



## AI-driven optimization of ethanol-powered internal combustion engines in alignment with multiple SDGs: A sustainable energy transition

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### ABSTRACT

With the escalating requirement for global sustainable energy solutions and the complexities linked with the complete transition to new technologies, internal combustion engines (ICEs) powered with biofuels like ethanol are gaining significance over time. However, problems linked to the performance and emissions of such ICEs necessitate accurate prediction and optimization. The study employed the integration of artificial neural networks (ANN) and multi-level historical design of response surface methodology (RSM) to address these challenges in alignment with the Sustainable Development Goals (SDGs). A single-cylinder spark ignition (SI) engine powered with ethanol-gasoline blends at different loads and speeds was used to gather data. Among six initially trained ANN models, the most efficient model with a regression coefficient ( $R^2$ ) of 0.9952 (training), 0.98579 (validation), 0.98847 (testing), and 0.99307 (overall) was employed to predict outputs such as brake power, brake specific fuel consumption (BSFC), brake thermal energy (BTE), concentration of carbon dioxide ( $\text{CO}_2$ ), carbon monoxide (CO), hydrocarbons (HC), and oxides of nitrogen  $\text{NO}_x$ . Predicted outputs were optimized by incorporating RSM. On implementing optimized conditions, it was observed that BP and BTE increased by 19.9%, and 29.8%, respectively. Additionally, CO, and HC emissions experienced substantial reductions of 28.1%, and 40.6%, respectively. This research can help engine producers and researchers make refined decisions and achieve improved performance and emissions. The study directly supports SDG 7, SDG 9, SDG 12, SDG 13, and SDG 17, which call for achieving affordable, clean energy, sustainable industrialization, responsible consumption, and production, taking action on climate change, and partnership to advance the SDGs as a whole respectively.

### Introduction

It is estimated that by 2050, there will be 9.2 billion people on the planet, with the transport industry potentially consuming over one-third of the world's energy and more than half of total oil production [1,2]. In line with the issues addressed by the Sustainable Development Goals (SDGs), this population upsurge and industrial expansion have resulted in the unavoidable depletion of conventional fuels and increasing threats to environmental sustainability, energy security, and economic stability. Alternative fuels such as biofuels and hydrogen for internal

combustion engines (ICEs) are thought to provide solutions to these problems [3–6]. Investigation of these alternative fuels directly promotes SDGs 7 (Affordable and Clean Energy) and 13 (Climate Action), which reinforce transitioning to sustainable and clean energy sources to address climate change. SDG 7 highlights the significance of switching from polluting and unsustainable energy sources to cleaner ones. Additionally, it assists in establishing a balance between addressing the urgent need to combat climate change, promoting economic growth, and fulfilling energy demands. [7–9]. However, the complete transition to new technologies encounters socio-technological obstacles and

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**Table 1**

Summary of researchers' work exploring techniques on SI engine performance and emissions with biofuel mixtures.

| Author Name and Reference | Fuel Blend                             | ANN | RSM | BP | BSFC | BTE | CO | CO <sub>2</sub> | HC | NO <sub>x</sub> |
|---------------------------|--|-----|-----|----|------|-----|----|-----------------|----|-----------------|
| Yücesu et al. [22]        | Gasoline, Ethanol, and Methanol        | ✓   | ✓   | ↑  | ↓    | –   | –  | –               | –  | –               |
| Simsek et al. [23]        | Gasoline, LPG, and Bio Gas             | –   | –   | –  | ↑    | ↑   | ↓  | ↓               | ↓  | ↑               |
| Najafi et al. [24]        | Gasoline, and Ethanol                  | ✓   | –   | ↑  | ↓    | ↑   | ↓  | ↑               | ↓  | ↑               |
| Uslu et al. [25]          | Gasoline and 1-amyI Alcohol            | ✓   | ✓   | –  | ↑    | ↑   | ↓  | –               | ↓  | ↓               |
| Barboza et al. [26]       | Gasoline hydrogen peroxide and ethanol | ✓   | ✓   | –  | –    | ↑   | ↓  | ↑               | ↓  | ↓               |
| Palani et al. [27]        | Gasoline, ethanol, n-butanol           | –   | ✓   | –  | ↑    | ↑   | ↓  | –               | ↓  | ↑               |
| Yusri et al. [28]         | Gasoline and secondary butyl alcohol   | –   | ✓   | ↑  | ↑    | ↑   | ↓  | ↑               | ↓  | ↓               |
| Kaliyaperumal et al. [29] | Gasoline and Gasohol/Hydrogen          | ✓   | –   | –  | ↑    | ↑   | ↓  | ↑               | ↓  | ↑               |
| Yaman et al. [30]         | Gasoline and 1-heptanol                | –   | ✓   | –  | ↑    | ↑   | ↓  | ↑               | ↓  | ↑               |

**Table 2**

E100 and E0's characteristics.

| Property   | Ethanol                          | Gasoline                       |
|--|----------------------------------|--------------------------------|
| Chemical Formula                                 | C <sub>2</sub> H <sub>5</sub> OH | C <sub>8</sub> H <sub>12</sub> |
| Composition (C, H, O) mass%                      | 52.17, 13.04, 34.78              | 87%, 13%, 0%                   |
| Calorific Value (MJ/kg)                          | 26.7                             | 46                             |
| Heat of evaporation (kJ/kg)                      | 904                              | 325                            |
| Stoichiometric A/F ratio                         | 9.0                              | 14.7                           |
| Oxygen content % mass                            | 34.8%                            | 0%                             |
| Density kg/m <sup>3</sup>                        | 789                              | 740                            |
| Flash Point (°C)                                 | 13                               | –43                            |
| Auto Ignition Temperature (°C)                   | 420                              | 270                            |
| Solubility in water (ml/100 ml H <sub>2</sub> O) | Infinitely soluble               | Infinitely soluble             |

**Table 3**

Test engine facets.

| Engine Parameter   | Value    |
|--|----------|
| Bore(mm)   | 68       |
| Stroke (mm)  | 45       |
| Displacement (cm <sup>3</sup> )                                  | 163      |
| Compression ratio  | 8.5:1    |
| Net power (kW/rpm)   | 3.6/3600 |
| Fuel tank capacity (Liters)                                      | 3.1      |
| Fuel consumption at constant rated power (Liter/hour) @ 3600 rpm | 1.4      |
| Engine Oil Capacity (Liters)                                     | 0.6      |

necessitates a significant investment. Hence, biofuel-powered internal combustion engines (ICEs) are expected to remain noteworthy [10–12]. Nevertheless, optimizing their parameters to comply with emissions regulations, ensure energy security, improve efficiency, and meet consumer expectations poses multifaceted challenges. The SGD 9 (Industry, Innovation, and Infrastructure) is aligned with these challenges, which focuses on sustainable industrialization, innovation, and infrastructure to empower environmental sustainability and economic growth [13–15]. Traditional methods involving precise instruments and costly experimentation are time-consuming. These issues are aligned with SDG 12 (Responsible Consumption and Production) [7,14,16]. Consequently, the development of substitute solutions is a pressing need that supports sustainable consumption and production practices. Computational modeling techniques have been used to identify the relationships between operating parameters and accurately predict numerous characteristics of internal combustion engines (ICEs), such as performance, combustion, and emissions [17]. Among these techniques, artificial neural networks (ANN) and response surface methodology (RSM) have emerged as prominent techniques that make accurate predictions and optimize by utilizing diverse input configurations, respectively [18–20]. Table 1 provides a summary of previous research conducted by various scholars employing different techniques for this purpose. An ANN efficiently handles numerical data with several variables that would be challenging otherwise. In contrast to conventional techniques, a well-trained neural network makes faster predictions, bypassing time-consuming and complex mathematical problem-solving as well as the

need for expensive and complex physical and computer models [21].

The performance of SI engines utilizing ethanol-methanol blends was determined by Kapusuz et al. [31]. The study shows that the mixture of 11% methanol and 1% ethanol by volume exhibited improved performance, yielding regression coefficients within the range of 0.931–0.990. Samet et al. [32] developed an ANN model to predict results for a diesel engine fueled with a diethyl ether blend up to 10%, achieving regression coefficients (R<sub>2</sub>) ranging from 0.964 to 0.9878 and mean relative error (MRE) values ranging from 0.51% to 4.8%. Khandal et al. [33] examined the performance of a diesel engine powered by a mixture of plastic pyrolysis oil, diesel, and ethanol by employing the ANN model. The ANN technique is also utilized by Shivakumar [34] to evaluate engine efficiency and emissions. The performance of the butanol-gasoline based SI engine was predicted by Liu et al. [35]. Moreover, Rezaei et al. [36], conducted a study and established that the ANN model showcased faster convergence and exceptional performance.

Table 1 showcases prior studies optimizing engines based on experimental data, rather than utilizing predicted data. In the present study, the ANN model efficiently predicted output values based on given inputs. These input-predicted output pairs were then optimized using the RSM technique. This integration significantly reduces the number of experimental runs. In scenarios where new, unseen input data is encountered, no longer a need to conduct expensive experiments to obtain corresponding outputs. Instead, the well-trained ANN model accurately predicts the required outputs and the RSM optimization process delivers optimal operating conditions for the engine. The research highlights how the ANN model's architecture influences performance. This methodology aids in identifying the most accurate and robust model for predicting engine operations. By considering a broader range of outputs, the research contributes to a more comprehensive understanding of the engine's operating parameters and opens new possibilities for optimizing engine operations.

The contribution of this research to achieving multiple SDGs simultaneously and fostering a sustainable and resilient future for the planet as a whole makes it distinctive. The integration of two cutting-edge computational techniques (ANN and multi-level RSM) to predict and optimize operations of the ethanol-powered engine offers a deeper comprehension of the complex interactions between fuel blends, engine performance, and environmental impact. This distinctive aspect of this study opens up exciting possibilities for dropping experimental runs and intricate mathematical modeling. The study represents a notable strive for affordable and clean energy, sustainable industrialization, responsible consumption and production, and climate action.

## Materials and methods

This section presents the preparation of fuel blends, experimental design for testing, ANN model development, and methods and definitions for RSM-based optimization.

