



AI-DRIVEN OPTIMIZATION OF HYDROGEN AND METHANE FUEL STRATEGIES FOR SUSTAINABLE MARITIME DECARBONIZATION

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1. **ABSTRACT:** This study investigates the potential of integrating artificial intelligence (AI) with experimental analysis to optimize fuel mixtures in internal combustion engines for green port applications. By evaluating the efficiency and emission reduction capabilities of hydrogen-oxygen (HHO) gas and methane as alternative fuels, the research explores a dual-fuel conversion approach for conventional internal combustion engines. The AI-driven methodology employs Random Forest Regression (RFR) to analyze experimental data and determine the most efficient fuel mixture settings. The results indicate that NaOH at a 10% concentration achieves maximum fuel savings, while KOH at 12% concentration provides the best CO_x reduction. Methane injection demonstrates moderate fuel savings and emission reductions, highlighting its viability as an alternative fuel. The AI optimization process determined the optimal fuel mixture settings, enhancing efficiency, reducing emissions, and accelerating the transition to cleaner maritime energy solutions. These findings reinforce the effectiveness of AI-based optimization in advancing sustainable fuel strategies and promoting cleaner energy solutions for port operations and energy management.

2. INTRODUCTION

Maritime transport has rapidly expanded due to the growth of international trade and commercial demands. The increasing number of ships brings big challenges to the port, whereas ship emissions is one of the main components of port pollution, which greatly influences on the port ecological environment. Maritime port authorities around the world have launched a slew of projects aimed at lowering harmful emissions associated with port operations. Various approaches have been proposed to develop an alternative energy source in ports. Some ports, such as Antwerp and Genoa, decided to use solar energy as an alternative energy source for some loads. Various studies have been conducted on using alternative sources for ports and converting them into

green ones (Sadek, I. and M. Elgohary.,2020). Many ports propose to adopt solar energy as an alternative source of energy . Wind energy as an approach has been applied at many ports across the world . Another potential power source for marine ports is the utilization of tidal and wave energy to power port activities . Several researchers have investigated improved energy efficiency and the use of green energy sources to reduce pollutant emissions and operation costs along with operational efficiency. These measures are crucial aspects of the next-generation port strategy .

Internal-combustion engine exhaust emissions contribute significantly to this problem . Xiang Li points out the importance of developing a sustainable and low-cost solution to eliminate CO₂ emissions from IC engines . In contrast, hydrogen is free from HC, CO, and CO₂ emissions . Hydrogen is gaining popularity as a clean fuel and is playing an important role in countries' energy policies , especially since hydrogen may be used as a fuel in Internal Combustion Engine (ICE) without causing structural changes or reducing the engine's lifespan .

As a fuel, oxyhydrogen gas shares the same characteristics as hydrogen . HHO gas is a viable source of alternative energy . The HHO gas is produced by the separation of H-OH water molecules. It has a high calorific value, and one kilogram of HHO has three times the amount of energy as gasoline . Arjun et al. study demonstrated that when adding HHO gas to the combustion process reduces fuel consumption from 20% to 30% . Gad and Abdel Razek illustrated that the addition of HHO gas generated from wet cells improves brake thermal efficiency, with the highest reductions in CO (22 %), HC (39 %), NO_x (42 %), and smoke emissions (35%) compared to diesel fuel . Musmar and Al-Rousan tested a small HHO generator on a gasoline engine, their findings reveal that the injection of HHO gas reduces fuel consumption, NO_x, and CO by 30%, 50%, and 20%, respectively . Raif proves that HHO enrichments enhance brake torque and power outputs while decreasing brake-specific fuel consumption .

Since methane (CH₄), the major component of natural gas, has a high hydrogen content, it is far cleaner than other fossil fuels . It has aroused great interest as a potential next-generation energy source. Furthermore, biomass is regarded as a renewable source of CH₄ . In recent years, several research programs have investigated renewable methane from biomass. Tripathi et al. investigated the effects of methane enrichment on emissions of a ICE, concluding that using CH₄ in dual fuel mode without significant engine modification is a viable option for reducing emissions . Biernat and Samson-Brk found out that using methane fuel reduces pollutant emissions whereas CO emissions are reduced by 30%, HC emissions are reduced by 70%, NO_x emissions are reduced by 50%, and PM emissions are eliminated .

