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A machine learning based multi-objective optimization for flue gas desulfurization enhancement in coal power plants

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ABSTRACT

Coal-fired power plants emit large quantities of hazardous pollutants including sulfur dioxide (SO_2), oxides of nitrogen (NO_X) and Mercury (Hg) that threaten environmental sustainability. Flue gas desulfurization (FGD) systems are widely deployed to reduce SO_2 emissions, yet their performance depends on large number of interacting operational variables, making real-time optimization challenging. This research aims to develop a practical, data-driven optimization framework for performance improvement of industrial-scale FGD systems. Artificial neural network (ANN) based process models have been trained for its proven capability to model complex nonlinear relationships in high-dimensional process data, and reasonable memory requirement for making excellent function approximate for real-life applications. Two years of continuous operational data from a 660 MW coal power plant were used to train ANN models that predict desulfurization efficiency, NOx, and Hg emissions based on key flue gas and slurry parameters. Monte Carlo sensitivity analysis showed that absorber slurry pH, inlet NOx concentration, and inlet dust concentration are the dominant factors for the three outputs, respectively. A Non-Dominated Sorting Genetic Algorithm II (NSGA-II) was applied to determine optimal operating settings under varying plant load scenarios, with the Technique for Order Preference by Similarity to Ideal Solution (TOPSIS) selecting the most balanced solutions. Results show that the optimized conditions improve SO_2 removal efficiency while reducing NOx and Hg emissions compared to conventional setpoints. The proposed framework offers a practical pathway for cleaner and more efficient operation of large-scale FGD systems, supporting the power sector's net-zero objectives.

Introduction

The ever-rising energy demand to support economic, social, and societal development drives the utilization of the available energy resources to ensure a secure and reliable energy supply. Fossil fuel-based power generation systems are technologically mature and widely used globally, however, these produce toxic and greenhouse gases, causing significant damage to the environmental sustainability and public health. Renewable energy driven power generation technologies are not quite reliable owing to its intermittent nature; thereby, the communities rely on the fossil-based energy systems to meet the energy demand [1–3].

Coal-fired power plants are a major source of hazardous flue gas emissions among thermal power plants [4]. Various flue gas cleaning technologies are installed in coal power plants which include selective catalytic reduction, low-NO_x burners, electro-static precipitators, and flue gas desulphurization (FGD) [4]. Generally, many input variables are associated with the operation control of these technologies. Furthermore, the variables have complex interactions; thereby, estimating the optimized value of the variables under various power generation modes is challenging [6,7].

Artificial intelligence-based data-driven algorithms are one of the smartest ways to model, predict, and control emissions concerning

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Nomenclature

AI	Artificial Intelligence
ANN	Artificial Neural Network
b1,b2	Bias terms in ANN hidden and output layers
FGD	Flue Gas Desulfurization
GA	Genetic Algorithm
Hg	Mercury
N	Number of data observations
NOx	Nitrogen Oxides
NSGA-II	Non-Dominated Sorting Genetic Algorithm II
O2	Oxygen concentration in inlet flue gas (%)
pH	Acidity/basicity of the absorber slurry
RMSE	Root Mean Square Error
R2	Coefficient of Determination
SO2	Sulfur Dioxide
SSE	Sum of Squared Errors
TOPSIS	Technique for Order Preference by Similarity to Ideal Solution
W1,W2	Weight matrices between ANN layers
Xi	Input variable value for observation i
$\hat{y}_i$	Predicted output value for observation i
y_i	Actual output value for observation i
$\bar{y}$	Mean of actual output values

research parameters [5,6]. Among these data-driven methods, artificial neural network (ANN) is one of AI's excellent function approximation algorithms. The model can learn from input-output data and be used to model complex nonlinear systems[7–9]. In the context of FGD system that is characterized by large input space and the nonlinear function space of the output variables, ANN can predict the desulphurization efficiency, Hg, and NO_x based on input variables such as flue gas flow rate, temperature, pH, and reagent dosage [10,11].

Several studies have been conducted to model and predict the flue gas emissions and control the operation of FGD. For instance, Jonathan et al. [12] employed the Bayesian regularized artificial neural network to accurately predict the mercury speciation in coal combustion flue gases, capturing up to 97 % of the variation. Sedat et al. [13], proposed ANN and image feature extraction method to estimate the flue gas temperature in another study. Feature extraction from two colour channels of the flame image was used to train the ANN regression model. Robert et al. [13], presented the combination of ANN and response surface method to model and analyze the performance evaluation of dry flue gas desulfurization. The results demonstrate very good accuracy of ANN model with high coefficient of determination (R^2) values and low root mean square error (RMSE) values indicating a reliable mapping of the dry flue gas desulfurization process.

Combining data-driven models and optimization techniques is an effective way to reduce the flue gas emissions due to effective operation optimization of the system, so different optimization algorithms have been employed along with ANN for that purpose. For instance, Wang et al. [14] proposed an improved genetic algorithm (GA) for optimizing the operation of FGD systems in a power plant. The results indicated that the proposed algorithm could reduce the operating cost of the FGD system by 10 % while meeting the regulatory standards for SO_2, Hg, and NOx removal efficiency. In another study, Kong et al. [15] used ANN and GA to optimize the operation of a wet FGD system in a coal-fired power plant and showed that the proposed approach can improve the removal efficiency of SO_2 and NO_x by 1.63 % and 2.08 %, respectively, while reducing the operating cost by 1.34 %. In another study by Uddin et al. [10], ANN was utilized to model SO_2, NO_x, Hg, and dust discharge from a wet FGD system and provided the effect of the input variables on the emissions discharge.

These studies demonstrate the effectiveness of using ANN for accurately predicting the removal efficiency of SO_2, Hg, and NO_x based on input variables. The combination of ANN and optimization algorithms is a promising approach to optimize the operation of flue gas desulfurization systems to remove SO_2, Hg, and NO_x. However, the above-cited studies mainly focus on lab-based work, which does not reflect how the model will perform during practical scenarios and operating conditions of industrial-scale FGD systems. In addition, in the literature cited above, the model-based sensitivity analysis showing the insight into the workings of FGD system is missing that can be of potential interest to the research and industrial community for operation excellence of industrial systems. Similarly, a few studies report the ANN based optimisation of FGD system for emissions reduction that can its improve the performance for emission removal from the flue gas.

To fill these gaps, the present work utilizes industrial data from a full-scale coal power plant's FGD system, compiling the facility's actual operating conditions. For this study, FGD system has been focused, because it is a widely adopted technology for SO_2 removal, and it's performance significantly makes an impact on overall plant emissions including NO_x and Hg. In addition, FGD involves multiple independent variables like (slurry flow rate, pH of slurry etc.,), which makes it a very good candidate for AI based optimization approach to improve emission control. The data-driven process models built on ANN algorithm are constructed to predict desulfurization efficiency, NO_x and Hg discharge by inlet dust (mg/Nm^3), inlet SO_2 (mg/Nm^3), inlet humidity (%), inlet O_2 (%), inlet NO_x (mg/Nm^3), inlet temperature (°C), pH (pH of absorber slurry) and slurry density (kg/m^3). The effectively developed ANN models can simulate the FGD system's response depending on input variable conditions. Subsequently, the sensitivity analysis of the ANN model shows insight into the most critical parameters affecting the considered output variables of FGD system. Since, the trained ANN models can predict the responses for the considered output variables of the FGD system, thus in the next step, the developed ANN models are deployed to formulate a multi-objective optimization problem that is solved by Non-Dominated Sorting Genetic Algorithm II (NSGA-II). The technique selects the optimum solution(s) for the multi-objective optimization problem for Order of Preference by Similarity to Ideal Solution (TOPSIS) method. This research presents the industrial-scale utilization of ANN model for the operation optimization of FGD systems that promotes operation excellence and can showcase the efficacy of ANN in improving the performance of industrial systems.

