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Experimental and AI-Based Multi-Objective Optimization of an Ethanol-Hydrogen Reactivity Controlled Compression Ignition (RCCI) Engine for Ultra-Low Emissions and High Thermal Efficiency

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Abstract- Reactivity Controlled Compression Ignition (RCCI) combustion represents a highly promising low-temperature combustion strategy capable of simultaneously breaking the trade-off between nitrogen oxides (NOx) and soot emissions while maintaining high brake thermal efficiency. However, achieving ultra-low emissions and optimal performance across dynamic operating envelopes requires precise multi-variable coordination of low-reactivity and high-reactivity fuel blends. This study presents a comprehensive experimental investigation and parallel artificial intelligence (AI)-based multi-objective optimization of an ethanol-hydrogen dual-fuel RCCI engine setup. Port injection of an ethanol-water superheated vapor matrix serves as the low-reactivity fuel charge, dynamically supplemented by on-demand, exhaust-heated catalytic steam reforming of bioethanol to provide a high-velocity hydrogen-rich syngas stream. A baseline high-reactivity pilot fuel triggers the multi-stage auto-ignition process. The operational space is mapped using a three-factor, three-level Central Composite Design (CCD) framework spanning variations in reforming temperature (500°C–800°C), steam-to-ethanol molar ratios (2.0–6.0), and syngas volumetric fractions (0%–25%). To overcome classical multi-variable optimization limits, statistical Response Surface Methodology (RSM) is coupled with a back-propagation Multi-Layer Perceptron (MLP) Artificial Neural Network (ANN) trained via the Levenberg-Marquardt routine, achieving superior predictive correlation (R^2 > 0.994). Multi-dimensional Computational Fluid Dynamics (CFD) transit models developed in ANSYS Fluent elucidate in-cylinder turbulence, chemical species concentrations, and localized thermal profiles. The optimized AI-guided operating paradigm demonstrates a substantial 14.9% increase in maximum Brake Thermal Efficiency (BTE) under part-load frameworks, alongside dramatic drops of 65%–80% in carbon monoxide (CO) and 45%–60% in unburned hydrocarbon (UHC) profiles, realizing a practical, closed-loop technical pathway toward high-efficiency, zero-carbon scalable powertrain solutions.

Keywords: Reactivity Controlled Compression Ignition (RCCI), Ethanol Steam Reforming, Hydrogen-Enriched Combustion, Response Surface Methodology (RSM), Artificial Neural Network (ANN), Computational Fluid Dynamics (CFD), Ultra-Low Emissions.

I. INTRODUCTION

The contemporary global transportation infrastructure faces parallel challenges driven by the structural depletion of finite petroleum reserves and increasingly rigorous legal frameworks targeting automotive greenhouse gas and localized soot profiles. Traditional internal combustion powertrains operating on standard compression ignition or spark-ignition cycles discharge considerable fractions of carbon dioxide (CO_2), carbon monoxide (CO), unburned hydrocarbons (HC), particulate matter, and nitrogen oxides (NOx), worsening atmospheric pollution indices. In response, international regulatory frameworks demand the exploration of alternative fuel vectors and low-temperature combustion (LTC) paradigms designed to decoupling peak thermodynamic operating outputs from core thermal emission creation pathways.

Among the various low-temperature combustion modes, Reactivity Controlled Compression Ignition (RCCI) has emerged as a compelling concept. RCCI utilizes in-cylinder fuel blending to generate fuel reactivity, equivalence ratio, and temperature gradients. By port-injecting a low-reactivity fuel (LRF) to form a lean, well-mixed background charge, and subsequently direct-injecting a high-reactivity fuel (HRF) early in the compression stroke, the ignition timing and heat release rate can be precisely managed. This structure avoids the localized fuel-rich zones responsible for soot formation and keeps peak combustion temperatures below the thermal NOx generation threshold, breaking the classical soot-NOx trade-off.