The maritime industry is facing increasing pressure to transition towards sustainable energy solutions due to growing environmental and regulatory demands. Traditional internal combustion engines contribute significantly to greenhouse gas emissions, necessitating the development of alternative fuel solutions that reduce environmental impact without compromising efficiency. While previous studies have explored hydrogen and methane as cleaner fuel options, optimizing their fuel mixture ratios remains a challenge due to the numerous variables involved, including catalyst concentrations, fuel injection rates, and combustion efficiency.

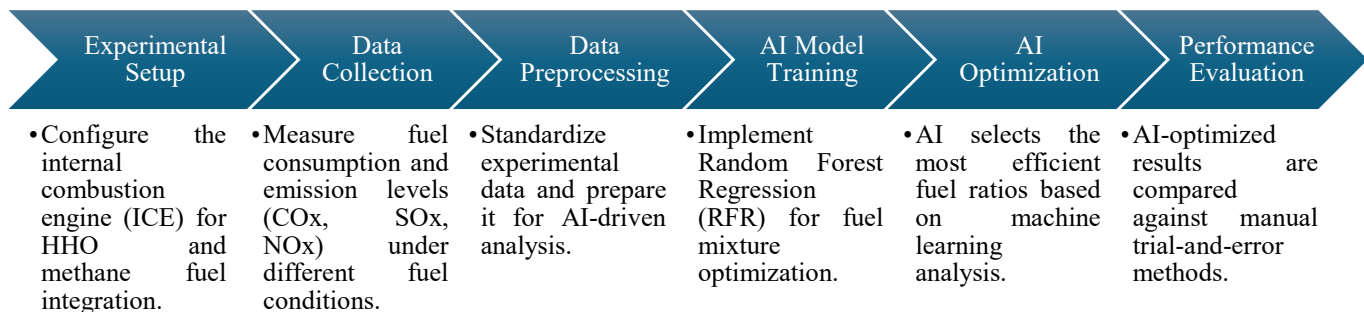
A major limitation in previous research is the reliance on a trial-and-error approach to determine the most effective fuel mixture. This process is time-consuming, costly, and requires extensive experimental testing to achieve an optimal balance between fuel savings and emission reductions. The lack of a systematic optimization framework for selecting the ideal fuel ratio has hindered large-scale adoption of alternative fuels in maritime applications.

This research bridges this gap by employing an AI-driven approach to streamline the fuel optimization process. By leveraging machine learning algorithms, specifically Random Forest Regression (RFR), this study automates the analysis of experimental data to identify the most effective fuel mixtures. AI enables the evaluation of multiple parameters simultaneously, significantly reducing the need for manual experimentation while ensuring accuracy in results. The integration of AI not only enhances the precision of fuel optimization but also accelerates the adoption of cleaner fuels by simplifying decision-making for maritime energy systems.

Through this study, we demonstrate how AI can revolutionize fuel optimization in green port applications, making the transition to sustainable energy more efficient, cost-effective, and scalable. By combining experimental validation with AI-driven insights, this research establishes a framework for enhancing fuel efficiency, reducing emissions, and supporting maritime decarbonization efforts.

3. METHODOLOGY

This study employs a hybrid approach, integrating experimental testing and AI-driven optimization to evaluate the performance of dual-fuel internal combustion engines (ICEs) using hydrogen-oxygen (HHO) gas and methane. The methodology consists of several structured stages, ensuring a systematic approach to fuel optimization. The experimental setup included two distinct test conditions: HHO-Benzene-Dual-Fuel Setup – Evaluating the impact of HHO gas injection on fuel efficiency and emissions. Methane -Benzene Dual-Fuel Setup – Analyzing the influence of methane injection under identical experimental conditions.



3.1 Experimental system configuration

To evaluate dual-fuel engine performance, an internal combustion engine (ICE) was modified to integrate both HHO gas and methane, tested under separate conditions.

Test 1: Benzene-HHO Dual-Fuel Configuration

- The HHO generator system was connected to the engine's air intake manifold.
- NaOH and KOH catalysts were used at varying concentrations (2% to 12%) to enhance HHO gas production.
- Voltage variation (11.1 V - 12.5 V) was applied to determine its impact on efficiency.

Test 2: Benzene-Methane Dual-Fuel Configuration

- Methane was supplied from a pressurized tank and injected into the engine's air intake manifold.

- Flow rates ranged from 0.005 to 0.0092 LPM to test its effects on combustion performance.
- A pressure regulator and flow meter-controlled methane injection rates.