### Formulation of fuel blends

In this study, ethanol was sourced from Shahmurad Ethanol Limited,

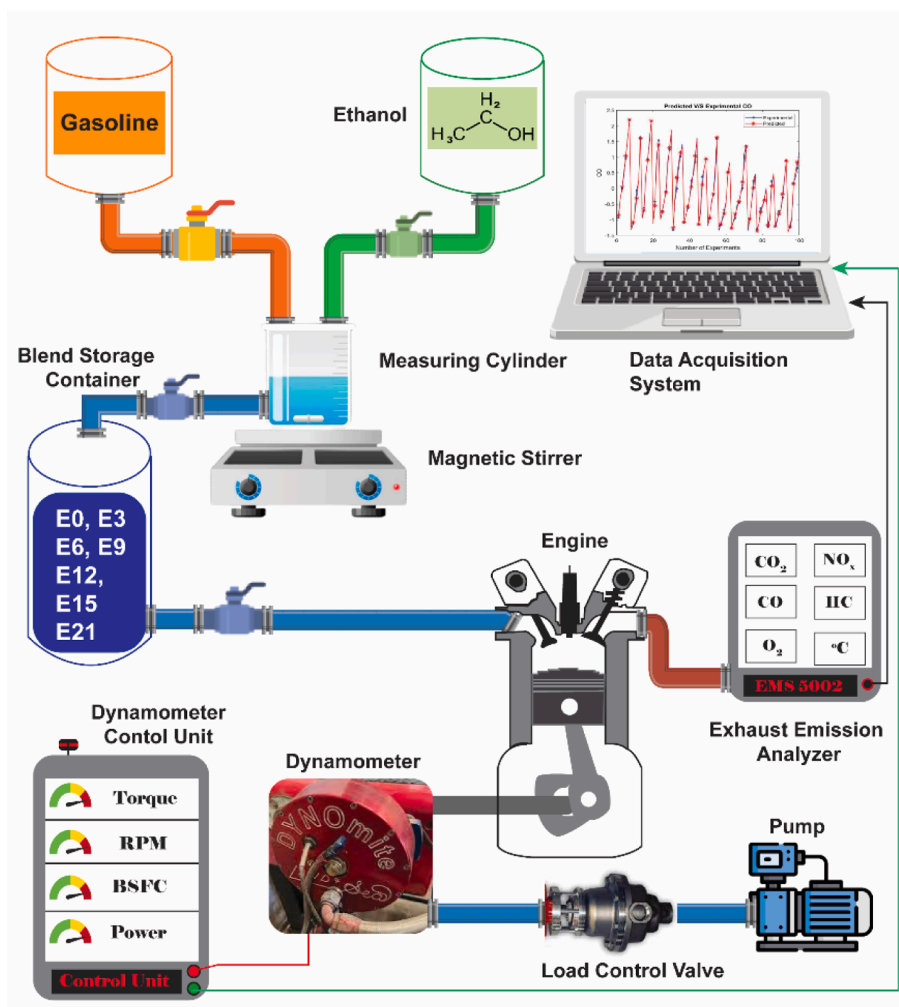


Fig. 1. The layout of the test rig and experimental configuration.

Table 4  
Comprehensive testing scheme.

| Factors                | Description                                 |
|------------------------|---|
| Fuel                   | E0, E3, E6, E9, E12, E15, E21               |
| Loads                  | 50% and 100%                                |
| Speed range            | 1300–3700 RPM (with an increase of 300 rpm) |
| Performance Parameters | Torque, BP, BSFC and BTE                    |
| Emission Parameters    | CO <sub>2</sub> , CO, HC, NO <sub>x</sub>   |
| Ambient Temperature    | 27°C  |
| Atmospheric Pressure   | 1 atm                                       |

Table 5  
Specification of ANN models structures.

| Specifications   | Description  |
|--|--|
| ANN-1HL-9 N, ANN-1HL-11, ANN-1HL-15 N, ANN-2HL-9 N, ANN-2HL-11 N, ANN-2HL-15 N | The digits designate the number of hidden layers and neurons in the hidden layer |
| Training Algorithm   | Levenberg-Marquardt  |
| Epochs   | 100  |
| In-Training Performance Plots  | Regression and error histograms  |
| Post-training performance parameters   | MRE, RMSE, and R <sup>2</sup>  |
| Data Distribution  | 70% Training, 15% (Testing) and 15% (validation)                                 |
| Stopping Criteria  | Minimization of mean square error  |

a principal ethanol producer in Pakistan, and gasoline was obtained from Pakistan State Oil (PSO). Gasoline was marked as the reference for all the blends. Table 2 outlines ethanol (E100) and gasoline (E0) attributes.

The ethanol was added to gasoline at various concentrations of 0%, 3%, 6%, 9%, 12%, 15%, 18%, and 21% by volume, resulting in fuel blends represented as E3, E6, E9, E12, E15, E18, and E21 respectively. Blends were continuously stirred using a magnetic stirrer for 15 min to ensure a fully homogeneous mixture of the fuels.

Experimental setup and testing plan

An air-cooled spark ignition (SI) engine with an overhead valve was used during this study. Table 3 presents the qualifications of the test engine.

For testing, the engine was connected through a mild steel shaft to a 7-inch Dynamite dynamometer, with a water-brake system. By utilizing EMS-5002 analyzer, emissions were quantified. A 500-ml measuring cylinder (0.5 ml grade) was used to measure fuel flow. The working fluid was water for applying loads through the piping system. The experimental setup schematic is illustrated in Fig. 1.

Data acquisition was accomplished using a system with signal conditioning circuitry to convert sensor signals into digital data. DYNO-MAX software measured engine performance, while the emissions measurement system covered a wide range of engine speeds for comprehensive data collection in different operating conditions. The

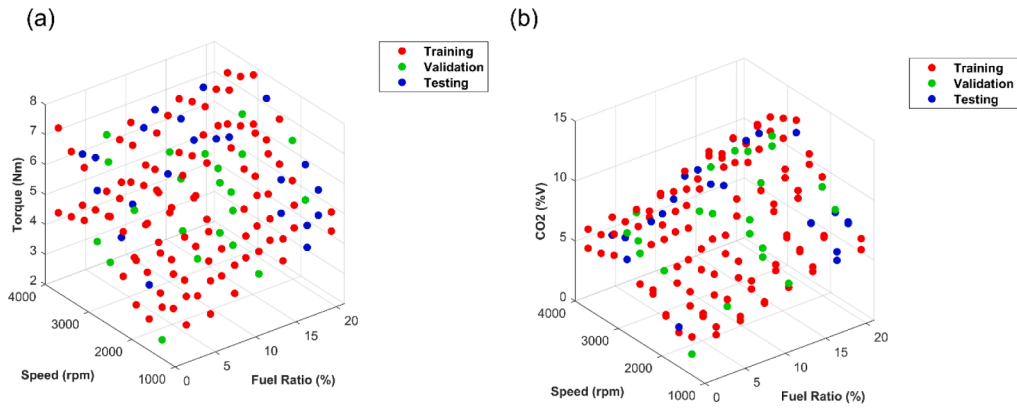


Fig. 2. Random distribution of data set for (a) torque and (b) CO<sub>2</sub>.

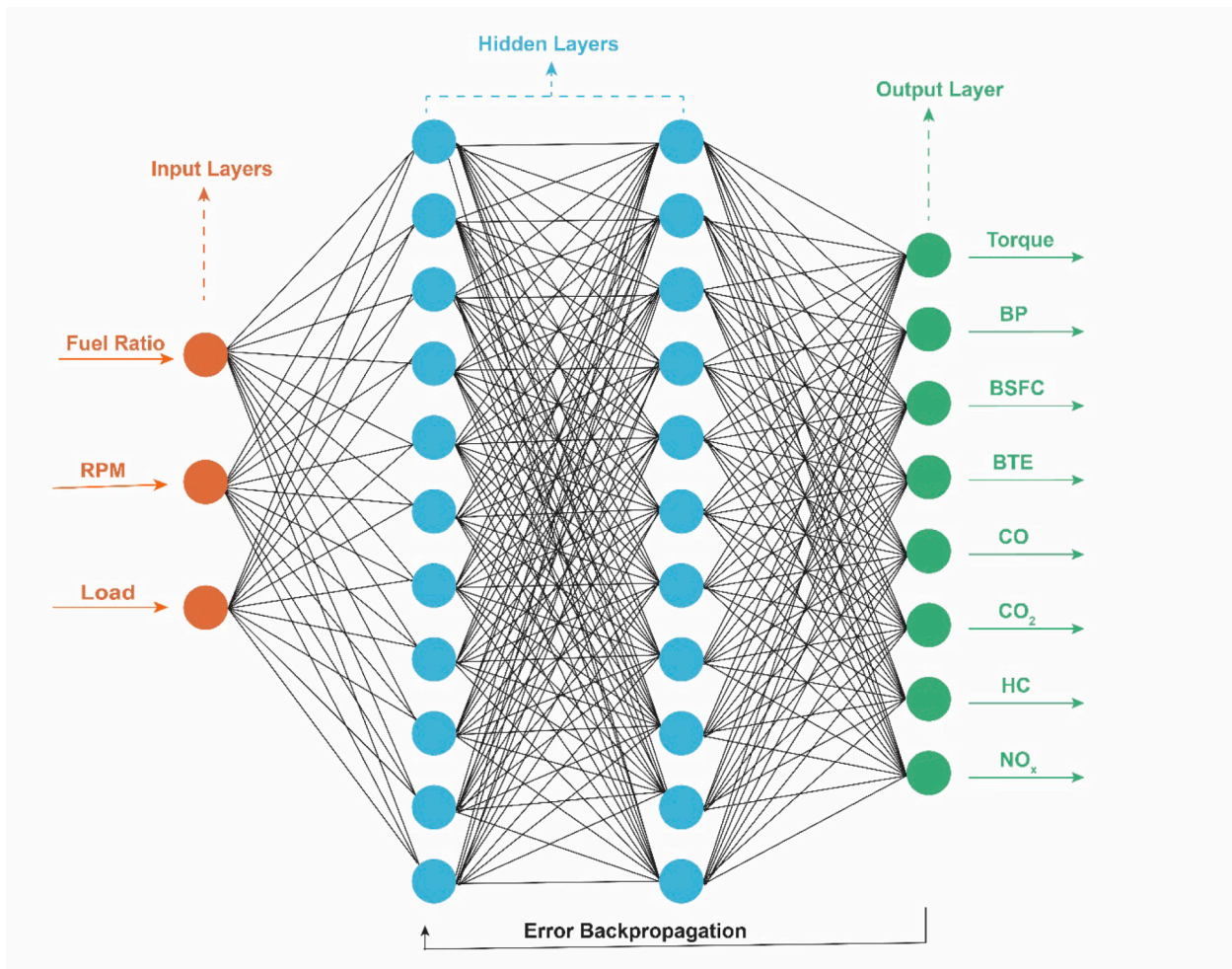


Fig. 3. Structure of ANN-2HL-11 N.