Methodology

The methodology adopted to carry out this study is shown in Fig. 1. In the first step, key operational variables of the Flue Gas Desulfurization (FGD) system were collected, including both process input parameters and critical environmental performance indicators such as desulfurization efficiency, NO_x emissions, and mercury (Hg) discharge. The statistical distribution of each variable was examined using histograms, providing a preliminary understanding of data variability and frequency across defined intervals. To assess potential multicollinearity among the input features, the Pearson correlation coefficient was employed, enabling the identification and subsequent elimination of highly collinear variables. This step is essential, as machine learning (ML) models typically exhibit improved generalizability and predictive accuracy when trained on non-redundant, independent input features.

Following data preprocessing, a suite of artificial intelligence (AI) based models was developed, with rigorous hyperparameter optimization conducted to enhance model performance. Comparative analysis of multiple learning algorithms was performed to identify the most accurate and robust predictive model. Once trained, the selected model was

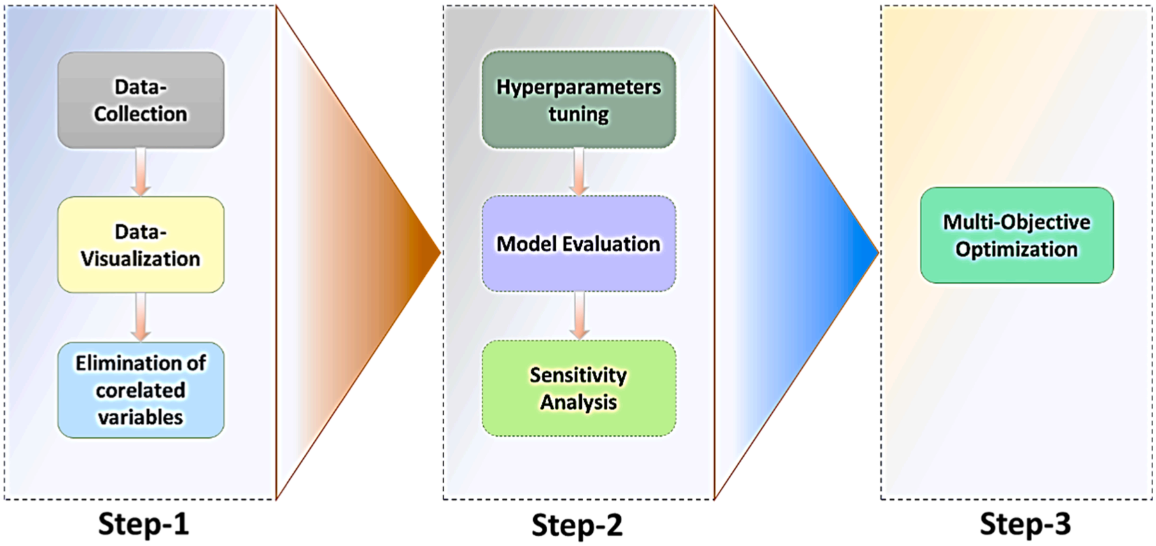

Fig. 1. Stepwise methodology flow sheet.

further examined to evaluate the relative importance of input variables in influencing target outputs, thereby offering interpretability and insights into the underlying system dynamics.

Subsequently, the trained AI model was integrated into a multi-objective optimization framework, wherein the conflicting objectives, such as maximizing desulfurization efficiency while minimizing NO_x and Hg emissions, were addressed simultaneously. The optimization was performed using a Pareto-based approach, and the Technique for Order Preference by Similarity to Ideal Solution (TOPSIS) method was applied to identify the most favourable operational strategy from the Pareto-optimal set.

In the second step, based on the input variables, an ANN model is trained to predict the three output variables: desulphurization efficiency, NO_x and Hg discharge. The predictive accuracy of the models is maintained by extensive hyperparameter tuning and model evaluation in the testing and validation phase. The predictive accuracy of ANN model is assessed using root-mean-squared-error (RMSE) and coefficient of determination (R^2) – the two statistical performance indicators widely used for the evaluation of model prediction [16,17]. Furthermore, Sensitivity analysis utilizing the Monte Carlo technique is conducted to assess the impact of input variables on the output variables. The details regarding Monte Carlo technique-based variables significance analysis are provided in [18].

In the third step, an optimization problem is defined to maximize the desulphurization efficiency and minimize NO_x and Hg discharge from the FGD system. Four operating scenarios for the optimization problem are constructed based on the minimum, middle, maximum and full operating ranges of selected input variables – the variables that represent the power generation mode of the power plant. NSGA-II method is an effective multi-objective optimization technique that requires reasonable computational resources and can estimate the optimized solutions for the complex objective function. TOPSIS is applied to select an optimized solution for the objective function. MATLAB 2021b software trains the ANN models, carrying out the sensitivity and multi-objective optimization analyses. The model-based optimization framework has been successfully applied in this work to determine the optimized solutions corresponding to different operating conditions that can be applied for real-time optimization of the processes.

Artificial Neural Network (ANN)

Artificial Neural Networks (ANNs) are advanced computational models inspired by the structure and functionality of biological neural systems [19,20]. An ANN typically consists of three hierarchical layers: the input layer, one or more hidden layers, and the output layer. The input layer receives and transmits the external data into the network, with the number of neurons corresponding directly to the number of input features. The hidden layers serve as the core computational units of the ANN, where each neuron processes information by computing a weighted sum of its inputs, applying a non-linear activation function, and passing the result forward through the network. The complexity of the problem being modelled typically influences both the number of hidden layers and the number of neurons within each layer [21]. Finally, the output layer generates the network's prediction or classification result, based on the learned representations and transformations from the preceding layers [23]. This architecture enables ANNs to capture complex, non-linear relationships in high-dimensional datasets, making them particularly suitable for modelling and optimization tasks in energy systems, such as the prediction and control of flue gas desulfurization (FGD) performance metrics, including SO_2 removal efficiency and pollutant emissions. The mathematical depiction of the information processing involved in creating an ANN model is provided as follows:

$$\widehat{Y}_i = f_2\left(\sum_{i=1}^{N} W_2\left[f_1\left(\sum_{i=1}^{N} X_i W_1 + b_1\right)\right] + b_2\right) \tag{1}$$

Here, X is a set of input variables and $i = 1, 2, 3, \ldots N$ equal to the number of observations associated with the number of input variables. W_1 and W_2 denote the weight connections originating from the input-hidden layer and the hidden-output layer of the Artificial Neural Network (ANN). Whereas, b_1 and b_2 as well as f_1 and f_2 are the bias and activation functions applied at ANN's hidden and output layers, respectively. As a result of information processing, the responses are simulated corresponding to the conditions of the input variables, which are represented as $\widehat{Y}$ [18].

Monte Carlo based significance analysis

We apply Monte Carlo technique to establish the feature importance on the predictions made by ANN. The feature importance analysis identifies significance features that influence the model-based prediction as per their feature importance. Monte Carlo technique is a robust choice of significance analysis since it comprehensively investigates the impact of features on the model-based predictions under large number of simulations [22,23]. The method works in changing the operating level of the desirable operating variable from its minimum to maximum values in a number of step sizes. In each step size, other operating variables are randomly changed between their operating levels. The procedure is repeated for all operating levels of the variable of interest for sensitivity analysis and the effect of variation in the operating levels of desirable operating variable on the output variable is computed. The same procedure is applied for all remaining input variables and the marginal effect of each operating variable on the change in the output variable is computed. This allows to establish the feature importance order that highlights the significance of operating variables towards the predictions made by the model. The reader may learn about the technique in more details in this paper [18].