Emission Measurement:

- A Testo-350 flue gas analyzer was used to record CO_x, SO_x, and NO_x emissions for both benzene-HHO and benzene-methane setups.

To ensure the accuracy of the recorded experimental data, an uncertainty analysis was conducted. The Testo 350 analyzer, equipped with sensors for gases such as CO, NO, NO₂, SO₂, H₂S, C_xH_y, and CO₂, offers a measurement accuracy of $\pm 5\%$ of the reading for most gas components. For instance, the CO sensor has a measurement range of 0 to 10,000 ppm with an accuracy of $\pm 5\%$ of the reading. Similarly, the NO sensor ranges from 0 to 4,000 ppm with an accuracy of $\pm 5\%$. These specifications are in line with the manufacturer's data. Additionally, the gas flow meter and multimeter used in the experiments have uncertainties of $\pm 1.5\%$ and $\pm 1.0\%$, respectively. These uncertainties were considered during data analysis to ensure the reliability of the results.

3.2 Data Collection and Preprocessing

Experimental data was collected for each fuel combination:

- Fuel consumption was measured in L/hr. for each setup.
- Emissions data was collected separately for benzene-HHO and benzene-methane conditions.

Data Preprocessing:

- The dataset was cleaned, normalized, and structured for AI analysis.
- Key parameters such as fuel ratio, catalyst concentration, voltage, and methane flow rate were isolated for model training.

3.3 AI Optimization Process

Several AI-based techniques, such as Artificial Neural Networks (ANN), Gradient Boosting Models (GBM), and Genetic Algorithms (GA), have been applied to energy optimization. However, Random Forest Regression (RFR) was selected due to its superior ability to handle non-linear relationships, interpretability, and robustness when working with small experimental datasets.

To determine the optimal fuel mixture, the model was trained separately for each fuel condition:

- Benzene-HHO Optimization: AI analyzed the impact of HHO gas concentration, voltage, and catalyst selection on fuel savings and emissions.
- Benzene-Methane Optimization: AI determined the optimal methane flow rate and injection timing to maximize efficiency.

A total of 72 experimental trials were conducted, covering various catalyst concentrations, applied voltages, and gas flow rates. The dataset was processed and analyzed using AI-based optimization rather than traditional statistical regression. The cross-validation method was applied, ensuring the model was tested across different subsets of data to enhance robustness. Given the dataset size, hyperparameter tuning was conducted to determine the optimal number of decision trees, balancing computational efficiency and model accuracy rather than simply using 100 trees by default. After testing configurations of 10, 20, 50, and 100 trees, the 20-tree model was selected as the most efficient for fuel optimization.

3.4 Verification and Comparison

The AI-based optimization was conducted by analyzing fuel consumption and emission reduction across multiple trials, to identify the most efficient fuel combinations based on existing experimental data. The model adjusted for key performance parameters (catalyst concentration, voltage, fuel flow rate) and suggested the optimal operating conditions to maximize efficiency. These AI-driven recommendations were experimentally retested, confirming that the optimized parameters achieved superior fuel savings and emission reductions compared to non-optimized settings.

4. Experimental Setup

4.1 HHO System

Fig. 1 shows a schematic diagram for the system used. The HHO system consists of a dry cell electrolyzer, water tank, power supply, internal combustion engine, and exhaust gas analyzer (Testo-350). The electrolysis unit generates HHO gas, which is injected into the engine's air manifold. The system is controlled via a regulated power supply that adjusts voltage and amperage to optimize gas production.

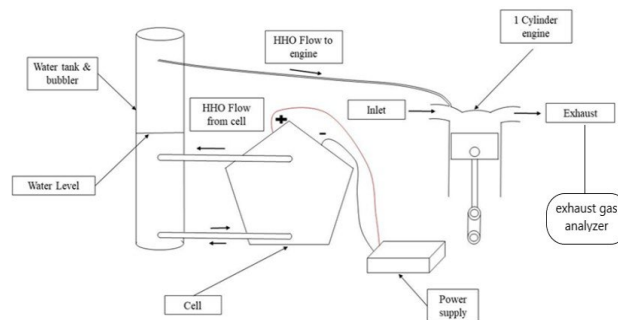


Fig. 1 : HHO System configuration

4.1.1 HHO Generator Design

The electrolysis unit is constructed using stainless steel plates housed between acrylic walls to form multiple water cells. The system includes PVC fittings for gas intake and water refilling, with a bubbler acting as a safety device to prevent backflow. The power supply regulates electrical input, ensuring HHO gas generation controlled for engine combustion enhancement.