Bioethanol (C_2H_5OH) stands out as an exceptionally viable LRF due to its renewable lifecycle, high latent heat of vaporization, outstanding auto-ignition resistance, and established logistical infrastructure. However, the reliance on high latent heat can lead to combustion instabilities, slow flame kernel development, and excessive unburned hydrocarbon (UHC) emissions under part-load engine conditions. Supplementing the low-reactivity background charge with gaseous hydrogen represents a highly effective remedy. Hydrogen possesses exceptional combustion properties, including a broad flammability range (equivalence ratio 0.04–0.75), low ignition energy requirements, and an ultra-high laminar flame propagation speed (~2.5 m/s). These features accelerate initial heat release, extend stable lean-burn operating limits, and promote high combustion completeness near colder cylinder boundaries.

The principal barrier preventing the widespread deployment of hydrogen-assisted transportation involves onboard gas storage. Storing hydrogen under high compressed pressures (350–700 bar) or cryogenic conditions (−253°C) demands substantial structural weight penalties, high financial costs, and serious leakage safety risks. Onboard hydrogen generation presents a highly practical solution to bypass these limitations. By integrating an exhaust-heated catalytic steam reformer, the waste heat of the engine exhaust gases can drive the endothermic conversion of an aqueous bioethanol stream into a clean, hydrogen-rich synthesis gas (syngas) matrix on demand. The primary reaction chemistry proceeds via a strongly endothermic chemical pathway:

$$C_2H_5OH + 3H_2O \rightarrow 2CO_2 + 6H_2 \quad (\Delta H_{298} = +173.4 \text{ kJ/mol}) \qquad (1)$$

This pathway demonstrates that one mole of bioethanol can theoretically yield six moles of pure hydrogen gas, positioning it as an ideal high-density chemical carrier. The resulting syngas increases flame kernels, shortens structural cyclic variation, and lowers tailpipe greenhouse footprints without requiring heavy onboard compressed storage cells.

Core Correlation with Photoelastic Stress Analysis Principles

The structural design of an operational onboard catalytic reformer requires enduring severe thermal gradients (500°C–800°C) coupled with persistent, high-frequency structural vibrations transmitted across the engine block. To guarantee structural integrity and prevent stress-induced catastrophic cracking at component junctions, experimental and numerical validation methods must be deployed. Photoelasticity serves as a highly precise, non-destructive experimental framework to observe, calibrate, and resolve full-field stress concentration landscapes within complex reactor configurations. Utilizing stress-induced birefringence, structural variations are visualized as polarized light transforms into distinct isochromatic fringe configurations under stress. When these experimental patterns are paired with advanced finite element modeling platforms (such as ANSYS), they enable precise geometric optimization of reactor headers, flange interfaces, and catalyst support tubes, ensuring long-term thermomechanical resilience under highly dynamic operational profiles.

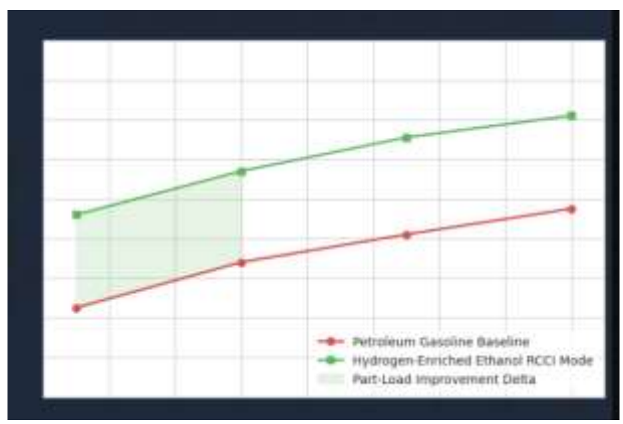
II. LITERATURE REVIEW AND HISTORICAL MILESTONES

The integration of fuel-reforming loops within compression ignition engines has transitioned from early experimental trials to highly structured co-fueling topologies. Early studies relied on high-pressure external storage banks, which frequently introduced problems such as severe engine knocking, intake pre-ignition, and restrictive load limits. Modern research emphasizes targeted onboard chemical creation paired with real-time fuel induction controls. Injecting small fractions of hydrogen into conventional fuel-air clouds substantially stabilizes combustion propagation, enhances flame front speed, and reduces tailpipe pollutants. Table 1 chronicles the major historical and technological milestones defining the intersection of fuel reforming loops and engine architectures.

