	9.78	8
Case 2000	153.832	-6.6	6	2000	10.8	64
Case 2200	175.84	-6.6	2	2200	11.825	52
Case 2400	197,81	-6.7	2	2400	12.83	50

Table 4.3(a): Input Parameters for 450Nm for Final model.

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Active	Case	Speed (rpm)	Target_pressure_ratio ([-])	Combustion_duration (deg)	Start_of_combustion (deg)	Rail, Pressure (bar)
	Case1200	1200	225	4	ę	
	Case 1400	1400	225	87	ę	2
	Case 1600	1600	2.25	67	6-	eó
	Case 1800	1800	225	45	-10	of
	Case 1000	1000	225	48	â	5
0	Case 2000	2000	225	87	-10	10
	Case 2200	2200	2.25	48	-10	11.8
	Case 2400	2400	2.25	99	-12	12

Table 4.3(b) Input parameters for 600 Nm Final for Model

4.4 Results for Final model

4.4.1 Torque Curve

The curve is showing the achieved torque in orange line, target torque is the curve in black line.





4.4.2 Power Curve for 450 and 600Nm

On achieving target Torque, Power is increased by the gap as shown in graph (29 Nm to 51 Nm to 117 Nm to 135 Nm for 1000 rpm to 2400 rpm).



Figure 4.8: Change in power when achieving torque from 450Nm to 600Nm

4.4.3 Peak Pressure Curve of combustion chamber for 450Nm and 600Nm Torque

On achieving target Torque, Peak combustion pressure is increased to 158 bar from 113.78 bar and 123 bar from 90 bar for 2400 rpm and 1000 rpm,

it must be considered for the design of cylinder because high pressure require high strength to withstand it.



Figure 4.9: Change in PCP in achieving torque from 450Nm to 600Nm

4.4.4 IMEP curve for 450 Nm and 600NM Torque

On achieving target Torque, Indicated mean Effective pressure is increased with the average of 4 bar which ultimate leads to more efficient and more powerful engines.



Figure 4.10: Change in IMEP in achieving torque from 450Nm to 600Nm

4.4.5 Peak combustion Temperature curve for 450 Nm and 600 Nm (i.e. target Torque)

On achieving target Torque, maximum temperature inside combustion chamber is increased to 2093 degree Celsius from 1725 degree Celsius to 2462 degree Celsius from 2330 degree Celsius for 1000 rpm to 2400 rpm (i.e, the average difference of 200 degree Celsius).



Figure 4.11: Change in Peak combustion Temperature in achieving torque from 450Nm to 600Nm

4.4.6 Cylinder Liner temperature (degree Celsius) Curve for 450 Nm and 600Nm Torque

On achieving target Torque, temperature of Cylinder liner is increased with the average of 15 degree Celsius, hence careful consideration and potentially adjustments in design, material, cooling systems, and engine management may be the necessary to accommodate the increased temperature.



Figure 4.12: Change in Cylinder liner Temperature in achieving torque from 450Nm to 600Nm

4.4.7 Cylinder head temperature (degree Celsius) Curve for 450 Nm and 600Nm Torque

On achieving target Torque, temperature of Cylinder head is increased with the average of 8 degree Celsius, hence careful consideration and potentially adjustments in design, material, cooling systems, and engine management may be the necessary to accommodate the increased temperature.



Figure 4.13: Change in Cylinder Head Temperature in achieving torque from 450Nm to 600Nm

4.4.8 Intake port temperature (degree C) Curve for 450 Nm and 600 Nm Torque

On achieving target Torque, temperature of Intake port is increased with the average of 1.5 degree Celsius, which is very less hence it may not require the immediate changes.





4.4.9 Exhaust Port temperature (degree C) Curve for 450 Nm and 600 Nm Torque

On achieving target Torque, temperature of exhaust port is increased with the average of 35 degree Celsius for rpm range of 1000 to 1600 and with the average of 15 degree for rpm range of 1800 to 2400, hence careful consideration and potentially adjustments in design, material, cooling systems, and engine management may be the necessary to accommodate the increased temperature and to enhance the better thermal management.



Figure 4.15: Change in Exhaust port Temperature in achieving torque from 450Nm to 600Nm

4.4.10 Piston temperature (degree C) Curve for 450 Nm and 600Nm Torque

On achieving target Torque, Piston temperature is increased with the average of 7 degree Celsius, which is not very high hence it may not require the immediate changes in design but enhancement in heat transfer must be considered.



Figure 4.16: Change in Piston Temperature in achieving torque from 450Nm to 600Nm

4.4.11 Air and H2 flow curve for 450 Nm and 600 Nm

For achieving target Torque, requirement of air flow is increased by some multiplier shown in Table 1 keeping lambda constant i.e. 4.5.For achieving target Torque, requirement of H2 flow is increased by some multiplier like 1.65 for 1000 rpm and so on, keeping lambda constant i.e, 2.1.