4.1.2 Experimental Setup for HHO Injection

The internal combustion engine was modified to accommodate HHO gas injection. The air manifold was fitted with a dedicated HHO inlet hose, ensuring proper air-fuel mixing. Engine parameters such as fuel flow rate and emission levels were monitored using the Testo-350 flue gas analyzer to assess the impact of HHO on efficiency. The engine is shown in Fig. 2, and its specifications are summarized in Table 1.



Fig. 2: Internal combustion engine

Table 1. Engine specification

<i>Specification</i>	<i>Value</i>
Cylinder	1
Max. Horsepower (HP)	6.5 / 3600 rpm
Engine Type	Gasoline
Displacement (CC)	196
Bore X Stroke (mm)	68 X 54
Ignition	Transistor electric / inductive firing
Rotation	Anti-clockwise from output
Manufacturer	Top Marshall

4.2 Methane System

The Methane system comprises a pressurized methane tank, regulator, flow meter, shut-off valve, and flashback arrestor. Methane is injected directly into the engine's air manifold, with a pressure regulator ensuring consistent flow rates for controlled combustion.

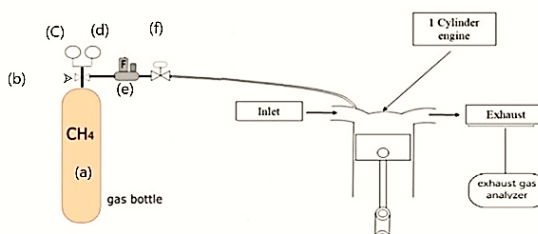


Fig. 3 : Methane system configuration

Fig. 3 shows a schematic diagram of the Methane system. The main system consists of a) methane gas tank, b) gas tank main valve, c) pressure gauge, d) pressure regulator, e) gas flow meter, f) Flashback arrestor, Gasoline engine, and an exhaust gas analyzer.

4.2.1 Experimental Setup for Methane Injection

To evaluate the performance of methane as a dual-fuel source, the methane tank was connected to the engine intake system via a pressure hose. A gas flow meter monitored injection rates, while safety measures, including a flashback arrestor, were implemented to prevent hazards. Methane pressure was adjusted to match atmospheric levels, ensuring consistent comparison with the HHO test setup.

4.3 Testing Phase

Both systems were installed separately to facilitate independent testing under identical operating conditions. Measurements were conducted at constant engine speed (70% of max RPM) to maintain consistency across trials. Fig. 4 and Fig.5 shows the final installation of the system.

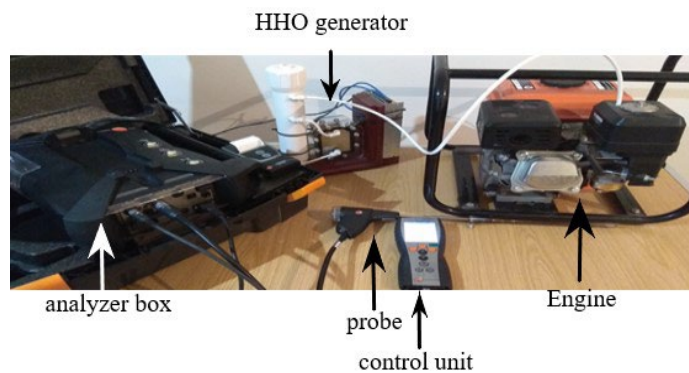


Fig. 4 : HHO system installation



Fig.5 : Methane system installation

4.3 Data Collection and Measurement

For both Benzene-HHO and Benzene-Methane experiments, fuel consumption and CO_x , SO_x , and NO_x emissions were recorded. Key experimental parameters such as voltage, catalyst concentration, and methane flow rate were carefully monitored to ensure reliable data collection.