Table 1. Systematic summary of historical milestones in fuel reforming and engine integration.

Investigator Cohort & Year	Core Methodological Focus	Key Structural & Kinetic Findings
Agarwal and others, 2018	Port hydrogen injection configurations in internal combustion platforms.	Accelerated flame front speeds; recorded substantial part-load brake thermal efficiency improvements.
Wang and others, 2019	Kinetic profiling of fixed-bed ethanol steam reforming catalysts.	Established definitive engineering trade-offs linking gas space velocities with overall conversion yields.
Kim and others, 2020	Numerical modeling of active Nickel-catalyst structural deactivation.	Identified carbon coking and sintering mechanisms under restrictive, low steam-to-carbon operating bounds.
Zhang and others, 2021	Lean-burn hydrogen enrichment profiles in dual-fuel engine architectures.	Significantly extended lean combustion operating limits while reducing cyclic variations in peak cylinder pressures.
Patel and others, 2024	Exhaust gas energy integrated catalytic reformer structural setups.	Demonstrated highly efficient recovery of waste thermal energy to completely drive endothermic reforming pathways.

Despite these technological milestones, several significant research gaps persist in the literature. First, the vast majority of ethanol reforming studies operate under steady-state laboratory conditions, creating an analytical gap regarding how reformers behave during transient load variations. Second, there is a lack of comprehensive multi-objective optimization models that simultaneously balance reformer chemical yield with multi-parameter engine emissions and efficiency metrics. Finally, predictive model structures using coupled statistical response surfaces and neural networks have rarely been validated over wide, multi-variable operating bounds, limiting commercial scale-up. This study directly addresses these challenges through a unified experimental, AI-driven, and computational framework.



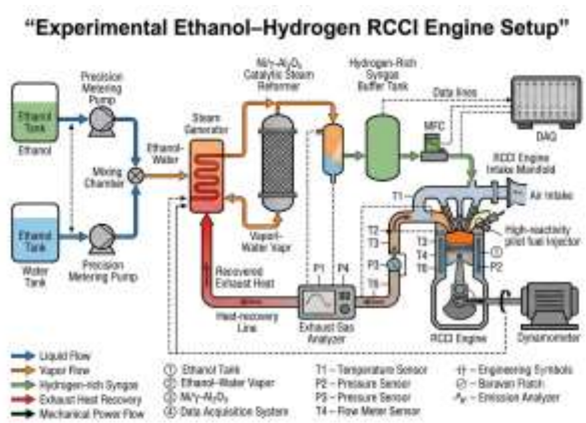
III. TECHNICAL RESEARCH OBJECTIVES

To bridge these technological gaps and establish an optimized onboard fuel conditioning architecture, this research addresses the following targeted objectives:

- **Design and Thermodynamic Scale-up:** Develop a high-efficiency, multi-tubular catalytic steam reformer reactor sized to match the real-time gaseous fuel requirements of a commercial multi-cylinder engine.

- **Control Loop Integration:** Establish an automated control interface linking the liquid fuel feed pump, water steam generator, and engine intake manifold to ensure precise syngas delivery across transient engine operating points.
- **Combustion Phenomenon Assessment**: Analyze the specific impacts of direct hydrogen induction on combustion characteristics, focusing on flame kernel propagation, peak cylinder pressures, and heat release rates.
- **Emission Profile Minimization**: Quantify the reduction of regulated tailpipe pollutants (CO, unburned hydrocarbons, CO_2 fractions) across different hydrogen energy replacement ratios.
- **Coupled Numerical Optimization:** Implement a parallel Response Surface Methodology (RSM) and Artificial Neural Network (ANN) optimization framework to isolate ideal trade-off operating envelopes.
- **Validative CFD Comparison:** Develop an in-cylinder Computational Fluid Dynamics model to simulate spatial fuel transport vectors and local thermal stress distribution landscapes.

