Gautam Panwar, 2026, 14:4
ISSN (Online): 2348-4098
ISSN (Print): 2395-4752

International Journal of Science, Engineering and Technology
An Open Access Journal

The ML based H2 blended fueled internal combustion engines: Optimization, challenges, and future directions

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Abstract- Engines running on hydrogen (H_2ICE) offer strong potential for reducing traditional fossil fuels while leveraging existing engine architectures. Hydrogen introduces key advantages, like high combustion efficiency, broad ignition ranges, and no carbon output. Yet problems such as the creation of NO_x, combustion instability, and storage limitations halt its widespread rollout. In this context, machine learning (ML) techniques provide a practical way for handling the complex and nonlinear behavior of hydrogen combustion systems. Complex setups, covering artificial neural networks (ANN), support vector regression (SVR), random forest (RF), and gradient boosting algorithms such as XGBoost, demonstrate strong capability at forecasting how the engine runs, optimizing operating conditions, and controlling emissions. This paper presents a comprehensive assessment of ML-assisted optimization of hydrogen engine systems, aimed at boosting output and lowering pollution. By combining hydrogen fuel with data-driven strategies, real-world gains in engine efficiency, stable operation, and reduced emissions can be achieved, supporting the transition to sustainable energy systems.

Keywords: Hydrogen-fueled internal combustion engines, ML, Combustion optimization.

I. INTRODUCTION

H2ICE have re-emerged as a viable option for low-carbon mobility, especially in niches where battery electric vehicles (BEV) face limitations with energy density, long charging times, and limited infrastructure. While BEV are at the heart of current electrification strategies, scaling them up is tough because of material availability, dependency on the grid, and performance issues in heavy-duty or long-haul situations. In this context hydrogen-fueled internal combustion engines serve as a transitional solution by sticking with existing engine designs while dropping carbon emissions significantly. Hydrogen combustion eliminates carbon dioxide emissions and achieves high thermal efficiency because of its wide flammability limits and rapid flame propagation.

However, these characteristics also introduce some significant challenges, like abnormal combustion phenomena such as pre-ignition and backfiring, along with increased NO_x emissions due to high in-cylinder temperatures. Even with its long history, significant advancements are still required to develop hydrogen-fueled engines that actually match or beat the performance, efficiency, and cost-effectiveness of conventional fossil-fuel systems. The historical evolution of hydrogen-enriched internal combustion engines is traced back in Figure 1, which breaks down key developmental phases from early conceptual combustion studies to modern advancements in ML-driven optimization and digital twin technologies. The timeline highlights major transitions, including foundational experiments, dual-fuel engine development, automotive prototype implementation, and recent advancements toward intelligent hydrogen engine systems, pulled from various literature sources.

A fundamental understanding of hydrogen combustion is essential, as there are naturally complex links between main engine variables, covering RPM, workload, air-fuel mix, and when the spark hits. Traditional physics-based and empirical models often fail to accurately model the complex and nonlinear interactions among engine parameters under different running states. Because of this, ML has become an effective alternative, allowing for data-driven modeling and more precise prediction of engine behavior with better computational efficiency.

Commonly used ML techniques, including ANN, RF, and SVR, have demonstrated strong capability in predicting critical combustion characteristics such as in-cylinder pressure, heat release rate, and emission formation, which supports real-time optimization and adaptive control of hydrogen engine systems [3,4,5]. Still, even with more people using ML in this domain, comprehensive comparative evaluations addressing model robustness, interpretability, and generalization in hydrogen-specific environments are still rare [1].

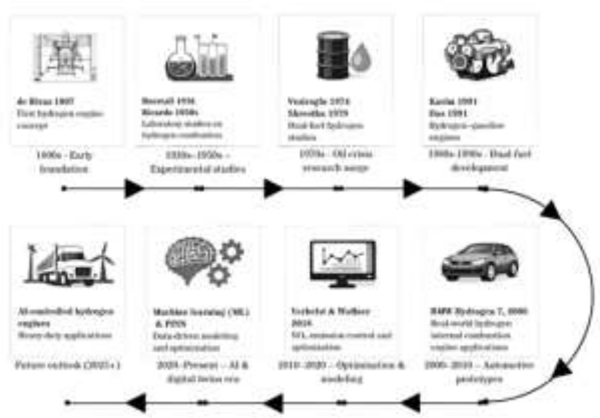

Fig.1. Timeline of evolution of hydrogen-enriched internal combustion engines.