Non-Dominated Sorting Genetic Algorithm II (NSGA-II)

The Genetic Algorithm (GA) is a population-based metaheuristic optimization technique inspired by the principles of natural selection and evolutionary biology. It operates through the iterative evolution of a population of candidate solutions, which are evaluated based on a predefined objective or fitness function. Each candidate, commonly encoded as a binary or real-valued chromosome, represents a potential solution in the decision space of the optimization problem [24]. The algorithm proceeds through a sequence of stochastic operators: selection, crossover, and mutation. During the selection phase, individuals with superior fitness, i.e., those that better satisfy the objective function, are preferentially chosen to contribute to the next generation. The crossover operator facilitates the exchange of genetic material between selected parent chromosomes, generating offspring that inherit characteristics from both parents. Mutation introduces random alterations to selected genes, thereby maintaining genetic diversity and enabling the exploration of new regions in the solution space [25]. This evolutionary framework allows GA to effectively navigate complex, high-dimensional, and non-convex optimization landscapes. As such, it has been extensively applied in energy systems engineering, including the optimization of flue gas desulfurization (FGD) processes, where multiple conflicting objectives such as SO_2 removal efficiency, NO_x emissions, and operational cost must be simultaneously balanced.

Through iterative application of selection, crossover, and mutation operators, Genetic Algorithms (GAs) progressively evolve a population of candidate solutions, with each generation typically exhibiting improved fitness relative to the previous one. This evolutionary cycle continues until a predefined termination criterion, such as a maximum number of generations or a satisfactory fitness threshold, is met. The stopping condition can vary based on the specific optimization problem [26]. The fundamental GA framework has undergone numerous enhancements, with alternative strategies for selection, crossover, and mutation developed to improve convergence speed and solution quality. These choices significantly influence algorithmic performance and are often tailored to the problem domain. Among evolutionary algorithms, those capable of maintaining population diversity and exploring multiple trade-offs simultaneously have become increasingly popular for solving complex multi-objective optimization problems [27].

One of the most widely adopted algorithms in this category is the Non-Dominated Sorting Genetic Algorithm II (NSGA-II). NSGA-II is particularly effective in handling multi-objective problems due to its fast non-dominated sorting mechanism and elitist strategy. In each generation, the population is classified into several non-dominated fronts based on Pareto dominance, and diversity is preserved using crowding distance metrics [28]. Offspring are generated using genetic operators and replace the lesser fit individuals, allowing the algorithm to converge efficiently toward a well-distributed Pareto front [29].

In this study, the trained ANN model has been embedded within the NSGA-II framework to predict system responses as part of the optimization loop. The parameters related to NSGA-II include size of population, mutation rate etc., which are set at the default values in the MATLAB. The resulting Pareto-optimal solutions represent various trade-offs between competing objectives, such as maximizing desulfurization efficiency while minimizing NO_x and Hg emissions. .

To facilitate decision-making, the Technique for Order Preference by Similarity to Ideal Solution (TOPSIS) is employed to identify the most favourable compromise solution from the Pareto set. Fig. 2 illustrates the integration of the ANN model within the multi-objective optimization architecture.

NSGA-offers a robust framework for optimizing the operational parameters of flue gas desulfurization (FGD) systems [30]. FGD processes are inherently complex, governed by multiple interacting input variables that influence both desulfurization efficiency and the release of secondary pollutants such as nitrogen oxides (NO_x) and mercury (Hg) [31]. These performance indicators typically exhibit trade-offs, making the optimization problem inherently multi-objective. NSGA-II effectively addresses this challenge by simultaneously maximizing SO_2 removal efficiency and minimizing NO_x and Hg emissions, thereby identifying a set of Pareto-optimal solutions that reflect the best possible compromises among conflicting environmental and operational objectives [32].

Evaluation criteria

Two statistical measures are deployed as an evaluation criterion to investigate the performance of the ANN model in making the predictions. It includes root-mean-squared-error (RMSE) and co-efficient of determination (R^2). The mathematical representation of R^2 and RMSE is given as:

$$R^2 = 1 - \frac{\sum_i^N (y_i - \hat{y}_i)^2}{\sum_i^N (y_i - \bar{y}_i)^2} \tag{2}$$

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N} (\hat{y}_i - y_i)^2} \tag{3}$$

here, y_i is the actual value to be simulated, whereas $\hat{y}_i$ is the model-simulated values for $i = 1,2, 3\ldots$, N. Whereas $\bar{y}_i$ is the mean of actual values of y_i. R2 is the measure of accuracy, and it varies from 0 to 1. On the other hand, RMSE is the error term that indicates the mean error present in the model predicted response.

Results and discussion

Data collection, visualization and processing

Flue gas desulphurization system is typically installed as an auxiliary system in the coal power plant. Limestone based slurry is sprayed on the flue gas entering the absorption tower of FGD system. The physical and chemical reactions between the limestone and the hazardous gases result in flue gas cleaning. More details about the working of FGD system can be found in [10]. In this research, we have considered flue gas system installed at a 660 MW coal power plant. The significant and causal operating variables model the desulphurization efficiency, NOx discharge and Hg discharge. The operational experience of the performance engineer has helped identify the critical and operationally relevant operating variables. The literature survey also suggests incorporating the operating variables corresponding to the flue gas and limestone slurry based operational variables [10,33–36]. Therefore, flue gas based operating variables: inlet dust (mg/Nm^3), inlet SO_2 (mg/Nm^3), inlet humidity (%), inlet O_2 (%), inlet NO_x (mg/Nm^3) and inlet temperature (°C), and limestone slurry-based variables: pH (pH of absorber slurry) and slurry density (kg/m^3) are taken to model the desulphurization efficiency, NO_x discharge, and Hg discharge from the flue gas desulphurization system.