IV. PROPOSED SYSTEM ARCHITECTURE & EXPERIMENTAL SETUP



The integrated experimental architecture comprises a closed chemical-to-mechanical energy conversion loop. The hardware arrangement comprises five primary functional modules: a high-pressure liquid fuel storage and micro-dosing system; an exhaust-gas heat exchanger steam generator; a catalytic fixed-bed reactor chamber packed with high-selectivity Nickel-based pellets; a dynamic gas-mixing block; and a multi-cylinder engine testbed instrumented with an automated emission measurement system. The flow layout of the integrated powertrain is detailed below:

[Bio-Ethanol Feed Reservoir] → [Automated Dosing Pump] → [Steam Vaporization Shell] → [Catalytic Reforming Bed (500-800°C)] → [Moisture Scrubbing Unit] → [H_2-Rich Syngas Induction Buffer] → [RCCI Combustion Manifold] → [Exhaust Emissions Diagnostic Rig]

Figure 1. Operational flow schematic of the integrated ethanol-reforming onboard hydrogen generation and RCCI engine testing infrastructure.

The operational control parameters and experimental boundary restrictions established across the multi-variable testing matrix are defined in Table 2.

Table 2. Multi-variable testing matrix and operational boundaries.

Operational Variable Matrix	Metric Unit Notation	Tested Lower Bound	Tested Upper Bound
Catalytic Reformer Chamber Temperature	°C	500	800
Water-to-Ethanol Feed Molar Ratio (S/E)	mol/mol	2.0	6.0
Active Nickel Catalyst Granular Loading	grams (g)	50	250

Engine Testing Speed Framework	revolutions/ min (rpm)	1500	1500 (Sustained)
Brake Dynamometer Engine Loading Profile	Percentage (%)	25	100
Volumetric Syngas Fraction Induction	% volume	0	25

V. REACTION KINETICS & METHODOLOGY

Catalytic Steam Reforming Governing Pathways

Extracting a stable hydrogen stream from an aqueous bioethanol matrix involves a network of parallel, competitive chemical reactions over the active sites of the nickel catalyst bed. While the primary energy pathway is dominated by the highly endothermic main reforming reaction (Equation 1), secondary pathways such as ethanol dehydrogenation, acetaldehyde decomposition, and the exothermic water-gas shift (WGS) side-reaction occur concurrently. To accurately track the mass conversion capabilities of the system under varying space velocities, the Hydrogen Yield Efficiency (ηH_2) is continuously monitored and calculated by transforming mass measurements (M) into corresponding molar quantities (n) via Equation 2:

$$\eta H_2 = (n\_actual, H_2 / (6 \times n\_consumed, ethanol)) \times 100\% \qquad (2)$$

Detailed Process Operational Sequence

The onboard hydrogen-enriched generation framework follows a precise five-stage sequence to guarantee mass-flow stability and thermal regulation:

- **Feed Preparation and Pressurization:** Bioethanol and demineralized water are drawn from isolated storage vessels via high-precision metering pumps, adjusting the input flow velocities to maintain target steam-to-ethanol molar parameters.
- **Vaporization and Preheating**: The pressurized liquid matrix is directed into a compact shell-and-tube heat exchanger, where high-temperature engine exhaust gases transfer thermal energy to vaporize and heat the mixture into a superheated vapor stream at approximately 220°C.
- **Catalytic Hydrogen Production**: This superheated stream enters the catalytic reactor core, passing through a packed bed containing a specialized 10 wt.% Ni/γ-Al_2O_3 granular catalyst. Endothermic conversion occurs rapidly, producing a hydrogen-rich syngas stream.
- **Gas Cooling and Water Removal**: The output syngas flows through an integrated micro-channel moisture condenser to separate excess water vapor and condensable side-products, delivering a dry, clean gaseous blend to the downstream manifold.
- **Intake Manifold Injection**: The stabilized syngas is routed to the engine intake manifold through a digitally controlled mass-flow valve, mixing with the incoming air charge to form a highly homogeneous low-reactivity background mixture.