engine testing involved no structural modifications. The engine speed was progressively increased from 1300 rpm to 3700 rpm in 300 rpm increments, with 50% and 100% loads applied. The steady-state operation was achieved using gasoline as the initial fuel. Blends were prepared shortly before testing to maintain consistency and prevent moisture accumulation. Three repetitions of each test were executed to gauge its accuracy, and average readings were recorded. Dynamite 2010 software accurately recorded speed and load values. Fuel consumption,

BSFC, BP, and BTE were calculated using heating values and density. Table 4 summarizes the testing scheme. (See Fig. 1.).

*Development of ANN models*

Using MATLAB software for formulating and executing ANN models offers several strengths and benefits [37]. The gathered dataset from the data acquisition system includes fuel ratio, load, RPM, torque, BP, BSFC,



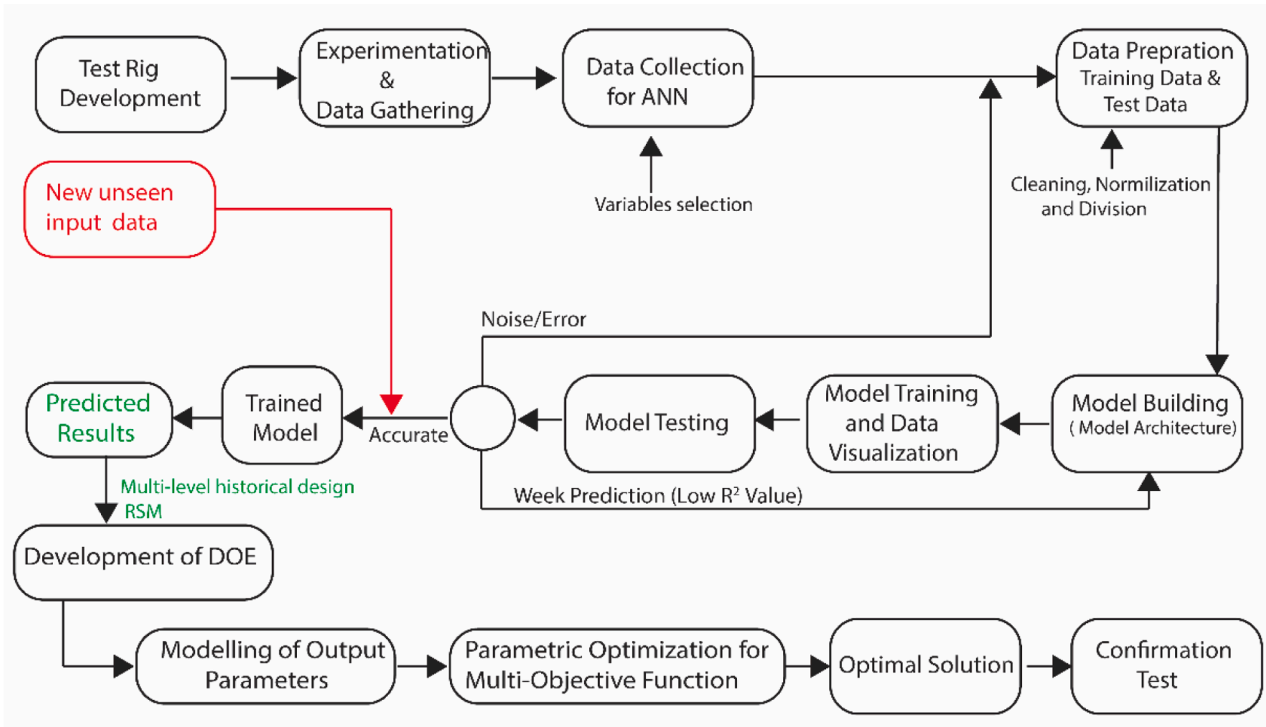


Fig. 4. Flow chart for the methodology of ANN-integrated RSM.

Table 6  
Model defining parameters.

| Numeric Factor | Units      | Subtype | Low Level  | High Level | Mean | Std. Dev. |       |
|----------------|------------|---------|------------|------------|------|-----------|-------|
| A              | Load       | %       | Continuous | 50         | 100  | 75        | 25.09 |
| B              | Speed      | rpm     | Continuous | 1300       | 3700 | 2500      | 777.3 |
| C              | Fuel Ratio | %       | Continuous | 0          | 21   | 10.50     | 6.69  |

Table 7  
R<sup>2</sup> for responses given by ANOVA.

| Response        | Adjusted R <sup>2</sup> | Predicted R <sup>2</sup> |
|-----------------|-------------------------|--------------------------|
| Torque          | 0.9379                  | 0.9332                   |
| BP              | 0.9797                  | 0.9774                   |
| BTE             | 0.7220                  | 0.7107                   |
| BSFC            | 0.6585                  | 0.6437                   |
| CO              | 0.9646                  | 0.9624                   |
| CO <sub>2</sub> | 0.7929                  | 0.7851                   |
| HC              | 0.9255                  | 0.9188                   |
| NO <sub>x</sub> | 0.9730                  | 0.9707                   |

Table 8  
P-values of model terms.

| Response        | A       | B       | C       | AB      | AC      | BC      |
|-----------------|---------|---------|---------|---------|---------|---------|
| Torque          | <0.0001 | <0.0001 | <0.0001 | 0.0095  | 0.0104  | <0.0001 |
| BP              | <0.0001 | <0.0001 | <0.0001 | <0.0001 | 0.8123  | <0.0001 |
| BTE             | <0.0001 | <0.0001 | 0.0073  | -       | -       | -       |
| BSFC            | <0.0001 | <0.0001 | 0.0196  | -       | -       | -       |
| CO              | <0.0001 | <0.0001 | <0.0001 | <0.0001 | <0.0001 | 0.6472  |
| CO <sub>2</sub> | <0.0001 | <0.0001 | <0.0001 | -       | -       | -       |
| HC              | <0.0001 | <0.0001 | <0.0001 | 0.041   | <0.0001 | 0.0187  |
| NO <sub>x</sub> | <0.0001 | <0.0001 | <0.0001 | 0.5922  | <0.0001 | 0.0002  |

A = Fuel ratio B = Engine load C = RPM

BTE, CO, CO<sub>2</sub>, HC, and NO<sub>x</sub> concentration. With a standard deviation of 1 and a mean of 0, the dataset was transformed by executing the ‘zscore’ argument in the z-score normalization. It ensures that all input features have equal weights during training. The transformation can shift the original range of values to include negative values or values greater than the original maximum. Z score for a data point is given by equation (1).

$$Z = \frac{(X - \mu)}{\sigma} \tag{1}$$

where X is the original value, μ is the mean of the data, and σ is the standard deviation. The connectivity and structure of an ANN model are dictated by its architecture [38,39]. Table 5 outlines the initial six different structures that were established and trained in the study. The 144 sets of experimental data were segregated into three distinct groups in this study. To facilitate the random selection of data points, the ‘divideind’ function was utilized to divide the data as 70% (100/144) for training, 15% (22/144) for validation, and 15% (22/144) for testing. To ensure an unbiased evaluation of the model’s performance and the trained model’s generalizability, the data must be carefully divided into these sets. The random distribution of the data set for torque and CO<sub>2</sub> is shown in Fig. 2. The trainlm function was employed for training, signifying the use of the Levenberg-Marquardt algorithm [40]. This algorithm empowers the effective handling of non-linear problems and rapid convergence by combining the benefits of the Gauss-Newton and

