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# AI-based evaluation of biofuel combustion performance and emission characteristics in gas turbines

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## ABSTRACT

The growing urgency for sustainable energy alternatives has accelerated research into biofuel utilization in gas turbine systems, where Artificial Intelligence (AI) offers transformative capabilities for performance assessment and emission prediction. This study investigates the AI-based assessment of biofuel performance parameters in gas turbine combustion systems with a focus on emission characterization. The primary objectives include evaluating the predictive accuracy of machine learning models for NOx and CO emissions and comparing the combustion efficiency of various biofuel blends against conventional Jet-A fuel. A quantitative secondary data analysis methodology was adopted, employing published experimental datasets (2019–2025) from the UCI Machine Learning Repository and peer-reviewed combustion studies, analysed using ANN, Random Forest, SVM, and LSTM algorithms. Two hypotheses were formulated: H1 states that AI-driven machine learning models achieve statistically significant prediction accuracy ($R^2 > 0.90$) for NOx and CO emissions from biofuel-fueled gas turbines; H2 states that biofuel blends (B20–B50) produce statistically significant reduction in CO emissions compared to conventional Jet-A fuel while maintaining thermal efficiency above 26%. The results confirm that the Random Forest model achieved $R^2 = 0.9792$ for NOx prediction, validating H1 ($t = 14.82$, $p < 0.001$). Biofuel blend B20 demonstrated 20.20% CO reduction with thermal efficiency of 27.80%, supporting H2 ($t = 8.67$, $p < 0.001$). It is concluded that AI-based predictive frameworks provide a reliable pathway for optimizing biofuel combustion and achieving emission reduction targets in gas turbine power generation.

**Keywords:** Artificial Intelligence, Biofuel Combustion, Gas Turbine Emissions, Machine Learning, NOx Prediction

## INTRODUCTION

The global energy landscape is undergoing a fundamental transformation driven by the twin imperatives of climate change mitigation and energy security. Gas turbines, which constitute a significant proportion of the world's power generation infrastructure, have traditionally relied on fossil fuels, contributing substantially to greenhouse gas emissions and atmospheric pollutants including Nitrogen Oxides (NOx) and Carbon Monoxide (CO). The International Energy Agency's Bioenergy Annual Report 2024 emphasized that biofuels are among the critical means to decarbonize power generation and transport sectors, yet deployment remains insufficient to meet net zero pathway targets [1]. In this context, the integration of biofuels into gas turbine combustion systems presents a compelling opportunity to reduce the carbon footprint while maintaining operational efficiency. Biofuels derived from renewable biomass sources, including vegetable oils, algae, and waste cooking oils, have demonstrated considerable potential as alternative fuels for gas turbine applications. The global biodiesel market, valued at approximately USD 32.09 billion in 2021, is projected to reach USD 189.7 billion by 2030, reflecting the expanding demand for sustainable fuel alternatives [2]. However, the combustion behavior of biofuels in gas turbines differs significantly from conventional fuels due to variations in calorific value, viscosity, and oxygen content. Biodiesel blends in micro gas turbine engines demonstrated lower CO emissions due to more complete combustion, while NOx and $CO_2$ emissions increased at higher engine speeds owing to elevated combustion temperatures [3]. Soy methyl ester, canola methyl ester, and recycled rapeseed methyl ester at B50 and B100 concentrations in a 30 kW gas turbine engine produced static thrust comparable to Jet-A while achieving 40% lower CO and 50% lower NO emissions [4]. The application of artificial intelligence and machine learning techniques has emerged as a powerful paradigm for predicting and optimizing combustion performance and emissions in gas turbine systems. A stacked ensemble machine learning model for predicting CO and NOx emissions from gas turbines outperformed classical algorithms, achieving RMSE reductions of 5.7% for NOx [5]. Kaya et al. introduced a benchmark predictive emissions monitoring system (PEMS) dataset collected over five years from a gas turbine in Turkey containing 36,733 hourly instances, achieving $R^2 = 0.83$ for NOx and $R^2 = 0.89$ for CO emissions [6]. The Turbo Expo 2025 conference highlighted that AI can navigate massive design spaces with hundreds of parameters, generating combustor design proposals meeting specific NOx emission limits, pressure drop specifications, and thermoacoustic stability criteria [7]. Despite these advancements, a notable gap exists in the systematic integration of AI-based assessment frameworks specifically tailored for biofuel performance evaluation in gas turbine combustion. Most existing studies have either focused exclusively on conventional fossil fuels or have applied limited machine learning algorithms without rigorous hypothesis-driven comparative analysis. Hosseini [8] noted in a comprehensive review that AI techniques have been utilized across various stages of biofuel production for improving prediction accuracy and process optimization, yet their specific application to gas turbine emission characterization with biofuel blends remains underexplored. dos Santos Coelho et al. demonstrated that deep forest regression models achieved $R^2 = 0.9647$ for CO emissions in gas turbines, indicating the substantial potential of advanced ML architectures [9]. This study addresses this critical gap by systematically evaluating AI-based predictive models for assessing biofuel combustion performance and emission characteristics in gas turbine systems through a rigorous hypothesis-testing framework, thereby contributing to the development of sustainable, data-driven energy solutions.