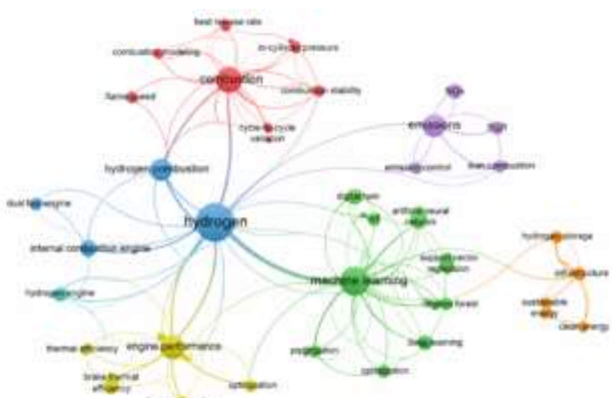

Fig.2. Keyword co-occurrence network illustrating ML applications in hydrogen production, generated using VOSviewer version 1.6.20.

Figure 2 presents the keyword co-occurrence network of ML applications in hydrogen production, made using VOSviewer version 1.6.20.

A growing body of research demonstrates the increasing role of ML in optimizing hydrogen engine performance and enabling intelligent energy systems. Zbikowski and Teodorczyk showed that ML models significantly improve prediction accuracy of combustion and emission traits in hydrogen-blended engines [3]. Wang and others reported that hydrogen addition enhances combustion efficiency but introduces challenges linked to abnormal combustion behavior [1].

Falfari and colleagues emphasized the viability of hydrogen as a near-term low-carbon option within current engine setups [2]. Jose's team developed an ML-based framework for optimizing mixtures, pointing out injection strategies' importance in achieving stable combustion [4]. Ofner and others showed that deep learning models are effective in detecting combustion anomalies like knocking [5]. Danciu and coworkers looked into how turbulent flow structures interact with hydrogen flame dynamics using data-driven methods [6]. Rohrhofer's group proposed neural network-based surrogate models to lower computational complexity in combustion simulations [7]. Zhu and others presented an automated ML framework to minimize cycle-to-cycle variations in hydrogen engines, boosting stability and efficiency [8].

Bekmyrza and collaborators explored integrating ML with IoT technologies for smart hydrogen infrastructure [9], while Nassar highlighted digital twin frameworks' role in real-time system optimization [10]. Also, Makki Abadi and Rashidi demonstrated the effectiveness of ML in optimizing hydrogen production processes [11], and Du provided a comprehensive review of ML applications across various hydrogen production methods [12]. These studies all show a shift toward intelligent, data-driven hydrogen energy systems. Although current research tends to focus on separate parts of hydrogen combustion or ML applications, this study provides an integrated analysis by methodically connecting combustion modeling, performance optimization, and emission control within a unified ML-assisted framework.

By doing this, it points out how these parts work together in driving efficient, stable, and low-emission hydrogen engine systems.

Unlike previous reviews that focus on individual aspects such as combustion modeling or emission prediction, this paper integrates combustion modeling, performance optimization, and emission control within a unified ML framework. The review also highlights emerging technologies including digital twins, PINN, and AutoML while identifying current research gaps and future research directions. To ensure a structured and comprehensive analysis, the review methodology adopted in this study is described below.

II. REVIEW METHODOLOGY

This review was conducted by collecting recent literature on hydrogen-fueled internal combustion engines and ML applications from major scientific databases, including IEEE Xplore, SpringerLink, ScienceDirect, MDPI, SAE, and Google Scholar. Publications from 2003 to 2025 were considered. The selected studies focused on combustion modeling, performance optimization, emission prediction, digital twins, and hydrogen production. Only relevant peer-reviewed journal articles and conference papers were included. The collected literature was analyzed to identify current trends, research gaps, challenges, and future research directions.