**Table 9**  
Performance metrics of ANN structures for each output.

| Output          | Performance Parameters | ANN Models Nomenclature |                |                |                 |                 |                |
|-----------------|------------------------|-------------------------|----------------|----------------|-----------------|-----------------|----------------|
|                 |                        | ANN-1HL-9 N             | ANN-1HL-11 N   | ANN-1HL-15 N   | ANN-2HL-9 N     | ANN-2HL-11 N    | ANN-2HL-15 N   |
| Torque          | R <sup>2</sup>         | 0.99292                 | 0.99415        | 0.99554        | 0.99560         | <b>0.99594</b>  | 0.99537        |
|                 | RMSE                   | 0.11553                 | 0.10089        | 0.09539        | 0.09821         | 0.09177         | <b>0.08847</b> |
|                 | MRE                    | -0.03516                | -0.02924       | -0.01398       | -0.01616        | <b>-0.03198</b> | -0.00464       |
| BP              | R <sup>2</sup>         | 0.99292                 | 0.99415        | 0.99554        | 0.99560         | <b>0.99594</b>  | 0.99537        |
|                 | RMSE                   | 0.11553                 | 0.10089        | 0.09539        | 0.09821         | <b>0.07177</b>  | 0.08847        |
|                 | MRE                    | -0.03516                | -0.01924       | -0.01398       | -0.01616        | <b>-0.03198</b> | -0.00464       |
| BSFC            | R <sup>2</sup>         | 0.99526                 | 0.99484        | 0.99524        | 0.99565         | <b>0.99596</b>  | 0.99541        |
|                 | RMSE                   | 1.79753                 | <b>1.67847</b> | 1.77320        | 1.79918         | 1.81497         | 1.68845        |
|                 | MRE                    | 0.11166                 | 0.00143        | -0.10810       | 0.17326         | <b>-0.80373</b> | 0.83854        |
| BTE             | R <sup>2</sup>         | 0.99373                 | 0.99065        | 0.99234        | 0.99383         | <b>0.99456</b>  | 0.99193        |
|                 | RMSE                   | 0.11524                 | 0.13483        | 0.12218        | 0.11056         | <b>0.10001</b>  | 0.12263        |
|                 | MRE                    | 0.40082                 | 0.36798        | -0.04032       | 0.44777         | <b>-0.13693</b> | 0.46470        |
| CO              | R                      | 0.99024                 | 0.99391        | 0.99460        | 0.99389         | <b>0.99653</b>  | 0.99406        |
|                 | RMSE                   | 0.14089                 | 0.11364        | <b>0.09876</b> | 0.10496         | 0.09897         | 0.09984        |
|                 | MRE                    | 0.86602                 | 0.61949        | -0.32298       | <b>-0.71277</b> | -0.27307        | -0.19510       |
| CO <sub>2</sub> | R <sup>2</sup>         | 0.98600                 | 0.98872        | 0.98925        | 0.99211         | <b>0.99504</b>  | 0.98386        |
|                 | RMSE                   | 0.16756                 | 0.14854        | 0.12987        | 0.13083         | 0.14154         | <b>0.11318</b> |
|                 | MRE                    | 0.65879                 | 0.37526        | 0.29761        | 0.43750         | <b>0.03063</b>  | 0.46725        |
| HC              | R <sup>2</sup>         | 0.99353                 | 0.98812        | 0.99432        | 0.99606         | <b>0.99709</b>  | 0.99318        |
|                 | RMSE                   | 0.11490                 | 0.14961        | 0.10801        | 0.08963         | <b>0.07541</b>  | 0.10987        |
|                 | MRE                    | 0.00968                 | 0.02983        | 0.06622        | <b>-0.02307</b> | 0.02929         | 0.03305        |
| NO <sub>x</sub> | R <sup>2</sup>         | 0.99507                 | 0.99501        | 0.99589        | 0.99587         | <b>0.99669</b>  | 0.99001        |
|                 | RMSE                   | 0.09964                 | 0.10013        | 0.09327        | 0.08748         | <b>0.07533</b>  | 0.08378        |
|                 | MRE                    | 0.15185                 | 0.14952        | <b>0.03383</b> | 0.20429         | 0.17002         | 0.26562        |

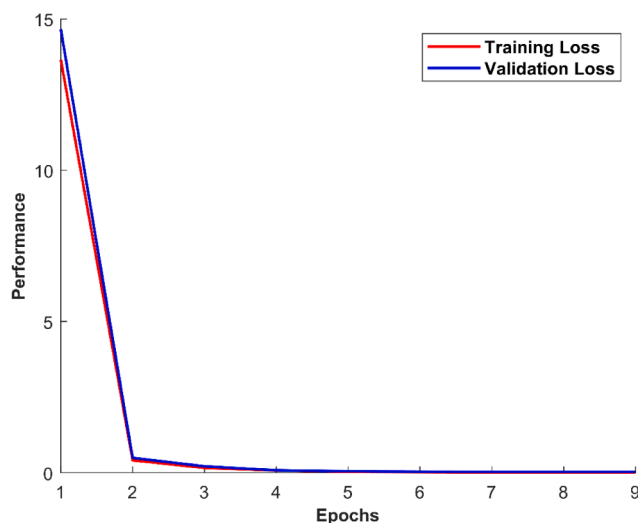


Fig. 5. Learning curves of the ANN-2HL-11 N model.

gradient descent methods. The ReLU (Rectified Linear Unit) activation function was employed, while sigmoid and tanh are also commonly used for similar problems [25,41–43]. Fig. 3 presents the structure of an ANN model consisting of two hidden layers with 11 neurons in each layer. A loss function was employed to compute the prediction error. The error was then propagated backward through the network by executing the backpropagation algorithm. Weights and biases were adjusted based on the gradient of the loss function concerning these parameters.

The adjusted weights and biases were then updated in each iteration using the optimization algorithm Adam. RMSprop is also well known [40,44]. By computing performance metrics such as R<sup>2</sup> (coefficient of determination), MSE, and RMSE, the consistency and precision of the models were quantified. An ANN model with a complex structure starts to memorize the training data instead of learning patterns (overfitting), and an ANN model with a structure that is not complex enough to capture the underlying pattern in the data leads to underfitting. Both problems have a negative influence on performance. In this study,

learning curves are plotted to check whether the model is overfitted, underfit, or a good fit. Once the ANN model was acceptable, engine performance and emissions were forecasted for unobserved data. By comparing the forecasted results with experimental values, the model’s dependability was confirmed.

*RSM methodology approach*

The current study is aimed at utilizing an ANN model to predict the optimal ethanol ratio, engine load, and speed and to attain efficient performance and reduced emissions. To accomplish this, the study incorporates RSM through Design-Expert version 13 was used for defining the multi-level historical design. Fuel ratio, engine load, and RPM were chosen as continuous numeric factors, while ANN estimated values of torque, BP, BTE, BSFC, CO, CO<sub>2</sub>, HC, and NO<sub>x</sub> were nominated as response variables. Fig. 4 presents a graphical understanding of the innovative methodology for this integration. The model-defining parameters are listed in Table 6.

The model attributes were evaluated by applying analysis of variance (ANOVA). A significance benchmark of a p-value less than 0.05 was used. Given the null hypothesis’s validity, the p-value signifies the probability of seeing test results as extreme as the observed ones. [25,45–47]. The ratio of squared deviations to individual sums of squares (SOS) was employed to compute the percentage contribution (PC%) of each model term. The F-value, a test statistic in ANOVA, specifies the overall worth of mean differences between groups. A large F-value suggests significant differences among group means if it exceeds the critical value [28].

The predicted R<sup>2</sup>, a reasonable agreement between the predicted and adjusted R<sup>2</sup>, and the p-value determine the selection of an appropriate model. R<sup>2</sup> values close to 1 specify a perfect linear curve. R<sup>2</sup> values from the ANOVA test are listed in Table 7, signifying good model fit and agreement with experimental data.

Table 8 provides insights into the significance of factors in the responses based on their corresponding p-values. At 95% confidence level, the study was carried out. By analyzing the p-values presented in Table 8, it becomes evident that the ethanol ratio, engine speed, and load have significant effects on all the responses.

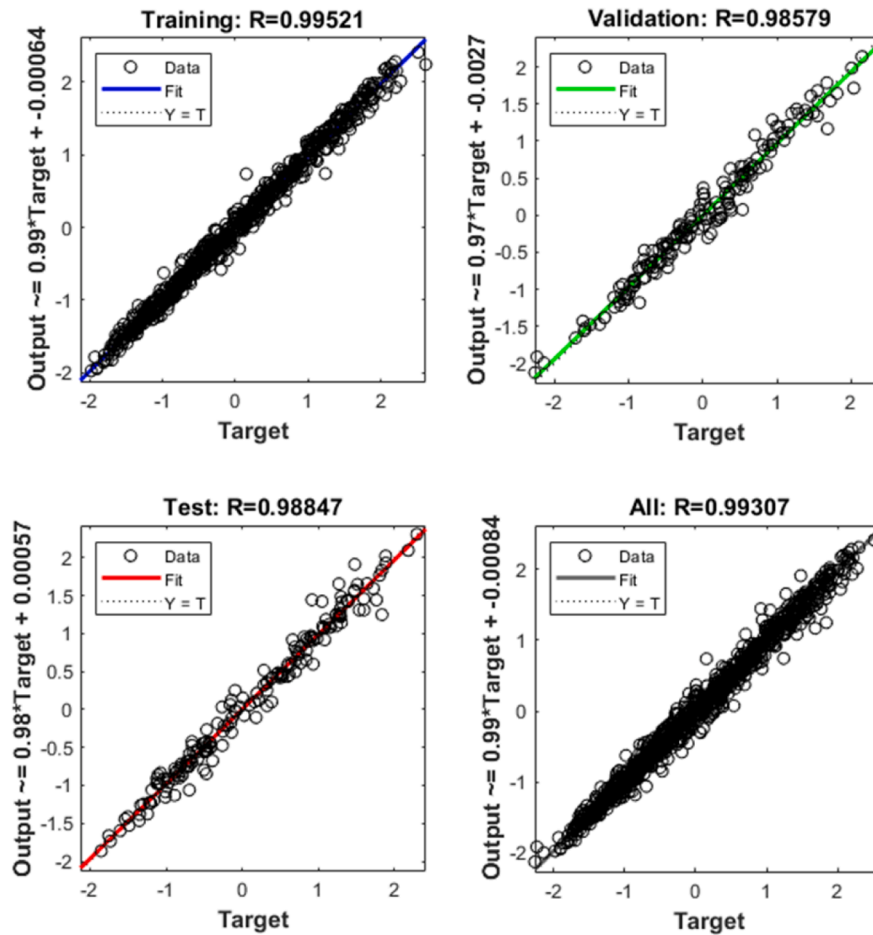


Fig. 6. Regression plots of the ANN-2HL-15 N model.

### 3 Results and discussions

This section presents the performance results of the ANNMs (ANN models), the prediction outcomes derived from the trained model, and the optimized results achieved using RSM.

#### Annms performance results

The ability of an ANN model to capture the complex relationships in the data has a significant dependence on the number of hidden layers and neurons. An ANN model with a complex structure starts to memorize the training data instead of learning patterns (overfitting), and an ANN model with a structure that is not complex enough to capture the underlying pattern in the data leads to underfitting. Both problems have a negative influence on performance. Table 9 presents three key metrics to evaluate each model's performance. The bold values are desired values, aiding in identifying the best-performing model.

Learning curves are shown in Fig. 5 which shows moderately high initial training and validation loss. The loss steadily declines and reaches a plateau when more training and validation instances are added.