## LITERATURE REVIEW

The intersection of biofuel technology, gas turbine combustion, and artificial intelligence has attracted significant scholarly attention in recent years. Awogbemi and Kallon [2] provided an extensive review of machine learning applications in biodiesel production processes, highlighting that ANN, RSM, and ANFIS have been successfully deployed to optimize conversion efficiency and predict fuel properties. Their analysis established that ML-based approaches outperform traditional statistical methods in handling the non-linear relationships inherent in biofuel production and combustion systems, achieving prediction accuracy improvements of 15–30% over conventional regression models. Extending this framework to gas turbine applications, Hoque et al. investigated NOx emission predictions through integrated data-driven machine learning approaches using the UCI gas turbine dataset and reported that ensemble models demonstrated superior accuracy, with Random Forest achieving 91.68%, XGBoost at 91.54%, and CATBoost exhibiting the highest accuracy at 92.76% [10]. In the domain of biofuel combustion characteristics in turbine systems, Aravind et al. examined hydrogen combustion dynamics in a tri-fuel engine operating with diesel, algae spirogyra methyl ester, and ditert-butyl peroxide, finding that the dual-fuel approach improved brake thermal efficiency by 2.6% while reducing CO emissions by 18% [11]. Roy et al. applied neural networks for reducing emissions and optimizing performance of hydrogen-biofuel compression ignition engines and confirmed that AI-driven optimization achieved prediction errors under 5% while maintaining engine performance parameters within acceptable ranges [12]. The study by Nogueira et al. on prediction of NOx and $CO_2$ emissions from an experimental dual-fuel engine using optimized random forest combined with feature engineering and SHAP-based explainability achieved $R^2$ values of 0.9811 for NOx and 0.9276 for $CO_2$, establishing random forest as a highly effective tool for emission prediction in multi-fuel combustion environments [13]. Regarding gas turbine-specific biofuel applications, Nascimento et al. conducted foundational work on biodiesel fuel in diesel micro-turbine engines, establishing through coupled modeling and experimental evaluation that biofuel blends maintained thermal efficiency within 2–3% of conventional fuels while demonstrating measurable CO emission reductions of 12–18% [14]. Nguyen Chi Thanh et al. demonstrated that a 30% microalgae biodiesel blend with nanoparticles in micro gas turbine engines reported the highest static thrust while substantially reducing fuel consumption rates due to high thermal efficiency [3]. Potts and Leontidis evaluated tabular machine learning methods for predicting gas turbine emissions, benchmarking gradient-boosted decision trees against deep learning architectures, and noted that Siemens Energy's Chemical Kinetics PEMS model utilized pilot/main fuel split, inlet air temperature, and inlet air pressure as primary parameters for emission calculation with industrially validated accuracy [15]. The advancement of deep learning architectures for emission prediction has been documented by several recent studies. A modified CNN-Bi-LSTM model with extrinsic attention mechanism developed for gas turbine emission prediction demonstrated $R^2$ values of 0.881 for NOx and 0.801 for CO, significantly outperforming conventional single-model approaches Environment, Development and Sustainability, 2026. Wang et al. proposed an innovative NOx emissions prediction model based on random forest feature selection and evolutionary Reformer architecture that yielded the highest $R^2$ alongside the lowest RMSE, MAE, and MSPE values compared to LSTM, GRU, and Transformer baselines [16]. The comprehensive review published in ACS Omega highlighted that AI models including support vector machines, ANFIS, and multilayer perceptrons optimize fuel performance across biomass conversion systems, with ANFIS achieving 94.2% prediction accuracy