III. ML-BASED OPTIMIZATION OF HYDROGEN ENGINES

ML is now a key tool used for addressing complex and nonlinear behavior of hydrogen-fueled internal combustion engines, primarily for combustion modeling, performance optimization, and emission control under changing running setups [1,4,5].

Combustion Modeling

ML is now a strong way for mapping out complex combustion processes in hydrogen-fueled internal combustion engines. Traditional physics-based methods usually fail to accurately model down the nonlinear links between running variables. Specifically, ML techniques like ANN, SVR, and deep learning models have shown they are effective in predicting key combustion characteristics. This covers in-cylinder pressure changes, temperature distribution, and heat release rates across different engine states.

Data-driven models learn these relationships from experimental and simulation datasets, improving prediction accuracy while reducing computational cost compared with conventional modeling approaches. Studies by Zbikowski and Teodorczyk [3] and Jose et al. [4] demonstrated that ML-based frameworks work in capturing combustion dynamics and improving mixture formation. Also, Ofner et al. [5] further show that deep learning techniques can detect abnormal combustion events such as knocking. On top of that, research on hydrogen flame behavior, such as that by Danciu et al. [6], and the development of surrogate combustion models by Rohrhofer et al. [7], highlight the increasing role of ML in real-time combustion prediction and control.

Performance Optimization

Using ML in hydrogen engine systems is vital for enhancing performance. Major metrics such as brake thermal efficiency (BTE) and specific fuel consumption depend on variables specifically when fuel is injected, ignition timing, and air-to-fuel ratio. Traditional trial-and-error tuning is time-consuming. Instead, ML models offer a systematic approach to identify optimal operating conditions based on data analysis.

Methods such as random forest regression, ANN-based optimization, and gradient boosting algorithms have been primarily used to model the complex interactions among engine parameters and to pinpoint optimal operating conditions across varying engine loads and speeds. Zhu et al. [8] showed that automated ML can reduce cycle-to-cycle variations, while Jose et al. [4] highlighted the importance of injection strategies for stable combustion. Also, combining ML models with optimization algorithms allows for adaptive and real-time engine control, which improves overall system performance and stability under changing conditions [1,8].

Emission Prediction and Control

Emission prediction and control are vital uses of ML in hydrogen-fueled engines. ML models can accurately predict emission levels like NOx, carbon monoxide (CO), and unburned hydrocarbons (HC) by capturing complex relationships between engine parameters and emission outputs. This enables better control strategies to reduce emissions. A major challenge in hydrogen engines is the trade-off between combustion efficiency and NOx emissions. ML-based multi-objective optimization approaches address this issue by identifying operating conditions that balance these competing goals. Table 1 presents a comparative analysis of hydrogen-enriched internal combustion engine studies across various fuel blends and engine configurations, highlighting their effects on performance and emissions.

Table 1. Comparative analysis of hydrogen-enriched internal combustion engine studies.

Blended fuel with H_2	Engine Type	Application	Performance	Reference
Hydrogen	Modified SI	Light-duty	High efficiency; increased NO_x emissions	[13]
Gasoline	PFI SI	Passenger	Increased efficiency; decreased CO_2 emissions	[14]
NG	Dual SI	Transport	Improved combustion; decreased HC, CO emissions	[15]
Diesel	CI	Heavy-duty	Increased efficiency; decreased NO_x emissions	[16]
Diesel	DI CI	Commercial	Improved combustion; decreased smoke	[17]
Diesel	CI	Stationary	Increased BTE; decreased carbon emissions	[18]
Methane	Lean SI	Low-emission	Increased lean efficiency; increased NO_x emissions	[19]
Gasoline	DI SI	Automotive	Increased efficiency; reduced fuel consumption	[20]
NG	Turbo SI	Urban	Stable combustion with increased emissions	[21]
EGR	SI	Controlled	Increased NO_x emissions; slight efficiency loss	[22]
Biodiesel	CI	Renewable	Improved combustion; decreased PM	[23]
Ethanol	SI	Clean vehicles	Increased efficiency; decreased emissions	[24]