A well-fitted model is indicated by the proximity of training and validation losses, with validation somewhat greater. This result emphasizes the significance of finding the right balance between model complexity and the capacity to generalize patterns from the data, avoiding both overfitting and underfitting and ultimately resulting in enhanced performance. Based on the regression plot, shown in Fig. 6 data points tend to cluster around the diagonal line and the ANN-2HL-11 N model achieves high R values of 0.99521 (training), 0.98579

(validation), 0.98847 (testing), and 0.99307 overall. This shows that the ANN-2HL-11 N model accurately captures underlying patterns and relationships, which reinforces its performance.

Predicted outputs were plotted against experimental values to thoroughly evaluate the performance and accuracy of the trained model. In Fig. 7(a) the model's performance throughout the training process is assessed for torque. These randomly selected 100 data points are the part of training set which is 70% (100/144) of the available dataset. The focus is on the relative position of predicted and experimental values of each experiment. Each experiment was performed for a different set of conditions. Therefore, there is no physical relationship between the variable values and the increasing number of experiments in this figure. The negative values of torque that were initially below the mean of the dataset are the result of Z-score normalization. Instead of focusing on the absolute values themselves, this shift towards negative values is more about the relative positions and distributions of the normalized data. The predicted and experimental values of torque for each experiment are closely located in Fig. 7 (a) which is graphical evidence of the performance metrics of ANN-2HL-11 N presented in Table 9. Once the ANN model was fully trained, Fig. 7 (b), displays the actual predicted and experimental values following reverse normalization. The entire data set of torque is clustered along a diagonal line (45 degrees). Fig. 7(c and d) presents similar trends for BP. Performance for BSFC, BTE, and emissions is assessed in Figs. 8, 9, and 10 respectively.

In these plots, the negative values for the BP, BTE, BSFC, and emissions are not interpreted as practically or physically negative values. Instead, they show how the normalized data points are positioned about the dataset's original mean. It is important to note that these plots aim to

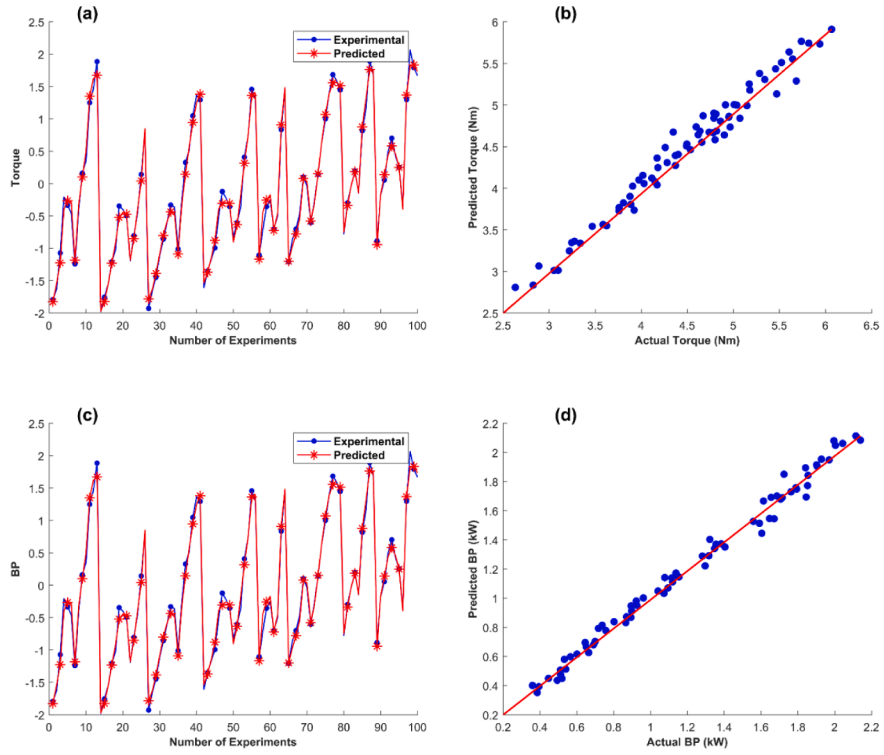


Fig. 7. Predicted values in comparison with experimental values of (a) normalized, and (b) actual torque dataset and, (c) normalized and (d) actual BP dataset.

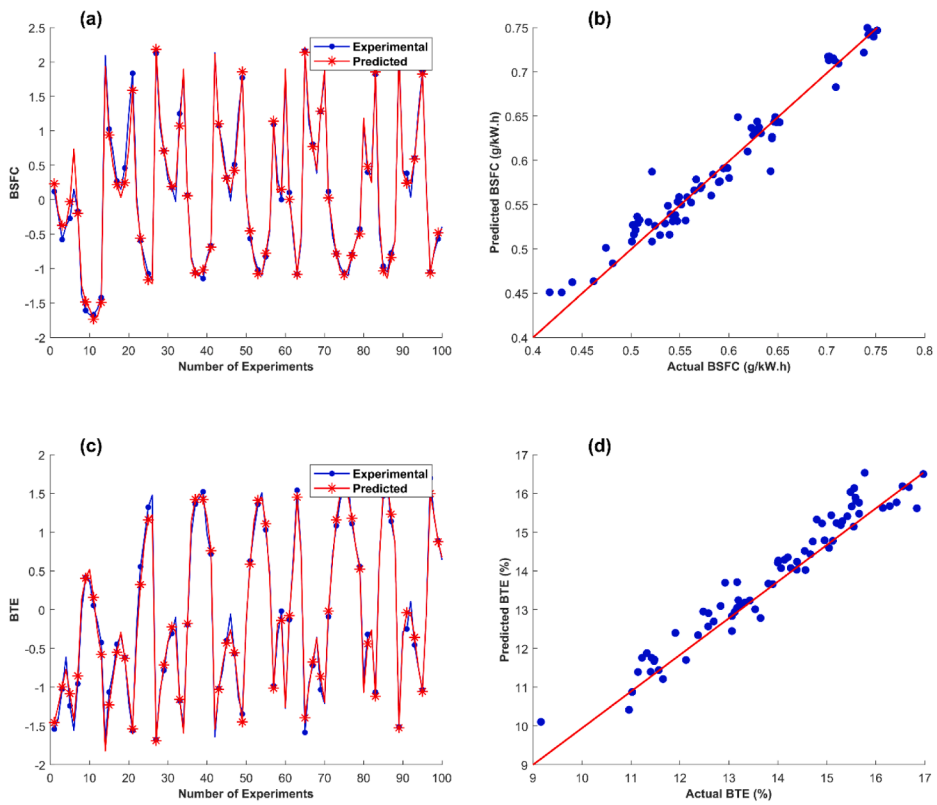


Fig. 8. Predicted values in comparison with experimental values of (a) normalized and (b) actual BSFC dataset, and (c) normalized, and (d) actual BTE dataset.



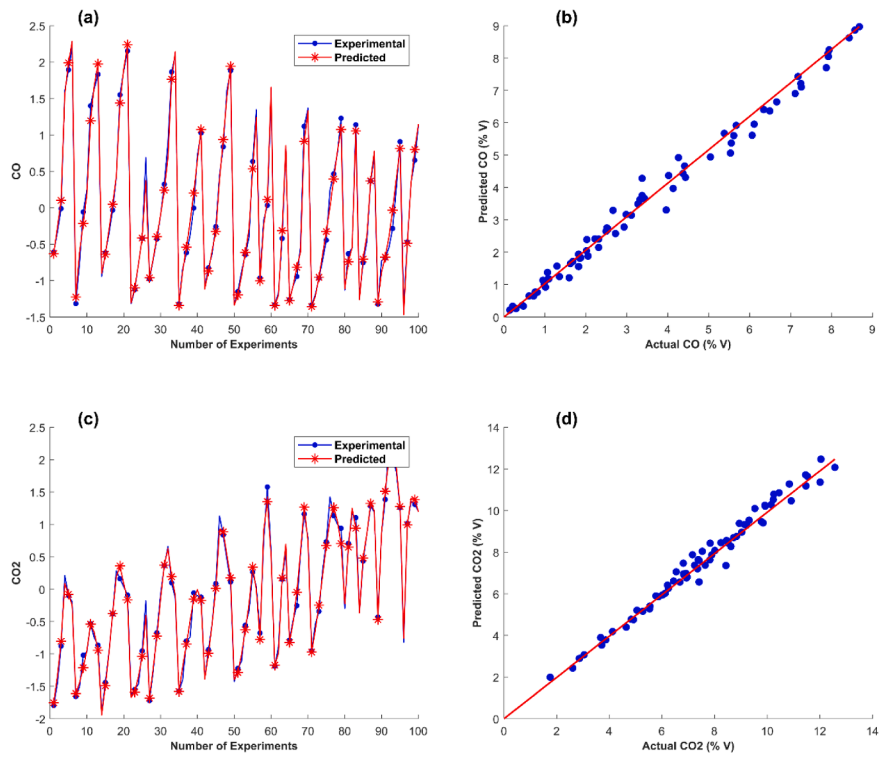


Fig. 9. Predicted values in comparison with experimental values of (a) normalized and (b) actual CO dataset, and (c) normalized, and (d) actual CO<sub>2</sub> dataset.