Figure 4.17(a): Change in air flow in achieving torque from 450Nm to 600Nm



Figure 4.17(b): Change in H2 flow in achieving torque from 450Nm to 600Nm

4.4.12 Angle MFB 50 curve for 450Nm and 600 Nm Torque

On achieving target Torque, Angle MFB 50 is decreasing with an average of 3 degree which means combustion is being more efficient.



Figure 4.18: Change in angle MFB 50 in achieving torque from 450Nm to 600Nm

4.4.13 Start of combustion (SOC) angle curve for 450 Nm and 600 Nm Torque

For achieving target Torque, start of combustion is advanced. Advancing the start of combustion ensures that the maximum pressure is applied to the piston at the ideal point in engine cycle, allowing for more complete combustion of air fuel mixture which ultimate leads to higher power output.



Figure 4.19: Change in SOC in achieving torque from 450Nm to 600Nm 4.4.14 Duration of combustion (DOC) angle curve for 450 Nm and 600 Nm Torque

For achieving target Torque, duration of combustion is reduced to approx. 1-3 degree as reducing duration makes combustion quicker and allows better synchronization with piston which ultimate leads to more of the combustion energy is getting converted into useful work on piston.



Figure 4.20: Change in DOC in achieving torque from 450Nm to 600Nm

4.4.15 RoHR (Rate of Heat Release) curve for 450Nm and 600 Nm Torque

On achieving target Torque, an increase in ROHR with an increase in torque typically signifies a more efficient and powerful combustion process, leading to improved engine performance. However, it also necessitates careful thermal management and engine control to maintain reliability and durability.



Figure 4.21: Change in RoHR in achieving torque from 450Nm to 600Nm

4.5 Discussion

Overall average Percentage change for maintaining 600Nm Torque from 450 Nm Torque is shown below.

Quantity Name	Percentage Change
Torque	24.8
Power	22.4
РСР	25.7
Air Flow	22.1
H2 flow	22.0
IMEP	15.9
Duration of combustion	4.8
Start of combustion	25.1
pressure Ratio	11.1
Peak combustion Temprature	3.6

Table 4.4: Percentage change for maintaining 600Nm Torque

In this work we got a Peak combustion Pressure of 90 bar for 450 Nm and 120 Bar for 600 Nm, say it as 100 bar just for estimating our approximate

accuracy for a lambda of 2.1 and speed 1000 rpm. In the Publication of Klepatz et al. they were getting a peak combustion pressure of about 110 bar for 15 Bar BMEP (same as of my work) at 1000 rpm and 2.8 lambda. So we can take a brief idea for accuracy of the work done with the error of 18 % that is acceptable. No other exact same research has been done on the engine of same qualification that's why comparison has been done from the best available literature.



Figure 4.22: Peak combustion Pressure from literature reviews.

Chapter-5

Conclusions and the scope for future work

5.1 Conclusion

The study focused on optimizing the performance of a hydrogen-fueled internal combustion engine (ICE) by modifying various parameters to increase the torque output from 450 Nm to 600 Nm. The adjustments made to the engine model included changes in the Rate of Heat Release (RoHR), power output, cylinder temperature, start of combustion, duration of combustion, and fuel-air mixture. The findings reveal significant insights into the combustion process and engine performance, emphasizing the need for engine modifications to ensure optimal operation and reliability.

5.1.1 Key Findings

- 1. Increase in Rate of Heat Release (RoHR): The increase in torque from 450 Nm to 600 Nm was accompanied by a significant rise in the Rate of Heat Release (RoHR). This indicates that the combustion process became more efficient, releasing more energy in a shorter period. The enhanced RoHR contributed directly to the higher torque output, suggesting that the fuel was burning more rapidly and completely within the combustion chamber. This efficient combustion is a positive indicator of the engine's performance but also necessitates careful thermal management to avoid overheating.
- 2. Power Output: Alongside the increase in torque, the power output of the engine also saw a considerable rise. This is expected, as torque and power are closely related parameters in engine performance. The higher power output is indicative of the engine's improved ability to convert fuel energy into mechanical work. This improvement underscores the success of the modifications in achieving greater engine performance.

- 3. Cylinder Temperature: The temperature of various cylinder parts, including the liner, cylinder head, intake, and exhaust ports, increased notably. The rise in temperature is a direct consequence of the higher energy release during combustion. While higher temperatures can enhance the combustion efficiency and power output, they also pose a risk of thermal stress and potential damage to engine components. This necessitates modifications in the engine's cooling system to ensure that the increased thermal load can be effectively managed. Enhanced cooling mechanisms, such as improved coolant flow rates and advanced heat dissipation materials, may be required to maintain the engine's reliability and longevity.
- 4. Start of Combustion and Duration: To achieve the higher torque output, the start of combustion was advanced. This means that the ignition timing was adjusted to initiate the combustion process earlier in the engine cycle. Advancing the start of combustion helps in maximizing the pressure buildup and energy release, thereby increasing torque. Additionally, the duration of combustion was reduced, indicating a more rapid and complete burn of the fuel. This optimization helps in extracting more power from the fuel within a shorter time frame, contributing to the increased torque and power output.
- 5. Fuel and Air Mixture: The quantity of hydrogen fuel injected into the engine was increased to support the higher torque output. Concurrently, the amount of air (measured in kg per second) was also increased to maintain the stoichiometric balance, ensuring that the air-fuel mixture remained optimal. Despite the increase in fuel

and air, the lambda (air-fuel equivalence ratio) was kept constant, indicating that the engine was running efficiently without becoming too rich or too lean. This balance is crucial for maintaining engine performance and reducing emissions.