for methane yield and MLP reducing carbon emission estimation error by 22% (ACS Omega, 2025). Ross-Veitía et al. applied multiple ML regression algorithms to predict CO, $CO_2$, and NOx emissions from industrial boilers using real operational data from twenty boilers, demonstrating that ensemble approaches consistently outperformed single-algorithm models [17]. These studies collectively underscore the transformative potential of AI in bridging the performance gap between biofuels and conventional fuels in gas turbine applications, while also revealing the need for hypothesis-driven investigations that rigorously quantify prediction reliability and emission reduction significance.

## OBJECTIVES

1. To evaluate and compare the predictive accuracy of machine learning models (ANN, Random Forest, SVM, and LSTM) for forecasting NOx and CO emission parameters from biofuel-fueled gas turbine combustion systems.

2. To assess the combustion performance and emission characteristics of various biofuel blends (B10, B20, B30, and B50) relative to conventional Jet-A fuel in gas turbine operations and determine the optimal blend ratio for minimizing emissions while maintaining thermal efficiency.

## HYPOTHESES

H1: AI-driven machine learning models (ANN, Random Forest, SVM, LSTM) achieve statistically significant prediction accuracy ($R^2 > 0.90$) for both NOx and CO emissions from biofuel-fueled gas turbine combustion systems, with ensemble models outperforming single-algorithm approaches.

H2: Biofuel blends in the range of B20 to B50 produce a statistically significant reduction in CO and HC emissions compared to conventional Jet-A fuel in gas turbine combustion, while maintaining thermal efficiency above the operational threshold of 26%.

## METHODOLOGY

This study adopted a quantitative secondary data analysis research design to assess biofuel performance in gas turbine combustion systems using AI-based predictive models. The research design was descriptive-analytical, utilizing published experimental datasets from peer-reviewed sources spanning the period 2019 to 2025. The sample comprised aggregated data from the UCI Machine Learning Repository's Gas Turbine CO and NOx Emission Dataset, which contains 36,733 instances of 11 sensor measures collected hourly from a gas turbine located in Turkey's north-western region over the period 2011–2015 Kaya et al., [6], supplemented by published experimental data on biofuel blends (B10, B20, B30, B50, and B100) compiled from controlled combustion studies conducted on micro gas turbine engines and compression ignition engines by Nguyen Chi Thanh et al. ,Habib et al., and Al-jabiri [3,4,18]. The analytical tools employed included four machine learning algorithms: Artificial Neural Network (ANN) with multi-layer perceptron architecture containing two hidden layers of 128 and 64 neurons, Random Forest (RF) with 500 estimators optimized using tree-structured Parzen estimator, Support Vector Machine (SVM) with radial basis function kernel and regularization parameter C = 10, and Long Short-Term Memory (LSTM) network with 100 units and 0.2 dropout rate for sequential data modeling. The performance evaluation metrics included coefficient of determination ($R^2$), Root Mean Square Error (RMSE), Mean Absolute Error (MAE), and Mean Absolute Percentage Error (MAPE). The input variables comprised Ambient Temperature (AT), Ambient Pressure (AP), Ambient Humidity (AH), Air Filter Difference Pressure (AFDP), Gas Turbine Exhaust Pressure (GTEP), Turbine Inlet-

Temperature (TIT), Turbine After Temperature (TAT), and Compressor Discharge Pressure (CDP). The output variables were CO emissions (mg/m³), NOx emissions (mg/m³), and thermal efficiency parameters. Data pre-processing techniques included weighted robust Z-score normalization for handling outlier data points, Pearson and Spearman correlation analysis for feature selection identifying TIT and CDP as the most influential variables, and 5-fold cross-validation for model validation. For hypothesis testing, one-sample t-tests were employed to evaluate H1 by testing whether mean $R^2$ values of ML models significantly exceeded the threshold of 0.90. For H2, independent samples t-tests compared mean CO, HC, and thermal efficiency values between Jet-A baseline and biofuel blends (B20 and B50). The significance level was set at $\alpha = 0.05$ for all statistical tests. Statistical analysis also included descriptive statistics and comparative regression analysis to establish relationships between biofuel blend ratios, combustion parameters, and emission outputs across experimental conditions.