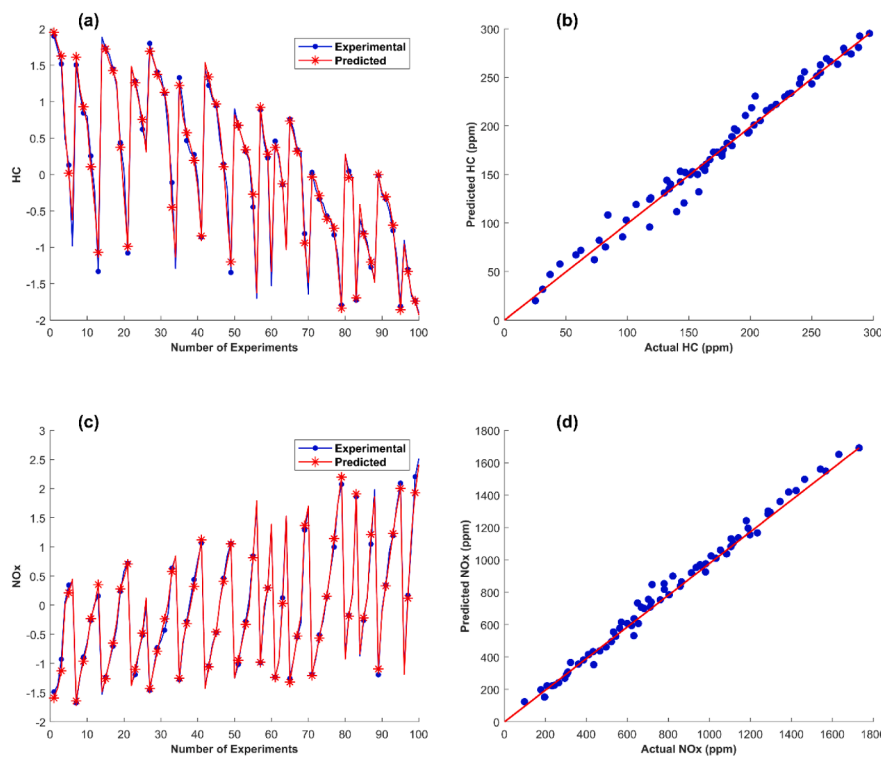
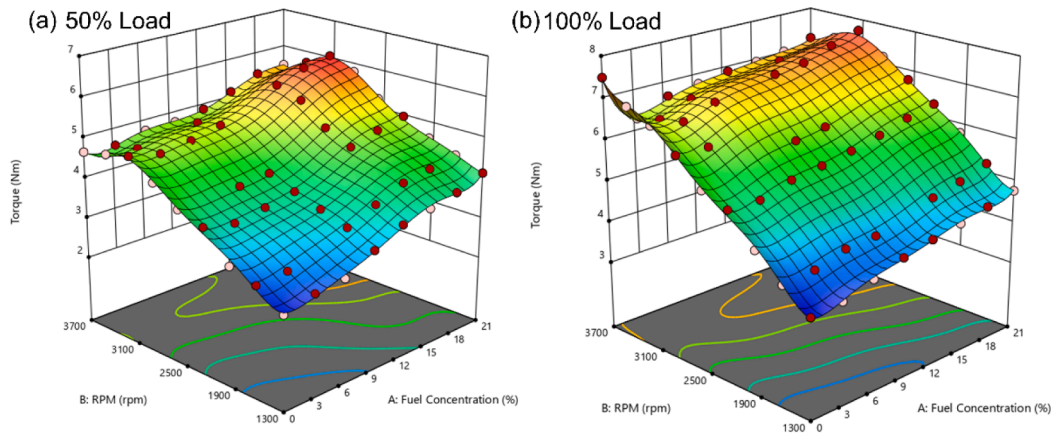


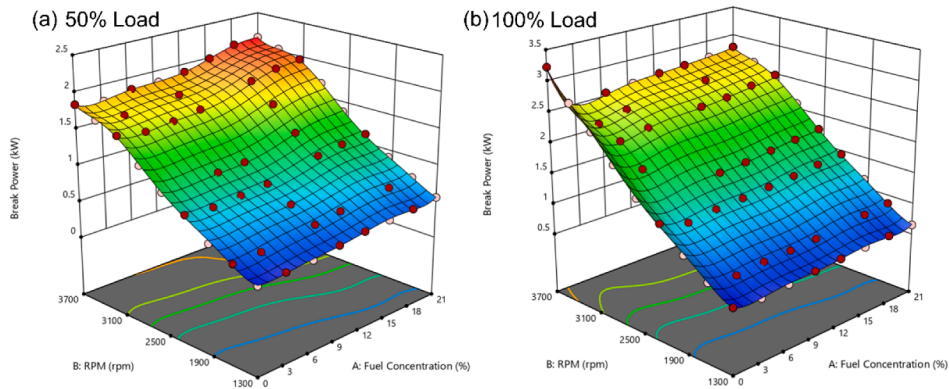
Fig. 10. Predicted values in comparison with experimental values of (a) normalized, and (b) actual HC dataset, and (c) normalized, and (d) actual NO<sub>x</sub> dataset.

**Table 10**  
Setup for optimization.

| Variable              | Optimization Criteria | Lower Limit | Upper Limit | Importance | Lower Weight | Upper Weight |
|-----------------------|-----------------------|-------------|-------------|------------|--------------|--------------|
| A: Fuel Concentration | is in range           | 0           | 21          | 3          | 1            | 1            |
| B: Load               | is in range           | 50          | 100         | 3          | 1            | 1            |
| C: RPM                | is in range           | 1300        | 3700        | 3          | 1            | 1            |
| Torque                | is in range           | 2.631       | 7.71142     | 3          | 1            | 1            |
| Brake Power           | maximize              | 0.35863     | 3.22758     | 3          | 1            | 1            |
| BSFC                  | minimize              | 0.30895     | 0.75138     | 3          | 1            | 1            |
| BE                    | maximize              | 9.15977     | 22.4894     | 3          | 1            | 1            |
| CO                    | is in range           | 0.0707      | 8.68        | 3          | 1            | 1            |
| CO <sub>2</sub>       | is in range           | 1.75        | 12.57       | 3          | 1            | 1            |
| HC                    | minimize              | 18.53       | 297         | 3          | 1            | 1            |
| NOx                   | is in range           | 97          | 1911.86     | 3          | 1            | 1            |



**Fig. 11.** Surface analysis of torque at (a) 50% load and at (b) 100% load.



**Fig. 12.** Surface analysis of BP at (a) 50% load and at (b) 100% load.

highlight the predictive model’s consistency in capturing trends and overall behavior. The close alignment between predicted and experimental values within the expected error range reaffirms the effectiveness of the model.

*Rsm-based optimization results*

To optimize the engine, BSFC, emissions, BTE, and BP were to be minimized and maximized while keeping all study factors within-range criterion. Table 10 demonstrates the defined limitations and optimization arrangement. Optimal model fitting and interpretation of the results depends on “Weight” and “Importance” in RSM. The weight allows for proper consideration of the variability and reliability of experimental data, while the importance helps identify the critical factors driving the

response variable. By providing valuable insights into the relationship between factors and responses, they contribute to the robustness and effectiveness of the RSM analysis.

In Fig. 11, the engine demonstrates lower torque output at 1300 rpm, attributed to reduced power generation at lower speeds, known as the “low-end torque” region. As RPM increases beyond this range for all fuel blends in the study, torque output consistently rises. It is attributed to enhanced energy input and output due to the faster burning of fuel at higher speeds [48,49]. At 100% load (Fig. 11(b)), the engine reaches its peak torque region around 3100 rpm, resulting in a 7.7 Nm for E21. However, beyond this region, as RPM continues to increase, torque output declines, known as the “fall-off” or “decline” in torque. As the engine encounters limitations in terms of intake flow, cylinder filling, frictional losses, valvetrain operation, exhaust backpressure, and

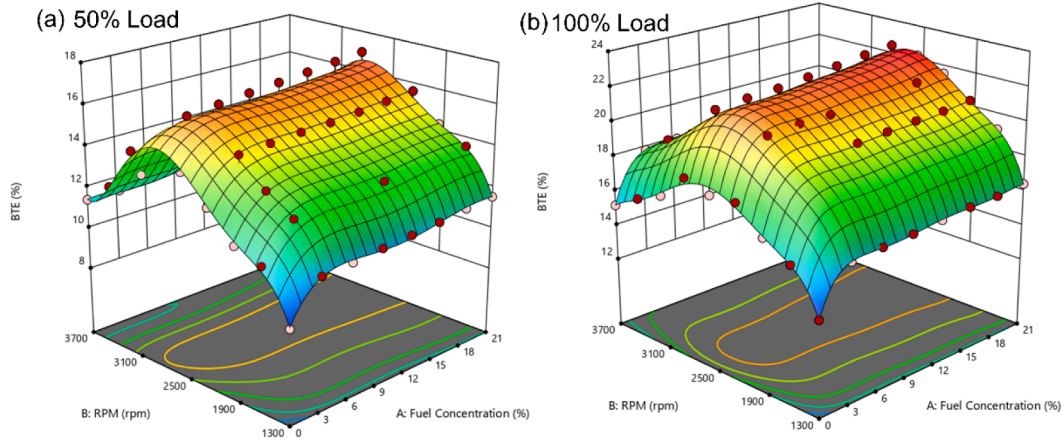


Fig. 13. Surface analysis of BTE at (a) 50% load and at (b) 100% load.

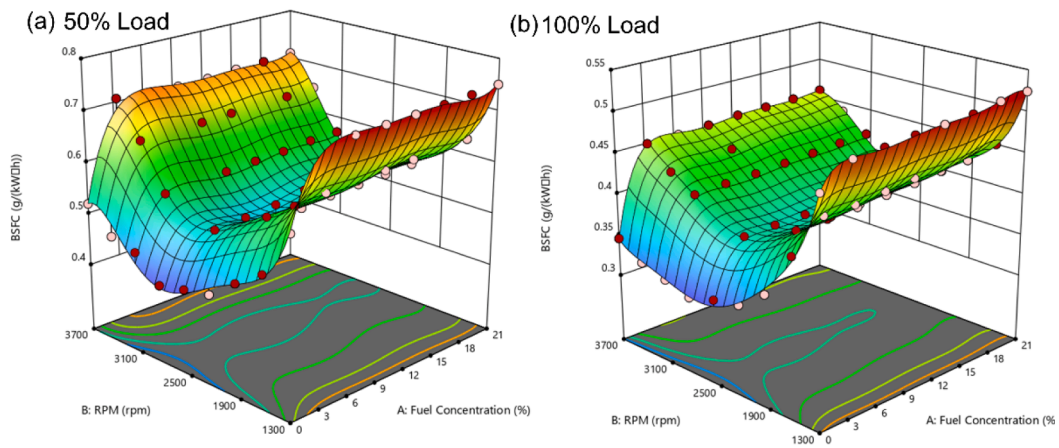


Fig. 14. Surface analysis of BSFC at (a) 50% load and at (b) 100% load.