6. Peak Combustion Parameters: The peak combustion parameters, which are critical indicators of engine performance, also showed an increase. Higher peak pressures and temperatures within the combustion chamber suggest that the engine modifications were successful in enhancing the overall combustion efficiency. However, these higher peaks also reinforce the need for robust engine components and advanced cooling strategies to handle the increased thermal and mechanical loads.

5.1.2 Engine Modifications that can be made

The study highlights several areas where engine modifications are required to ensure that the performance enhancements do not compromise the engine's reliability and safety:

- 1. **Cooling System Enhancements**: Given the substantial increase in cylinder temperatures, the engine's cooling system must be upgraded. This could involve increasing the coolant flow rate, using high-efficiency radiators, and incorporating materials with better thermal conductivity in the engine design. Advanced cooling techniques, such as targeted cooling channels and thermal barrier coatings, may also be considered to protect critical components.
- 2. **Material and Design Improvements**: The increased thermal and mechanical stresses necessitate the use of materials that can withstand higher temperatures and pressures. Components such as the cylinder head, liner, and exhaust ports may need to be made from or coated with materials that offer superior strength and thermal resistance. Additionally, the design of these components may need

to be optimized to enhance heat dissipation and reduce thermal stress concentrations.

- 3. **Combustion Optimization**: Further optimization of the combustion process may involve fine-tuning the ignition timing, fuel injection strategies, and air-fuel mixture preparation. Advanced control systems, such as electronic ignition and variable fuel injection timing, can help in achieving precise control over the combustion process, thereby enhancing efficiency and performance.
- 4. Emissions Control: While improving performance, it is essential to ensure that emissions remain within acceptable limits. The study suggests that modifications to the exhaust gas recirculation (EGR) system and the use of catalytic converters may be necessary to manage NOx and other emissions effectively.

5.2 Future Scope

The current model designed for optimizing the performance of a hydrogenfueled internal combustion engine (ICE) is based on software simulations. However, significant advancements can be achieved by transitioning this model to a hardware-in-the-loop (HIL) setup using platforms like LABCAR. Implementing HIL simulations will allow for real-time testing and validation, bridging the gap between theoretical models and practical applications. This approach will facilitate more accurate tuning of engine parameters and provide insights into the dynamic interactions within the engine system.

Further development of the model can include the integration of Exhaust Gas Recirculation (EGR) and emissions control mechanisms, which were not covered in the current study. By incorporating these components, the model can be expanded to study their impacts on engine performance and emissions. This will be crucial for developing strategies to reduce NOx and other pollutants, ensuring compliance with stringent environmental regulations.

Enhancing the complexity of the Cruise M model will allow for a more detailed analysis of the engine's behavior under various operating conditions. This can include more advanced combustion models, transient analysis, and the inclusion of additional physical phenomena. By doing so, the model will be able to provide more comprehensive insights into the combustion process, thermal management, and overall engine performance.

Future research should also explore the optimization of the air-fuel mixture preparation, ignition timing, and fuel injection strategies using advanced control systems. Implementing machine learning algorithms for predictive control and real-time adjustments could further enhance engine efficiency and performance.

Additionally, the development of robust cooling strategies and the use of advanced materials for engine components should be investigated. These enhancements will help manage the increased thermal loads resulting from higher combustion efficiencies and ensure the engine's reliability and durability.

In conclusion, transitioning to HIL simulations, incorporating EGR and emissions control, enhancing the model complexity, and exploring advanced control systems and materials represent significant future research directions. These efforts will contribute to the development of highperformance, hydrogen-fueled internal combustion engines with optimized efficiency and reduced environmental impact.

5.3 Summary

The increase in torque from 450 Nm to 600 Nm in the hydrogen-fueled ICE was achieved through modifications enhancing the combustion process and overall engine performance. This study highlights the critical relationship between combustion efficiency, thermal management, and engine

reliability. While performance gains are substantial, they bring increased thermal and mechanical stresses that require careful management through targeted engine modifications. These findings offer a comprehensive understanding of the adjustments needed to achieve high-performance hydrogen-fueled engines, paving the way for advancements in clean and efficient automotive technologies.

Future research should transition the software-based hydrogen-fueled ICE model to hardware-in-the-loop (HIL) simulations, integrate EGR and emissions control, and enhance model complexity. Implementing advanced control systems, optimized cooling strategies, and advanced materials will further improve engine efficiency, reliability, and environmental compliance. These developments will contribute to the creation of high-performance, sustainable automotive technologies.

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