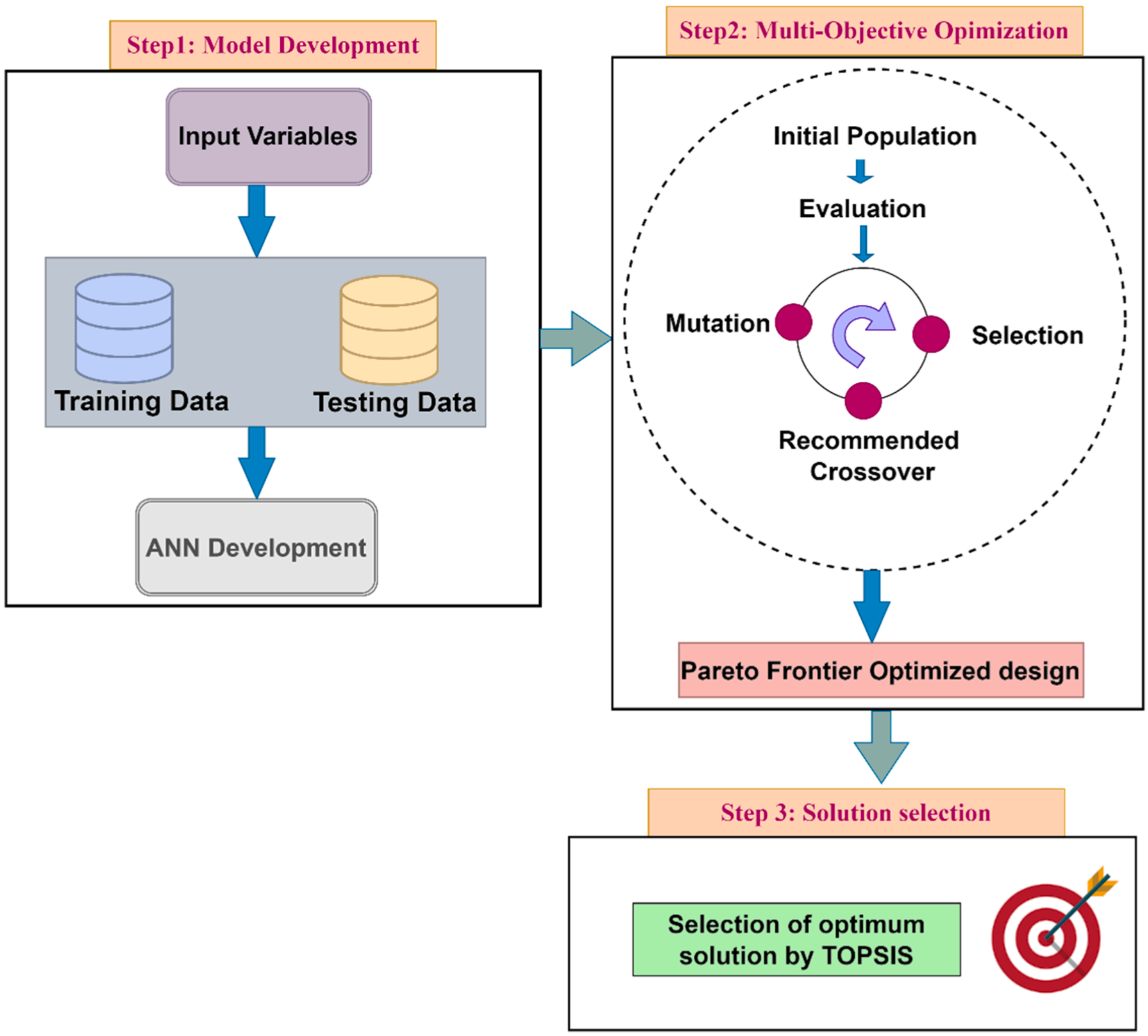

Fig. 2. Schematic flow diagram for three-step methodology for the selection of optimum solution.

The operational data for the FGD system were recorded via the plant's Supervisory Information System (SIS) over a prolonged period of continuous operation. The observations during the shut-down state of the power plant, malfunctioning of sensors, sensor calibration and faulty observations which are observed significantly away from the normal data occurrence, have been removed. We take data samples at different operating months to account for seasonal variation on the performance of FGD system. Data visualisation techniques including scatter plots have been made to locate the outliers (lie significantly away from the main data distribution), faulty operating zones in the measurements (horizontal lines meaning sensor is recording constant values) [37]. The visual inspection is robust to removal of useful data observations which sometime are observed at the tails of data distribution but accurately identify the outliers [37]. In total, 715 sequential observations (time--stamped records of 5 min interval for capturing the process dynamics) of the input and output variables were collected that capture the wide operating space of operating variables. This dataset captures the full range of normal operating conditions across different seasons and load levels. The distribution of each variable is shown in Fig. 3, indicating that the data points cover the entire operating range without significant gaps. Such continuity and breadth in the data ensure that the trained model and subsequent analyses are based on representative real-world operating behaviour.

The important point to note here is that the variables have continuous data distribution on the operating ranges, and no empty zones are observed along the data distribution profiles of the variables. Thus, a good data distribution and reasonable frequency count are kept for both input-output variables, which is essential for building a flexible machine learning (ML) model for the predictive and optimization analyses.

Identification of linear-dependent input variables

To ensure stable operation and optimal performance of the flue gas desulfurization (FGD) system, key process control variables are maintained at designated setpoints. These variables are continuously recorded at multiple locations along the process for monitoring and control purposes. However, such operational data often contain redundancies due to potential linear dependencies among variables. Since multicollinearity can adversely affect performance and interpretability of machine learning models, it is essential to identify and eliminate correlated features [18].

In this work, the Pearson correlation coefficient has been employed to evaluate the linear relationships among input and output variables. The resulting correlation heat map, shown in Fig. 4, reveals that most variable pairs exhibit coefficients near zero, indicating weak or no linear correlation. The correlation coefficients range from −0.66 to 0.61, suggesting an overall absence of strong linear dependence, except between NO_x discharge and inlet NO_x concentration. As a result, all selected input features are considered sufficiently independent and were retained for machine learning model development.

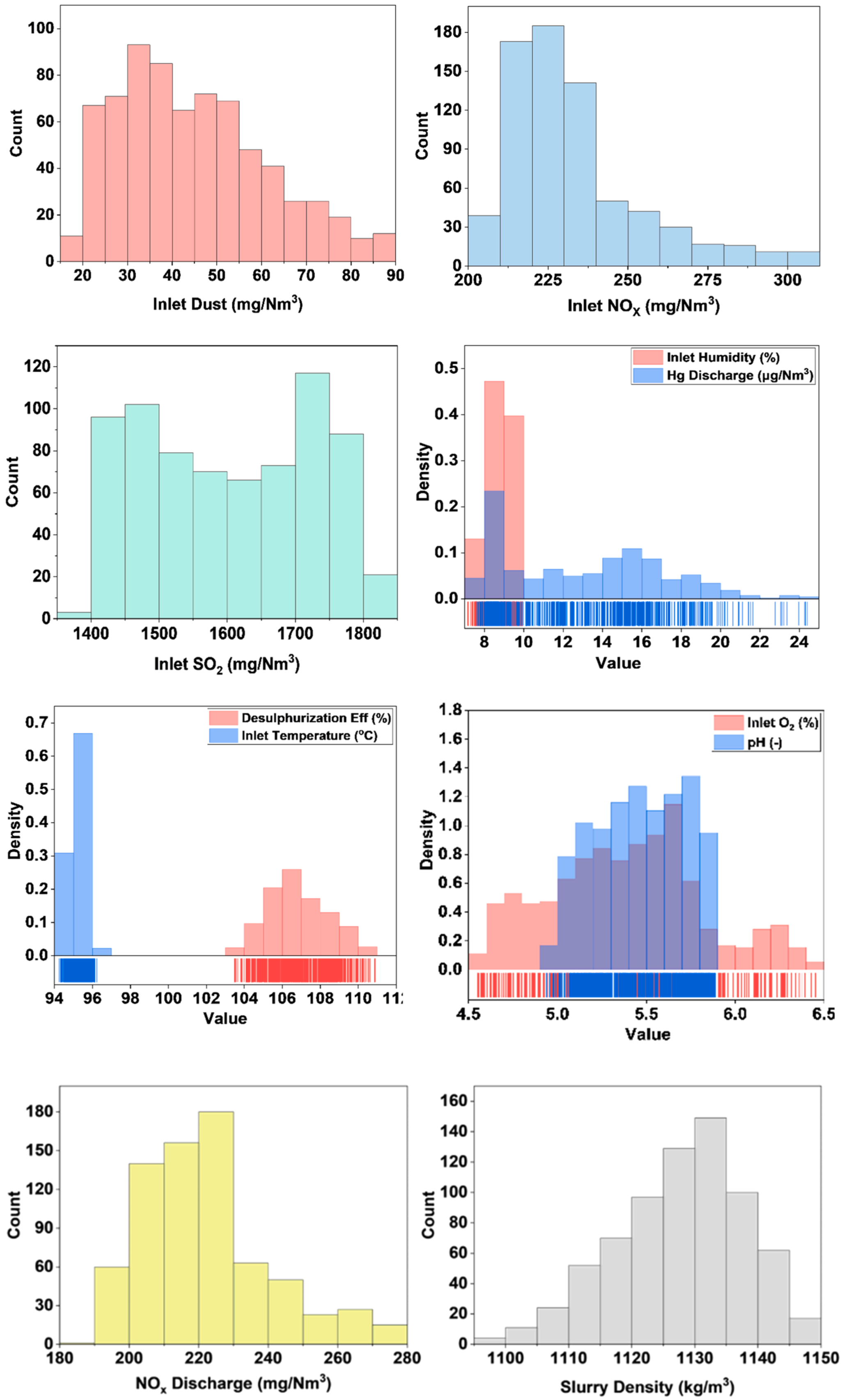

Fig. 3. Data-distribution space of the input and output variables taken from the flue gas desulphurization system. The input variables will model desulphurization efficiency, NOx discharge, and Hg discharge.