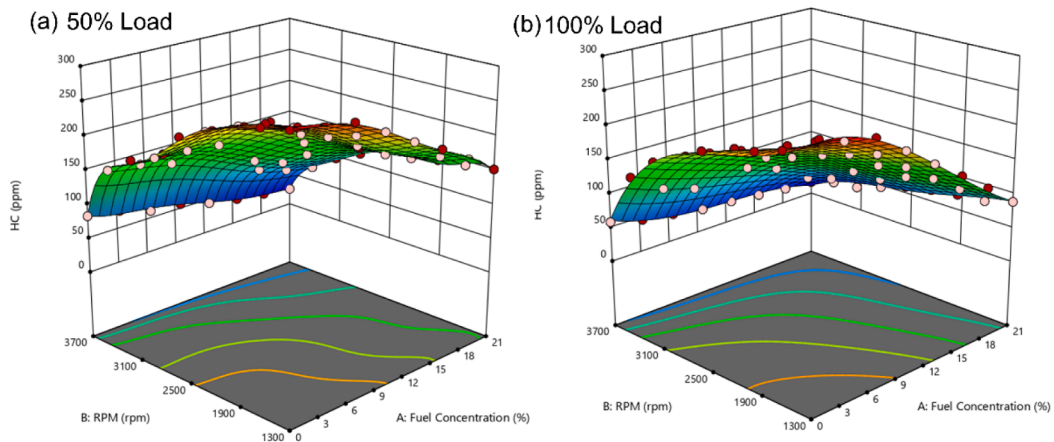


Fig. 15. Surface analysis of torque at (a) 50% load and at (b) 100% load.

mechanical stress [50]. The ethanol ratio consistently increases torque, attributed to ethanol’s higher-octane rating, better air–fuel mixture, cooling effect, and ability to achieve higher compression ratios. Increasing the ethanol ratio from 0% to 21% at 100% load and 3100 rpm, resulted in a 16.86% increase in torque.

In Fig. 12, it can be observed that at lower speeds, the engine demonstrates a comparatively lower BP. By increasing the RPM to a specific

range, the BP increases. Enriching ethanol increases density, smooths combustion (due to oxygen), and boost BP, but higher concentrations decrease calorific value and BP [51]. Maximum brake was observed for increasing the ethanol ratio from 0% to 18% at 100% load and 3100 rpm, which resulted in a 23.70% increase in BP.

Fig. 13 demonstrates that the BTE increases within a specific RPM range, reaching its highest value of 22.49% at 2800 rpm and 100% load

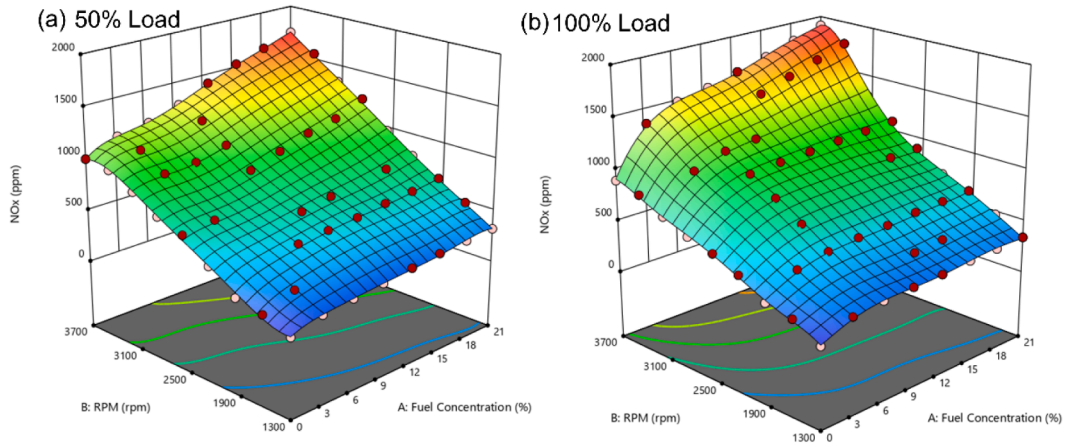


Fig. 16. Surface analysis of torque at (a) 50% load and at (b) 100% load.

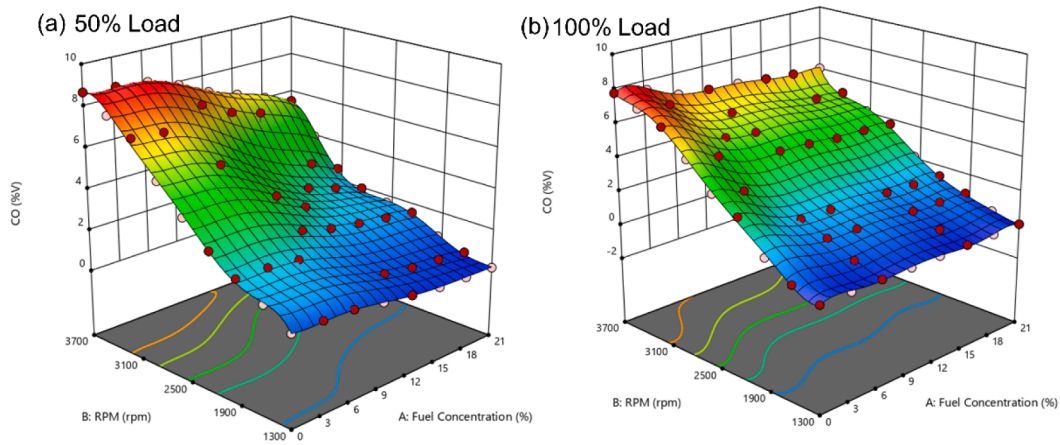


Fig. 17. Surface analysis of CO at (a) 50% load and at (b) 100% load.

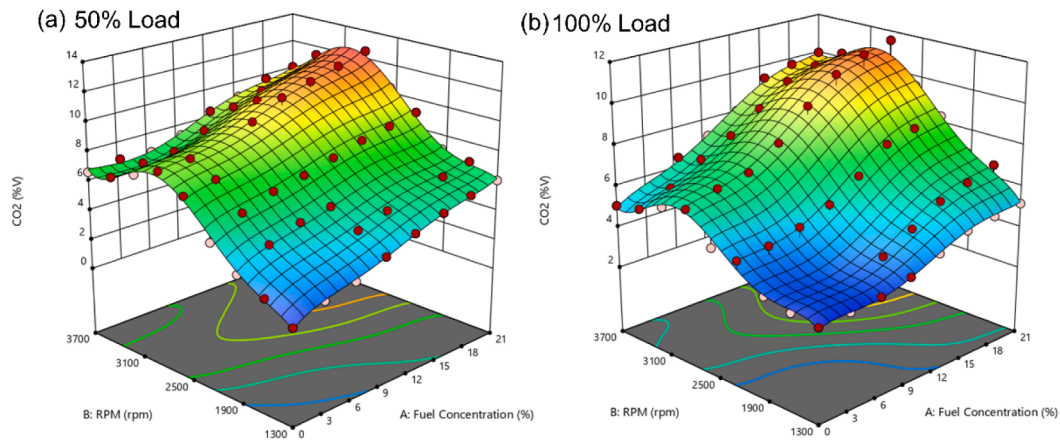


Fig. 18. Surface analysis of CO<sub>2</sub> at (a) 50% load and at (b) 100% load.

for E21. Increasing the engine speed from 1300 rpm to 2800 rpm leads to a significant 26.8% improvement in BTE. However, BTE starts to decline at speeds above 2800 rpm. Lean mixtures at lower speeds increase BTE, but faster and abrupt combustion at higher speeds decreases BTE [27]. BTE shows an upward trend with higher ethanol ratios, especially when the ratio rises from 0% to 6%, resulting in a higher-octane rating and compression ratio and increased BP and BTE.

In Fig. 14, the BSFC initially decreases as RPM increases within a specific range, but beyond that range, it starts to rise. Lower speeds result in a decrease in BSFC due to a substantial increase in BP. However, at higher speeds, the swift and unexpected combustion leads to a rapid increase in BSFC [52]. For instance, increasing the engine speed from 1300 rpm to 2800 rpm at 100% load for E3 led to a 26% decrease in BSFC. At speeds higher than 2800 rpm, BSFC began to increase. The



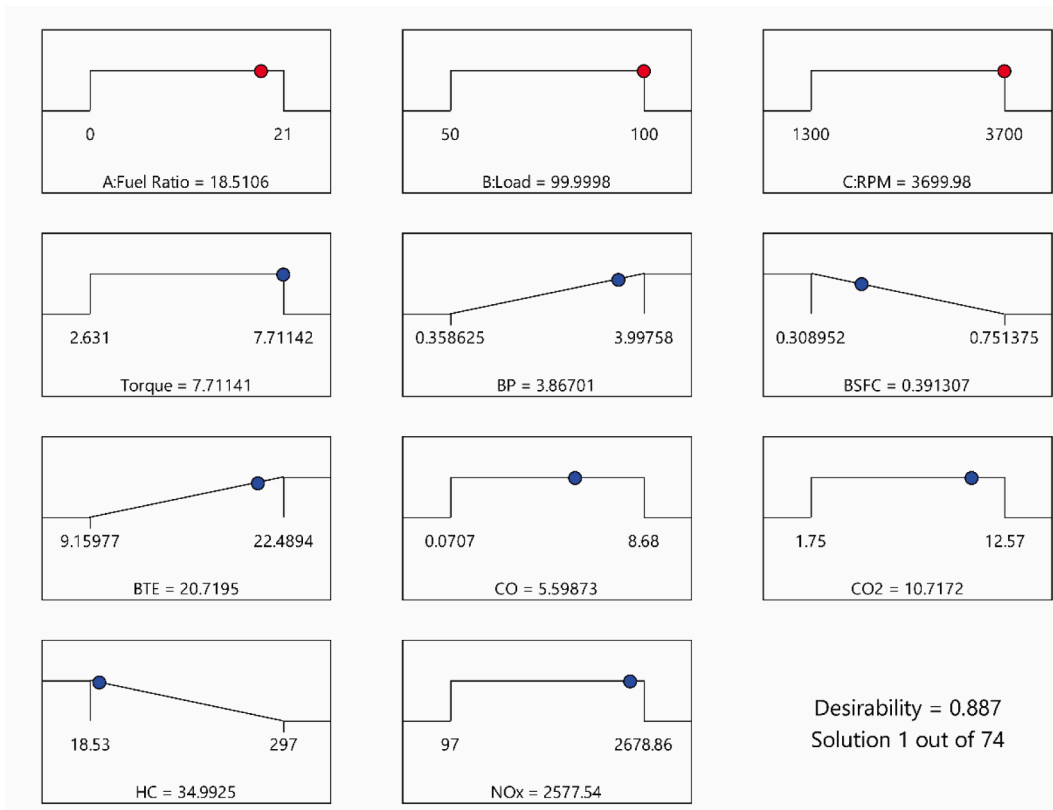


Fig. 19. Ramp chart displaying the optimal operational parameters for the engine.