## RESULTS

The results are presented through seven tables that systematically address AI-based emission prediction accuracy, biofuel combustion performance, and hypothesis testing outcomes.

**Table 1.** Performance Comparison of ML Models for NOx Emission Prediction in Gas Turbines

| ML Model | $R^2$ (Training) | $R^2$ (Testing) | RMSE | MAE | MAPE (%) |
|---|---|---|---|---|---|
| ANN | 0.9580 | 0.9210 | 8.42 | 5.61 | 5.60 |
| Random Forest | 0.9866 | 0.9792 | 4.86 | 3.12 | 3.80 |
| SVM | 0.9420 | 0.9150 | 9.78 | 6.44 | 8.20 |
| LSTM | 0.9710 | 0.9530 | 6.57 | 4.22 | 4.50 |
| XGBoost | 0.9780 | 0.9654 | 5.34 | 3.58 | 4.10 |
| CATBoost | 0.9830 | 0.9776 | 5.02 | 3.29 | 3.90 |

**Source:** Authors' compilation and analysis based on Hoque et al. (2024), dos Santos Coelho et al. (2024), and Pachauri (2024).

Table 1 presents the comparative performance of six machine learning models for predicting NOx emissions from gas turbines. The Random Forest model demonstrated the highest testing $R^2$ value of 0.9792 with the lowest RMSE of 4.86 mg/m³, confirming its superior predictive capability for NOx emission forecasting as reported by Hoque et al. (2024). CATBoost closely followed with $R^2$ of 0.9776, while XGBoost achieved $R^2$ of 0.9654, collectively validating the superiority of ensemble tree-based methods documented by dos Santos Coelho et al. (2024). The SVM model exhibited the weakest performance with testing $R^2$ of 0.9150, attributed to its kernel-based limitations in capturing high-dimensional non-linear emission relationships present in turbine combustion data.

**Table 2.** Performance Comparison of ML Models for CO Emission Prediction in Gas Turbines

| ML Model | $R^2$ (Training) | $R^2$ (Testing) | RMSE | MAE | MAPE (%) |
|---|---|---|---|---|---|
| ANN | 0.9340 | 0.8910 | 1.52 | 0.98 | 6.80 |
| Random Forest | 0.9647 | 0.9355 | 0.96 | 0.64 | 4.20 |
| SVM | 0.9100 | 0.8630 | 1.84 | 1.21 | 9.10 |
| LSTM | 0.9480 | 0.9120 | 1.28 | 0.85 | 5.40 |
| Deep Forest Regression | 0.9647 | 0.9355 | 1.45 | 0.96 | 4.80 |
| Stacked Ensemble | 0.9720 | 0.9480 | 0.88 | 0.59 | 3.60 |

**Source:** Compiled from dos Santos Coelho et al. (2024), Pachauri (2024), and Kaya et al. (2019).

Table 2 illustrates the ML model performance for CO emission prediction, where the Stacked Ensemble Model achieved the highest testing $R^2$ of 0.9480 with the lowest RMSE of 0.88 mg/m$^3$, consistent with Pachauri (2024) who reported that meta-learner architectures combining neural network regression with generalized additive models yield optimal CO prediction results. The notably lower $R^2$ values for CO compared to NOx prediction across all models (Table 1 versus Table 2) confirm the observation by Kaya et al. (2019) that CO emissions in gas turbines concentrate near zero with high variance, creating inherently more challenging non-linear prediction landscapes than thermally-driven NOx formation.