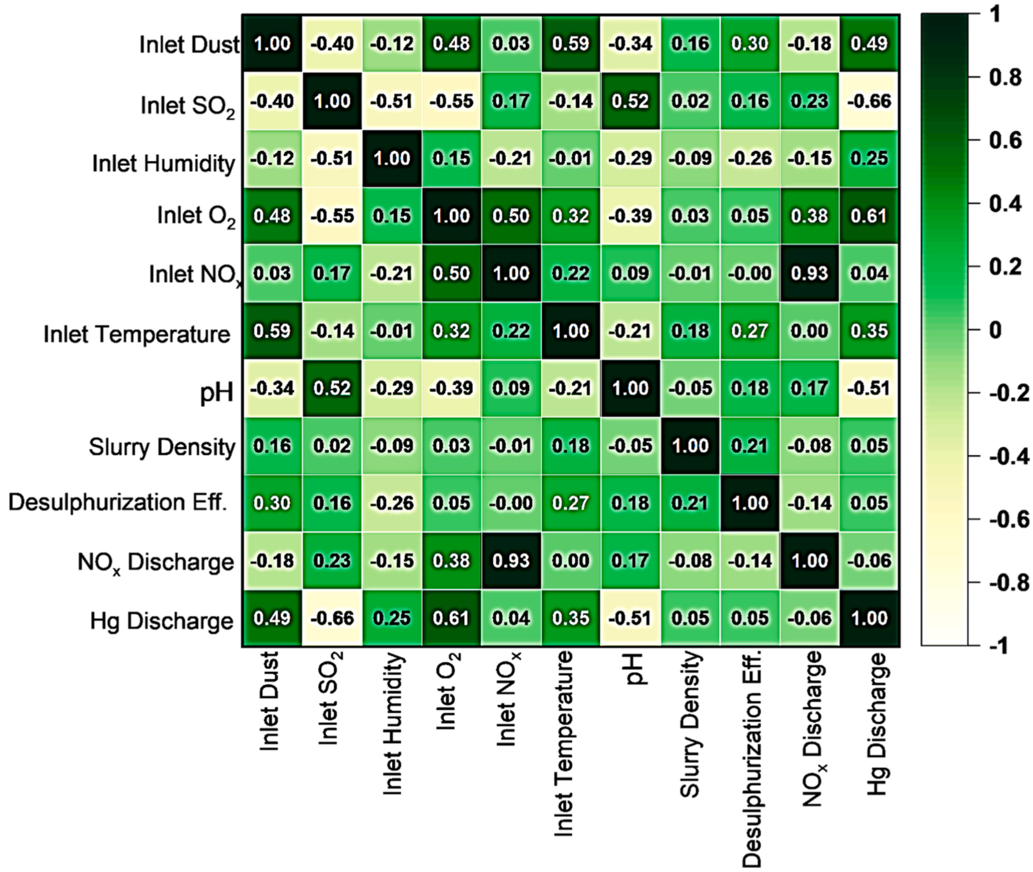

Fig. 4. Pearson correlation coefficient-based heat map for the input-output variables.

Development of ANN model

The predictive performance of ANN models is highly dependent on the appropriate tuning of key hyperparameters, particularly the number of hidden layers and the number of neurons within each layer [38]. Literature suggests that a single hidden layer with a sufficient number of neurons is often adequate to capture nonlinear behaviours in process data [39]. As a result, a shallow ANN architecture was used in this study to model the output variables of the flue gas desulfurization (FGD) system. The number of neurons in the hidden layer was varied from 8 to 20, guided by empirical recommendations that suggest selecting between 1x to 2.5x the number of input features[40,41]. Model performance was evaluated using established metrics to identify the optimal network configuration, i.e., number of neurons in the hidden layer.

The dataset was partitioned into training, validation, and testing subsets with an 80:10:10 split ratio to ensure reliable model development and evaluation. A hyperbolic tangent (*tanh*) activation function was applied to the hidden layer to capture non-linearity, while a linear activation function was used at the output layer to maintain continuity in regression outputs [42]. A learning rate of 0.01 was adopted, consistent with standard practice, to balance convergence speed and stability during weight and bias updates [17,43]. The Levenberg-Marquardt algorithm was employed for training, given its superior convergence properties and low memory requirements. The objective function of the model was defined using the sum of squared errors (SSE), which is effective for minimizing regression loss in function approximation tasks [44]. To prevent overfitting, early stopping criteria were implemented. Training was halted when either the gradient fell below 1×10^{-7}, the validation performance failed to improve for 10 consecutive iterations, or a maximum of 10,000 training epochs was reached. These criteria ensured optimized adjustment of network parameters while maintaining generalization capability.

The performance of the ANN model during training, validation, and testing was evaluated for varying numbers of hidden layer neurons, an essential hyperparameter influencing model accuracy. Fig. 5 presents the predictive performance of the ANN across different network configurations for the three output variables: desulfurization efficiency, NO_x discharge, and Hg discharge.

Fig. 5(a–c) illustrates the variations in the coefficient of determination (R^2) and root mean square error (RMSE) with respect to the number of hidden neurons for each output. Specifically, for desulfurization efficiency (Fig. 5a), the R^2 values ranged from 0.86 to 0.92, while RMSE varied between 0.15 % and 0.18 %, indicating a high level of predictive accuracy and generalization across the tested configurations.

Closely observing the performance of the model by the defined evaluation criteria, it is determined that ANN model, which has 14 hidden layer neurons (hyperparameter of ANN model) has comparatively better predictive performance ($R^2_{train} = 0.90$, $R^2_{test} = 0.90$, $R^2_{val} = 0.89$ & $RMSE_{train} = 0.16$ %, $RMSE_{test} = 0.18$ %, $RMSE_{val} = 0.16$ %) compared with those of other models. Similarly, the comparative performance analysis for NO_x and Hg reveals that ANN model having 10 and 20 neurons in the hidden layer are the better predictive approximate for the two output variables. R^2 and RMSE for NO_x discharge is as follows: $R^2_{train} = 0.98$, $R^2_{test} = 0.98$, $R^2_{val} = 0.97$ & $RMSE_{train} = 4.1$ mg/Nm^3, $RMSE_{test} = 3.5$ mg/Nm^3, $RMSE_{val} = 3.7$ mg/Nm^3. Whereas R^2 and RMSE for Hg discharge is as follows: $R^2_{train} = 0.93$, $R^2_{test} = 0.91$, $R^2_{val} = 0.92$ & $RMSE_{train} = 1.49$ μg/Nm^3, $RMSE_{test} = 1.72$ μg/Nm^3, $RMSE_{val} = 1.53$ μg/Nm^3. These results clearly demonstrate that the appropriate selection of hidden layer neurons significantly enhances model accuracy and generalization. The comparative analysis supports the identification of optimal ANN architectures tailored to each target output variable in the flue gas desulfurization system.