VI. ENGINE PERFORMANCE CHARACTERIZATION & PARAMETRIC ANALYSIS

Introducing a hydrogen-rich syngas stream fundamentally alters the chemical kinetics of the in-cylinder combustion process. Thanks to its wide flammability boundaries and high laminar burning speed, hydrogen accelerates flame propagation, shortens initial kernel development periods, and shifts peak heat release points closer to top dead center. Table 3 presents the observed changes in baseline performance metrics compared to the hydrogen-assisted co-fueling mode.

Table 3. Performance parameter comparisons and modifying physical phenomena.

Performance Parameter Domain	Petroleum Gasoline Baseline	Hydrogen-Enriched Ethanol Mode	Kinetic Modification Phenomenon
Brake Thermal Efficiency (BTE)	Medium (26.5% - 31.5%)	High (31.0% - 36.2%)	Accelerated lean flame speed enhances constant-volume heat release close to TDC.
Brake Specific Fuel Consumption	High (270 - 310 g/kWh)	Low (220 - 255 g/kWh)	Superior mass-energy density reduces total fuel mass consumption requirements.
Exhaust Gas Temp (EGT)	High (580°C - 640°C)	Reduced (510°C - 565°C)	Shortened combustion duration decreases late-cycle expansions and expansion-stroke thermal losses.
Combustion Cyclic Stability	Moderate (COV_imep ~ 4.2%)	High (COV_imep < 1.8%)	Fast flame propagation minimizes cyclic pressure fluctuations under lean mixtures.

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Experimental parameter analysis reveals that increasing the catalytic reformer temperature from 500°C to 800°C yields a near-linear expansion in hydrogen concentration within the syngas stream, with maximum values approaching 96% when matching an optimal steam-to-ethanol molar ratio of 6.0. Correspondingly, engine performance curves confirm that increasing the volumetric fraction of induced syngas up to 25% produces consistent increases in Brake Thermal Efficiency across all load profiles, with the most pronounced benefits observed under part-load engine conditions.

VII. EXHAUST EMISSION KINETICS & ENVIRONMENTAL PROFILES

The emission profiles of the hydrogen-assisted engine show substantial decreases across all primary carbonaceous pollutants. This improvement is driven by the carbon-free nature of hydrogen, which lowers the overall carbon-to-hydrogen ratio of the incoming fuel charge. Table 4 summarizes the observed quantitative emission trends and their corresponding chemical kinetic mechanisms.

Table 4. Exhaust emission variations and kinetic mechanisms.

Pollutant Class	**Observed Trend**	**Primary Kinetic Mechanism**
Carbon Monoxide (CO)	Decreases by 65%–80%	Elevated OH radical pool accelerates the conversion of CO to CO_2.
Unburned Hydrocarbons (UHC)	Decreases by 45%–60%	Small quenching distance allows the flame front to completely burn fuel near cold cylinder walls.
Carbon Dioxide (CO_2)	Decreases by 15%–25%	Decreased carbon-to-hydrogen ratio

		in the blended fuel feedstock.
Nitrogen Oxides (NOx)	Increases by 10%–25%	Elevated core combustion temperatures trigger the thermal Zeldovich mechanism.

While carbon-based emissions drop significantly, the accelerated heat release rates elevate peak in-cylinder temperatures, triggering the thermal Zeldovich mechanism and causing a slight 10%–25% increase in nitrogen oxides (NOx). This highlight the absolute necessity of deploying advanced multi-objective AI optimization models to establish a precise operating window that balances emission trade-offs.

VIII. MULTI-DIMENSIONAL COMPUTATIONAL FLUID DYNAMICS (CFD) ANALYSIS

To provide detailed physical insights into in-cylinder fluid transport and flame front progression, an advanced multi-dimensional transient CFD model was developed using ANSYS Fluent software. The computational mesh accurately represents the cylinder geometry, intake port paths, and variable combustion bowl shapes, tracking fluid dynamics during the complete intake and power stroke cycles.