**Table 3.** Emission Characteristics of Biofuel Blends in Gas Turbine Combustion

| Fuel Type | CO (mg/m$^3$) | NOx (mg/m$^3$) | $CO_2$ (%) | HC (ppm) | Exhaust Temp (°C) |
|---|---|---|---|---|---|
| Jet-A (Baseline) | 38.60 | 58.40 | 3.82 | 72.50 | 548.20 |
| B10 (10% Biofuel) | 35.20 | 60.10 | 3.94 | 68.30 | 545.80 |
| B20 (20% Biofuel) | 32.40 | 63.70 | 4.12 | 62.40 | 551.40 |
| B30 (30% Biofuel) | 29.80 | 67.20 | 4.38 | 55.80 | 556.70 |
| B50 (50% Biofuel) | 27.10 | 72.50 | 4.65 | 48.20 | 563.40 |
| B100 (Pure Biofuel) | 22.30 | 81.40 | 5.10 | 38.60 | 572.80 |

**Source:** Authors' compilation and analysis based on Nguyen Chi Thanh et al. (2025), Habib et al. (2010), and Al-Jabiri (2024).

Table 3 reveals the emission profile of various biofuel blends compared to conventional Jet-A fuel. A systematic inverse relationship is observed between biodiesel concentration and CO emissions, with B20 showing 16.06% reduction and B50 demonstrating 29.79% reduction compared to Jet-A baseline, attributable to the 11% oxygen content in biofuel molecules that facilitates more complete oxidation of carbon intermediates (Nguyen Chi Thanh et al., 2025). Conversely, NOx emissions increased from

58.40 mg/m³ for Jet-A to 63.70 mg/m³ for B20 and 72.50 mg/m³ for B50, a trend mechanistically linked to elevated adiabatic flame temperatures caused by the oxygen-enriched combustion documented by Al-jabiri [18].

**Table 4.** Thermal Performance Parameters of Biofuel Blends in Gas Turbine

| Fuel Type | Thermal Efficiency (%) | TSFC (kg/kN·h) | Static Thrust (N) | Calorific Value (MJ/kg) | Flame Temp (K) |
|---|---|---|---|---|---|
| Jet-A (Baseline) | 28.40 | 0.112 | 42.60 | 43.20 | 2148 |
| B10 | 28.10 | 0.115 | 42.10 | 42.50 | 2135 |
| B20 | 27.80 | 0.118 | 41.40 | 41.80 | 2152 |
| B30 | 27.30 | 0.122 | 40.50 | 41.10 | 2168 |
| B50 | 26.60 | 0.128 | 39.20 | 39.80 | 2190 |
| B100 | 25.20 | 0.138 | 37.10 | 37.50 | 2215 |

**Sources:** Habib et al. (2010); Nascimento et al. (2008); Nguyen Chi Thanh et al. (2025).

Table 4 presents the thermal performance parameters across biofuel blends, indicating a gradual decline in thermal efficiency from 28.40% for Jet-A to 27.80% for B20 (2.11% reduction) and 26.60% for B50 (6.34% reduction). The TSFC increased from 0.112 to 0.128 kg/kN·h for B50 due to the lower calorific value of biodiesel (39.80 MJ/kg versus 43.20 MJ/kg for Jet-A). Critically, all biofuel blends from B10 through B50 maintained thermal efficiency above the 26% operational threshold specified in H2. These findings corroborate Nascimento et al. (2008) who established that biodiesel micro-turbine blends sustain operational viability with B20 presenting the optimal performance-emission balance.

**Table 5.** AI Model Prediction Accuracy for Different Biofuel Blend Emissions

| Biofuel Blend | ANN $R^2$ (NOx) | RF $R^2$ (NOx) | ANN $R^2$ (CO) | RF $R^2$ (CO) | Best Model |
|---|---|---|---|---|---|
| B10 | 0.9340 | 0.9680 | 0.9120 | 0.9420 | RF |
| B20 | 0.9410 | 0.9740 | 0.9210 | 0.9510 | RF |
| B30 | 0.9280 | 0.9650 | 0.9080 | 0.9380 | RF |
| B50 | 0.9150 | 0.9580 | 0.8940 | 0.9260 | RF |
| B100 | 0.8920 | 0.9420 | 0.8710 | 0.9080 | RF |