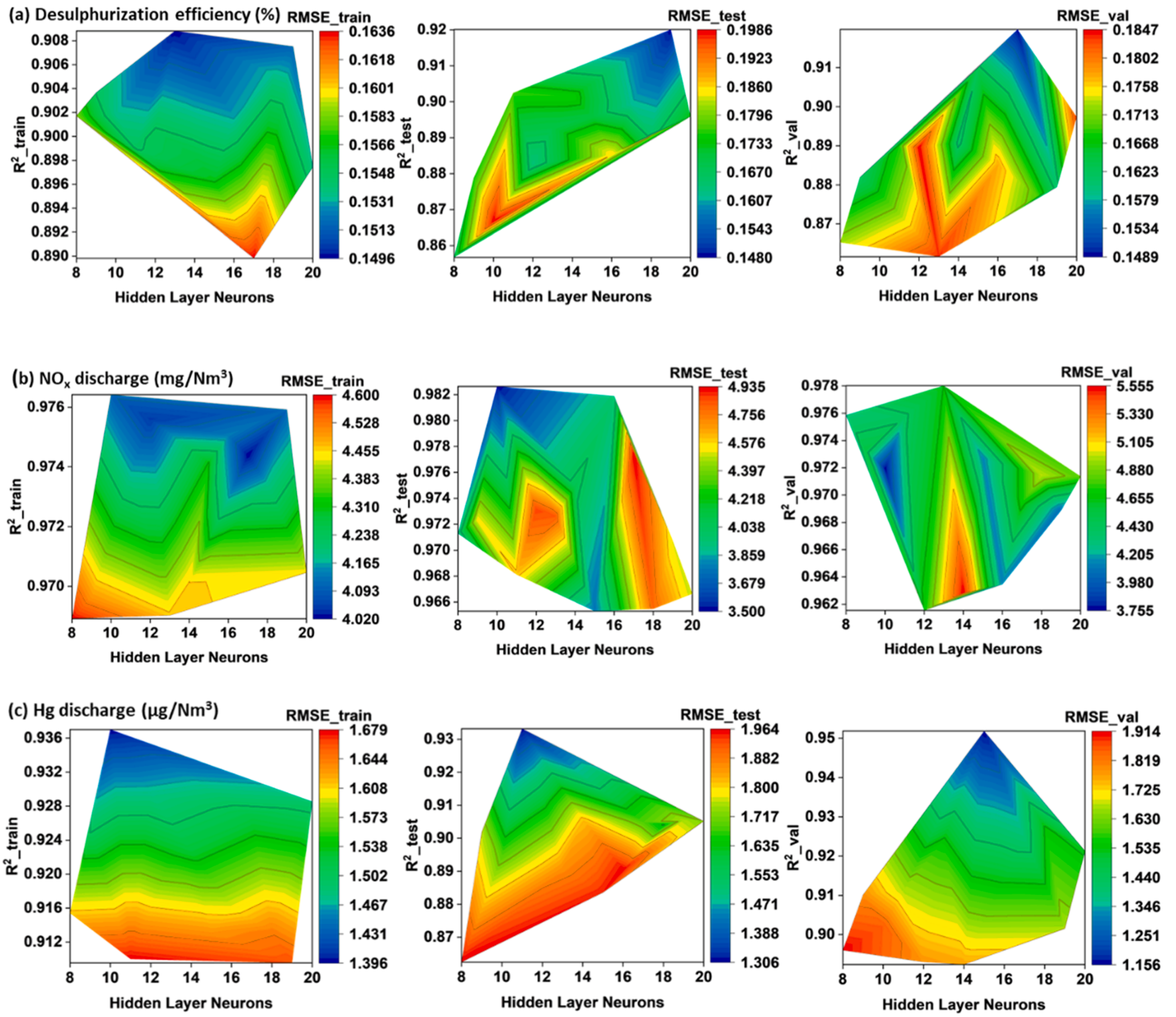

Fig. 5. Development of ANN model under training, testing and validation phase with respect to hidden layer neurons for a) desulphurization efficiency, b) NOx discharge, and c) Hg discharge.

Monte Carlo technique-based sensitivity analysis

Since the ANN model operate as black-box models, it is essential to assess the influence of individual input parameters on model outputs to enhance interpretability. Sensitivity analysis is widely used to quantify the relative importance of input variables. In this study, a Monte Carlo-based sensitivity analysis was employed to systematically evaluate the contribution of each input parameter to the prediction of output variables. This approach enables a statistically robust ranking of input significance, thereby providing insights into the underlying process dynamics and guiding informed decision-making for operational optimization [45].

The percentage influence of input variables on the three target outputs—desulfurization efficiency (%), NO_x discharge (mg/Nm^3), and Hg discharge ($\mu g/Nm^3$), is presented in Fig. 6(a–c). For desulfurization efficiency, pH emerged as the most influential parameter, contributing 45.5 % to the model's predictive capability. This strong dependence is attributed to the alkaline nature of the absorber slurry, which facilitates SO_2 removal through acid-base reactions and subsequent physico-chemical interactions [46]. Inlet dust loading (18.8 %) and flue gas humidity (14.2 %) were identified as the next most significant inputs. Humidity enhances SO_2 solubilization and reaction kinetics, while excessive dust can impair slurry reactivity by fouling or poisoning the active surface. Consequently, routine monitoring and maintenance of slurry quality are critical for sustaining desulfurization efficiency.

In the case of NO_x discharge, inlet NO_x concentration was the dominant input, accounting for 92.3 % of the model's sensitivity, indicating that downstream FGD processes have minimal effect on NO_x removal. The next key contributors were inlet dust (5.2 %) and SO_2 (2.2 %). Dust may indirectly affect NO_x emissions by altering slurry characteristics, while SO_2 can participate in the side reactions with NO_x species, although marginally [47] Similarly, for Hg discharge, inlet dust exhibited the highest significance (42.4 %), likely due to its role in adsorbing mercury species during particulate capture. Inlet SO_2 (27.2 %) also showed a strong influence, as it participates in redox and complexation reactions that facilitate Hg removal [48]. Inlet O_2 was the third most significant parameter (15.2 %), acting as an oxidizing agent that can promote the re-emission of elemental mercury (Hg^o) from the absorber slurry by destabilizing dissolved mercury complexes [49].

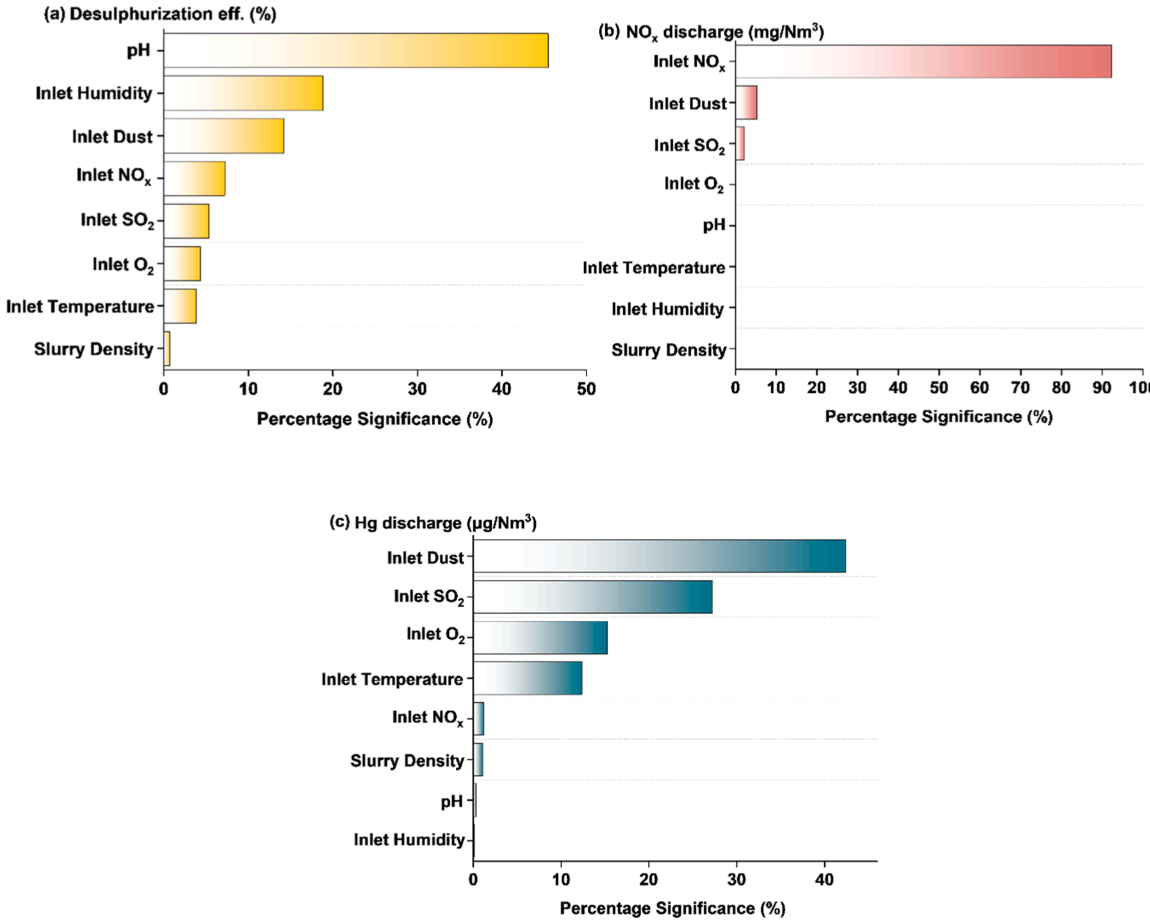

Fig. 6. Monte Carlo technique-based input variables significance for the three target output variables a) desulphurization efficiency (%), b) NOx discharge (mg/Nm3) and c) Hg discharge (µg/Nm3).