For the most part, hydrogen enrichment enhances combustion efficiency and reduces carbon-based emissions; however, it may also lead to increased NOx formation depending on operating conditions. Ofner et al. [5] and Zbikowski and Teodorczyk [3] demonstrated that it works in predicting emissions. Zhu et al. [8] highlight their role in making combustion more stable and reducing variability. Also, combining ML with control techniques like exhaust gas recirculation (EGR), adaptive ignition timing, and real-time monitoring systems can significantly reduce emission levels without major impacts on performance. This integration supports the development of cleaner hydrogen-based propulsion systems [2,3,9]. Despite these advancements, significant gaps still exist in the generalization, interpretability, and real-time applicability of ML models in hydrogen engine systems.

IV. CHALLENGES & FUTURE DIRECTIONS

Despite showing promise as a green fuel option, hydrogen faces several engineering and operational challenges that stall its use within internal combustion engines. Combustion instability and significant cycle-to-cycle variations stem from hydrogen's large burn range and quick ignition speed. This frequently leads to abnormal combustion events like pre-ignition, backfiring, and swift pressure climbs. These effects increase mechanical strain and reduce engine durability. Even small changes in mixture composition can destabilize engine performance and lower efficiency. To fix these issues, we need effective control strategies and predictive modeling techniques that can keep combustion stable under varying operating conditions [2,6].

Another drawback is the emission paradox connected with hydrogen combustion. Even though hydrogen eliminates carbon-heavy exhaust, intense heat from the fire can lead to NOx. This sparks a balancing act pairing how well it runs and its green footprint. Usual methods for cutting tailpipe output, like EGR and after-treatment systems, bring more intricacy and cost. Thus, there is a growing demand for smart optimization frameworks that can balance efficiency and emission standards across different operating scenarios [3,8].

Material compatibility is still a big worry as hydrogen's small molecular size allows it to diffuse into metal parts, causing hydrogen embrittlement and weakening structures under repeated stress. Also, its low viscosity and lack of lubrication speed up component wear, while high diffusivity increases leakage risks in standard sealing systems. These issues show we need hydrogen-compatible materials, better sealing technologies, and solid durability assessment methods [2,3].

Looking at the broad system, the mass implementation of hydrogen technologies is held back by significant challenges in storage, transportation, and network growth. The poor energy storage density of hydrogen needs high-pressure compression or cryogenic liquefaction, which both require massive power and bring about safety fears. Also, a limited refueling infrastructure limits everyday usage. Future moves will likely depend on the integration of digital technologies, such as IoT-enabled sensors, digital twins, and ML models that incorporate physics. These technologies facilitate real-time monitoring, predictive maintenance, and adaptive control. Specifically, the integration of PINN within digital twin frameworks offers a promising approach for enabling accurate, interpretable, and real-time optimization of hydrogen energy systems [9–12].

V. CONCLUSION

ML and artificial intelligence are reshaping the development of hydrogen-based energy systems by allowing for data-driven optimization past traditional trial-and-error methods. In hydrogen-powered internal combustion engines, ML effectively predicts combustion dynamics, optimizing engine settings, and controlling emissions well, even under complex conditions. High-level models like graph neural networks (GNN), PINN, and hybrid AutoML methods also enhance hydrogen production processes, system monitoring, and infrastructure optimization.

But, the large-scale deployment of hydrogen technologies requires addressing key challenges related to combustion stability, emission control, material durability, and infrastructure limitations. Because of this, combining physics-based knowledge with ML models is vital for increasing reliability, understanding, and real-world deployment. Altogether, the integration of ML, new materials, and digital technologies provides a pathway for bridging laboratory research with large-scale industrial efforts. This enables the development of efficient, safe, and sustainable hydrogen energy systems.

VI. DECLARATIONS

Conflict of Interest
The authors declare that there is no conflict of interest.

Funding
No external funding was received for this work.

Data Availability
No datasets were generated or analysed during this study.

Author Contributions
All authors contributed to the conceptualization, literature review, manuscript writing, editing, and final approval of the manuscript.

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