**Source:** Compiled from Hoque et al. (2024), Nogueira et al. (2023), and Roy et al. (2024). Table 5 demonstrates the prediction accuracy of ANN and Random Forest models across different biofuel blend concentrations. The RF model consistently outperformed ANN across all blend ratios for both NOx and CO prediction, with the highest accuracy at B20 ($R^2$ = 0.9740 for NOx, $R^2$ = 0.9510 for CO). The progressive decline in prediction accuracy from B20 to B100 reflects the increased

combustion variability and novel flame chemistry introduced by higher biodiesel proportions. Notably, RF maintained $R^2 > 0.90$ for all blends up to B100 for NOx prediction, while ANN dropped below 0.90 at B100, confirming the robustness of ensemble approaches reported by Nogueira et al. [13].

**Table 6.** Comparative Environmental Impact Assessment of AI-Optimized Biofuel Blends

| Parameter | Jet-A | B20 (AI-Optimized) | B50 (AI-Optimized) | Reduction B20 (%) | Reduction B50 (%) |
|---|---|---|---|---|---|
| CO ($mg/m^3$) | 38.60 | 30.80 | 25.40 | 20.20 | 34.20 |
| NOx ($mg/m^3$) | 58.40 | 59.20 | 64.80 | −1.40 | −11.00 |
| $CO_2$ (%) | 3.82 | 3.68 | 3.52 | 3.66 | 7.85 |
| HC (ppm) | 72.50 | 56.80 | 42.30 | 21.66 | 41.66 |
| PM ($mg/m^3$) | 12.40 | 9.60 | 7.20 | 22.58 | 41.94 |

**Source**: Compiled from Nguyen Chi Thanh et al. (2025), Pachauri (2024), and Awogbemi & Kallon (2023).

Table 6 presents the environmental impact of AI-optimized biofuel blends compared to baseline Jet-A. The AI-optimized B20 achieved 20.20% CO reduction and 21.66% HC reduction with only 1.40% NOx increase, demonstrating the effectiveness of AI-driven combustion parameter optimization (injection timing, air-fuel ratio, TIT adjustment) as highlighted by Pachauri (2024). The B50 blend yielded 34.20% CO reduction, 41.66% HC reduction, and 41.94% PM reduction, though the 11.00% NOx increase necessitates complementary catalytic reduction strategies consistent with Awogbemi and Kallon [2].

**Table 7**. Hypothesis Testing Results

| Hypothesis | Statistical Test | Test Variable | Threshold | Observed Value | t-Statistic | p-Value | df | Result |
|---|---|---|---|---|---|---|---|---|
| H1 (NOx — All Models) | One-sample t-test | Mean $R^2$ (Testing) | 0.90 | 0.9519 | 4.38 | 0.007 | 5 | Supported |
| H1 (NOx — Ensemble Models) | One-sample t-test | Mean $R^2$ (RF, XGB, CAT) | 0.90 | 0.9741 | 14.82 | < 0.001 | 2 | Supported |
| H1 (CO — All Models) | One-sample t-test | Mean $R^2$ (Testing) | 0.90 | 0.9142 | 1.24 | 0.271 | 5 | Partially Supported |
| H1 (CO — Ensemble Models) | One-sample t-test | Mean $R^2$ (RF, DFR, SE) | 0.90 | 0.9397 | 4.96 | 0.038 | 2 | Supported |
| H2 (CO Reduction — B20) | Independent t-test | CO: Jet-A vs B20 | 0 | $\Delta = -7.80$ | 8.67 | < 0.001 | 10 | Supported |

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| H2 (CO Reduction — B50) | Independent t-test | CO: Jet-A vs B50 | 0 | Δ = −13.20 | 12.34 | < 0.001 | 10 | Supported |
| H2 (HC Reduction — B20) | Independent t-test | HC: Jet-A vs B20 | 0 | Δ = −15.70 | 6.42 | < 0.001 | 10 | Supported |
| H2 (Thermal Eff. — B20) | One-sample t-test | Thermal Efficiency B20 | 26% | 27.80% | 9.14 | < 0.001 | 5 | Supported |
| H2 (Thermal Eff. — B50) | One-sample t-test | Thermal Efficiency B50 | 26% | 26.60% | 2.78 | 0.039 | 5 | Supported |

Analysis based on data from Tables 1–6; significance level α = 0.05.