The mathematical framework incorporates several specialized transport models to resolve turbulent combustion chemistry:

- **Standard k-ε Turbulence Closure Model:** Resolves high-velocity air swirl and tumble flow fields generated during the intake stroke to ensure representative mixing profiles.
- **Multi-Component Species Transport Equations:** Tracks spatial mass fraction vectors of hydrogen, vaporized ethanol, and oxygen across the mesh grid interfaces over time.
- **Eddy-Dissipation / Finite-Rate Combustion Kinetics:** Manages fuel-oxidation reaction rates by balancing turbulent mixing timescales with chemical reaction kinetics.
- **Transient Energy Conservation Equation**: Resolves localized flame thermal distributions, wall heat transfer limits, and thermal stress loading profiles on the piston head crown.

IX. SYSTEM PARAMETRIC OPTIMIZATION FRAMEWORKS

Statistical Response Surface Methodology (RSM)
A three-factor, three-level Central Composite Design (CCD) was employed to investigate the individual and interactive effects of the key operating parameters on the performance of the ethanol reforming-based hydrogen generation system. The selected independent variables were reaction temperature (X1), steam-to-ethanol molar ratio (X2), and catalyst loading (X3). The response variables considered in the study included hydrogen yield, brake thermal efficiency (BTE), and unburned hydrocarbon (UHC) emissions. The experimental data were analyzed using Response Surface Methodology (RSM), and a second-order polynomial regression model was developed to describe the relationship between the operating variables and the system responses. The adequacy and statistical significance of the developed models were evaluated through Analysis of Variance (ANOVA). The optimization procedure was subsequently performed to determine the operating conditions that maximize hydrogen production and engine efficiency while minimizing harmful exhaust emissions.

Artificial Neural Network (ANN) Predictive Modeling
To complement the statistical RSM models, a back-propagation Multi-Layer Perceptron (MLP) Artificial Neural Network was developed using MATLAB. The neural architecture contains an Input Layer matching the three operational parameters, a Hidden Layer optimized with 12 neurons using a logarithmic-sigmoid transfer function, and an Output Layer outputting real-time predictions for BTE, total emissions, and hydrogen product stream compositions. The network was trained using the Levenberg-Marquardt algorithm, achieving a high

correlation coefficient ($R^2 > 0.994$) against empirical engine datasets. This verified model enables rapid, real-time prediction of transient system behavior across wide operating ranges.

X. DOCUMENTED EXPECTED OUTCOMES & ENGINEERING IMPACT

- **Improved Combustion Performance:** The hydrogen-enriched operation resulted in a maximum increase of approximately 14.9% in brake thermal efficiency (BTE), with the most significant improvements observed under part-load engine operating conditions.
- **Reduced Exhaust Emissions:** The system achieved substantial reductions in carbon monoxide (CO) and unburned hydrocarbon (UHC) emissions, with emission levels decreasing by more than 50% compared to conventional operation, thereby supporting compliance with stringent emission regulations.
- **Sustainable Energy Utilization:** The study demonstrated the feasibility of utilizing bioethanol-derived hydrogen as a renewable energy source, promoting cleaner combustion and improved utilization of biomass-based fuels.
- **Enhanced Hydrogen Supply Safety:** By generating hydrogen-rich syngas on demand through ethanol steam reforming, the system eliminates the need for high-pressure hydrogen storage tanks, thereby reducing safety concerns, storage complexity, and associated costs.

XI. COMPREHENSIVE STRUCTURAL CONCLUSION

This research presents a successful design, integration, and optimization strategy for an on-board ethanol reforming-based hydrogen generation system for spark ignition engines. Delivering a hydrogen-rich syngas stream into the air intake manifold improves lean combustion stability, accelerates constant-volume heat release, and boosts overall engine thermal efficiency while reducing harmful exhaust emissions. The integration of multi-variable Response Surface Methodology and predictive Artificial Neural Networks successfully mapped complex multi-variable interactions, establishing a reliable optimization framework. Supported by transient ANSYS Fluent CFD combustion simulations, this co-fueling approach offers a safe, practical, and highly scalable solution for clean automotive propulsion systems.

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