Multi-objective optimization analysis

The modelled output variables in this study exhibit distinct operational objectives: desulfurization efficiency is to be maximized, while NO_x and Hg discharges are to be minimized. These contrasting goals form the basis for the formulation of a multi-objective optimization problem, aimed at enhancing pollutant removal performance while minimizing harmful emissions from the flue gas desulfurization (FGD) system.

The multi-objective optimization problem is defined as follows:

Objective function: f = max (desulphurization efficiency) + min (NO_x discharge + Hg discharge)

Subjected to:

$18 \leq$ *Initial dust* $(mg/Nm^3) \leq 89$
$1387 \leq$ *Initial* SO_2 $(mg/Nm^3) \leq 1831$
$7.1 \leq$ *Initial Humidity* $(\%) \leq 10.0$
$4.5 \leq$ *Initial* O_2 $(\%) \leq 6.5$
$205 \leq$ *Initial* NO_x $(mg/Nm^3) \leq 307$
$103 \leq$ *In Temperature* $(^\circ C) \leq 111$
$4.9 \leq \mathrm{pH} \leq 5.9$
$1096 \leq$ *Slurry Density* $(kg/m^3) \leq 1148$

Variable bounds were established to define the solution space for the multi-objective optimization problem. Recognizing that the flue gas desulfurization (FGD) system operates under varying inlet conditions depending on the power plant's load, four representative operating scenarios were developed. These scenarios reflect the minimum, intermediate, maximum, and full operational ranges of key flue gas parameters namely, inlet dust, SO_2, and NO_x concentrations representing different emission load conditions entering the scrubber unit.

Here, the 'maximum' emission load scenario corresponds to a high plant load condition with the key inlet parameters (such as dust, SO_2, and NOx concentrations) fixed at their upper bound values. In contrast, the 'full-range' scenario imposes no fixed load – instead, all input variables are free to vary across their entire allowable ranges to identify a global optimum. This distinction allows us to examine both a specific peak-load optimization and an unconstrained optimization covering all operating conditions.

For each scenario, the optimization problem was solved using the Non-dominated Sorting Genetic Algorithm II (NSGA-II), with the remaining input variables allowed to vary across their full admissible ranges. The parameters related with the population size and mutation rate etc. are set at default values as provided in MATLAB. This approach enabled the identification of optimal operating conditions for the FGD system under varying emission loads. To select the most suitable trade-off solution from the Pareto front generated by NSGA-II, the Technique for Order Preference by Similarity to Ideal Solution (TOPSIS) was employed. The TOPSIS-selected solutions, representing the optimal compromise among conflicting objectives, are highlighted as red points in Fig. 7. The NSGA-II parameter settings were adopted from validated literature to ensure convergence and computational efficiency, thereby enhancing the reliability of the optimization results [50].

Low-load scenario: Fig. 7. (a) the Pareto-optimal solutions corresponding to a low emission load scenario, defined by inlet dust, SO_2, and NO_x concentrations of 18 mg/Nm^3, 1387 mg/Nm^3, and 205 mg/Nm^3, respectively. Under this operating condition, the optimal trade-off solution selected via the TOPSIS method indicates that all three output objectives, maximized desulfurization efficiency and minimized NO_x

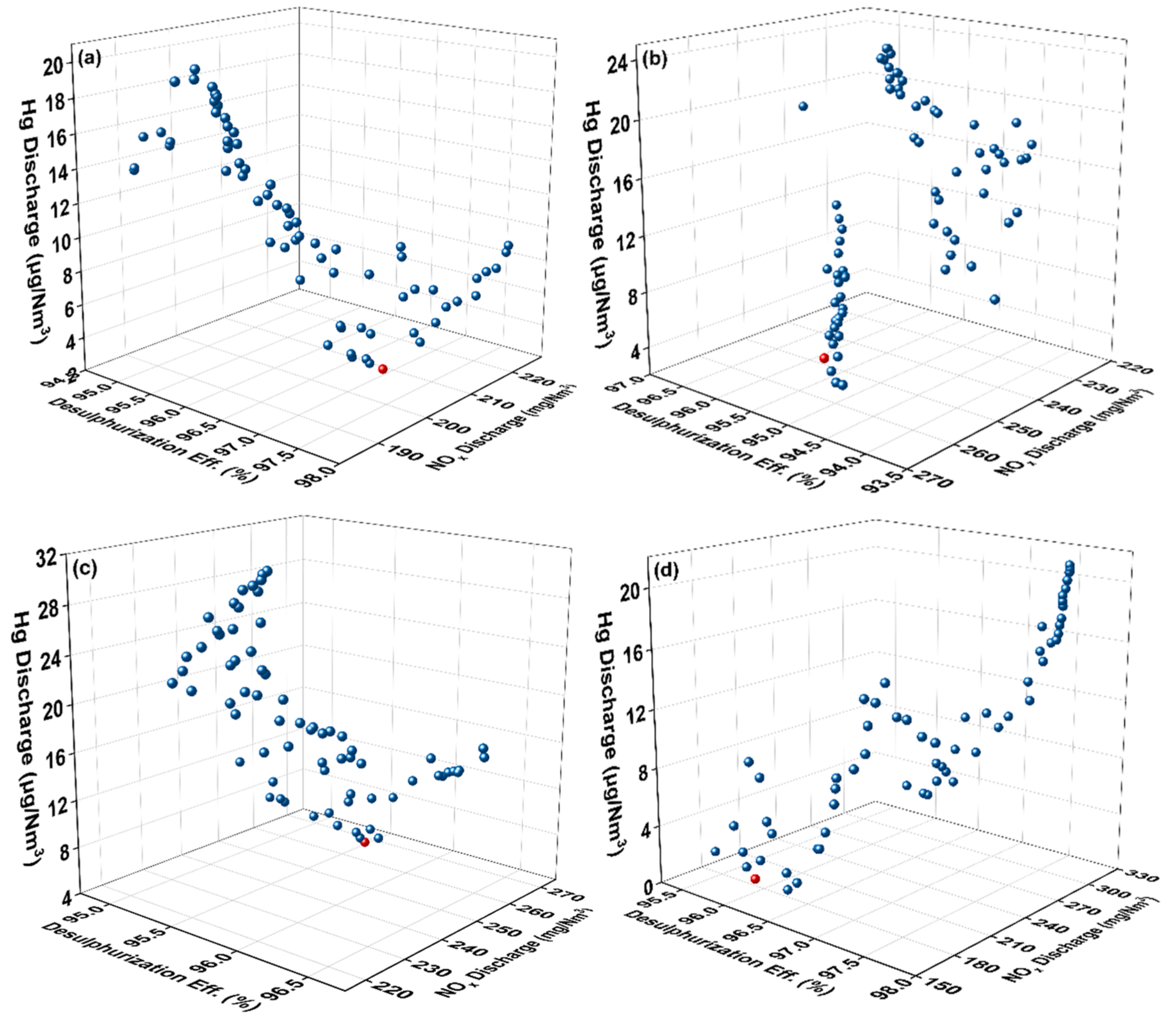

Fig. 7. The optimal solution estimated by NSGA-II under different operating values taken from the operating range of inlet dust, inlet SO2, and inlet NOx as a) minimum, b) middle, c) maximum, and d) full operating range. The optimal solution is selected by TOPSIS and is shown by red spot.

and Hg discharges, can be achieved by setting the input variables to the following values: inlet humidity at 7.2 %, inlet O_2 concentration at 6.2 %, flue gas temperature at 111 °C, pH at 5.0, and slurry density at 1144 kg/m^3. Notably, pH, a critical control parameter in the FGD process, is optimized near its lower operational limit, reflecting its dominant influence even under minimal emission load conditions. Likewise, maintaining slurry density at 1144 kg/m^3 supports enhanced gas–liquid contact and effective SO_2 absorption. These findings suggest that optimal system performance can be sustained through coordinated control of key input parameters, even during low-load operating scenarios.