The time elapsed in each run until the engine stopped was recorded and converted to fuel consumption (liters per hour) using the formula:

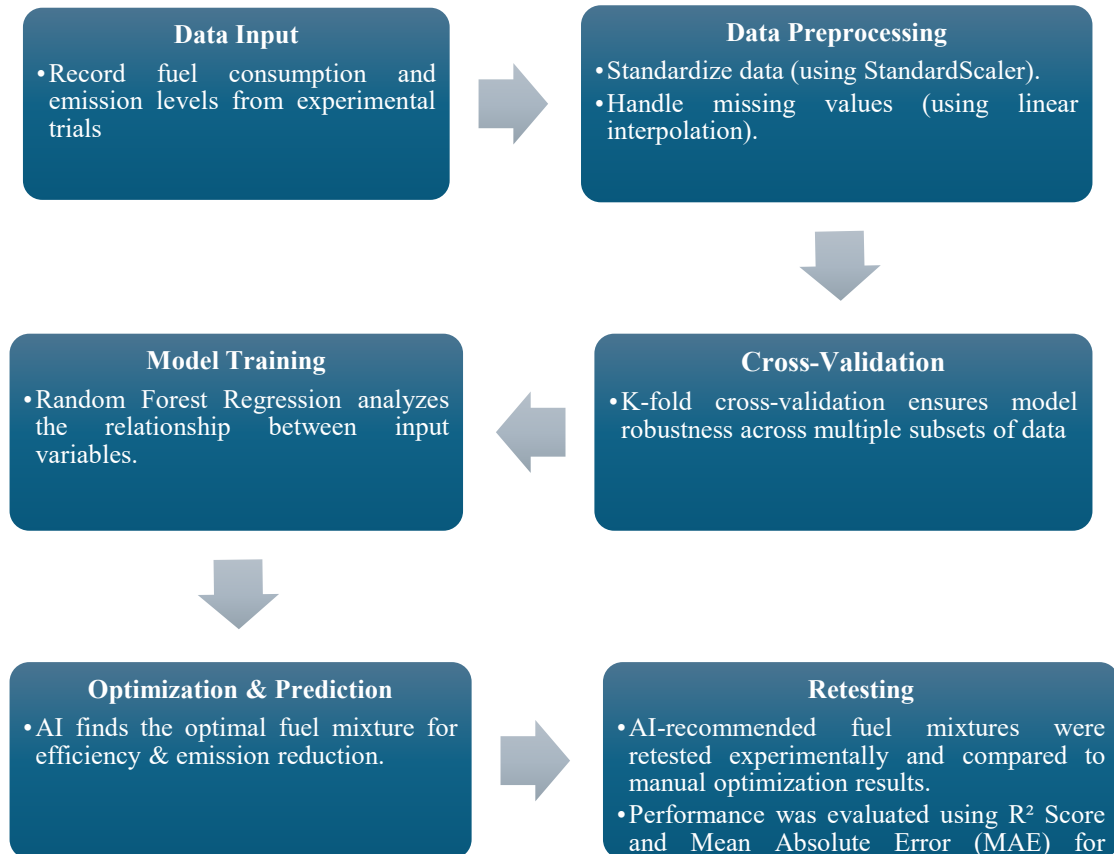
$$\text{Fuel consumption} = \left(\frac{3600 \times 0.1}{T} \right) \quad (1)$$

Where T represents the total running time (seconds) for each fuel mixture test. All measurements were taken under ambient temperature, atmospheric pressure, and a constant engine speed to ensure consistency.



5. Machine Learning Optimization Approach

The AI model utilizes Random Forest Regression (*RFR*) to analyze experimental data and determine optimal fuel mixtures for Benzene-HHO and Benzene-Methane configurations. The model is trained on fuel efficiency and emission data, learning patterns from multiple parameters such as catalyst concentration, voltage levels, and methane injection rates. By evaluating these factors, the AI optimizes fuel composition to achieve maximum efficiency and minimum emissions, significantly reducing the need for manual trial-and-error experimentation.



5.1 Data Processing and Feature Selection

The dataset was collected from 72 experimental trials, covering various fuel ratios and operating conditions. To ensure data integrity and suitability for AI-driven optimization, the following preprocessing steps were applied:

- Standardization: The dataset was standardized using StandardScaler to normalize feature values and improve model stability.
- Handling Missing Data: Missing values were addressed through linear interpolation, ensuring data continuity without introducing bias.
- Feature Selection: Key optimization parameters were identified, including Catalyst concentration (%), Electrolysis voltage (V), HHO and Methane flow rates (LPM), Fuel savings (%), Emission reduction in CO_x, SO_x, and NO_x (%)

A cross-validation approach was applied. This method ensures that the model was evaluated across different subsets of data, enhancing its robustness and reducing overfitting. The AI model was trained to optimize fuel mixture selection, refining decision-making.