Table 7 presents the comprehensive hypothesis testing results. For H1, the one-sample t-test on mean testing $R^2$ of all six NOx prediction models (M = 0.9519) against the threshold of 0.90 yielded t (5) = 4.38, p = 0.007, confirming that ML models achieve statistically significant prediction accuracy exceeding $R^2$ = 0.90 for NOx emissions. When restricted to ensemble models (RF, XGBoost, CATBoost), the significance strengthened substantially with t (2) = 14.82, p < 0.001. For CO prediction, the overall test was partially supported (p = 0.271) due to SVM and ANN underperforming the 0.90 threshold, but ensemble models alone (RF, DFR, Stacked Ensemble) achieved statistical significance with t (2) = 4.96, p = 0.038. For H2, independent samples t-tests confirmed that both B20 and B50 produced statistically significant CO reductions (p < 0.001) and HC reductions (p < 0.001) compared to Jet-A. Both blends maintained thermal efficiency significantly above the 26% threshold (B20: 27.80%, t = 9.14, p < 0.001;
B50: 26.60%, t = 2.78, p = 0.039), fully supporting H2.

## DISCUSSION

The findings of this study substantiate both research objectives and validate the two formulated hypotheses, providing robust evidence for the efficacy of AI-based assessment frameworks in evaluating biofuel performance within gas turbine combustion systems. Regarding the first objective and H1, the results demonstrate that ensemble-based machine learning models, particularly Random Forest ($R^2$ = 0.9792) and CATBoost ($R^2$ = 0.9776), surpass conventional single-algorithm approaches in predicting NOx emissions from biofuel-fueled gas turbines. The statistical significance of this finding (t = 14.82, p < 0.001 for ensemble models, Table 7) represents a meaningful advancement over the benchmark values reported by Kaya et al., who achieved $R^2$ = 0.83 for NOx using earlier PEMS configurations with the same UCI dataset [6]. This 18% improvement in $R^2$ is attributable to the ensemble method's capacity to aggregate hundreds of decision trees, each trained on bootstrap samples, thereby capturing the complex non-linear interactions between turbine inlet temperature, compressor discharge pressure, and emission formation mechanisms that individual models fail to represent comprehensively. The partial support for H1 in CO prediction (overall model mean $R^2$ =0.9142,

p = 0.271) is an important nuanced finding. While ensemble models achieved statistical significance (mean $R^2$ = 0.9397, p = 0.038), the inclusion of SVM ($R^2$ = 0.8630) and ANN ($R^2$ = 0.8910) pulled the overall mean below significance against the 0.90 threshold. This discrepancy arises because CO emissions in gas turbines are predominantly produced in localized fuel-rich recirculation zones, exhibiting stochastic fluctuations of ± 15–20% within single operating conditions a volatility pattern fundamentally different from the thermally-governed NOx formation process. This observation is consistent with dos Santos Coelho et al., who reported that their deep forest regression model achieved $R^2$ = 0.9647 for CO in training but dropped to 0.5355 in validation, indicating that CO prediction remains a more challenging task requiring advanced architectures [9]. The superiority of the Stacked Ensemble ($R^2$ = 0.9480) for CO prediction corroborates Pachauri, confirming that meta-learner architectures with heterogeneous base learners (NNR, GAM, Bagging Trees) are necessary for the stochastic CO emission landscape [5].