Table 11  
Results of the confirmation test.

|                 | Torque | BP   | BTE   | BSFC  | CO  | CO <sub>2</sub> | HC    | NO <sub>x</sub> |
|-----------------|--------|------|-------|-------|-----|-----------------|-------|-----------------|
| Optimized Value | 7.71   | 3.87 | 20.72 | 0.391 | 5.6 | 6.01            | 34.99 | 2577.5          |
| Test Value      | 7.92   | 3.99 | 21.24 | 0.379 | 5.8 | 6.23            | 33.69 | 2489.9          |
| Error (%)       | 2.8    | 3.3  | 2.5   | 3.1   | 3.5 | 3.6             | 3.7   | 3.4             |

Table 12  
Outputs comparison at optimal operating conditions with pure gasoline fuel.

|              | Torque (Nm) | BP (kW) | BTE (%) | BSFC (kg/kW.h) | CO (% V) | HC (ppm) | NO <sub>x</sub> (ppm) |
|--------------|-------------|---------|---------|----------------|----------|----------|-----------------------|
| E0           | 7.0         | 3.23    | 15.96   | 0.346          | 7.79     | 58.41    | 1819                  |
| E18.5        | 7.71        | 3.87    | 20.72   | 0.391          | 5.6      | 34.99    | 2577.5                |
| % Difference | 9.4         | 19.9    | 29.8    | 12.9           | - 28.1   | - 40.1   | 41.7%                 |

Table 13  
Assessment of ANN and RSM model performances.

|                 | ANN<br>R <sup>2</sup> | MRE     | RSME   | RSM<br>R <sup>2</sup> | MRE     | RSME   |
|-----------------|-----------------------|---------|--------|-----------------------|---------|--------|
| Torque          | 0.9959                | -0.0319 | 0.0917 | 0.9162                | -0.0345 | 0.0991 |
| BP              | 0.9959                | -0.0717 | 0.0319 | 0.9063                | -0.0782 | 0.0348 |
| BSFC            | 0.9959                | -1.8149 | 0.8037 | 0.9162                | -1.9601 | 0.8680 |
| BTE             | 0.9945                | -0.1000 | 0.1369 | 0.8951                | -0.1100 | 0.1506 |
| CO              | 0.9965                | -0.0989 | 0.2730 | 0.8669                | -0.1118 | 0.3085 |
| CO <sub>2</sub> | 0.9950                | 0.1415  | 0.0306 | 0.8855                | 0.1571  | 0.0339 |
| HC              | 0.9970                | 0.0754  | 0.0292 | 0.8973                | 0.0829  | 0.0322 |
| NO <sub>x</sub> | 0.9966                | 0.0753  | 0.1700 | 0.9867                | 0.0760  | 0.1717 |

lowest BSFC value occurred at 2800 rpm and 100% load. Moreover, increasing the ethanol ratio from 0% to 21% at 100% load and 2800 rpm resulted in a 19.5% increase in BSFC. The increase in BSFC is due to

ethanol's lower energy content and different stoichiometric air-fuel ratio requirements compared to gasoline and its altered combustion characteristics [53–55].

A reduction in HC concentration is shown in Fig. 15 as the ethanol ratio and RPM increase. The lowest recorded HC value of 8.53 ppm occurred at 3700 rpm and 100% load for E21. This can be attributed to the higher oxygen content in the fuel, resulting in a relative increase in the air-fuel ratio (AFR) and subsequently reducing HC emissions. When the engine speed increased from 1300 rpm to 2800 rpm and the fuel ratio changed from E0 to E21, there was a significant reduction of approximately 46.31% in HC concentration. Fig. 16 demonstrates an increase in NO<sub>x</sub> concentrations as the ethanol ratio and RPM increase. The level of NO<sub>x</sub> emissions is influenced by exhaust temperature, which escalates with load and speed [56]. It is evident that as the ethanol content in the fuel rises, so does the emission of NO<sub>x</sub>. Accelerated fuel combustion leads to higher flame temperatures, contributing to increased NO<sub>x</sub> [57,58].

Increasing the ethanol concentration in the gasoline-ethanol blend, as depicted in Fig. 17, leads to a noticeable decrease in CO emissions [59,60]. This is attributed to improved combustion completeness and a shift towards a stoichiometric air–fuel ratio. At 1300 rpm and 100% load, the lowest CO emission was observed for E21, with a significant reduction of 32.21% when the ethanol ratio increased from 0% to 21%. Fig. 18 shows that lower RPMs result in lower CO<sub>2</sub> emissions due to reduced fuel consumption at lower power outputs. As RPM increases, CO<sub>2</sub> emissions rise as the engine operates at higher power outputs, leading to increased fuel consumption. However, beyond 2800 rpm, engine efficiency decreases, leading to reduced fuel consumption and lower CO<sub>2</sub> emissions.

Fig. 19 illustrates ramp chart displaying the optimal operational parameters for the engine. The optimal operating conditions for the engine were determined to be an ethanol volume fraction of 18.5%, an engine speed of 3699.9 rpm, and a 100% load setting.

Under these conditions, the engine exhibited favorable performance and emission characteristics, including torque of 7.71 Nm, BP of 3.87 kW, BSFC of 0.391 kg/kW.h, BTE of 20.72%, and low emissions of CO (5.6 % V), CO<sub>2</sub> (10.71 % V), HC (34.99 ppm), and NO<sub>x</sub> (2577.5 ppm). The calculated composite desirability (D) value of 0.887 validates the optimized model, indicating that the engine responses have been accurately optimized. Operating the engine at the identified parameters would yield the most desirable results, aligning with the objectives of the study. Experimental verification of the optimized results was conducted through a confirmation test and results are summarized in Table 11.

The outputs comparison for the engine running at 3700 rpm, 100% load, and 18.5% ethanol at the same speed and load condition but purely fueled with gasoline is shown in Table 12. The positive values indicate a percentage increase and a negative sign indicates a percentage reduction. The performance matrices between ANN and RSM are compared in Table 13. The ANN model exhibits high R<sup>2</sup>, low MRE, and RSME than RSM.

## Conclusion

The ANN-2HL-15 N model was considered the best model among the six trained models. The model demonstrated exceptional efficiency, with high R<sup>2</sup> values of 0.9952 (training), 0.98579 (validation), 0.98847 (testing), and 0.99307 (overall). It also exhibited the lowest RMSE and MSE values and provided accurate predictions within the range of actual experimental results. The MRE ranged from 0.047% to 0.40%. These results highlight the ANN model's potential for precisely predicting operational effectiveness and discharge levels in small-scale single-cylinder SI engines. The predicted operational parameters and the discharged pollutants were then optimized by integrating a multi-level historical design of RSM.

An ethanol volume fraction of 18.5 %, engine speed of 3700 rpm, and 100% load were identified as optimal operating conditions. Noteworthy improvements resulted from applying these conditions compared to running the engine on gasoline. Specifically, BP and BTE increased by 19.9%, and 29.8%, respectively. Additionally, CO, and HC emissions experienced substantial reductions of 28.1%, and 40.6%, respectively. The increased oxygen and hydrogen content in the blend led to improved combustion, resulting in higher heat generation and elevated emission gas temperatures. Therefore 41.7% increase in NO<sub>x</sub> emissions was observed. As the test results and optimized values are closely associated, this research has affirmed its resilience for forecasting and optimizing.

The results of this study, which looks at the emissions and performance of the ICE fueled by ethanol, are in line with SDGs 7 and 13. Regarding optimization and prediction, the distinctive combination of ANN and RSM encourages sustainable industrialization, more conscientious consumption, and more ethical production patterns. All these are crucial components of SDGs 9 and 12. To make refined decisions and

achieve improved performance and emissions, this research can benefit engine producers and researchers. This alliance between scholars and industry stakeholders supports SDG 17 (Partnerships for the Goals), which also encourages knowledge-sharing to advance the SDGs as a whole.

For future research, dynamic model adaptation has the potential to enhance the capabilities of the established ANN model for ethanol-powered ICEs. Dynamic optimization of such ICEs by utilizing a real-time monitoring and control system along with an ANN predictive model can further enhance performance and reduce emissions. It reinforces the significance of the study by including varying conditions in transient states for the optimization process. Efficiency can be enhanced further by powertrains that combine ethanol utilization with electric energy.

## CRediT authorship contribution statement

**Muhammad Usman:** Conceptualization, Validation, Writing – review & editing, Supervision. **Muhammad Kashif Jamil:** Conceptualization, Methodology. **Waqar Muhammad Ashraf:** Software, Formal analysis. **Syed Saqib:** Validation, Supervision. **Touqeer Ahmad:** Methodology, Software. **Yasser Fouad:** Resources, Writing – review & editing, Funding acquisition. **Husnain Raza:** Formal analysis, Writing – original draft. **Umar Ashfaq:** Investigation, Writing – original draft. **Aamir Pervaiz:** Investigation, Resources.

## Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

## Data availability

No data was used for the research described in the article.

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