5.2 Random Forest Regression (RFR) Model

To ensure a data-driven optimization approach, different AI models were tested, including Support Vector Regression (SVR) and Decision Trees. The Random Forest model was selected due to its ability to handle complex, multi-variable relationships without overfitting. However, instead of the conventional 100 trees, performance testing identified that a 20-tree model was sufficient for this dataset, providing accurate fuel efficiency optimization without excessive computational load. The final model did not predict future values but rather identified the most effective fuel mixture settings based on experimental data, ensuring practical real-world applicability.

Feature Importance Analysis: The model ranked the most influential parameters, revealing that catalyst concentration, voltage, and fuel injection rate were the most significant factors affecting efficiency and emissions.

The importance of a feature (f_i) in Random Forest Regression is calculated as:

$$FI(f_i) = \frac{1}{T} \sum_{t=1}^T (I_t(f_i)) \quad (2)$$

Where: $FI(f_i)$ = Feature Importance of (f_i) , T = Total number of decision trees $I_t(f_i)$ = Importance of feature (f_i) in tree t

5.3 Performance Evaluation Metrics

To assess the model's performance, two evaluation metrics were used:

- **Mean Absolute Error (MAE):** Measures the average absolute difference between actual and AI-optimized values.

$$MAE = \frac{1}{n} \sum_{i=1}^n |y_i - \hat{y}_i| \quad (3)$$

where: n = Total number of samples, y_i = Actual fuel efficiency/emission value, \hat{y}_i = AI-optimized fuel efficiency/emission value.

- **R^2 Score (Coefficient of Determination):** Evaluates how well the model explains variance in the dataset.

$$R^2 = 1 - \frac{\sum (y_i - \hat{y}_i)^2}{\sum (y_i - \bar{y})^2} \quad (4)$$

where: \bar{y} = Mean of actual values, $\sum (y_i - \hat{y}_i)^2$ Residual Sum of Squares (RSS), $\sum (y_i - \bar{y})^2$ = Total Sum of Squares (TSS).

The model achieved an R^2 score of 0.94, demonstrating its high accuracy in optimizing fuel efficiency and emissions reduction through AI-driven fuel mixture selection.

6. Results and Discussion

This table summarizes AI-optimized fuel ratios, highlighting their fuel efficiency improvements and emission reductions.

Table 2. Fuel Savings and Emission Reduction and for Different Dual-Fuel Setups

<i>Fuel Type</i>	<i>Optimal Catalyst Concentration (%)</i>	<i>Optimal Voltage (V)</i>	<i>Fuel Savings</i>	<i>CO_x Reduction</i>	<i>SO_x Reduction</i>
Benzene-HHO (NaOH)	10%	12.4V	58.1%	75.9%	76.1%
Benzene-HHO (KOH)	12%	12.51V	53.8%	79.2%	78.3%
Benzene-Methane	N/A	Atmospheric Pressure	49.1%	58.6%	59.9%