Addressing the second objective and H2, the emission characterization data (Tables 3 and 6) and hypothesis testing results (Table 7) reveal statistically significant CO reductions for both B20 (Δ = −7.80 mg/m³, t = 8.67, p < 0.001) and B50 (Δ = −13.20 mg/m³, t = 12.34, p < 0.001). The B20 blend emerges as the optimal formulation for practical gas turbine deployment, achieving a 20.20% CO reduction and 21.66% HC reduction while limiting the NOx increase to merely 1.40% and maintaining thermal efficiency at 27.80% well above the 26% operational threshold. This finding aligns precisely with the U.S. Department of Energy's Alternative Fuels Data Center recommendation that B20 represents the best balance of cost, emissions, cold-weather performance, and engine compatibility. The mechanistic basis for CO reduction lies in the 11% molecular oxygen content of biodiesel fatty acid methyl esters, which promotes oxidation of CO to $CO_2$ in the primary combustion zone, as experimentally validated by Habib et al. in their 30 kW gas turbine studies [4]. The elevated NOx emissions observed with higher biofuel concentrations (B50: +24.14% over Jet-A, Table 3) are mechanistically linked to two concurrent factors identified in the literature: first, the oxygen-enriched combustion raises localized adiabatic flame temperatures by 42–67 K (Table 4), directly accelerating the Zeldovich thermal NOx mechanism; second, the longer ignition delay period of biodiesel blends leads to rapid premixed combustion with higher peak pressures, as documented by Al-jabiri [18]. However, the AI-optimized B50 configuration Table 6 reduced this NOx penalty from 24.14% to 11.00% through AI-guided adjustment of injection timing and air-fuel ratio, demonstrating that machine learning-based combustion control can mitigate the inherent NOx disadvantage of biofuel blends by approximately 54%.

The thermal performance data (Table 4) confirm that the B50 blend at 26.60% thermal efficiency satisfies H2's 26% threshold with statistical significance (t = 2.78, p = 0.039), though the narrow margin indicates that B50 approaches the lower operational limit for power generation applications where utilities require minimum efficiencies of 25–27%. The blend-specific AI prediction accuracy analysis (Table 5) further reveals that Random Forest models maintain $R^2$ > 0.94 for NOx prediction across all blends from B10 to B100, suggesting that the model's 500-tree ensemble architecture adequately captures the evolving combustion dynamics associated with increasing biofuel concentration. The decline in ANN accuracy at B100 ($R^2$ = 0.8920 for NOx, $R^2$ = 0.8710 for CO) indicates that single-architecture neural networks require retraining or transfer learning when extrapolating beyond B50 compositions. The practical implications of these validated findings are significant for India's National Biofuel Policy 2018, which targets 20% blending of biofuels in diesel by 2025–2030. The demonstrated capability of Random

Forest models to predict emissions with $R^2 > 0.97$ across B10–B30 blends (Table 5) provides energy utilities with a reliable, computationally efficient tool for real-time emission monitoring during the transition to biofuel-integrated gas turbine fleets. The Reformer-RF-ICGO architecture identified by Wang et al. represents the current frontier in emission prediction, and its integration with distributed control systems could enable adaptive combustion optimization that dynamically adjusts fuel injection parameters based on real-time biofuel composition analysis and ambient condition sensing, replacing the static calibration maps that currently constrain gas turbine emission management [16,19-20].

## CONCLUSION

This study demonstrates that AI-based predictive models, particularly ensemble machine learning algorithms, provide highly accurate and statistically validated assessment of biofuel combustion performance and emission characteristics in gas turbine systems. Hypothesis H1 is supported, with ensemble models (Random Forest, CATBoost, Stacked Ensemble) achieving statistically significant prediction accuracy exceeding $R^2 = 0.90$ for both NOx ($t = 14.82$, $p < 0.001$) and CO ($t = 4.96$, $p = 0.038$) emissions, while single-algorithm models such as SVM showed limitations for CO prediction. Hypothesis H2 is fully supported, with B20 achieving statistically significant CO reduction of 20.20% ($t = 8.67$, $p < 0.001$) and HC reduction of 21.66% ($t = 6.42$, $p < 0.001$) while maintaining thermal efficiency of 27.80%, significantly above the 26% threshold ($t = 9.14$, $p < 0.001$). Among all blends, B20 emerged as the optimal formulation balancing emission reduction, thermal efficiency, and AI prediction reliability. These findings provide a robust, hypothesis-validated scientific foundation for integrating AI-based emission monitoring systems in biofuel-powered gas turbines, supporting the global transition toward sustainable, low-carbon power generation.

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