Mid-load scenario: Fig 7(b) corresponds to medium emission scenario, at an intermediate emission level (inlet dust ~53 mg/Nm^3, SO_2 ~1609 mg/Nm^3, NO_x ~256 mg/Nm^3), NSGA-II with TOPSIS results inc optimal set-points of approximately: humidity 9.0 %, O_2 4.6 %, flue gas temperature 111 °C, pH 5.7, and slurry density 1104 kg/m^3. It indicates that compared to the low-load case, the absorber slurry's optimal pH is higher, reflecting the need for increased alkalinity to neutralize the greater SO_2 burden at mid loads. The required slurry density is slightly lower than in the low-load scenario, indicating that under moderate loads, adequate SO_2 capture can be achieved without pushing slurry concentration to its upper limit.

Maximum-load scenario: For the peak load condition (inlet dust ~88 mg/Nm^3, SO_2 ~1831 mg/Nm^3, NO_x ~307 mg/Nm^3), the optimization suggests optimal inputs of around: humidity 7.3 %, O_2 6.3 %, temperature 111 °C, pH 5.3, and slurry density 1105 kg/m^3. This high-load optimum continues the trend of elevated pH set-points (relative to the low-load case) to handle increased SO_2 levels, while the slurry density remains near the values seen at mid load. Under maximum emission stress, the model finds that maintaining a moderately high pH and a slurry density around ~1100 kg/m^3 provides the best trade-off for sustaining desulfurization efficiency and controlling NO_x/Hg emissions.

Full-range scenario: In the unconstrained optimization scenario (with all inputs free over their full ranges), the algorithm identifies a balanced optimal configuration: inlet dust ~32 mg/Nm^3, SO_2 ~1719 mg/Nm^3, NO_x ~209 mg/Nm^3, humidity ~7.3 %, O_2 ~5.3 %, temperature ~110.8 °C, pH ~5.4, and slurry density ~1130 kg/m^3. Interestingly, none of the inlet pollutant concentrations in this solution are at their extreme minimum or maximum, indicating that the globally optimal trade-off involves moderate values for some inputs. This suggests that running the system at either extreme low or high emissions may not yield the best overall performance without sacrificing one of the objectives. The chosen compromise values (for instance, a mid-level inlet dust concentration) allow the FGD to operate efficiently across competing goals.

Across these scenarios, clear patterns emerge linking optimal FGD settings to the unit's load. As the emission load increases, the optimal absorber slurry pH generally needs to be higher (from ~5.0 at low load to ~5.7 at intermediate load and ~5.3 at peak load), consistent with the requirement for greater alkalinity to scrub higher SO_2 volumes. Slurry density, which influences gas–liquid contact and byproduct handling, also varies with load: the optimal values tend to hover around

1100–1130 kg/m^3 under mid to high loads, ensuring sufficient SO_2 absorption capacity while preventing excessive solids that could hinder separation. At the lowest load, a higher slurry density was optimal, likely to maximize contact efficiency even when pollutant levels are low.

These findings underscore the importance of adaptive, model-based control. As a power plant's load (and thus emission input) changes, the FGD's ideal operating conditions must shift accordingly. Compared with conventional operation—where plant operators manually adjust set-points or rely on fixed rule-based control—our load-aware optimization method offers clear advantages. Manual and rule-based strategies often struggle to adapt to rapid changes in flue gas composition or load conditions, leading to sub-optimal SO_2 removal and higher reagent consumption. In contrast, previous studies have shown that advanced model-based and AI-driven optimization approaches achieve better tracking of target values, faster recovery from disturbances, and reduced operator workload, ultimately improving pollutant removal efficiency and overall system performance in wet-FGD and coal-fired boiler applications[51,30,31,52]. This scenario-based optimization approach therefore provides practical guidance, enabling operators to proactively adjust parameters like slurry pH and density in response to changing load conditions.

Overall, the ANN-driven multi-objective optimization framework proves capable of guiding real-time adjustments in FGD operation, ensuring that pollutant removal efficiency is maximized, and emissions are minimized across a wide range of operating scenarios.

Conclusion

The coal combustion in the power plants releases environmental pollutants that cause the deterioration of the environment and damage public health. By integrating artificial neural networks (ANN), Monte Carlo-based sensitivity analysis, and the NSGA-II multi-objective optimization algorithm, the framework successfully identified optimal control strategies for minimizing NO_x and Hg discharges while maximizing desulfurization efficiency under varying emission load scenarios. The results demonstrate the effectiveness of AI-driven approaches in managing complex, interactive process variables and provide a foundation for real-time, data-informed operational decision-making in emission control systems. The main findings of this study are summarized in the points given below:

- An ANN-based process model was developed to accurately map complex nonlinear relationships between FGD input parameters and output responses (desulfurization efficiency, NO_x, and Hg emissions), enabling data-driven process optimization.
- Monte Carlo sensitivity analysis identified pH, inlet NO_x, and inlet dust as the most influential variables for desulfurization efficiency (45.5 %), NO_x discharge (92.3 %), and Hg discharge (42.4 %), respectively.
- A multi-objective optimization framework using NSGA-II, combined with TOPSIS based decision-making, effectively determined optimal input settings across multiple emission load scenarios, demonstrating adaptability under dynamic and broad operating conditions.
- The results confirm that pH and slurry density require targeted control, especially under higher emission loads, to maintain FGD performance, reflecting the importance of chemical and physical interactions in the absorber unit.
- The proposed AI-driven optimization strategy supports real-time, scenario-based operation of FGD systems, offering a scalable solution for cleaner and more efficient power plant emission control.

Future work and recommendations

Future work should focus on implementing a range of machine learning algorithms, such as support vector machines, random forests, and deep learning models, in combination with both deterministic and evolutionary optimization techniques, in order to establish a comprehensive benchmark for FGD system performance. Expanding the dataset to include longer temporal spans and multiple power plants will improve the generalizability of the models and enable transfer learning opportunities. Moreover, integration of real-time plant data with online optimization frameworks can transform the proposed methodology into an adaptive decision-support tool for operators. Future studies should also extend sensitivity and uncertainty analyses using advanced probabilistic methods, ensuring the robustness of optimization outcomes under data variability. Finally, coupling economic and environmental objectives within the optimization framework, followed by pilot-scale or industrial demonstrations, will be essential to validate the practical deployment of AI-driven FGD optimization strategies in coal-fired power plants.

CRediT authorship contribution statement

Fahid Riaz: Writing – review & editing, Writing – original draft, Visualization, Validation, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Conceptualization. **Muhammad Rizwan Awan:** Writing – review & editing, Visualization, Validation, Methodology, Formal analysis, Data curation. **Hafiz Zahid Nabi:** Writing – review & editing, Visualization, Investigation, Formal analysis, Data curation. **Ghulam Moeen Uddin:** Validation, Methodology, Data curation. **Muhammad Sultan:** Validation, Data curation. **Muhammad Asim:** Writing – review & editing, Supervision, Project administration, Investigation, Conceptualization.

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.

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Data availability

Data will be made available on request.

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