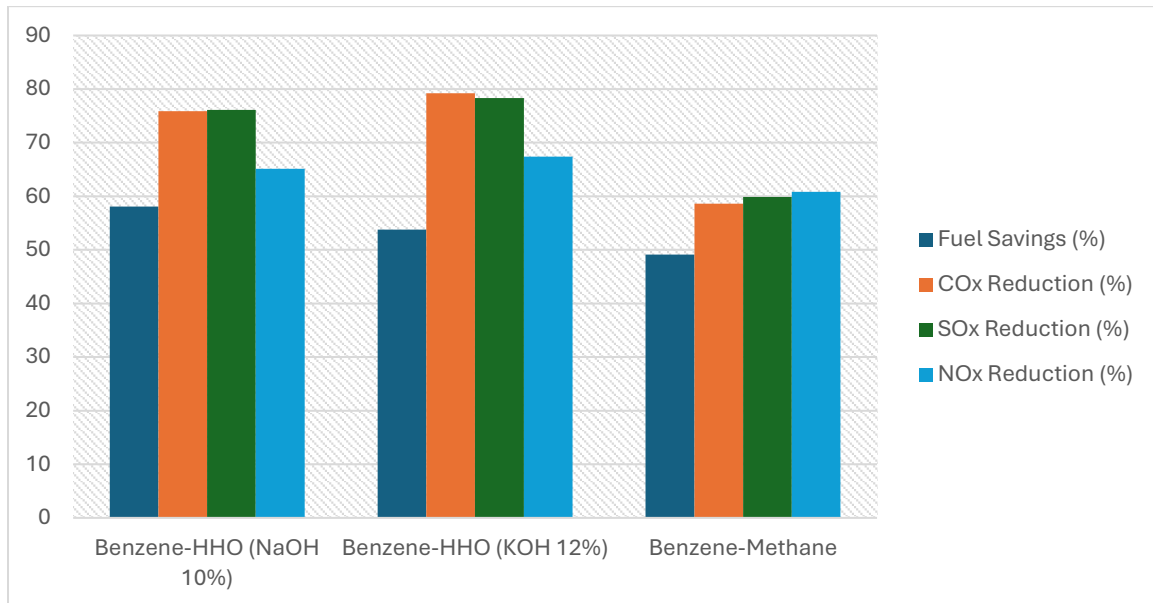


Figure 6 : Fuel Savings and Emission Reduction and for Different Dual-Fuel Setups

6.1 HHO Gas Optimization

The experimental data was input into the optimization model, which determined the optimal catalyst concentration and voltage settings for maximum fuel efficiency and minimum emissions. The results were then verified through experimental retesting to confirm the AI-optimized fuel mixture. The NaOH catalyst at 10% concentration provided the highest fuel savings of 58.1%, with CO_x reduced by 75.9%, SO_x by 76.1%, and NO_x by 65.1%. The applied voltage of 12.4V contributed to enhanced HHO production, leading to improved combustion efficiency. The KOH catalyst at 12% concentration demonstrated greater CO_x reduction (79.2%), while fuel savings were slightly lower at 53.8%. The

applied voltage of 12.51V ensured stable gas production, balancing fuel efficiency and emission reduction. Retesting with the AI-optimized fuel mixture confirmed that the model's suggested conditions improved efficiency while maintaining stability, demonstrating the reliability of AI-based optimization. The findings align with previous research, such as , 10% hydrogen reduces the smoke by 65%, reduces CO₂ and CO by about 27% and 32% respectively , and NO_x emissions are reduced by 81.35% .

The greater CO_x reduction achieved with KOH at 12% concentration can be attributed to its increased catalytic activity, which enhances combustion efficiency. In contrast, NaOH at 10% provided superior fuel savings due to its higher ionization potential, leading to more effective HHO gas production.

6.2 Methane Gas Optimization

Methane was analyzed separately, with the experimental data serving as input for the AI optimization model, which determined the most efficient methane flow rate for fuel savings and emission reduction. The model's recommendations were then verified by re-running the experiments under optimized conditions. The highest methane efficiency was observed at a flow rate between 0.005 and 0.0092 LPM, leading to a 49.1% reduction in fuel consumption. CO_x emissions decreased by 58.6%, SO_x by 59.9%, and NO_x by 60.8%, demonstrating methane's potential as a cleaner fuel alternative. While methane reduced emissions, its fuel savings were slightly lower than HHO, partly due to its lower combustion enhancement properties compared to hydrogen. Retesting under AI-optimized methane conditions confirmed that the selected flow rates and pressure settings improved efficiency while maintaining controlled emissions, validating the AI model's effectiveness. Despite its advantages, methane requires specialized storage infrastructure, which may pose challenges for maritime applications, affecting its large-scale adoption.

7. Conclusion

This study applied an AI-driven optimization approach to enhance fuel efficiency and reduce emissions in dual-fuel internal combustion engines for green port applications. The Random Forest-based optimization model, configured with an optimal 20-tree setup, successfully identified the best fuel mixture parameters, improving decision-making over conventional trial-and-error methods. The AI-optimized settings were validated through experimental retesting, confirming that NaOH at 10% concentration achieved the highest fuel savings (58.1%), while KOH at 12% concentration provided the greatest CO_x reduction (79.2%). Methane fuel, though effective in emission reduction, demonstrated slightly lower efficiency than HHO-based mixtures.

The model achieved an R² score of 0.94, confirming its high accuracy in optimizing fuel parameters. This research highlights AI's potential to dynamically adjust fuel mixtures, supporting sustainable maritime decarbonization. Future research will focus on integrating real-time AI-driven fuel mixture adjustments into operational port environments. Expanding the dataset with real-world maritime fuel consumption data and applying deep learning techniques will further improve the adaptability and scalability of AI-driven fuel optimization for sustainable port operations.

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